Advanced Quantum Theory

AMATH473/673, PHYS454

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Introduction

Quantum theory, together with general relativity, represents humanity's so-far deepest understanding of the laws of nature. And quantum phenomena are not rare or difficult to observe. In fact, we experience quantum phenomena constantly! For example, the very stability of the desk at which you are sitting now has its origin in a quantum phenomenon. This is because atoms are mostly empty space and the only reason why atoms don't collapse is due to the uncertainty relations. Namely, the uncertainty relations imply that it costs plenty of momentum (and therefore energy) to compress atoms. Also, for example, the spectrum of sunlight is shaped by quantum effects - if Planck's constant were smaller, the sun would be bluer.

Over the past century, the understanding of quantum phenomena has led to a number of applications which have profoundly impacted society, applications ranging from nuclear power, lasers, transistors and photovoltaic cells, to the use of MRI in medicine. Ever new sophisticated applications of quantum phenomena are being developed, among them, for example, quantum computers which have the potential to revolutionize information processing.

Also on the level of pure discovery, significant progress is currently being made, for example, in the field of cosmology, where both quantum effects and general relativistic effects are important: high-precision astronomical data obtained by satellite telescopes over the past 15 years show that the statistical distribution of matter in the universe agrees with great precision with the distribution which quantum theory predicts to have arisen from quantum fluctuations shortly after the big bang. All structure in the universe, and ultimately therefore also we, appear to have originated in quantum fluctuations.

The aim of this course is to explain the mathematical structure underlying all quantum theories and to apply it to the relatively simple case of nonrelativistic quantum mechanics. Nonrelativistic quantum mechanics is the quantum theory that replaces Newton's mechanics. The more advanced quantum theory of fields, which is necessary for example to describe the ubiquitous particle creation and annihilation processes, is beyond the scope of this course, though of course I can't help but describe some of it. For example, the first chapter of these notes, up to section 1.5, describes the history of quantum theory as far as we will cover it in this course. The introduction goes on, however, with a historical overview that outlines the further developments, from relativistic quantum mechanics to quantum field theory and on to the modern day quest for a theory of quantum gravity with applications in quantum cosmology. Quantum theory is still very much a work in progress and original ideas are needed as much as ever!

Note: This course prepares for a number of graduate courses, for example, the graduate course Quantum Field Theory for Cosmology (AMATH872/PHYS785) that I normally teach every other year.

Chapter 1

A brief history of quantum theory

1.1 The classical period

At the end of the 19th century, it seemed that the basic laws of nature had been found. The world appeared to be a mechanical clockwork running according to Newton's laws of mechanics. Light appeared to be fully explained by the Faraday-Maxwell theory of electromagnetism which held that light was a wave phenomenon. Also, for example, heat had been understood as a form of energy. Together, the then known theories constituted "Classical Physics". Classical physics was so successful that it appeared that theoretical physics was almost complete, the only task left being to add more digits of precision. At that time, young Max Planck, for example, was an undergraduate student at the University of Munich. One of his instructors there was Philipp von Jolly. In the spirit of the time then, von Jolly advised Planck against a career in physics. Planck stuck with it though and became one of those whose work overthrew classical physics.

1.2 Planck and the "Ultraviolet Catastrophe"

The limits to the validity of classical physics first became apparent in measurements of the spectrum of heat radiation. It had been known that very hot objects, such as a smith's hot iron, are emitting light. They do because matter consists of charged particles whose motion makes them act like little antennas that emit and absorb electromagnetic waves.

This of course also means that even relatively cold objects emit and absorb electromagnetic radiation. Their heat radiation is not visible to us because it too weak and mostly of too long wavelength for our eyes to see, but the heat radiatioin even of cold objects is easily measurable with instruments.

Black objects are those that absorb electromagnetic radiation (of whichever frequency range under consideration) most easily and by time reversal symmetry they are therefore also the objects that emit electromagnetic heat radiation of that frequency range most readily. For that reason, for example, tea in a tea pot that is black cools down faster than tea in a white or reflecting tea pot.

Now in the late 1800s, when researchers had completed the theorioes of classical physics, they were finally ready to try to calculate the spectrum of the radiation emitted by black bodies. To everybody's surprise, the calculations, which were first performed by Rayleigh and Jeans, predicted far more emission of waves of short wavelengths (such as ultraviolet and shorter wavelengths) than what experimental measurements seemed to indicate.

Actually, this was not a small discrepancy: the laws of classical physics were found to predict that any object would actually emit an infinite amount of heat radiation in an arbitrarily short time. Roughly speaking, this was because, according to classical physics and its equipartition theorem, as a system (such as a cup of tea) is left alone and starts to thermally equilibrate, every physical degree of freedom, such as the kinetic energy of an atom or molecule - or such as the energy of an electromagnetic wave of a given wavelength - should acquire an average energy of $kT/2$. Here, k is the Boltzmann constant and T the temperature in Kelvin. This prediction, however, was problematic because there are infinitely many wavelengths and each was supposed to acquire $kT/2$. Even if we put the hot cup of tea in a metal box of finite size that there is a limit to how large the wavelengths of electromagnetic field can be, there is no limit to how short the wavelengths can be. Hence, the prediction of classical physics that even the just the heat of a simple hot cup of tea should excite electromagnetic waves, i.e., that it should emit an infinite amount of heat radiation of arbitrarily short wavelengths.

At first, this was not seen as a reason to doubt the laws of classical physics. It seemed obvious that this nonsensical prediction could only be due to an error in the calculation. Eventually, however, as time passed and nobody appeared to be able to find a flaw in the calculation, the problem became considered serious enough to be called the "ultraviolet catastrophe". Planck decided to study this problem.

1.3 Discovery of h

From about 1890 to 1900, Planck dedicated himself to thoroughly analyzing all assumptions and steps in the calculations of Rayleigh and Jeans. To his great disappointment and confusion he too did not find an error. In the year 1900, Planck then learned of a new precision measurement of the heat radiation spectrum. Those measurements were precise enough to allow curve fitting. By that time, Planck had so much experience with the calculations of heat radiation that on the same day that he first saw the curve of the heat radiation spectrum he correctly *guessed* the formula for the frequency spectrum of heat radiation, i.e., the formula that is today called Planck's formula. After two further months of trying he was able to derive his formula from a simple but rather strange hypothesis. Planck's hypothesis was that matter cannot radiate energy continually, but only in discrete portions of energy which he called “quanta”.

Concretely, Planck postulated that light of frequency f could only be emitted in discrete packets of energy, with each packet, or quantum, carrying the energy $E_q = hf$. Planck found that the value of this constant, h, must be about 6.6 10^{-34}Kg m^2/s for the prediction of the heat radiation spectrum to come out right. The reason why this cures the ultraviolet catastrophe is that it means that electromagnetic waves of very short wavelengths are energetically expensive: Unlike in classical physics where a wave can have a very small amplitude and therefore small energy, now we have that to excite a wave of frequency f, at least the amount of energy hf must be invested to create at least one quantum (i.e., photon) of that wavelength. The equipartition law of classical physics is broken thereby:

We said that the charges that make up the cup of tea have random motions and therefore act like currents in an antenna, creating electromagnetic waves. Now, if these charges, acting like antennas, want to emit a photon of frequency f, they must muster the energy hf. But the charges only possess a typical energy, due to their thermal motion, of the order of kT. The charges that make up the cup of tea are, therefore, statistically unlikely to muster enough energy to create photons whose energy hf exceeds kT. This is why the spectrum of a lit candle of a few hundred degrees peaks in the red and then falls of quickly for higher frequencies. It’s also why the spectrum of sunlight, at 6000 degrees, peaks in the green and then falls of quickly towards the ultraviolet.

Planck’s quantum hypothesis was in clear contradiction to classical physics: light was supposed to consist of continuous waves. After all, light was known to be able to produce interference patterns[1]. The quantum hypothesis was perceived so radical, therefore, that most researchers, including Planck himself, still expected to find an explanation of the quantum hypothesis within classical physics.

1.4 Mounting evidence for the fundamental importance of h

The significance of Planck’s constant was at first controversial and even Planck was hesitant to view his quantum hypothesis as anything more than a mathematical trick that would presumably find some explanation within a continuum theory eventually. Einstein, however, was prepared to take Planck’s finding at face value and in 1906, Einstein used it to quantitatively explain the photoelectric effect: Light can kick electrons

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[1] It is easy to see these interference patterns: in a dark room, have a candle burning on a desk, then sit a few meters away from it. Close one of your eyes and hold a hair in front of your other eye, about 1cm in front of the eye, vertically. Align the hair with the flame of the candle. Do you see an interference pattern, i.e., the flame plus copies of it to its left and right? From the apparent distance between the copies of the flame and the distance of the hair to the flame you can work out the ratio of the thickness of the hair to the wavelength of the light.

out of a metal's surface. Classical physics predicted that this ability depends on the brightness of the light. Einstein's quantum physics correctly explained that it instead depends on the color of the light: Einstein's radical idea was that light of frequency f comes in quanta, i.e., in packets of energy hf. Then, he reasoned, the light's energy packets must be of high enough energy and therefore of high enough frequency to be able to free electrons from the metal. Einstein's explanation of the photoelectric effect is the only result for which he was awarded a Nobel prize.

At about the same time, work by Rutherford and others had shown that atoms consist of charged particles which had to be assumed to be orbiting another. This had led to another deep crisis for classical physics: If matter consisted of charged particles that orbit another, how could matter ever be stable? When a duck swims in circles in a pond, it continually makes waves and the production of those waves costs the duck some energy. Similarly, an electron that orbits a nucleus should continually create electromagnetic waves. Just like the duck, also the electron should lose energy as it radiates off electromagnetic waves. A quick calculation showed that any orbiting electron should rather quickly lose its energy and therefore fall into the nucleus. According to classical physics, therefore, matter would not be stable and we could not exist.

Finally, in 1913, Bohr was able to start explaining the stability of atoms. However, to this end he too had to make a radical hypothesis involving Planck's constant h: Bohr hypothesized that, in addition to Newton's laws, the orbiting particles should obey a strange new equation. The new equation says that a certain quantity calculated from the particle's motion (the so called "action" from the action principle), can occur only in integer multiples of h. In this way, only certain orbits would be allowed. In particular, there would be a smallest orbit of some finite size, and this would be the explanation of the stability of atoms. Bohr's hypothesis also helped to explain another observation which had been made, namely that atoms absorb and emit light preferably at certain discrete frequencies.

1.5 The discovery of quantum theory

Planck's quantum hypothesis, Einstein's light quanta hypothesis and Bohr's new equation for the hydrogen atom all contained Planck's h in an essential way, and none of this could be explained within the laws of classical physics. Physicists, therefore, came to suspect that the laws of classical physics might have to be changed according to some overarching new principle, in which h would play a crucial role. They were looking for a new kind of physics, a quantum physics. The theoretical task at hand was enormous: One would need to find a successor to Newton's mechanics, which would be called quantum mechanics. And, one would need to find a successor to Faraday and Maxwell's electromagnetism, which would be called quantum electrodynamics. The new quantum theory would have to reproduce all the successes of classical physics while at the same time explaining in a unified way all the quantum phenomena, from Planck's heat radiation formula, to the stability and the absorbtion and emission spectra of atoms.

This task took more than twenty years of intense experimental and theoretical research by numerous researchers. Finally, in 1925, it was Werner Heisenberg who first found "quantum mechanics", the successor to Newton's mechanics. (At the time, Heisenberg was a 23 year old postdoctoral fellow with a Rockefeller grant at Bohr's institute in Copenhagen). Soon after, Erwin Schrödinger found a simpler formulation of quantum mechanics which turned out to be equivalent. Shortly after, Dirac was able to fully clarify the mathematical structure of quantum mechanics, thereby finally revealing the deep principles that underlie quantum theory. Dirac's textbook "Principles of Quantum Mechanics" is a key classic.

The new theory of "Quantum Mechanics", being the successor to Newton's mechanics, correctly described how objects move under the influence of electromagnetic forces. For example, it described how electrons and protons move under the influence of their mutual electromagnetic attraction. Thereby, quantum mechanics explained the stability of atoms and the details of their energy spectra. In fact, quantum mechanics was soon applied to explain the periodic table and the chemical bonds.

What was still needed, however, was the quantum theory of those electromagnetic forces, i.e., the quantum theoretic successor to Faraday and Maxwell's electromagnetism. Planck's heat radiation formula was still not explained from first principles! Fortunately, the discovery of quantum mechanics had already revealed most of the deep principles that underlie quantum theory. Following those principles, Maxwell's theory of electromagnetism was "quantized" to arrive at quantum electrodynamics so that Planck's formula for the heat radiation spectrum could be derived.

It then became clear that quantum mechanics, i.e., the quantization of classical mechanics, was merely the starting point. Somehow, quantum mechanics would have to be upgraded to become consistent with the brand new theory of relativity which Einstein had discovered! And then it would have to be covariantly combined with the quantization of electrodynamics in order to be able to describe both matter and radiation and their interactions.

1.6 Relativistic quantum mechanics

Already by around 1900, Lorentz, Einstein and others had realized that Newton's mechanics, with its assumptions of an absolute space and time, was in fact incompatible with Faraday and Maxwell's theory of electromagnetism, for reasons unrelated to quantum theory, thereby contributing to the crisis of classical physics. In a daring move, Einstein accepted Faraday and Maxwell's relatively new theory of electromagnetism as superior and questioned the validity of Newton's notion of absolute space and time:

Maxwell was able to calculate the speed of electromagnetic waves from first principles, and found it to match with the measured speed of light. His calculations also showed, however, that a traveller with some large constant velocity would find the same speed of light. (Today we would say that this is because the Maxwell equations are covariant).

At the time, this was rather surprising as it clearly contradicted Newton's classical mechanics which says that velocities are simply additive. For example, according to Newton, a passenger who walks forward at $v_1 = 5$km/h in a train travelling at $v_2 = 100$km/h has a speed of $v_3 = v_1 + v_2 = 105$km/h relative to the ground. In fact, she does not. Her speed to the ground is $v_3 = (v_1 + v_2)/(1 + v_1 v_2/c^2) = 104.9999994...$km/h. Today, the nonadditivity of velocities is an easy-to-measure everyday phenomenon which is built into GPS systems, for example. At the time, the nonadditivity of velocities was first confirmed experimentally by Michelson and Moreley, who compared the speed of two light rays travelling parallel and orthogonal to the motion of the earth around the sun. The new theory that explained it all was of course Einstein's special relativity. By 1916, Einstein developed the theory further into general relativity, which superseded Newton's laws of gravity. General relativity very elegantly explains gravity as curvature of space-time.

Historically, the discovery of relativity therefore happened more or less simultaneously with the discovery of quantum theory. Yet, the two theories were developed virtually independently of another. In actual experiments, special relativity effects seemed of little importance to quantum mechanical effects and vice versa. For example, it was easy to estimate that an electron which orbits the nucleus of a hydrogen atom would travel at most at speeds smaller than one percent of the speed of light. Also, since gravity is extremely weak compared to the electromagnetic forces that rule the atom it was clear that general relativity would be even less important than special relativity for those early quantum mechanical studies. Conversely, the uncertainty principle appeared irrelevant at the astrophysical scales where general relativity was applied.

Nevertheless, soon after quantum mechanics had been found in 1925 it became apparent that at least the tiny special relativistic effect of the speed of an electron orbiting a nucleus was indeed measurable. This meant that there was experimental guidance for the development of an improved version of quantum mechanics that would be compatible with special relativity. Indeed, Klein, Gordon, Dirac and others soon developed "relativistic quantum mechanics[2]". Dirac's analysis, in particular, led him to correctly predict surprising magnetic properties of electrons, and it led him to correctly predict the existence and properties of antiparticles such as the positron!

However, the fact that particles are able to create and annihilate another in collisions, which had clearly been observed, was beyond the power of even relativistic quantum mechanics. It was clear that a significant enlargement of the framework of quantum theory was needed.

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[2] This relativistic quantum mechanics is an improvement of quantum mechanics which is consistent merely with *special* relativity. The search for a quantum theory that is consistent also with general relativity is still on today.

1.7 Quantum field theory

The way forward was called “second quantization”. The starting observation was that, in quantum mechanics, the wave functions behave completely deterministically, namely according to the Schrödinger equation. Given the initial wave function, one can calculate its evolution with absolute certainty. It was felt that to be able to predict the evolution of something, here the wavefunction, with absolute certainty was unusual for a quantum theory. The idea of second quantization was, therefore, to apply quantum theory to quantum theory itself. To this end, the quantum mechanical wave functions were to be treated as classical fields, much like the classical electromagnetic fields. Then, the aim was to find the quantum version of those fields. Since quantum theory was to be applied to the wave functions themselves, the amplitudes of wave functions would no longer be numbers but they would be operators instead. (An operator is a linear map on an infinite dimensional vector space). As a consequence, in quantum field theory, the amplitudes of the wave functions would be subject to uncertainty relations. One should not be able to be sure of the values of the wave function, nor should one be able to be sure of the norm of the wave function. In quantum mechanics, the normalization of the wave function to norm 1 means that there is exactly one particle, somewhere. In second quantization with its uncertainty principles, one could generally no longer be sure how many particles there are. Roughly speaking, it is in this way that the quantum fluctuations of the wave functions themselves would then account for the creation and annihilation of particles[3].

The problem of finding a quantum theory for fields had of course already been encountered when one had first tried to find the quantum theoretic successor to Faraday and Maxwell’s electrodynamics (which was consistent with special relativity from the start). As it turned out, guided by the general principles underlying quantum mechanics the quantum theory of the electromagnetic fields alone was not too hard to find. Following these lines, one was eventually able to write down a unifying quantum theory both of charged particles and their antiparticles, and also of their interaction through electromagnetic quanta, i.e., photons. While this theory succeeded well in describing all the interactions, including particle annihilation and creation processes, it did yield much more than one had bargained for. The reason was that, since now the particle number was no longer conserved, the time-energy uncertainty principle made it possible for short time intervals that energy (and therefore all kinds of particles) could be virtually “borrowed” from the vacuum.

As a consequence, the new quantum field theory, called quantum electrodynamics, necessarily predicted that, for example, that an electron would sometimes spontaneously borrow energy from the vacuum to emit a photon which it then usually quickly reabsorbs. During its brief existence, this so-called “virtual” photon even has a chance to split into a virtual electron-positron pair which shortly after annihilates to

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[3] Yes, third and higher quantization has been considered, but with no particular successes so far.

become the virtual photon again. In fact, the virtual electron (or the positron) during its short existence, might actually emit and quickly reabsorb a virtual photon. That photon, might briefly split into an electron positron pair, etc etc ad infinitum. Even more intriguing is that even without a real electron to start with, the vacuum alone is predicted to have virtual particles continually appearing and disappearing! All of this happens under the veil of the time-energy uncertainty principle.

It turned out that the quantum field theory's predictions was in good agreement with experimental results for the very simplest interactions. It was hoped that when taking into account also the predicted virtual processes hidden under the veil of the time-energy uncertainty principle, the accuracy of the predictions would increase even further.

Not so! These calculations typically yielded divergent integrals and so, at first, one only obtained seemingly meaningless predictions of infinite numbers. It took the combined efforts of numerous scientists, such as Feynman, Tomanaga, Weisskopf, Dyson and others, over about twenty years, to solve this problem.

It turned out that those calculations that had yielded infinities did make sense after all, if one suitably recalibrated the parameters of the theory, such as the fundamental masses and charges. This process of recalibration, called renormalization, also occurs in condensed matter physics, where it is easier to understand intuitively: Consider an electron that is traveling through a crystal. It has the usual mass and charge. But if you want to influence the electron's motion you will find that the traveling electron behaves as if it had a several times larger mass and a smaller charge. That's because the electron slightly deforms the crystal by slightly displacing the positive and negative charges that it passes by. It is these deformations of the crystal, which travel with the electron, which make the electron behave as if it were heavier and they also shield its charge. Also, the closer we get to the electron with our measurement device, the less is its charge shielded, i.e., the more we see of the bare charge of the electron.

The key lesson here is that the masses and charges that one observes in a crystal are generally not the "bare" masses and charges that the particles fundamentally possesses. The observed masses and charges even depend on how closely one looks at the electron.

Now when fundamental particles travel through the vacuum, then they deform the distribution of those virtual particles that pop in and out of existence under the veil of the time-energy uncertainty principle. Again, this makes particles behave as if they had a different mass and a different charge. The masses and charges that are observed are not the "bare" masses and charges that the particles fundamentally possess. The observed masses and charges actually depend again on how closely one looks at the particles, i.e., at what energy one observes them, say with an accelerator. In quantum field theory, it turns out that the bare masses and charges may formally even tend to zero or be divergent. This is okay, as long as the predicted measured values come out right.

1.8 Renormalization

Technically, if you like to know the gist of renormalization already, renormalization consists of the following steps: First, artificially render all predictions finite, say by cutting off the divergent integrals. It turned out that this can be achieved by postulating the existence of a smallest possible distance ϵ between any two particles and by calculating virtual processes accordingly. Next, adjust the parameters of the theory (charges, masses etc) such that a handful of predictions come out in agreement with experiment (namely as many as there are free parameters such as masses and charges in the theory). Now let $\epsilon \to 0$, while at the same time letting the bare parameters of the theory run so that the same handful of predictions comes out right. (The parameters of the theory will thereby usually tend to 0 or ∞.) Crucially, all other (infinitely many!) possible predictions of the theory will now also come out finite in the limit $\epsilon \to 0$ - and they can be compared to experiment. Indeed, predictions so-obtained through renormalization, for example for the energy levels of the hydrogen atom, match the experimental results to more than a dozen digits behind the comma!

Of course, renormalization has always been seen as mathematically and conceptually unsatisfactory. Nevertheless, it did open the door to the successful application of quantum field theory for the description of all the many species of particles that have been discovered since, from neutrinos and muons to quarks.

It is important also to mention two developments related to quantum field theory: First, on the applied side, it turned out that quantum field theoretic methods can also be used for the description of wave phenomena in solids. These are crucial, for example, for the understanding of superconductivity. Second, on the theoretical side, Feynman in his work on quantum electrodynamics, found an equivalent but very insightful and mathematically powerful new formulation for the principles of quantum theory, called the path integral formulation. I will briefly outline the path integral formulation of quantum mechanics later in this course.

1.9 Beyond quantum field theory?

Today, quantum field theory has served as the basis of elementary particle physics (and therefore as the basis for the description of all that we are made of) for about fifty years. Even though numerous new particles and even new forces have been discovered over the years, quantum field theory itself never needed to undergo any fundamental changes. Similarly successful has been Einstein's general relativity, which has now served as the basis of all gravitational physics for over 80 years. Even the most sophisticated experiments seem to merely confirm the validity of quantum field theory and general relativity with more and more precision.

Could it be, therefore, that these two theories constitute the final laws of nature and that this is all there is? Should one discourage students from a career in the subject?

Certainly not! In fact, the situation resembles in many ways the situation at the time Planck was a student. We have two highly successful theories - but they are inconsistent! As long as we consider gravity to be a fixed background for quantum theory some calculations can be performed. Hawking's prediction of black hole radiation is of this kind. However, once we fully take into account the dynamics of general relativity, we face a problem: The predictions of infinities in quantum field theory appear to persist. In the renormalization procedure, the limit $\epsilon \to 0$ does no longer seem to work (not for lack of trying!).

This problem is very deep. Many believe that this indicates that there actually exists a finite shortest length, ϵ, in nature, much like there is a finite fastest speed. Indeed, if we put together what we know from general relativity and what we know from quantum theory, we can conclude that we cannot even in principle devise an experimental operation that would allow us to resolve distances as small as about $10^{-35}m$, which is the so-called Planck scale:

Consider the task of resolving some very small structure. To this end, we need to shine on it some probing particles of very short wavelength. Due to quantum theory, the shorter the wavelength, the higher is the energy uncertainty of the probing particle. According to general relativity, energy gravitates and curves space. Thus, the probing particles will randomly curve space to the extent of their energy uncertainty. Assume now that a distance of $10^{-35}m$ or smaller is to be resolved. A short calculation shows that to this end the probing particles would have to be of such short wavelength, i.e., of such high energy uncertainty that they would significantly curve and thereby randomly disturb the region that they are meant to probe. It therefore appears that the very notion of distance loses operational meaning at distances of about $10^{-35}m$.

In order to describe the structure of space-time and matter at such small scales we will need a unifying theory of quantum gravity. Much effort is being put into this. In this field of research, it is widely expected that within the unified quantum gravity theory there will be a need for renormalization, but not for infinite renormalization. This yet-to-be found theory of quantum gravity may also solve several other major problems of quantum theory. In particular, it could yield an explanation for the particular masses and charges of the elementary particles, and perhaps even an explanation for the statistical nature of quantum theoretical predictions.

A very concrete major problem awaiting resolution in the theory of quantum gravity is the derivation of the cosmological constant, which represents the energy of the vacuum. Quantum field theory predicts the vacuum to possess significant amounts of energy due to vacuum fluctuations: Each field can be mathematically decomposed into a collection of quantum theoretical harmonic oscillators, each of which contributes a finite ground state energy of $\hbar\omega/2$. General relativity predicts that the vacuum energy should gravitate, just like any other form of energy.

Evidence from recent astronomical observations of the expansion rate of the universe indicates that the cosmological constant has a small but nonzero value. How much vacuum energy does quantum field theory predict? Straightforwardly, quantum field theory predicts the vacuum energy density to be infinite. If we augment quantum field theory by the assumption that the Planck length is the shortest length in nature, then quantum field theory predicts a very large vacuum energy. In fact, it is by a factor of about 10^{120} larger than what is experimentally observed. This is the today's "ultraviolet catastrophe". It appears that whoever tries to reconcile quantum theory with general relativity must be prepared to question the very foundations of all we know of the laws of nature. Original ideas are needed that may be no less radical than those of Planck or Einstein. Current attempts are, for example, string theory and loop quantum gravity.

1.10 Experiment and theory

In the past, progress in the search for the theory of quantum gravity has been severely hampered by the fact that one cannot actually build a microscope with sufficiently strong resolving power to probe Planck scale physics. Even the best microscopes today, namely particle accelerators, can resolve distances only down to at most 10^{-20}m, which is still many orders of magnitude away from the Planck scale of $10^{-35}m$. Of course, guidance from experiments is not strictly necessary, as Einstein demonstrated when he first developed general relativity. Nevertheless, any candidate theory must be tested experimentally before it can be given any credence.

In this context, an important recent realization was that there are possibilities for experimental access to the Planck scale other than through accelerators! One possibility could be the study of the very highly energetic cosmic rays that occasionally hit and locally briefly light up the earth's atmosphere. Another recently much discussed possibility arises from the simple fact that the universe itself was once very small and has dramatically expanded since. The idea is, roughly speaking, that if the early expansion was rapid enough then the universe might have acted as a microscope by stretching out everything to a much larger size. Astronomical evidence obtained over the past few years indicate that this did happen.

The statistical distribution of matter in the universe is currently being measured with great precision, both by direct observation of the distribution of galaxies, and through the measurement of the cosmic microwave background. Experimental evidence is mounting for the theory that the matter distribution in the universe agrees with what one would expect if it originated as tiny primordial quantum fluctuations - which were inflated to cosmic size by a very rapid initial expansion of the universe! It appears that the universe itself has acted as a giant microscope that enlarged initially small quantum phenomena into an image on our night sky! It is just possible that even the as yet unknown quantum phenomena of Planck length size have left an imprint in this image. Some of my own research is in this area. See, for example, this paper: https://doi.org/10.1103/PhysRevLett.119.031301. New satellite based telescopes are currently further exploring these phenomena.

Chapter 2

Classical mechanics in Hamiltonian form

2.1 Newton's laws for classical mechanics cannot be upgraded

When physicists first tried to find the laws of quantum mechanics they knew from experiments that Planck's constant h would have to play an important role in those laws. Imagine yourself in the situation of these physicists. How would you go about guessing the laws of quantum mechanics? Clearly, quantum mechanics would have to strongly resemble classical mechanics. After all, quantum mechanics should be an improvement over classical mechanics. Thus, it would have to reproduce all the successful predictions of classical mechanics, from the motion of the planets to the forces in a car's transmission. So how if we try to carefully improve one or several Newton's three axioms of classical mechanics by suitably introducing Planck's constant?

For example, could it be that $F = ma$ should really be $F = ma + h$ instead? After all, h is such a small number that one could imagine that this correction term might have been overlooked for a long time. However, this attempt surely can't be right on the trivial grounds that h does not have the right units: F and ma have the units Kgm/s^2 while the units of h are Kgm^2/s. But then, could the correct second law perhaps be $F = ma(1 + h/xp)$? The units would match. Also this attempt can't be right because whenever x or p are small, the term h/xp would be enormous, and we could therefore not have overlooked this term for all the hundreds of years since Newton. Similarly, also $F = ma(1 + xp/h)$ can't be right because for the values of x and p that we encounter in daily life the term xp/h would usually be big enough to have been seen.

In fact, no attempt to improve on Newton's laws in such a manner works. This is why historically this search for the laws of quantum mechanics actually took a quarter century! When the first formulations of quantum mechanics were eventually found by

Heisenberg and Schrödinger, they did not at all look similar to classical mechanics.

It was Dirac who first clarified the mathematical structure of quantum mechanics and thereby its relation to classical mechanics. Dirac remembered that a more abstract formulation of classical mechanics than Newton's had long been developed, namely Hamiltonian's formulation of classical mechanics. Hamilton's formulation of classical mechanics made use of a mathematical tool called Poisson brackets. Dirac showed that the laws of classical mechanics, once formulated in their Hamiltonian form, can be repaired by suitably introducing h into its equations, thereby yielding quantum mechanics correctly. In this way, Dirac was able to show how quantum mechanics naturally supersedes classical mechanics while reproducing the successes of classical mechanics. We will follow Dirac in this course[1].

2.2 Levels of abstraction

In order to follow Dirac's thinking, let us consider the levels of abstraction in mathematical physics: Ideally, one starts from abstract laws of nature and at the end one obtains concrete number predictions for measurement outcomes. In the middle, there is usually a hierarchy of mathematical problems that one has to solve.

In particular, in Newton's formulation of classical mechanics one starts by writing down the equations of motion for the system at hand. The equations of motion will generally contain terms of the type $m\ddot{x}$ and will therefore of the type of differential equations. We begin our calculation by solving those differential equations, to obtain functions. These functions we then solve for variables. From those variables we eventually obtain some concrete numbers that we can compare with a measurement value. The hierarchy of abstraction is, therefore:

$$\begin{array}{c}\text{Differential equations}\\ \Downarrow\\ \text{Functions}\\ \Downarrow\\ \text{Variables}\\ \Downarrow\\ \text{Numbers}\end{array}$$

This begs the question if there is a level of abstraction above that of differential equations? Namely, can the differential equations of motion be obtained as the *solution* of

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[1] In his paper introducing the Schrödinger equation, Schrödinger already tried to motivate his equation by an analogy with some aspect of Hamilton's work (the so called Hamilton Jacobi theory). This argument did not hold up. But, another part of Schrödinger's intuition was right on: His intuition was that the discreteness in quantum mechanics (e.g., of the energy levels of atoms and molecules) has its mathematical origin in the usual discreteness of the resonance frequencies of wave phenomena.

some higher level mathematical problem? The answer is yes, as Dirac remembered: Already in the first half of the 19th century, Lagrange, Hamilton and others had found this higher level formulation of classical mechanics. Their methods had proven useful for solving the dynamics of complicated systems, and some of those methods are still being used, for example, for the calculation of satellite trajectories. Dirac thought that if Newton's formulation of classical mechanics was not upgradable, it might be worth investigating if the higher level formulation of Hamilton might be upgradable to obtain quantum mechanics. Dirac succeeded and was thereby able to clearly display the similarities and differences between classical mechanics and the quantum mechanics of Heisenberg and Schrödinger. To see this is our first goal in this course.

Remark: For completeness, I should mention that there are two equivalent ways to present classical mechanics on this higher level of abstraction: One is due to Hamilton and one is due to Lagrange. Lagrange's formulation of classical mechanics is also upgradable, i.e., that there is a simple way to introduce h to obtain quantum mechanics from it, as Feynman first realized in the 1940s. In this way, Feynman discovered a whole new formulation of quantum mechanics, which is called the path integral formulation. I will explain Feynman's formulation of quantum mechanics later in the course.

2.3 Classical mechanics in Hamiltonian formulation

2.3.1 The energy function H contains all information

What was Hamilton's higher level of abstraction? How can classical mechanics be formulated so that Newton's differential equations of motion are themselves the solution of a higher level mathematical problem? Hamilton's crucial observation was the following: the expression for the total energy of a system already contains the complete information about that system! In particular, if we know a system's energy function, then we can derive from it the differential equations of motion of that system. In Hamilton's formulation of classical mechanics the highest level description of a system is therefore through its energy function. The expression for the total energy of a system is also called the Hamiltonian. The hierarchy of abstraction is now:

$$\begin{gathered}\text{Hamiltonians}\\ \Downarrow\\ \text{Differential equations}\\ \Downarrow\\ \text{Functions}\\ \Downarrow\\ \text{Variables}\\ \Downarrow\\ \text{Numbers}\end{gathered}$$

As a very simple example, let us consider a system of two point[2] masses, m_1 and m_2, which are connected by a spring with spring constant k. We write their respective position vectors as $\vec{x}^{(r)} = (x_1^{(r)}, x_2^{(r)}, x_3^{(r)})$ and their momentum vectors as $\vec{p}^{(r)} = (p_1^{(r)}, p_2^{(r)}, p_3^{(r)})$, where r is 1 or 2 respectively (we will omit the superscript ${}^{(r)}$ when we talk about one mass only). The positions and momenta are of course functions of time. Let us, therefore, keep in mind that for example $x_3^{(1)}$ is just a short hand notation for the function $x_3^{(1)}(t)$. Since this is a simple system, it is easy to write down its equations of motion:

$$\frac{d}{dt}\,x_i^{(r)} = \frac{p_i^{(r)}}{m_r} \tag{2.1}$$

$$\frac{d}{dt}\,p_i^{(1)} = -k(x_i^{(1)} - x_i^{(2)}) \tag{2.2}$$

$$\frac{d}{dt}\,p_i^{(2)} = -k(x_i^{(2)} - x_i^{(1)}) \tag{2.3}$$

Here, $r \in \{1,2\}$ labels the objects and $i \in \{1,2,3\}$ labels their coordinates. Hamilton's great insight was that these equations of motion (as well as those of arbitrarily complicated systems) can all be *derived* from just one piece of information, namely the expression for the system's total energy H alone! This is to say that Hamilton discovered that the expression for the total energy is what we now call the generator of the time evolution. The Hamiltonian H, i.e., the total energy of the system, is the kinetic energy plus the potential energy. In our example:

$$H = \frac{\left(\vec{p}^{(1)}\right)^2}{2m_1} + \frac{\left(\vec{p}^{(2)}\right)^2}{2m_2} + \frac{k}{2}\left(\vec{x}^{(1)} - \vec{x}^{(2)}\right)^2 \tag{2.4}$$

Here, $\left(\vec{p}^{(1)}\right)^2 = \sum_{i=1}^{3}\left(p_i^{(1)}\right)^2$ etc. Now imagine that the system in question is instead a complicated contraption with plenty of wheels, gears, discs, levers, weights, strings, masses, bells and whistles. Using Newton's laws it is possible to determine the equations of motion for that system but it will be complicated and will typically involve drawing lots of diagrams with forces. Hamilton's method promises a lot of simplification here. We just write down the sum of all kinetic and potential energies, which is generally not so difficult, and then Hamilton's methods should yield the equations of motion straightforwardly. In practice we won't be interested in complicated contraptions. We'll be interested in systems such as molecules, quantum computers or quantum fields, which all can be quite complicated too.

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[2] In this course, we will always restrict attention to point masses: all known noncomposite particles, namely the three types of electrons and neutrinos, six types of quarks, the W and Z particles (which transmit the weak force responsible for radioactivity), the gluons (which transmit the strong force responsible for the nuclear force) and the photon are all point-like as far as we know.

But what is the technique with which one can derive the equations of motion from a Hamiltonian, for example, Eqs.2.1-2.3 from Eq.2.4? Exactly how does the generator, H, of the time evolution generate the time evolution equations Eqs.2.1-2.3?

2.3.2 The Poisson bracket

The general procedure by which the equations of motion can be derived from a Hamiltonian H requires the use of a powerful mathematical operation, called "Poisson bracket"[3]:

The Poisson bracket is a particular kind of multiplication: Assume that f and g are polynomials in terms of the positions and momenta of the system, say $f = -2p_1$ and $g = 3x_1^2 + 7p_3^4 - 2x_2^3p_1^3 + 6$. Then, the Poisson bracket of f and g is written as $\{f, g\}$ and the evaluation of the bracket will yield another polynomial in terms of the position and momenta of the system. In this case:

$$\{-2p_1\ ,\ 3x_1^2 + 7p_3^4 - 2x_2^3p_1^3 + 6\} = 12x_1 \tag{2.5}$$

But how does one evaluate such a Poisson bracket to obtain this answer? The rules for evaluating Poisson brackets are tailor-made for mechanics. There are two sets of rules:

A) By definition, for each particle, the Poisson brackets of the positions and momenta are:

$$\begin{aligned} \{x_i, p_j\} &= \delta_{i,j} &(2.6)\\ \{x_i, x_j\} &= 0 &(2.7)\\ \{p_i, p_j\} &= 0 &(2.8)\end{aligned}$$

for all $i, j \in \{1, 2, 3\}$. Here, $\delta_{i,j}$ is the Kronecker delta, which is 1 if $i = j$ and is 0 if $i \neq j$. But these are only the Poisson brackets between linear terms. How to evaluate then the Poisson bracket between two polynomials? The second set of rules allow us to reduce this general case to the case of the Poisson brackets between linear terms:

B) By definition, the Poisson bracket of two arbitrary expressions in the positions and momenta, $f(x, p)$ and $g(x, p)$, obey the following rules:

$$\begin{aligned} \{f, g\} &= -\{g, f\} && \text{antisymmetry} &(2.9)\\ \{cf, g\} &= c\,\{f, g\}, \quad \text{for any number } c && \text{linearity} &(2.10)\\ \{f, g + h\} &= \{f, g\} + \{f, h\} && \text{addition rule} &(2.11)\end{aligned}$$

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[3] Remark: In elementary particle physics there is a yet higher level of abstraction, which allows one to *derive* Hamiltonians. The new level is that of so-called "symmetry groups". The Poisson bracket operation plays an essential role also in the definition of symmetry groups. (Candidate quantum gravity theories such as string theory aim to derive these symmetry groups from a yet higher level of abstraction which is hoped to be the top level.)

$$\begin{aligned} \{f,gh\} &= \{f,g\}h + g\{f,h\} && \text{product rule} \qquad (2.12) \\ 0 &= \{f,\{g,h\}\} + \{h,\{f,g\}\} + \{g,\{h,f\}\} && \text{Jacobi id.} \qquad (2.13) \end{aligned}$$

Let us postpone the explanation for why these definitions had to be chosen in exactly this way[4]. For now, note that an immediate consequence of these rules is that the Poisson bracket of a number always vanishes:

$$\{c,f\} = 0 \qquad \text{if } c \text{ is a number} \qquad (2.14)$$

The point of the second set of rules is that we can use them to successively break down the evaluation of a Poisson bracket like that of Eq.2.5 into sums and products of expressions that can be evaluated by using the first set of rules, Eqs.2.6,2.7,2.8. Using the product rule we immediately obtain, for example:

$$\{x_3, p_3^2\} = \{x_3,p_3\}p_3 + p_3\{x_3,p_3\} = 1p_3 + p_3 1 = 2p_3 \qquad (2.15)$$

Here now is the first set of exercises. These exercises, and all exercises up until Sec.2.3.5 are to be solved using only the above axioms for the Poisson bracket. In Sec.2.3.5, we will introduce a representation of the Poisson bracket in terms of derivatives[5]. You can use this representation only for the exercises from Sec.2.3.5 onward.

Exercise 2.1 *Prove Eq.2.14.*

Exercise 2.2 *Show that* $\{f,f\} = 0$ *for any* f.

Exercise 2.3 *Assume that* n *is a positive integer. Evaluate* $\{x_1, p_1^n\}$.

Exercise 2.4 *Verify Eq.2.5.*

Exercise 2.5 *Show that the Poisson bracket is not associative by giving a counter example.*

So far, we defined the Poisson brackets of polynomials in the positions and momenta of one point mass only. Let us now consider the general case of a system of n point masses, $m^{(r)}$ with position vectors $\vec{x}^{(r)} = (x_1^{(r)}, x_2^{(r)}, x_3^{(r)})$ and momentum vectors $\vec{p}^{(r)} = (p_1^{(r)}, p_2^{(r)}, p_3^{(r)})$, where $r \in \{1, 2, ..., n\}$. How can we evaluate the Poisson brackets of

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[4] If the product rule already reminds you of the product rule for derivatives (i.e., the Leibniz rule) this is not an accident. As we will see, the Poisson bracket can in fact be viewed as a sophisticated generalization of the notion of derivative.

[5] The abstract, axiomatically-defined Poisson bracket that we defined above may sometimes be a bit tedious to evaluate but it is very powerful because of its abstractness. As Dirac first showed, this abstract, axiomatically-defined Poisson bracket is the exact same in classical and quantum mechanics. As we will see in Sec.2.3.5, there is a representation of this abstract Poisson bracket in terms of derivatives, which is more convenient to work with but this representation only works in classical mechanics.

expressions that involve all those positions and momentum variables? To this end, we need to define what the Poisson brackets in between positions and momenta of different particles should be. They are defined to be simply zero. Therefore, to summarize, we define the basic Poisson brackets of n masses as

$$\begin{aligned} \{x_i^{(r)}, p_j^{(s)}\} &= \delta_{i,j}\ \delta_{r,s} && (2.16)\\ \{x_i^{(r)}, x_j^{(s)}\} &= 0 && (2.17)\\ \{p_i^{(r)}, p_j^{(s)}\} &= 0 && (2.18) \end{aligned}$$

where $r, s \in \{1, 2, ..., n\}$ and $i, j \in \{1, 2, 3\}$. The evaluation rules of Eqs.2.9-2.13 are defined to stay just the same.

Remark: In preparation for the next exercise, let's remember something important about how mathematics works: Mathematics is about structures. Whenever the same structure occurs somewhere, we call it by the same name.

For example, one such structure is called a group. A group is the structure where we have a set, S, whose elements have an operation that takes any two elements as input and outputs an element of S. Let's call that operation γ. So if $s_1, s_2 \in S$, then $\gamma(s_1, s_2) \in S$. For S to be called a group, the operation γ must obey these three conditions:

1. If $s_2, s_2, s_3 \in S$ then $\gamma(\gamma(s_1, s_2), s_3) = \gamma(s_1, \gamma(s_2, s_3))$ (associativity).
2. There exists an element, let's call it $e \in S$, for which $\gamma(e, s) = \gamma(s, e) = s$ for all $s \in S$ (neutral element).
3. For each $s \in S$, there exists an element, let's call it $s' \in S$, so that $ss' = e = s's$ (inverse).

Here are some examples of groups:

- The set $S := \mathbb{R}$ of real numbers with γ being addition: $\gamma(s_1, s_2) := s_1 + s_2$.
- The set, $S := M(15, \mathbb{C})$ of 15×15 complex matrices for which γ is matrix addition: $\gamma(s_1, s_2) := s_1 + s_2$.
- The set, $S := GL(7)$ of invertible 7×7 matrices for which γ is matrix multiplication: $\gamma(s_1, s_2) := s_1 s_2$.
- The set $SO(3)$ of rotations in three dimensions with γ being the concatenation of the two rotations: $\gamma(s_1, s_2) := s_2 \circ s_1$, i.e., we perform first rotation s_1 and then rotation s_2.

Here we can see mathematical abstraction at work: All these examples are examples of a structure called a group. Whatever we can prove for all groups, i.e., by using only the three conditions 1,2,3 above, will automatically be true for all groups. This is what makes mathematics so powerful. Whatever we manage to prove for a structure will automatically be true for all occurrences of that structure.

This works on many levels. For example, you may wonder whether the last example above, the group $SO(3)$, should have been written in terms of 3×3 matrices. Actually no, because $SO(3)$ is its own group. $SO(3)$ has infinitely many representations in terms of $n \times n$ matrices, i.e., while the case $n = 3$ is particularly important in practice, it is only a special case. In other words, $SO(3)$ is actually its own structure and it has many occurrences. Some occurrences of this structure, or 'representations' are in terms of matrices, some are in terms of operators and some have to do with spin and cannot be properly visualized. But as always in mathematics, whatever we can prove for the abstract structure, we automatically know to be true for all of its representations.

Exercise 2.6 *Mathematically, the set of polynomials in positions and momenta is an example of a structure that is called a Poisson algebra. A general Poisson algebra is a vector space with two extra multiplications: One multiplication which makes the vector space into an associative algebra, and one (non-associative) multiplication* $\{,\}$*, called the Lie bracket, which makes the vector space into what is called a Lie algebra. If the two multiplications are in a certain sense compatible then the set is said to be a Poisson algebra. Look up and state the axioms of a) a Lie algebra, b) an associative algebra and c) a Poisson algebra. Give your source(s). The source is to be a textbook, and not a site such as Wikipedia. Wikipedia is anonymous and therefore often inaccurate. Write out the answer and make sure you understand the answer. Such material is considered examinable.*

2.3.3 The Hamilton equations

Let us recall why we introduced the Poisson bracket: A technique that uses the Poisson bracket is supposed to allow us to *derive* all the differential equations of motion of a system from the just one piece of information, namely from the expression of the total energy of the system, i.e., from its Hamiltonian.

To see how this works, let us consider an arbitrary polynomial f in terms of the positions and momentum variables $x_i^{(r)}, p_j^{(s)}$ of the system in question, for example, something like $f = 7x_2^{(3)}\left(x_3^{(1)}\right)^3 - 2\cos(4t^2)(p_1^{(1)})^7 + 3/2$. This f depends on time for two reasons: There is an explicit dependence on time through the cosine term, and there is an implicit dependence on time because the positions and momenta generally depend on time. According to Hamilton's formalism, the equation of motion for f is then given by:

$$\frac{df}{dt} = \{f, H\} + \frac{\partial f}{\partial t} \tag{2.19}$$

Here, the notation $\partial f/\partial t$ denotes differentiation of f with respect to only its explicit time dependence. In the example above it is the derivative of the time dependence in the term $\cos(4t^2)$.

Eq.2.19 is a famous equation which is called the Hamilton equation. Why is it famous? If you know how to evaluate Poisson brackets then the Hamilton equation Eq.2.19 encodes for you all of classical mechanics! Namely, given H, equation Eq.2.19 yields the differential equation of motion for any entity f by the simple procedure of evaluating the Poisson bracket on its right hand side.

If f is dependent on time only through x and p (say if we choose for f a polynomial in x and p's with constant coefficients) then $\partial f/\partial t = 0$ and Hamilton's equation simplifies to:

$$\frac{d}{dt} f \ = \ \{f, H\} \tag{2.20}$$

In the remainder of this book, unless otherwise specified, we will always choose our functions f, g, h to have no explicit dependence on time, i.e., they will depend on time only implicitly, namely through the time dependence of the x and p's. In particular, the most important choices for f are of this kind: $f = x_i^{(r)}$ or $f = p_i^{(r)}$. For these choices of f we immediately obtain the fundamental equations of motion:

$$\frac{d}{dt} x_i^{(r)} \ = \ \{x_i^{(r)}, H\} \tag{2.21}$$

$$\frac{d}{dt} p_i^{(r)} \ = \ \{p_i^{(r)}, H\} \tag{2.22}$$

Here is a concrete example: A single free particle of mass m possesses only kinetic energy. Its Hamiltonian is:

$$H = \sum_{j=1}^{3} \frac{p_j^2}{2m} \tag{2.23}$$

By using this H in Eqs.2.21,2.22, we obtain the following equations of motion for the positions and momenta:

$$\frac{d}{dt} x_i \ = \ \left\{ x_i \ , \ \sum_{j=1}^{3} \frac{p_j^2}{2m} \right\} \ = \ \frac{p_i}{m} \tag{2.24}$$

and

$$\frac{d}{dt} p_i \ = \ \left\{ p_i \ , \ \sum_{j=1}^{3} \frac{p_j^2}{2m} \right\} \ = \ 0 \tag{2.25}$$

They agree with what was expected: $p_i = m\dot{x}_i$ and $\ddot{x}_i = 0$, where the dot indicates the time derivative. For another example, consider again the system of two point masses

m_1, m_2 which are connected by a spring with spring constant k. Its Hamiltonian H was given in Eq.2.4. By using this H in Eqs.2.21,2.22 we should now be able to derive the system's equations of motion (as given in Eqs.2.1-2.3). Indeed:

$$\begin{aligned} \frac{d}{dt}\, x_i^{(r)} &= \{x_i^{(r)}, H\} && (2.26)\\ &= \frac{p_i^{(r)}}{m_r} && (2.27) \end{aligned}$$

$$\begin{aligned} \frac{d}{dt}\, p_i^{(1)} &= \{p_i^{(1)}, H\} && (2.28)\\ &= -k(x_i^{(1)} - x_i^{(2)}) && (2.29) \end{aligned}$$

$$\begin{aligned} \frac{d}{dt}\, p_i^{(2)} &= \{p_i^{(2)}, H\} && (2.30)\\ &= -k(x_i^{(2)} - x_i^{(1)}) && (2.31) \end{aligned}$$

Let us omit the proof that Hamilton's formulation of classical mechanics always yields the same equations of motion as Newton's.

Exercise 2.7 *Consider $f = gh$, where g and h are some polynomial expressions in the position and momentum variables. There are two ways to calculate df/dt: Either we use the Leibniz rule, i.e., $\dot{f} = \dot{g}h + g\dot{h}$, and apply Eq.2.20 to both $\dot{g}$ and $\dot{h}$, or we apply Eq.2.20 directly to gh and use the product rule (Eq.2.12) for Poisson brackets. Prove that both methods yield the same result.*

This exercise shows that a property of the derivative on the left hand side of Eq.2.20 determines a rule for how the Poisson bracket had to be defined. In fact, such requirements of consistency are the main reason why the Poisson bracket is defined the way it is.

Exercise 2.8 *Use Eq.2.13 to prove that:*

$$\frac{d}{dt}\,\{f, g\} = \{\dot{f}, g\} + \{f, \dot{g}\} \tag{2.32}$$

2.3.4 Symmetries and Conservation laws

Our reason for reviewing the Hamiltonian formulation of mechanics is that it will be useful for the study of quantum mechanics. Before we get to that, however, let us ask why the Hamiltonian formulation of mechanics was useful for classical mechanics. It was, after all, developed more than half a century before quantum mechanics.

Sure, it was fine to be able to derive all the differential equations of motion from the one unifying equation. Namely, if for simplicity, we are now assuming that $f(x,p)$ is chosen not to have any explicit dependence on time, the universal Hamilton equation which expresses the differential equation of all variables f, is:

$$\dot{f} \;=\; \{f, H\} \tag{2.33}$$

Ultimately, however, one obtains this way just the same equations of motion as Newton's methods would yield. Was there any practical advantage to using Hamilton's formulation of mechanics? Indeed, there is an important practical advantage: The main advantage of Hamilton's formulation of mechanics is that it gives us powerful methods for studying conserved quantities, such as the energy or angular momentum. In general, for complicated systems (such as planetary systems, for example), there can be much more complicated conserved quantities than these. To know conserved quantities usually significantly helps in solving the dynamics of complicated systems. This feature of Hamilton's formulation of mechanics will carry over to quantum mechanics, so studying it here will later help us also in quantum mechanics.

Consider a polynomial f in x and p's with constant coefficients. Then, $\partial f/\partial t = 0$ and Eq.2.33 applies. We can easily read off from Eq.2.33 that *any such f is conserved in time if and only if its Poisson bracket with the Hamiltonian vanishes:*

$$\{f, H\} = 0 \quad \Rightarrow \quad \dot{f} = 0 \tag{2.34}$$

Consider, for example, a free particle. Its Hamiltonian is given in Eq.2.23. We expect of course that its momenta p_i are conserved. Indeed:

$$\dot{p}_i = \left\{ p_i, \sum_{j=1}^{3} p_j^2/2m \right\} = 0 \tag{2.35}$$

For another example, consider a system whose Hamiltonian is any polynomial in x's and p's with constant coefficients. The proof that this system's energy is conserved is now fairly trivial to see (using Axiom Eq.2.9):

$$\dot{H} = \{H, H\} = 0 \tag{2.36}$$

I mentioned that in order to be able to find solutions to the equations of motion of complicated real-life systems it is often crucial to find as many conserved quantities as possible. Here is an example. Consider a 3-dimensional isotropic (i.e., rotation invariant) harmonic oscillator. Because of its symmetry under rotations, it angular momentum is conserved. But this oscillator has actually a much larger symmetry and therefore more conserved quantities. This is because a harmonic oscillator, being of the form $x^2 + p^2$ also possesses rotation symmetry in phase space. I will here only remark that this means that the 3-dimensional isotropic harmonic oscillator possesses $SO(3)$ rotational symmetry as well as a larger $SU(3)$ symmetry.

Powerful methods for discovering symmetries and constructing the implied conserved quantities for arbitrary systems have been developed on the basis of Eq.2.33 and the Poisson bracket. A key technique is that of so-called canonical transformations, i.e., of changes variables for which the Poisson brackets remain the same. You can find these methods in classical mechanics texts under the keywords "canonical transformations" and "Hamilton Jacobi theory".

In fact, Poisson bracket methods reveal a very deep one-to-one correspondence between conserved quantities and so-called symmetries. For example, the statement that an experiment on a system gives the same result no matter when we perform the experiment, is the statement of a "symmetry" which is called time-translation invariance symmetry. In practice, it means that the Hamiltonian of the system does not explicitly depend on time: $\partial H/\partial t = 0$. As we just saw, this implies energy conservation: $dH/dt = 0$.

Similarly, the statement that an experiment on a system gives the same result wherever we perform the experiment is the statement of space-translation symmetry. It implies and is implied by momentum conservation. Further, the statement that an experiment on a system gives the same result whatever the angular orientation of the experiment is the statement of rotation symmetry. It implies and is implied by angular momentum conservation.

These are examples of the Noether theorem, of Emmi Noether. Her theorem plays a crucial role both in practical applications, and in fundamental physics[6]. We will later come back to Noether's theorem.

Exercise 2.9 *Show that if H is a polynomial in the positions and momenta with arbitrary (and possibly time-dependent) coefficients, it is true that $dH/dt = \partial H/\partial t$.*

Exercise 2.10 *Consider the system with the Hamiltonian of Eq.2.4. Show that the total momentum is conserved, i.e., that $p_i^{(1)} + p_i^{(2)}$ is conserved for all i.*

2.3.5 A representation of the Poisson bracket

In principle, we can evaluate any Poisson bracket $\{f, g\}$ by using the rules Eqs.2.6-2.12 if, as we assume, f and g are polynomials or well-behaved power series in the position and momentum variables. This is because the product rule allows us to break Poisson brackets that contain polynomials into factors of Poisson brackets that contain polynomials of lower degree. Repeating the process, we are eventually left with having

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[6] Mathematically, symmetries are described as groups (for example, the composition of two rotations yields a rotation and to every rotation there is an inverse rotation). In elementary particle physics, symmetry groups are one abstraction level higher than Hamiltonians: It has turned out that the complicated Hamiltonians which describe the fundamental forces, i.e., the electromagnetic, weak and strong force, are essentially derivable as being the simplest Hamiltonians associated with with three elementary symmetry groups.

to evaluate only Poisson brackets of linear terms, which can easily be evaluated using the first set of rules.

This is all good and fine but when f or g contain high or even infinite powers of the position and momentum variables, then the evaluation of the Poisson bracket $\{f, g\}$ can become rather tedious and cumbersome.

For practical purposes it is of interest, therefore, to have a shortcut for the evaluation of Poisson brackets. Indeed, for complicated f and g, the Poisson bracket $\{f, g\}$ can be evaluated usually faster by the following formula:

$$\{f, g\} = \sum_{r=1}^{n} \sum_{i=1}^{3} \left(\frac{\partial f}{\partial x_i^{(r)}} \frac{\partial g}{\partial p_i^{(r)}} - \frac{\partial f}{\partial p_i^{(r)}} \frac{\partial g}{\partial x_i^{(r)}} \right) \tag{2.37}$$

Exercise 2.11 *Use Eq.2.37 to evaluate* $\{x^8 p^6, x^3 p^4\}$.

Exercise 2.12 *Show that Eq.2.37 is indeed a representation of the Poisson bracket, i.e., that it always yields the correct answer. To this end, check that it obeys Eqs.2.9-2.13 and Eqs.2.16-2.18 (except: no need to check the Jacobi identity as that would be straightforward but too tedious).*

Exercise 2.13 *Find the representation of the Hamilton equations Eq.2.19 and Eqs.2.21, 2.22 obtained by using Eq.2.37.*

Remark: Some textbooks start with these representations of the Hamilton equations, along with the representation Eq.2.37 of the Poisson bracket - without reference to the Hamilton equations' more abstract origin in Eq.2.19 and Eqs.2.21, 2.22. This is unfortunate because those representations using Eq.2.37 do not carry over to quantum mechanics, while the more abstract equations Eq.2.19 and Eqs.2.21, 2.22 will carry over to quantum mechanics unchanged, as we will see!

2.4 Summary: The laws of classical mechanics

We already discussed that quantum mechanics must have strong similarities with classical mechanics, since it must reproduce all the successes of classical mechanics. This suggested that the laws of quantum mechanics might be a slight modification of Newton's laws which would somehow contain Planck's constant h. Since this did not work, we reformulated the laws of classical mechanics on a higher level of abstraction, namely in Hamilton's form. Before we now try to guess the laws of quantum mechanics, let us restate Hamilton's formulation of classical mechanics very carefully:

The starting point is the energy function H of the system in question. It is called the Hamiltonian, and it is an expression in terms of the position and momentum variables of the system. Then, assume we are interested in the time evolution of some quantity f which is also a polynomial in the x and p's (say with constant coefficients). Then we can derive the equation of motion for f through:

$$\frac{d}{dt}\,f \;=\; \{f, H\} \tag{2.38}$$

In particular, f can be chosen to be any one of the position and momentum variables of the system, and we obtain their equations of motion as Eqs.2.21,2.22. In order to obtain explicit differential equations from Eqs.2.38,2.21,2.22 we evaluate the Poisson bracket on its right hand side. To this end, we use the definitions Eqs.2.6-2.13. The so-obtained differential equations are then solved to obtain the positions $x_i^{(r)}(t)$ and momenta $p_i^{(r)}(t)$ as functions of time.

We note that the Poisson bracket which is defined by the axioms Eqs.2.6-2.12 possesses an often convenient explicit representation through Eq.2.37. We need to keep in mind, however, that Eq.2.37 merely provides a convenient shortcut for evaluating the Poisson bracket. This shortcut only works in classical mechanics. In quantum mechanics, there will also be a representation of the Poisson bracket but it will look very different from Eq.2.37.

2.5 Classical field theory

This section is a mere comment. In classical mechanics, the dynamical variables are the positions of particles, together with their velocities or momenta. For each particle there are three degrees of freedom of position and momenta.

In a field theory, such as Maxwell's theory, positions (and momenta) are not dynamical variables. After all, unlike a particle that moves around, a field can be everywhere at the same time. In the case of a field theory, what is dynamical is its amplitude.

Consider say a scalar field ϕ. At every point x in space it has an amplitude $\phi(x,t)$ that changes in time with a 'velocity' of $\dot{\phi}(x,t)$ which we may call the canonically conjugate momentum field: $\pi(x,t) := \dot{\phi}(x,t)$. Unlike the three degrees of freedom that particle possesses, a field therefore possesses uncountably many degrees of freedom, one at each position x. Now one can define the Poisson brackets of the first kind for them in analogy to the Poisson brackets for particles:

$$\{\phi(x,t), \pi(x',t)\} \;=\; \delta^3(x-x') \tag{2.39}$$

$$\{\phi(x,t), \phi(x',t)\} \;=\; 0 \tag{2.40}$$

$$\{\pi(x,t), \pi(x',t)\} \;=\; 0 \tag{2.41}$$

Here, $\delta^3(x-x')$ is the three dimensional Dirac delta distribution. The second set of axioms for the Poisson bracket is unchanged, i.e., it is still given by Eqs.2.9-2.13.

There is also a representation of the Poisson bracket for fields in terms of derivatives but we won't cover it here (can you guess it?). The energy of the classical field, i.e., its Hamiltonian, is:

$$H(\phi, \pi) = \int d^3x \, \frac{1}{2} \left(\pi(x,t)^2 + \sum_{i=1}^{3} (\partial_i \phi(x,t))^2 + m^2 \phi(x,t)^2 \right) \tag{2.42}$$

The Hamilton equation Eq.2.38 is unchanged.

Exercise 2.14 *(Bonus question) Derive the equations of motion for $\phi(x,t)$ and $\pi(x,t)$, i.e., choose $f = \phi(x,t)$ or $f = \pi(x,t)$ in Eq.2.38. Combine these two differential equations by eliminating $\pi(x,t)$ to obtain one differential equation for $\phi(x,t)$ which contains up to the second time derivatives.*

The combined equation is the so-called Klein Gordon equation. The Dirac equation and the Maxwell equations can be treated similarly, although with some small extra complications because the amplitudes of these fields are not scalar but are vectorial and spinorial respectively.

Chapter 3

Quantum mechanics in Hamiltonian form

We formulated the laws of classical mechanics on a higher level of abstraction, as summarized in Sec.2.4 because classical mechanics appeared to be not upgradeable when written in Newton's formulation. We are now ready to upgrade the more abstract Hamiltonian laws of classical mechanics to obtain quantum mechanics. A modification is needed which is a small enough to preserve all the successes of classical mechanics while it must also introduce h in order to correctly predict quantum mechanical effects.

For example, could it be that Eq.2.38 needs to be modified to obtain quantum mechanics? Could the correct equation be, say, $\frac{d}{dt}\,f = \{f, H\} + h$ or $\frac{d}{dt}\,f = \{f + h^2/f, H\}$, where h is Planck's constant? Those two equations can't be right, of course, already because the units generally don't match. Could it be then that to obtain quantum mechanics we will have to change the definitions for the Poisson bracket? Could it be that the definition Eq.2.12 needs to be changed? This, of course, is unlikely too because the definitions for the Poisson bracket were fixed by consistency conditions (recall, e.g., Exercise 2.7). The structure of our Poisson algebra is quite tightly constrained.

No, the necessary upgrade of the Hamiltonian formalism is actually much more subtle! Let us remember that when we defined the Poisson algebra structure in the previous section we did not make any assumptions about the mathematical nature of the functions $x(t)$ and $p(t)$ (let us omit writing out the indices). In particular, we did not make the assumption that these functions are number-valued. We can start with a Hamiltonian, i.e., a polynomial in the x and p and then by using the rules of the Poisson bracket we can derive the differential equations of motion. In the process, we never need to assume that the functions $x(t)$ and $p(t)$ are number valued. Could it be that the $x(t)$ and $p(t)$ need not be number valued and that this holds the key to upgrading classical mechanics to obtain quantum mechanics? Actually yes!

Before we get to this, we have to consider though that we actually did assume the x and p to be number valued at one specific point at the very end of the previous chapter. There, we wrote down a convenient representation of the Poisson bracket in

Eq.2.37, and there we needed the x and p to be number-valued - because to use this convenient representation we needed to be able to differentiate with respect to the x and p. We can conclude from this that if allowing the $x(t)$ and $p(t)$ to be something else than number valued is the key to upgrading to quantum mechanics, then the Poisson bracket will not be representable any more through Eq.2.37.

In fact, as we will see, this is how it will play out. Everything we did in the previous chapter, except for the representation Eq.2.37 will still exactly hold true in quantum mechanics. In particular, the differential equations of motion derived from the Hamiltonian will look exactly the same in quantum and classical mechanics. That's because they are derived from the same Hamiltonian polynomial in the x and p by using the same rules for the Poisson bracket. But then, if not in the equations of motion, how does the upgrade involve h at all?

3.1 Reconsidering the nature of observables

At this point, let us reconsider the very basics: How do the symbols we write on paper relate to real systems? We measure a system with concrete measurement devices in the lab, for example, devices for the measurement of positions and devices for the measurement of momenta. As usual, we invent for each kind of measurement a symbol, say $x_i^{(r)}$ and $p_i^{(r)}$. At this stage we need to be careful not to over-interpret these symbols. At this stage, these symbols have nothing to do (yet) with numbers, vectors, matrices, operators or bananas. Instead, these symbols are merely names for kinds of measurement. We need to find out more about the nature of these $x_i^{(r)}$ and $p_i^{(r)}$.

Now according to our everyday experience, the operation of a position measurement device does not interfere with the operation of a momentum measurement device: it seems that we can always measure both, positions and momenta. For example, GPS units are able to tell both position and velocity at the same time to considerable accuracy. It is tempting to assume, therefore, that there is no limit, in principle, to how accurately positions and velocities can be determined. And that would mean that we can let each of the symbols $x_i^{(r)}(t)$ and $p_i^{(r)}(t)$ stand for its measurement devices's output number at time t.

It is at this very point, namely when we make the assumption that positions and momenta can be accurately measured simultaneously, that we make the assumption that the symbols $x_i^{(r)}(t)$ and $p_i^{(r)}(t)$ can be represented mathematically as number-valued functions of time. And number-valued functions have the property of being commutative:

$$x_i^{(r)} p_j^{(s)} - p_j^{(s)} x_i^{(r)} \ = \ 0 \tag{3.1}$$

Since measurement values cannot be just any number but always come out real, we also have the law:

$$\left(x_i^{(r)}\right)^* = x_i^{(r)} \qquad \text{and} \qquad \left(p_j^{(s)}\right)^* = p_j^{(s)} \tag{3.2}$$

Similarly, we have $H^* = H$. Technically, the *-operation is an example of was is called an involution.

Exercise 3.1 *Find and list the defining property of an involution and give your source. The source is to be a textbook, and not a site such as Wikipedia. That's because Wikipedia is anonymous and therefore often inaccurate. Write out the answer and make sure you understand the answer. Such material is considered examinable.*

The statements above, namely that position and momentum measurements are compatible and come out as real numbers are indeed a nontrivial part of the laws of classical mechanics. For completeness we should have included them in the summary of classical mechanics in Sec.2.4.

A reality property of the form of Eq.3.2 will still be true in quantum mechanics. But the commutativity property expressed in Eq.3.1 and its underlying assumption that the operation of position and momentum measurement devices do not interfere with another needs to be abandoned and upgraded. It turns out that position and momentum measurements are like taking a shower and working out at the gym. It matters in which sequence one does them:

$$\text{gym}\cdot\text{shower - shower}\cdot\text{gym} = \text{sweat} \tag{3.3}$$

3.2 The canonical commutation relations

For the remainder of this course, we will need a way to make it transparent in every equation whether a variable is number valued or not. To this end, we will decorate variables that may not be number valued with a hat, for example, $\hat{H}, \hat{p}, \hat{x}$, or more specifically $\hat{x}_i^{(r)}$ and $\hat{p}_i^{(r)}$ for each position and momentum measurement device. Now how can the interference of the measurement devices mathematically be expressed as properties of the symbols $\hat{x}_i^{(r)}$ and $\hat{p}_i^{(r)}$?

According to classical mechanics one would be able to operate all measurement devices all the time and they would not interfere with another. We could therefore choose the $\hat{x}_i^{(r)}(t)$ and $\hat{p}_i^{(r)}(t)$ to stand for the number-valued outcomes of those measurements as functions of time. Crucially, the fact that we can't actually know positions and momenta simultaneously means that we can no longer choose the $\hat{x}_i^{(r)}(t)$ and $\hat{p}_i^{(r)}(t)$ to stand simply for number-valued outcomes of those measurements as functions of time.

Mathematically, it was the commutativity law of Eq.3.1 which expressed that in classical mechanics the symbols $\hat{x}_i^{(r)}(t)$ and $\hat{p}_i^{(r)}(t)$ can be represented as number valued functions. Could it be that Eq.3.1 has to be modified to include h so that the $\hat{x}_i^{(r)}(t)$ and $\hat{p}_i^{(r)}(t)$ become non-commutative and therefore can no longer be number-valued functions?

Are position and momentum measurements noncommuting similar to how doing sports and having a shower don't commute?

It was Dirac who first realized that all of the Poisson algebra structure that we defined above can be kept (and therefore the ability to derive the equations of motion), while changing just one little thing: allowing the symbols $\hat{x}_i^{(r)}(t)$ and $\hat{p}_i^{(r)}(t)$ to be noncommutative in a very particular way.

Before we can follow Dirac's argument, let us first reconsider the product rule for the Poisson bracket:

$$\{f, gh\} = \{f, g\}h + g\{f, h\} \tag{3.4}$$

Using the antisymmetry rule, $\{f, g\} = -\ \{g, f\}$, the product rule can be rewritten in this form:

$$\{gh, f\} = \{g, f\}h + g\{h, f\} \tag{3.5}$$

Using Eqs.3.4,3.5, we can now follow Dirac's argument for why the Poisson algebra structure imposes strict conditions on the form that any noncommutativity can take. Dirac considered the Poisson bracket

$$\{\hat{u}_1\hat{u}_2, \hat{v}_1\hat{v}_2\} \tag{3.6}$$

where $\hat{u}_1, \hat{u}_2, \hat{v}_1, \hat{v}_2$ are arbitrary polynomials in the variables $\hat{x}_i^{(r)}$ and $\hat{p}_j^{(s)}$. Expression Eq.3.6 can be decomposed into simpler Poisson brackets in two ways, namely using first Eq.3.4 and then Eq.3.5, or vice versa. And, of course, any noncommutativity of the $\hat{x}_i^{(r)}$ and $\hat{p}_j^{(s)}$ has to be such that both ways yield the same outcome:

$$\begin{aligned} \{\hat{u}_1\hat{u}_2, \hat{v}_1\hat{v}_2\} &= \hat{u}_1\{\hat{u}_2, \hat{v}_1\hat{v}_2\} + \{\hat{u}_1, \hat{v}_1\hat{v}_2\}\hat{u}_2 \\ &= \hat{u}_1(\hat{v}_1\{\hat{u}_2, \hat{v}_2\} + \{\hat{u}_2, \hat{v}_1\}\hat{v}_2) + (\hat{v}_1\{\hat{u}_1, \hat{v}_2\} + \{\hat{u}_1, \hat{v}_1\}\hat{v}_2)\hat{u}_2 \end{aligned} \tag{3.7}$$

must agree with:

$$\begin{aligned} \{\hat{u}_1\hat{u}_2, \hat{v}_1\hat{v}_2\} &= \hat{v}_1\{\hat{u}_1\hat{u}_2, \hat{v}_2\} + \{\hat{u}_1\hat{u}_2, \hat{v}_1\}\hat{v}_2 \\ &= \hat{v}_1(\hat{u}_1\{\hat{u}_2, \hat{v}_2\} + \{\hat{u}_1, \hat{v}_2\}\hat{u}_2) + (\hat{u}_1\{\hat{u}_2, \hat{v}_1\} + \{\hat{u}_1, \hat{v}_1\}\hat{u}_2)\hat{v}_2 \end{aligned} \tag{3.8}$$

We can, therefore, conclude that, independently of whether or not we have commutativity, it must always be true that:

$$\{\hat{u}_1, \hat{v}_1\}(\hat{v}_2\hat{u}_2 - \hat{u}_2\hat{v}_2) = (\hat{v}_1\hat{u}_1 - \hat{u}_1\hat{v}_1)\{\hat{u}_2, \hat{v}_2\} \tag{3.9}$$

And this equation has to be true for all possible choices of $\hat{u}_1, \hat{u}_2, \hat{v}_1, \hat{v}_2$. How can we ensure this? As is easy to check, Eq.3.9 will be true[1] if we require all expressions $\hat{u}, \hat{v}$ in the position and momentum variables obey:

$$\hat{v}\hat{u} - \hat{u}\hat{v} = k\{\hat{u}, \hat{v}\} \tag{3.10}$$

---

[1] We will not show here that, vice versa, *only* the condition Eq.3.10 ensures that Eq.3.9 holds true. If you are interested, there is plenty of literature on the topic of "quantization".

with k being some constant that commutes with everything. This is because in this case, the left and right hand sides of Eq.3.9 are automatically identical. But what value does k take? Of course, the case $k = 0$ would be classical mechanics, because it implies that all expressions in the positions and momenta commute.

However, it turns out that in order to eventually yield the correct experimental predictions (we will later see how), we have to set $k = -ih/2\pi$, i.e., we have

$$\hat{u}\hat{v} - \hat{v}\hat{u} = i\hbar\{\hat{u}, \hat{v}\} \tag{3.11}$$

where we used the convenient definition:

$$\hbar = \frac{h}{2\pi} \tag{3.12}$$

In particular, choosing for $\hat{u}$ and $\hat{v}$ the variables $x_i^{(r)}$ and $p_j^{(s)}$, and using Eqs.2.6-2.8, we now obtain the quantum mechanical commutation relations for n particles:

$$\begin{aligned}
\hat{x}_i^{(r)}\hat{p}_j^{(s)} - \hat{p}_j^{(s)}\hat{x}_i^{(r)} &= i\hbar\ \delta_{i,j}\delta_{r,s} &(3.13)\\
\hat{x}_i^{(r)}\hat{x}_j^{(s)} - \hat{x}_j^{(s)}\hat{x}_i^{(r)} &= 0 &(3.14)\\
\hat{p}_i^{(r)}\hat{p}_j^{(s)} - \hat{p}_j^{(s)}\hat{p}_i^{(r)} &= 0 &(3.15)
\end{aligned}$$

Let us keep in mind that we did not modify the rules of the Poisson bracket. We still have:

$$\begin{aligned}
\{\hat{x}_i, \hat{p}_j\} &= \delta_{i,j} &(3.16)\\
\{\hat{x}_i, \hat{x}_j\} &= 0 &(3.17)\\
\{\hat{p}_i, \hat{p}_j\} &= 0 &(3.18)
\end{aligned}$$

$$\begin{aligned}
\{f, g\} &= -\{g, f\} & &\text{antisymmetry} &(3.19)\\
\{cf, g\} &= c\,\{f, g\}, \quad \text{for any number } c & &\text{linearity} &(3.20)\\
\{f, g + h\} &= \{f, g\} + \{f, h\} & &\text{addition rule} &(3.21)\\
\{f, gh\} &= \{f, g\}h + g\{f, h\} & &\text{product rule} &(3.22)\\
0 &= \{f, \{g, h\}\} + \{h, \{f, g\}\} + \{g, \{h, f\}\} & &\text{Jacobi id.} &(3.23)
\end{aligned}$$

Because the rules for the Poisson bracket did not change with the upgrade to quantum mechanics, one arrives in quantum mechanics at the same equations of motion as in classical mechanics. This is as long as one does not unnecessarily commute any variables.

The equations Eqs.3.13-3.15 are called the “Canonical Commutation Relations” (CCRs). The appearance of the imaginary unit i will be necessary to ensure that measurements are predicted as real numbers, as we will see below. Eqs.3.14,3.15 express that position measurements among another and momentum measurements among another do not interfere. Only positions and momenta of the same particle and in the same direction, i.e., for $i = j$ and $r = s$, are noncommutative.

In conclusion, we upgrade classical mechanics to quantum mechanics by first formulating classical mechanics in Hamiltonian form to identify the Poisson algebra structure. Then, we realize that while keeping all the rules for the Poisson bracket intact, there is still the freedom to make the associative multiplication in the Poisson algebra noncommutative, parametrized by some constant k. Nature chose the modulus of k to be nonzero though very small, namely $\hbar$. The fact that the Poisson bracket stays the same when quantizing explains why quantum mechanics has the same equation of motion as does classical mechanics. The fact that $\hbar$ is so small explains why it took long to discover quantum mechanics.

In spite of the tremendous similarity between classical and quantum mechanics from this perspective, quantum mechanical calculations will in practise look rather different from classical calculations. This is because they will require representations of the $\hat{x}_i^{(r)}(t)$ and $\hat{p}_i^{(r)}(t)$ variables as explicit non-number valued mathematical entities that obey the commutation relations. Even though there is only a slight noncommutativity in the Poisson algebra of quantum mechanics its representations will necessarily look quite different from the representation of the classical commutative Poisson algebra. This will explain why the Schrödinger equation looks rather different from Newton's equations.

3.3 From the Hamiltonian to the equations of motion

In quantum mechanics, as in classical mechanics, the energy function $\hat{H}$ encodes all information about the system. It is still called the Hamiltonian and it is in general some polynomial (or well-behaved power series) in the positions and momenta $\hat{x}_i^{(r)}$ and $\hat{p}_i^{(r)}$ of the system. In quantum mechanics, the sequence of steps that lead from the Hamiltonian down to concrete number predictions for experiments can be drawn schematically in this form:

$$\begin{array}{c}\text{Hamiltonian}\\ \Downarrow\\ \text{Equations of motion}\\ \Downarrow\\ \text{Differential equations}\\ \Downarrow\\ \text{Non-number-valued functions}\\ \Downarrow\\ \text{Number-valued functions}\end{array}$$

$$\Downarrow$$

Number predictions

So far, we can perform the first step, namely the derivation of the equations of motion from the Hamiltonian: Assume that we are interested in the time evolution of some $\hat{f}$ which is a polynomial in the $\hat{x}$ and $\hat{p}$'s (say with constant coefficients). Then we can derive the equation of motion for $\hat{f}$ through:

$$\frac{d}{dt}\,\hat{f} \;=\; \{\hat{f},\hat{H}\} \tag{3.24}$$

where $\{,\}$ is the usual Poisson bracket, as defined in Eqs.2.6-2.12. In particular, $\hat{f}$ can be chosen to be any one of the position and momentum variables of the system, so that we obtain for their equations of motion, exactly as in Eqs.2.21,2.22:

$$\frac{d}{dt}\,\hat{x}_i^{(r)} \;=\; \{\hat{x}_i^{(r)},\hat{H}\} \tag{3.25}$$

$$\frac{d}{dt}\,\hat{p}_i^{(r)} \;=\; \{\hat{p}_i^{(r)},\hat{H}\} \tag{3.26}$$

By evaluating the Poisson bracket on the right hand side of Eqs.3.25,3.26 these equations of motion then become differential equations for the entities $\hat{x}_i^{(r)}(t)$ and $\hat{p}_i^{(r)}(t)$. Clearly, the resulting equations of motion will be analogous to those of classical mechanics. The entities $\hat{x}_i^{(r)}(t)$ and $\hat{p}_i^{(r)}(t)$ must also still obey Eq.3.2, which in quantum mechanics is usually written as:

$$\left(\hat{x}_i^{(r)}\right)^\dagger = \hat{x}_i^{(r)} \qquad \text{and} \qquad \left(\hat{p}_j^{(s)}\right)^\dagger = \hat{p}_j^{(s)} \tag{3.27}$$

We will call any polynomial or well-behaved power series $\hat{f}$ in the $\hat{x}$ and $\hat{p}$ an "observable", if it obeys $\hat{f}^\dagger = \hat{f}$. As we will see later, the condition $\hat{f}^\dagger = \hat{f}$ will indeed imply that measurement outcomes are predicted as real numbers. In addition to the position variables $\hat{x}_i^{(r)}(t)$ and momentum variables $\hat{p}_j^{(s)}(t)$ also, e.g., the energy $\hat{H}(t)$ and the angular momentum variables $\hat{L}_i(t)$ are observables.

While classical mechanics requires the Poisson algebra to be commutative, quantum mechanics requires that the equations of motion be solved by entities $\hat{x}_i^{(r)}(t)$ and $\hat{p}_i^{(r)}(t)$ which are noncommutative:

$$\hat{x}_i^{(r)}\hat{p}_j^{(s)} - \hat{p}_j^{(s)}\hat{x}_i^{(r)} \;=\; i\hbar\;\delta_{i,j}\delta_{r,s} \tag{3.28}$$

$$\hat{x}_i^{(r)}\hat{x}_j^{(s)} - \hat{x}_j^{(s)}\hat{x}_i^{(r)} \;=\; 0 \tag{3.29}$$

$$\hat{p}_i^{(r)}\hat{p}_j^{(s)} - \hat{p}_j^{(s)}\hat{p}_i^{(r)} \;=\; 0 \tag{3.30}$$

Technically, we will, therefore, need to solve differential equations of motion with noncommutative entities. In practice, the task is then to start from the top level of abstraction, the Hamiltonian of a system, then working one's way down by calculating the equations of motion, and then solving them to obtain something from which eventually predictions can be made of numbers that can be measured in experiments on the system. In the next section, we will investigate what kind of noncommutative mathematical objects, such as, for example, matrices, may represent the position and momentum variables.

Exercise 3.2 *For classical mechanics, formula Eq.2.37 provided a convenient representation of the Poisson bracket. However, Eq.2.37 is not a valid representation of the Poisson bracket in the case of quantum mechanics. In quantum mechanics, we have a (not so convenient) representation of the Poisson bracket through Eq.3.11:*

$$\{\hat{u},\hat{v}\} = \frac{1}{i\hbar}(\hat{u}\hat{v}-\hat{v}\hat{u}) \tag{3.31}$$

Use this representation, and the canonical commutation relations to evaluate the Poisson bracket $\{\hat{x}^2,\hat{p}\}$.

Let us introduce an often-used notation, called "the commutator":

$$[A,B] \ := \ A\ B \ - \ B\ A \tag{3.32}$$

For simplicity, assume that $\hat{H}$ and $\hat{f}$ are polynomials in the positions and momenta which depend on time only through their dependence on the $\hat{x}$ and $\hat{p}$. Then the Hamilton equation Eq.3.24 holds and takes the form:

$$i\hbar\,\frac{d}{dt}\,\hat{f}(t) \ = \ [\hat{f}(t),\hat{H}] \tag{3.33}$$

$$\tag{3.34}$$

and, in particular:

$$\begin{aligned} i\hbar\,\frac{d}{dt}\,\hat{x}_i^{(r)}(t) \ &= \ [\hat{x}_i^{(r)}(t),\hat{H}] \\ i\hbar\,\frac{d}{dt}\,\hat{p}_i^{(r)}(t) \ &= \ [\hat{p}_i^{(r)}(t),\hat{H}] \end{aligned} \tag{3.35}$$

These equations are called the Heisenberg equations of motion.

Remark: The particular method by which in the past few sections we upgraded classical mechanics to quantum mechanics is called canonical quantization. I covered it in some detail because of its importance: Essentially the same method was used to find quantum electrodynamics starting from Faraday and Maxwell's electromagnetism. All the quantum field theories of elementary particles can be derived this way. Even string theory and most other modern attempts at finding the unifying theory of quantum gravity try to employ canonical quantization. I should mention too that the problem of canonical quantization for constrained classical systems was also pioneered by Dirac but is still not fully understood. A simple example of a constrained system would be a particle that is constrained to move on a curved surface. The most important constrained system is general relativity.

Exercise 3.3 *Reconsider the system with the Hamiltonian Eq.2.4, which consists of two particles that are attracted to another through a harmonic force (a force which is proportional to their distance). In practice, for example the force that binds diatomic molecules and the force that keeps nucleons (i.e., neutrons and protons) inside a nucleus are approximately harmonic for small oscillations. In those cases, the effect of* $\hbar$ *cannot be neglected. One obtains the correct quantum theoretic Hamiltonian from the classical Hamiltonian of Eq.2.4 by simply placing hats on the* x *and* p*'s. Find explicitly all the equations of motion which the* $\hat{x}_i^{(r)}$ *and* $\hat{p}_j^{(r)}$ *(where* $r \in \{1,2\}$*) of this system must obey.*

Exercise 3.4 *To obtain the quantum Hamiltonian from the classical Hamiltonian and vice versa by placing or removing hats on the* x *and* p*'s is generally not as straightforward as in the previous exercise! Namely, there can occur so-called "ordering ambiguities": Consider the two Hamiltonians* $\hat{H}_1 = \hat{p}^2/2m + a(\hat{x}^2\hat{p}\hat{x} - \hat{x}\hat{p}\hat{x}^2)$ *and* $\hat{H}_2 = \hat{p}^2/2m + b(\hat{p}\hat{x}\hat{p}^2 - \hat{p}^2\hat{x}\hat{p})$ *where* a *and* b *are constants with appropriate units. Check whether or not these two Hamiltonians are the same in classical mechanics. Also find all choices of* a, b *for which the two Hamiltonians are the same in quantum mechanics.*

Exercise 3.5 *Find a Hamiltonian which contains at least one thousand powers of* $\hat{x}$ *and which also agrees with the Hamiltonian* $\hat{H}_1$ *of the previous exercise in classical mechanics. Make sure that your Hamiltonian is formally hermitean, i.e., that it obeys* $\hat{H}^\dagger = \hat{H}$*. Help: To ensure hermiticity, you can symmetrize. For example,* $\hat{x}\hat{p}^2$ *is not hermitean but* $(\hat{x}\hat{p}^2 + \hat{p}^2\hat{x})/2$ *is hermitean.*

Remark: In quantum theory, the choice of Hamiltonian always has an ordering ambiguity because one could always add to the Hamiltonian any extra terms that are proportional to $(\hat{x}\hat{p} - \hat{p}\hat{x})$ because those terms don't affect what the Hamiltonian is in classical mechanics. In principle, experiments are needed to decide which Hamiltonian is the correct one. In practice, the simplest choice is usually the correct choice. The simplest choice is obtained by symmetrizing the given classical Hamiltonian and then not adding any extra terms that are proportional to $\hat{x}\hat{p} - \hat{p}\hat{x}$. This is called the Weyl ordered Hamiltonian.

3.4 From the Hamiltonian to predictions of numbers

In the framework of classical mechanics we know how to descend from the most abstract level, where the system is described simply by giving its Hamiltonian H, down to the concrete level of predicting numbers for measurement outcomes. Now we will have to develop methods for descending in quantum mechanics from the level of the Hamiltonian down to the concrete predictions of numbers in experiments.

In the previous section, we already took the first step: we found that we can use the Hamiltonian to derive the differential equations of motion of the system. Since the Poisson brackets have not changed as we went from classical to quantum mechanics, the equations of motion are the same as those of classical mechanics[2].

The big change compared to classical mechanics, is that now the position and momentum variables $\hat{x}_i^{(r)}(t)$ and $\hat{p}_j^{(s)}(t)$ are noncommutative according to Eqs.3.28-3.30, and that they, therefore, can no longer be represented by number-valued functions of time. This means that the equations of motion can no longer be interpreted as differential equations for number-valued functions!

But we need to find a way to descend the ladder of abstractions all the way from the Hamiltonian on the top of the ladder down to concrete predictions of numbers at the bottom of the ladder. To that end, in order now to be able to solve the equations of motion as explicit differential equations, the $\hat{x}_i^{(r)}(t)$ and $\hat{p}_j^{(s)}(t)$ must be viewed as functions of time whose values are some kind of noncommutative mathematical objects. What kind of mathematical objects could these be?

3.4.1 Linear maps

Actually, *every* mathematical object can be viewed as a map, if need be, as a trivial map. For example the number 5 can be identified with the map that maps everything to 5. So let us look at maps. Let's try to represent the symbols $\hat{x}_i^{(r)}(t)$ and $\hat{p}_j^{(s)}(t)$ as some kind of explicit map-valued functions of time. A simple kind of maps is the linear maps. And they can be noncommutative! So this looks promising.

For example, any square matrix that acts on a finite-dimensional vector space of column vectors represents a linear map. And square matrices are generally noncommutative! In principle, we need the matrices to be square matrices so that they map back into the same vector space, so that we can multiply any two matrices on the same vector space. As we will see later, with some precautions, we can also consider infinite-by-infinite matrices that act as linear maps on infinite-dimensional vector spaces.

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[2] Except for the ordering ambiguity: when going from the classical to the quantum Hamiltonian we could (if we had any experimental reason to do so) add to the quantum Hamiltonian any hermitean terms that are proportional to $\hbar$, such as terms like $ig(\hat{x})(\hat{x}\hat{p}-\hat{p}\hat{x})\hat{g}(\hat{x})$ where g is some polynomial in $\hat{x}$.

There are actually many kinds of linear maps and they may not act on vector spaces of column vectors at all!

Let us consider, for example, the infinite-dimensional vector space $V := C^7(\mathbb{R})$ of seven times continuously differentiable functions on the real line. The set V forms a vector space because it obeys the defining axioms of a vector space: in brief, one can suitably add any two elements of V and get an element of V and one can suitably multiply any element of V with a number and get an element of V.

Exercise 3.6 *Find and list the precise axioms that a set has to obey to be called a vector space.*

Definition: *A map on a vector space that is infinite dimensional is called an operator.*

For example, the derivative operator, D, acts on functions in V in this way:

$$D : g(\lambda) \to \frac{d}{d\lambda} g(\lambda) \tag{3.36}$$

The operator D is a linear operator, i.e., it is a linear map, because it obeys $\partial_\lambda\ (c\, g(\lambda)) = c\ \partial_\lambda g(\lambda)$ for all numbers c and because $\partial_\lambda(g_1(\lambda) + g_2(\lambda)) = \partial_\lambda g_1(\lambda) + \partial_\lambda g_2(\lambda)$. Here, in order to simplify the notation, we introduced the notation: $\partial_\lambda := \frac{d}{d\lambda}$

Exercise 3.7 *Check whether or not the multiplication operator, M, which maps $M : g(\lambda) \to \lambda g(\lambda)$ is a linear operator.*

Exercise 3.8 *Show that the two operators D and M on V do not commute, namely by calculating $(DM - MD)g(\lambda)$.*

Exercise 3.9 *Check whether or not the operator Q which acts on functions in V as $Q : g(\lambda) \to \lambda^5 g(\lambda)$ is a linear operator.*

3.4.2 Choices of representation

We have just seen examples of linear maps and, since they generally do not commute, they may be useful for representing the variables $\hat{x}_i^{(r)}(t)$ and $\hat{p}_j^{(s)}(t)$ as explicit mathematical objects. And this is what we need to be able to descend further down the ladder of abstractions, down to predictions of numbers for measurement outcomes.

But could it be that one should use representations of the $\hat{x}_i^{(r)}(t)$ and $\hat{p}_j^{(s)}(t)$ as nonlinear maps instead? Non-linear representations have been considered in the literature. There are articles by Steven Weinberg, for example, on this topic. This work has shown, however, that any attempt at using nonlinear spaces or nonlinear operators to define quantum theories generally leads to physically incorrect predictions. We will, therefore, here only consider linear representations.

Now that we have settled on representations of the variables $\hat{x}_i^{(r)}(t)$ and $\hat{p}_j^{(s)}(t)$ as linear operators, we still have plenty of choice, because there are so many vector spaces and so many linear operators on them. And this leads to a worry: could it happen that we invest great effort in developing one particular kind of representation of the variables $\hat{x}_i^{(r)}(t)$ and $\hat{p}_j^{(s)}(t)$ as operators, say as matrices, and then it turns out that we have bet on the wrong horse? Maybe, we should have instead developed a representation of the $\hat{x}_i^{(r)}(t)$ and $\hat{p}_j^{(s)}(t)$ as, for example, multiplication and differentiation operators?

Fortunately, essentially[3] all linear representations of variables $\hat{x}_i^{(r)}(t)$ and $\hat{p}_j^{(s)}(t)$ that obey the canonical commutation relations are equivalent, i.e., they lead to the exact same predictions! This is the content of the Stone von Neumann theorem, which we will later cover more precisely. Technically, as we will see, all linear representations are the same, up to a change of basis in the vector space. It may seem strange that, for example, a space of column vectors with countably infinitely many entries could be isomorphic to some space of functions on the real line. But this is what will turn out to be the case[4]!

So to recapitulate: our task is to solve the equations of motion, the hermiticity conditions and the canonical commutation relations for $\hat{x}_i^{(r)}(t)$ and $\hat{p}_j^{(s)}(t)$ as linear-map-valued (instead of number-valued) functions of time.

We now know that the choice of which kind of linear representation we use will ultimately not matter when calculating physical predictions.

As our first choice, let us, therefore, use the most concrete kind of linear maps to represent the $\hat{x}_i^{(r)}(t)$ and $\hat{p}_j^{(s)}(t)$, namely, let us try to represent them as matrix-valued functions in time. Historically, quantum mechanics was actually first written down in terms of matrix-valued functions, back in June 1925 when the young Heisenberg had some quiet time while escaping his hay fever on the island of Helgoland in the North Sea.

3.4.3 A matrix representation

Let us now find out how the variables $\hat{x}_i^{(r)}(t)$ and $\hat{p}_j^{(s)}(t)$ can be represented as matrix-valued functions in time, and how, therefore, the abstract equations of motion can be represented as explicit matrix differential equations for matrix-valued functions of time. To keep the number of indices in check, we will restrict ourselves here to the case of just one $\hat{x}(t)$ and one $\hat{p}(t)$ operator.

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[3] There is a small subtlety, arising from the fact that, as we'll see later, the $\hat{x}$ and $\hat{p}$ are what are called unbounded operators. This leaves some loopholes, in principle, but nature does not appear to make use of those.

[4] If you want to know the essence already: the space of functions will be the set of equivalence classes of square-integrable functions, two functions being in the same equivalence class if their difference has vanishing integral over its norm squared. In this space of equivalence classes one can find bases of countably infinitely many basis vectors.

The canonical commutation relations are of course to hold at all times. To begin with, let us ask whether it is possible to find two $N \times N$ matrices $\hat{x}(t_0)$ and $\hat{p}(t_0)$ so that at the starting time, t_0, of the experiment the canonical commutation relations hold:

$$\hat{x}(t_0)\,\hat{p}(t_0)\, - \hat{p}(t_0)\,\hat{x}(t_0) \;=\; i\hbar\,\mathbf{1} \tag{3.37}$$

Here, $\mathbf{1}$ is the identity matrix. At this point it is useful to remember that the trace of matrices $\mathrm{Tr}(A) = \sum_n A_{n,n}$ is linear and cyclic:

$$\mathrm{Tr}(A+B) = \mathrm{Tr}(A) + \mathrm{Tr}(B) \quad \text{and} \quad \mathrm{Tr}(AB) = \mathrm{Tr}(BA) \tag{3.38}$$

Exercise 3.10 *Verify Eqs.3.38 by writing the matrices in an orthonormal basis, i.e., with indices, and by then evaluating the trace by summing up the matrix elements on the diagonal.*

We see that the trace of the left hand side of Eq.3.37 vanishes, while the trace of the right hand side is $i\hbar N$. Thus, there are in fact no $N \times N$ matrices, i.e., there are no finite-dimensional matrices $\hat{x}(t_0)$ and $\hat{p}(t_0)$ that obey the commutation relation Eq.3.37! For infinite dimensional matrices, however, the trace may be ill-defined on both sides, and our argument then does not apply. In fact, there exist infinite-dimensional matrices which do obey the commutation relation.

In order to find such matrices we start by defining the $\infty \times \infty$ dimensional matrix:

$$a_{n,m} = \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \\ 0 & 0 & \sqrt{2} & 0 & 0 & \\ 0 & 0 & 0 & \sqrt{3} & 0 & \\ 0 & 0 & 0 & 0 & \sqrt{4} & \\ 0 & 0 & 0 & 0 & 0 & \\ & & & & & \ddots \end{pmatrix}_{n,m} \tag{3.39}$$

The hermitean conjugate is:

$$a^{\dagger}_{n,m} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \\ \sqrt{1} & 0 & 0 & 0 & 0 & \\ 0 & \sqrt{2} & 0 & 0 & 0 & \\ 0 & 0 & \sqrt{3} & 0 & 0 & \\ 0 & 0 & 0 & \sqrt{4} & 0 & \\ & & & & & \ddots \end{pmatrix}_{n,m} \tag{3.40}$$

Their commutation commutation relation is:

$$aa^{\dagger} - a^{\dagger}a \;=\; \mathbf{1} \tag{3.41}$$

Since they are not numbers, we should decorate a and $a^\dagger$ with hats but traditionally one doesn't put hats on these operators.

Remark: *In case you are wondering because you feel that you have seen similar things before: fundamentally, these operators a and $a^\dagger$ have absolutely nothing to do with harmonic oscillators. What we are currently doing will be good for any choice of system, not just harmonic oscillators. We are currently developing a representation of the variables $\hat{x}(t)$ and $\hat{p}(t)$ as matrices and this representation will, of course, be good for any arbitrary choice of Hamiltonian*[5]*.*

Exercise 3.11 *Verify Eq.3.41.*

Using a and $a^\dagger$, we can now represent $\hat{x}(t_0)$ and $\hat{p}(t_0)$ as matrices that obey the canonical commutation relation, namely by defining:

$$\hat{x}(t_0) = L(a^\dagger + a) \tag{3.42}$$

and

$$\hat{p}(t_0) = \frac{i\hbar}{2L}(a^\dagger - a) \tag{3.43}$$

Here, L is some arbitrary real number with units of length, which we need because $\hat{x}$ has a unit of length while a and $a^\dagger$ do not have units. The definitions are such that the realness conditions Eqs.3.27 are obeyed, i.e., such that the matrices are formally[6] hermitean: $\hat{x}^\dagger(t_0) = \hat{x}(t_0)$ and $\hat{p}^\dagger(t_0) = \hat{p}(t_0)$.

Exercise 3.12 *Verify that the two matrices defined in Eqs.3.42,3.43 with the help of Eqs.3.39,3.40, are formally hermitean. I am using the term "formally" here to indicate that, for the purposes of this exercise, you need not worry about potential subtleties that may arise because these matrices are infinite dimensional.*

Exercise 3.13 *Show that the hermitean conjugation of matrices reverses the order, i.e., that if A and B are linear maps, then $(AB)^\dagger = B^\dagger A^\dagger$. To this end, write out the matrices with indices and use that hermitean conjugating a matrix means transposing and complex conjugating it.*

Technically, † is a map from the Poisson algebra into itself which is called an involution because it is its own inverse. Because it also reverses the order it is called an "anti" algebra mapping: First multiplying and then applying † is the same as first applying † and then multiplying, up to the reversal of the order.

We see, therefore, why the imaginary unit i appeared in the canonical commutation relations: If we apply † to the commutation relations $\hat{x}\hat{p} - \hat{p}\hat{x} = k\mathbf{1}$ we obtain $\hat{p}\hat{x} - \hat{p}\hat{x} = k^*\mathbf{1}$, i.e., we obtain $k = -k^*$. Thus, k has to be imaginary. And of course it is: $k = i\hbar$.

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[5] Still, it is true also that the use of the a and $a^\dagger$ will be particularly convenient when considering the special case of harmonic oscillators.

[6] I am writing here "formally" hermitean, because the issue of whether a matrix is hermitean, symmetric or self-adjoint is quite subtle for infinite-dimensional matrices, as we will see later.

3.4.4 Example: Solving the equations of motion for a free particle with matrix-valued functions

In the case of the free particle which moves in one dimension, the Hamiltonian is $\hat{H} = \hat{p}^2/2m$. The Hamilton equations or, equivalently, the Heisenberg equations, yield the abstract equations of motion:

$$\frac{d}{dt}\hat{x}(t) = \frac{1}{m}\hat{p}(t) \tag{3.44}$$

$$\frac{d}{dt}\hat{p}(t) = 0 \tag{3.45}$$

Let us view these equations as matrix equations. Using the results of the previous section, it becomes clear that these equations are solved through

$$\hat{x}(t) = \hat{x}(t_0) + \frac{(t-t_0)}{m}\hat{p}(t_0) \tag{3.46}$$

and

$$\hat{p}(t) = \hat{p}(t_0), \tag{3.47}$$

where $\hat{x}(t_0)$ and $\hat{p}(t_0)$ are the matrices of Eqs.3.42,3.43. Concretely, by substituting in the matrices a and $a^\dagger$, we have:

$$\hat{x}(t)_{n,m} = \begin{pmatrix} 0 & \sqrt{1}\left(L - \frac{i\hbar(t-t_0)}{2Lm}\right) & 0 & \\ \sqrt{1}\left(L + \frac{i\hbar(t-t_0)}{2Lm}\right) & 0 & \sqrt{2}\left(L - \frac{i\hbar(t-t_0)}{2Lm}\right) & \\ 0 & \sqrt{2}\left(L + \frac{i\hbar(t-t_0)}{2Lm}\right) & 0 & \\ & & & \ddots \end{pmatrix} \tag{3.48}$$

$$\hat{p}(t)_{n,m} = \begin{pmatrix} 0 & -\sqrt{1}\frac{i\hbar}{2L} & 0 & \\ \sqrt{1}\frac{i\hbar}{2L} & 0 & -\sqrt{2}\frac{i\hbar}{2L} & \\ 0 & \sqrt{2}\frac{i\hbar}{2L} & 0 & \\ & & & \ddots \end{pmatrix} \tag{3.49}$$

For simplicity, not all the many zeros in these matrices are shown. The only nonzero terms are immediately to the left and right of the diagonal.

Exercise 3.14 *Show that the matrices $\hat{x}(t)$ and $\hat{p}(t)$ obey at all times $t > t_0$ all the quantum mechanical conditions, i.e., the equations of motion, the hermiticity condition, and the commutation relation.*

Remark: We had constructed the representation in such a way that the commutation relation and the hermiticity condition hold at the initial time t_0. Having solved the equations of motion we found that the commutation relation and the hermiticity conditions continue to hold at all times t. This is nontrivial but it is not a coincidence. As we will soon see, the quantum mechanical time evolution of all systems[7] preserves the commutation relations and hermiticity. The preservation of the commutation relations is of course the preservation of the Poisson bracket. And we have in classical and quantum mechanics that the Poisson brackets between the positions and momenta are preserved by the dynamics through the Hamilton equation: $d/dt\ \{\hat{x},\hat{p}\} = \{\{\hat{x},\hat{p}\},\hat{H}\} = \{1,\hat{H}\} = 0$. We can also turn the logic around. Assume we know nothing about Hamiltonians and about the dynamics of quantum systems. Except, we may want to assume that, whatever the time evolution is, it must preserve the Poisson algebra structure, i.e., we require that the Poisson brackets be conserved in time. The structure of the Poisson algebra then demands (we don't show this explicitly here) that the time evolution must be generated through an equation of the type of the Hamilton equation, by some generator which we may call H, and which we may then as well call the Hamiltonian.

3.4.5 Example: Solving the equations of motion for a harmonic oscillator with matrix-valued functions

The vibrational degree of freedom of a diatomic molecule such as HF, CO or HCl can be described as a harmonic oscillator (as long as the oscillations are small). Now let x stand for the deviation from the equilibrium distance between the two nuclei. This distance oscillates harmonically and is described by this effective Hamiltonian of the form of a harmonic oscillator:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2 \tag{3.50}$$

The term "Effective Hamiltonian" expresses the fact that this Hamiltonian is not really the exact Hamiltonian but that it is a good approximation to the Hamiltonian in the regime of low energies (i.e., of small oscillations) that we are considering here. By the way, how do we know that the true Hamiltonian is not simply a harmonic oscillator? Easy: we know from experiments that diatomic molecules will, for example, split apart at sufficiently high temperatures, i.e., that they do not have infinite binding energy. A harmonic oscillator potential, however, just keeps going up faster with distance and therefore if you tried to pull apart the two particles in the diatomic molecule, they would just get pulled together more and more strongly. Diatomic molecules could never be split if they were truly harmonically bound.

So then if we know that the true potential is not harmonic, how do we know that a harmonic potential is a good approximation at low energies? That's because

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[7] With the possible exception of systems that involve black hole horizons or other gravitational horizons or singularities.

any potential $V(x)$ is normally well described by a smooth function $V(x)$ with a minimum at, say x_0, around which we can Taylor expand the potential: $V(x) = V(x_0) + V'(x_0)(x - x_0) + \frac{1}{2}V"(x_0)(x - x_0)^2 + ...$ Here, $V'(x_0) = 0$ because x_0 is assumed to be the minimum and therefore in the regime of small oscillations, where x is close to x_0, any potential starts out quadratic, i.e., as a harmonic oscillator.

Now let us remember that the matrix-valued functions $\hat{x}(t)$ and $\hat{p}(t)$ that we want to solve the harmonic oscillator problem Eq.3.50 have to obey three conditions, as always in quantum theory. First, the matrix-valued functions $\hat{x}(t)$ and $\hat{p}(t)$ must obey the equations of motion of the harmonic oscillator given in Eq.3.50. Second, they must be hermitean, $\hat{x}(t) = \hat{x}^\dagger(t)$ and $\hat{p}(t) = \hat{p}^\dagger(t)$. Third, they must obey the canonical commutation relation $[\hat{x}(t), \hat{p}(t)] = i\hbar 1$ (where 1 is now to be represented by the identity matrix).

Now the first problem would seem easy to solve: we know that the equations of motion are solved any linear combination of $\sin(\omega t)$ and $\cos(\omega t)$. But these are just number-valued functions and cannot by themselves obey the commutation relations! On the other hand, we do have matrices a and $a^\dagger$ that are beautifully noncommutative. But they are constant in time and therefore cannot alone describe the dynamics given by the equations of motion. This suggests that we try to construct the solution by combining the a and $a^\dagger$ matrices with the sine and cosine solutions. Let's try this ansatz[8]

$$\hat{x}(t) = \xi(t)a + \xi^*(t)a^\dagger, \tag{3.51}$$

and let us choose $\xi(t)$ to be a linear combination of the sine and cosine solutions to the equations of motion:

$$\xi(t) := r\sin(\omega t) + s\cos(\omega t) \tag{3.52}$$

Here, for now, r and s can be any complex numbers. By the way, whenever one makes an ansatz of this kind (and one often does, especially in quantum field theory), then $\xi(t)$ is called a mode function. The task now is to find out if we can find coefficients r and s such that the matrix-valued function $\hat{x}(t)$ and the corresponding $\hat{p}(t) = m\dot{\hat{x}}(t)$ obey the equations of motion, are hermitean and obey the canonical commutation relation.

Exercise 3.15 *Show that for any arbitrary choice of complex numbers r, s, the matrix-valued functions $\hat{x}(t)$ and $\hat{p}(t)$ defined through Eqs.3.51,3.52 obey the equations of motion at all time.*

Exercise 3.16 *Show that, again for any arbitrary choice of complex numbers r, s, the matrix-valued functions $\hat{x}(t)$ and $\hat{p}(t)$ defined through Eqs.3.51,3.52 obey the hermiticity conditions at all time.*

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[8] An ansatz is an educated guess.

Exercise 3.17 *Find the equation that the complex numbers* r, s *have to obey so that the matrix-valued functions* $\hat{x}(t)$ *and* $\hat{p}(t)$ *defined through Eqs.3.51,3.52 obey the canonical commutation relations at all time. This equation for* r, s *is called the Wronskian condition and it has many solutions. Give an example of a pair of complex numbers* r, s *that obey the Wronskian condition and write down* $\hat{x}(t)$ *explicitly with these values for* r, s *filled in.*

Since there are many pairs r, s that obey the Wronskian condition, our ansatz given by Eqs.3.51,3.52 allows us to generate many solutions! We knew that there are always many linear representations of $\hat{x}(t)$ and $\hat{p}(t)$ in quantum theory (and that they are all physically equivalent because they are all related by changes of bases). Here, with our ansatz we have found already infinitely many of these representations of $\hat{x}(t)$ and $\hat{p}(t)$ for the harmonic oscillator. Actually, among the representations that we just found, some representations are particularly convenient and most of the time one uses one of those. These choices of r, s turn out to be convenient because the matrix-representation of the Hamiltonian $\hat{H}(t)$ is much simpler for clever choices of r, s than for other choices.

Exercise 3.18 *Use Eqs.3.51,3.52 to express the Hamiltonian in terms of functions and the operators* $a, a^\dagger$. *There should be terms proportional to* a^2, *to* $(a^\dagger)^2, aa^\dagger$ *and* $a^\dagger a$.

Exercise 3.19 *It turns out that it is possible to choose the coefficients* r *and* s *so that the terms in the Hamiltonian which are proportional to* a^2 *and* $(a^\dagger)^2$ *drop out. Find the condition which the equation that* r *and* s *have to obey for this to happen. Choose a pair of complex numbers* r, s *such that the Hamiltonian simplifies this way, and of course such that the Wronskian condition is obeyed. Write down* $\hat{H}(t)$ *as an explicit matrix for this choice of* r, s. *It should be a diagonal matrix.*

Remark: Notice that this convenient choice of r, s depends on the parameters m and ω of the harmonic oscillator. This means that each harmonic oscillator has its own optimal choices of parameters r, s. Making such wise choices of the parameters r, s is particularly useful in quantum field theory where each wavevector (and therefore frequency ω) of a quantum field has its own harmonic oscillator degree of freedom, and should therefore best have its own convenient choice of r, s that diagonalizes its Hamiltonian.

3.4.6 From matrix-valued functions to number predictions

Let us assume now that we have solved a quantum mechanical problem in the sense that we have found explicit matrix-valued functions $\hat{x}_i^{(r)}(t)$ and $\hat{p}_j^{(j)}(t)$ which obey the canonical commutation relations, the hermiticity conditions, and the equations of motion. For example, the quantum mechanical problem of the free particle in one dimension is solved by the matrix-valued functions given in Eqs.3.48,3.49.

How then are we to further descend the ladder of abstraction, down to the most concrete level, namely that of predictions of numbers that will be measured in experiments? How can we extract from those matrix-valued functions the information which will let us predict the outcome of say a position or a momentum measurement at some time t?

To this end, assume that we have solved the dynamics, i.e., that we have calculated $\hat{x}(t)$ and $\hat{p}(t)$ as explicit matrix-valued functions of time. Then we can also immediately write down the time evolution of any polynomial $f(\hat{x}(t), \hat{p}(t))$ of the $\hat{x}(t)$ and $\hat{p}(t)$ that we may be interested in. For example, we can write down the time evolution of the Hamiltonian $\hat{H}(\hat{x}(t), \hat{p}(t))$ or say the first component of the angular momentum: $\hat{L}_3(t) = \hat{x}_2(t)\hat{p}_3(t) - \hat{p}_2(t)\hat{x}_3(t)$.

Mathematically, the problem now boils boils down to this question: Given such a matrix valued function $\hat{f}(\hat{x}(t), \hat{p}(t))$, let us pick a time t. Then $\hat{f}(\hat{x}(t), \hat{p}(t))$ at the time t is an explicit infinite-by-infinite matrix. How can we extract from that matrix a prediction for the number-valued outcome, $\bar{f}(t)$, of an experiment that measures $\hat{f}$? For example, say we want to measure the position at time t. Given the matrix $\hat{x}(t)$ by what method can we extract from that matrix a prediction for the position $\bar{x}(t)$?

To find that method, let us start with the observation that the method by which we extract a number-valued prediction $\bar{f}(t)$ from a matrix $\hat{f}(t)$ should not depend on the basis in which we write down the matrix $\hat{f}(t)$. The reason is that a change of basis in a vector space yields merely another way to write down the same linear map. And physical predictions should not depend on any human choice of how (i.e., in which basis) to write down a map. This means that $\bar{f}(t)$ should be a scalar formed from the matrix $\hat{f}(t)$.

Now how can one get a scalar from a matrix? By using the scalar product of course. So assume that we are given two column vectors with coefficients ψ_i and ϕ_i. Then

$$\sum_{n,m=1}^{\infty} \psi_n^* \hat{f}_{n,m}(t) \phi_m \tag{3.53}$$

is scalar. Could this be the prediction for the measurement outcome? No this cannot be quite right because this quantity is generally complex while measurement outcomes are of course always real numbers. This leaves us with the conjecture that the predicted value, which we will denote by $\bar{f}(t)$ for a measurement of $\hat{f}(t)$ at time t, is[9] of the form:

$$\bar{f}(t) = \sum_{n,m=1}^{\infty} \psi_n^* \hat{f}_{n,m}(t)\psi_m \tag{3.54}$$

Now that we are using the same vector left and right, this number is guaranteed to be real for all quantities $\hat{f}$ which are hermitean, $\hat{f}^\dagger = \hat{f}$, i.e., for all quantities that in classical mechanics are real-valued, as it should be.

Let us check that Eq.3.54 always comes out real if $\hat{f}$ is what is called an observable, i.e., if $\hat{f}$ obeys $\hat{f}^\dagger = \hat{f}$, i.e., if $\hat{f}_{s,r}^* = \hat{f}_{r,s}$. Indeed[10]:

$$\bar{f}(t)^* = \left(\sum_{r,s=1}^{\infty} \psi_r^* \hat{f}_{r,s}(t)\psi_s\right)^* = \sum_{r,s=1}^{\infty} \psi_r \hat{f}_{r,s}^*(t)\psi_s^* = \sum_{r,s=1}^{\infty} \psi_s^* \hat{f}_{s,r}(t)\psi_r = \bar{f}(t) \tag{3.55}$$

So this works! And, for example, the predictions for measurements at time t of the position, momentum, angular momentum or energy are, therefore:

$$\bar{x}(t) = \sum_{n,m=1}^{\infty} \psi_n^* \hat{x}_{n,m}(t)\psi_m \tag{3.56}$$

$$\bar{p}(t) = \sum_{n,m=1}^{\infty} \psi_n^* \hat{p}_{n,m}(t)\psi_m \tag{3.57}$$

$$\bar{L}^{(i)}(t) = \sum_{n,m=1}^{\infty} \psi_n^* \hat{L}_{n,m}^{(i)}(t)\psi_m \tag{3.58}$$

$$\bar{H}(t) = \sum_{n,m=1}^{\infty} \psi_n^* \hat{H}_{n,m}(t)\psi_m \tag{3.59}$$

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[9] There is a more general possibility: clearly, $\bar{f}$ should depend on $\hat{f}$ linearly (they have the same units) and this leaves the possibility that $\bar{f}(t) = \text{Tr}(\rho\hat{f}(t)) = \sum_{i,j}\rho_{i,j}\hat{f}_{j,i}(t)$ where ρ is some hermitean matrix. As we will see, we will make use of this possibility when describing a system whose initial conditions we are not quite sure of, where we can only give probabilities of initial conditions, i.e., where we don't even know for sure even the initial expectation values of the various observables. In this case, we say that the system is described by a mixed state and the matrix ρ is called the mixed state matrix. The term "mixed" is used because the uncertainties in predictions then have mixed origins - both from quantum effects but also from our ignorance of the system to start with. What we consider so far are so-called pure states ψ, which are the special case where $\rho_{i,j} = \psi_i^*\psi_j$. For general ρ, the normalization condition $\sum_i \psi_i^*\psi_i = 1$ is replaced by $\text{Tr}(\rho) = 1$.

[10] This argument is correct for finite-dimensional matrices only. Quantum mechanics requires infinite-dimensional matrices where the sums are infinite sums and analytic issues therefore arise. That there is a fundamental difference between finite and infinite-dimensional vector spaces we saw earlier when we found that the canonical commutation relations do not possess finite-dimensional representations. We will, therefore, later revisit the issue of hermiticity.

3.5 Initial conditions

In order to obtain those scalar functions for predictions, $\bar{f}(t)$, we had to introduce a complex vector with infinitely many coefficients!

$$\psi_n = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \vdots \end{pmatrix} \tag{3.60}$$

We are free to choose ψ, and it is a convention to choose a vector ψ of unit length, i.e., for which $\sum_n^\infty \psi_n^* \psi_n = 1$. We call such vectors normalized. For example, the vector ψ could be given by:

$$\psi_n = \frac{1}{5} \begin{pmatrix} 4 \\ 3i \\ 0 \\ 0 \\ \vdots \end{pmatrix} \tag{3.61}$$

There are, of course, infinitely many choices for such vectors ψ. But what does making a choice of such a vector ψ mean? What is the physics of that choice?

Obviously the choice of ψ determines the predictions that we make for **all** possible measurements at any time t! The choice of ψ in fact even determines what the expected outcome is for measurements at the initial time t_0! And this last observation reveals what the choice of the vector ψ means physically: the choice of ψ is the choice of initial conditions!

Remember that when we solved the equations of motion to obtain those matrix-valued functions $\hat{x}(t)$ and $\hat{p}(t)$, we did not have an opportunity to specify the initial conditions of the experimental setup. We did not have an opportunity to specify, for example, whether the particle was initially, i.e., at the time t_0, fast or slow, or where the particle was at the initial time t_0.

Now we have an opportunity to specify how the system started off at time t_0: The choice of ψ encodes our specification of the initial state of the system: by choosing a vector ψ we are choosing an experimental starting condition at time t_0. Namely, by choosing ψ, we are choosing what measurement outcomes to expect if we measure *any arbitrary observable,* $\hat{f}$, right at the initial time t_0. Since there are infinitely many observables, it is plausible that we get to choose infinitely coefficients in ψ to fix their initial conditions. For example, some of these observables are:

$$\bar{x}(t_0) = \sum_{n,m=1}^{\infty} \psi_n^* \hat{x}_{n,m}(t_0) \psi_m \tag{3.62}$$

$$\bar{p}(t_0) = \sum_{n,m=1}^{\infty} \psi_n^* \hat{p}_{n,m}(t_0) \psi_m \tag{3.63}$$

$$\bar{L}^{(i)}(t_0) = \sum_{n,m=1}^{\infty} \psi_n^* \hat{L}^{(i)}_{n,m}(t_0)\psi_m \tag{3.64}$$

$$\bar{H}(t_0) = \sum_{n,m=1}^{\infty} \psi_n^* \hat{H}_{n,m}(t_0)\psi_m \tag{3.65}$$

And of course also for any $\hat{f}$ obeying $\hat{f}^\dagger = \hat{f}$, we have

$$\bar{f}(t_0) = \sum_{n,m=1}^{\infty} \psi_n^* \hat{f}_{n,m}(t_0)\psi_m \tag{3.66}$$

3.6 Emergence of probabilities

The fact that we have equations of motion and that initial conditions are to be specified is not unusual of course, because this is also what one does in classical mechanics. But what seems unusual here is that we have to specify so many initial conditions. In order to choose a vector ψ that describes the initial state of our quantum system, we get to choose its infinitely many coefficients ψ_i (with the only constraint being that ψ should be normalized). Why are there so many initial conditions? In classical mechanics, it sufficed to specify the initial position and the initial momentum and that determined the initial state completely! And from that initial condition you could then calculate $x(t)$ and $p(t)$. And, in classical mechanics, once you have $x(t)$ and $p(t)$ you automatically also have the predictions for any $f(x(t), p(t))$.

So let us ask: in quantum mechanics, does it really matter which values we choose for the infinitely many coefficients of ψ or do perhaps only two of these coefficients matter? Isn't it the case that once we can make a prediction $\bar{x}(t)$ and $\bar{p}(t)$ we can also predict any $\bar{f}(\hat{x}(t), \hat{p}(t))$? If that were true, then this should be true:

$$\bar{f}(\hat{x}(t), \hat{p}(t)) = f(\bar{x}(t), \bar{p}(t)) \tag{3.67}$$

Actually, this equation does generally not hold in quantum mechanics! Mathematically, it is because, for example, when A is a square matrix and v is a vector then generally $v^\dagger A^n v \neq (v^\dagger A v)^n$. Therefore, just because we have a prediction for the position and the momentum does not mean that we have a prediction for other measurements such as the energy or the angular momentum!

Exercise 3.20 *Give a counter example for Eq.3.67. To this end, write out Eq.3.67 explicitly, i.e., in matrix form, for the case* $\hat{f}(\hat{x}(t), \hat{p}(t)) = \hat{x}^2$. *Then choose a suitable normalized* ψ *so that Eq.3.67 is seen to be violated. (It is not difficult to find such a* ψ*, almost every one will do.)*

On one hand, this explains why, mathematically, we have to specify so many initial conditions in quantum mechanics, namely all those coefficients ψ_i. But what is the physics of this?

To see this, let us have a closer look at the observation that knowing the number-valued predictions $\bar{x}(t), \bar{p}(t)$ does not alone suffice to make predictions of the outcome of other measurements $\bar{f}$. Namely, this means, in particular, that even if we have a prediction for, say, the position, $\bar{x}(t)$, we actually don't automatically have also a prediction for the square of the position: $\overline{x^2}(t)$.

From the perspective of classical mechanics this is weird. If we have a prediction for the position shouldn't we have a prediction for the square of it too? Well yes. Except, if the prediction is not certain, if it has some statistical spread or uncertainty. Then, even in classical physics, the square of the expectation value of a measurement need not be the expectation value of the square. In fact, as is well known, the statistical variance $(\Delta(Q))^2$ of any variable Q is defined as the difference between the two

$$(\Delta(Q))^2 := \overline{\left(Q - \bar{Q}\right)^2} = \overline{Q^2} - \bar{Q}^2 \tag{3.68}$$

which, as the middle term shows, is also the mean of the squared deviation from the mean. ΔQ is called the uncertainty in Q.

Now in quantum mechanics, if $\hat{f}$ is an observable, i.e., if it is hermitean, so is $\hat{f}^2$. This is because if $\hat{f}^\dagger = \hat{f}$ then $(\hat{f}^2)^\dagger = \hat{f}^2$. And it is important that in quantum mechanics they are independent observables. For example, their initial values can be specified independently. This is because, as always in statistics, we generally have $\overline{f^2} \neq \bar{f}^2$. The average of some squared numbers is rarely the same as the square of the average of those numbers: generally, e.g. $(a_1^2 + a_2^2)/2 \neq ((a_1 + a_2)/2)^2$. Interestingly, this means that quantum mechanics also allows us to calculate the variance in the set of measurement outcomes of each observable $\hat{f}$, namely through this mean value:

$$(\Delta f(t))^2 = \overline{(f(t) - \bar{f}(t))^2} = \overline{f^2(t)} - \bar{f}^2 \tag{3.69}$$

For example, from Eq.3.69:

$$(\Delta x(t))^2 = \sum_{r,s,t=1}^{\infty} \psi_r^* \hat{x}_{r,s} \hat{x}_{s,t} \psi_t - \left(\sum_{u,v=1}^{\infty} (\psi_u^* \hat{x}_{u,v} \psi_v) \right)^2 \tag{3.70}$$

Here, the number $\hat{x}_{r,s}$ is the matrix element of the matrix $\hat{x}$ with indices r, s. Similarly, given ψ, also all the higher moments of the probability distributions of positions and momenta are predictable, such as $\overline{x^n}(t)$ and $\overline{p^n}(t)$.

What we have found, therefore, is that in quantum mechanics, since the predictions generally (i.e., except for special cases) obey

$$\bar{f}(\hat{x}(t), \hat{p}(t)) \neq f(\bar{x}(t), \bar{p}(t)), \tag{3.71}$$

the predictions should come with uncertainty. They should be statistical. Our predictions for observables $\bar{f}(t)$ such as $\bar{x}(t), \bar{p}(t), \bar{H}(t), \bar{L}_i(t)$, ... can only be predictions for expectation values. There will generally be a spread of outcomes, i.e., there will be nontrivial variances. This crucial finding, namely that the predicted expectation values of observables $\hat{f}$ are largely independent, also explains why it takes so many numbers, namely all the coefficients ψ_i to specify initial conditions in quantum mechanics. In effect, one has to specify all the initial expectation values of all the possible observables. And there are infinitely many polynomials $\hat{f}(\hat{x},\hat{p})$ that obey $\hat{f}(\hat{x},\hat{p})^\dagger = \hat{f}(\hat{x},\hat{p})$. In effect, we need to specify so many initial conditions because we need to fix an entire probability distribution.

We therefore arrive at this interpretation: Assume we run an ensemble of experiments, each with the same initial experimental setup, i.e., all described by the same initial state vector ψ. Then, having calculated the solutions to the equations of motion as in Eqs.3.48,3.49, we can calculate the mean of any observable $\bar{f}(t)$, such as, for example, position $\bar{x}(t)$ and momentum $\bar{p}(t)$ that will be measured in an ensemble of measurements by using Eqs.3.56,3.57. In fact, we can only predict means. But this also includes the ability to predict the variance of any variable, because the variance of an observable is a mean value too, as Eq.3.69 shows.

Remark: Also for systems of many particles, such as a molecule, all observables $\hat{f}(t)$, such as $\hat{x}_i^{(r)}$ and $\hat{p}_j^{(s)}$, can be represented as matrices acting in the same vector space. The choice of ψ in this vector space determines how all the constituent particles start off, because all $\bar{f}(t_0)$ are determined, including, e.g., $\bar{x}_i^{(r)}(t_0) = \sum_i \psi_i^* \hat{x}_i^{(r)}(t_0)\psi_i$ etc.

Remark: We say that ψ is the so-called *state vector* of the system. It is clear from Eqs.3.54 that if two state vectors ψ and ϕ differ only by a phase, $\psi_n = e^{i\alpha}\phi_n$ for all n, then they yield the same predictions and are, therefore, describing the same state. The state vector of any system is defined only up to an overall phase.

Remark: Conversely, assume we prepare an experimental setup for which we know the ensemble mean values at initial time $\bar{f}(t)$ for all observables $\hat{f}$:

$$\bar{x}(t_0) = a_1, \quad \bar{p}(t_0) = a_2, \quad \overline{x^2}(t_0) = a_3, \quad \overline{p^2}(t_0) = a_4, \quad \overline{x^3}(t_0) = a_5, \quad ... \tag{3.72}$$

There are, clearly, infinitely many observables $\hat{f}$ (with $\hat{f}^\dagger = \hat{f}$) whose initial values can be specified. Which ψ describes a system with so-specified initial conditions? ψ can be calculated from Eqs.3.72, which are infinitely many equations for the unknown vector components $\{\psi_i\}$ in terms of the given coefficients $\{a_j\}$:

$$\sum_{i,j} \psi_i^* \hat{x}_{i,j}(t_0)\psi_j = a_1, \qquad \sum_{i,j} \psi_i^* \hat{p}_{i,j}(t_0)\psi_j = a_2, \qquad \sum_{i,j,k} \psi_i^* \hat{x}_{i,k}\hat{x}_{k,j}(t_0)\psi_j = a_3, \quad ... \tag{3.73}$$

Mathematically, we are dealing with a so-called moment problem. We must ask, in particular, what conditions the coefficients $\{a_i\}$ must obey for there to exist a matching state ψ. Physically, this is the question which initial conditions can actually occur in an experimental setup. We anticipate, of course, that the $\{a_i\}$ cannot be chosen completely arbitrarily because some observables are interfering variables. This question will later lead us to Heisenberg's famous uncertainty relations.

Exercise 3.21 *Verify that ψ of Eq.3.61 is normalized. For this choice of ψ, calculate explicitly the expectation values $\bar{x}(t), \bar{p}(t)$ as well as the uncertainties in those predictions, i.e., the standard deviations $\Delta x(t)$ and $\Delta p(t)$ for the free particle. Your results should show that neither the position nor the momentum are predicted with certainty at any time, not even at the initial time t_0. The fact that $\Delta x(t)$ grows in time expresses that a momentum uncertainty over time leads to increasing position uncertainty. $\Delta p(t)$ remains constant in time, expressing that the momentum of a free particle, no matter what value it has, remains unchanged.*

Finally, we also have to conclude that if we measure our system at time say t_1 then we gain information and we have to update our initial state vector accordingly to a new initial state vector ψ' which is such as to encode our knowledge of the initial state of the system at t_1. We will later revisit the question of this so-called wave function collapse.

Exercise 3.22 *Spell out the step of the second equality in Eq.3.68.*

3.7 The Hilbert space of quantum mechanics, and Dirac's notation

In the previous sections, we solved the equations of motion for matrix-valued functions $\hat{x}(t)_{ij}$ and $\hat{p}(t)_{ij}$. And, of course, once we have the $\hat{x}(t)_{ij}$ and $\hat{p}(t)_{ij}$, we can easily calculate from them the matrix-valued function of time $\hat{f}(t)_{ij}$ for every observable $\hat{f}$, i.e., for every polynomial in the $\hat{x}$ and $\hat{p}$ that obeys $\hat{f} = \hat{f}^\dagger$.

We also found out how to specify initial conditions, namely by choosing vector coefficients ψ_i. Of course, the coefficients ψ_i themselves are numbers and not vectors. The ψ_i are the coefficients of an abstract vector. Following Dirac, we will call that abstract vector a "ket" and denote by $|\psi\rangle$. By working with column vectors and matrices, we have implicitly chosen a basis in the vector space. Let us give these basis vectors the names $|b_n\rangle$, for $n = 1, 2, ...$

The fact that the numbers ψ_i are the coefficients of $|\psi\rangle$ in the basis $\{|b_n\rangle\}_{n=1}^{\infty}$ that we have implicitly chosen is expressed in the equation:

$$|\psi\rangle = \sum_n \psi_n |b_n\rangle \tag{3.74}$$

Therefore, the abstract vector $|\psi\rangle$ is an element of the abstract vector space of initial state vectors. Once we choose a basis, then the abstract vector $|\psi\rangle$ has a unique collection of coefficients ψ_n that expand $|\psi\rangle$ in that basis. The coefficients ψ_n are usually arranged in a column and that column of numbers is also being called a *column vector.* But keep in mind that this column is really just the collection of the numbers ψ_n. This *column vector* of coefficients is not the state vector $|\psi\rangle$. Instead, one says that the column vector of the coefficients *represents* the abstract initial state vector $|\psi\rangle$ in the basis $\{|b_n\rangle\}_{n=1}^{\infty}$.

Similarly, the matrix elements $\hat{x}(t)_{ij}$ themselves are of course simply numbers. They are the coefficients of the abstract linear map $\hat{x}(t)$ from the vector space into itself, in the basis $\{|b_n\rangle\}_{n=1}^{\infty}$. We say that the matrices, such as $(\hat{x}(t)_{ij})_{i,j=1}^{\infty}$ provide a *representation* of the abstract operator $\hat{x}(t)$ that maps the abstract vector space of initial state vectors into itself. Whenever then we change basis in the vector space, as we will freely do later, then this implies a corresponding change of the coefficients of the matrices $\hat{x}(t)_{ij}, \hat{p}(t)_{ij}$, ..., $\hat{f}(t)_{ij}$ as well as the coefficients ψ_i of the vector ψ. The abstract initial state vector $|\psi\rangle$ and the abstract operators such as $\hat{x}(t), \hat{p}(t)$ and $\hat{f}(t)$ stay the same as we change the choice of basis. But their representation in terms of column vectors and matrices will change[11].

The representations that we have used so far have been so-called discrete representations, i.e., representations that use a basis of countably many, i.e., discretely-labeled basis vectors $\{|b_n\rangle\}_{n=1}^{\infty}$. One of the perks of working with infinite-dimensional vector spaces is that they also admit so-called continuous representations. One may loosely think of these representations as using a set of continuously-labeled basis $\{|b_\lambda\rangle\}_{\lambda\in K}$ where $K = \mathbb{R}$ or $K \subset \mathbb{R}$. It is also possible to have representations using bases that are in part discrete and in part continuous[12]. This means that the way that concrete quantum mechanical calculations look like can depend very much on which basis one chooses to work with, i.e., on the choice of representation.

Always, however, the number-valued predictions of expectation values of a quantum theory only depend on the abstract operators $\hat{x}(t), \hat{p}(t)$,... and on the abstract vectors ψ. The predictions, $\bar{x}(t), \bar{p}(t)$, ... $\bar{f}(t)$ are scalars, i.e., they are basis independent. Choices of basis, i.e., choices of representation are merely issues of convenience.

Let us now study what ultimately matters, namely the abstract structure of the vector space of initial state vectors and the structure of the abstract operators acting as maps on this abstract vector space.

3.7.1 Hilbert spaces

We begin by reviewing the definition of a complex vector space. In brief, a complex vector space is a set, $\mathcal{H}$, which is an abelian group over the complex numbers:

Definition: Any set $\mathcal{H}$ is called a *complex vector space,* if

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[11] Notice that we can always rotate any basis so that in the new basis the vector $|\psi\rangle$ is the vector with the coefficients $\psi_i = \delta_{i,0}$. This is usually not convenient but it is possible.

[12] For example, the eigenbasis of the Hamiltonian of the Hydrogen atom is of this form, containing a countable number of eigenstates that are bound states and an uncountable number of eigenstates that are scattering states.

a) it possesses an operation $\mathcal{H} \times \mathcal{H} \to \mathcal{H}$ called "addition" which obeys the rules for a commutative (i.e., also called abelian) group and if

b) the set $\mathcal{H}$ has a multiplication $\mathbb{C} \times \mathcal{H} \to \mathcal{H}$ obeying the following axioms for all $|v\rangle, |w\rangle \in \mathcal{H}$ and for all $\alpha, \beta \in \mathbb{C}$:

$$\begin{aligned}
(\alpha+\beta)|v\rangle &= \alpha|v\rangle + \beta|v\rangle && (3.75)\\
\alpha(|v\rangle + |w\rangle) &= \alpha|v\rangle + \alpha|w\rangle && (3.76)\\
(\alpha\beta)|v\rangle &= \alpha(\beta|v\rangle) && (3.77)\\
1|v\rangle &= |v\rangle && (3.78)
\end{aligned}$$

Notice that *every* set obeying these axioms is a complex vector space. To illustrate this point, consider, for example, the set of 3×2 matrices with complex entries. We can add such matrices and we can multiply them with complex numbers. It is easy to check that the above axioms are obeyed, so this set is a complex vector space. Also, consider, for example, the set of complex-valued continuous functions on $\mathbb{R}^4$, such as $g(x_1, x_2, x_3, x_4) = x_1 \cos(x_2 x_3^x) e^{ix_2x_4}$ or $h(x_1, x_2, x_3, x_4) = x_1 + i(x_2 + x_4^3)$. We can add such functions and we can multiply them with complex numbers and we will always get yet another continuous function on $\mathbb{R}^4$. It is easy to check that the set of complex-valued continuous functions on $\mathbb{R}^4$ is a complex vector space (which is infinite dimensional). Also, and this will be very important, given any complex vector space one can construct another complex vector space, called the dual vector space, $\mathcal{H}^*$.

Definition: For any complex vector space, $\mathcal{H}$, we define the complex vector space called its *dual space*, $\mathcal{H}^*$, as the set of continuous[13] linear maps $\hat{v} \to \mathbb{C}$. We call the elements of $\mathcal{H}^*$ "bra" vectors and use the notation $\langle r| \in \mathcal{H}^*$. They linearly map elements of $\mathcal{H}$ into complex numbers:

$$\begin{aligned}
\langle r| : &\quad \mathcal{H} \to \mathbb{C} && (3.79)\\
\langle r| : &\quad |v\rangle \to \langle r|v\rangle && (3.80)
\end{aligned}$$

That they are linear maps means:

$$\langle r| : \quad (\alpha|v\rangle + \beta|w\rangle) \to \alpha\langle r|v\rangle + \beta\langle r|w\rangle \qquad (3.81)$$

Exercise 3.23 *Verify that $\mathcal{H}^*$ is a complex vector space.*

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[13] Aren't all linear maps continuous? Well no, not necessarily in infinite-dimensional spaces! Consider for example the map $\phi : \mathcal{H} \to \mathbb{C}$ that maps vectors $|\psi\rangle$ into numbers through $|\psi\rangle \to \phi(|\psi\rangle) := \sum_n n!\psi_n$ in some basis. The map ϕ is clearly a map from the vector space into the complex numbers that is linear. But ϕ is not continuous. To see this, consider that arbitrarily small changes to the vector $|\psi\rangle$ (i.e., to the coefficients ψ_n) can change $\phi(|\psi\rangle)$ arbitrarily strongly.

Definition: A complex vector space is said to possess a *scalar product* or also called *inner product* if it possesses a map $\mathcal{H} \times \mathcal{H} \to \mathbb{C}$ that obeys certain conditions that we'll discuss below. So an inner product takes two vectors in $\mathcal{H}$ and maps then into a number. Equivalently, a vector space with an inner product is a vector space that possesses a map $\mathcal{H} \to \mathcal{H}^*$ obeying certain conditions. How does this yield an inner product of two vectors in $\mathcal{H}$? Take the first vector, map it into a vector in $\mathcal{H}^*$ and then use that dual vector to linearly map the second vector in $\mathcal{H}$ to obtain a number, which is then the value of the inner product.

Concretely, such a map is usually denoted by $^\dagger : \mathcal{H} \to \mathcal{H}^*$ and it is called a hermitean conjugation map. We can use the hermitean conjugation map to map any element $|v\rangle \in \mathcal{H}$ into an element in $|v\rangle^\dagger \in \mathcal{H}^*$. One could give this image of the vector $|v\rangle$ any name but one traditionally chooses to call it by the same name as its pre-image: $\langle v| := |v\rangle^\dagger \in \mathcal{H}^*$. The hermitian conjugation map is required to be what is called anti-linear, i.e., linear but with a complex conjugation:

$$^\dagger : \quad \mathcal{H} \to \mathcal{H}^* \tag{3.82}$$

$$^\dagger : \quad r|v\rangle + s|w\rangle \to r^*\langle v| + s^*\langle w| \qquad \forall |v\rangle, |w\rangle \in \mathcal{H}, \forall r, s \in \mathbb{C} \tag{3.83}$$

What then is the list of requirements that defines an inner product, or scalar product? A scalar product is required to map any two vectors $|v\rangle, |w\rangle \in \mathcal{H}$ into a complex number denoted by $\langle v|w\rangle \in \mathbb{C}$, obeying these conditions:

$$\langle u| \left(\alpha|v\rangle + \beta|w\rangle\right) = \alpha\langle u|v\rangle + \beta\langle u|w\rangle \tag{3.84}$$

$$\langle v|w\rangle^* = \langle w|v\rangle \tag{3.85}$$

$$\langle v|v\rangle \geq 0 \tag{3.86}$$

$$\langle v|v\rangle = 0 \quad \text{only if} \quad |v\rangle = 0 \tag{3.87}$$

Definition: A complex vector space equipped with a scalar product is called a unitary vector space or inner product space or also pre-Hilbert space.

Definition: The "length" or "norm", $||\ |v\rangle||$, of a vector $|v\rangle \in \mathcal{H}$ is defined as $||\ |v\rangle|| = \langle v|v\rangle^{1/2}$. We say that $|v\rangle$ is normalized if $||\ |v\rangle|| = 1$.

Definition: The distance $d(|v\rangle, |w\rangle)$ between two vectors is defined as $||(|v\rangle - |w\rangle)||$.

Since quantum mechanics requires infinite-dimensional representations, we will have to be concerned with sequences of vectors and their convergence. For example, if we are to make sense of a series such as Eq.3.74 we need to define what it means to sum up an infinite number of basis vectors.

Definition: We say that a sequence of vectors $|v_n\rangle$ converges (namely to some vector $|v\rangle$), and we write $\lim_{n\to\infty} |v_n\rangle = |v\rangle$, iff (i.e., if and only if) it is true that

$\lim_{n\to\infty} d(|v_n\rangle, |v\rangle) = 0$.

Definition: A sequence $\{|v_n\rangle\}$ is called fundamental (or Cauchy), if and only if $\lim_{n,m\to\infty} d(|v_n\rangle, |v_m\rangle) = 0$. By this is meant that $\forall\epsilon > 0$, $\exists R$ so that $\forall n, m > R$: $d(|\hat{v}_n\rangle, |v_m\rangle) < \epsilon$.

Definition: A pre-Hilbert space is called a Hilbert space if all its fundamental sequences converge[14].

Remark: Since the distance to a vector of infinite length would be infinite, no sequence could converge to a vector of infinite length. All vectors in a Hilbert space have finite length.

How then, do these abstract concepts relate to the concrete vector components ψ_n and explicit matrix elements $\hat{x}_{r,s}, \hat{p}_{r,s}$ and $\hat{f}_{r,s}$?

To see this connection, we need the concept of Hilbert basis:

3.7.2 Hilbert bases

Definition: We say that a set of orthonormal vectors $\{|b_n\rangle\}$, i.e., a set of vectors obeying $\langle b_n|b_m\rangle = \delta_{n,m}$, is a Hilbert basis for $\mathcal{H}$, if all $|\psi\rangle \in \mathcal{H}$ have a unique representation of the form:

$$|\psi\rangle = \sum_n \psi_n |b_n\rangle \tag{3.88}$$

Definition: A Hilbert space $\mathcal{H}$ is called "separable", if it possesses a countable Hilbert basis.

Are they big enough for quantum mechanics? Yes, actually we know already that in quantum mechanics we can work with a separable Hilbert because we have succeeded

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[14] This means that in order to obtain a Hilbert space from a given pre-Hilbert space it may be necessary to add new elements to it - for the Cauchy sequences to converge to - until every Cauchy sequence has an element to converge to. This is similar to how the set of real numbers $\mathbb{R}$ is obtained from the set of rational numbers, $\mathbb{Q}$: There are Cauchy sequences in $\mathbb{Q}$ which have no rational number to converge to. Consider, for example, the sequence of rational numbers s_n where $s_n = trunk_n(\sqrt{2})$, namely, s_n is given by the first n digits of $\sqrt{2}$. Clearly, the sequence (s_n) is a Cauchy sequence but it does not converge to any number in $\mathbb{Q}$. That's because $\sqrt{2} \notin \mathbb{Q}$. So we add $\sqrt{2}$ and all other such irrational numbers to finally obtain $\mathbb{R}$. Now you may say yes but coming from $\mathbb{Q}$ we don't know what, for example, $\sqrt{2}$ is. How can we add it to $\mathbb{Q}$ then? Good that you ask! Here is roughly how you can do it. Consider all Cauchy sequences that seem to want to converge to the same point, say $\sqrt{2}$. How do we know that two Cauchy sequences want to converge to the same point? When their difference converges to zero. All these Cauchy sequences that want to converge to the same point in that sense form an equivalence class of sequences. We can call that equivalence class $\sqrt{2}$. In this way, any real number is really a set of equivalence classes of Cauchy sequences, where the elements within an equivalence class all converge to the same point (in the sense above). The completion of a pre-Hilbert space to obtain a Hilbert space is analogous.

above in representing the canonical commutation relations in a representation of matrices and column vectors. In fact, in quantum mechanics, it always suffices to consider a separable Hilbert space. Separable Hilbert spaces are the smallest Hilbert spaces after finite-dimensional Hilbert spaces. Recall that there are different kinds of infinity: following Cantor, we say that two sets have the same number of elements, or have the same "cardinality", if their elements can be mapped bijectively into another. For example, there are just as many even numbers, as there are natural numbers, as there are rational numbers. There are, however, many more real numbers, i.e., their cardinality is higher. Quantum field theory does appear to require nonseparable Hilbert spaces whose bases have the cardinality of the real numbers. If nature possesses a shortest length scale then a separable Hilbert space could suffice for quantum field theory as well.

Theorem: All Hilbert bases of a given Hilbert space have the same cardinality.

This theorem implies for quantum mechanics, because we know its Hilbert space is separable, that all its Hilbert bases are countable. This means that whatever Hilbert basis we may choose, our vectors will always be represented as column vectors and our $\hat{x}, \hat{p}$ and general $\hat{f}$ will be represented as matrices. It also means that the Hilbert space of a single 1-dimensional harmonic oscillator has the same dimension (namely countable infinity) as does the Hilbert space of a space ship[15].

As we will see later, there is a way to use what amounts to a continuous basis, but these come at the cost of the "basis vectors" having infinite length and therefore not being in the Hilbert space.

3.7.3 Discrete wave functions and matrix representations

Following up on Eq.3.88, it is important now to note that the coefficients ψ_n of the vector $|\psi\rangle$ in the $\{|b_n\rangle\}$ basis can be calculated through the scalar products:

$$\psi_n = \langle b_n|\psi\rangle \tag{3.89}$$

Eq.3.89 is easily verified by applying $\langle b_m|$ from the left in Eq.3.88:

$$\langle b_m|\psi\rangle \quad = \quad \langle b_m|\sum_n \psi_n|b_n\rangle$$

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[15] Following up on previous comments: In quantum field theory, which supersedes quantum mechanics, the Hilbert space is, in principle, non-separable. That's because every wave vector, of which there are continuously infinitely many, has its own harmonic oscillator. To avoid this problem, in practice we can consider a finite region of spacetime so that the set of wave vectors becomes discrete. If we further consider only wavelengths larger than some very small cutoff then only finitely many wave vectors remain and the Hilbert space is then separable. It is generally considered likely that there is a smallest length scale in nature, due to quantum gravity effects.

$$\begin{aligned} &= \sum_n \psi_n \langle b_m|b_n\rangle \\ &= \sum_n \psi_n \delta_{n,m} \\ &= \psi_m \end{aligned}$$

Definition: We call the set of coefficients $\psi_n = \langle b_n|\psi\rangle$ the "wave function" of the state $|\psi\rangle$ in the basis $\{|b_n\rangle\}$.

Remark: We have not yet introduced "continuous bases" such as the "position basis" $|x\rangle$ because they come with another set of issues to discuss. But it may be worth mentioning already that for them the corresponding definition will be: We call the set of coefficients $\psi(x) = \langle x|\psi\rangle$ the "wave function" of the state $|\psi\rangle$ in the basis of the $|x\rangle$.

A very useful observation is that the elements $|b_n\rangle$ of any Hilbert basis can be used to provide a representation of the identity map in this way:

$$\mathbf{1} = \sum_{\mathrm{n}} |\mathrm{b_n}\rangle\langle \mathrm{b_n}| \tag{3.90}$$

This is called the resolution of the identity in terms of the basis vectors $|b_n\rangle$. For example, using Eq.3.89:

$$\mathbf{1}|\psi\rangle = \sum_{\mathrm{n}=1}^{\infty} |\mathrm{b_n}\rangle\langle \mathrm{b_n}|\psi\rangle = \sum_{\mathrm{n}} \psi_{\mathrm{n}}|\mathrm{b_n}\rangle \tag{3.91}$$

Resolutions of the identity are commonly used for the important task of turning abstract equations into equations for concrete matrices and concrete vector coefficients. For example, let us insert the identity in the expression for the length of a vector:

$$\begin{aligned} \langle\psi|\psi\rangle &= \langle\psi|1|\psi\rangle && (3.92) \\ &= \sum_n \langle\psi|b_n\rangle\langle b_n|\psi\rangle && (3.93) \\ &= \sum_n \psi_n^* \psi_n && (3.94) \end{aligned}$$

Since all vectors $|\psi\rangle \in \mathcal{H}$ are of finite length, we conclude that the vector components must be square summable:

$$\sum_n \psi_n^* \psi_n < \infty \tag{3.95}$$

Further, if matrix elements $\hat{f}_{r,s}$ are given in the $\{|b_n\rangle\}$ basis, then they define a linear map $\hat{f}$:

$$\hat{f} = \sum_{r,s=1}^{\infty} |b_r\rangle\ f_{r,s}\ \langle b_s| \tag{3.96}$$

Conversely, the matrix elements of a linear map $\hat{f}$ in the basis of the $|b_n\rangle$ can be calculated as scalar products:

$$\hat{f}_{r,s} = \langle b_r|\hat{f}|b_s\rangle \tag{3.97}$$

This equation follows from Eq.3.96 by applying to it $\langle b_n|$ and $|b_m\rangle$ from the left and right respectively.

3.7.4 The domain of operators

We need to be careful because in infinite-dimensional Hilbert spaces linear maps normally cannot be allowed to act on all vectors of the Hilbert space! This is because if $|\psi\rangle \in \mathcal{H}$ and if therefore $\sum_n \psi_n^*\psi_n < \infty$, this does not imply that $\hat{f}|\psi\rangle \in \mathcal{H}$. This is because the coefficients $\phi_n = \sum_m \hat{f}_{n,m}\psi_m$ may not be square summable: $\sum_n \phi_n^*\phi_n =$ divergent, i.e., we may have $|\phi\rangle \notin \mathcal{H}$.

For example, consider this matrix:

$$(f)_{n,m} := \begin{pmatrix} 1^2 & 0 & 0 & 0 & \\ 0 & 2^2 & 0 & 0 & \\ 0 & 0 & 3^2 & 0 & \\ 0 & 0 & 0 & 4^2 & \\ & & & & \ddots \end{pmatrix}_{n,m} \tag{3.98}$$

The column vector[16]

$$(\psi)_n = \begin{pmatrix} 1/1 \\ 1/2 \\ 1/3 \\ 1/4 \\ \vdots \end{pmatrix}_n \tag{3.99}$$

is square summable[17]. Therefore, the coefficients ψ_n define a vector $|\psi\rangle \in \mathcal{H}$. Now the action of the matrix $(f)_{n,m}$ on this column vector would yield a column vector with the components $\phi_n = \sum_{m=1}^{\infty} f_{nm}\psi_m = n$. But the length of this column vector ϕ would be infinite because $\sum_{n=1}^{\infty} n^2 = \infty$. Therefore, the numbers ϕ_n cannot be the coefficients of any vector in the Hilbert space relative to any basis. Therefore, the abstract operator $\hat{f}$ defined by the matrix above cannot be allowed to act on the abstract Hilbert space vector $|\psi\rangle$ defined by the column vector above (namely because it would map it outside the Hilbert space).

Definition: We call the set $D_f \subseteq \mathcal{H}$ of vectors on which $\hat{f}$ is allowed to act the *domain* of $\hat{f}$. In general, we have some freedom in choosing the domain of an operator. But

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[16] Keep in mind that this so-called 'column vector' is really just the collection of the coefficients of an abstract Hilbert space vector relative to a choice of basis.

[17] Namely, $\sum_{n=1}^{\infty} 1/n^2 = \pi^2/6$. In the year 1735, Leonard Euler, who was 28 at the time, was the first to solve this tough old problem and that started his fame.

we have to keep in mind that domains must always be chosen such that the image of every vector in the domain is also inside the Hilbert space:

$$\forall |v\rangle \in D_f : \hat{f}|v\rangle \in \mathcal{H} \tag{3.100}$$

Note that we can allow the matrix $(\hat{f})_{n,m}$ of Eq.3.98 to act, for example, on all column vectors which possess only finitely many nonzero components, i.e., all the corresponding states are in the domain of the linear map $\hat{f} = \sum_{n,m} \hat{f}_{n,m}|b_n\rangle\langle b_m|$ that is defined by the matrix elements of Eq.3.98. But of course the domain of this $\hat{f}$ can be made a little larger by allowing it to act on vectors with infinitely many nonzero coefficients that, however, have to decay fast enough.

Exercise 3.24 *Let us consider how large we can make the domain $D_f \subset \mathcal{H}$ of the operator $\hat{f}$ defined in Eq.3.98. Concretely, how fast do the coefficients ψ_n of $|\psi\rangle$ have to decay, as $n \to \infty$. For this exercise, assume that the coefficients $|\psi_n|$ scale as n^s for $n \to \infty$. What then are the allowed values for s? Hint: The so-called Dirichlet series representation of the Riemann zeta function $\zeta(r) := \sum_{n=1}^{\infty} 1/n^r$ diverges for $r \leq 1$ but converges for $r > 1$.*

3.7.5 Changes of basis

Using the Dirac bra-ket notation, we can now rewrite equations such as Eq.3.54 in a much more compact form:

$$\bar{f}(t) = \langle\psi|\hat{f}(t)|\psi\rangle \tag{3.101}$$

We can easily recover Eq.3.54 from Eq.3.101, simply by twice inserting the resolution of the identity:

$$\begin{aligned}
\bar{f}(t) &= \langle\psi|\hat{f}(t)|\psi\rangle & (3.102)\\
&= \langle\psi|1\hat{f}(t)1|\psi\rangle & (3.103)\\
&= \sum_{n,m=1}^{\infty} \langle\psi|b_n\rangle\langle b_n|\hat{f}|b_m\rangle\langle b_m|\psi\rangle & (3.104)\\
&= \sum_{n,m=1}^{\infty} \psi_n^* f_{n,m} \psi_m & (3.105)
\end{aligned}$$

The beauty of Dirac's notation is that it does not refer to any particular choice of basis. If we do want to work in a particular basis, say $\{|b_n\rangle\}_{n=1}^{\infty}$ then we can simply suitably insert resolutions of the identity in terms of the basis vectors. If we then wish to change basis then we can do this by inserting resolutions of the identity for the new basis, say $\{|c_n\rangle\}_{n=1}^{\infty}$:

$$\bar{f}(t) = \langle\psi|\hat{f}(t)|\psi\rangle \tag{3.106}$$

$$= \sum_{n,m} \langle\psi|b_n\rangle\langle b_n|\hat{f}|b_m\rangle\langle b_m|\psi\rangle \qquad (3.107)$$

$$= \sum_{n,m} \langle\psi|1|b_n\rangle\langle b_n|1\hat{f}1|b_m\rangle\langle b_m|1|\psi\rangle \qquad (3.108)$$

$$= \sum_{n,m,r,s,u,v} \langle\psi|c_r\rangle\langle c_r|b_n\rangle\langle b_n|c_s\rangle\langle c_s|\hat{f}|c_u\rangle\langle c_u|b_m\rangle\langle b_m|c_v\rangle\langle c_v|\psi\rangle \qquad (3.109)$$

Let us denote the linear map that maps the basis vectors of one basis into the basis vectors of the other basis by $\hat{U}$:

$$\hat{U}: \ |b_n\rangle \to \hat{U}|b_n\rangle = |c_n\rangle \qquad (3.110)$$

Since $\hat{U}$ is a linear map, it can be written in the form:

$$\hat{U} = \sum_{r,s} |b_r\rangle \ U_{rs} \ \langle b_s| \qquad (3.111)$$

Applying $\langle b_m|$ to the right of $\hat{U}|b_n\rangle = |c_n\rangle$ we can now identify the change of basis coefficents of Eq.3.109 as the matrix elements of $\hat{U}$:

$$\langle b_m|c_n\rangle = U_{mn} \qquad (3.112)$$

Exercise 3.25 *By comparing Eqs.3.108 and Eq.3.109, find out how to express the wave function of $|\psi\rangle$ in the b basis in terms of its wave function in the c basis, using the matrix of $\hat{U}$. Also express the representation of $\hat{f}$ as a matrix in the b basis in terms of its representation as a matrix in the c basis, using the matrix representation of $\hat{U}$. Finally write Eq.3.109 in terms of a row vector, some matrices and a column vector.*

Exercise 3.26 *Assume that the basis vectors $|b_n\rangle$ are orthonormal. Show that if the new vectors $|c_n\rangle$ are to be an orthonormal basis too then $\hat{U}$ has to obey $\hat{U}^\dagger = \hat{U}^{-1}$. This means that $\hat{U}$ is what is called a unitary operator.*

Definition: An operator that obeys $\hat{U}^\dagger = \hat{U}^{-1}$ is called a unitary operator.

Remark: *In real vector spaces, matrices R that obey $R^t = R^{-1}$ are called rotation matrices because they rotate orthonormal basis vectors into orthonormal basis vectors. Here, we are working with Hilbert spaces, i.e., with complex vector spaces. Here, as Eq.3.110 shows, the unitaries play the role of rotations of orthonormal basis vectors into orthonormal basis vectors. Notice that R^t is defined through $R^t_{nm} = R_{mn}$, i.e., it is the transpose of R. In contrast, $U^\dagger$ is the transposed and also complex conjugated of U, i.e., it obeys $U^\dagger_{nm} = (U_{mn})^*$.*

In Dirac's notation it is clear that all the physical predictions $\bar{f}(t) = \langle\psi|\hat{f}|\psi\rangle$ only depend on $\hat{f}(t)$, which is a linear map, and on the choice of state vector $|\psi\rangle$. The predictions do not depend on the basis which we choose in the vector space while the coefficients ψ_n of $|\psi\rangle$ as a column vector and the matrix elements $\hat{f}_{r,s}$ of $\hat{f}(t)$ as a matrix strongly depend on the choice of basis.

Recall, in particular, that when we represented $\hat{x}$ and $\hat{p}$ using the matrices a and $a^\dagger$, in Eqs.3.42,3.43 we encountered the arbitrary constant L. In fact, the very choice of matrices a and $a^\dagger$ was merely convenient, but not unique. In general, there are infinitely many solutions to the quantum mechanical equations of motion, canonical commutation relations and hermiticity conditions in terms of matrix-valued functions. As we mentioned already, the Stone von Neumann theorem assures us that all those different matrix-valued function solutions to the quantum mechanical problem merely differ by a choice of basis. All physical predictions $\bar{f}(t)$ are obtained basis independently and are, therefore, identical.

Exercise 3.27 *Assume that* $b, b^\dagger$ *are linear maps on a Hilbert space and are obeying* $[b, b^\dagger] = \mathbf{1}$, *where* $\mathbf{1}$ *is the identity map. Assume that there is a normalized*[18] *vector, which we denote by* $|0\rangle$, *which obeys* $b|0\rangle = 0$. *Show that the vector* $|z\rangle$ *which is defined through* $|z\rangle = e^{zb^\dagger}|0\rangle$ *is an eigenvector of* b *if* z *is any complex number. These vectors are related to so-called coherent states which are of practical importance, for example, in quantum optics (light is often found in a similar quantum state). These states are also of importance regarding the problem of "decoherence" in quantum measurement theory, as we will discuss later.*

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[18] Notice that $|0\rangle$ is normalized, i.e., that it is of length one. This means that, in spite of its misleading (but usual) name, $|0\rangle$ is certainly not the zero-length vector of the Hilbert space.

Chapter 4

Eigenbases of Observables and the Spectral Theorem

We saw that quantum mechanics requires its Hilbert spaces to be infinite dimensional. The reason was that if commutation relations of the form $[\hat{x}, \hat{p}] = i\hbar 1$ had a representation in terms of N-dimensional matrices then the trace could be taken on both sides of the equation, yielding the contradiction $0 = i\hbar N$.

Exercise 4.1 *Are there any values of β for which the commutation relation $[\hat{x}, \hat{p}] = i\hbar(1 + \beta\hat{p}^2)$ may possess a finite-dimensional Hilbert space representation?*

We will now study in more detail the properties that operators in infinite-dimensional Hilbert spaces can possess. In particular, we know that every self-adjoint matrix $\hat{Q}$ *in a finite-dimensional Hilbert space* can be diagonalized, i.e., that there exists an orthonormal basis of eigenvectors of $\hat{Q}$ in the Hilbert space. The situation is more subtle in infinite dimensions, as the full spectral theorem for self-adjoint operators on general Hilbert spaces shows. Physicists speak of self-adjoint operators that possess non-normalizable eigenvectors which are not in the Hilbert space. What is the underlying mathematics?

4.1 Self-adjointness

What we have to look out for when defining self-adjointness in the infinite-dimensional case is that an operator can only act on those Hilbert space vectors that it maps into vectors that are in the Hilbert space, i.e., that are again normalizable. Since this requirement is nontrivial in infinite dimensional Hilbert spaces, the domain $D_{\hat{Q}}$ of an operator $\hat{Q}$, i.e., the set of vectors on which it is allowed to act can be smaller than the entire the Hilbert space.

Actually, for an operator on an infinite-dimensional Hilbert space it happens easily that its domain is smaller than the Hilbert space. For example, recall the operator

$\hat{Q}$ whose matrix representation in a Hilbert basis is diagonal with the diagonal entries being $1, 2^5, 3^5, 4^5, ...$, and consider the vector with the coefficients $(1, 1/2, 1/3, 1/4, ...)$ in the same basis. The vector is is in the Hilbert space because its coefficients are square-summable. But this vector is not in the domain of the operator $\hat{Q}$. That's because the image of our vector would be the vector with the coefficients $(1, 2^4, 3^4, 4^4, ...)$ and this vector is not normalizable and therefore not in the Hilbert space.

As a consequence, in the case of infinite-dimensional Hilbert spaces we have to carefully define the domain of all operators. Here is the definition of what we mean by the adjoint operator of an operator $\hat{Q}$, which is careful enough to be applicable also for infinite-dimensional Hilbert spaces:

Definition (adjoint operator): Assume that $\hat{Q}$ is an operator on a Hilbert space $\mathcal{H}$ with domain $D_{\hat{Q}}$, the domain being the maximal set of Hilbert space vectors that $\hat{Q}$ maps into the Hilbert space. Then the domain of the adjoint operator, denoted $\hat{Q}^\dagger$ is:

$$D_{\hat{Q}^\dagger} = \left\{ |\phi\rangle \in \mathcal{H} \mid \exists \ |\varphi\rangle \in \mathcal{H} \ \text{ so that } \ \langle\varphi|\psi\rangle = \langle\phi|\hat{Q}|\psi\rangle \ \ \forall |\psi\rangle \in D_{\hat{Q}} \right\} \tag{4.1}$$

Then, $\hat{Q}^\dagger$ is defined to act on its domain as:

$$\hat{Q}^\dagger|\phi\rangle = |\varphi\rangle \tag{4.2}$$

Definition (self-adjoint operator): An operator $\hat{Q}$ is called self-adjoint if it is the same operator as its adjoint, and this includes that the requirement that their domains agree: $D_{\hat{Q}} = D_{\hat{Q}^\dagger}$.

4.2 The spectrum of an operator

Going back to the basics, we begin by reviewing the concept of eigenvector.

Definition (eigenvector): For an operator $\hat{Q}$ on a Hilbert space $\mathcal{H}$ (finite or infinite dimensional), an eigenvector is any vector $|\psi\rangle \in D_Q \subset \mathcal{H}$ for which there is a number λ, called an eigenvalue, such that:

$$\hat{Q}|\psi\rangle = \lambda|\psi\rangle \tag{4.3}$$

The notions of eigenvector and eigenvalue are useful for infinite-dimensional Hilbert spaces too but we need the more general notions of spectrum and spectral resolution. To arrive at these notions, it will be useful to rewrite Eq.4.3 in this form:

$$(\hat{Q} - \lambda 1)|\psi\rangle = 0 \tag{4.4}$$

This equation shows us that the eigenvector $|\psi\rangle$ is a vector that the operator $(\hat{Q} - \lambda 1)$ maps into the zero-vector. As a consequence, the operator $(\hat{Q} - \lambda 1)$ maps any set of vectors that differ only by multiples of the vector $|\psi\rangle$ to the same vector. Therefore, we can draw the important conclusion that if λ is an eigenvalue of $\hat{Q}$, then the operator $(\hat{Q} - \lambda 1)$ is not invertible[1].

This is a very important observation because we can now refer to eigenvalues without referring to eigenvectors! That will come in handy when we want to deal with what would be eigenvectors if they weren't non-normalizable. We are now ready to define the spectrum of an operator on a Hilbert space $\mathcal{H}$.

Definition (spectrum): For any operator $\hat{Q}$ on a Hilbert space $\mathcal{H}$, any number $\lambda \in \mathbb{C}$ is said to be in the spectrum of $\hat{Q}$, if the operator $(\hat{Q} - \lambda 1)$ does not possess an inverse that is defined on the entire Hilbert space H.

According to this definition, eigenvalues clearly are part of the spectrum because for them, as we just saw, $(\hat{Q} - \lambda 1)$ does not possess an inverse. We define:

Definition (point spectrum): The set of eigenvalues forms the subset of the spectrum that is called the point spectrum.

So what other values can there possibly be in the spectrum, besides eigenvalues? The answer is that - in infinite-dimensional Hilbert spaces - in can happen that there are values λ for which $(\hat{Q} - \lambda 1)$ does have an inverse $(\hat{Q} - \lambda 1)^{-1}$, but this inverse cannot be defined on the entire Hilbert space $\mathcal{H}$, i.e., its domain is smaller than the Hilbert space. By the way, $(\hat{Q} - \lambda 1)^{-1}$ is also called the resolvent.

Definition (continuous spectrum): The set of $\lambda \in \mathbb{C}$ for which (a) the resolvent $(\hat{Q} - \lambda 1)^{-1}$ exists but (b) the domain of $(\hat{Q} - \lambda 1)^{-1}$ is smaller than $\mathcal{H}$ and (c) no Hilbert space vector is orthogonal to the domain of the resolvent, forms the subset of the spectrum that is called the continuous spectrum.

Definition (residual spectrum): In principle, for arbitrary operators $\hat{Q}$ on a Hilbert space, there is also the possibility that (a) $(\hat{Q} - \lambda 1)^{-1}$ exists but (b) the domain of $(\hat{Q} - \lambda 1)^{-1}$ is smaller than $\mathcal{H}$ and (c) there are Hilbert space vectors orthogonal to the domain of $(\hat{Q} - \lambda 1)^{-1}$ (in this case, we say that the domain of $(\hat{Q} - \lambda 1)^{-1}$ is not dense in $\mathcal{H}$). The set of these λ forms what is called the residual spectrum of $\hat{Q}$.

Proposition: The residual spectrum of self-adjoint and unitary operators is the empty set.

Therefore, we won't be concerned much with residual spectra.

Remark: It can be shown that the values in the continuous spectrum never arise as isolated points (unlike in the case of the point spectrum) but that they arise in continuous intervals, hence the naming.

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[1] Technically, the operator is not injective. Let's recall the relevant definitions: A map is called injective (or one-to-one) if every element of the target set is hit at most once. Injectivity is the condition needed for invertibility. A map is called surjective (or onto) if every element of the target set is hit at least once. A map is called bijective if it is both injective and surjective, i.e., if every element of the target set is hit exactly once.

It is clear that the values of the continuous spectrum are not eigenvalues because eigenvalues possess eigenvectors in the Hilbert space. Instead, we have:

Definition (approximate eigenvalues): The elements, λ, of the continuous spectrum are called approximate eigenvalues.

This terminology is justified because it can be shown that:

Proposition: If λ is in the continuous spectrum, i.e., if it is an approximate eigenvalue, then:

$$\forall \epsilon > 0 \quad \exists |\psi\rangle \in \mathcal{H} \quad \text{with} \;\; || \; |\psi\rangle \; || = 1 \;\; \text{so that} \;\; ||(\hat{Q} - \lambda 1)|\psi\rangle|| < \epsilon \tag{4.5}$$

Therefore, there will always be Hilbert space vectors that approximate what would be eigenvectors arbitrarily closely, namely in the sense of Eq.4.5. It is in this sense that one speaks of an approximate eigenvalue having an approximate eigenvector or an improper eigenvector or a non-normalizable eigenvector.

In quantum mechanics, there are plenty of operators which possess a continuous spectrum, such as the position and momentum operators. We see here already that these operators will not have eigenvectors for their continuous spectrum. However the fact that the continuous spectrum consists of approximate eigenvalues will translate into the important statement that their "eigenfunctions", such as Dirac deltas, can always be approximated with square integrable functions. For example, the Dirac delta can be approximated in this way:

$$\int_a^b f(x) \; \delta(x) \; dx = \lim_{\epsilon \to 0} \int_a^b f(x) \; \frac{\epsilon}{\pi} \frac{1}{x^2 + \epsilon^2} \; dx \tag{4.6}$$

Terminology (bound and scattering states): In quantum mechanics, one often encounters operators that possess both a point spectrum and a continuous spectrum. For example, the Hamilton operators for systems such as an atom or a molecule will have both a point spectrum and a continuous spectrum. This is because these systems have bound states and scattering states. For example, the electron of a Hydrogen atom is not able to escape a nucleus if it is in a low energy eigenstate. Its wave function decays away from the nucleus and is normalizable. The energy levels of bound states belong to the point spectrum and are discrete, therefore. However, we can also shoot an electron very fast by a proton. Since we can do so with arbitrary increments of the energy we expect that this is the case of the continuous spectrum. And yes, in this case, the wave function is coming in from infinitely far, getting scattered off the proton and also spreading away infinitely far. Such wave functions are not normalizable. If they are energy eigenstates they can therefore only be approximate eigenvectors and belong to the continuous spectrum.

4.3 The spectral theorem for self-adjoint operators

Theorem (Spectral theorem for self-adjoint operators): Assume that $\hat{f}$ is a self-adjoint operator: $\hat{f} = \hat{f}^\dagger$. Then, the spectrum of $\hat{f}$ is real and consists of a point spectrum or a continuous spectrum, or both. The operator $\hat{f}$ possesses an eigenbasis consisting of a discrete set of eigenvectors corresponding to the eigenvalues from the point spectrum and a continuous set of approximate eigenvectors corresponding to the continuous spectrum.

Exercise 4.2 *Assume that $|\psi\rangle$ is an eigenvector of a self-adjoint operator $\hat{f}$ with eigenvalue λ. Show that λ is real.*

Definition: Instead of the terms eigenvectors and approximate eigenvectors, one sometimes also speaks of proper and improper eigenvectors respectively.

In the case of self-adjoint operators on finite-dimensional Hilbert spaces, the spectrum consists purely of a point spectrum because in finite dimensional Hilbert spaces all vectors can be normalized. The spectral theorem in finite dimensions guarantees that the corresponding eigenvectors span the Hilbert space. For example, consider a self-adjoint operator $\hat{Q}$ in an N-dimensional Hilbert space and its eigenbasis $\{|q_n\rangle\}_{n=1}^N$ and the corresponding (point) spectrum of eigenvalues $q_1, ..., q_N$. In this case, it is easy to write down a resolution of the identity by summing over the values of the spectrum:

$$1 \;=\; \sum_{n=1}^{N} |q_n\rangle\langle q_n| \tag{4.7}$$

Similarly, we have the spectral representation of $\hat{Q}$:

$$\hat{Q} \;=\; \sum_{n=1}^{N} q_n \; |q_n\rangle\langle q_n| \tag{4.8}$$

On infinite-dimensional Hilbert spaces, however, the spectra will generally contain both continuous and discrete parts. Resolutions of the identity and spectral representations of operators should therefore contain also integrals. In practice, most physicists simply write down sums and integrals as needed with a tacit understanding that there may be subtleties.

But there is a mathematically rigorous way to treat these sums and integrals in a unified way, namely through the notion of Stieltjes integral which we will come back to in Sec.6.2.

4.3.1 Case 1: The self-adjoint operator $\hat{f}$ possesses only a point spectrum

We covered this case before. Let's do a quick review and close with an important new definition at the end of the section. So there is then an eigenbasis $\{|f_n\rangle\}$ of vectors obeying:

$$\hat{f}\ |f_n\rangle = f_n\ |f_n\rangle \quad \text{and} \quad \langle f_n|f_m\rangle = \delta_{nm} \tag{4.9}$$

We can sum them up to obtain a resolution of the identity:

$$\mathbf{1} = \sum_n |f_n\rangle\langle f_n| \tag{4.10}$$

It allows us to quickly expand vectors in the eigenbasis of $\hat{f}$:

$$|\psi\rangle = \mathbf{1}|\psi\rangle = \sum_n |f_n\rangle\langle f_n|\psi\rangle = \sum_n \psi_n|f_n\rangle \tag{4.11}$$

In the last step we used this definition:

Definition: The collection of numbers $\psi_n = \langle f_n|\psi\rangle$ is called the wave function of the state $|\psi\rangle$ in the eigenbasis of $\hat{f}$.

Notice that it is a function of n which takes only discrete values because the spectrum is here discrete. Later, in the case of the continuous spectrum, the wave function will be defined over the continuous spectrum.

The resolution of the identity also allows us to quickly expand arbitrary operators, $\hat{g}$, in the eigenbasis of $\hat{f}$:

$$\hat{g} = \mathbf{1}\hat{g}\mathbf{1} = \sum_{n,m} |f_n\rangle\langle f_n|\hat{g}|f_m\rangle\langle f_m| = \sum_{n,m} g_{nm}|f_n\rangle\langle f_m| \tag{4.12}$$

In the last step we used this definition:

Definition: We call $g_{nm} := \langle f_n|\hat{g}|f_m\rangle$ the matrix elements of the operator $\hat{g}$ in the eigenbasis of $\hat{f}$.

For example, if we choose for $\hat{g}$ to be $\hat{g} = \hat{f}$ then we obtain

$$f_{nm} = \langle f_n|\hat{f}|f_m\rangle = f_n\ \langle f_n|f_n\rangle = f_n\ \delta_{nm} \tag{4.13}$$

i.e., $\hat{f}$ is diagonal in its own eigenbasis, as expected. For illustration, let us also express an equation, say

$$|\phi\rangle = \hat{g}|\psi\rangle \tag{4.14}$$

in the $\hat{f}$ eigenbasis. We begin by multiplying the equation with $\langle f_r|$ from the left:

$$\langle f_r|\phi\rangle = \langle f_r|\hat{g}|\psi\rangle \tag{4.15}$$

Therefore:

$$\langle f_r|\phi\rangle = \langle f_r|\hat{g}\mathbf{1}|\psi\rangle = \sum_n \langle f_r|\hat{g}|f_n\rangle\langle f_n|\psi\rangle \tag{4.16}$$

We obtain the following equation for explicit column vectors (the wave functions) and a matrix:

$$\phi_r = \sum_n g_{r,n}\psi_n \tag{4.17}$$

We obtained these expansions of vectors and operators and their equations in eigenbases by using the resolution of the identity. It it will be very useful later also to consider partial resolutions of the identity, namely by not summing all the way:

Definition: We define a partial resolution of the identity:

$$\hat{E}_N := \sum_n^N |f_n\rangle\langle f_n| \tag{4.18}$$

Clearly, in the limit, we obtain the resolution of the identity:

$$\lim_{N\to\infty} \hat{E}_N = \mathbf{1} \tag{4.19}$$

It will be important later that each $\hat{E}_N$ is an operator, defined on the entire Hilbert space, which is a projector, namely, that it obeys $\hat{E}_N = \hat{E}_N^\dagger$ and $\hat{E}_N^2 = \hat{E}_N$.

Definition: An operator $\hat{P}$ is called a projector if it is self-adjoint, and obeys: $\hat{P}^2 = \hat{P}$.

Exercise 4.3 *Show that $\hat{E}_N$ is a projector.*

We now come to case 2 of the spectral theorem:

4.3.2 Case 2: The spectrum of $\hat{f}$ is purely continuous

In this case, let us give the spectrum a name:

$$J := \mathrm{spec}(\hat{f}) \subseteq \mathbb{R} \tag{4.20}$$

Notice that J can be a subset of the real line but it can also be the full real line. J can also consist of several disconnected pieces[2]. To start with, let us use the notation that is common in physics. In physics notation, $\hat{f}$ has a basis of approximate eigenvectors $\{|f\rangle\}_{f\in J}$ that are continuum normalized

$$\langle f|f'\rangle = \delta(f-f') \tag{4.21}$$

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[2] For example, the Hamiltonian of electrons in a periodic potential, e.g., in a crystal, tends to possess a continuous spectrum that consists of several disjoint stretches, called bands. Insulators, semiconductors and conductors are distinguished by the degree to which the states in the highest energetically accessible band are filled with electrons.

and yield a resolution of the identity:

$$\mathbf{1} = \int_J |f\rangle\langle f| \; df \tag{4.22}$$

Similarly to case 1 where $\hat{f}$ possesses only a purely point spectrum, here too we obtain wave functions for states and matrix elements for operators:

$$|\psi\rangle = \mathbf{1}|\psi\rangle = \int_J |f\rangle\langle f|\psi\rangle \; df = \int_J \psi(f) \; |f\rangle \tag{4.23}$$

In the last step we used this definition:

Definition: We call $\psi(f) := \langle f|\psi\rangle$ the wave function of the state $|\psi\rangle$ in the eigenbasis of $\hat{f}$. Here, f runs through the spectrum of $\hat{f}$.

Further, we obtain for operators:

$$\hat{g} = \mathbf{1}\hat{g}\mathbf{1} = \int_J\int_J |f\rangle\langle f|\hat{g}|f'\rangle\langle f'| \; df \; df' = \int_J\int_J g(f,f')|f\rangle\langle f'| \; df \; df' \tag{4.24}$$

In the last step we used this definition:

Definition: We call $g(f,f') := \langle f|\hat{g}|f'\rangle$ the matrix elements of $\hat{g}$ in the eigenbasis of $\hat{f}$. We may also sometimes use the notation $g_{f,f'}$ for $g(f,f')$. The function $g(f,f')$ is also called the integral kernel of $\hat{g}$ in the continuous eigenbasis of $\hat{f}$.

Notice that $g_{f,f'}$ behaves like a matrix with continuous rather than discrete indices. In fact, everything is the same as for a matrix, except that summations over indices are now integrations.

For example, let us express the equation $|\phi\rangle = \hat{g}|\psi\rangle$ in the $\hat{f}$ eigenbasis, as in the discussion of case 1 above. Now, however, we pick an operator $\hat{f}$ whose spectrum is continuous. We begin by multiplying the equation with $\langle\hat{f}|$ from the left:

$$\langle f|\phi\rangle = \langle f|\hat{g}|\psi\rangle \tag{4.25}$$

Therefore:

$$\langle f|\phi\rangle = \langle f|\hat{g}\mathbf{1}|\psi\rangle = \int_J \langle f|\hat{g}|f'\rangle\langle f'|\psi\rangle \; df' \tag{4.26}$$

We obtain the following equation for explicit column vectors (the wave functions) and a matrix, though now all indices are continuous:

$$\phi(f) = \int_J g(f,f')\psi(f') \; df' \tag{4.27}$$

Let us also quickly consider the matrix elements, i.e., the integral kernel, of $\hat{f}$ in its eigenbasis, in the case where the spectrum is continuous:

$$f(f,f') = \langle f|\hat{f}|f'\rangle = f'\langle f|f'\rangle = f' \; \delta(f-f') \tag{4.28}$$

Therefore:

$$\hat{f} = \int_J\int_J f' \; \delta(f-f')|f\rangle\langle f'| \; df \; df' = \int_J f|f\rangle\langle f| \; df \tag{4.29}$$

4.3.3 Case 3: The self-adjoint operator $\hat{f}$ has a point spectrum and a continuous spectrum

In this case, we have:

$$\mathbf{1} = \sum_n |f_n\rangle\langle f_n| + \int_J |f\rangle\langle f| \, df \tag{4.30}$$

$$\hat{f} = \sum_n f_n \, |f_n\rangle\langle f_n| + \int_J f \, |f\rangle\langle f| \, df \tag{4.31}$$

Exercise 4.4 *Derive the expression for the abstract equation* $|\phi\rangle = \hat{g}|\psi\rangle$ *in this basis.*

Exercise 4.5 *Look up and state the complete spectrum of the Hamiltonian of the Hydrogen atom (without spin or higher order corrections of any form). Give the exact source in a textbook.*

Hint: Essentially every textbook on quantum mechanics treats the Hydrogen atom. What do they do, from our perspective? They start with the Hamiltonian of the Hydrogen atom, expressed in the position basis. Then they calculate the eigenbasis of the Hamiltonian, i.e., they calculate the energy eigenstate's wave functions in the position basis. They are the wave functions of the Hydrogen orbitals. In principle, it's just like we will calculate in Ch.**??** the eigenstates of the position operator in the eigenbasis of a harmonic oscillator and vice versa. But never mind the details of this. It's not what the question is about.

The question is merely about the spectrum of the Hamiltonian of the Hydrogen atom. What are the proper eigenvalues and what are the approximate eigenvalues? I.e., the task is for you to learn to read the literature with the new mathematical and physical insights in the background. The question is to thereby find out the point spectrum and also the continuous spectrum of the Hamiltonian of the Hydrogen atom. Yes, the Hamiltonian of the Hydrogen atom has both types of spectrum. If your textbook doesn't mention the continuous spectrum (whose eigenfunctions describes electrons that are not bound to the proton but merely scatter off it), check another textbook. Regarding the point spectrum, do list also how often each eigenvalue occurs. Remember that eigenvalues can be degenerate, i.e., the eigenspace to an eigenvalue can be multi-dimensional. I.e., list the dimension of each eigenvalue's eigenspace. No need to list the wave functions of the Hamiltonian's eigenvectors.

Comment: We can see here why a smart phone battery demands about 5V from the USB charger and why nuclear fuel can release about a million times more energy per kilo fuel than a chemical fuel such as oil or coal does:

You'll find that the spacing of the first energy levels of the Hydrogen atom is usually given in a unit of energy that is called an electronvolt, [eV]. By definition, 1 eV is the amount of energy that an electron gains when you let it travel between two electrodes that have a voltage bias of 1 Volt between them. The larger spacings between the discrete energy levels (belonging to bound states) of the Hydrogen atom, and of molecules in general, is in the range of a few eV. This is the reason why batteries and photovoltaic cells operate at the voltage levels of a few eV. All chemical and biochemical reactions operate in the range of just a few eV too.

The formation of a molecules of Vitamin D, for example, happens to require an amount of energy, namely about 4.2 eV, that is in the upper range in the field of biochemistry and the other molecules of our bodies just don't have that kind of large energy gap available! That's why we need to consume vitamin D or make it using ultraviolet-B sunlight. UV-B photons that carry the required 4.2eV of energy needed to make Vitamin D molecules have a wavelength of about 295nm. We can't see sunlight of such short wavelength. Ultraviolet light is bluer than blue or even violet, which is why it is called ultraviolet. Sunlight scatters of air molecules through Rayleigh scattering and that effect is the stronger the smaller the wavelength. That's why during the day the sky is full of scattered light - which is blue. UV-B light makes it all the way down to the surface essentially only when the sun stands steeper in the sky than about 45 degrees. Else, it's just scattered around and away. So that's why we get enough vitamin D from sunlight only is the summer. In the winter, it's good to have vitamin D supplements. You know, the tablets that taste like dust. Yummy!

Now atomic nuclei also have a Hamiltonian. These nuclei can be excited so that they vibrate (point spectrum) or so that they split apart into non-bound fragments (continuous spectrum). The typical energy gaps in the spectra of nuclei are 1 MeV. That's why you can get roughly on the order of a million times more energy out of a kilo of plutonium than out of a litre of oil. Still, I am not advocating for nuclear energy. Why? The tremendous amount of energy in nuclear fuel also means that unlike a chemical fire that runs out of energy in a few days, radioactive contamination can easily spew radioactive radiation energy for millions of days (depending on the element of course). I flew over Fukushima. It's terrible.

4.4 The spectral theorem for unitary operators

The spectral theorem for self-adjoint operators $\hat{f}$ translates directly into a spectral theorem for unitary operators, i.e., for operators obeying $U^\dagger = U^{-1}$. This is because there is a bijective map, called the Cayley transform, that maps every self-adjoint operator into a unitary operator and vice versa:

$$\hat{U} := (\hat{f} - i\mathbf{1})(\hat{f} + i\mathbf{1})^{-1} \tag{4.32}$$

Exercise 4.6 *Show that $\hat{U}$ is unitary.*

The Cayley transform is invertible:

$$\hat{f} = -i(\hat{U} - 1)^{-1}(\hat{U} + 1) \tag{4.33}$$

Clearly, in the eigenbasis of $\hat{f}$, where $\hat{f}$ is diagonal, also $\hat{U}$ is diagonal. This means that $\hat{f}$ and $\hat{U}$ possess the same eigenvectors and approximate eigenvectors, with the same multiplicities (i.e. with the same dimension of the eigenspaces). Further, since both operators are simultaneously diagonal, if $r \in \mathbb{R}$ is in the spectrum of $\hat{f}$, then $\alpha = (r - i)(r + i)^{-1}$ (which is a Moebius transform of r), is in the spectrum of $\hat{U}$.

Exercise 4.7 *Show that each α is a complex number on the unit circle of the complex plane, i.e., that its modulus squared is $\alpha\alpha^* = 1$.*

Therefore, the spectral theorem for self-adjoint operators implies a corresponding spectral theorem for unitary operators. They too only possess a point and or a continuous spectrum, with corresponding eigenvectors and approximate eigenvectors.

Remark: You may wonder why we here did we not use exponentiation to obtain a unitary operator for any self-adjoint operator, through $\tilde{U} := \exp(i\hat{f})$. The reason is that, while we could use exponentiation, it has a drawback. The drawback is that the exponentiation map is not invertible because of the periodicity of $\exp(ir)$. Multiple eigenvalues of $\hat{f}$ could map into one eigenvalue for $\tilde{U}$. The Cayley transform is invertible, i.e., it maps each unitary operator uniquely to a self-adjoint operator and vice versa.

The most general spectral theorem is for normal operators: The spectral theorem naturally generalizes beyond self-adjoint and unitary operators, namely to all operators that are called normal. An operator $\hat{Q}$ is called normal if it commutes with its adjoint, i.e., if $[\hat{Q}, \hat{Q}^\dagger] = 0$. For example, the operators a and $a^\dagger$ that obey $[a, a^\dagger] = 1$ are clearly not normal. Indeed, the eigenstates of a that you calculated in Exercise 3.27, the so-called coherent states, can be shown to be not orthogonal to another.

Exercise 4.8 *Assume that $\hat{f}$ is a self-adjoint operator with a purely point spectrum $\{f_n\}$. Further assume that $\hat{U}$ is the Cayley transform of f. Determine whether or not the operator $\hat{Q} := \hat{f} + \hat{U}$ is a normal operator. If not, why not? If yes, what is the spectrum of $\hat{Q}$?*

Chapter 5

The position, momentum and energy representations

5.1 The eigenbasis of the position operator

We had found a representation of the position operator (parametrized by a parameter L that specifies the unit of length) in Eqs.3.42,3.48:

$$\hat{x}_{n,m} = \begin{pmatrix} 0 & \sqrt{1}L & 0 & 0 & \\ \sqrt{1}L & 0 & \sqrt{2}L & 0 & \\ 0 & \sqrt{2}L & 0 & \sqrt{3}L & \\ 0 & 0 & \sqrt{3}L & 0 & \\ & & & & \ddots \end{pmatrix}_{n,m} \tag{5.1}$$

Here, the subscript n, m indicates the matrix element in the $(n+1)$'st row and $(m+1)$'st column, because we will count from 0. We are here obviously dealing with a discrete, i.e., countable, basis. Let us call these basis vectors $|E_n\rangle$ for $n = 0, 1, 2, 3, ...$. Then we have

$$\langle E_n|\hat{x}|E_m\rangle = \hat{x}_{n,m} \tag{5.2}$$

and

$$\hat{x} = \sum_{n,m=0}^{\infty} |E_n\rangle \hat{x}_{n,m} \langle E_m| \tag{5.3}$$

Clearly, $\hat{x}$ is not diagonal in the $\{|E_n\rangle\}$ basis. Now to find a basis in which $\hat{x}$ is diagonal, i.e., to find an eigenbasis of $\hat{x}$, we need to find the solutions to the eigenvalue equation:

$$\hat{x}|x\rangle = x|x\rangle \tag{5.4}$$

To this end, we first act with $\langle E_n|$ from the left to obtain:

$$\langle E_n|\hat{x}|x\rangle = x\langle E_n|x\rangle \tag{5.5}$$

Inserting a resolution of the identity we obtain a concrete eigenvalue equation in a basis:

$$\sum_{m=0}^{\infty} \langle E_n|\hat{x}|E_m\rangle\langle E_m|x\rangle = x\langle E_n|x\rangle \tag{5.6}$$

We know the matrix elements $\langle E_n|\hat{x}|E_m\rangle$ of the position operator, namely

$$\langle E_n|\hat{x}|E_m\rangle = L\begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \\ \sqrt{1} & 0 & \sqrt{2} & 0 & 0 & \\ 0 & \sqrt{2} & 0 & \sqrt{3} & 0 & \\ 0 & 0 & \sqrt{3} & 0 & \sqrt{4} & \\ 0 & 0 & 0 & \sqrt{4} & 0 & \\ & & & & & \ddots \end{pmatrix}_{n,m} \tag{5.7}$$

and our task is to determine for which real eigenvalues x there exists a column vector that is an eigenvector. Its components are then the wave function $\langle E_n|x\rangle$ for a position eigenstate $|\hat{x}\rangle$ in the $\{|E_n\rangle\}$ basis. Once we have these wave functions, $\langle E_n|x\rangle$, of position eigenstates, we can write down the position eigenvectors $|x\rangle$ themselves in the basis $\{|E_n\rangle\}$:

$$|x\rangle = \sum_n |E_n\rangle\langle E_n|x\rangle \tag{5.8}$$

Now Eq.5.6 yields an equation for each $n \in \{0, 1, 2, ...\}$. These equations are

$$L\sqrt{1}\langle E_1|x\rangle = x\langle E_0|x\rangle \tag{5.9}$$

$$L\sqrt{1}\langle E_0|x\rangle + L\sqrt{2}\langle E_2|x\rangle = x\langle E_1|x\rangle \tag{5.10}$$

$$L\sqrt{2}\langle E_1|x\rangle + L\sqrt{3}\langle E_3|x\rangle = x\langle E_2|x\rangle \tag{5.11}$$

and so on. We have arrived at a recursion for the coefficients $\langle E_n|x\rangle$ which gives us a solution, i.e., a full set of coefficients $\langle E_n|x\rangle$ for any choice of x! This is because once we pick an arbitrary value for the first coefficient, $\langle E_0|x\rangle$, we can then calculate the second coefficient, namely $\langle E_1|x\rangle$. From these two we can calculate the third, $\langle E_2|x\rangle$. In this way, iteratively, all $\langle E_n|x\rangle$ are determined and can be calculated. An important conclusion we can draw from this is that no matter what value for x we try, we always find an eigenvector for it! This means that the spectrum of $\hat{x}$ is the real line: $\text{spec}(\hat{x}) = \mathbb{R}$.

The recursion problem can be solved in closed form. Without proof (which is straightforward but tedious) we only state the result:

$$\langle E_n|x\rangle = \frac{e^{-\frac{x^2}{4L^2}}}{\sqrt{\pi^{1/2}2^n(n)!}}\, H_n\left(\frac{x}{\sqrt{2}L}\right) \tag{5.12}$$

Here, H_n is the n'th Hermite polynomial, defined through:

$$H_n(z) \;:=\; (-1)^n \; e^{z^2} \; \frac{d^n}{dz^n} \; e^{-z^2} \tag{5.13}$$

But then, didn't we have for each eigenvalue x a choice in what value we wanted to give to the first coefficient, $\langle E_0|x\rangle$? Yes we did. In the equation Eq.5.12, can we make this choice such that the eigenvectors $|x\rangle$ come out normalizable? Here, let us remember that we just established that the spectrum is the real line and is, therefore, purely continuous. From the spectral theorem, we conclude that the eigenvectors $|\hat{x}\rangle$ are not normalizable. Instead, therefore, the choice of the first coefficient is made for each x such that the resulting eigenvectors come out to be what is called *continuum normalized.* Namely, one can show that with Eq.5.12, we have:

$$\langle x|x'\rangle = \sum_{n=0}^{\infty} \langle x|n\rangle\langle n|x'\rangle = \delta(x-x') \tag{5.14}$$

Therefore, we have now found the wave function $\langle E_n|x\rangle$ of each position eigenstate $|x\rangle$ in the basis $\{|E_n\rangle\}_n$. In fact, we have inadvertently also obtained the position wave functions of the eigenstates of harmonic oscillators! To see this, let us briefly review aspects of the harmonic oscillator.

5.2 The energy eigenbasis of a harmonic oscillator

Following up on Exercise (3.19), we express the harmonic oscillator's Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2 \tag{5.15}$$

in terms of operators $a, a^\dagger$ which obey $[a, a^\dagger] = 1$. In the $\{|E_n\rangle\}$ basis, these operators have the matrix elements given in Eqs.3.39,3.40. We make again the ansatz:

$$\hat{x} = L(a^\dagger + a), \qquad \hat{p} = iK(a^\dagger - a) \quad \text{with} \quad L, K \in \mathbb{R} \tag{5.16}$$

So far, the parameters L and K are still arbitrary real numbers. The ansatz needs to solve the hermiticity conditions $\hat{x} = \hat{x}^\dagger$ and $\hat{p} = \hat{p}^\dagger$ and it obviously does. A little calculation shows that this ansatz also succeeds in solving the canonical commutation relations $[\hat{x}, \hat{p}] = i1$, namely if we choose $K = (2L)^{-1}$ which we will henceforth do. Now, only L is still left as a free parameter in our ansatz. (For now, let us not worry about the time evolution and consider only one arbitrary point in time.) Therefore, we have found a valid way of writing $\hat{x}$ and $\hat{p}$.

At this point we are still free to choose any real value for L and, in principle, any value of L is as good as any other. Let us now express the Hamiltonian in terms of the $a, a^\dagger$ operators:

$$\hat{H} = \frac{-1}{2m\;4L^2}\left((a^\dagger)^2 - a^\dagger a - aa^\dagger + a^2\right) + \frac{m\omega^2 L^2}{2}\left((a^\dagger)^2 + a^\dagger a + aa^\dagger + a^2\right) \tag{5.17}$$

We notice that we can make the $(a^\dagger)^2$ and a^2 terms cancel by choosing L so that the prefactors match, i.e., so that

$$\frac{1}{8mL^2} = \frac{m\omega^2 L^2}{2} \tag{5.18}$$

which is solved by:

$$L = (2m\omega)^{-1/2} \tag{5.19}$$

We conclude that for every harmonic oscillator, when expressing the $\hat{x}$ and $\hat{p}$ operators in terms of a and $a^\dagger$, there is an especially convenient choice of L :

$$\hat{x} = \frac{1}{\sqrt{2m\omega}}(a^\dagger + a), \qquad \hat{p} = i\sqrt{\frac{m\omega}{2}}(a^\dagger - a) \tag{5.20}$$

This is because with this choice of L, the form of the oscillator's Hamiltonian, after a short calculation, simplifies to:

$$\hat{H} = \hbar\omega(a^\dagger a + 1/2) \tag{5.21}$$

How does this help us to find the spectrum of $\hat{H}$? Recall that we know the matrix elements $a_{n,m} = \langle E_n|a|E_m\rangle$ and $a^\dagger_{n,m} = \langle E_n|a^\dagger|E_m\rangle$ of the operators a and $a^\dagger$ in the basis $\{|E_0\rangle, |E_1\rangle, |E_2\rangle, |E_3\rangle, ...\}$, namely:

$$a_{n,m} = \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \\ 0 & 0 & \sqrt{2} & 0 & 0 & \\ 0 & 0 & 0 & \sqrt{3} & 0 & \\ 0 & 0 & 0 & 0 & \sqrt{4} & \\ 0 & 0 & 0 & 0 & 0 & \\ & & & & & \ddots \end{pmatrix}_{n,m} \tag{5.22}$$

The hermitean conjugate is:

$$a^\dagger_{n,m} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \\ \sqrt{1} & 0 & 0 & 0 & 0 & \\ 0 & \sqrt{2} & 0 & 0 & 0 & \\ 0 & 0 & \sqrt{3} & 0 & 0 & \\ 0 & 0 & 0 & \sqrt{4} & 0 & \\ & & & & & \ddots \end{pmatrix}_{n,m} \tag{5.23}$$

Clearly then, the matrix elements of the so-called number operator $\hat{N} := a^\dagger a$ in the basis $\{|E_0\rangle, |E_1\rangle, ...\}$ are

$$\hat{N}_{n,m} = (a^\dagger a)_{n,m} = n\ \delta_{n,m} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \\ 0 & 1 & 0 & 0 & 0 & \\ 0 & 0 & 2 & 0 & 0 & \\ 0 & 0 & 0 & 3 & 0 & \\ 0 & 0 & 0 & 0 & 4 & \\ & & & & & \ddots \end{pmatrix}_{n,m} \tag{5.24}$$

Clearly, $\hat{N}$ is a self-adjoint operator, $\hat{N}^\dagger = \hat{N}$, since it is diagonal in the basis $\{|E_0\rangle, |E_1\rangle, ...\}$ and is, therefore, diagonalizable. Since

$$\hat{H} = \hbar\omega(\hat{N} + 1/2) \tag{5.25}$$

we have that the Hamiltonian is diagonal in the basis $\{|E_0\rangle, |E_1\rangle, ...\}$, i.e., that $\hat{H}|E_n\rangle = E_n|E_n\rangle$, and that its eigenvalues are $E_n = \hbar\omega(n + 1/2)$ for $n \in \{0, 1, 2, ...\}$. The spectrum of the Hamiltonian of a harmonic oscillator is, therefore, purely a point spectrum.

Therefore, this Hamiltonian reads in its eigenbasis:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2 = \sum_{n=0}^{\infty} E_n|E_n\rangle\langle E_n| \tag{5.26}$$

The state $|E_n\rangle$ can therefore also be interpreted the n'th excited state of a harmonic oscillator with frequency ω. Now what is the position wave function of the n'th eigenstate of this harmonic oscillator? By definition it is given by $\langle x|E_n\rangle$. But we have $\langle x|E_n\rangle = (\langle E_n|x\rangle)^* = \langle E_n|x\rangle$ because $\langle E_n|x\rangle$ is real. This means that we have inadvertently also obtained the position wave functions of the eigenstates of the harmonic oscillator!

Exercise 5.1 *Consider the harmonic oscillator of above, choose $L = (2m\omega)^{-1/2}$ and assume that the oscillator system is in this state:*

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|E_0\rangle - |E_1\rangle) \tag{5.27}$$

Calculate $\bar{H}$ and $\bar{x}$ and the position wave function $\psi(x) := \langle x|\psi\rangle$.

5.3 The position representation

We established that the spectrum of $\hat{x}$ is $\mathbb{R}$, with each of these approximate eigenvalues coming with a corresponding approximate (i.e., non-normalizable) eigenvector $\{|x\rangle\}_{x\in\mathbb{R}}$. This means that we have a new resolution of the identity[1]:

$$\mathbf{1} = \int_{\mathbb{R}} |x\rangle\langle x| \; dx \tag{5.28}$$

It allows us to express arbitrary states in the eigenbasis of $\hat{x}$, i.e., we can now calculate:

$$|\psi\rangle = \int_{\mathbb{R}} |x\rangle\langle x|\psi\rangle \; dx = \int_{\mathbb{R}} \psi(x) \; |x\rangle \; dx \tag{5.29}$$

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[1] We are here using physicists' notation. The functional analytic details of operators with continuous spectra will be in an Appendix.

Here, $\psi(x) = \langle x|\psi\rangle$ is the position wave function of the state $|\psi\rangle$. Further, we can now calculate the scalar product of states in the position basis:

$$\langle\psi|\phi\rangle = \langle\psi|\mathbf{1}|\phi\rangle = \int_{\mathbb{R}} \langle\psi|x\rangle\langle x|\phi\rangle\ dx = \int_{\mathbb{R}} \psi(x)^*\phi(x)\ dx \tag{5.30}$$

For example, the normalization condition of a state $|\psi\rangle$ takes the form:

$$1 = \langle\psi|\psi\rangle = \int_{\mathbb{R}} \psi(x)^*\psi(x)\ dx \tag{5.31}$$

Operators can be expanded in the position eigenbasis by inserting resolutions of the identity:

$$\hat{f} = \mathbf{1}\hat{f}\mathbf{1} = \int_{\mathbb{R}}\int_{\mathbb{R}} |x\rangle\langle x|\hat{f}|x'\rangle\langle x'|\ dx\ dx' = \int_{\mathbb{R}}\int_{\mathbb{R}} f(x,x')|x\rangle\langle x'|\ dx\ dx' \tag{5.32}$$

Here, the $f(x,x') = \langle x|\hat{f}|x'\rangle$ are called the matrix elements of $\hat{f}$ in the position representation. Of course, since x is a continuous rather than a discrete index for the matrix elements, we are not really dealing with a conventional matrix here. While the term matrix element is commonly used in the physics literature, the alternative terminology in proper mathematical language is to say that $f(x,x')$ is the *integral kernel* of $\hat{f}$ in the position eigenbasis.

Definition: If $\hat{f}$ is an operator, and $\{|\lambda\rangle\}$ is a continuous basis (such as the position eigenbasis) then we call $f(\lambda,\lambda') := \langle\lambda|\hat{f}|\lambda'\rangle$ the matrix elements of $\hat{f}$ in the $\{|\lambda\rangle\}$ basis. Of course, $f(\lambda,\lambda')$, which could also be written as $f_{\lambda,\lambda'}$, is a matrix whose two indices take continuous values. When such a 'matrix' acts on a vector then the common index needs to be integrated instead of summed: $\langle\lambda|\hat{f}|\psi\rangle = \int f(\lambda,\lambda')\psi(\lambda')d\lambda'$. For this reason, $f(\lambda,\lambda')$ is also called the integral kernel of $\hat{f}$ in the $\{|\lambda\rangle\}$ basis.

For example, for the operator $\hat{f} = \hat{x}$ we find that its integral kernel,

$$\hat{x}(x,x') = \langle x|\hat{x}|x'\rangle = x\langle x|x'\rangle = x\delta(x-x'), \tag{5.33}$$

is diagonal in the sense that the kernel vanishes off the diagonal, i.e., for $x \neq x'$. Let us also express the position operator in the position basis:

$$\hat{x} = \hat{x}1 = \int_{\mathbb{R}} \hat{x}\ |x\rangle\langle x|\ dx = \int_{\mathbb{R}} x\ |x\rangle\langle x|\ dx \tag{5.34}$$

Let us now calculate the momentum operator's matrix elements in the position representation:

$$\hat{p}(x,x') = \langle x|\hat{p}|x'\rangle = \sum_{n,m}\langle x|E_n\rangle\langle E_n|\hat{p}|E_m\rangle\langle E_m|x'\rangle = i\hbar\frac{d}{dx'}\delta(x-x') \tag{5.35}$$

Here, we inserted resolutions of the identity in terms of the eigenbasis $\{|E_n\rangle\}$ of a harmonic oscillator. This is useful because we already know the matrix elements $\langle n|\hat{p}|m\rangle$ of $\hat{p}$ explicitly from Eqs.5.20,5.22,5.23 and we know the coefficients $\langle E_n|x\rangle$ from Eq.5.12. The last step, i.e., to work out the sums over n and m is quite tedious and we skip the details here.

But what is the derivative of the Dirac delta? The Dirac delta itself is defined to obey:

$$\int_{\mathbb{R}} f(x)\delta(x-x')\ dx = f(x') \tag{5.36}$$

Now for the derivative of the Dirac delta we obtain via integration by parts:

$$\int_{\mathbb{R}} f(x)\frac{d}{dx}\delta(x-x')\ dx = -\int_{\mathbb{R}} \left(\frac{d}{dx}f(x)\right)\ \delta(x-x')\ dx = -\frac{df}{dx}(x') \tag{5.37}$$

We now obtain the operator $\hat{p}$ in the position representation:

$$\hat{p} = \int_{\mathbb{R}}\int_{\mathbb{R}} i\hbar\left(\frac{d}{dx'}\delta(x-x')\right)|x\rangle\langle x'|\ dx\ dx' \tag{5.38}$$

Remember that already in Eqs.3.48,3.49, we had found a representation of the operators $\hat{x}$ and $\hat{p}$ as infinite-by-infinite matrices. Now, with Eqs.5.33,5.35, we have found a representation of $\hat{x}$ and $\hat{p}$ in a continuous basis, namely in the eigenbasis of the position operator.

5.4 Shorthand notation for operators acting on wave functions

Let us consider an operator Q that maps a vector $|\psi\rangle$ into a vector $|\phi\rangle = Q|\psi\rangle$. Since $|\psi\rangle$ and $|\phi\rangle$ both possess position wave functions, namely $\psi(x)$ and $\phi(x)$, we have that Q also induces a map of wave functions into wave functions, namely $\hat{Q} : \psi(x) \to \phi(x)$. This is conveniently described by an important shorthand notation:

Definition: We denote the induced action of an operator on a wave function by a dot. For example, an operator $\hat{Q}$ acts on a state $|\psi\rangle$ by mapping it into a state $|\phi\rangle$, i.e., we have $|\phi\rangle = \hat{Q}|\psi\rangle$. If we choose some basis $\{|\lambda\rangle\}$, this also means that $\hat{Q}$ maps the wave function $\psi(\lambda)$ into the wave function $\phi(\lambda)$. We write this as:

$$\phi(\lambda) = \hat{Q}.\psi(\lambda) \tag{5.39}$$

For example, in the case of the position operator and the position eigenbasis:

$$\phi(x) = \langle x|\phi\rangle = \langle x|\hat{x}|\psi\rangle = x\langle x|\psi\rangle = x\psi(x) \tag{5.40}$$

In the shorthand notation, we can therefore write that the action of the position operator on position wave functions is:

$$\hat{x}.\psi(x) = x\psi(x) \tag{5.41}$$

What then is the action of $\hat{p}$ on position wave functions? Abstractly, we have $|\varphi\rangle = \hat{p}|\psi\rangle$. In the position eigenbasis, this is:

$$\begin{aligned}
\phi(x) &= \langle x|\phi\rangle = \langle x|\hat{p}|\psi\rangle && (5.42)\\
&= \int_{\mathbb{R}} \langle x|\hat{p}|x'\rangle\langle x'|\psi\rangle \; dx' && (5.43)\\
&= \int_{\mathbb{R}} i\hbar \left(\frac{d}{dx'}\delta(x-x')\right) \psi(x') \; dx' && (5.44)\\
&= -i\hbar \int_{\mathbb{R}} \delta(x-x') \; \frac{d}{dx'}\psi(x') \; dx' + i\hbar \left[\delta(x-x')\psi(x')\right]_{x'=-\infty}^{x'=\infty} && (5.45)\\
&= -i\hbar\frac{d}{dx}\psi(x) && (5.46)
\end{aligned}$$

This means that in the shorthand notation we can write:

$$\hat{p}.\psi(x) = -i\hbar\frac{d}{dx}\psi(x) \tag{5.47}$$

Exercise 5.2 *Verify the canonical commutation relation in the position representation, i.e., verify that, for all (differentiable) wave functions $\psi(x)$:*

$$(\hat{x}\hat{p} - \hat{p}\hat{x} - i\hbar 1).\psi(x) = 0 \tag{5.48}$$

5.5 The momentum representation

Similar to how we diagonalized the position operator, we could now calculate also the momentum operator's eigenbasis. Namely, we could diagonalize the momentum operator's matrix representation Eq.3.49 in the $\{|E_n\rangle\}_{n=0}^{\infty}$ basis of a harmonic oscillator. Instead, it will be more convenient to calculate the momentum operator's spectrum and eigenbasis by diagonalizing it in the position representation. Concretely, let us solve the eigenvector equation

$$\hat{p}|p\rangle = p|p\rangle \tag{5.49}$$

in the position basis, i.e., with the momentum eigenvector $|p\rangle$ written in the form:

$$|p\rangle = \mathbf{1}|p\rangle = \int_{\mathbb{R}} |x\rangle\langle x|p\rangle \; dx \tag{5.50}$$

Here, $\langle x|p\rangle$ is the wave function of the momentum eigenvector $|p\rangle$ to eigenvalue p in the position basis. If we can calculate $\langle x|p\rangle$, then we have the momentum eigenvector $|p\rangle$ through Eq.5.50. From Eq.5.49 we obtain:

$$\langle x|\hat{p}\mathbf{1}|p\rangle = p\ \langle x|p\rangle \tag{5.51}$$

$$\int_{\mathbb{R}} \langle x|\hat{p}|x'\rangle\langle x'|p\rangle\ dx' = p\ \langle x|p\rangle \tag{5.52}$$

$$\int_{\mathbb{R}} i\hbar \left(\frac{d}{dx'}\delta(x-x')\right) \langle x'|p\rangle\ dx' = p\ \langle x|p\rangle \tag{5.53}$$

$$\int_{\mathbb{R}} -i\hbar\delta(x-x')\frac{d}{dx'}\langle x'|p\rangle\ dx' = p\ \langle x|p\rangle \tag{5.54}$$

Therefore, the function $\langle x|p\rangle$ must obey:

$$-i\hbar\ \frac{d}{dx}\ \langle x|p\rangle = p\ \langle x|p\rangle \tag{5.55}$$

Notice that we could have found immediately that Eq.5.49 translates into Eq.5.55 in the position basis by using the shorthand notation Eq.5.47. Clearly, the solution to Eq.5.55 is:

$$\langle x|p\rangle = N\ e^{\frac{ixp}{\hbar}} \tag{5.56}$$

Since, therefore, we are able to find an eigenvector $|p\rangle$ for each value $p \in \mathbb{R}$, we can conclude that $\text{spec}(\hat{p}) = \mathbb{R}$. The spectrum is, therefore, continuous and the approximate eigenfunctions $\langle x|p\rangle$ therefore require continuum normalization:

$$\begin{aligned}
\delta(p-p') &= \langle p|p'\rangle && (5.57)\\
&= \int_{\mathbb{R}} \langle p|x\rangle\langle x|p'\rangle\ dx && (5.58)\\
&= \int_{\mathbb{R}} N^*\ e^{\frac{-ixp}{\hbar}}\ N\ e^{\frac{ixp'}{\hbar}}\ dx && (5.59)\\
&= N^*N \int_{\mathbb{R}} e^{\frac{ix}{\hbar}(p-p')}\ dx && (5.60)
\end{aligned}$$

At this point we use the fact that

$$\int_{\mathbb{R}} e^{iab}\ da = 2\pi\ \delta(b) \tag{5.61}$$

to conclude that $N = (2\pi\hbar)^{-1/2}$. We obtain the continuum normalized position eigenfunctions of the momentum eigenvectors:

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}\ e^{\frac{ixp}{\hbar}} \tag{5.62}$$

Notice that this also yields the momentum wave functions of the position eigenvectors:

$$\langle p|x\rangle = \langle x|p\rangle^* = \frac{1}{\sqrt{2\pi\hbar}}\ e^{\frac{-ixp}{\hbar}} \tag{5.63}$$

We obtain, analogously to the calculation for $\hat{x}$ before, a resolution of the identity and a spectral resolution of the momentum operator:

$$\mathbf{1} = \int_{\mathbb{R}} |p\rangle\langle p|\ dp, \qquad \text{and} \qquad \hat{p} = \int_{\mathbb{R}} p\ |p\rangle\langle p|\ dp \tag{5.64}$$

The momentum wave function of a state $|\psi\rangle$ is then obtained from:

$$|\psi\rangle = \mathbf{1}|\psi\rangle = \int_{\mathbb{R}} |p\rangle\langle p|\psi\rangle\ dp = \int_{\mathbb{R}} \tilde{\psi}(p)\ |p\rangle\ dp \tag{5.65}$$

Here, $\tilde{\psi}(p) := \langle p|\psi\rangle$ is a common notation for the momentum wave function. The scalar product of two states is now calculated through

$$\langle\phi|\psi\rangle = \int_{\mathbb{R}} \langle\phi|p\rangle\langle p|\psi\rangle\ dp = \int_{\mathbb{R}} \tilde{\phi}(p)^*\tilde{\psi}(p)\ dp \tag{5.66}$$

We can now derive how the momentum wave function $\tilde{\psi}(p)$ can be expressed in terms of the position wave function $\psi(x)$:

$$\begin{aligned} \tilde{\psi}(p) &= \langle p|\psi\rangle && (5.67)\\ &= \int_{-\infty}^{\infty} \langle p|x\rangle\langle x|\psi\rangle dx && (5.68)\\ &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x)\ e^{\frac{-ixp}{\hbar}}\ dx && (5.69) \end{aligned}$$

We conclude that the position and momentum representations (i.e., bases) are related by Fourier transformation. Similarly, as we saw earlier, the position eigenbasis and the eigenbasis of the Hamiltonian of a harmonic oscillator are related by a Hermite transformation. Analogously, any two choices of (appropriately orthonormalized) bases are related by a transformation that implements the unitary change of basis.

Exercise 5.3 *Derive the action of $\hat{x}$ and $\hat{p}$ on momentum wave functions, i.e., derive the short hand notation $\hat{x}.\tilde{\psi}(p) =?\tilde{\psi}(p)$ and $\hat{p}.\tilde{\psi}(p) =?\tilde{\psi}(p)$ analogously to how we derived the short hand notation for the position representation.*

5.6 Energy representations: bound states and scattering states

Consider an arbitrary quantum system with Hamiltonian $\hat{H}$. Since $\hat{H}$ is normally self-adjoint, it possesses an eigenbasis, the so-called energy eigenbasis. Let us denote the normalizable and nonnormalizable eigenvectors of $\hat{H}$ by $|E_\mu\rangle$ where μ is an index that runs through a continuous, a discrete or a mixed index set, as the case may be. Remember that, the Hamiltonians of some systems possess a purely discrete spectrum, as is the case for the harmonic oscillator. The Hamiltonians of other systems are purely continuous, as for example, that of the free particle. The spectrum can also consist of a discrete and a continuous spectrum, as, for example, the spectrum of the Hamiltonian of the hydrogen atom. What does this mathematical property of the spectrum being discrete or continuous make correspond to, physically?

To see the physical difference, let us recall that eigenvalues E_n of $\hat{H}$ that are in the point spectrum $E_n \in \text{spec}_{discr.}(\hat{H})$ come with eigenvectors $|E_n\rangle$ that are normalizable and that, in contrast, the approximate eigenvalues $E \in \text{spec}_{cont.}(\hat{H})$ of the continuous spectrum, the so-called approximate eigenvalues, come with non-normalizable approximate eigenvectors $|E\rangle$. Let us consider these normalizable and non-normalizable vectors in the position eigenbasis, i.e., $\psi_{E_n}(x) = \langle x|E_n\rangle$ and $\psi_E(x) = \langle x|E\rangle$ respectively.

Since each state $|E_n\rangle$ is normalizable, $\langle E_n|E_n\rangle = 1$, we have from Eq.5.31 that its position wave function is square integrable:

$$\int_{-\infty}^{\infty} \psi_{E_n}(x)^* \psi_{E_n}(x)\ dx = 1 \tag{5.70}$$

This implies that the wave function must decay quickly towards ±∞. For this reason, particles described by such a wave function are fairly localized and we say that they are in a bound state. This could be, for example, an electron bound to a proton, described by one of Hydrogen's orbital wave functions. In contrast, the wave functions $\psi_E(x)$ belonging to states of the continuous spectrum are not normalizable and describe particles that are entirely delocalized, much like plane waves. These eigenstates of the Hamiltonian describe particles that come in from infinity, interact with our system, perhaps change direction a bit and then go away out to infinity. The states of the continuous spectrum of the Hamiltonian are, therefore, also called scattering states. The Hamiltonians of electrons that orbit the nuclei of an atom or a molecule always possess both a discrete energy spectrum and above it also a continuous energy spectrum that reaches up to infinite energies. This is because the electrons can be bound to the nuclei at discrete energy levels, until at sufficiently high energies the nuclei can no longer hold on to the particle and the particle merely scatters off the nuclei.

There is a classical analog in the solar system. Comets are in bound states around the sun. In contrast, the extra-solar rock called Oumuamua, for example, had much more kinetic energy than a comet and it only scattered off our solar system when it visited our solar system in 2017. Similarly, the hydrogen atom's well known discrete energy levels constitute only the point spectrum. The Hamiltonian of an electron interacting with a proton also possesses a continuous spectrum which ranges from 0 to infinity.

Chapter 6

Continuous versus discrete in quantum mechanics

6.1 It takes only a countable infinite amount of information to specify a quantum state

Let us review how it can be that a state $|\psi\rangle$ can be specified by both, an uncountable amount or also by a countable amount of coefficients. Namely, $|\psi\rangle$ can be specified through uncountably many numbers $\psi(x) = \langle x|\psi\rangle$, where x runs through all the uncountably infinitely many real numbers, or also through the countably infinitely many numbers $\psi_n = \langle n|\psi\rangle$ where n runs through a countably infinite number of integers.

The answer is subtle. The countably many coefficients ψ_n really do suffice to specify $|\psi\rangle$ because $|\psi\rangle = \sum_{n=1}^{\infty} \psi_n|n\rangle$. Therefore, when we instead describe $|\psi\rangle$ through the uncountably infinitely many data $\psi(x) \ \ \forall x \in \mathbb{R}$ this description must possess a large redundancy. Indeed, there are many wave functions that describe the same state!

Consider two wave functions $\psi(x)$ and $\phi(x)$ which are exactly the same for all $x \in \mathbb{R}$, except at a finite number of points $x_1, x_2, ..., x_N$, where they differ, for example, $\phi(x_2) = 77$ but $\psi(x_2) = -3.2$. Any such pairs of wave functions $\psi(x)$ and $\phi(x)$ are actually physically equivalent in the sense that the predictions come out the same. The reason is that when we calculate an expectation value with either $\psi(x)$ or $\phi(x)$ the prediction always comes out to be the same. Consider, for example, the position expectation value: $\bar{x} = \int \psi^*(x)x\psi(x) = \int \phi^*(x)x\phi(x)$. The reason is that the value of an integral is insensitive to changing the value of its integrand function at a finite number of points.

Why? It's because when you integrate, i.e., when you calculate the area under a curve, then if you make the integrand function have a spike at one isolated point, this does not have any effect on the area under the curve. A spike at a single point doesn't affect the area under the curve because such a spike is just a line and lines don't have area. If you are interested in the details of the integration theory behind this, look up the notion of Lebesgue integration.

So in conclusion, since we can add isolated spikes everywhere on the x axis, each position wave function has uncountably infinitely many brother and sister position wave functions that differ only at individual points and that are indistinguishable under the integral and are, therefore, also indistinguishable in the calculation of any expectation value. So they are physically equivalent.

Each individual state $|\psi\rangle$, possesses, therefore, an equivalence class of uncountably infinitely many position wave functions. What is specified by $|\psi\rangle$ is merely the equivalence class, but not any particular wave function in it. This can pose a problem when wanting to differentiate the wave function. That's because wherever the wave function is not differentiable because of one of those spikes, we can only differentiate before and after the spike but there is no derivative at the spike. That's not a problem under the integrals because it happens only at isolated points, but it's tedious. Therefore, in practice, we always choose the most differentiable member of the equivalence class. I know, all these things are often not spelled out in textbooks, as many authors just follow the herd. But in this course we are not afraid to dig somewhat deeper into what's really going on.

So the redundancy in the form of wave functions grouping into large equivalence classes for each state is why it is that a(n) (equivalence class of) position wave function $\psi(x)$ can be specified by just giving countably many data, such as the data $\{\psi_n\}$ for $n = 1, 2, ...$ Namely, by specifying, for example, the ψ_n we obtain $|\psi\rangle = \sum_{n=1}^{\infty} \psi_n |n\rangle$ and from it we obtain a $\psi(x) = \langle x|\psi\rangle$. Let us remember that it is not the unique $\psi(x)$ that we obtain in this way. It's just the differentiable member of a whole equivalence class of wave functions, such as $\phi(x)$ that would describe the exact same physics.

6.2 Stieltjes integration explains the Dirac delta

Definition (Stieltjes integral): The Stieltjes integral

$$\int_a^b f(x)\ dm(x) \tag{6.1}$$

requires an integrand, i.e., a function $f(x)$ to be integrated over and a function $m(x)$, called the integrator (or measure) which is monotonically increasing (i.e., which obeys $m(x_2) \geq m(x_1)$ when $x_2 > x_1$). The integration is performed by considering partitions $x_0 < x_1 < x_2 < ... < x_n$ of the interval $[a, b]$, i.e., $x_0 = a$ and $x_n = b$. We then define:

$$\int_a^b f(x)\ dm(x) := \lim_{\epsilon \to 0} \sum_i f(\tilde{x}_i)\ (m(x_{i+1}) - m(x_i)) \tag{6.2}$$

Here, $f(\tilde{x}_i)$ is f evaluated at an arbitrary point in the i'th interval: $\tilde{x}_i \in [x_i, x_{i+1}]$ and the limit is the limit in which the maximum spacing, ϵ occurring in a sequence of partitionings goes to zero. Notice that if the integrator function is constant, then the integral vanishes. Also, if we add any constant to the integrator function $m(x)$, this makes no difference to the integral because only differences of its values occur in Eq.6.2.

Now how does the Stieltjes integral relate to ordinary integration?

Proposition: Assume that the integrator function is differentiable and that the derivative $m'(x)$ of $m(x)$ is continuous. Then the Stieltjes integral can be expressed in terms of the ordinary integral:

$$\int_a^b f(x)\ dm(x) = \int_a^b f(x)\ \frac{dm(x)}{dx}\ dx \tag{6.3}$$

So in particular, if we choose the integrator function to be $m(x) = x$ then we have $dm/dx = 1$ and we recover the ordinary integral over f.

But what then is the advantage of the Stieltjes integration method? The key advantage is that we can do more types of integrals now because the integrator function m need not have a continuous derivative! For example, consider the case of m being a Heaviside step function:

$$m(x) = \theta(x) = \begin{cases} 0 & \text{if } x < 0 \\ 1/2 & \text{if } x = 0 \\ 1 & \text{if } x > 0 \end{cases} \tag{6.4}$$

Assuming that $a < 0 < b$ and applying the definition Eq.6.2 shows that the Stieltjes integral in this case yields:

$$\int_a^b f(x)\ dm(x) = f(0) \tag{6.5}$$

For comparison, the Dirac delta is defined to be the mathematical object that obeys:

$$\int_a^b f(x)\ \delta(x) dx = f(0) \tag{6.6}$$

Comparing with Eq.6.3, we now see that the Dirac delta behaves like the derivative of the Heaviside function

$$\frac{d}{dx}\ \theta(x) = \delta(x) \tag{6.7}$$

This equation is commonly stated but let us keep in mind that, strictly speaking, this equation holds when functions are being integrated over using the Stieltjes integration method.

Exercise 6.1 *Explain Eq.6.5 using a sketch of the plot of a function and a partitioning of the integration interval.*

Similarly, we can generate a sum by using an integrator function with multiple steps. For example, $m(x) = \sum_i \theta(x - x_i)$ yields.

$$\int_a^b f(x)\ dm(x) = \sum_i f(x_i) \tag{6.8}$$

More generally, by using an integrator function that is in some parts of the real line smooth and in some parts of the real line it has steps of various sizes, one single Stieltjes integral can express arbitrarily complicated combinations of sums and Riemann integrals.

Exercise 6.2 *Sketch the graph of an integrator function* $m(x)$ *which integrates over the intervals* $[3, 6]$ *and* $[9, 11]$ *and sums over the values of the integrand at the points* $x = 5$ *and* $x = 6$*.*

Let us recall why we here introduce the Stieltjes integral. It is because it allows us to avoid using the Dirac delta. Of course, we could bring back the Dirac delta. For example, using the Dirac Delta, we could rewrite Eq.6.8:

$$\int_a^b f(x)\ dm(x) = \int_a^b f(x)\ \frac{dm(x)}{dx}\ dx = \int_a^b f(x)\ \sum_i \delta(x - x_i)\ dx = \sum_i f(x_i) \tag{6.9}$$

In practice, working with the Dirac delta is indeed convenient, even though it is not a function but is instead what is called a distribution[1]. The reason why we need a way to work without using the Dirac delta is that when it comes to integrating not over functions but integrating over operators, then we need to be able to work with operator-valued functions, such as $|x\rangle\langle x|$ rather than working with operator-valued distributions such as $\delta(x)$. The problem with "operator" such as $|x\rangle\langle x|$ is that they are not really operators because, for example, we cannot multiply them onto themselves: $|x\rangle\langle x|x\rangle\langle x| = \delta(0)|x\rangle\langle x|$ is undefined.

The Dirac delta is a distributional generalization of a number-valued function. But we would here need distributional generalizations also of vector- and operator-valued functions too, because this would come up in resolutions of the identity and in spectral representations of observables. Even if in practice one works with operator-valued distributions as if there were no subtlety, it is good to know, at least in principle, how things can be put on a solid footing by using the Stieltjes integral.

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[1] A distribution such as the Dirac delta can be viewed as a continuous linear map from a specified space of functions to numbers. For example, the Dirac delta in $\int f(x)\ \delta(x - x_0)\ dx$ maps the function f linearly into the number $f(x_0)$. For details, see, e.g., the appendix on distributions in Messiah's book on quantum mechanics. Distributions can also be viewed as elements of a type of Hilbert space called a Sobolev space, in which the inner product involves derivatives.

6.3 The Stieltjes integral explains operators such as $|x\rangle\langle x|$.

In order to make sense of expressions such as $|x\rangle\langle x|$, let us first define the notion of a partial resolution of the identity:

Definition: Assume that $\hat{f}$ is a self-adjoint operator whose spectrum is purely continuous and consists of the entire real line. Then we define the partial resolution of the identity in the eigenbasis of $\hat{f}$ in this way:

$$\hat{E}(f) := \int_{-\infty}^{f} |\tilde{f}\rangle\langle\tilde{f}| \; d\tilde{f} \tag{6.10}$$

We recover the full resolution of the identity as:

$$\mathbf{1} = \hat{E}(\infty) = \lim_{f\to\infty} \int_{-\infty}^{f} |\tilde{f}\rangle\langle\tilde{f}| \; d\tilde{f} \tag{6.11}$$

The partial resolution of the identity in Eq.6.10 has the advantage that we can differentiate it with respect to the integration boundary:

$$\frac{d\hat{E}(f)}{df} = |f\rangle\langle f| \tag{6.12}$$

So now we have found an expression for the object that we are interested in: $|x\rangle\langle x|$. How does this help? Let us rewrite the resolution of the identity:

$$\mathbf{1} = \int_{\mathbb{R}} |f\rangle\langle f| = \int_{\mathbb{R}} \frac{d\hat{E}(f)}{df} \; df \tag{6.13}$$

From this, we now obtain, in the Stieltjes sense:

$$\mathbf{1} = \int_{\mathbb{R}} d\hat{E}(f) \tag{6.14}$$

And similarly:

$$\hat{f} = \int_{\mathbb{R}} f \; d\hat{E}(f) \tag{6.15}$$

Why are Eqs.6.14,6.15 useful? Remember that, in keeping with physics notation, we used expressions such as $|f\rangle\langle f|$ which are actually ill defined if $|f\rangle$ is an improper or 'approximate' eigenvector. For example, its square is infinite: $|f\rangle\langle f|f\rangle\langle f| = \delta(0)\,|f\rangle\langle f|$.

It would seem that so far not much is gained. Doesn't Eq.6.14 still make use of $|f\rangle\langle f|$? It does not! Let us look at the definition of the Stieltjes integral in Eq.6.2 again. The role of $m(x)$ there is played here by $\hat{E}(f)$. Notice that in Eq.6.2 only evaluations of $m(x)$ occur and that there is no need to evaluate its derivative $dm(x)/dx$ ever. Similarly here, in Eqs.6.14,6.15, only $\hat{E}(f)$ occurs but not anymore its derivative (which would be $|f\rangle\langle f|$).

And $\hat{E}(f)$ is a perfectly well-behaved operator! One can show that for every value of f it is a projector. For this reason, Eqs.6.14,6.15 are at the heart of the rigorous mathematical formulations and applications of the spectral theorem.

In fact, while in the current section we only considered the case where the spectrum of $\hat{f}$ is the real line, the spectrum of a self-adjoint operator can of course contain arbitrary continuous and discrete parts. The Stieltjes integral takes care of this automatically, i.e., we no longer have to use a mix of sums and integrals. All we need is the Stieltjes integrals Eqs.6.14,6.15 over the full real line. In them, the summations of the point spectrum, see, e.g., Eqs.4.30,4.31, arise, as usual for Stieltjes integrals, through discontinuities in the integrator function $\hat{E}(f)$. The continuous spectrum is where the integrator function changes continuously and on stretches of $\mathbb{R}$ where there is no continuous or point spectrum, the integrator function $\hat{E}(f)$ is constant.

Chapter 7

Uncertainty principles

7.1 The Heisenberg uncertainty relations

To solve a quantum mechanical problem is to choose or determine the initial state vector $|\psi\rangle$ and to calculate the position and momentum operators $\hat{x}(t), \hat{p}(t)$ subject to the equations of motion, the canonical commutation relations and subject to the hermiticity conditions $\hat{x}(t) = \hat{x}(t)^\dagger$ and $\hat{p}(t) = \hat{p}(t)^\dagger$.

Once the $\hat{x}(t), \hat{p}(t)$ (usually with indices indicating dimensions and particle number) and the initial state vector $|\psi\rangle$ of the system are known, we can calculate everything: Consider any observable $\hat{f}(t)$, i.e., any polynomials or well-behaved power series in the positions and momenta obeying $\hat{f}^\dagger(t) = \hat{f}(t)$. Then we can calculate its ensemble expectation values $\bar{f}(t) = \langle\psi|\hat{f}(t)|\psi\rangle$. Here, the term ensemble expectation value means the average outcome of the measurement of the observable $\hat{f}(t)$ if the same experiment (i.e., with the same initial conditions) is either repeated many times, or is performed many times simultaneously. An ensemble of experimental runs can be an ensemble in time or an ensemble in space.

Now if $\hat{f}(t)$ is an observable, i.e., if it obeys $\hat{f}(t) = \hat{f}(t)^\dagger$ then also $\hat{f}(t)^2$ is an observable, i.e., it obeys $\hat{f}(t)^2 = (\hat{f}(t)^2)^\dagger$. Thus, for any observable $\hat{f}(t)$ we can predict not only its ensemble average $\bar{f}(t)$, but we can also predict the ensemble average value $\overline{f^2}(t)$ of the square of that observable.

In classical mechanics, this would not be surprising. For example, when the initial conditions for throwing an object (such as a ball or a particle) are known then the distance that the object will fly (say in vacuum) before hitting the ground is an observable that can be predicted. Let's say the prediction is $50m$. Well then clearly we can also predict the square of that distance: It will be $2500m^2$. Since in classical mechanics we are sure about the distance we are also sure about the square of the distance.

In quantum mechanics, we saw that the prediction for the squares of the distance measurements is generally not the square of the prediction for the distance measurements! Knowing the average outcome of the measurement of an observable does not automatically tell us the average outcome of the square of that observable: In general (i.e., in most cases), we have $\bar{f}^2 \neq \overline{f^2}$. This means that the predictions cannot be certain, there must be a spread of the measurement outcomes. For example, the measurement outcomes for the distance might be 49m, 50m and 51m with probabilities 1/3 each. Then the prediction is 50m but the predicted square of the distances is then $(49^2 + 50^2 + 51^2)/3\ m^2 = (2500 + 2/3)m^2$.

We conclude that quantum mechanics implies that when performing an ensemble of identical experiments, each time measuring $\hat{f}$ at the end, then the measurement values for f must have a spread. Only this way can we have that $\bar{f}^2 \neq \overline{f^2}$. The predictions of quantum mechanics are generally probabilistic. We can only predict the outcome of a measurement with certainty if the observable in question happens to obey $\bar{f}^2 = \overline{f^2}$.

The extent to which the equation $\bar{f}^2 = \overline{f^2}$ is violated quantifies how large the spread of the outcomes of the $\hat{f}$ measurements will be in an ensemble of experimental runs.

In fact the difference between the left hand side and the right hand side of that equation coincides with the variance of the measurement outcomes. Remember that the variance of a statistical distribution is the average of the squared deviation from the average. Here, in Dirac notation:

$$\begin{aligned}
(\Delta f(t))^2 &= \overline{(\hat{f}(t) - \overline{f}(t))^2} && (7.1)\\
&= \langle\psi| \left(\hat{f}(t) - \langle\psi|\hat{f}(t)|\psi\rangle\right)^2 |\psi\rangle && (7.2)\\
&= \langle\psi|\hat{f}^2(t)|\psi\rangle - \langle\psi|\hat{f}|\psi\rangle^2 && (7.3)\\
&= \overline{f(t)^2} - \overline{f(t)}^2 && (7.4)
\end{aligned}$$

We can now derive Heisenberg's famous uncertainty relations for the variances and the square roots of the variances (the so called standard deviation) between any pairs of observables:

Proposition: Assume $\hat{f}(t)$ and $\hat{g}(t)$ are observables and assume that the system is in the state $|\psi\rangle$. Then:

$$\Delta f(t)\ \Delta g(t)\ \geq\ \frac{1}{2}|\langle\psi|[\hat{f}(t), \hat{g}(t)]|\psi\rangle| \tag{7.5}$$

In particular, we have for all states $|\psi\rangle$:

$$\Delta x(t)\ \Delta p(t)\ \geq\ \frac{1}{2}|\langle\psi|i\hbar|\psi\rangle| = \frac{\hbar}{2} \tag{7.6}$$

In this way, the noncommutativity of the positions and momenta directly imply that in a state in which the position $\bar{x}(t)$ is predicted sharply, i.e., with small standard deviation $\Delta x(t)$, the prediction $\bar{p}(t)$ of the momentum must come with a correspondingly large standard deviation $\Delta p(t)$, and vice versa. In general, we have of course:

$$\Delta x_i^{(r)}(t)\ \Delta p_j^{(s)}(t)\ \geq\ \frac{\hbar}{2}\ \delta_{i,j}\delta_{r,s} \tag{7.7}$$

Recall that initial conditions can be posed by specifying the mean values $\bar{f}(t_0), \bar{g}(t_0)$ etc. of all observables $\hat{f}(t_0), \hat{g}(t_0)$ including their arbitrary powers. We asked under which conditions so-posed initial conditions determine a state $|\psi\rangle$. We see now that the Heisenberg uncertainty relations impose restrictions on which so-described initial conditions can occur.

Proof of the Heisenberg uncertainty principle: Assume $|\psi\rangle$ is normalized and assume that $\hat{f}$ and $\hat{g}$ are observables at some time t. (To keep the formulas from getting too long we will simply write $\hat{g}, \hat{f}$ instead of $\hat{g}(t), \hat{f}(t)$). We start by considering the vector

$$|\phi\rangle = \Big(\hat{f} - \bar{f}\mathbf{1} + \mathrm{i}\alpha(\hat{\mathrm{g}} - \bar{\mathrm{g}}\mathbf{1})\Big)\,|\psi\rangle \tag{7.8}$$

where α is an arbitrary real number. No vector's norm is negative. In particular, $\langle\phi|\phi\rangle \geq 0$, i.e.:

$$\langle\psi|\,\Big((\hat{f} - \bar{f}\mathbf{1}) - \mathrm{i}\alpha(\hat{\mathrm{g}} - \bar{\mathrm{g}}\mathbf{1})\Big)\,\Big((\hat{f} - \bar{f}\mathbf{1}) + \mathrm{i}\alpha(\hat{\mathrm{g}} - \bar{\mathrm{g}}\mathbf{1})\Big)\,|\psi\rangle \geq 0 \tag{7.9}$$

Thus:

$$\langle\psi|(\hat{f} - \bar{f}\mathbf{1})^2|\psi\rangle + \alpha^2\langle\psi|(\hat{\mathrm{g}} - \bar{\mathrm{g}}\mathbf{1})^2|\psi\rangle + \alpha\langle\psi|\mathrm{i}(\hat{\mathrm{f}}\hat{\mathrm{g}} - \hat{\mathrm{g}}\hat{\mathrm{f}})|\psi\rangle \geq 0 \tag{7.10}$$

Therefore:

$$(\Delta f)^2 + \alpha^2(\Delta g)^2 + \alpha\langle\psi|i[\hat{f},\hat{g}]|\psi\rangle \geq 0 \tag{7.11}$$

Thus, completing the squares for α:

$$(\Delta f)^2 + (\Delta g)^2\left(\alpha + \frac{\langle\psi|i[\hat{f},\hat{g}]|\psi\rangle}{2(\Delta g)^2}\right)^2 - \frac{\Big(\langle\psi|i[\hat{f},\hat{g}]|\psi\rangle\Big)^2}{\left(2(\Delta g)^2\right)^2}\,(\Delta g)^2 \geq 0 \tag{7.12}$$

In the last step, we assumed[1] that $\Delta g \neq 0$. We observe that if we were to choose α very large, then the big bracket is large and the inequality is trivially obeyed. Conversely, for any given $|\psi\rangle$, we obtain the most stringent inequality for the standard deviations by choosing α such that the big bracket vanishes, i.e., if we choose $\alpha = -\langle\psi|i[\hat{f},\hat{g}]|\psi\rangle/(2(\Delta g)^2)$. We obtain:

$$(\Delta f)^2(\Delta g)^2 - \frac{\langle\psi|i[\hat{f},\hat{g}]|\psi\rangle^2}{4} \geq 0 \tag{7.13}$$

and therefore, finally:

$$\Delta f(t)\ \Delta g(t)\ \geq\ \frac{1}{2}|\langle\psi|[\hat{f}(t),\hat{g}(t)]|\psi\rangle| \tag{7.14}$$

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[1] If $\Delta g = 0$ then it depends on whether or not also $\langle\psi|i[\hat{f},\hat{g}]|\psi\rangle$ is zero. First, we observe that $\langle\psi|i[\hat{f},\hat{g}]|\psi\rangle$ is a real number because $\Big(i[\hat{f},\hat{g}]\Big)^\dagger = i[\hat{f},\hat{g}]$. Now if $\Delta g = 0$ and $\langle\psi|i[\hat{f},\hat{g}]|\psi\rangle = 0$, then Eq.7.11 implies no condition on Δf. If, however, $\Delta g = 0$ and $\langle\psi|i[\hat{f},\hat{g}]|\psi\rangle \neq 0$, then $\Delta f = +\infty$ because it must then be larger than any positive real number (since α can be chosen arbitrarily).

Exercise 7.1 *There are indications from studies of quantum gravity*[2]*, that the uncertainty relation between positions and momenta acquire corrections due to gravity effects and should be of the form:* $\Delta x\Delta p \geq \frac{\hbar}{2}(1+\beta(\Delta p)^2+...)$*, where* β *is a small positive number. (a) Show that this type of uncertainty relation arises if the canonical commutation relation is modified to read* $[\hat{x},\hat{p}] = i\hbar(1+\beta\hat{p}^2)$*. (b) Sketch the modified uncertainty relation* $\Delta x\Delta p \geq \frac{\hbar}{2}(1+\beta(\Delta p)^2)$ *in the* Δp *versus* Δx *plane. (c) Show that this resulting uncertainty relation implies that the uncertainty in position can never be smaller than* $\Delta x_{min} = \hbar\sqrt{\beta}$*.*

Technical remark: In this case, the position observables $\hat{x}$ cannot possess eigenvectors nor close approximations to eigenvectors, because they would have vanishing position uncertainty. Such $\hat{x}$ therefore cannot be diagonalizable and therefore, by the so-called spectral theorem, they cannot be self-adjoint (i.e., the domains of x and $x^\dagger$ do not coincide). Such position operators are what is called symmetric operators, i.e., they obey only the bare minimum condition on an observable namely that all its expectation values are real: $\hat{f}$ is called symmetric iff $\langle\psi|\hat{f}|\psi\rangle \in \mathbb{R}\ \forall|\psi\rangle \in D_{\hat{f}}$. In linear algebra, i.e., when the Hilbert spaces are finite dimensional, the notions of self-adjoint operator and symmetric operator coincide. In infinite-dimensional Hilbert spaces, all self-adjoint operators are also symmetric but not all symmetric operators are self-adjoint. In the international mathematical literature, the definitions of self-adjoint operator and symmetric operator are generally agreed upon. Unfortunately, however, there is no agreement on the definition of the term hermitean operator, which can mean either self-adjoint or symmetric operator, depending on the author. In the physics literature, the term hermitean is often used but its definition is rarely specified. Here, we will use the hermitean operator as synonymous to symmetric operator. The term describes the bare minimum requirement on any observable: Its expectation values must be real. We will write $\hat{f} = \hat{f}^\dagger$ with the tacit understanding that the domains of $\hat{f}$ and $\hat{f}^\dagger$ may not coincide.

7.2 The time and energy uncertainty relation

We have seen that in quantum mechanics the position coordinates are observables whose uncertainties can be calculated through $\Delta x = \langle\psi|(\hat{x}-\langle\psi|\hat{x}|\psi\rangle)^2|\psi\rangle^{1/2}$. In contrast, quantum mechanics treats the time coordinate t as a mere parameter. Therefore,

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[2] Gravity comes in this way: Momentum, just like energy, gravitates by curving space. Assume that we want to measure positions very precisely, i.e., we try to make Δx very small. This, however, leads to a large momentum uncertainty Δp and therefore ultimately to a large uncertainty in the curvature of space at the location where we try to resolve the position. It can be shown that if Δx were about $10^{-35}m$ or smaller, the resulting curvature uncertainty would significantly disturb the precision of the position predictions. Thus, in simple models, a finite lower bound $\approx 10^{-35}m$ to the uncertainty in positions is expected. The critical length $10^{-35}m$ is called the Planck length. In my thesis, I happened to find the first Hilbert space representations for such minimal-length uncertainty relations. A lot of follow-up papers (about two a week) are calculating the impact on atoms, black holes and cosmology.

if we are looking to derive an uncertainty relation that involves time, we first need to clarify what we mean by an uncertainty Δt in time.

To this end, consider an observable $\hat{f}(t)$. Its expectation value, $\bar{f}(t)$, and its uncertainty $\Delta f(t)$ generally change over time.

Now consider that we prepare an ensemble (i.e., a collection) of identical experiments, all starting with the same initial condition. Let's say that in a sub-ensemble we measure the observable $\hat{f}$ at a time t_0 and in the remaining cases of the ensemble we measure the observable at a time $t_0+\Delta t$. The individual outcomes of the measurements of $\hat{f}(t_0)$ will generally differ from the outcomes of the individual measurements of $\hat{f}(t_0+\Delta t)$. There are two reasons for this. One reason is that the system has evolved from time t_0 to time $t_0+\Delta t$ and so the expectation values $\hat{f}(t_0)$ and $\hat{f}(t_0+\Delta t)$ are generally different and so of course the typical measurement outcomes are different at the two times. The other reason why the measurements generally differ at the times t_0 and $t_0+\Delta t$ is that there are quantum fluctuations, namely as predicted by $\Delta f(t_0)$ and $\Delta f(t_0+\Delta t)$.

This leads to the question which of the two reasons is the dominant one. And that depends! If we choose a short Δt then the system will not have had much time to evolve and therefore $\bar{f}(t_0)$ and $\bar{f}(t_0+\Delta t)$ are still approximately the same. This means that the differing outcomes of the measurements of $\hat{f}$ at t_0 and at $t_0+\Delta t$ are almost entirely due to quantum fluctuations. If one the other hand, we make Δt very large then the system had time to evolve significantly and the expectation values $\bar{f}(t_0)$ and $\bar{f}(t_0+\Delta)$ can therefore differ significantly. In this case the difference between the individual outcomes of the individual measurements of $\hat{f}$ at t_0 or $t_0+\Delta t$ are almost entirely due to the evolution of the system and not due to the quantum fluctuations.

There must be a Δt that is the threshold between the two cases! Namely, starting from some time t_0, how much time, Δt do we have to wait until the expectation value of $\hat{f}$ has changed appreciably, i.e., until it exceeds the quantum uncertainty? That time is crucial: it is the time we have to wait to be able to see the evolution of a quantum system in spite of the presence of quantum noise!

Concretely, we need to determine the amount of time, Δt, that it takes for the expectation value $\bar{f}(t)$ to change by the average standard deviation $\overline{\Delta f}$. Here, we define the average standard deviation as the time-average over the standard deviation from t_0 to $t_0+\Delta t$:

$$\overline{\Delta f} := \frac{\int_{t_0}^{t_0+\Delta t} \Delta f(t)\ dt}{\Delta t} \tag{7.15}$$

We want to determine that amount of time Δt that it takes for the change of the expectation value $\bar{f}$ to start exceeding $\overline{\Delta f}$, because that's the amount of time it takes for change due to the dynamics of the system to dominate over the quantum noise. So we are looking for that amount of time Δt for which:

$$|\bar{f}(t_0+\Delta t)-\bar{f}(t_0)| = \overline{\Delta f} \tag{7.16}$$

Combining Eqs.7.15,7.16, we obtain for the critical Δt:

$$\Delta t = \frac{\int_{t_0}^{t_0+\Delta t} \Delta f(t)\ dt}{|\bar{f}(t_0+\Delta t) - \bar{f}(t)|} \tag{7.17}$$

Interestingly, quantum mechanics implies a fundamental relation between the amount of time, Δt, that it takes for an expectation value $\bar{f}$ to change by more than the average quantum fluctuation and the uncertainty in the energy ΔH. Namely, assuming that the Hamiltonian does not depend on time[3], we obtain:

$$\Delta f(t) \Delta H \geq \frac{1}{2} \left| \langle\psi|[\hat{f}(t), \hat{H}]|\psi\rangle \right| \tag{7.18}$$

and

$$\frac{d\hat{f}(t)}{dt} = \frac{1}{i\hbar}\ [\hat{f}(t), \hat{H}] \tag{7.19}$$

we obtain:

$$\Delta f(t) \Delta H \geq \frac{\hbar}{2} \left| \langle\psi| \frac{d\hat{f}(t)}{dt} |\psi\rangle \right| = \frac{\hbar}{2} \left| \frac{d}{dt} \langle\psi|\hat{f}(t)|\psi\rangle \right| \tag{7.20}$$

We used that the initial state vector $|\psi\rangle$ does not depend on time. We obtain:

$$\Delta f(t) \Delta H \geq \frac{\hbar}{2} \left| \frac{d\bar{f}(t)}{dt} \right| \tag{7.21}$$

Integrating over time, we obtain:

$$\begin{aligned} \Delta H \int_{t_0}^{t_0+\Delta t} \Delta f(t)\ dt \ &\geq\ \frac{\hbar}{2} \int_{t_0}^{t_0+\Delta t} \left| \frac{d\bar{f}(t)}{dt} \right|\ dt \\ &\geq\ \frac{\hbar}{2} \left| \int_{t_0}^{t_0+\Delta t} \frac{d\bar{f}(t)}{dt}\ dt \right| = \frac{\hbar}{2} |\bar{f}(t_0+\Delta t) - \bar{f}(t_0)| \end{aligned} \tag{7.22}$$

Now inserting Eq.7.17 we finally obtain the time-energy uncertainty relation:

$$\Delta t\ \Delta H\ \geq\ \frac{\hbar}{2} \tag{7.23}$$

It is quite remarkable that this uncertainty relation looks so similar to that between position and momentum! And, notice that all dependence on the choice of $\hat{f}$ has dropped out. What this means is that if the energy of a system has uncertainty ΔH then for *every* observable $\hat{f}$ it takes at least an amount of time Δt that obeys Eq.7.23 for the mean value $\bar{f}$ of the observable to change appreciably, i.e., for it to change by at

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[3] Of course, if we allow ourselves to change the Hamiltonian arbitrarily then we can make observables change arbitrarily quickly too.

least the average uncertainty $\overline{\Delta f}$. In the extreme case where we know the energy of a system precisely, then none of its observables possesses any time variation. Consider, for example, a system in its lowest energy state, say a hydrogen atom. If we know that the hydrogen atom is in its lowest energy state and if we are sure, therefore, what its energy is, $\Delta H = 0$, then none of the observables $\hat{f}$ of the hydrogen atom changes over time! For example, there is definitely no observable rotation of the electron about the proton in any way - because *all* observables' expectation values are constant. Conversely, if a system is to possess any observables $\hat{f}$ which do change appreciably on a short time scale Δt, for example, if we want to run a fast quantum computer, then the system must be in a state in which its energy is uncertain by a large amount ΔH, obeying Eq.7.23.

Exercise 7.2 *Ultimately, every clock is a quantum system, with the clock's pointer or display consisting of one or more observables of the system. Even small quantum systems such as a nucleus, an electron, atom or molecule have been made to serve as clocks. Assume now that you want to use a small system, such as a molecule, as a clock by observing how one of its observables changes over time. Assume that your quantum clock possess a discrete and bounded*[4] *energy spectrum* $E_1 \leq E_2 \leq E_3 \leq ... \leq E_{max}$ *with* $E_{max} - E_1 = 1eV$ *(1eV=1 electronvolt) which is a typical energy scale in atomic physics. (a) Calculate the maximum uncertainty in energy,* ΔE *that your quantum clock can possess. (b) Calculate the maximally achievable accuracy for such a clock. I.e., what is the shortest time interval (in units of seconds) within which any observable property of the clock could change its expectation value by a standard deviation?*

7.3 The impact of quantum uncertainty on the dynamics

The fact that, in general, $(\bar{f})^n \neq \overline{f^n}$ is also important for the dynamics of quantum systems because, as we will see, it implies that quantum mechanical mean values such as $\bar{x}(t)$ and $\bar{p}(t)$ do not follow the same equations of motion as the classical positions and momenta $x(t)$ and $p(t)$.

We begin by considering the special cases in which, in spite of all the subtleties of quantum mechanics, the mean values $\bar{x}_i^{(r)}, \bar{p}_j^{(s)}$ of the positions and momenta sometimes do obey exactly the same equations of motion as the those of Newton. Consider, for example, the harmonic oscillator $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{k}{2}\hat{x}^2$. Using the Heisenberg equations, we obtain

$$\frac{d\hat{x}}{dt} = \frac{\hat{p}}{m} \quad \text{and} \quad \frac{d\hat{p}}{dt} = -k\hat{x} \tag{7.24}$$

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[4] The energy could be bounded for several reasons. For example, your quantum clock could be a molecule that is such that if you were to supply any more energy that E_{max} to your quantum clock, it would break up, i.e., you would reach the continuous spectrum.

and, therefore:

$$\langle\psi|\frac{d\hat{x}}{dt}|\psi\rangle = \langle\psi|\frac{\hat{p}}{m}|\psi\rangle \quad \text{and} \quad \langle\psi|\frac{d\hat{p}}{dt}|\psi\rangle = -k\langle\psi|\hat{x}|\psi\rangle \tag{7.25}$$

Since the state $|\psi\rangle$ does not depend on time, we obtain these Ehrenfest equations:

$$\frac{d\bar{x}}{dt} = \frac{\bar{p}}{m} \quad \text{and} \quad \frac{d\bar{p}}{dt} = -k\bar{x} \tag{7.26}$$

The number-valued mean values $\bar{x}(t), \bar{p}(t)$ therefore obey the classical Newton equations! This means that without even solving the canonical commutation relations, equations of motion and hermiticity conditions for matrix-valued functions we can quickly solve Eqs.7.26 the same we would classically to obtain that $\bar{x}(t)$ and $\bar{p}(t)$ oscillate with frequency $\omega = \sqrt{k/m}$.

This is all very useful, also because many systems can be approximated as a harmonic oscillator near the minimum of their potential. However, for general quantum systems, the mean values $\bar{x}(t)$ and $\bar{p}(t)$ do not obey Newton's equations. Consider, for example, the non-harmonic oscillator $\hat{H} = \frac{\hat{p}^2}{2m} + \alpha\hat{x}^4$, which leads to

$$\frac{d\hat{x}}{dt} = \frac{\hat{p}}{m} \quad \text{and} \quad \frac{d\hat{p}}{dt} = -4\alpha\hat{x}^3 \tag{7.27}$$

and, therefore:

$$\frac{d}{dt}\langle\psi|\hat{x}|\psi\rangle = \langle\psi|\frac{\hat{p}}{m}|\psi\rangle \quad \text{and} \quad \frac{d}{dt}\langle\psi|\hat{p}|\psi\rangle = -4\alpha\langle\psi|\hat{x}^3|\psi\rangle \tag{7.28}$$

We obtain these equations for the expectation values:

$$\frac{d\bar{x}}{dt} = \frac{\bar{p}}{m} \quad \text{and} \quad \frac{d\bar{p}}{dt} = -4\alpha\overline{x^3} \tag{7.29}$$

We remember now that, in general, $\langle\psi|\hat{x}^3|\psi\rangle \neq \langle\psi|\hat{x}|\psi\rangle^3$, i.e., $\overline{x^3} \neq \bar{x}^3$. Therefore, the equations Eqs.7.29 do not match Newton's equations, which would have to be: $\frac{d\bar{x}}{dt} = \frac{\bar{p}}{m}$ and $\frac{d\bar{p}}{dt} = -4\alpha\bar{x}^3$.

We now observe that the equations for the mean values $\bar{x}_i^{(r)}(t)$ and $\bar{p}_j^{(s)}(t)$ of positions and momenta obey Newton's equation only if the Hamiltonian is a polynomial of degree at most two in the positions and momenta.

The proof is simple. The Hamilton equations hold true also in quantum mechanics:

$$\frac{d\hat{x}_i^{(r)}(t)}{dt} = \{\hat{x}_i^{(r)}(t), \hat{H}\} = \hat{f}(\hat{x},\hat{p}) \quad \text{and} \quad \frac{d\hat{p}_i^{(r)}(t)}{dt} = \{\hat{p}_i^{(r)}(t), \hat{H}\} = \hat{g}(\hat{x},\hat{p}) \tag{7.30}$$

Here, $\hat{x}, \hat{p}$ stand for all position and momentum variables. If $\hat{H}$ is a polynomial of degree ≤ 2 in the positions and momenta, then the right hand sides $\hat{f}(\hat{x},\hat{p}), \hat{g}(\hat{x},\hat{p})$ of these equations are linear functions in the positions and momenta. This implies that $\overline{f(\hat{x},\hat{p})} = f(\bar{x},\bar{p})$ and $\overline{g(\hat{x},\hat{p})} = g(\bar{x},\bar{p})$, so that we obtain that the expectation values obey equations whose form is identical to Newton's equations:

$$\frac{d\bar{x}_i^{(r)}}{dt} = f(\bar{x},\bar{p}) \qquad \text{and} \qquad \frac{d\bar{p}_j^{(s)}}{dt} = g(\bar{x},\bar{p}) \tag{7.31}$$

Remark: Examples of such systems are free particles, particles in harmonic oscillator potentials as well as particles exposed to constant electromagnetic fields.

Remark: For Hamiltonians of the form $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$ where V is not a polynomial of degree ≤ 2, the dynamics of the mean values of positions and momenta is generally quite different from Newton's dynamics. However, if the particle is well-localized, then the variance $(\Delta x)^2$ is small, i.e., we have $(\Delta x)^2 = \overline{x^2} - \bar{x}^2 \approx 0$ and, more generally: $\overline{x^n} \approx \bar{x}^n$. We conclude that as long as such a particle is well localized, its position and momentum expectation values $\bar{x}(t)$ and $\bar{p}(t)$ approximately obey the Newton equations.

Remark: The fact that the lowest eigenvalue of the harmonic oscillator's Hamiltonian is larger than zero (we calculated it in a previous exercise) can be explained, similarly, intuitively: a classical particle in a harmonic oscillator has as its lowest energy state the state in which it is at rest at the origin. A particle in the lowest energy state of a harmonic oscillator has a position spread, i.e., $\Delta x > 0$ for that state (if it were zero, Δp would have to be infinite). This means that the particle sees the potential not only at the origin but also a bit to either side, where it is elevated. It therefore sees in effect a finite average value of the potential even when it is in the lowest energy state.

Chapter 8

Pictures of the time evolution

8.1 The time-evolution operator

A system of N particles possesses $3N$ degrees of freedom in the sense that it has $3N$ pairs of position and momentum observables $\hat{x}_i^{(r)}, \hat{p}_j^{(s)}$. These obey the $6N$ equations of motion Eqs.3.35,3.35, which are in practice $6N$ coupled differential equations for $3N$ matrix-valued functions of time. Obviously it becomes very difficult to solve all those equations if N is large. Fortunately, there is a technique that allows us to avoid having to solve all that many differential equations: In fact, it suffices to solve just one differential equation of motion for just one matrix-valued function $\hat{U}(t)$!

Definition: The solution, $\hat{U}(t)$, to the equations

$$i\hbar\frac{d}{dt}\hat{U}(t) \;=\; \hat{U}(t)\hat{H}(t) \tag{8.1}$$

and

$$\hat{U}(t_0) \;=\; \mathbf{1} \tag{8.2}$$

where **1** is the identity matrix (or identity map) is called the system's time-evolution operator.

Proposition: Assume we have found matrices $\hat{x}_i^{(r)}(t_0), \hat{p}_j^{(s)}(t_0)$ which obey the canonical commutation relations and hermiticity conditions at the initial time t_0. Then, the solutions $\hat{x}_i^{(r)}(t), \hat{p}_j^{(s)}(t)$ can easily be obtained from the time-evolution operator:

$$\hat{x}_i^{(r)}(t) \;=\; \hat{U}^\dagger(t)\hat{x}_i^{(r)}(t_0)\hat{U}(t) \tag{8.3}$$

$$\hat{p}_j^{(s)}(t) \;=\; \hat{U}^\dagger(t)\hat{p}_j^{(s)}(t_0)\hat{U}(t) \tag{8.4}$$

Proof: The proof is straightforward. For example, let us check that the $\hat{x}(t)$ defined in terms of the initial $\hat{x}(t_0)$ and the time evolution operator in equation Eq.8.3 does obey the correct equation of motion:

$$\begin{aligned}
i\hbar\frac{d}{dt}\hat{x}(t) &= i\hbar\frac{d}{dt}\left(\hat{U}^\dagger(t)\hat{x}(t_0)\hat{U}(t)\right) \\
&= i\hbar\left(\dot{\hat{U}}^\dagger(t)\hat{x}(t_0)\hat{U}(t)+\hat{U}^\dagger(t)\hat{x}(t_0)\dot{\hat{U}}(t)\right) \\
&= -\hat{H}(t)\hat{U}^\dagger(t)\hat{x}(t_0)\hat{U}(t)+\hat{U}^\dagger(t)\hat{x}(t_0)\hat{U}(t)\hat{H}(t) \\
&\quad \text{(we used that} \quad i\hbar\dot{\hat{U}}=\hat{U}\hat{H} \ \text{ implies } \ -i\hbar\dot{\hat{U}}^\dagger=\hat{H}\hat{U}^\dagger) \\
&= -\hat{H}(t)\hat{x}(t)+\hat{x}(t)\hat{H}(t) \\
&= [\hat{x}(t),\hat{H}(t)] \qquad (8.5)
\end{aligned}$$

The proof for $\hat{p}(t)$ is similar.

Exercise 8.1 *Assume that $\hat{f}(t)$ is any observable which does not explicitly depend on time (i.e., which is a polynomial or a well-behaved power series in the position and momentum operators with constant coefficients). Show that the time evolution of any such $\hat{f}(t)$ is given by:*

$$\hat{f}(t) = \hat{U}^\dagger(t)\hat{f}(t_0)\hat{U}(t) \qquad (8.6)$$

Later we will see that the time evolution also automatically conserves the hermiticity conditions and the canonical commutation relations.

Remark: Not only does the Hamiltonian determine the time-evolution operator $\hat{U}(t)$, but conversely $\hat{U}(t)$ also determines the Hamiltonian. From Eq.8.1, we obtain:

$$\hat{H}(t)=i\hbar\hat{U}^{-1}(t)\frac{d}{dt}\hat{U}(t) \qquad (8.7)$$

Finally, let us remember that the Hamiltonian encodes all there is to know about a given system. Once we know the Hamiltonian, all equations of motion can be derived. Eq.8.7 shows that also the time-evolution operator encodes all information about a quantum system. This observation is the starting point in Feynman's formulation of quantum mechanics which we will discuss later in the course.

8.1.1 Calculating $\hat{U}(t)$

We are left with having to solve Eqs.8.1,8.2. For systems whose Hamiltonian $\hat{H}$ does not depend on time we can immediately write down the solution! Namely:

$$\hat{U}(t)=e^{\frac{1}{i\hbar}(t-t_0)\hat{H}} \qquad (8.8)$$

Of course, to make sense of this formula, we need to define what we mean by the exponentiation of a matrix or operator. This is easy. We exponentiate matrices the same way that we exponentiate numbers, namely through the power series: $e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!}$. In our case:

$$\hat{U}(t) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{(t-t_0)}{i\hbar} \right)^n \hat{H}^n \tag{8.9}$$

Here, we also defined that the zero'th power of the matrix $\hat{H}$ is the identity matrix: $\hat{H}^0 = \mathbf{1}$. This ensures that the initial condition Eq.8.2 holds true for the $\hat{U}(t)$ defined by Eq.8.9. Let us check that also Eq. 8.1 is obeyed:

$$i\hbar \frac{d}{dt} \hat{U}(t) = \frac{i\hbar}{i\hbar} e^{\frac{1}{i\hbar}(t-t_0)\hat{H}} \hat{H} = \hat{U}(t)\hat{H} \tag{8.10}$$

In the main step, we differentiated the power series Eq.8.9 term by term.

We must ask whether there is any chance that we could actually sum up this power series for a given Hamiltonian matrix $\hat{H}$. The answer is yes: First of all, if we are given a Hamiltonian which happens to be a diagonal matrix then its exponentiation is easy to obtain $\hat{U}(t)$! That is because if

$$\hat{H} = \begin{pmatrix} E_1 & 0 & 0 & 0 & \\ 0 & E_2 & 0 & 0 & \\ 0 & 0 & E_3 & 0 & \\ 0 & 0 & 0 & E_4 & \\ & & & & \ddots \end{pmatrix} \tag{8.11}$$

then

$$\hat{H}^n = \begin{pmatrix} E_1^n & 0 & 0 & 0 & \\ 0 & E_2^n & 0 & 0 & \\ 0 & 0 & E_3^n & 0 & \\ 0 & 0 & 0 & E_4^n & \\ & & & & \ddots \end{pmatrix} \tag{8.12}$$

and, therefore:

$$\hat{U}(t) = \begin{pmatrix} e^{\frac{(t-t_0)}{i\hbar}E_1} & 0 & 0 & 0 & \\ 0 & e^{\frac{(t-t_0)}{i\hbar}E_2} & 0 & 0 & \\ 0 & 0 & e^{\frac{(t-t_0)}{i\hbar}E_3} & 0 & \\ 0 & 0 & 0 & e^{\frac{(t-t_0)}{i\hbar}E_4} & \\ & & & & \ddots \end{pmatrix} \tag{8.13}$$

Of course, if $\hat{H}$ is given as a non-diagonal matrix, then the calculation of its arbitrary powers to obtain $\hat{U}(t)$ may not be doable. However, Hamiltonians are self-adjoint operators and for those there is always a basis in which they are diagonal. The problem of finding a basis in which a time-independent Hamiltonian is diagonal is, therefore, of great practical importance and various methods to this end have been devised.

In practice, Hamiltonians often possess an explicit time-dependence. For example, when working with nuclei, atoms or molecules in a quantum computer, the experimenter may want to be able to turn a knob to change and control the energy levels of nuclei, atoms or molecules so that, for example, the gaps between certain energy levels can be made at will to go in or out of resonance with incoming photons. To manipulate the energy levels of a nucleus, atom or molecule requires that the Hamiltonian has parameters in it that can be tuned externally. This can be achieved by applying from the outside, for example, a suitable magnetic or electric field whose strengths can be changed at will. For example, for a free charged particle exposed to a classical electromagnetic field the Hamiltonian $\hat{H} = \hat{p}^2/2m$ becomes:

$$\hat{H} = \frac{1}{2m}\ \left(\hat{\vec{p}} + \frac{e}{c}\ \vec{A}(\hat{\vec{x}},t)\right)^2 - e\Phi(\hat{\vec{x}},t) \tag{8.14}$$

Here, the vector potential $\vec{A}$ and the potential Φ can be made to suitably change over time. When the application of an external electric field changes the energy levels of an atom or molecule, it is called the Stark effect. When the application of an external magnetic field changes the energy levels of an atom or molecule then it is called a Zeeman effect[1]. We have to keep in mind, however, that there are limitations to the validity of Eq.8.14. In particular, the electromagnetic field is itself a quantum system and therefore the $\vec{A}$ and Φ should obey suitable field commutation relations and be operator valued[2]. We will later see why it is that the electromagnetic field often behaves approximately as if it were a classical field, justifying that Eq.8.14 is then a good approximation.

Given that time-dependent Hamiltonians are important, for example, for the control of quantum systems, the question must be addressed if one can give a closed formula for the time evolution operator $\hat{U}(t)$ also for systems whose Hamiltonian, $\hat{H}(t)$, is time dependent. The answer is yes, but it is complicated because the Hamiltonian $\hat{H}(t_1)$ at a time t_1 and the Hamiltonian $\hat{H}(t_2)$ at time t_2 are then generally quite different and have no reason to commute with another! The time-evolution operator is then:

$$\hat{U}(t) = Te^{\frac{1}{i\hbar}\int_{t_0}^{t}\hat{H}(t)\ dt} \tag{8.15}$$

Its simple looks are deceiving. Here, T is the so-called time-ordering operator. Applied to a product of Hamiltonians it orders them with respect to time:

$$T\left(\hat{H}(t_1)\hat{H}(t_2)...\hat{H}(t_n)\right) = \hat{H}(\tilde{t}_1)\hat{H}(\tilde{t}_2)...\hat{H}(\tilde{t}_n) \tag{8.16}$$

The set of times $\{\tilde{t}_i\}_{i=1}^n$ is the same as the set of times $\{t_i\}_{i=1}^n$, but it is ordered: $\tilde{t}_1 \leq \tilde{t}_2 \leq ... \leq \tilde{t}_n$. So, for example:

$$T\left(\hat{H}(3.4s)\hat{H}(4.1s)\hat{H}(2.7s)\right) = \hat{H}(2.7s)\hat{H}(3.4s)\hat{H}(4.1s). \tag{8.17}$$

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[1] The Zeeman effect is used to measure, for example, magnetic fields in far away galaxies: these fields change the absorption and transmission spectra of light that passes through gases in the galaxies.

[2] The full quantum theory of the electromagnetic field is called quantum electrodynamics.

The time ordering operator T is needed because $\hat{H}(t)$ and $\hat{U}(t)$ generally don't commute when $\hat{H}(t)$ depends on time. Explicitly, Eq.8.15 reads:

$$\hat{U}(t) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{1}{i\hbar}\right)^n \int_{t_0}^{t} \int_{t_0}^{t} ... \int_{t_0}^{t} T\left(\hat{H}(t_1)\hat{H}(t_2)...\hat{H}(t_n)\right) \, dt_1 \, dt_2 \, ... \, dt_n \tag{8.18}$$

Exercise 8.2 *Bonus question: Show that Eq.8.18 solves Eq.8.1, i.e., show that, in this way, we achieve that differentiation of* $\hat{U}(t)$ *yields a factor of* $\hat{H}(t)$ *to the right* of $\hat{U}(t)$.

Of course, if $\hat{H}$ does not depend on time, we recover the formula Eq.8.9 for $\hat{U}(t)$. Notice that if $\hat{H}$ does not depend on time the Hamiltonian commutes with $\hat{U}(t)$, because the Hamiltonian $\hat{H}$ commutes with any power of itself (as does every matrix: $[A, A^n] = 0$).

8.1.2 Significance of $\hat{U}(t)$

The general expression for the time-evolution operator $\hat{U}(t)$ given in Eq.8.18 is of course difficult to use in practical calculations. But it can be very useful for abstract studies. For example, it can be used to show that the time-evolution operator is unitary, i.e., that it obeys:

$$\hat{U}(t)^\dagger = \hat{U}(t)^{-1} \tag{8.19}$$

In the simpler case of Eq.8.9 this is easy to see:

$$\begin{aligned}
\hat{U}(t)^\dagger &= \left(\sum_{m=0}^{\infty} \frac{1}{m!} \left(\frac{(t-t_0)\hat{H}}{i\hbar}\right)^m\right)^\dagger && (8.20)\\
&= \sum_{m=0}^{\infty} \frac{1}{m!} \left(-\frac{(t-t_0)\hat{H}}{i\hbar}\right)^m && (8.21)\\
&= \hat{U}(t)^{-1} && (8.22)
\end{aligned}$$

The last step is justified because even for power series of matrices we have $e^A e^{-A} = 1$. The reason is that there is only one matrix A involved, i.e., noncommutativity does not come into play and the power series in the matrix A therefore behaves just like a power series in a number. The fact that the time evolution operator $\hat{U}(t)$ is unitary[3] is in many ways of great mathematical and physical significance[4]. In particular, this fact allows us to prove:

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[3] If a number obeys $u^* = u^{-1}$ the number must be a phase, i.e., it must be of the form $e^{i\alpha}$ for a real α. Unitary operators behave in many ways like phases. In particular, there is always a basis in which a given unitary operator is diagonal. Then, its diagonal elements are all phases. We saw an example of this in Eq.8.13.

[4] Possible exceptions to the unitarity of time evolution are being considered for the case of black holes horizons. There is a conundrum because unitary matrices are always invertible, but a fall into

Proposition: Assume that $\hat{x}_i^{(r)}(t_0)$ and $\hat{p}_j^{(s)}(t_0)$ obey the canonical commutation relations and the hermiticity conditions at the initial time t_0. Then, the quantum mechanical time evolution operator $\hat{U}(t)$ yields $\hat{x}_i^{(r)}(t)$ and $\hat{p}_j^{(s)}(t)$ which obey the canonical commutation relations and the hermiticity conditions at all subsequent times.

Proof: In the case of the hermiticity conditions we have to show, for example, that $\left(\hat{x}_i^{(r)}(t)\right)^\dagger = \hat{x}_i^{(r)}(t)$. Indeed:

$$\begin{aligned}
\left(\hat{x}_i^{(r)}(t)\right)^\dagger &= \left(\hat{U}^\dagger(t)\hat{x}_i^{(r)}(t_0)\hat{U}(t)\right)^\dagger && (8.23)\\
&= \hat{U}^\dagger(t)\left(\hat{x}_i^{(r)}(t_0)\right)^\dagger\hat{U}(t) && (8.24)\\
&= \hat{U}^\dagger(t)\hat{x}_i^{(r)}(t_0)\hat{U}(t) && (8.25)\\
&= \hat{x}_i^{(r)}(t) && (8.26)
\end{aligned}$$

Similarly, any $\hat{f}$ obeying $\hat{f}(t_0) = \hat{f}^\dagger(t_0)$ will also obey $\hat{f}(t) = \hat{f}^\dagger(t)$ for all subsequent t.

Exercise 8.3 *(a) Use the time evolution operator to prove that the canonical commutation relations are conserved, i.e., that, for example,* $[\hat{x}(t_0), \hat{p}(t_0)] = i\hbar$ *implies* $[\hat{x}(t), \hat{p}(t)] = i\hbar$ *for all* t. *(b) Consider the possibility that (due to quantum gravity effects) at some time* t_0 *the* xp *commutation relations take the form* $[\hat{x}(t_0), \hat{p}(t_0)] = i\hbar(1+\beta\hat{p}(t_0)^2)$ *(where* β *is a small positive constant). Assume that the Hamiltonian is self-adjoint, i.e., that the time evolution operator is still unitary. Will these commutation relations be conserved under the time evolution? (Remark: such commutation relations would imply that gravity induces a corresponding change in the Poisson brackets between the* $\hat{x}$ *and* $\hat{p}$*).*

Exercise 8.4 *Consider a system with a Hamiltonian that has no explicit time dependence. Assume that we prepare the system in a state so that its energy at the initial time* t_0 *is known precisely.* **a)** *Show that the energy of the system will stay sharp, i.e., without uncertainty, at that value.* **b)** *Consider now the specific example of a harmonic oscillator system. Its positions and momenta evolve according to Eqs.7.26. Given the time-energy uncertainty relations, what more can you conclude for the time-evolution of* $\bar{x}(t)$ *and* $\bar{p}(t)$ *if the system is in a state with vanishing uncertainty in the energy?*

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a black hole appears to be nonreversible. I think it could be that the resolution of the conundrum will involve time evolution that is described not by a unitary operator but by a merely isometric operator. Isometric operators preserve the hermiticity and canonical commutation relations without being invertible. In finite dimensional Hilbert spaces, isometry and unitarity are the same. Unitary and isometric operators are closely related (namely via the so-called Cayley transform) to self-adjoint and symmetric operators respectively, which we discussed before.

8.2 The pictures of time evolution

8.2.1 The Heisenberg picture

We had found that to solve a quantum mechanical problem of N particles we can solve the $6N$ equations of motion Eqs.3.35,3.35 for its $6N$ basic observables $\hat{x}_i^{(r)}(t), \hat{p}_j^{(s)}(t)$. In practice, this requires solving $6N$ coupled differential equations for infinite by infinite matrices. This method goes back all the way to when Heisenberg first discovered quantum mechanics. When working this way, we say we are working in the "Heisenberg picture".

In the last section we saw that the number of matrix differential equations that need to be solved in the Heisenberg picture, namely $6N$, can be reduced to a single differential equation, namely Eq.8.1 for the time-evolution operator, $\hat{U}(t)$. The time evolution of the $6N$ observables $\hat{x}_i^{(r)}(t), \hat{p}_j^{(s)}(t)$ is then immediately obtained through Eqs.8.3,8.4.

In fact, the computational effort in solving a quantum mechanical problem can be further reduced. Namely, instead of solving this one matrix differential equation, it actually suffices to solve just one vector-differential equation:

8.2.2 The Schrödinger picture

A key observation about the mathematics of quantum mechanics is that we never directly measure either the matrix elements $\hat{f}(t)_{n,m}$ of an observable $\hat{f}(t)$ nor do we ever directly measure the vector components ψ_n of the system's state vector $|\psi\rangle$. We can only measure the scalar expectation values $\bar{f}(t) = \langle\psi|\hat{f}(t)|\psi\rangle = \sum_{n,m} \psi_n^* \hat{f}(t)_{n,m}\psi_m$. The deeper reason for this is that physical predictions cannot depend on the basis which we choose in the vector space. Of course, only scalars are basis independent, while vector and matrix components depend on the choice of basis in the vector space.

Therefore, in order to make physical predictions, our primary goal is to find the measurable functions $\bar{f}(t)$. And there is a shortcut to calculating these! To see this, first we use

$$\hat{f}(t) = \hat{U}^\dagger(t)\hat{f}(t_0)\hat{U}(t) \tag{8.27}$$

to write $\bar{f}(t)$ in the form:

$$\begin{aligned}
\bar{f}(t) &= \langle\psi| \left(\hat{U}^\dagger(t)\hat{f}(t_0)\hat{U}(t)\right) |\psi\rangle && (8.28)\\
&= \sum_{i,j,n,m} \psi_i^* \left(\hat{U}^\dagger_{i,j}(t)\hat{f}_{j,n}(t_0)\hat{U}_{n,m}(t)\right) \psi_m && (8.29)
\end{aligned}$$

Since the multiplication of matrices and their action on vectors is associative, i.e., $a(bc) = (ab)c$, we can place the brackets also differently:

$$\bar{f}(t) = \left(\langle\psi|\hat{U}^\dagger(t)\right) \hat{f}(t_0) \left(\hat{U}(t)|\psi\rangle\right) \tag{8.30}$$

$$= \sum_{i,j,n,m} \left(\psi_i^* \hat{U}^\dagger_{i,j}(t)\right) \hat{f}_{j,n}(t_0) \left(\hat{U}_{n,m}(t)\psi_m\right) \tag{8.31}$$

This suggests to define time-dependent states $|\psi(t)\rangle$:

$$|\psi(t)\rangle = \hat{U}(t)|\psi\rangle \tag{8.32}$$

These states are called "Schrödinger states", as opposed to the time-independent states $|\psi\rangle$ that we have dealt with so far and that are called "Heisenberg states". From Eq.8.2 we have that at the initial time t_0 the Schrödinger state starts out as identical to the Heisenberg state: $|\psi(t_0)\rangle = |\psi\rangle$.

Using the Schrödinger states we have:

$$\bar{f}(t) = \langle\psi(t)|\hat{f}(t_0)|\psi(t)\rangle \tag{8.33}$$

So we have now reformulated the calculation of $\bar{f}(t)$ so that we no longer need to know the time evolution of any observable $\hat{f}(t)$. It suffices to know the operators $\hat{f}(t_0)$ of an observable only at the initial time.

Now, however, we need instead to calculate the time-dependent vectors $|\psi(t)\rangle$. Have we really gained any advantage? Don't we still first have to calculate $\hat{U}(t)$ to then obtain $|\psi(t)\rangle$ through Eq.8.32? Actually, no, there is a way to calculate $|\psi(t)\rangle$ without calculating $\hat{U}(t)$ first. To see this, let us rewrite the differential equation Eq.8.1 for $\hat{U}(t)$, using $\hat{U}^\dagger(t)\hat{U}(t) = 1$, to obtain:

$$i\hbar\frac{d}{dt}\hat{U}(t) = \hat{U}(t)\hat{H}(t)\hat{U}^\dagger(t)\hat{U}(t) \tag{8.34}$$

Applying this equation to the Heisenberg state $|\psi\rangle$ we obtain:

$$i\hbar\frac{d}{dt}\hat{U}(t)|\psi\rangle = \hat{U}(t)\hat{H}(t)\hat{U}^\dagger(t)\hat{U}(t)|\psi\rangle \tag{8.35}$$

This yields for the Schrödinger state $|\psi(t)\rangle$:

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = \hat{U}(t)\hat{H}(t)\hat{U}^\dagger(t)|\psi(t)\rangle \tag{8.36}$$

This suggests to define:

$$\hat{H}_S(t) = \hat{U}(t)\hat{H}(t)\hat{U}^\dagger(t) \tag{8.37}$$

The operator $\hat{H}_s(t)$ is called the "Hamilton operator in the Schrödinger picture". With this definition, we conclude that the time-dependent Schrödinger state $|\psi(t)\rangle$ can be calculated by solving the differential equation:

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = \hat{H}_S(t)|\psi(t)\rangle \tag{8.38}$$

This is the famous Schrödinger equation. It is a differential equation for a vector-valued function, namely $|\psi(t)\rangle$. It is, therefore, a good deal simpler than the differential equations for matrix-valued functions that we had dealt with so far. Choosing a Hilbert basis, the Schrödinger equation reads in components:

$$i\hbar\frac{d}{dt}\psi_n(t) = \sum_m \hat{H}_S(t)_{n,m}\psi(t)_m \tag{8.39}$$

Once we obtain the Schrödinger state $|\psi(t)\rangle$, the prediction for the mean value of any observable $\hat{f}$ follows from:

$$\bar{f}(t) = \langle\psi(t)|\hat{f}(t_0)|\psi(t)\rangle \tag{8.40}$$

$$= \sum_{n,m} \psi_n^*(t)\hat{f}_{n,m}(t_0)\psi_m(t) \tag{8.41}$$

Of course, in order to be able to solve the Schrödinger equation we first need to know the Hamiltonian $\hat{H}_S(t)$ in the Schrödinger picture. And we found in Eq.8.37 that the Schrödinger picture Hamiltonian $\hat{H}_S(t)$ generally differs from the Heisenberg picture Hamiltonian $\hat{H}(t)$. If quantization of classical mechanics primarily yields the Heisenberg operator, then we now have to ask how we can find the Schrödinger Hamiltonian. Will we have to first calculate the unitary time evolution operator $\hat{U}(t)$ so that we can then use Eq.8.37? Having to first calculate the time evolution operator would of course defeat the purpose - because the whole point of using the Schrödinger picture is to avoid having to calculate an operator-valued function $\hat{U}(t)$ and instead only having to calculate a vector-valued function $|\psi(t)\rangle$.

Indeed, there is a direct way to obtain the Schrödinger Hamiltonian from the Heisenberg Hamiltonian: In Eq.8.37, the Heisenberg Hamiltonian is, as always, a polynomial or suitable power series of the position and momentum operators (with generally time-dependent coefficients). Therefore:

$$\hat{H}_S(t) = \hat{U}(t)\hat{H}(\hat{x}(t),\hat{p}(t),t)\hat{U}^\dagger(t) \tag{8.42}$$

Since $\hat{U}^\dagger(t)\hat{U}(t) = 1$, we can also write:

$$\hat{H}_S(t) = \hat{H}\left(\hat{U}(t)\hat{x}(t)\hat{U}^\dagger(t), \hat{U}(t)\hat{p}(t)\hat{U}^\dagger(t), t\right) \tag{8.43}$$

For example, $\hat{U}(t)\left(\hat{p}(t)\hat{p}(t)\right)\hat{U}^\dagger(t) = \left(\hat{U}(t)\hat{p}(t)\hat{U}^\dagger(t)\right)\left(\hat{U}(t)\hat{p}(t)\hat{U}^\dagger(t)\right)$.
Now from Eqs.8.3,8.4 we have

$$\hat{U}(t)\hat{x}(t)\hat{U}^\dagger(t) = \hat{x}(t_0) \quad \text{and} \quad \hat{U}(t)\hat{p}(t)\hat{U}^\dagger(t) = \hat{p}(t_0) \tag{8.44}$$

so that we finally obtain:

$$\hat{H}_S(t) = \hat{H}\left(\hat{x}(t_0), \hat{p}(t_0), t\right) \tag{8.45}$$

We conclude that the Schrödinger Hamiltonian is the exact same polynomial or power series in the position and momentum operators as the Heisenberg Hamiltonian, i.e., its polynomial or power series has the same generally time-dependent coefficients. The only difference is that the position and momentum operators in the Schrödinger Hamiltonian are frozen at the initial time.

Finally, let us recall the equation of motion for the time evolution operator:

$$i\hbar\frac{d}{dt}\hat{U}(t) = \hat{U}(t)\hat{H}(t) \tag{8.46}$$

Using Eq.8.37, which is also $\hat{H}(t) = \hat{U}^\dagger(t)\hat{H}_S(t)\hat{U}(t)$, in Eq.8.46, we find that $\hat{U}(t)$ can also be calculated directly from the Schrödinger Hamiltonian, namely through:

$$i\hbar\frac{d}{dt}\hat{U}(t) = \hat{H}_S(t)\hat{U}(t) \tag{8.47}$$

Notice that, in the similar equation Eq.8.1 for calculating $\hat{U}(t)$ from the Heisenberg[5] Hamiltonian $\hat{H}(t)$, the order on the right hand side is reversed.

Exercise 8.5 *Eq.8.37 shows that, in general, $\hat{H} \neq \hat{H}_S$ because in general the Heisenberg Hamiltonian does not commute with the time evolution operator. And this is because time-dependent Heisenberg Hamiltonians generally don't even commute with themselves at different times. Show that if the Heisenberg Hamiltonian $\hat{H}$ does not explicitly depend on time (i.e., if it is a polynomial in the $\hat{x}$ and $\hat{p}$ with time-independent coefficients, i.e., if we do not introduce an explicit time-dependence manually) then it coincides with the Schrödinger Hamiltonian.*

Exercise 8.6 *Assuming that $\hat{f}$ is an observable that has no explicit time dependence (i.e., that depends on time only through the operators $\hat{x}(t)$ and $\hat{p}(t)$), show that the following equation holds true in the Schrödinger picture and in the Heisenberg picture:*

$$i\hbar\frac{d}{dt}\,\langle\psi|\hat{f}|\psi\rangle = \langle\psi|[\hat{f},\hat{H}]|\psi\rangle \tag{8.48}$$

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[5] For simplicity we will keep denoting the Heisenberg Hamiltonian $\hat{H}(t)$ instead of $\hat{H}_H(t)$

The Schrödinger equation in the position representation

Since we now have the resolution of the identity in the position eigenbasis, we can use it to express the abstract Schrödinger equation

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle \tag{8.49}$$

in the position basis. For example, for the harmonic oscillator we have

$$i\hbar\ \frac{d}{dt}|\psi(t)\rangle = \left(\frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2\right)|\psi(t)\rangle \tag{8.50}$$

and therefore:

$$i\hbar\ \langle x|\frac{d}{dt}|\psi(t)\rangle = \langle x|\left(\frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2\right)|\psi(t)\rangle \tag{8.51}$$

On the left hand side, we can pull the time derivative before the matrix element because $\langle x|$ is constant in time, since we are here working in the Schrödinger picture. On the right hand side, we insert resolutions of the identity in terms of the position eigenbasis. Then we use the definition $\psi(x,t) = \langle x|\psi(t)\rangle$ and our knowledge of the matrix elements of $\hat{x}$ and $\hat{p}$ from Eqs.5.33,5.35 to obtain:

$$\begin{aligned}
i\hbar\ \frac{d}{dt}\langle x|\psi(t)\rangle &= \langle x|\left(\frac{1}{2m}\hat{p}\mathbf{1}\hat{p}\mathbf{1} + \frac{m\omega^2}{2}\hat{x}^2\right)|\psi(t)\rangle \qquad (8.52)\\
&= \int_{\mathbb{R}}\int_{\mathbb{R}} \frac{1}{2m}\ \langle x|\hat{p}|x'\rangle\langle x'|\hat{p}|x''\rangle\langle x''|\psi(t)\rangle\ dx'\ dx'' + \frac{m\omega^2}{2}\ \langle x|\hat{x}^2|\psi(t)\rangle\\
&= \int_{\mathbb{R}}\int_{\mathbb{R}} \frac{1}{2m}\ i\hbar\left[\frac{d}{dx'}\delta(x-x')\right]\left[i\hbar\frac{d}{dx''}\delta(x'-x'')\right]\psi(x'',t)\ dx'\ dx''\\
&\quad +\frac{m\omega^2}{2}\ x^2\psi(x,t)\\
&= \int_{\mathbb{R}}\int_{\mathbb{R}} \frac{-\hbar^2}{2m}\ \left[\frac{d}{dx'}\delta(x-x')\right]\delta(x'-x'')\frac{-d}{dx''}\psi(x'',t)\ dx'\ dx''\\
&\quad +\frac{m\omega^2}{2}\ x^2\psi(x,t)\\
&= \int_{\mathbb{R}} \frac{-\hbar^2}{2m}\ \left[\frac{d}{dx'}\delta(x-x')\right]\frac{-d}{dx'}\psi(x',t)\ dx' + \frac{m\omega^2}{2}\ x^2\psi(x,t)\\
&= \int_{\mathbb{R}} \frac{-\hbar^2}{2m}\ \delta(x-x')\frac{d^2}{dx'^2}\psi(x',t)\ dx' + \frac{m\omega^2}{2}\ x^2\psi(x,t)\\
&= \frac{-\hbar^2}{2m}\ \frac{d^2}{dx^2}\psi(x,t)\ dx' + \frac{m\omega^2}{2}\ x^2\psi(x,t)
\end{aligned}$$

Therefore, we finally arrive at a Schrödinger equation in the position representation:

$$i\hbar\frac{d}{dt}\psi(x,t) = \frac{-\hbar^2}{2m}\ \frac{d^2}{dx^2}\psi(x,t) + \frac{m\omega^2}{2}\ x^2\psi(x,t) \tag{8.53}$$

That this calculation was a little tedious shows how useful the shortcut notation of Eqs.5.41,5.47 is in comparison. Using the shortcut notation, we can immediately go from the abstract Schrödinger equation Eq.8.50 to the one in the position basis, Eq.8.53. To this end, we use the shorthand notation to quickly express any abstract Schrödinger equation

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = \hat{H}(\hat{x},\hat{p})|\psi(t)\rangle, \tag{8.54}$$

such as Eq.8.50, in the position representation:

$$i\hbar\frac{d}{dt}\psi(x,t) = \hat{H}(\hat{x}.,\hat{p}.)\psi(x,t) \tag{8.55}$$

And, therefore, with the shortcut notations Eqs.5.41,5.47, we immediately obtain the Schrödinger equation in the position representation:

$$i\hbar\frac{d}{dt}\psi(x,t) = \hat{H}\left(x,-i\hbar\frac{d}{dx}\right)\psi(x,t) \tag{8.56}$$

which in the above example of the harmonic oscillator, is directly Eq.8.53.

8.2.3 The Dirac picture

Let us remember that when working in the "Heisenberg picture", we calculate predictions $\bar{f}(t)$ through:

$$\bar{f}(t) = \langle\psi|\hat{f}(t)|\psi\rangle = \langle\psi|\left(\hat{U}^\dagger(t)\hat{f}(t_0)\hat{U}(t)\right)|\psi\rangle \tag{8.57}$$

To this end, we have to solve the Heisenberg equation $i\hbar\frac{d}{dt}\hat{f}(t) = [\hat{f}(t),\hat{H}(t)]$ (at least for the basic position and momentum operators) to obtain the time-dependent operators $\hat{f}(t)$. The state $|\psi\rangle$ is time independent. In contrast, when working in the "Schrödinger picture", we calculate predictions $\bar{f}(t)$ through:

$$\bar{f}(t) = \langle\psi(t)|\hat{f}(t_0)|\psi(t)\rangle = \left(\langle\psi|\hat{U}^\dagger(t)\right)\hat{f}(t_0)\left(\hat{U}(t)|\psi\rangle\right) \tag{8.58}$$

Here, we have to solve the Schrödinger equation $i\hbar\frac{d}{dt}|\psi(t)\rangle = \hat{H}_S(t)|\psi(t)\rangle$, to obtain the time-dependent states $|\psi(t)\rangle$. The position and momentum operators are time independent.

One might think that it is always easiest to work in the Schrödinger picture, because in it we have to solve merely a vector differential equation rather than a matrix differential equation. Actually, under certain circumstances, it is possible to further simplify the calculation of the predictions, $\bar{f}(t)$. This is, when the system possesses a Schrödinger Hamiltonian $H_s(t)$ which consists of two parts

$$\hat{H}_S(t) = \hat{H}_S^{(e)}(t) + \hat{H}_S^{(d)}(t) \tag{8.59}$$

where $\hat{H}_S^{(e)}(t)$ is an easy-to-handle Hamiltonian (hence the superscript $^{(e)}$) and $\hat{H}_S^{(d)}(t)$ is a Hamiltonian that is difficult to handle (hence the superscript $^{(d)}$). For example, $\hat{H}_S^{(e)}(t)$ might be the Hamiltonian that contains only the kinetic energy terms of a bunch of particles, and $\hat{H}_S^{(d)}(t)$ could contain terms that describe complicated interactions of these particles. Or, $\hat{H}_S^{(e)}(t)$ might describe the time evolution of a gate within a quantum computer. The additional term $\hat{H}_S^{(d)}(t)$ might describe a special kind of interaction that the gate has with its environment. In such cases one would often call $\hat{H}_S^{(e)}(t)$ a "free" Hamiltonian while calling $\hat{H}_S^{(d)}(t)$ an "interaction Hamiltonian". So if the interaction Hamiltonian $\hat{H}_S^{(d)}(t)$ were absent we could easily solve the dynamics of the system in either the Heisenberg or the Schrödinger picture. Only the presence of $\hat{H}_S^{(d)}(t)$ makes it difficult to calculate $\bar{f}(t)$.

This raises the question: Is there a way that we can make use of the fact that $\hat{H}_S^{(e)}(t)$ is easy, i.e., that we can easily obtain the time-evolution operator $\hat{U}^{(e)}(t)$ that solves:

$$i\hbar\frac{d}{dt}\hat{U}^{(e)}(t) = \hat{H}_S^{(e)}(t)\hat{U}^{(e)}(t) \tag{8.60}$$

The answer is yes: As Dirac first recognized, we can choose to work in what is called the "Dirac picture" which is also called the "interaction picture". Just like the Heisenberg and the Schrödinger pictures, also the Dirac picture is obtained by a clever bracketing in the expression:

$$\bar{f}(t) = \langle\psi|\hat{U}^{\dagger}(t)\hat{f}(t_0)\hat{U}(t)|\psi\rangle \tag{8.61}$$

(For simplicity, let us continue to consider only observables $\hat{f}(t)$ which do not possess an explicit manually-introduced time dependence). Namely, to obtain the Dirac picture, the time evolution operator in this expression is first written as the product of two evolution operators. One will be bracketed so that it goes with the state and one will be bracketed so that it goes with the observables.

The overall idea for Dirac picture is that the simple time evolution according to $\hat{H}^{(e)}(t)$ is given to the operators through an equation similar to the Heisenberg equation. The remaining, more difficult time evolution is then given to the state vectors through an equation similar to the Schrödinger equation.

We begin by defining the unitary operator $\hat{U}'(t)$ that expresses the difference between the full time evolution and the simple time evolution of only the easy-to-handle part of the Hamiltonian:

$$\hat{U}'(t) := \hat{U}^{(e)\dagger}(t)\hat{U}(t) \tag{8.62}$$

Notice that in the special case where the full Hamiltonian consists of only the easy-to-handle Hamiltonian, i.e., if $\hat{H}_S(t) = \hat{H}_S^{(e)}(t)$, then $\hat{U}(t) = \hat{U}^{(e)}(t)$ and therefore $\hat{U}'(t) = 1$.

Exercise 8.7 *Show that $\hat{U}'(t)$ is unitary.*

From Eq.8.62, we have:

$$\hat{U}(t) = \hat{U}^{(e)}(t)\hat{U}'(t) \tag{8.63}$$

Inserted into Eq.8.61, we obtain:

$$\bar{f}(t) = \langle\psi|\hat{U}'^{\dagger}(t)\hat{U}^{(e)\dagger}(t)\hat{f}(t_0)\hat{U}^{(e)}(t)\hat{U}'(t)|\psi\rangle \tag{8.64}$$

Now in order to obtain the Dirac picture, we choose to place brackets this way:

$$\bar{f}(t) = \Big(\langle\psi|\hat{U}'^{\dagger}(t)\Big)\Big(\hat{U}^{(e)\dagger}(t)\hat{f}(t_0)\hat{U}^{(e)}(t)\Big)\Big(\hat{U}'(t)|\psi\rangle\Big) \tag{8.65}$$

Accordingly, we define the operators and states in the Dirac picture through:

$$\hat{f}_D(t) = \hat{U}^{(e)\dagger}(t)\hat{f}(t_0)\hat{U}^{(e)}(t) \tag{8.66}$$

and

$$|\psi(t)\rangle_D = \hat{U}'(t)|\psi\rangle \tag{8.67}$$

In the Dirac picture, the time evolution operator $\hat{U}^{(e)}(t)$ solves Eq.8.60 and is by assumption easy to obtain. Therefore, $\hat{f}_D(t)$ is by assumption easy to obtain via Eq.8.66. Similar to the Heisenberg picture, the $\hat{f}_D(t)$ obey this equation:

$$i\hbar\frac{d}{dt}\hat{f}_D(t) = [\hat{f}_D(t), \hat{H}_D^{(e)}(t)] \tag{8.68}$$

as is easy to show from Eq.8.66. Notice that, in $H_D^{(d)}(t)$, the position and momentum operators possess the time evolution of the Dirac picture, i.e., they evolve according to Eq.8.66, as do all observables in the Dirac picture.

Now, the remaining part of the time evolution, namely the by assumption more difficult to handle part is described through the time evolution of the Dirac states. As we will now see, this time evolution is governed by an equation that is similar to a Schrödinger equation:

Proposition: The time evolution of the states $|\psi(t)\rangle_D$ in the Dirac picture obeys the equations

$$i\hbar\frac{d}{dt}|\psi(t)\rangle_D = \hat{H}_D^{(d)}|\psi(t)\rangle_D \tag{8.69}$$

$$|\psi(t_0)\rangle_D = |\psi\rangle \tag{8.70}$$

where $\hat{H}_D^{(d)}$ is given by:

$$\hat{H}_D^{(d)}(t) = \hat{U}^{(e)\dagger}(t)\hat{H}_S^{(d)}(t)\hat{U}^{(e)}(t) \tag{8.71}$$

In $\hat{H}_D^{(d)}$, (as we saw for $\hat{H}_D^{(e)}(t)$ above) the position and momentum operators evolve according to the Dirac picture, i.e., according to the time evolution generated by the easy-to-handle part of the Hamiltonian: From Eq.8.66 we see that $\hat{H}_D^{(d)}(t)$ is the same polynomial or power series in the positions and momenta as is $\hat{H}_S^{(d)}(t)$ - except that in $\hat{H}_D^{(d)}(t)$ the position and momentum operators evolve according to the easy time evolution operator $\hat{U}^{(e)}$. Since, in the Dirac picture, all observables evolve according the easy time evolution operator $\hat{U}^{(e)}$, we can also say that $\hat{H}_D^{(d)}(t)$ is obtained by taking $\hat{H}_S^{(d)}(t)$ and writing it in the Dirac picture, i.e., by letting its operators evolve according to the easy time evolution.

Proof: We begin with:

$$i\hbar\frac{d}{dt}\hat{U}(t) = \hat{H}_S(t)\hat{U}(t) \tag{8.72}$$

Therefore, with the dot denoting the time derivative:

$$\begin{aligned}
i\hbar\left(\dot{\hat{U}}^{(e)}\hat{U}' + \hat{U}^{(e)}\dot{\hat{U}}'\right) &= \left(\hat{H}_S^{(e)} + H_S^{(d)}\right)\hat{U}^{(e)}\hat{U}' \\
i\hbar\dot{\hat{U}}^{(e)}\hat{U}' + i\hbar\hat{U}^{(e)}\dot{\hat{U}}' &= i\hbar\dot{\hat{U}}^{(e)}\hat{U}^{(e)\dagger}\hat{U}^{(e)}\hat{U}' + \hat{H}_S^{(d)}\hat{U}^{(e)}\hat{U}' \\
i\hbar\hat{U}^{(e)}\dot{\hat{U}}' &= \hat{H}_S^{(d)}\hat{U}^{(e)}\hat{U}' \\
i\hbar\dot{\hat{U}}' &= \hat{U}^{(e)\dagger}\hat{H}_S^{(d)}\hat{U}^{(e)}\hat{U}' \\
i\hbar\dot{\hat{U}}' &= \hat{H}_D^{(d)}\hat{U}' \\
i\hbar\dot{\hat{U}}'|\psi\rangle &= \hat{H}_D^{(d)}\hat{U}'|\psi\rangle \\
i\hbar\frac{d}{dt}|\psi(t)\rangle_D &= \hat{H}_D^{(d)}|\psi(t)\rangle_D
\end{aligned}$$

To summarize, in the Dirac picture, we first split the Hamiltonian as in Eq.8.59 into an "easy" and a "difficult" Hamiltonian. We let the operators $\hat{f}_D(t)$ evolve according to the easy Hamiltonian as given by Eqs.8.60,8.66 and we let the states $|\psi(t)\rangle_D$ evolve with respect to the difficult Hamiltonian according to Eqs.8.69,8.71. All predictions are then obtained through

$$\bar{f}(t) = {}_D\langle\psi(t)|\hat{f}_D(t)|\psi(t)\rangle_D \tag{8.73}$$

where ${}_D\langle\psi(t)|$ denotes the dual (i.e., bra-) vector to $|\psi(t)\rangle_D$.

For example, consider the Schrödinger Hamiltonian

$$\hat{H}_S(t) := \frac{\hat{p}(t_0)^2}{2m} + \frac{m\omega^2}{2}\ \hat{x}(t_0)^2 + e^{-\alpha t^2}\ \hat{p}(t_0)\hat{x}(t_0)^3\hat{p}(t_0) \tag{8.74}$$

In this case, the first two terms amount to a harmonic oscillator, which, on its own, is solvable. We could, therefore, work with these definitions for the Dirac picture:

$$\hat{H}_S^{(e)}(t) \ := \ \frac{\hat{p}(t_0)^2}{2m} + \frac{m\omega^2}{2}\ \hat{x}(t_0)^2 \tag{8.75}$$

$$\hat{H}_S^{(d)}(t) \ := \ e^{-\alpha t^2}\ \hat{p}(t_0)\hat{x}(t_0)^3\hat{p}(t_0) \tag{8.76}$$

In practice, the Dirac picture is in fact used ubiquitously. For example, when studying the interaction between an atom and the quantized electromagnetic field, the easy-to-handle part of the total Hamiltonian consists of the Hamiltonian of the atom and the Hamiltonian of the electromagnetic field. The difficult-to-handle part of the total Hamiltonian is the part that describes the interaction between the photon field and the atom.

8.2.4 The Feynman picture

So far, we saw that the Heisenberg, Schrödinger and Dirac pictures are obtained by suitably bracketing in the general expression for the calculation of quantum theoretic predictions[6]:

$$\begin{aligned}
\bar{f}(t) &= \langle\psi|\hat{U}^\dagger(t)\hat{f}(t_0)\hat{U}(t)|\psi\rangle && (8.77)\\
&= \langle\psi|\left(\hat{U}^\dagger(t)\hat{f}(t_0)\hat{U}(t)\right)|\psi\rangle && \text{(Heisenberg picture)}\\
&= \left(\langle\psi|\hat{U}^\dagger(t)\right)\hat{f}(t_0)\left(\hat{U}(t)|\psi\rangle\right) && \text{(Schrödinger picture)}\\
&= \langle\psi|\hat{U}'^\dagger(t)\hat{U}^{(e)\dagger}(t)\hat{f}(t_0)\hat{U}^{(e)}(t)\hat{U}'(t)|\psi\rangle\\
&= \left(\langle\psi|\hat{U}'^\dagger(t)\right)\left(\hat{U}^{(e)\dagger}(t)\hat{f}(t_0)\hat{U}^{(e)}(t)\right)\left(\hat{U}'(t)|\psi\rangle\right) && \text{(Dirac picture)}
\end{aligned}$$

In the Heisenberg, Schrödinger and Dirac pictures we avoid calculating the time evolution operator, $\hat{U}(t)$, by bracketing it either with the states or with the observables or with both. Instead of solving the equation of motion Eq.8.60 for $\hat{U}(t)$, we then need solve the Heisenberg or Schrödinger equations or the corresponding equations in the Dirac picture[7].

In contrast, the Feynman picture consists of calculating the time evolution operator $\hat{U}(t)$. Once we have $\hat{U}(t)$, we can then calculate all predictions $\bar{f}(t)$ with the states and observables frozen at the initial time, using Eq.8.77:

$$\bar{f}(t) = \langle\psi|\hat{U}^\dagger(t)\hat{f}(t_0)\hat{U}(t)|\psi\rangle \qquad \text{(Feynman picture)}$$

When written in a basis, the Feynman picture is called the Green's function method and we will study it now. Later in the course, we will return to the Green's function method to see that the Feynman picture goes very much further and in fact offers a complete re-formulation of quantum theory.

---

[6] The formalism applies, unchanged, to all quantum theories, including quantum field theories where the Dirac picture is normally used. The the free evolution of all particles described by an "easy" Hamiltonian while the particle interactions are described by a "difficult" Hamiltonian.

[7] The term Dirac equation exists but refers to a relativistic wave equation that is unrelated to the Dirac picture.

The Green's function method

We have studied how to represent observables and states in various representations, such as the position and momentum eigenbases. Let us now consider the time-evolution operator in representations. The time evolution operator in a representation is called a Green's function[8].

But why would we want to calculate a time evolution operator? Solving for $\hat{U}(t)$ is to solve for an operator-valued function of time. Normally, solving the Schrödinger equation is easier because it is an equation of motion for a vector-valued function $|\psi(t)\rangle$. One reason why it is sometimes useful to solve for the time evolution operator is that finding $\hat{U}(t)$ means solving the quantum mechanical problem for all initial conditions at once. In contrast, the Schrödinger equation must be solved for each initial condition separately. Namely, in the Schrödinger picture, we have to solve

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \hat{H}_S|\psi(t)\rangle \tag{8.78}$$

separately for each initial condition

$$|\psi(t_0)\rangle = |\psi_0\rangle \tag{8.79}$$

In contrast, assume we calculated the time-evolution operator $\hat{U}(t)$ that obeys:

$$i\hbar \frac{d}{dt} \hat{U}(t) = \hat{H}_S(t)\hat{U}(t) \quad \text{and} \quad \hat{U}(t_0) = \mathbf{1} \tag{8.80}$$

Then, using $\hat{U}(t)$ we can immediately obtain $|\psi(t)\rangle$ for all initial conditions any initial state $|\psi_0\rangle$:

$$|\psi(t)\rangle = \hat{U}(t)|\psi_0\rangle \tag{8.81}$$

With this motivation for studying the time evolution operator in mind, let us consider the form this takes in a basis.

Definition: For any basis $\{|\lambda\rangle\}_{\lambda\in\Lambda}$ we call the matrix elements

$$G(\lambda,\lambda',t) := \langle\lambda|\hat{U}(t)|\lambda'\rangle \tag{8.82}$$

the Green's function in the basis $\{|\lambda\rangle\}$. Here, the values λ run through the entire index set Λ that labels the basis.

Often, one considers the Green's function in the position basis:

$$G(x,x',t) := \langle x|\hat{U}(t)|x'\rangle \tag{8.83}$$

---

[8] Green was actually primarily a miller by profession and he did science on the side. Cayley by the way was primarily a lawyer and he wrote almost a thousand scientific papers.

We are now ready to repeat the basis-independent arguments Eqs.8.78-8.81 in the position representation. To this end, in principle, we need to multiply these basis-independent equations from the left by $\langle x|$ and we need to insert resolutions of the identity of the position eigenbasis between any two operators and between any operator and a state vector. In this way, a number of integrals arise from the resolutions of the identity and a number of Dirac deltas (and their derivative) arise from the matrix elements of $\hat{x}$ and $\hat{p}$ in the position basis. Fortunately, we can speed up these calculations by using the shorthand notation that we introduced in Sec.5.4.

Namely, in the Schrödinger picture, we need to solve the Schrödinger equation

$$i\hbar\ \frac{d}{dt}\psi(x,t) = \hat{H}_S(\hat{x}.,\hat{p}.)\psi(x,t) \tag{8.84}$$

which is, remembering the shorthand dot notation:

$$i\hbar\ \frac{d}{dt}\psi(x,t) = \hat{H}_S(x,-i\hbar\frac{d}{dx})\ \psi(x,t) \tag{8.85}$$

And we need to solve it separately for each initial condition:

$$\psi(x,t_0) = \psi_0(x) \tag{8.86}$$

Instead, writing Eqs.8.80,8.81 in the position basis we can solve the Schrödinger equation for all initial conditions $\psi_0(x)$ at once:

Proposition: Consider the solution $G(x,x',t)$ of the differential equation

$$i\hbar\ \frac{d}{dt}\ G(x,x',t) = \hat{H}_S(x,-i\hbar\frac{d}{dx})\ G(x,x',t) \tag{8.87}$$

with the initial condition

$$G(x,x',t_0) = \delta(x-x'). \tag{8.88}$$

Notice that this means that $G(x,x',t)$ is the Green's function in the position basis. Using $G(x,x',t)$, the time-dependent solution $\psi(x,t)$ for any initial condition $\psi_0(x)$ is then obtained through:

$$\psi(x,t) = \int_{\mathbb{R}} G(x,x',t)\ \psi_0(x')\ dx' \tag{8.89}$$

You may wonder why this is called a solution. Don't we still have to perform an integral to obtain $\psi(x,t)$? The answer is that, in physics, a problem such as solving for a quantum system's evolution, is usually considered solved once the end result is reduced to the performing of an integral over known functions. This because an integral can usually be done straightforwardly either analytically or numerically without requiring any further creativity.

Exercise 8.8 *Show that* $\psi(x,t)$ *of Eq.8.89 does obey the Schrödinger equation Eq.8.84 and the initial condition Eq.8.86.*

Example: For the harmonic oscillator with

$$\hat{H}_S = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2 \tag{8.90}$$

the Green's function obeys:

$$i\hbar\frac{d}{dt}G(x,x',t) = \left(\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{m\omega^2}{2}x^2\right)G(x,x',t) \quad \text{and} \quad G(x,x',t_0) = \delta(x-x') \tag{8.91}$$

Setting $t_0 = 0$, the solution can be shown to be:

$$G(x,x',t) = \left(\frac{m\omega}{2\pi i\hbar\sin(\omega t)}\right)^{1/2} e^{\frac{im\omega}{2\hbar\sin(\omega t)}\left(\left(x^2+x'^2\right)\cos(\omega t)-2xx'\right)} \tag{8.92}$$

Using this Green's function, we can now calculate the time evolution of the wave function of any arbitrary initial state without needing to solve any further differential equation, namely merely by performing an integral:

$$\psi(x,t) = \int_{\mathbb{R}} G(x,x',t)\psi_0(x')dx' \tag{8.93}$$

Of course, once we know $G(x,x',t)$ (and therefore $\hat{U}(t)$), we can similarly use it instead to immediately calculate the time evolution of all operators in the Heisenberg picture, if desired.

Remark: Since the Hamiltonian of the harmonic oscillator is quadratic in both $\hat{x}$ and $\hat{p}$, its evolution has periodicity and, in suitable units, circular symmetry (in classical phase space). This leads to a curious special case for the time evolution that we can read off from the Green's function: Let us consider the time t_q where $\omega t_q = \pi/2$, i.e., the time when one quarter period is up. At that time, $\cos(\omega t_q) = 0$ and, therefore, $G(x,x',t_q) \propto e^{ic_2xx'}$, i.e., the Green's function reduces to a Fourier factor! Concretely:

$$\begin{aligned} \psi(x,t_q) &= \int_{\mathbb{R}} G(x,x',t_q)\psi_0(x')dx' && (8.94) \\ &= \int_{\mathbb{R}} \left(\frac{m\omega}{2\pi i\hbar}\right)^{1/2} e^{\frac{-im\omega}{\hbar}xx'}\psi_0(x')dx' && (8.95) \end{aligned}$$

This means that the wave function of a harmonic oscillator is initially some arbitrary square integrable function $\psi_0(x)$, then a quarter period later, the position wave function has evolved into its Fourier transform, up to a constant prefactor. One can, therefore, use a quantum harmonic oscillator to quickly Fourier transform any wavefunction - it only takes a quarter period. By the way, fast ways of Fourier transforming (though not usually done in this way) are important in quantum computing. For example, in Shor's algorithm for the factoring of integers.

Chapter 9

Measurements and state collapse

9.1 Ideal measurements

Assume that at a time t_m, a quantum system is in a state $|\psi\rangle$ and we measure an observable $\hat{f}$. Let us call the number that we obtained the measurement outcome f_m. In practice, there can be many engineering obstacles to measuring accurately. We will disregard these engineering obstacles and we will instead assume that we performed an ideal measurement. By an ideal measurement is meant a measurement whose outcome can be trusted completely, in the sense that if, right after the time t_m we perform a repeat measurement of the observable $\hat{f}$, we can be certain to find the same measurement value f_m again.

This means that, when we make an ideal measurement and find the measurement value f, then right after the measurement the state of the system must be a state, $|\psi_{after}\rangle$, for which the expectation value is $\bar{f} = f_m$ and for which the uncertainty is $\Delta f = 0$.

This means that a measurement can change the state of a quantum system. We say that the state $|\psi\rangle$ of the system just prior to the measurement collapses to become a new state $|\psi_{after}\rangle$ right after the measurement. The term "collapse" is used because if we assume that the measurement happens at a point in time, then the change of state happens instantaneously at that time.

9.2 State collapse

But how can it be that because of a measurement the state suddenly collapses into a new state? This is not the usual smooth type of unitary time evolution! Yes, according to classical mechanics, in principle we could perform an ideal measurement where we have everything completely under control and where we could arrange, therefore, that the measurement process does not significantly disturb the measured system. But the fact that in reality even an ideal measurement can change the state (though it doesn't have to) should not be surprising. That's because a measurement requires some kind of interaction and in quantum theory, because of the uncertainty principle, we cannot have everything perfectly under control, as we will see later.

Concerning the fact that the state's collapse is not governed by the usual kind of smooth unitary evolution described by the unitary time-evolution operator, let us remember that we have so far only considered the quantum mechanics of isolated systems. The systems that we developed the Heisenberg and Schrödinger equations for can be arbitrarily large - but we have not investigated at all yet what happens when our quantum system is coupled to some other system externally. Now during the duration of a measurement process our system is not isolated and therefore it actually cannot be described by the Heisenberg or Schrödinger equation. The time evolution of our system is not governed by a unitary time evolution operator during the measurement process!

Instead, the evolution of a quantum system that interacts with some other system is governed by what is called a quantum channel[1], and that mathematical framework will allow us to calculate also the processes that happen during a measurement.

For now, let us draw an important conclusion from the fact that right after an ideal measurement of $\hat{f}$ that found a value f_m, the new state of the system must be a state, $|\psi_{after}\rangle$, for which the expectation value is $\bar{f} = f_m$ and for which the uncertainty is $\Delta f = 0$. Namely, we can draw the conclusion that after the measurement, the state $|\psi_{after}\rangle$ of the system is an eigenstate of $\hat{f}$ with the eigenvalue f_m. To see this, we use that $|\psi_{after}\rangle$ must be such that the uncertainty in $\hat{f}$ vanishes:

$$\begin{aligned} 0 &= (\Delta f)^2 && (9.1)\\ &= \langle\psi_{after}|\left(\hat{f} - \langle\psi_{after}|\hat{f}|\psi_{after}\rangle\right)^2 |\psi_{after}\rangle && (9.2)\\ &= \left[\langle\psi_{after}|\left(\hat{f} - \langle\psi_{after}|\hat{f}|\psi_{after}\rangle\right)\right]\ \left[\left(\hat{f} - \langle\psi_{after}|\hat{f}|\psi_{after}\rangle\right)|\psi_{after}\rangle\right] && (9.3)\\ &= \langle\phi|\phi\rangle && (9.4) \end{aligned}$$

where

$$|\varphi\rangle = \left(\hat{f} - \langle\psi_{after}|\hat{f}|\psi_{after}\rangle\right)|\psi_{after}\rangle \qquad (9.5)$$

Since the length of this vector vanishes, $||\ |\varphi\rangle\ || = 0$, we can conclude that $|\varphi\rangle = 0$ and therefore that:

$$\hat{f}|\psi_{after}\rangle = f_m|\psi_{after}\rangle \qquad (9.6)$$

---

[1] You may wonder if this quantum channel is something beyond quantum mechanics. Fortunately, it is not. We can can calculate such quantum channels simply by pursuing the usual quantum mechanical study using the Schrödinger or Heisenberg equations as we have done all along so far. As we'll see later, we just have to apply the laws of quantum mechanics to the total quantum system that consists of our to-be-measured system plus the quantum system that is the measuring device. This is because that total system can be an isolated system and so our methods apply.

Here, we were able to use $\langle\psi_{after}|\hat{f}|\psi_{after}\rangle = f_m$ because we performed an ideal measurement. Therefore, due to the measurement, the state $|\psi\rangle$ of the system collapses into a state $|\psi_{after}\rangle$ which is an eigenstate of the measured observable, with the eigenvalue being the value that was found in the measurement.

Corollary: An important conclusion that we can draw from the above is that an ideal measurement of an observable $\hat{f}$ can only ever produce a measurement outcome value f_m that is among the eigenvalues of the operator $\hat{f}$, i.e., the measurement outcomes must be elements of the spectrum of our observable: $f_m \in \mathrm{spec}(\hat{f})$. For example, the set of eigenvalues of the quantized harmonic oscillator consists of the values $E_n = \hbar\omega(n + 1/2)$ with $n = 0, 1, 2, ...$ An ideal measurement of the energy of a harmonic oscillator can therefore only ever find any one of these values E_n and the state right after the measurement can therefore only ever be one of the energy eigenstates, i.e., $|\psi_{after}\rangle = |E_n\rangle$ for some positive integer m.

9.3 Probability for finding measurement outcomes: the Born rule

Let us now assume again that the state of the system before the measurement is $|\psi\rangle$. What then is the probability that if we perform an ideal measurement, we will find the system in a particular eigenstate $|\psi_{after}\rangle = |f_j\rangle$? So far, we have only seen how to calculate expectation values. How can we calculate a probability? Fortunately, such probabilities are simply expectation values of a particular kind of observables. We can, therefore, use our knowledge of how to calculate expectation values of observables to obtain these probabilities. Namely, let us consider this observable:

$$\hat{Q} := |f_j\rangle\langle f_j| \tag{9.7}$$

This operator can be called an observable because it is, obviously, self-adjoint: $\hat{Q}^\dagger = \hat{Q}$. Assume we have a measurement apparatus that allows us to measure the observable $\hat{Q}$. By the corollary above, the possible measurement outcomes are the eigenvalues of $\hat{Q}$. The spectrum of $\hat{Q}$ is easy to determine because $\hat{Q}$ is actually diagonal in the eigenbasis of $\hat{f}$:

$$\hat{Q}|f_i\rangle = |f_j\rangle\langle f_j|f_i\rangle = \delta_{i,j}\ |f_i\rangle \tag{9.8}$$

Therefore, the eigenbasis $\{|f_i\rangle\}$ of $\hat{f}$ is also an eigenbasis of $\hat{Q}$ but the eigenvalues of $\hat{Q}$ are only 0 and 1. From the corollary above we can conclude, therefore, that when we measure the observable $\hat{Q}$, then the only possible outcomes can be the values 0 or 1. Now given that the state of the system is $|\psi\rangle$ right before the measurement, we can use our methods to calculate the expectation value of the outcome of measuring the observable $\hat{Q}$ in an ensemble of measurements:

$$\bar{Q} = \langle\psi|\hat{Q}|\psi\rangle = \langle\psi|f_j\rangle\langle f_j|\psi\rangle = |\langle f_j|\psi\rangle|^2 \tag{9.9}$$

Since the outcome of every individual measurement of $\hat{Q}$ is either zero or one, depending on whether we find the state $|f_j\rangle$ or not, the expectation value $\bar{Q}$ is actually the probability for finding the state $|f_j\rangle$.

Corollary: We can now draw the important conclusion that when a system is in a pure state $|\psi\rangle$ then if we measure whether or not the system is in state $|\phi\rangle$ then the probability that we will find it to be in the state $|\phi\rangle$ is given by

$$\text{probability} = |\langle\phi|\psi\rangle|^2 \tag{9.10}$$

This is called the Born rule.

9.4 1-bit measurements

The observable $\hat{Q} = |f_n\rangle\langle f_n|$ and more generally any observable of the form $\hat{Q} = |\phi\rangle\langle\phi|$ is an example of a projection operator. Let us recall the definition of projection operators: An operator $\hat{P}$ is called a projection operator, or projector, if it obeys:

$$\hat{P} = \hat{P}^\dagger \qquad \text{and} \qquad \hat{P}^2 = \hat{P} \tag{9.11}$$

Since projection operators are self-adjoint, the spectral theorem tells us that they can be diagonalized. Let us calculate which possible eigenvalues, q, projection operators can possess:

$$q|q\rangle = \hat{Q}|q\rangle = \hat{Q}^2|q\rangle = q^2|q\rangle \tag{9.12}$$

Since $q = q^2$ implies that $q \in \{0, 1\}$, we conclude that the eigenvalues of a projector can only be 0 or 1. This also means that when measuring an observable that is a projector, there are only those two possible measurement outcomes. These are 1-bit measurements.

Exercise 9.1 *Assume that spec($\hat{Q}$) $= \{0, 1\}$ for a normal operator $\hat{Q}$. Does this mean that $\hat{Q}$ is a projector, and why?*

The observable $\hat{Q} = |f_j\rangle\langle f_j|$ of the previous section is a projection operator because it obeys the conditions Eqs.9.11. Since $\hat{Q}|\psi\rangle = (\langle f_j|\psi\rangle)|f_j\rangle$, which is a vector proportional to $|f_j\rangle$, we say that $\hat{Q}$ is the projection operator onto the eigenspace of $\hat{f}$ with eigenvector $|f_j\rangle$.

Now assume that we measure the observable $\hat{Q}$ and find the eigenvalue 1. We can then write:

$$|\psi_{after}\rangle = \frac{1}{||\ \hat{Q}|\psi\rangle\ ||}\ \hat{Q}|\psi\rangle \tag{9.13}$$

The denominator is needed to ensure that $|\psi_{after}\rangle$ is normalized. Now what if we measure $\hat{Q}$ and find the outcome 0? To see what happens then, let us consider the observable $\hat{R} := \mathbb{1} - \hat{Q}$. $\hat{R}$ is a projector and it is the 1-bit observable that is complementary to $\hat{Q}$ in the sense that it yields 1 when measuring $\hat{Q}$ yields 0 and vice versa (and $\hat{Q}$ and $\hat{R}$ can be measured simultaneously because they commute). Since, therefore, measuring 0 for $\hat{Q}$ means measuring 1 for $\hat{R}$, we can conclude that the state then collapses into the state:

$$\begin{aligned} |\psi_{after}\rangle &= \frac{1}{||\ \hat{R}|\psi\rangle\ ||}\ \hat{R}|\psi\rangle && (9.14) \\ &= \frac{1}{||\ (\mathbb{1} - \hat{Q})|\psi\rangle\ ||}\ (\mathbb{1} - \hat{Q})|\psi\rangle && (9.15) \end{aligned}$$

We notice that, because the denominators contain $|\psi\rangle$, the state collapse from the state $|\psi\rangle$ before the measurement to the state $|\psi_{after}\rangle$ after the measurement is a nonlinear map. This shows that the state collapse cannot be described by a unitary (and therefore linear) operator of the kind that would arise from the equation of motion for the time evolution operator in an isolated quantum system. As we will later see, the collapse is part of the unitary evolution of the larger quantum system consisting of our system and the measurement apparatus. When both are quantum mechanically described, the measurement process can be described as the interaction between two subsystems.

9.5 The case of degenerate eigenspaces

Let us now consider the case that the measurement value $f_j \in \mathbb{R}$ that was measured is an eigenvalue of $\hat{f}$ which is degenerate, i.e., the eigenspace of $\hat{f}$ with eigenvalue f_j is N-dimensional with $N > 1$. Let the vectors $\{|f_{j_a}\rangle\}_{a=1}^{N}$ be an orthonormal eigenbasis of that eigenspace. We can then define the projector $\hat{Q}$ onto that eigenspace:

$$\hat{Q} := \sum_{a=1}^{N} |f_{j_a}\rangle\langle f_{j_a}| \tag{9.16}$$

Exercise 9.2 *Verify that this operator $\hat{Q}$ is a projector.*

Definition: We say that a projector is of rank N, if (as is the case here), the dimension of its image is N.

Notice that, since $\hat{Q}$ is a projector, it is still a 1-bit observable and its measurement outcomes are 0 or 1. By the same reasoning as previously for the rank 1 projectors, the expectation value $\bar{Q}$ is the probability for finding the measurement outcome f_n in a measurement of $\hat{f}$. Also, analogous to the case where the eigenvalue f_j was non-degenerate, the collapse of the state $|\psi\rangle$ can be expressed using $\hat{Q}$:

$$|\psi_{after}\rangle = \frac{1}{||\ \hat{Q}|\psi\rangle\ ||}\ \hat{Q}|\psi\rangle \tag{9.17}$$

As before, the denominator is needed to make sure that $|\psi_{after}\rangle$ is normalized.

Exercise 9.3 *Let us check that the prescription Eq.9.17 describes the collapse correctly. To see this we need to check if it obeys the condition that it describes the outcome of an ideal measurement, i.e., of a measurement that, when immediately repeated, will yield the same result. Show that when the collapse described by Eq.9.17 is applied twice, it yields the same state as after the first application.*

Notice that every projector, $\hat{Q}$ is a 1-bit observable. In particular, the sum in Eq.9.16 can be chosen to contain infinitely many terms, and the sum can also be replaced by an integral, for continuously labeled vectors.

Exercise 9.4 *(a) Consider a free electron in one dimension. Write down the 1-bit observable* $\hat{Q}$ *which yields the measurement outcome* 1 *if the electron is measured in the interval* $[x_a, x_b]$ *and* 0 *if it is found outside this interval. (b) Consider a one-dimensional harmonic oscillator. Write down the 1-bit observable* $\hat{Q}$ *which yields the measurement outcome* 1 *if the energy of the oscillator is up to* $7\hbar\omega/2$ *and is* 0 *if the energy is above* $7\hbar\omega/2$.

9.6 Successive versus simultaneous measurements

Let us consider the time evolution in the Schrödinger picture. The dynamics of our system is then described as the dynamics of the state vector. We start at a time t_0 with the system in a state $|\psi_0\rangle$. Then the state evolves in time, $|\psi(t)\rangle$, according to the Schrödinger equation until a time t_1 when a measurement of some observable $\hat{f}$ is performed. An outcome, $f_m \in \text{spec}(\hat{f})$, is found with probability $\bar{Q} := \langle\psi(t_1)|\hat{Q}|\psi(t_1)\rangle$ where $\hat{Q}$ is the projector onto the eigenspace of $\hat{f}$ with eigenvalue f_m. The measurement takes a short amount of time, ϵ. The state $|\psi(t_1+\epsilon)\rangle$ immediately after the measurement is:

$$|\psi(t_1+\epsilon)\rangle = \frac{1}{||\ \hat{Q}|\psi(t_1)\rangle\ ||}\ \hat{Q}|\psi(t_1)\rangle \tag{9.18}$$

The system is then again evolving according to the Schrödinger equation until a time t_2 when we perform the measurement of a second observable, say $\hat{g}$. An outcome, $g_m \in \text{spec}(\hat{g})$, is found with probability $\bar{Q} := \langle\psi(t_2)|\hat{Q}|\psi(t_2)\rangle$ where $\hat{Q}$ is the projector onto the eigenspace of $\hat{g}$ with eigenvalue g_m. The state $|\psi(t_2+\epsilon)\rangle$ immediately after the second measurement (again of some small duration ϵ') is

$$|\psi(t_2+\epsilon')\rangle = \frac{1}{||\ \hat{Q}|\psi(t_2)\rangle\ ||}\ \hat{Q}|\psi(t_2)\rangle \tag{9.19}$$

After that, the state proceeds to evolve according to the Schrödinger equation until the next measurement, and so on. As we will later discuss, these measurements can be described as interactions of our system with the rest of the world. Vice versa, when the system interacts with the rest of the world this can generally be seen as measurements of the system.

An important special case is the case where we measure $\hat{g}$ so soon after measuring f that the Schrödinger time evolution of the state between the two measurements is negligible. In this case, are we justified to say we measured $\hat{f}$ and $\hat{g}$ simultaneously?

The answer depends on whether $\hat{f}$ and $\hat{g}$ commute with another or not. Let us first assume that $[\hat{f}, \hat{g}] \neq 0$. In this case, their respective projection operators $\hat{Q}$ generally do not commute. This means that it makes a difference whether we first measure $\hat{f}$ and then $\hat{g}$ or vice versa. For this reason, we cannot claim that we measure $\hat{f}$ and $\hat{g}$ simultaneously. One must be before the other because the result of the two projections depends on the order of the projections.

Now let us assume that $[\hat{f}, \hat{g}] = 0$. In this case, their respective projection operators $\hat{Q}$ do not commute. This means that it makes no difference whether we first measure $\hat{f}$ and then $\hat{g}$ or vice versa. For this reason, we can measure $\hat{f}$ and $\hat{g}$ simultaneously. If in experiments, we are not absolutely accurate and sometimes we measure one a little bit earlier than the other or vice versa, it makes no difference because the two wave function collapses of the two measurements commute. In this sense, commuting observables correspond to compatible measurements, i.e., to measurements that can be performed simultaneously.

In general, we are able to measure any number of observables $\hat{f}^{(i)}$ simultaneously, if they commute:

$$[\hat{f}^{(i)}, \hat{f}^{(j)}] = 0 \tag{9.20}$$

Intuitively, this is because for commuting observables the uncertainty principle poses no constraints on measuring them simultaneously. If two observables commute there is no obstruction to finding states for which the uncertainty in both observables vanishes at the same time because the uncertainty relation for commuting observables is trivially $\Delta\hat{f}^{(i)}\Delta\hat{f}^{(j)} \geq 0$. Technically, the key point is that commuting observables can be jointly diagonalized:

Proposition: Self-adjoint matrices can be simultaneously diagonalized if and only if they commute.

Proof: Assume that they can be jointly diagonalized. In this case, they are simultaneously diagonal in a basis (their joint eigenbasis) and they do, therefore, commute. This proves one direction of the proposition. To see the other direction, assume they commute. First, diagonalize $\hat{f}^{(1)}$. Pick the degenerate subspace V to an eigenvalue, say λ. I.e., we have that $\hat{f}^{(1)}|\phi\rangle = \lambda|\phi\rangle$ for all $|\phi\rangle \in V$. We now show that $\hat{f}^{(2)}$ maps this eigenspace into itself: $\hat{f}^{(2)} : V \to V$. This is important because it means that $\hat{f}^{(2)}$ is represented on V as a self-adjoint matrix. We have to show that if $|\phi\rangle \in V$ then also $\hat{f}^{(2)}|\phi\rangle \in V$, i.e., we have to show that $\hat{f}^{(1)}\left(\hat{f}^{(2)}|\phi\rangle\right) = \lambda\left(\hat{f}^{(2)}|\phi\rangle\right)$. But this is the case because $\hat{f}^{(1)}$ and $\hat{f}^{(2)}$ commute:

$$\hat{f}^{(1)}\hat{f}^{(2)}|\phi\rangle = \hat{f}^{(2)}\hat{f}^{(1)}|\phi\rangle = \hat{f}^{(2)}\lambda|\phi\rangle = \lambda\left(\hat{f}^{(2)}|\phi\rangle\right) \tag{9.21}$$

Now that we know that $\hat{f}^{(2)}$ maps V into itself and is therefore a self-adjoint matrix on V, we know from the spectral theorem for self-adjoint operators that there exists a basis in that subspace that diagonalizes $\hat{f}^{(2)}$. If there is still a degenerate subspace, we proceed by also diagonalizing a third commuting observable $\hat{f}^{(3)}$, and so on. This completes the proof of the proposition.

State collapse: Let us now assume that the system is in a state $|\psi\rangle$ and we then measure r commuting observables simultaneously. Let us call the r measurement outcomes $f^{(1)}_{m_1}, f^{(2)}_{m_2}, ..., f^{(3)}_{m_r}$. What is the state collapse? Each measurement contributes a projection operator $\hat{Q}_{f^{(i)}}$. After the r simultaneous measurements, the state $|\psi\rangle$ is collapsed into the state:

$$|\psi_{after}\rangle = \frac{1}{||\ \prod_{i=1}^{r} \hat{Q}_{f^{(i)}} |\psi\rangle\ ||} \prod_{i=1}^{r} \hat{Q}_{f^{(i)}} |\psi\rangle \tag{9.22}$$

The prefactor has to be this factor to make $|\psi_{after}\rangle$ normalized. Notice that the sequence of operators in the product does not matter because the projectors $\hat{Q}_{f^{(i)}}$ commute. This is because the r commuting observables $\hat{f}^{(i)}$ and therefore their projectors are all diagonal in the same joint eigenbasis.

Maximal sets of commuting observables. After simultaneously measuring a sufficiently large set of r commuting observables $\hat{f}^{(1)}, \hat{f}^{(2)}, ..., \hat{f}^{(r)}$ and obtaining r measurement values $f^{(1)}, f^{(2)}, ..., f^{(r)}$, the state $|\psi_{after}\rangle$ that the system collapses into is fully characterized by the r measured eigenvalues, i.e., i.e., joint eigenspaces of all these observables are all one-dimensional. These joint eigenvectors are then commonly denoted by their joint eigenvalues:

$$|\psi_{after}\rangle = |f^{(1)}, f^{(2)}, ..., f^{(r)}\rangle \tag{9.23}$$

Remark: In the quantum mechanics of a finite number of particles, there always exist finite maximal sets of commuting observables. When such a set of observables is measured simultaneously, any state collapses onto one-dimensional subspaces. Measuring more commuting observables would not bring more information in this case: In Eq.9.22, we would be multiplying more projectors but any additional projectors would merely act as the identity on the already one-dimensional space on which the other projectors are already projecting.

Remark: In quantum mechanics, in principle, even just one suitably-chosen observable $\hat{f}$ suffices to perform a complete measurement, i.e., a measurement that projects the state onto a one dimensional subspace. Any observable $\hat{f}$ whose spectrum is nondegenerate will do. In practice, however, it is often convenient to measure several commuting observables at the same time.

In the quantum mechanics of N particles in three dimensions, a maximal set of commuting observables is, for example, given by the set of their $3N$ momentum operators.

For an electron in the Hydrogen atom (omitting the spin for now), a maximal set is also $(\hat{H}, \hat{L}^2, \hat{L}_3)$ and their joint eigenvectors are then denoted by $|f^{(1)}, f^{(2)}, f^{(3)}\rangle = |E_n, l, m\rangle$.

9.7 States versus state vectors

Comment regarding the uniqueness of $|\psi_{after}\rangle$: The vector $|\psi_{after}\rangle$, because it has to be normalized, $\langle\psi_{after}|\psi_{after}\rangle = 1$, is unique only up to a phase: If $|\psi_{after}\rangle$ is a normalized eigenvector to the eigenvalue f, then so is $e^{i\alpha}|\psi_{after}\rangle$ for any $\alpha \in \mathbb{R}$. It does not matter which of these vectors we pick to represent the state after the measurement because these vectors all yield the same predictions for every observable, $\hat{g}$:

$$\bar{g} = \langle\psi_{after}|\hat{g}|\psi_{after}\rangle = \langle\psi_{after}|e^{-i\alpha}\ \hat{g}\ e^{i\alpha}|\psi_{after}\rangle \tag{9.24}$$

We say that these vectors represent the same state, i.e., a state is actually an equivalence class of normalized vectors that differ only by a phase.

For completeness, I should mention that there are very special cases when such phases can actually matter. These are cases where the Hamiltonian has a set of parameters and when in this parameter space the topology is nontrivial (e.g. if there are forbidden regions in this parameter space). This leads to so-called topological phases such as the so-called Berry phase. Such phases are currently of great interest in efforts to develop quantum computers. The reason is that quantum computers are generally vulnerable to small environmental disturbances but topological structures are global and therefore less susceptible to small perturbations.

Chapter 10

Mixed states

So far in this course, we always assumed that the state $|\psi\rangle$ of the system is known. In this case, the prediction for an observable $\hat{f}$ is calculated through:

$$\bar{f} = \langle\psi|\hat{f}|\psi\rangle \tag{10.1}$$

In these lucky circumstances, where we know the state of the system for sure, we say that the state of the system is a *pure state.*

In practice, however, the state is usually not known for sure and we can at best assign probabilities to the system being one of many states. In this general case, we say that the system is in a *mixed state.* A mixed state, therefore, describes not only the state of the system per se but also our state of knowledge about the system.

There are two main situations in which we can determine the probabilities for what state a system may be in. One of them is case where the system has been in contact with a thermal bath of known temperature. Roughly speaking, the system will be the less likely to be in a particular state, the higher the energy is in this state. And, the higher the temperature, the higher is the probability that the system is in a high energy state nevertheless. We will later calculate the exact probabilities as a function of the state's energy and as a function of the temperature of the heat bath.

The second situation in which it is straightforward to calculate the probabilities for which state a system is in, is right after an observable of a system has been measured. That's because we can calculate probabilities of measurement outcomes and we can, therefore, calculate the probabilities for the states that the system will be in after the measurement. Of course, these probabilities become certainties once we read the output of the measurement apparatus. Nevertheless, keeping track of the probabilities can be important, especially if, for all measurement outcomes, we let the system continue its evolution after the measurement.

Regarding the dynamics of the system, when we know only the probabilities for the states that a system may be in, it is clear that we need to keep track of the dynamics of pure each state that the system may be in. This means that we will need to study the evolution of mixed states. For this purpose, how can we describe mixed states efficiently?

10.1 Density matrix

Let us assume that our system is in a mixed state. Concretely then, let us denote the probability for our system to be in one of the states $|b_n\rangle$ of a Hilbert basis $\{|b_n\rangle\}_n$ by $\rho_n \in [0,1]$:

$$\rho_n = \text{probability}(|b_n\rangle) \tag{10.2}$$

The probabilities have to sum up to one:

$$\sum_n \rho_n = 1 \tag{10.3}$$

When the state of the system is a mixed state, the expectation value of an observable $\hat{f}$ is of course the arithmetic mean of the expectation values for each of the $|b_n\rangle$:

$$\bar{f} = \sum_n \rho_n \langle b_n|\hat{f}|b_n\rangle \tag{10.4}$$

For book keeping purposes, let us now define the so-called density operator for the mixed state:

Definition: We use the coefficients ρ_n of a mixed state to define the so-called *density operator* or *density matrix* $\hat{\rho}$*:*

$$\hat{\rho} := \sum_n \rho_n \ |b_n\rangle\langle b_n| \tag{10.5}$$

Since the operator $\hat{\rho}$ describes the mixed state, it is common to call $\hat{\rho}$ itself the mixed state. We see that, by construction, $\hat{\rho}$ possesses a basis in which it is diagonal and possesses only real eigenvalues. We can conclude, therefore, that $\hat{\rho}$ is a self-adjoint operator.

Proposition: Assuming that a system is in a mixed state $\hat{\rho}$, we can now express all predictions $\bar{f}$ for observables $\hat{f}$, i.e., Eq.10.4 in a compact form:

$$\bar{f} = \text{Tr}\left(\hat{\rho}\hat{f}\right) \tag{10.6}$$

Let us recall that all predictions of quantum theory are predictions of expectation values $\bar{f}$ for observables $\hat{f}$ and that these $\bar{f}$ must be scalars because measurement outcomes cannot depend on human choices of bases. Notice that $\bar{f}$ in Eq.10.6 is indeed basis-independent. This is because the trace, i.e., the sum over the diagonal elements of an operator A can be evaluated in any Hilbert basis, for example, in the $\{|b_n\rangle\}_n$ basis:

$$\mathrm{Tr}(A) = \sum_n \langle b_n|A|b_n\rangle \tag{10.7}$$

We can now prove Eq.10.6 by using Eq.10.4:

$$\begin{aligned}
\mathrm{Tr}(\hat\rho\hat f) &= \sum_n \langle b_n|\hat\rho\hat f|b_n\rangle && (10.8)\\
&= \sum_n \langle b_n|\sum_m \rho_m|b_m\rangle\langle b_m|\hat f|b_n\rangle && (10.9)\\
&= \sum_{n,m} \rho_m\delta_{n,m}\langle b_m|\hat f|b_n\rangle && (10.10)\\
&= \sum_n \rho_n\langle b_n|\hat f|b_n\rangle && (10.11)\\
&= \bar f && (10.12)
\end{aligned}$$

Exercise 10.1 *(a) Prove that Tr*$(\hat\rho) = 1$*. (b) Prove that Tr*$(\hat\rho^2) \leq 1$ *and that Tr*$(\hat\rho^2) = 1$ *if and only if* $\hat\rho$ *is the density operator of a pure state.*

Any self-adjoint operator $\hat\rho$ whose spectrum is discrete, and for which $\mathrm{spec}(\hat\rho) \subset [0, 1]$ and $\mathrm{Tr}(\hat\rho) = 1$ can be viewed as a density operator of a mixed state. To see this, we can diagonalize $\hat\rho$ to obtain Eq.10.5.

Let us briefly return to pure states, i.e., to the situation where we know for sure that the system is in some particular state that we may call $|\psi\rangle$. Let us rename that state $|b_1\rangle := |\psi\rangle$ and let us add arbitrary orthonomal vectors $\{|b_n\rangle\}_{n=2}^\infty$ so that $\{|b_n\rangle\}_{n=1}^\infty$ is a Hilbert basis. We can, therefore, view any pure state as the special case of a mixed state whose probability distribution $\{\rho_n\}$ is particularly simple: $\rho_n = \delta_{n,1}$. This means that, if a system is in a pure state $|b_1\rangle$ or $|\psi\rangle$ then its density operator is a projector of rank 1:

$$\begin{aligned}
\hat\rho &= |b_1\rangle\langle b_1| && (10.13)\\
&= |\psi\rangle\langle\psi| && (10.14)
\end{aligned}$$

Correspondingly, the way that we now calculate predictions for mixed states, $\bar f = \mathrm{Tr}(\hat f\hat\rho)$ reduces for pure states $\hat\rho = |\psi\rangle\langle\psi|$ to the old way of calculating predictions for pure states, namely $\bar f = \langle\psi|\hat f|\psi\rangle$. Indeed:

$$\begin{aligned}
\bar f &= \mathrm{Tr}(\hat\rho\hat f) && (10.15)\\
&= \mathrm{Tr}(|\psi\rangle\langle\psi|\hat f) && (10.16)\\
&= \sum_n \langle b_n|\psi\rangle\langle\psi|\hat f|b_n\rangle && (10.17)
\end{aligned}$$

$$= \sum_n \langle\psi|\hat{f}|b_n\rangle\langle b_n|\psi\rangle \tag{10.18}$$

$$= \langle\psi|\hat{f}|\psi\rangle \tag{10.19}$$

Here, $\{|b_n\rangle\}_n$ is any Hilbert basis.

The reason why mixed states are called mixed is that in this case the randomness in the outcome of predictions has mixed origins. On one hand, the outcome of measurements is still unpredictable because of quantum fluctuations. On the other hand, the outcome of measurements is also uncertain because we don't know with certainty which state vector describes the system.

10.2 Dynamics of a mixed state

Let us now consider that a quantum mechanical system is at a time t_0 in a mixed state described by a matrix $\hat{\rho}$. Recall that, depending on the basis one may choose, $\hat{\rho}$ may or may not be diagonal. But one can always choose a Hilbert basis $\{|b_n\rangle\}_n$ so that $\hat{\rho}$ is diagonal, because $\hat{\rho}$ is self-adjoint. The system can therefore be viewed as being in the state $|b_n\rangle$ with probability ρ_n.

Now assume that we let the system evolve for $t > t_0$ while being isolated from any environment. In the Schrödinger picture, whichever state $|b_n\rangle$ our systems is in at time t_0, it will evolve according to the Schrödinger equation as a state $|b_n(t)\rangle$ for $t > t_0$. We don't know which state the system is actually in but we do know the system's initial mixed state density operator $\hat{\rho}(t_0)$. Using the Schrödinger equation, one can show that the density operator obeys the so-called von Neumann equation:

$$i\hbar\frac{d}{dt}\ \hat{\rho}(t) = [\hat{H}_S(t), \hat{\rho}(t)] \tag{10.20}$$

Exercise 10.2 *Use the Schrödinger equation and the definition of the density operator to prove the von Neumann equation Eq.10.20.*

How does $\hat{\rho}$ evolve in the Heisenberg picture? Not at all since then only the observables evolve.

10.3 How to quantify the mixedness

Sometimes, we may be relatively sure about which state vector describes the system and at other times we may be very uncertain. For example, intuitively, it is clear that a system exposed to an environment that is very cold is likely to be found in of the lowest energy states. If it is instead exposed to a hot environment then there will be a fair probability to find it high energy states.

Concretely, let us assume that we know the complete set of probabilities $\{\rho_n\}$ for the system to be described by any one of the vectors $|b_n\rangle$ of a Hilbert basis $\{|b_n\rangle\}$. Given these data, i.e., given the density matrix, $\hat{\rho}$, how can we quantify how certain or uncertain we are about the true state the system is in? The answer is that our ignorance is best quantified by the so-called von Neumann entropy[1]

$$S_{vN}[\{\rho_n\}] := -\sum_n \rho_n \ln \rho_n \tag{10.21}$$

We can re-write the von Neumann entropy in a basis-independent form:

$$S_{vN}[\hat{\rho}] = -\mathrm{Tr}\left(\hat{\rho}\ln(\hat{\rho})\right) \tag{10.22}$$

Remark: Methods for defining a function of an operator ("Functional Calculus"). In Eq.10.22, we need to define the logarithm of an operator. Remember that, when we need to define a function of an operator, one method is to use the Taylor expansion of that function together with the fact that we do know how to take powers of an operator. This method works as long as the function in question possesses a Taylor expansion and as long as the eigenvalues of the operator don't exceed the radius of convergence of the Taylor expansion. The full set on conditions for non-normal operators is nontrivial. Here in Eq.10.22, however, we need to define the logarithm of an operator and the logarithm does not even possess a Taylor expansion about zero (and neither does the function $x\ln(x)$). Fortunately, we can use here another method for defining the function of an operator. This method can be applied to any operator that is normal, i.e., which commutes with its adjoint, i.e., which, by the spectral theorem, can be diagonalized. The method consists in defining the function of the operator in the eigenbasis of the operator, by applying the function on each eigenvalue. This method can be applied to define the logarithm of $\ln(\hat{\rho})$ because $\hat{\rho}$ is self-adjoint and therefore normal.

Exercise 10.3 *Prove Eq.10.22 using Eq.10.21.*

10.4 Shannon entropy

But what is the origin of the von Neumann entropy formula? Actually, the problem of how to quantify how much ignorance is expressed in an arbitrary (classical) probability distribution $\{\rho_n\}_n$ is an old problem that occurs with any conventional probability distribution. The solution is that the natural measure of the ignorance expressed by a probability distribution is given by its Shannon entropy. The von Neumann entropy of the probability distribution of states is just a special case of a Shannon entropy (which

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[1] Given that $\ln(0) = -\infty$, does this formula have a problem if one or some of the ρ_i vanish? It is actually not a problem because the terms in the von Neumann formula are $\rho_n \ln(\rho_n)$ and such a term behaves well in that limit: $\lim_{\rho_n\to 0^+} \rho_n \ln(\rho_n) = 0$. Therefore, we set $\rho_n \ln(\rho_n) = 0$ if $\rho_n = 0$.

is why we will henceforth drop the subscript in S_{vN} and denote it simply by S.

Definition: For any probability distribution $\{\rho_n\}_n$, independently of whether it arises in quantum mechanics, in Las Vegas or elsewhere, i.e., for any set of numbers obeying $\rho_n \in [0,1]$ and $\sum_n \rho_n = 1$, its Shannon entropy is defined as:

$$S[\{\rho_n\}] := -\sum_n \rho_n \ \ln \rho_n \tag{10.23}$$

But why is the Shannon entropy a good definition? First, it passes a simple test. Assume that only one of the ρ_n, say ρ_{n_0}, is nonzero. In this case, the sum in the Shannon entropy has only one term: $S[\{\rho_n\}_n] = -\rho_{n_0} \ln \rho_{n_0}$. And that term vanishes too because $\rho_{n_0} = 1$ and therefore $\ln \rho_{n_0} = 0$. This means that when we are sure of the outcome, i.e., when we have zero uncertainty, then the Shannon entropy indeed yields the value of zero as it should be.

But, of course, many other definitions would also yield that result. For example the 27th power of the Shannon entropy would. So why should we quantify the amount of uncertainty or ignorance that is contained in a probability distribution through the particular formula given in Eq.10.23?

To derive Eq.10.23, Shannon considered two independent systems (classical systems in his case) with independent probability distributions, say $\{\rho_i\}$ and $\{\rho'_j\}$. Shannon's ingenious insight was that, whatever the formula $S[\{\rho_n\}]$ is, it has to be such that the ignorance about independent probability distributions is additive. If we have the amount of ignorance S about one system and the amount of ignorance S' about another, independent system, then the amount of ignorance that we have about the combined system should be $S_{tot} = S + S'$.

Concretely, if $\{\rho_n\}$ and $\{\rho'_m\}$ are the individual probabilities for the states n and m of the two independent systems respectively, then the probability that if we check both systems at once that the joint outcome is the pair of outcomes (n,m) is given by the product of the probabilities:

$$\tilde{\rho}_{n,m} = \rho_n \ \rho'_m \tag{10.24}$$

The numbers $\rho_{n,m}$ form the probability distribution of the combined system. Now we have the two individual probability distributions plus the probability distribution of the total system. Notice that the new probability distribution $\tilde{\rho}_{n,m}$ has a double index (n,m) but it works just the same way as a single index. For example, we still have that the sum of the probabilities add up to one, only that we now have to sum over the double index: $\sum_{n,m=1} \tilde{\rho}_{n,m} = 1$ (as is easy to check). Shannon stipulated that whatever the definition of the ignorance, S, for a probability distribution is, it should have the property of being additive:

$$S[\{\tilde{\rho}_{n,m}\}] = S[\{\rho_i\}] + S[\{\rho'_j\}] \tag{10.25}$$

Exercise 10.4 *Use Eq.10.24 to show that the Shannon entropy definition Eq.10.23 obeys the additivity condition Eq.10.25. Hint: the ignorance about the combined system,* $S[\{\tilde{\rho}_{n,m}\}]$*, is calculated with the same formula, namely:*

$$S[\{\tilde{\rho}_{n,m}\}] = -\sum_{n,m} \tilde{\rho}_{n,m}\ \ln(\tilde{\rho}_{n,m}) \tag{10.26}$$

Also, you may use that $1 = \sum_n \rho_n = \sum_m \rho'_m = \sum_{n,m} \tilde{\rho}_{n,m}$.

To be precise, the Shannon entropy definition in Eq.10.23 is not the only definition that satisfies Eq.10.25. Instead, we could have also defined an entropy with the logarithm to some base $a > 0$ that is different from e:

$$S_a[\{\rho_n\}] := -\sum_n \rho_n\ \log_a \rho_n \tag{10.27}$$

Using the fact that $\log_a b = \ln(b)/\ln(a)$ we have that this would yield merely a rescaling of the entropy:

$$S_b[\{\rho_n\}] = \log_b(a)\ S_a[\{\rho_n\}] \tag{10.28}$$

So which value of a we choose to define the entropy does not matter much. Still, what does the choice of the value a correspond to?

It turns out that a has a beautiful interpretation: the amount of ignorance, i.e., the entropy, S, is the number of questions - of the type that possess a possible outcomes - that we would need to have answered to remove our ignorance.

To see this, let us consider the special case of a finite and uniform probability distribution $\rho_n := 1/N$ for $n = 1, ..., N$. So this is the special case where our system can be in N different states and each state has the same probability, $1/N$. Further, let's assume that N is a power of 2, say $N = 2^r$. Now in this case, how many binary questions (i.e., questions with $a = 2$ possible outcomes) do we need to have answered to find out in which of the N possible states our system is in? The answer is r. Why? It's because any integer from 1 to N can be written as a binary string of r bits. Now let us calculate the Shannon entropy S_2 for this probability distribution:

$$S_2[\{\rho_n\}] = -\sum_n \frac{1}{N} \log_2\left(\frac{1}{N}\right) = \log_2(N) = r \tag{10.29}$$

So the Shannon entropy S_2 is indeed the number of binary questions that would need to be answered to remove our ignorance, i.e., to tell us which state the system is in.

Now what if instead we use questions that allow $a = 3$ three possible answers? In that case, we could go through the same calculation as above but we would need to require that N is a power of 3, say $N = 3^u$. Then we can conclude that any integer between 1 and N can be represented by a string of u so-called trits (which are like bits but have three possible values). We conclude that, therefore, S_3 of a probability distribution is the number of questions with three possible outcomes that we would need to have answered to specify the exact state that our system is in. One can prove:

Proposition: The entropy $S_a[\{\rho_n\}]$ of a probablity distribution quantifies the ignorance as the number of questions with a possible answers that would need to be answered to remove the ignorance about the state. We are here ignoring the fact that the number of questions should be an integer.

Remark: In our arguments to arrive at the number of bits or trits etc, we used probability distributions that are uniform, i.e., where all states are equally likely. In the case where the probability distribution is non-uniform, the statement about the number of questions that need to be asked is still true but it's not as easy to see. For example, when there are N states but some states very rarely occur, then this will effectively reduce the number of questions that need to be asked[2]. Uniform probability distributions possess the maximal entropy. For a full explanation of how to interpret the of number questions in the case of nonuniform probability distributions, I recommend the famous text by Shannon and Weaver: Mathematical Theory of Communication. This is one of the most influential books of all times because it started information theory. Have a look also at the important notion of Kolmogorov complexity which describes how much information there is in a file by asking how much it can be compressed.

Definition: We say that the entropy $S_a[\{\rho_n\}]$ measures the ignorance in units of *bits* if $a = 2$, *nats* if $a = e$, *trits* if $a = 3$ and *decimals* if $a = 10$. In physics one usually uses the unit of nats, i.e., one chooses the base e in the logarithm. Ultimately, whether we measure ignorance in bits, trits, decimals or nats is arbitrary because, as we saw in Eq.10.28, the difference choices merely differ by a constant prefactor in front of the entropy. So to measure distances in bits or nats is like measuring say distances in kilometers or miles[3].

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[2] This is in effect because there are clever choices for which questions to ask in order to exploit the rarity. This is intimately related to the concept of data compression: in maximally compressed data, all symbols occur equally likely because any unequal probability distributon could be exploited for further compression. By the way we are here of course talking about lossless data compression. Lossy data compression, such as that employed most frequently for images and sound does not relate as closely to measuring the information content in a file.

[3] However, there is ultimately a fundamental difference between bits and nats on one hand and kilometers and miles on the other hand. This is because the very notion of length should break down at the Planck scale of about $10^{-35}m$, as we discussed earlier (and so will notions of distances in time). This can happen because ultimately, our notion of distance stems from everyday experiences and we are not used to quantum fluctuating spacetime effects in our experience at ordinary scales. A priori, there is no reason to think that notions that we formed on the basis of everyday experiences hold up under extreme conditions. Now the notion of information is different. No matter how counter-intuitive processes become at extremely small scales, it is to be expected that it always makes sense to ask how much information is needed to describe the situation and how it evolves. The notion of information and its units of bits, nats etc are in this sense more robust than notions such as distance and its

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units of km or miles. It could be that physics ultimately needs to be fully reformulated in (quantum) information-theoretic terms.

Chapter 11

Thermal states

11.1 Methods for determining density matrices

In the previous chapter, we introduced the notion of density matrix, ρ, to describe situations in which we do not know the state of the system for sure and where instead we assign probabilities to the states that the system may be in. But this then leads to the question of how one can determine these probabilities. How do we find out what the density matrix is for a quantum system?

A very powerful and very often used technique for determining the density matrix, $\hat{\rho}$, of a quantum system is based on information theory. It is based on the principle that the less we know about a particle, the larger is the von Neumann entropy of its density matrix. The technique consists of calculating $\hat{\rho}$ as that density matrix which possesses the maximum von Neumann entropy (expressing our complete ignorance), subject to the constraints that we do generally know a few things about the density matrix $\hat{\rho}$ of the quantum system. Mathematically, the technique consists of treating this as a problem of constrained optimization by using Lagrange multipliers.

To obtain an example for the information-theoretic methods of obtaining the density matrix of a quantum system, we could consider, for example, diatomic molecules[1] such

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[1] The full system of a diatomic molecule such as O_2 with all its electrons and the two nuclei has many degrees of freedom. Interestingly, the relative motion of the two nuclei can often be treated separately. Why? Don't the nuclei also interact with the electrons? The answer is that yes the two nuclei do interact with the electrons but the nuclei are thousands of times heavier than the electrons and therefore much slower. The two nuclei are like two lazy whales surrounded by lots of quick little electron fish. To the lazy nuclei the electrons just look like some negatively charged cloud that surrounds them. The two oxygen nuclei are bound together by the negatively charged electron clouds that act like glue, so that the nuclei can't get too far from another. But the oxygen nuclei also cannot get to close to another because of the repulsion due to their equal charges. As a consequence, the distance between the two nuclei will generally oscillate around the equilibrium position. We will here not spend the time to mathematically justify it but the upshot is that one can show that the relative motion of the two oxygen nuclei can be described as a quantum system where $\hat{x}_i$ operators $i = 1, 2, 3$ describe the distance vector between the nuclei. The Hamiltonian has a kinetic term $\vec{\hat{p}}^{\,2}/2m$ (with m

as the O_2 molecules that float around in the air.

Concretely, we start by writing down facts that we do know about the density matrix $\hat{\rho}$, with each fact being written down as an equation. These equations are called the constraint equations. Then we set up a function Q consisting of the von Neumann entropy and the constraints added with Lagrange multipliers. Then we solve that optimization problem.

In the example of an O_2 molecule in air, what do we know about its density matrix? We know that the molecule is being kicked around like a soccer ball in the interactions with its neighbors in the air. In these interactions, sometimes the O_2 molecule will receive energy and go into a higher-energetic state, sometimes it may drop to a lower-energetic state and give away energy. For us, there is no way of knowing which pure state the O_2 molecule may be in at any moment.

But if we assume that the air is of uniform temperature and if we assume that the O_2 molecule has been in the air for a while then we can conclude that the probabilities for finding the O_2 molecule in the various states have stabilized, i.e., that they are no longer changing. In this case, we say that our system, here the O_2 molecule, has *thermalized*. Here we have the first fact that we know about the density matrix of the O_2 molecule: After thermalization (which happens very fast for a small system such as an O_2 molecule in air), the density matrix is no longer changing:

$$d\hat{\rho}/dt = 0 \tag{11.1}$$

Further, we also know about our O_2 molecule that the expectation value of its energy is not infinite but is some finite value, that we may call $\bar{E}$. This means that we have a second equation that the density matrix must fulfill:

$$\bar{E} = \text{Tr}(\hat{\rho}\hat{H}) \tag{11.2}$$

Finally, a third fact that we know about the density matrix is that, as always, it must have trace 1:

$$\text{Tr}(\hat{\rho}) = 1. \tag{11.3}$$

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being a reduced mass) plus a potential term $V(\hat{x})$. From the perspective of the slow nuclei, all the fast and complicated dynamics of the electrons is simply reduced to the existence of this potential that binds them together. Now that potential has its minimum at the equilibrium distance where the nuclei as much repel as attract another. The potential increases to the left and right of that special distance. For a diatomic system like this we therefore always obtain some quantum oscillator. The potential $V(\hat{x})$ can be Taylor expanded around the equilibrium distance. The linear term will vanish because we are expanding around the minimum of the potential. The quadratic terms in the expansion would give a harmonic potential but there are generally also higher order terms. We obtain that our system is some 3-dimensional nonharmonic oscillator, which means that the energy levels will generally not be equidistantly spaced. In this system the nuclei will vibrate against each other and they will also generally rotate around each other. If the system receives too much energy, the O_2 molecule breaks apart. Mathematically, this is described by the potential flattening and the spectrum becoming continuous above some energy. We will assume that the energies don't suffice for that, i.e., we will assume the heat bath to be not too hot. For example, at room temperature, O_2 is essentially stable.

These facts now fully determine the density matrix of our O_2 molecule. More generally, we can determine the density matrix of any system for which conditions Eqs.11.1,11.2,11.3 hold. Let us first state the result and then prove it.

11.2 Thermal equilibrium states

Definition: We will call any system whose Hamiltonian has a purely discrete spectrum and for which conditions Eqs.11.1,11.2,11.3 hold a "test system". We use the term test because such systems don't affect their environment much, they only test it. We require that the spectrum be discrete so that we can form traces[2]. We will call a test system's environment (such as the air in the case of the O_2 molecule) its *heat bath.*

Proposition: Consider a test system that is exposed to a heat bath environment of fixed temperature T. Then, after thermalization, the test system is in the thermal state described by this density operator:

$$\hat{\rho} = \frac{1}{\mathrm{Tr}\left(e^{-\frac{\hat{H}}{kT}}\right)}\ e^{-\frac{\hat{H}}{kT}} \tag{11.4}$$

We see here that $\hat{\rho}$ is an exponential function of the Hamiltonian. The fraction is a mere numerical pre-factor that will plays the rôle of a normalization factor that makes sure that $\mathrm{Tr}(\hat{\rho}) = 1$. Further, k here is the Boltzmann constant. It is the conversion factor between Kelvins and Joules. The units of T are Kelvins but kT is an energy and the units of kT are Joules.

Definition: (Partition function) The function

$$Z(T) := \mathrm{Tr}\left(e^{-\frac{\hat{H}}{kT}}\right) \tag{11.5}$$

is called the *partition function.*

It is convenient to introduce a new variable, the so-called inverse temperature:

$$\beta := \frac{1}{kT} \tag{11.6}$$

We then have:

$$\hat{\rho} = \frac{1}{\mathrm{Tr}\left(e^{-\beta\hat{H}}\right)}\ e^{-\beta\hat{H}} \tag{11.7}$$

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[2] Recall that when a Hamiltonian has a continuous spectrum it means that there are non-normalizable states corresponding to unbound particles, such as plane waves. We can ensure that the spectrum of the Hamiltonian is discrete by assuming that our system is in a large box because that prevents the existence of unbound states. Since the box may be chosen as large as trillions of light years across, this box regularization, also called *infrared regularization,* is a harmless technical tool that does not impact practical physical predictions.

Remark: Notice that for high temperatures, i.e., for $\beta \to 0$, $\hat{\rho}$ becomes closer and closer to the identity matrix, i.e., all states become more and more equally likely.

Exercise 11.1 *Show that, conversely, as the temperature is driven to zero, $\beta \to \infty$, the density matrix tends towards the pure ground state of the Hamiltonian.*

11.3 Thermal states are states of maximum ignorance

Let us now derive the formula Eq.11.7 for the thermal state of a test system by using the information-theoretic strategy that we described above. First, we remember that all the information that we do have about the mixed state $\hat{\rho}$ of our test system is contained in Eqs.11.1,11.2,11.3.

Beyond that we know nothing about the state that the test system may be in. This latter statement is not an empty statement! That's because it means that the density operator of the test system should possess the maximal von Neumann entropy allowed, given the constraints expressed in Eqs.11.1,11.2,11.3.

This allows us to set up a concrete maximization problem for the entropy of the test system while using Lagrange multipliers to implement the two constraints. Namely, we need to find the operator $\hat{\rho}$ and numbers λ and μ (the Lagrange multipliers) that extremize the expression:

$$Q(\hat{\rho}, \mu, \lambda) := -\mathrm{Tr}(\hat{\rho} \ln \hat{\rho}) - \lambda(\mathrm{Tr}(\hat{\rho}\hat{H}) - \bar{E}) - \mu\,(\mathrm{Tr}(\hat{\rho}) - 1) \tag{11.8}$$

By setting the derivatives with respect to λ and μ to zero we obtain, as it should be, the constraints:

$$\mathrm{Tr}(\hat{\rho}\hat{H}) = \bar{E} \qquad \text{and} \qquad \mathrm{Tr}(\hat{\rho}) = 1 \tag{11.9}$$

Finally, we set the derivative with respect to $\hat{\rho}$ equal to zero and obtain:

$$-\ln(\hat{\rho}) - \mathbf{1} - \lambda\hat{\mathrm{H}} - \mu\mathbf{1} = 0 \tag{11.10}$$

Did we just differentiate with respect to an operator? Here is how we can do this in this special case. From the condition of thermal equilibrium, Eq.11.1, and using the von Neumann equation that describes the evolution of the density matrix in the Schrödinger picture[3], Eq.10.20, it follows that

$$[\hat{H}_S(t), \hat{\rho}(t)] = 0 \tag{11.11}$$

Now we remember that any two self-adjoint matrices $A = A^\dagger$ and $B = B^\dagger$ have eigenbases[4], say $A|a_n\rangle = a_n|a_n\rangle$ and $B|b_n\rangle = b_n|b_n\rangle$. It is a theorem that if these operators also obey $[A, B] = 0$ then they possess a joint eigenbasis, i.e., $|a_n\rangle = |b_n\rangle\ \forall n$.

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[3] In the Heisenberg picture the pure states don't evolve and therefore the micxed states don't either. In the Heisenberg picture, all the dynamics in the observables.

[4] We postpone the consideration of cases of continuous spectra.

Therefore, we can consider Eq.11.8 in the joint eigenbasis of $\hat{\rho}$ and of $\hat{H}$ so that all matrices are diagonal. Then, by differentiating Eq.11.8 with respect to the diagonal elements of $\hat{\rho}$, setting the resulting equations to zero and collecting these equations as one matrix equation, we obtain Eq.11.10. Now from Eq.11.10, defining $\mu' := \mu + 1$, we obtain:

$$\hat{\rho} = e^{-\mu' \mathbf{1} - \lambda \hat{\mathrm{H}}} = e^{-\mu'}\ e^{-\lambda \hat{H}} \tag{11.12}$$

We still need to implement the constraints Eq.11.2 and Eq.11.3 and these two constraints will fix the two variables λ and μ'. First, from the normalization constraint, Eq.11.3, we obtain:

$$\mathrm{Tr}(\hat{\rho}) = e^{-\mu'}\ \mathrm{Tr}(e^{-\lambda \hat{H}}) = 1 \tag{11.13}$$

Therefore

$$e^{-\mu'} = \frac{1}{\mathrm{Tr}(e^{-\lambda \hat{H}})} \tag{11.14}$$

so that we obtain:

$$\hat{\rho} = \frac{1}{\mathrm{Tr}(e^{-\lambda \hat{H}})}\ e^{-\lambda \hat{H}} \tag{11.15}$$

Now the energy constraint $\bar{E} = \mathrm{Tr}(\hat{\rho}\hat{H})$ will allow us also to determine the λ. Namely, the energy constraint is

$$\bar{E} = \frac{1}{\mathrm{Tr}(e^{-\lambda \hat{H}})}\ \mathrm{Tr}(\hat{H}\ e^{-\lambda \hat{H}}) \tag{11.16}$$

Concretely, in the eigenbasis of $\hat{\rho}$ and $\hat{H}$, with $\hat{H}|E_n\rangle = E_n|E_n\rangle$, the energy constraint becomes:

$$\bar{E} = \frac{\sum_n E_n\ e^{-\lambda E_n}}{\sum_m e^{-\lambda E_m}} \tag{11.17}$$

Now what does this tell us about the physics of λ? It tells us that, whatever the precise physical rôle of λ is, it should have something to do with the temperature of the test system's heat bath environment. The intuition is that if we want our test system to have a certain energy expectation value $\bar{E}$ then the parameter λ of the heat bath may be adjusted to provide for that. Could it be that λ is the temperature? Almost!

If we want $\bar{E}$ to be large, then the temperature of the heat bath (e.g. the air around our O_2 molecule) must be high, and vice versa. Each temperature corresponds to an energy expectation value and vice versa. Now we have just seen that the energy expectation value $\bar{E}$ depends on the parameter λ that arose as a Lagrange multiplier. So shouldn't λ be the temperature? Here is why it is not the temperature:

Exercise 11.2 *Differentiate Eq.11.16 with respect to λ and show that this derivative is always ≤ 0. Hint: Recall the definition of the variance (of the energy).*

From the result of the exercise, namely that $\bar{E}$ increases as λ is decreasing, we conclude that λ cannot be the temperature. But it could be and is in fact its inverse:

Definition (temperature): We obtained in Eq.11.17 a fundamental relationship between the energy expectation value of a test system and the Lagrange multiplier λ. The Lagrange multiplier λ is called the inverse temperature β, i.e., we have $\beta = \lambda$.

Remark: In this course, we left behind classical mechanics and are building up quantum mechanics from scratch. We can define what we mean by the notion of temperature in the way we derived it above.

Now from Eqs.11.6,11.15 and with $\lambda = \beta$, we finally proved the expression Eq.11.4 for the density operator of a test system in a thermal environment:

$$\hat{\rho} = \frac{1}{\mathrm{Tr}\left(e^{-\frac{\hat{H}}{kT}}\right)}\ e^{-\frac{\hat{H}}{kT}} \tag{11.18}$$

Exercise 11.3 *Consider a quantum harmonic oscillator of frequency* ω *in a thermal environment with temperature* T*. a) Calculate its thermal state* $\hat{\rho}$*. b) Explicitly calculate the energy expectation value* $\bar{E}(\beta)$ *as a function of the inverse temperature* β*. Hint: Consider using the geometric series* $\sum_{n=0}^{\infty} e^{-\alpha n} = \sum_{n=0}^{\infty} \left(e^{-\alpha}\right)^n = 1/(1-e^{-\alpha})$ *which holds for all* $\alpha > 0$*. Also the derivative of this equation with respect to* α *is useful.*

Definition (the freezing out of degrees of freedom): In the calculation of part b) of this exercise, the result will show that the energy expectation value $\bar{E}$ depends on the oscillator frequency ω. For large ω, the energy expectation $\bar{E}$ value drops off sharply. There is an intuitive explanation: Consider a harmonic oscillator with large frequency ω. Its first excited state is energetically the amount $\hbar\omega$ above the ground state. If the harmonic oscillator is placed in a relatively cold environment, i.e., if $\hbar\omega \gg kT$, then its random interactions with the cold environmental particles are likely insufficient to excite our test system. It is likely to stay in the ground state. When a test system's lowest energy gap is so large compared to the temperature that the test system is very unlikely to get excited by the environment then we say that the degrees of freedom of the test system are *frozen out.* The test system is almost guaranteed to be in its ground state, in spite of being in contact with an environment.

Remark (ultraviolet catastrophe): Remember that the first strong hint that classical mechanics is in trouble came from the calculation of the thermal radiation spectrum. The spectrum came out to be divergent. Ultimately, this divergence can be traced back the equipartition theorem of classical mechanics. For harmonic oscillators the equipartition theorem says that each classical harmonic oscillator that is exposed to a thermal environment will have an energy expectation value of kT, independently of the frequency of the harmonic oscillator. Now as we discussed earlier, the electromagnetic field when Fourier decomposed, consists of infinitely many harmonic oscillators, namely oscillators for each wave vector. This means that there are infinitely many oscillators, of arbitrarily high frequencies, each acquiring kT of thermal energy in thermal equilibrium. This predicts an infinite energy density in the electromagnetic field, at every nonzero temperature. That was the original ultraviolet catastrophe.

Planck solved the problem when he calculated what amounts to part b) of the above exercise: He found that in quantum theory, equipartition does not hold. Instead, the harmonic oscillators of the electromagnetic field which have very high frequencies are effectively frozen out: they contribute very little to the total energy density in the electromagnetic field.

Chapter 12

Composite quantum systems

As we mentioned before, there are two instances in which we can calculate the density matrix of a system relatively straightforwardly. One instance is where the system in question has thermalized with a heat bath. The other instance is when the system in question is being measured or interacted with.

12.1 Beyond thermal baths

In the previous chapter, we discussed how the density matrix of a system can be obtained when the system has interacted with a thermal bath long enough to equilibrate, i.e., for its density matrix to no longer change. It turned out that in this case, it is not necessary to study the quantum mechanics of the heat bath. Instead, we found that an information-theoretic strategy is sufficient to obtain the density matrix:

Calculate $\hat{\rho}$ as that density matrix which expresses maximum ignorance of the state of the system subject to the constraints that we do know a number of properties of the density matrix. In fact, this information-theoretic strategy is successful also in more complicated situations, for example, when our system is able to exchange particles with the heat bath.

This method of calculating density matrices is very useful because, in practice, quantum mechanical systems are generally exposed to a heat bath, even if we try to avoid this. For example, we may place our quantum system, let's say an atom, in a closed box that we have pumped empty of other particles. Even then, our atom will be exposed to a heat bath. This is because as long as the walls of the box have some temperature above zero, particles and photons will evaporate from (and condense back to) the wall, thereby filling the box with a heat bath whose temperature is of the same temperature as the walls of the box. Every quantum system is, therefore, prone to become mixed by interacting with its environment. This is why, to minimize this source of mixedness, quantum experiments and quantum technologies such as quantum computing often operate at extremely low temperatures.

In what follows, let us assume again, as we tacitly did before the section on thermal states, that our quantum system is sufficiently isolated in a sufficiently cool environment so that the system's interactions with the environment are negligible on the time scale that we consider. In this case, a system that is initially prepared in a pure state can become mixed due to a measurement or interaction.

12.2 Mixedness arising from interaction

An important circumstance in which we can calculate the density matrix of a system is when we run an ensemble of experiments after the measurement of an observable $\hat{f}$. This is because, knowing the state of the system before the measurement, we can calculate the probabilities for the measurement outcomes of the $\hat{f}$ measurement. We can calculate, therefore, the probabilities for the system to collapse into any one of the $|f_n\rangle$, i.e., we can calculate the density matrix for the mixed state that the system is in after the measurement. (To keep things simple, we assume that the spectrum of $\hat{f}$ is purely discrete and nondegenerate. The generalization to the case with arbitrary spectra is straightforward.)

Of course, if we were not to run an ensemble but considered an individual run of the experiment then after reading off the measurement outcome from the display of the measurement apparatus, the system would be in a pure state. However, often needs to consider the entire ensemble and in which case the mixed density matrix of the ensemble is needed.

To see this, let us remember that there is no minimum size for a measurement apparatus. This also means that for a state vector to collapse, human observers are not necessary. Any measurement device, no matter how small, can collapse the state of a system. Even a single stray particle that strikes our quantum system can serve as a measurement device that collapses the state of our system. For example, our quantum system of interest could be an atom. Then even when just a single stray electron or a single stray photon could be scattering off of our atom and thereby learn some observable $\hat{f}$ about our atom.

Of course, the electron will not bring any measuring equipment, notebooks and internet connection along for its interaction with the atom. But the electron will measure the atom in the sense that after its collision with the atom, it will carry some information about the atom, such as roughly where it was and how fast it was: if we could find and measure the atom before and after the collision, we could learn such information about the atom. This is why the stray particle in effect performs a measurement on our system and therefore collapses its state.

Which observable, $\hat{f}$, it is that the stray particle measures about our atom depends on the initial state of the stray particle and it depends on the type of interaction it has with our atom, as we will discuss in detail later. The outcome is that, by effectively performing a measurement $\hat{f}$ on our system, the stray particle collapses the state of our atom. Of course, when this happens, we humans generally don't ever learn what this electron or photon has measured (unless we design a suitable apparatus to catch and measure it). Therefore, we have to treat our atom as having been measured and the measurement outcome as not being known. This means that we have to describe our atom as being in a mixed state after it was struck by the stray particle.

The fact that any even small system can measure a quantum system means of course that quantum systems are very susceptible to being measured. After all, any quantum system is usually surrounded by particles that could interact with it. Therefore, we often have the situation that a quantum system evolves unitarily according the Schrödinger equation only in between interactions with its environment.

12.3 The collapse picture of interactions

Let us now summarize mathematically how, in an ensemble of experiments, a system collapses from a pure to a mixed state when being measured. The measurement could be by an apparatus or by a system as small as a stray particle. It will be convenient to use the Schrödinger picture for this discussion.

The scenario is that we run an ensemble of experiments where at a time t_0 we prepare the system always in the same pure state $|\psi_0\rangle$. Then we let the system evolve undisturbed until an observable $\hat{f}$ is being measured (e.g. by a stray particle) during a short time interval $[t_1, t_1 + \epsilon]$. Then the probability that the state right after the measurement of $\hat{f}$, at the time $t_1 + \epsilon$ collapsed to $|f_n\rangle$ is given by:

$$p_n := |\langle f_n|\psi(t_1)\rangle|^2 \tag{12.1}$$

Independent of the measurement outcome, i.e., independently of which state the system collapsed into, we always (i.e., for all experiments in the ensemble) let the collapsed states evolve further. Now, at the starting time $(t_1 + \epsilon)$, our system is in a mixed state described by this density matrix:

$$\rho(t_1 + \epsilon) = \sum_n p_n |f_n\rangle\langle f_n| \tag{12.2}$$

At a later time, t_2, another observable $\hat{g}$ could be measured, e.g. again by a stray particle. We can then predict the ensemble average value $\bar{g}(t_2)$ through:

$$\bar{g}(t_2) = \mathrm{Tr}(\rho(t_2)\hat{g}) \tag{12.3}$$

Here, the density matrix $\rho(t_2)$ is obtained by solving the von Neumann equation of motion with Eq.12.2 as the initial condition. We can also predict the probability for individual measurement outcomes g_n and therefore the collapses in to states $|g_n\rangle$, i.e., we can calculate the density matrix of the system after the second measurement.

In conclusion, we see here how a system can collapse into new mixed states whenever it is being measured. We assumed here that the measurement outcome is either not known, as in the case of a measurement by a stray particle or that irrespective of the recorded measurement outcome, the evolution is continued for the entire ensemble of experiments.

However, so far two questions have remained open here. One is the question of how to find out what observable a stray particle would measure. The second question is how the sudden state collapse can be explained as being part of the usual smooth quantum mechanical evolution according to the Schrödinger equation. In order to answer these questions, we will have to treat both, our system, and the apparatus (or e.g. stray particle) that measures it as quantum mechanical systems that are together forming a bigger quantum mechanical system.

In this way, we can re-examine the measurement process, namely as a process of an interaction between two subsystems of a quantum system.

12.4 Heisenberg cuts

As far as we know, everything in the universe behaves quantum mechanically. This means that we can choose to describe any subset of the universe as one quantum system and consider the rest of the universe as belonging to the "environment" of our quantum system. We can make the part of the universe that we consider to be our quantum system of interest larger or smaller, as we please.

So let us assume that have conceptually carved out a part of the universe and consider it to be our quantum system. We then consider the rest of the universe as its environment. The conceptual cut that separates the quantum system that we carved out from the rest of the universe is called the Heisenberg cut. That we can make any Heisenberg cut that we want is tremendously useful. For example, shifting the Heisenberg cut allows us to better understand the process by which a the state of a quantum system collapses when the quantum system is measured.

How so? By considering two different Heisenberg cuts, we can describe a measurement process in two complementary ways: First, there is the Heisenberg cut that we have implicitly used all along. This is the Heisenberg cut around our system of interest, such as an atom. The stray particle that measures our atom is part of the rest of the universe. With this Heisenberg cut, the measurement process induced a non-unitary evolution of the density matrix of the electron.

To see this, let us briefly review why a unitary time evolution can evolve pure states only into pure but never mixed states: First, let us recall that a density operator is pure if it can be brought into the form:

$$\hat{\rho} = |\psi\rangle\langle\psi| \tag{12.4}$$

Let us assume a system is in such a pure state initially. After a unitary time evolution

$$|\psi\rangle \rightarrow |\phi\rangle = \hat{U}|\psi\rangle \tag{12.5}$$

the state is

$$\hat{\rho}' = \hat{U}|\psi\rangle\langle\psi|\hat{U}^\dagger = |\phi\rangle\langle\phi| \tag{12.6}$$

which is still the density matrix of a state that is pure.

But if quantum mechanics, whose evolution is always unitary, describes everything, how can it then describe that the state of say an atom evolves from a pure to a mixed state when struck by a stray particle? Do we need physics beyond the Schrödinger equation to describe the nonunitary evolution during a measurement process? The answer is no. To see why we will expand or *dilate* the Heisenberg cut to include the stray particle (or whichever other measurement device we may be using):

Namely, let us now choose an alternative, second Heisenberg cut, namely the cut that now includes the quantum system that we were originally interested in (e.g., an atom) plus the stray particle (or other measurement apparatus). They are now both within the new Heisenberg cut and together they form one quantum system with its own Schrödinger equation. What is the benefit of the new Heisenberg cut? The tremendous advantage of the new Heisenberg cut is that the interaction between the atom and the measurement apparatus (or stray particle) is no longer a measurement process that the environment performs on our electron. No, now the same process is merely an interaction between two parts of a single larger (or dilated) quantum system. This larger quantum system is fully described by its Schrödinger equation. Therefore, the dilated quantum system follows unitary evolution! No physics beyond the Schrödinger equation is now needed.

We will study this dynamics in detail later. For now, we can anticipate that quantum mechanics is self-contained and no new rules beyond the Schrödinger equation are required to describe measurements in this sense. This is because the interaction of our electron with the remnant atom can be fully described by the Schrödinger equation. The price to pay was that it's not just the Schrödinger equation for our electron alone! Now it's the Schrödinger equation for the electron plus the atom that interacts with the electron.

To conclude, what we do in order to calculate through such a measurement process is to change the Heisenberg cut to a larger, dilated, system. This total system has its own Schrödinger equation and as long as there is no outside interference with this total system, it will evolve unitarily. The Hamiltonian governing the evolution of this larger system is, as always, the sum of all the energies involved: It is, therefore, the sum of the free Hamiltonian of our system, $\hat{H}_{sys}$, plus the free Hamiltonian of our measurement device (such as a stray particle), $\hat{H}_{mea}$, plus a Hamiltonian $\hat{H}_{int}$ that describes the energies involved in their interaction:

$$\hat{H}_{total} = \hat{H}_{sys} + \hat{H}_{mea} + \hat{H}_{int} \tag{12.7}$$

For example, the free Hamiltonians could be of the simple form $\hat{p}^2/2m$ and the interaction Hamiltonian may be describing (roughly), for example, some electrostatic attraction, say $\hat{H}_{int} = -\alpha/|\hat{x}_{el} - \hat{x}_a|$ (assuming for simplicity that the atom is charged).

Now when the interaction between our electron and the atom takes place it is simply part of the unitary evolution within this larger system. There is no collapse from the perspective of this larger combined system.

This will allow us to calculate the collapse or more precisely the pure-to-mixed state transition from the perspective of the electron in all detail! Namely, the strategy is this: First we solve for the unitary time evolution of the combined system. Then we analyze what the unitary time evolution of the big system implies for the subsystem of only the electron. In the process we will gain insights into the interplay of the notions of measurement, decoherence, pure and mixed states and into the deep role that entanglement plays in this.

But first we need to find out how to construct the Hilbert space of a dilated, i.e., composite system and how the operators, such as the Hamiltonians and other observables act on it. That this is somewhat nontrivial becomes clear if we reconsider this sum of the free plus interaction energies of above: $\hat{H}_{total} = \hat{H}_{sys} + \hat{H}_{mea} + \hat{H}_{int}$. One often finds a formula like this in the literature but in this form the formula is actually abbreviated and as it stands it is not quite correct: The three Hamiltonians act on different Hilbert spaces and therefore cannot be added. As we will see, the correct way to write the sum of the Hamiltonians, so that they all act on the same Hilbert space, namely that of the large system is

$$\hat{H}_{total} = \hat{H}_{sys} \otimes 1 + 1 \otimes \hat{H}_{mea} + \hat{H}_{int} \tag{12.8}$$

So we need the notion of tensor product.

Remark: Instead of combining two systems A and B into a combined system AB, one can also start with the large system and divide it into two subsystems. To this end we would use that the observables of one subsystem commute with the observables of the other subsystem, which implies that observables of the two subsystems can be jointly diagonalized. The mathematical structure - the so-called tensor product - that results form dividing a large system into two in this way is of course the same as the tensor product obtained by combining the two subsystems to form the large system.

12.5 Combining quantum systems via tensor products

Beyond the motivation to better understand measurement and decoherence processes, there are many more situations where we may want to combine quantum systems: For example, we may want to consider the combined quantum system of an atom and the quantum system of the electromagnetic field. By working in the larger quantum system that contains them both, we can calculate emission and absorption processes. Or we may want to study how the interplay of subsystems forms a larger system, such as how atoms form molecules or crystals.

Let us, therefore, now consider two quantum systems that we will call systems A and B. Each quantum system has its Hilbert space of states that we denote $\mathcal{H}^{(A)}$ and $\mathcal{H}^{(B)}$ respectively. System A has its Hamiltonian, $\hat{H}^{(A)}$ and observables $\hat{f}^{(A)}$ that all act on the Hilbert space $\mathcal{H}^{(A)}$. Similarly, system B has its Hamiltonian, $\hat{H}^{(B)}$ and observables $\hat{f}^{(B)}$ that act on the Hilbert space $\mathcal{H}^{(B)}$. Now instead of considering the two systems separately, let us choose the Heisenberg cut around both of them such that we obtain one quantum system which consists of the two subsystems A and B.

12.5.1 The tensor product of Hilbert spaces

Let us first ask what is the Hilbert space of the combined system. The Hilbert space of the combined system is what is called the tensor product of the two subsystems' Hilbert spaces and the notation is:

$$\mathcal{H}^{(AB)} := \mathcal{H}^{(A)} \otimes \mathcal{H}^{(B)} \tag{12.9}$$

But what is the right hand side, what is $\otimes$? To define the right hand side, i.e., to define $\mathcal{H}^{(A)} \otimes \mathcal{H}^{(B)}$ we first need to explain what the elements of $\mathcal{H}^{(A)} \otimes \mathcal{H}^{(B)}$ are. To begin with, for any pair of vectors $|\psi\rangle \in \mathcal{H}^{(A)}$ and $|\phi\rangle \in \mathcal{H}^{(B)}$ we define the expression:

$$|\psi\rangle \otimes |\phi\rangle \tag{12.10}$$

Each such expression is, by definition, an element of our new Hilbert space $\mathcal{H}^{(A)} \otimes \mathcal{H}^{(B)}$. And, because $\mathcal{H}^{(A)} \otimes \mathcal{H}^{(B)}$ should obey the axioms of a Hilbert space we must now also include all finite linear combinations of such pairs in $\mathcal{H}^{(A)} \otimes \mathcal{H}^{(B)}$:

$$\sum_i |\psi_i\rangle \otimes |\phi_i\rangle \quad \in \quad \mathcal{H}^{(A)} \otimes \mathcal{H}^{(B)} \tag{12.11}$$

In order for $\mathcal{H}^{(A)} \otimes \mathcal{H}^{(B)}$ to be a linear vector space, the tensor product must be defined to obey these rules for all $\alpha, \alpha_1, \alpha_2 \in \mathbb{C}$:

$$\alpha\left(|\psi\rangle \otimes |\phi\rangle\right) = (\alpha|\psi\rangle) \otimes |\phi\rangle = |\psi\rangle \otimes (\alpha|\phi\rangle) \tag{12.12}$$

$$(\alpha_1|\psi_1\rangle + \alpha_2|\psi_2\rangle) \otimes |\phi\rangle = \alpha_1|\psi_1\rangle \otimes |\phi\rangle + \alpha_2|\psi_2\rangle \otimes |\phi\rangle \tag{12.13}$$

$$|\psi\rangle \otimes (\alpha_1|\phi_1\rangle + \alpha_2|\phi_2\rangle) = \alpha_1|\psi\rangle \otimes |\phi_1\rangle + \alpha_2|\psi\rangle \otimes |\phi_2\rangle \tag{12.14}$$

We are now ready for an important definition:

Definition: Any state $|\Omega\rangle \in \mathcal{H}^{(AB)}$ which can be written in the form of a single product,

$$|\Omega\rangle = |\psi\rangle \otimes |\phi\rangle \tag{12.15}$$

is called an *unentangled state.* Any state $|\Omega\rangle$ that cannot be written in this way, i.e., that requires a sum of terms,

$$|\Omega\rangle = \sum_i |\psi_i\rangle \otimes |\phi_i\rangle \tag{12.16}$$

is called an *entangled* state.

Remark: Notice that, for example, the state $|\Omega\rangle \in \mathcal{H}^{(AB)}$ given by

$$|\Omega\rangle = |\psi\rangle \otimes |\phi\rangle + |\psi\rangle \otimes |\varphi\rangle \tag{12.17}$$

is actually unentangled. That's because, by Eq.12.13, it can be written as a simple product:

$$|\Omega\rangle = |\psi\rangle \otimes |\xi\rangle \tag{12.18}$$

with $|\xi\rangle = |\phi\rangle + |\varphi\rangle$.

Definition: We denote the dual Hilbert space by $\mathcal{H}^{(AB)*}$. Its elements are given by all expressions of the form

$$\langle\psi| \otimes \langle\phi| \tag{12.19}$$

and their finite linear combinations.

Hermitean conjugation is now defined through:

$$(|\psi\rangle \otimes |\phi\rangle)^\dagger := \langle\psi| \otimes \langle\phi| \tag{12.20}$$

The inner product between the vectors $|\psi_1\rangle \otimes |\phi_1\rangle$ and $|\psi_2\rangle \otimes |\phi_2\rangle$ is then defined through

$$(\langle\psi_1| \otimes \langle\phi_1|)\,(|\psi_2\rangle \otimes |\phi_2\rangle) = \langle\psi_1|\psi_2\rangle\langle\phi_1|\phi_2\rangle \tag{12.21}$$

and it extends by linearity to the inner product of all elements of $\mathcal{H}^{(AB)}$ (which may be linear combinations of vectors of the form $|\psi\rangle \otimes |\phi\rangle$). Now that we have the inner product between vectors in $\mathcal{H}^{(AB)}$, we can also calculate, as usual for Hilbert spaces, the length or what is also called the norm of vectors $|\varphi\rangle \in \mathcal{H}^{(AB)}$ through $||\ |\varphi\rangle\ || := \langle\varphi|\varphi\rangle^{1/2}$. And using the norm we can calculate the distance between two vectors in $\mathcal{H}^{(AB)}$ as usual through: $d\,(|\varphi_1\rangle, |\varphi_2\rangle) := ||\ |\varphi_1\rangle - |\varphi_2\rangle\ ||$. Using the notion of distance, following standard procedure for the construction of Hilbert spaces, we can define the Cauchy sequences. Similar again to how one completes the set of rational numbers to obtain the set of real numbers we now add to the Hilbert space all the sequences of vectors that are Cauchy sequences with respect to this distance. In this way, the construction of the Hilbert space $\mathcal{H}^{(AB)}$ is completed and one can verify that all the Hilbert space axioms hold for $\mathcal{H}^{(AB)}$.

12.5.2 The tensor product of operators

Now that we have the Hilbert space $\mathcal{H}^{(AB)}$ of the combined system AB, let us ask how arbitrary operators $\hat{f}^{(A)}$ and $\hat{f}^{(B)}$ of the subsystems A and B can be made to act on that bigger Hilbert space. To this end, let us first remember that operators form a vector space: That's simply because any linear combination of operators is again an operator. But if the operators of system A form a vector space and the operators of system B form a vector space then we can form the tensor product of these two vector spaces, i.e., we can form tensor products of operators, again with linearity rules analogous to those of Eqs.12.12,12.13,12.14 but now for the vector space of operators:

$$\alpha\left(\hat{f}^{(A)} \otimes \hat{f}^{(B)}\right) = \left(\alpha \hat{f}^{(A)}\right) \otimes \hat{f}^{(B)} = \hat{f}^{(A)} \otimes \left(\alpha \hat{f}^{(B)}\right) \tag{12.22}$$

$$\left(\alpha_1 \hat{f}_1^{(A)} + \alpha_2 \hat{f}_2^{(A)}\right) \otimes \hat{f}^{(B)} = \alpha_1 \hat{f}_1^{(A)} \otimes \hat{f}^{(B)} + \alpha_2 \hat{f}_2^{(A)} \otimes \hat{f}^{(B)} \tag{12.23}$$

$$\hat{f}^{(A)} \otimes \left(\alpha_1 \hat{f}_1^{(B)} + \alpha_2 \hat{f}_2^{(B)}\right) = \alpha_1 \hat{f}^{(A)} \otimes \hat{f}_1^{(B)} + \alpha_2 \hat{f}^{(A)} \otimes \hat{f}_2^{(B)} \tag{12.24}$$

Remark: We will not need to make vector spaces of operators into Hilbert spaces, i.e., at this stage we will not need an inner product on these spaces. The vector space structure with its linearity is all we need here.

Now we can answer the question of how, e.g., the measurement outcomes of an observable $\hat{f}^{(A)}$ of system A can be predicted when working in the Hilbert space of the combined system $\mathcal{H}^{(AB)}$. The problem is that $\hat{f}^{(A)}$ acts on $\mathcal{H}^{(A)}$ but not on $\mathcal{H}^{(AB)}$.

The answer is that if $\hat{f}^{(A)}$ is an observable on the Hilbert space $\mathcal{H}^{(A)}$, then the operator $\hat{f}^{(A)} \otimes 1$ acts on the total Hilbert space $\mathcal{H}^{(AB)}$ and represents the observable in the larger system. Its action is:

$$\left(\hat{f}^{(A)} \otimes 1\right)(|\psi\rangle \otimes |\phi\rangle) = \left(\hat{f}^{(A)}|\psi\rangle\right) \otimes |\phi\rangle \tag{12.25}$$

Let us verify this by calculating the expectation value of $\hat{f}^{(A)}$ both within system A

$$\langle\psi|\hat{f}^{(A)}|\psi\rangle = \bar{f}^{(A)} \tag{12.26}$$

and as part of the bigger system AB:

$$(\langle\psi| \otimes \langle\phi|)\left(\hat{f}^{(A)} \otimes 1\right)(|\psi\rangle \otimes |\phi\rangle) = \langle\psi|\hat{f}^{(A)}|\psi\rangle\langle\phi|\phi\rangle = \langle\psi|\hat{f}^{(A)}|\psi\rangle = \bar{f}^{(A)} \tag{12.27}$$

More generally, we have that if two operators $\hat{A}$ and $\hat{B}$ act on the Hilbert spaces $\mathcal{H}^{(A)}$ and $\mathcal{H}^{(B)}$ respectively, then their tensor product is an operator that acts on elements of $\mathcal{H}^{(AB)}$ in this way:

$$\left(\hat{A} \otimes \hat{B}\right)(|\psi\rangle \otimes |\phi\rangle) = \left(\hat{A}|\psi\rangle\right) \otimes \left(\hat{B}|\phi\rangle\right) \tag{12.28}$$

The general case is obtained by linearity. Remember that the generic case involves generic vectors of the combined Hilbert space and these are linear combinations of pairs of vectors, as described in Eq.12.11. And, a generic operator on the Hilbert space of the combined system AB will have the form of a linear combination of products:

$$\hat{W}^{(AB)} = \sum_r \hat{A}_r \otimes \hat{B}_r \tag{12.29}$$

An example is the sum of the Hamiltonians that we discussed at the end of Sec.12.4:

$$\hat{H}_{total} = \hat{H}_{el} \otimes 1 + 1 \otimes \hat{H}_a + \hat{H}_{int} \tag{12.30}$$

12.5.3 Bases

Assume that the vectors $|a_n\rangle \in \mathcal{H}^{(A)}$ form a Hilbert basis $\{|a_n\rangle\}_n$ of $\mathcal{H}^{(A)}$. Similarly, assume that the vectors $|b_n\rangle \in \mathcal{H}^{(B)}$ form a Hilbert basis $\{|b_n\rangle\}_n$ of $\mathcal{H}^{(B)}$. Then one can show that the following vectors form a Hilbert basis of the Hilbert space $\mathcal{H}^{(AB)}$of the combined system:

$$\{|a_n\rangle \otimes |b_m\rangle\}_{n,m} \tag{12.31}$$

This means that every vector in the combined system, $|\Gamma\rangle \in \mathcal{H}^{(AB)}$, can be expanded in this basis

$$|\Gamma\rangle = \sum_{n,m} \Gamma_{n,m} |a_n\rangle \otimes |b_m\rangle \tag{12.32}$$

where:

$$\Gamma_{n,m} = (\langle a_n| \otimes \langle b_m|)\,|\Gamma\rangle \tag{12.33}$$

Remark: The Hilbert space of the system AB, just like any other Hilbert space, possesses infinitely many bases and in general there is no need to pick a basis of the product kind above. For example, we could use the eigenbasis $\{|\Lambda_n\rangle\}_n$ any self-adjoint operator $\hat{\Lambda}$ on $\mathcal{H}^{(AB)}$.

Continuing with the basis $\{|a_n\rangle \otimes |b_m\rangle\}_{n,m}$ made out of the product of basis vectors of the subsystems, we obtain a resolution of the identity in the combined Hilbert space:

$$1 = \sum_{n,m} (|a_n\rangle \otimes |b_m\rangle)\,(\langle a_n| \otimes \langle b_m|) \tag{12.34}$$

Remark: In the literature, it is common not to write the tensor product symbol $\otimes$, i.e., it is understood that $|\psi\rangle|\phi\rangle = |\psi\rangle \otimes |\phi\rangle$ (which is similar to how one usually does not write out the product symbol: $ab = a \cdot b$. Actually, I already used that abbreviated notation in Eq.12.34: An expression such as $|\psi\rangle\langle\phi|$ is really shorthand: $|\psi\rangle\langle\phi| = |\psi\rangle \otimes \langle\phi|$, and it lives in $|\psi\rangle \otimes \langle\phi| \in \mathcal{H} \otimes \mathcal{H}^*$.

Finally, how can we expand an arbitrary operator $\hat{f}^{(AB)}$ of the combined quantum system in a basis of the combined system? First, using the basis $\{|\Lambda_n\rangle\}_n$ we obtain as usual:

$$\hat{f}^{(AB)} = \sum_{r,s} f^{(AB)}_{r,s} |\Lambda_r\rangle\langle\Lambda_s| \tag{12.35}$$

If we use a basis obtained from products of basis vectors of the subsystems then we obtain:

$$\hat{f}^{(AB)} = \sum_{i,j,k,l} f^{(AB)}_{i,j,k,l} \left(|a_i\rangle \otimes |b_j\rangle\right) \left(\langle a_k| \otimes \langle b_l|\right) \tag{12.36}$$

Chapter 13

Change of Heisenberg cut turns entanglement into mixedness

Our aim is now to calculate from the properties of system AB the properties of one of its subsystems, let's say subsystem A. Concretely, the aim is to calculate from knowledge of the state $\hat{\rho}^{(AB)}(t)$ of the composite system AB the state $\rho^{(A)}(t)$ of subsystem A. The density operator $\rho^{(A)}(t)$ of the subsystem A of a composite system AB will be called the *reduced density operator.*

The key technical tool for calculating the reduced density operator of the subsystem A from the density operator of the larger system AB is the so-called partial trace. Let us begin by briefly reviewing the usual trace.

13.1 Review: traces

First, let us recall that in order to calculate the expectation value of an observable $\hat{f}^{(AB)}$ for an arbitrary state of the quantum system AB, we have, as always, the equation $\bar{f}^{(AB)} = \mathrm{Tr}(\hat{f}^{(AB)}\hat{\rho}^{(AB)})$. The trace can be calculated in any Hilbert basis, say some Hilbert basis denoted by $\{|\Lambda_r\rangle\}$. Or, we can use the Hilbert basis $\{|a_n\rangle\otimes|b_m\rangle\}$ obtained from Hilbert bases of the subsystems A and B. We obtain, equivalently:

$$\begin{aligned} \mathrm{Tr}(\hat{f}^{(AB)}) &= \sum_r \langle\Lambda_r|\hat{f}^{(AB)}|\Lambda_r\rangle && (13.1)\\ &= \sum_{n,m} \left(\langle a_n|\otimes\langle b_m|\right)\hat{f}^{(AB)}\left(|a_n\rangle\otimes|b_m\rangle\right) && (13.2)\end{aligned}$$

Exercise 13.1 *Assume that the density operator of system A is $\hat{\rho}^{(A)}$ and that $\hat{f}^{(A)}$ is an observable in system A. Then the prediction for $\bar{f}^{(A)}$ is given as always by $\bar{f} =$ Tr$(\hat{\rho}^{(A)}\hat{f}^{(A)})$. Now assume that the density operator of a combined system AB happens* *to be of the form* $\hat\rho^{(AB)} = \hat\rho^{(A)} \otimes \hat\rho^{(B)}$*. Show that the operator* $\hat f^{(A)} \otimes 1$ *represents the observable* $\hat f^{(A)}$ *on the larger system AB, which means that the prediction* $\bar f^{(A)}$ *can also be calculated within the large system AB, namely as the expectation value of the observable* $\hat f^{(A)} \otimes 1$*. I.e., the task is to show that* $\bar f^{(A)} = Tr\left(\hat\rho^{(AB)}(\hat f^{(A)} \otimes 1)\right)$.

In exercise Ex.13.1, we showed that an observable $\hat f^{(A)}$ of the subsystem A is also an observable in the total system AB, namely $\hat f^{(A)} \otimes 1$. Now the question arises: How can we instead start from knowledge of $\hat\rho^{(AB)}$ and calculate from it the so-called reduced density matrix $\hat\rho^{(A)}$ so that we can then calculate the predictions $\bar f^{(A)}$ directly in the Hilbert space A as $\bar f^{(A)} = \mathrm{Tr}(\hat\rho^{(A)}\hat f^{(A)})$?

13.2 Partial traces

A key new concept that arises when considering quantum systems and their subsystems is the notion of partial trace. It is obtained by taking the trace over only the Hilbert space of one of the subsystems:

Definition: (Partial trace) Consider an operator $\hat f^{(AB)}$ of combined quantum system. Its *partial trace* over the Hilbert space $\mathcal{H}^{(B)}$ is an operator on the Hilbert space $\mathcal{H}^{(A)}$:

$$\begin{aligned}
\mathrm{Tr}_B(\hat f^{(AB)}) &:= \sum_r \langle b_r|\hat f^{(AB)}|b_r\rangle && (13.3)\\
&= \sum_r \langle b_r|\left(\sum_{ijkl} \hat f_{ijkl}\left(|a_i\rangle\otimes|b_j\rangle\right)\left(\langle a_k|\otimes\langle b_l|\right)\right)|b_r\rangle && (13.4)\\
&= \sum_{rijkl} f_{ijkl}\delta_{rj}\delta_{rl}|a_i\rangle\langle a_k| && (13.5)\\
&= \sum_{rik} f_{irkr}|a_i\rangle\langle a_k| && (13.6)
\end{aligned}$$

Technically, in Eq.13.3, $\langle b_r|$ is shorthand notation for what is really $\mathbf{1}\otimes\langle b_r|$. Here, the tensor product is the tensor product of two linear maps. One of the two linear maps is the map $\mathbf{1}$ which maps each vector in the Hilbert space $\mathcal{H}^{(A)}$ into itself. The other linear map is $\langle b_r|$. Remember that $\langle b_r|$, being a dual vector, is a linear map from the Hilbert space $\mathcal{H}^{(B)}$ into the complex numbers. Similarly, in Eq.13.3, $|b_r\rangle$ is shorthand notation for what is really $\mathbf{1}\otimes|b_r\rangle$, with $|b_r\rangle$ being a linear map that maps vectors in $\mathcal{H}^{(A)*}$ into the complex numbers.

In effect, the partial trace sets the operators' indices for the second Hilbert space equal and sums over them - analogous to summing over the diagonal, but only for the second Hilbert space. The end result is an operator on the Hilbert space $\mathcal{H}^{(A)}$. Analogously, the partial trace over the Hilbert space $\mathcal{H}^{(A)}$ yields an operator on the

Hilbert space $\mathcal{H}^{(B)}$.

Proposition: Assume that $\hat{S}^{(AB)}$ is an operator on the Hilbert space $\mathcal{H}^{(AB)}$. Then define $\hat{g}^{(A)} := \mathrm{Tr}_B\left(S^{(AB)}\right)$. Assume that $\hat{f}^{(A)}$ is an operator on the Hilbert space $\mathcal{H}^{(A)}$. Then the partial trace obeys:

$$\mathrm{Tr}\left(\left(\hat{f}^{(A)} \otimes 1\right) \hat{S}^{(AB)}\right) = \mathrm{Tr}\left(\hat{f}^{(A)}\hat{g}^{(A)}\right) \tag{13.7}$$

Exercise 13.2 *Prove the proposition above. Hint: Notice that the trace on the left hand side is a trace in the large Hilbert space $\mathcal{H}^{(AB)}$ while the trace on the right hand side is a trace over only the Hilbert space $\mathcal{H}^{(A)}$.*

13.3 How to calculate the state of a subsystem

Definition: (Reduced density operator) Assume $\hat{\rho}^{(AB)}$ is the density operator acting on the Hilbert space $\mathcal{H}^{(AB)}$ of a composite system AB. Then the so-called *reduced density operator,* which acts on the Hilbert space $\mathcal{H}^{(A)}$ of subsystem A is by definition obtained by tracing out subsystem B:

$$\hat{\rho}^{(A)} := \mathrm{Tr}_B\left(\hat{\rho}^{(AB)}\right) \tag{13.8}$$

From this, along with the proposition of Eq.13.7, we obtain an important consequence:

Corollary: Assume that a composite system AB is in an arbitrary state $\hat{\rho}^{(AB)}$. Consider an observable $\hat{f}^{(A)}$ of subsystem A. Then, the expectation value $\bar{f}^{(A)}$ can be calculated in two ways, corresponding to the two different Heisenberg cuts. If we work with the large Heisenberg cut that encompasses the system AB, then we can use that the observable $\hat{f}^{(A)}$ of subsystem A is represented in the large system AB by the operator $\hat{f}^{(A)} \otimes 1$ which acts on the Hilbert space $\mathcal{H}^{(AB)}$. So with the large Heisenberg cut we obtain the prediction for $\bar{f}^{(A)}$ through:

$$\bar{f}^{(A)} = \mathrm{Tr}\left((\hat{f}^{(A)} \otimes 1)\hat{\rho}^{(AB)}\right) \tag{13.9}$$

But we can also work with the Heisenberg cut that encompasses only subsystem A. We can then use the proposition of Eq.13.7 to calculate the prediction $\bar{f}^{(A)}$ through:

$$\bar{f}^{(A)} = \mathrm{Tr}\left(\hat{f}^{(A)}\hat{\rho}^{(A)}\right) \quad \text{where} \quad \hat{\rho}^{(A)} = \mathrm{Tr}_B(\hat{\rho}^{(AB)}) \tag{13.10}$$

Since this is true for all observables of system A we can conclude that when a composite system AB is in an arbitrary[1] state $\hat{\rho}^{(AB)}$ then the subsystem A is in the state $\hat{\rho}^{(A)} =$

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[1] Notice that here $\hat{\rho}^{(AB)}$ is a completely arbitrary density matrix (i.e., self-adjoint and with $\mathrm{Tr}(\hat{\rho}^{(AB)}) = 1$) that, unlike in the earlier exercise Ex.13.1, does not need to be of the form $\hat{\rho}^{(AB)} = \hat{\rho}^{(A)} \otimes \hat{\rho}^{(B)}$ which would mean that $\hat{\rho}^{(AB)}$ is unentangled. So, in particular, the density matrix $\hat{\rho}^{(AB)}$ is allowed to be entangled or unentangled, and of course also mixed or pure.

$\mathrm{Tr}_B(\hat{\rho}^{(AB)})$. We can conclude this because the predictions $\bar{f}^{(A)}$ for *all* observables $\hat{f}^{(A)}$ of system A come out right if we assume that system A is in the state $\hat{\rho}^{(A)}$. The same is true of course with the rôles of systems A and B exchanged: when a composite system AB is in an arbitrary state $\hat{\rho}^{(AB)}$ then the subsystem B is in the state $\hat{\rho}^{(B)} = \mathrm{Tr}_A(\hat{\rho}^{(AB)})$.

13.4 Entangled subsystems are mixed subsystems

In our analysis now, we will always assume[2] that the system AB is in a pure state, $|\Omega\rangle$. Our aim is to find out under which circumstances the density matrix $\hat{\rho}^{(A)}$ of a subsystem is pure.

The first case that we will consider is the case case in which the system AB is unentangled, i.e., the case in which $|\Omega\rangle$ is of the form:

$$|\Omega\rangle = |\psi\rangle|\phi\rangle \tag{13.11}$$

For convenience, as is often done in the literature, we dropped the tensor product symbol $\otimes$. The density matrix of the pure and unentangled system AB is then:

$$\hat{\rho}^{(AB)} = |\Omega\rangle\langle\Omega| = |\psi\rangle|\phi\rangle\langle\psi|\langle\phi| \tag{13.12}$$

From Eq.13.10 we know that the density matrix $\hat{\rho}^{(A)}$ of subsystem A is the reduced density matrix obtained by taking the partial trace over the Hilbert space of system B. Using an arbitrary Hilbert basis $\{|b_n\rangle\}$ of $\mathcal{H}^{(B)}$ we obtain:

$$\begin{aligned}
\hat{\rho}^{(A)} &= \mathrm{Tr}_B(\hat{\rho}^{(AB)}) && (13.13)\\
&= \sum_n \langle b_n|\left(|\psi\rangle|\phi\rangle\langle\psi|\langle\phi|\right)|b_n\rangle && (13.14)\\
&= \sum_n |\psi\rangle\langle b_n|\phi\rangle\langle\psi|\langle\phi|b_n\rangle && (13.15)\\
&= \sum_n |\psi\rangle\langle\psi|\langle\phi|b_n\rangle\langle b_n|\phi\rangle && (13.16)\\
&= |\psi\rangle\langle\psi|\langle\phi|\phi\rangle && (13.17)\\
&= |\psi\rangle\langle\psi| \qquad \text{(a pure state)} && (13.18)
\end{aligned}$$

We arrive at the important conclusion that if the state $\hat{\rho}^{(AB)}$ of a composite system AB is unentangled then the state of its subsystem, $\hat{\rho}^{(A)}$, is pure. Since we could interchange the rôles of subsystems A and B here, this also means that the state $\hat{\rho}^{(B)}$ of subsystem B is pure, namely: $\hat{\rho}^{(B)} = |\phi\rangle\langle\phi|$.

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[2] The so-called Stinespring dilation theorem shows that if need be it is always possible to enlarge a mixed system's Heisenberg cut (in practice or just mathematically) so that it becomes the subsystem of a larger system which is in a pure state.

Now conversely, let us assume that the subsystem A is in a pure state $\hat{\rho}^{(A)} = |\psi\rangle\langle\psi|$. Does this mean that the state

$$|\Omega\rangle = \sum_{n,m} \Omega_{n,m} |a_n\rangle |b_m\rangle \tag{13.19}$$

of the composite system AB must be unentangled if pure? We have:

$$\begin{aligned}
\hat{\rho}^{(A)} &= |\psi\rangle\langle\psi| && (13.20)\\
&= \mathrm{Tr}_B \left(|\Omega\rangle\langle\Omega| \right) && (13.21)\\
&= \mathrm{Tr}_B \left(\sum_{n_1,m_1,n_2,m_2} \Omega_{n_1,m_1} \Omega^*_{n_2,m_2} |a_{n_1}\rangle |b_{m_1}\rangle \langle a_{n_2}| \langle b_{m_2}| \right) && (13.22)\\
&= \sum_m \langle b_m| \left(\sum_{n_1,m_1,n_2,m_2} \Omega_{n_1,m_1} \Omega^*_{n_2,m_2} |a_{n_1}\rangle |b_{m_1}\rangle \langle a_{n_2}| \langle b_{m_2}| \right) |b_m\rangle && (13.23)\\
&= \sum_{n_1,n_2,m} \Omega_{n_1,m} \Omega^*_{n_2,m} |a_{n_1}\rangle \langle a_{n_2}| && (13.24)
\end{aligned}$$

Here, the Hilbert bases $\{|a_n\rangle\}$ and $\{|b_n\rangle\}$ of the Hilbert spaces $\mathcal{H}^{(A)}$ and $\mathcal{H}^{(B)}$ can be chosen arbitrarily. But there is a particularly useful choice for us now: let us choose the Hilbert basis $\{|a_n\rangle\}$ of $\mathcal{H}^{(A)}$ so that $|a_1\rangle = |\psi\rangle$. We then have from Eqs.13.20,13.24:

$$|a_1\rangle\langle a_1| = \sum_{n_1,n_2,m} \Omega_{n_1,m} \Omega^*_{n_2,m} |a_{n_1}\rangle \langle a_{n_2}| \tag{13.25}$$

Therefore:

$$\sum_m \Omega_{n_1,m} \Omega^*_{n_2,m} = \delta_{n_1,1} \delta_{n_2,1} \tag{13.26}$$

Choosing $n_1 = n_2 = n$, we obtain:

$$\sum_m |\Omega_{n,m}|^2 = 0 \quad \forall n > 1 \tag{13.27}$$

When this sum of positive terms vanishes, each term must vanish. As a consequence, $\Omega_{n,m}$ has this form:

$$\Omega_{n,m} = \delta_{n_1,1} \omega_m \tag{13.28}$$

Thus:

$$\begin{aligned}
|\Omega\rangle &= \sum_{n,m} \omega_m \delta_{n,1} |a_n\rangle |b_m\rangle = \sum_m |a_1\rangle \omega_m |b_m\rangle && (13.29)\\
&= |a_1\rangle |v\rangle \quad \text{where} \quad |v\rangle := \sum_m \omega_m |b_m\rangle && (13.30)
\end{aligned}$$

Since $|\Omega\rangle = |a_1\rangle|v\rangle$ is an unentangled state, as we set out to prove, we can now summarize our findings in this way:

Summary: Consider a composite system AB which is in a pure state $|\Omega\rangle \in \mathcal{H}^{(AB)}$. Then, subsystem A is in a pure state if and only if system AB is unentangled. Therefore, system A is in a mixed state, if and only if system AB is entangled. Since we can interchange the rôles of subsystems A and B in our calculations above, the same statements hold for subsystem B: System B is in a mixed state if and only if system AB is entangled.

Discussion: This finding means something rather curious for any composite system AB that is in a pure state that is entangled: In this case, even though AB is in a pure state, i.e., even though we know exactly what state the system AB is in, we are unsure about the exact pure state that a part of it, namely system A, is in, and we have to describe the state $\tilde{\rho}^{(A)}$ as mixed.

This is curious because we are used to thinking that if we know all there is to be known about a system, say a house, then we know all about its parts, such as the kitchen. In quantum theory that's not so! The process of dividing up a quantum system AB into constituent parts A and B can introduce mixedness! Intuitively, this is because information about of the total system, namely its entanglement is stored nonlocally, i.e., it is distributed over the subsystems. If we draw our Heisenberg cut around a subsystem, this information is lost, making the state of the subsystem mixed.

Conversely, an alternative way of looking at this phenomenon is this: assume each of two subsystems A,B is in a mixed state. If we draw the Heisenberg cut so as to include both of them at once then this larger system AB can be (though it does not need to be) in a pure state. In fact, as the so-called Stinespring dilation theorem shows, for every system A that is in a mixed state, one can either physically find or at least mathematically define a partner system B such that the combined, so called *dilated* system AB, is in a pure state.

Comment: Consider a system A that interacts with an experimenter. The experimenter and his or her equipment are all made of quantum particles and so we may describe the experimenter and their equipment collectively as system B. Now system A may be in a mixed state while system AB is in an entangled but pure state. Therefore, from the experimenter's perspective, the Heisenberg cut is drawn around system A alone and the mixedness of the state of A expresses classical uncertainty. However, for an observer outside of system AB, system AB is in a pure state. From the perspective of such an observer, all that happens in system A, including all of its randomness, is of quantum origin. This means that one observer's classical uncertainty can actually be another observer's quantum uncertainty! It depends on which sides of Heisenberg cuts these observers are!

Example: An instance of this phenomenon is Schrödinger's cat. In this example, we have a cat in a spaceship. The poor cat is rigged up to a system that will kill it when a radioactive atom decays. Here, the cat is system A. System B is the rest of the spaceship, including, in particular, the killing machine, the astronauts and all the rest that makes up the spaceship. Now assume that the spaceship is flying through completely empty space so that it doesn't interact with anything[3] and that, therefore, if the spaceship starts in a pure state it will unitarily evolve and stay in a pure state. In the meantime, the killing machine in the spaceship may or may not be triggered by a radioactive decay. The astronauts on board will see the cat live or die. These are the only two possibilities for the astronauts on board of the spaceship. If an ensemble of such experiment is performed then according to the astronauts on these spaceships, there are probabilities for the cat to be dead or alive at any given time. But for observers outside the spaceship, the spaceship will always follow the exact same unitary evolution! In every run of an ensemble of these experiments, the evolution of the spaceship and its contents will be following the exact same evolution - described by pure state density matrix that evolves unitarily. For the the outside observers, therefore, the cat is neither dead or alive - until they interact with the spaceship by opening it and looking inside.

Exercise 13.3 *Consider two systems, A and B, with Hilbert spaces* $\mathcal{H}^{(A)}$ *and* $\mathcal{H}^{(B)}$ *which each are only two-dimensional. Assume that* $\{|a_1\rangle, |a_2\rangle\}$ *and* $\{|b_1\rangle, |b_2\rangle\}$ *are orthonormal bases of the Hilbert spaces* $\mathcal{H}^{(A)}$ *and* $\mathcal{H}^{(B)}$ *respectively. Assume that the composite system AB is in a pure state* $|\Omega\rangle \in \mathcal{H}^{(AB)}$ *given by:*

$$|\Omega\rangle := \alpha(|a_1\rangle|b_2\rangle + 3|a_2\rangle|b_1\rangle) \tag{13.31}$$

Here, $\alpha \in \mathbb{R}$ *is a constant so that* $|\Omega\rangle$ *is normalized:* $\langle\Omega|\Omega\rangle = 1$.

a) Calculate α.

b) Is $|\Omega\rangle$ *an entangled or unentangled state?*

c) Calculate the density matrix $\hat{\rho}^{(A)}$ *of subsystem A. Is it pure or mixed? Hint: you can use your reply to b).*

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[3] In practice, this is of course not possible because the universe is filled, for example, with the photons of the cosmic microwave background radiation and will incessantly interact with any spaceship. However, it is possible to create setups in which small systems such as molecules that propagate inside a empty cavity without significant interactions for an appreciable amount of time. Similarly, a house and its kitchen are never fully isolated from an environment.

Chapter 14

Amounts of entanglement and mixedness

14.1 Entanglement entropy

In practice, in particular, for applications in quantum computing, quantum cryptography, quantum communication but also in quantum gravity, it is often important not only to know whether or not two systems A and B are entangled but it is also important to quantify how much two systems A and B are entangled. We have seen that for the composite system AB, if it is in a pure state, its two subsystems A and B are entangled if and only if they are in mixed states. This means that we can use the mixedness of the systems A and B to quantify how entangled they are!

Definition: (Entanglement entropy) Assume that a system AB is in a pure state $\hat{\rho}^{(AB)}$. Then the reduced state $\tilde{\rho}^{(A)}$ of system A is generally in a mixed state, and its mixedness is naturally quantified by its von Neumann entropy $S = -\text{Tr}\left(\tilde{\rho}^{(A)}\ln(\tilde{\rho}^{(A)})\right)$. Since this entropy has its origin in the entanglement present in the state $\hat{\rho}^{(AB)}$, it is also called the *entanglement entropy* of the state of system AB. It vanishes if and only if the state of AB is unentangled.

Given that we defined the entanglement entropy of system AB as the von Neumann entropy of system A we have to ask whether the entanglement entropy is well defined. What if we chose to define the entanglement entropy as the von Neumann entropy of subsystem B instead? After all, systems A and B could be very different. In particular, they could be of very different sizes, for example, their Hilbert spaces could be of different dimensions. Shouldn't we expect that their von Neumann entropies are generally different? It turns out that the von Neumann entropies of systems A and B are actually always the same - assuming as we here do - that the system AB is in a pure state.

Proposition: (The entanglement entropy is well defined) Assume that system

AB is a pure state. Then the von Neumann entropies of the subsystems A and B coincide.

Proof: As is easily seen in the eigenbasis of the density operator, the von Neumann entropy only depends on the nonzero eigenvalues. It suffices, therefore, to show that the reduced states of A and B possess the same nonzero eigenvalues, including multiplicities. To this end, let us now show that for every eigenvector $|\phi\rangle$ of $\tilde{\rho}^{(A)}$ with nonzero eigenvalue λ there is an eigenvector $|\psi\rangle$ of $\tilde{\rho}^{(B)}$ with the same eigenvalue, λ. To prove this, let us recall that $\hat{\rho}^{(A)} = \mathrm{Tr}_B(|\Omega\rangle\langle\Omega|)$ and $\hat{\rho}^{(B)} = \mathrm{Tr}_A(|\Omega\rangle\langle\Omega|)$ mean in a basis, say $\{|a_n\rangle|b_m\rangle\}_{n,m}$ that

$$\hat{\rho}^{(A)}_{n_1,n_2} = \sum_m \Omega_{n_1,m}\Omega^*_{n_2,m} \qquad \text{and} \qquad \hat{\rho}^{(B)}_{m_1,m_2} = \sum_n \Omega_{n,m_1}\Omega^*_{n,m_2} \tag{14.1}$$

Here, $\Omega_{n,m} = (\langle a_n|\langle b_m|)|\Omega\rangle$. Now assume that

$$\hat{\rho}^{(A)}|\phi\rangle = \lambda|\phi\rangle, \qquad \text{i.e.,} \qquad \sum_{n_2} \hat{\rho}^{(A)}_{n_1,n_2}\phi_{n_2} = \lambda\phi_{n_1} \tag{14.2}$$

which is, explicitly:

$$\sum_{n_2,m} \Omega_{n_1,m}\Omega^*_{n_2,m}\phi_{n_2} = \lambda\phi_{n_1} \tag{14.3}$$

Complex conjugation yields:

$$\sum_{n_2,m} \Omega^*_{n_1,m}\Omega_{n_2,m}\phi^*_{n_2} = \lambda\phi^*_{n_1} \tag{14.4}$$

Now the claim is that the vector $|\psi\rangle \in \mathcal{H}^{(B)}$ whose coefficients are defined to be

$$\psi_m := \sum_n \Omega_{n,m}\phi^*_n \tag{14.5}$$

is eigenvector to $\hat{\rho}^{(B)}$ with eigenvalue λ, i.e., $\hat{\rho}^{(B)}|\psi\rangle = \lambda|\psi\rangle$. In a basis, what we have to check is that:

$$\sum_{m_2} \hat{\rho}^{(B)}_{m_1,m_2}\psi_{m_2} = \lambda\psi_{m_1} \tag{14.6}$$

Concretely, we therefore need to check that:

$$\sum_{m_2,n,\tilde{n}} \Omega_{n,m_1}\Omega^*_{n,m_2}\Omega_{\tilde{n},m_2}\phi^*_{\tilde{n}} = \lambda \sum_{\tilde{n}} \Omega_{\tilde{n},m_1}\phi^*_{\tilde{n}} \tag{14.7}$$

This equation holds true because of Eq.14.4.

Remark: (multi-partite entanglement) The case where the composite system AB is itself in a mixed state offers new surprises. In this case, the entanglement entropies of

A and B can differ. Correspondingly, a new kind of entropic quantity, called quantum discord, appears beyond the entanglement entropy. How can this be? I will not go into the technical details about quantum discord here but it is instructive to get some intuition for what it is: There is a way to look at quantum discord that shows that it is just entanglement - but of a bigger system. Namely, assume that system AB is in a mixed state. Then, we can always dilate our system (in theory or practically), i.e., we can always enlarge the Heisenberg cut to encompass a bigger system ABC which is in a pure state. Tracing over C then gives us back our mixed state for AB. Now system ABC, which is in a pure state, can be entangled in many ways. A tri-partite system's state is unentangled only if it can be brought in the form $|\Xi\rangle = |\psi\rangle \otimes |\phi\rangle \otimes |\varphi\rangle$. In general, however, a tri-partite state $|\Xi\rangle$ can exhibit entanglement between any two of its subsystems and even also genuine tri-partite entanglement that does not include bi-partitie entanglement (Can you come up with such a state?). It turns out (we showed it in https://arxiv.org/pdf/1212.3275.pdf) that discord in a system AB consists of the remnant of tripartite and bipartite entanglement in a dilated system ABC after tracing over system C. The main message here is that quantum mechanics has much more than 2-partite entanglement to offer. In general, multi-partite entanglement in a composite system will leave an imprint in the mixedness and entanglement of a state obtained by tracing over one or several subsystems.

Remark: (mixed states have elevated energy) We can now draw an important conclusion: Assume that system AB is in its ground state, which is a pure state. Then it is possible (namely if the state of AB is entangled) that subsystem A is in a mixed state. But that means that system A is not in its ground state - because its ground state would be a pure state. So if system A is in a mixed state then its energy expectation value is higher than that of the ground state. This situation is very common from practical quantum computing in the lab (where there can be an interplay of cooling and entanglement) all the way to Hawking radiation. Here is (very roughly) how Hawking radiation arises:

Remark: (Hawking radiation) Consider the quantum system of fields in empty space. The ground state is the vacuum state where there are no particles. Now assume that there is a black hole. Let us call the quantum fields living on the outside system A and those living inside system B. Let us call the system consisting of the quantum fields both inside and outside the system AB. Living outside the black hole, we cannot observe what is inside, so we trace over system B. Our system is the outside system, A. One can show that the reduced density operator $\hat{\rho}^{(A)}$ of the quantum fields outside the black hole is then a mixed state. So the quantum fields on the outside of the black hole are not in their ground state, i.e., not in the vacuum state, so there are particles. It turns out that $\hat{\rho}^{(A)}$ is a thermal state. So there is thermal radiation outside the black hole, and is conjectured that, therefore, black holes radiate the so-called Hawking radiation (although it was originally very differently derived). It is an important open question to what extent the entanglement entropy of the outside of a black hole quantifies the amount of information that is lost because it fell into the black hole.

Exercise 14.1 *We have seen in this chapter that interactions with a nontrivial interaction Hamiltonian* $\hat{H}^{(AB)}$ *will produce a unitary time evolution operator* $\hat{U}^{(AB)}(t)$ *that will generally entangle the two subsystems A and B. However, suitable interactions can also disentangle the two systems again! That's because any unitary operator has an inverse. (And, for example, any time evolution operator's inverse could be obtained by swapping out its Hamiltonian by its negative.) So let us study an example evolution. To this end, let us take two systems A and B that each have a two-dimensional Hilbert space, spanned by orthonormal bases* $\{|a_1\rangle, |a_2\rangle\}$ *and* $\{|b_1\rangle, |b_2\rangle\}$*. Assume that the time evolution of the composite system AB is given by this time-evolution operator:*

$$\begin{aligned} \hat{U}^{(AB)}(t) \;&:=\; |a_1\rangle|b_2\rangle\langle a_1|\langle b_2| + |a_2\rangle|b_1\rangle\langle a_2|\langle b_1| && (14.8)\\ &\quad + \sin(\omega t)|a_2\rangle|b_2\rangle\langle a_1|\langle b_1| - i\sin(\omega t)|a_1\rangle|b_1\rangle\langle a_2|\langle b_2| && (14.9)\\ &\quad + i\cos(\omega t)|a_2\rangle|b_2\rangle\langle a_2|\langle b_2| + \cos(\omega t)|a_1\rangle|b_1\rangle\langle a_1|\langle b_1| && (14.10)\end{aligned}$$

Further assume that the initial state of system AB is given by:

$$|\Omega(t_0)\rangle = |a_1\rangle|b_1\rangle \tag{14.11}$$

a) Show that $\hat{U}(t)$ *is unitary.*

b) Calculate $\hat{\rho}^{(AB)}(t)$*.*

c) Use the result of b) to calculate $\hat{\rho}^{(A)}(t)$*.*

d) We saw that the amount of entanglement between A and B is directly related to the amount of mixedness of system A. How much system A is mixed can be determined by calculating the entanglement entropy, i.e., by calculating the von Neumann entropy of $\hat{\rho}^{(A)}(t)$*. The von Neumann entropy has a direct information-theoretic interpretation but it is somewhat difficult to calculate (because taking the log of* $\hat{\rho}^{(A)}(t)$ *generally requires us to diagonalize* $\hat{\rho}^{(A)}(t)$ *first). Fortunately, we found in Sec.14.2 that there is also a simpler way to quantify the mixedness of a density matrix, namely by calculating the so-called purity measure* $P[\hat{\rho}] = Tr[\hat{\rho}^2]$*. Calculate, therefore, the purity measure* $P[\hat{\rho}^{(A)}(t)]$ *and sketch a plot of it as a function of time.*

e) Remember that how much an interaction is entangling depends also on the initial state and remember that for some initial states the interaction may not be entangling at all. Now in our example here, if the initial state were instead $|\Omega(t_0)\rangle = |a_1\rangle|b_2\rangle$*, what would then be the purity measure of* $\hat{\rho}^{(A)}$ *as a function of time? Hint: In this case, there is a quick way to get the answer.*

14.2 Purity: a simpler measure of mixedness and entanglement

Let us reconsider how we can check for and quantify the purity of a state ρ. We can measure the purity of a state by calculating its von Neumann entropy $S_a[\rho] = -\mathrm{Tr}(\rho \log_a(\rho))$. The key advantage of the von Neumann entropy as a way to measure to purity of a state is that it possesses a direct information-theoretic interpretation, namely as the number questions with a possible outcomes that need to be answered to remove all ignorance about which pure state the system is in. A disadvantage of the von Neumann entropy is, however, that it is comparatively difficult to calculate. This is because in order to be able to evaluate its logarithm it is usually necessary to diagonalize the density matrix.

There is an alternative way to quantify the purity or mixedness of a state and therefore also to quantify the entanglement a subsystem has with another subsystem if both together form a system that is in a pure state. It is not as directly information-theoretic but it is much simpler to evaluate because it does not require us to diagonalize the density matrix. To arrive at this simple method, let us remember that every density operator is self-adjoint and in its eigenbasis takes the form:

$$\hat{\rho} = \sum_n \rho_n |a_n\rangle\langle a_n| \tag{14.12}$$

Here, the eigenvalues $\rho_n \in [0,1]$ are the probabilities for finding the system in one of the states $|a_n\rangle$. The ρ_n sum up to one: $\sum_n \rho_n = 1$. Now by definition, a state is pure if we know that the system is described by one Hilbert space vector, for example, $|a_7\rangle$, with certainty, i.e., if the density operator in its eigenbasis takes the form $\hat{\rho} = |a_7\rangle\langle a_7|$. This means that all the eigenvalues are zero except for one eigenvalue which is 1.

We notice now that the density operators $\hat{\rho}$ which are pure, i.e., which have one eigenvalue being one and all the other eigenvalues vanishing are exactly those density operators which obey:

$$\hat{\rho}^2 = \hat{\rho} \tag{14.13}$$

Therefore, to test whether or not a density matrix is pure we only need to check if it remains the same when squared!

Also, we can quantify how mixed a state is by calculating the so called *purity measure:* $P[\hat{\rho}] := Tr(\hat{\rho}^2)$.

Exercise 14.2 *Assume a system possesses a Hilbert space that is N-dimensional. Which state ρ is its least pure, i.e., which is its maximally mixed state, and what is the value of the purity $P[\rho]$ of that state?*

So far, we have established that the purity, $P[\rho]$, is a good measure of how mixed the state of a system is. But can $P[\rho^{(A)}]$ also serve to measure the amount of entanglement between systems A and B, similar to the entanglement entropy? To this end, we need to show, just as we did for the entanglement entropy, that $P[\rho^{(A)}] = P[\rho^{(B)}]$. This, however, is clearly the case because, as we showed above, the spectra and degeneracies of $\rho^{(A)}$ and $\rho^{(B)}$ agree, except for the eigenvalue 0, which doesn't contribute to the purity measure.

Chapter 15

Measurements are interactions

15.1 How interactions generate entanglement

We will now investigate the time evolution of two subsystems that interact with each other. To this end, let us assume that at an initial time, say $t = 0$, we prepare two independent systems A and B in pure states $|\phi(t_0)\rangle$ and $|\psi(t_0)\rangle$ respectively. We know from Sec.13.4 that the composite system AB is then in this pure and unentangled state:

$$|\Omega(t_0)\rangle = |\phi(t_0)\rangle \otimes |\psi(t_0)\rangle. \tag{15.1}$$

Let us now assume that the two systems first evolve freely towards another then briefly interact with another, and then freely drift away from another.

Let us remember how this all unfolds when we draw the Heisenberg cut around just system A. The state $\hat{\rho}^{(A)}(t)$ is initially pure and starts out evolving unitarily according to its Hamiltonian $\hat{H}^{(A)}$. Then, system A briefly interacts with B, and then continues to evolve freely according to its free Hamiltonian $H^{(A)}$. During the interaction, B was affected by A and, therefore, learned something about A (such as, e.g., A's position). Therefore, B in effect measured something observable about A, thereby collapsing A's state. Let us assume that B is a random particle from the environment (e.g., a remnant gas particle). This means that we don't learn exactly which was the outcome of B's measurement on A. Since, therefore, we don't know which state it is that system A collapsed into during the measurement, we need to describe the state $\hat{\rho}^{(A)}(t)$ of A right after the interaction as a mixed state. When the measurement is over and system A is again moving freely, its density matrix $\hat{\rho}^{(A)}(t)$ will again evolve unitarily according to the von Neumann equation. The evolution of $\hat{\rho}^{(A)}(t)$ from pure to mixed during the interaction remains mysterious here. That's because during the interaction, system A does not evolve according to just its Hamiltonian. The evolution of a density matrix from pure to mixed can never be described by a unitary evolution since, as we saw earlier, unitary evolution cannot change the eigenvalues of any operator, including the density operator[1].

To remedy this situation, let us now look at this same evolution using the Heisenberg cut that includes the full system AB. Namely, we can calculate the evolution of the state $|\Omega\rangle$ according to the Schrödinger equation

$$i\hbar\frac{d}{dt}|\Omega(t)\rangle = \hat{H}^{(AB)}_{total}(t)|\Omega(t)\rangle \tag{15.2}$$

where

$$\hat{H}^{(AB)}_{total}(t) = \hat{H}^{(A)}_{free}(t)\otimes 1 + 1\otimes\hat{H}^{(B)}_{free}(t) + \hat{H}^{(AB)}_{interaction}(t) \tag{15.3}$$

For example, if A and B are two electrons, the free Hamiltonians could be just the kinetic energies of the two electrons A and B:

$$\hat{H}^{(A)}_{free} = \frac{\hat{\vec{p}}^{\,2}_A}{2m_A}, \qquad \hat{H}^{(B)}_{free} = \frac{\hat{\vec{p}}^{\,2}_B}{2m_B} \tag{15.4}$$

Then the interaction Hamiltonian, which contains operators acting on both particles' Hilbert spaces, could be, for example, the electrostatic interaction energy[2]:

$$\hat{H}^{(AB)}_{interaction}(t) = \frac{\alpha}{\sqrt{(\hat{\vec{x}}_A\otimes 1 - 1\otimes\hat{\vec{x}}_B)^2}} \tag{15.5}$$

Here, α a real constant. Now since in this case the total Hamiltonian is time independent, the time evolution operator is obtained simply by exponentiation (no time-ordering required):

$$\begin{aligned}\hat{U}(t)^{(AB)} &= e^{\frac{-i(t-t_0)}{\hbar}\hat{H}^{(AB)}_{total}} && (15.6)\\ &= e^{\frac{-i(t-t_0)}{\hbar}\left(\hat{H}^{(A)}_{free}\otimes 1+1\otimes\hat{H}^{(B)}_{free}+\hat{H}^{(AB)}_{interaction}\right)} && (15.7)\end{aligned}$$

Let us assume that, initially, the particles are so far apart that the interaction Hamiltonian contributes negligibly. This means that the evolution starts out simple:

$$\hat{U}(t)^{(AB)} = e^{\frac{-i(t-t_0)}{\hbar}\left(\hat{H}^{(A)}_{free}\otimes 1+1\otimes\hat{H}^{(B)}_{free}\right)} \tag{15.8}$$

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[1] Such generalized evolutions can be studied of course, and they go by the name of 'completely positive trace preserving maps', or 'quantum channel'.

[2] How is this nontrivial function of an operator defined? Remember that we saw two ways to define a function, say $g(\hat{Q})$, of an operator, $\hat{Q}$. First, if the function g possesses a Taylor expansion, say $g(\lambda) = \sum_{n=0}^{\infty} g^{(n)}(0)\lambda^n/n!$, then we can define $g(\hat{Q})$ as the Taylor expansion $g(\hat{Q}) = \sum_{n=0}^{\infty} g^{(n)}(0)\hat{Q}^n/n!$. However, many functions do not possess such a Taylor expansion, or their spectrum or norm may exceed the radius of convergence of the Taylor expansion. For example, the function $g(\lambda) = \lambda\ln(\lambda)$ that occurs in the definition of the von Neumann entropy and the function $g(\lambda) = (\lambda^2)^{-1/2}$ that arises here both do not possess a Taylor expansion around zero (since their derivatives diverge at zero). This is where the second method is useful, assuming that the operator $\hat{Q}$ is a normal operator, i.e., assuming that $[\hat{Q},\hat{Q}^\dagger] = 0$. In this case, the spectral theorem applies and we can diagonalize $\hat{Q}$. Then, in the eigenbasis of $\hat{Q}$, we can define $g(\hat{Q})$ by applying g to each of the eigenvalues on the diagonal.

$$= e^{\frac{-i(t-t_0)}{\hbar}\hat{H}^{(A)}_{free}\otimes 1} \; e^{\frac{-i(t-t_0)}{\hbar} \; 1\otimes\hat{H}^{(B)}_{free}} \tag{15.9}$$

$$= \left(e^{\frac{-i(t-t_0)}{\hbar}\hat{H}^{(A)}_{free}} \otimes 1\right)\left(1 \otimes e^{\frac{-i(t-t_0)}{\hbar} \; \hat{H}^{(B)}_{free}}\right) \tag{15.10}$$

$$= e^{\frac{-i(t-t_0)}{\hbar}\hat{H}^{(A)}_{free}} \otimes e^{\frac{-i(t-t_0)}{\hbar}\hat{H}^{(B)}_{free}} \tag{15.11}$$

We obtain these factorizations because $[\hat{H}^{(A)}_{free}(t) \otimes 1, 1 \otimes \hat{H}^{(B)}_{free}(t)] = 0$ and so they behave under exponentiation just like numbers do. As a consequence, we have:

$$|\Omega(t)\rangle = \hat{U}(t)^{(AB)}|\Omega(t_0)\rangle \tag{15.12}$$

$$= \left(e^{\frac{-i(t-t_0)}{\hbar}\hat{H}^{(A)}_{free}(t)} \otimes e^{\frac{-i(t-t_0)}{\hbar}\hat{H}^{(B)}_{free}(t)}\right)|\phi(t_0)\rangle \otimes |\psi(t_0)\rangle \tag{15.13}$$

$$= \left(e^{\frac{-i(t-t_0)}{\hbar}\hat{H}^{(A)}_{free}(t)}|\phi(t_0)\rangle\right) \otimes \left(e^{\frac{-i(t-t_0)}{\hbar}\hat{H}^{(B)}_{free}(t)}|\psi(t_0)\rangle\right) \tag{15.14}$$

$$= |\phi(t)\rangle \otimes |\psi(t)\rangle \tag{15.15}$$

We conclude that as long as the interaction Hamiltonian is negligible, the state $|\Omega(t)\rangle$ of AB remains unentangled because it can continue to be written in this product form. From our results of the previous sections, this also means that the reduced state $\tilde{\rho}^{(A)} = \mathrm{Tr}_B(\hat{\rho}^{(AB)})$ of system A remains a pure state. The evolution of system A is unitary and indeed follows the free Schrödinger equation of system A.

What, however, happens when the interaction term becomes important? In this case we have that:

$$|\Omega(t)\rangle = \hat{U}(t)^{(AB)}|\Omega(t_0)\rangle \tag{15.16}$$

$$= e^{\frac{-i(t-t_0)}{\hbar}\left(\hat{H}^{(A)}_{free}(t)\otimes 1+1\otimes\hat{H}^{(B)}_{free}(t)+\hat{H}^{(AB)}_{interaction}(t)\right)}|\phi(t_0)\rangle \otimes |\psi(t_0)\rangle$$

$$= \sum_{n=0}^{\infty}\frac{(-i)^n(t-t_0)^n}{\hbar^n n!}\left(\hat{H}^{(A)}_{free}\otimes 1 + 1\otimes\hat{H}^{(B)}_{free} + \hat{H}^{(AB)}_{interaction}\right)^n |\phi(t_0)\rangle \otimes |\psi(t_0)\rangle$$

Now, since $\hat{H}^{(AB)}_{interaction}$ does generally not commute with either $\hat{H}^{(A)}_{free}$ or $\hat{H}^{(B)}_{free}$, these terms no longer factorize. This means that $|\Omega(t)\rangle$ is generally not the tensor product of two vectors but is a sum of such terms. In other words, the interaction Hamiltonian causes the initially unentangled state $|\Omega(t_0)\rangle = |\phi(t_0)\rangle \otimes |\psi(t_0)\rangle$ to evolve into an entangled state $|\Omega(t)\rangle$ during the time interval that the interaction Hamiltonian is important, i.e., while A and B are significantly interacting.

The key advantage of having chosen this larger Heisenberg cut is that we can calculate, in this way, the density matrix

$$\hat{\rho}^{(AB)}(t) = |\Omega(t)\rangle\langle\Omega(t)| \tag{15.17}$$

for all times, from the start through the interaction and later. This is because the full system AB is not interacting with any other system, and therefore its evolution is unitary and follows the von Neumann equation of the full Hamiltonian. Crucially, we can now use the results of the previous sections to calculate the density matrix of system A at all times, before, *during* and after the interaction between A and B, through:

$$\hat{\rho}^{(A)}(t) = \mathrm{Tr}_B(\hat{\rho}^{(AB)}(t)) \tag{15.18}$$

Since $\hat{\rho}^{(AB)}(t))$ becomes entangled in the interaction, we conclude from our earlier results, that at the same time $\hat{\rho}^{(A)}(t)$ indeed becomes mixed. And now, using this larger Heisenberg cut, we use Eq.15.18, to calculate exactly how $\hat{\rho}^{(A)}(t)$ evolves, even during the interaction while it goes from pure to mixed.

To summarize, we calculated the unitary time evolution of the pure state $|\Omega(t)\rangle$ of system AB and obtain the state $\hat{\rho}^{(A)}(t)$ of A as the reduced state density operator. What, from the perspective of a Heisenberg cut around A is a *measurement* by B is from the perspective of a Heisenberg cut around AB a unitary evolution that involves an *interaction* between A and B. But are measurements and interactions always in one-to-one correspondence? Is every interaction a measurement? For a subtle reason, this is not the case!

15.2 Interactions without measurements

It is possible that systems A and B strongly interact and, nevertheless, they may not get entangled and so their individual evolutions can remain unitary! To see how this can happen, let us consider the case where the interaction energy is dominant so that we can neglect the free Hamiltonians $\hat{H}^{(A)}_{free}$ and $\hat{H}^{(A)}_{free}$.

Alternatively, if this is not a good approximation, we can also always choose to work in the Dirac picture instead of the Schrödinger picture. In fact, this is what the Dirac picture was invented for and it is therefore also called the interaction picture! Remember that to use the Dirac picture, we need to make a choice of what we consider to be the easy and what the difficult part of the total Hamiltonian. We of course choose the interaction Hamiltonian to be the difficult part

$$\hat{H}_d := \hat{H}^{(AB)}_{interaction} \tag{15.19}$$

and the remaining free Hamiltonians to be the easy part:

$$\hat{H}_e := \hat{H}^{(A)}_{free} \otimes 1 + 1 \otimes \hat{H}^{(B)}_{free} \tag{15.20}$$

Either way, whether we work in the Schrödinger picture and assume that the interaction term dominates over the free Hamiltonians, or whether we work in the Dirac picture (which always works), the states will evolve according to only the interaction Hamiltonian $\hat{H}^{(AB)}_{interaction}$. Our question, therefore, becomes whether or not every nontrivial interaction Hamiltonian entangles.

To study this question, let us consider first the trivial case where the interaction Hamiltonian is of the form:

$$\hat{H}^{(AB)}_{interaction} = \hat{Q} \otimes 1 \tag{15.21}$$

Here, Q is a self-adjoint operator of system A. Clearly, the time evolution operator then factorizes: $\hat{U}(t)^{(AB)} = e^{\frac{-i(t-t_0)}{\hbar}\hat{Q}} \otimes 1$. Therefore, the time-evolved state $|\Omega(t)\rangle$ keeps factorizing and, therefore, system A remains in a pure state. Of course, a Hamiltonian of the form of Eq.15.21 is quite trivial. However, consider now an interaction Hamiltonian of the form

$$\hat{H}^{(AB)}_{interaction} = \hat{Q} \otimes \hat{R} \tag{15.22}$$

where $\hat{R}$ is a nontrivial self-adjoint operator of system B. This interaction Hamiltonian can entangle and will in general entangle:

$$\begin{aligned} |\Omega(t)\rangle &= e^{\frac{-i(t-t_0)}{\hbar}\hat{Q}\otimes\hat{R}}|\phi(t_0)\rangle \otimes |\psi(t_0)\rangle && (15.23) \\ &= \sum_{n=0}^{\infty} \frac{(-i)^n(t-t_0)^n}{\hbar^n n!} \left(\hat{Q}\otimes\hat{R}\right)^n |\phi(t_0)\rangle \otimes |\psi(t_0)\rangle && (15.24) \end{aligned}$$

We see that the resulting state vector $|\Omega(t)\rangle$ is generally not simply the tensor product of two vectors as would be required if $|\Omega(t)\rangle$ were to be unentangled. Let us now consider the interesting case, however, that $|\psi(t_0)\rangle$ is an eigenstate to $\hat{R}$, i.e., the case where $\hat{R}|\psi(t_0)\rangle = \lambda|\psi(t_0)\rangle$. In this case, the interaction Hamiltonian's action can be written in a much simplified form:

$$\begin{aligned} \hat{H}^{(AB)}_{interaction}|\phi(t_0)\rangle \otimes |\psi(t_0)\rangle &= (\hat{Q}\otimes\hat{R})|\phi(t_0)\rangle \otimes |\psi(t_0)\rangle && (15.25) \\ &= \lambda(\hat{Q}\otimes 1)|\phi(t_0)\rangle \otimes |\psi(t_0)\rangle && (15.26) \end{aligned}$$

From earlier we can conclude that, in this case, even though the interaction may be strong, it is not entangling. The subsystems remain pure, i.e., they evolve unitarily. In practice it often happens that the state, say $|\psi(t_0)\rangle$ of a subsystem is not quite an eigenstate of the interaction Hamiltonian, say $\hat{R}$, but that it is almost an eigenstate. This happens, in particular if the state $|\psi(t_0)\rangle$ is a coherent or a squeezed state for which the uncertainty ΔR can be very small. (Recall that coherent and squeezed states are at the boundary of the uncertainty relation). In this case, $|\psi(t_0)\rangle$ is approximately an eigenvector of $\hat{R}$ and Eq.15.26 holds approximately. Therefore, the interaction is only very little entangling and the evolution of the subsystems remains almost unitary. The situation described above is common.

Remark: Why classical fields can be put into the Schrödinger equation. For example, when we write a classical electromagnetic fields into the Schrödinger equation for an electron, we ought to, in principle, consider the fact that we have here the interaction between two quantum systems: the quantum system A which consists of the electron and the quantum system B which consists of the electromagnetic field.

These two systems interact, often strongly, and so it ought to be expected that these two systems decohere each other, and that, therefore, none of the two subsystems evolves unitarily on its own. In practice, however, one treats the electromagnetic field as a classical field in the electron's Hamiltonian and treats the evolution of the electron as unitary. How can this be a good approximation? The reason is that the dynamics of electromagnetic fields is such that they tend to be in coherent states with small uncertainties in the field amplitudes (compared to the expectation values of the field amplitudes). The quantized electromagnetic field is, therefore, approximately in an eigenstate of the interaction Hamiltonian (which contains the field amplitude operators) between the electron and the electromagnetic field. This is why an electron in background electromagnetic fields evolves usually almost unitarily and why we can often replace quantized electromagnetic fields by their classical expectation values. In the field of quantum optics one often considers so-called non-classical light for which this approximation does not hold. In this case the quantum nature of light is important, and can be used, for example, for purposes of quantum communication using quantum cryptography and for quantum computing.

Chapter 16

Composition of identical systems

We are used to thinking that everything ages, for example, humans, birds, machines and rocks. While that is true it appears also to be true that the elementary particles that everything is made out of do not age! For example, there are no electrons that grow wrinkles, protons don't grow long white beards. We cannot even make a scratch on an elementary particle. Elementary particles of the same kind appear to be indistinguishable. As a consequence, also larger systems, such as Hydrogen atoms, can be indistinguishable.

The indistinguishability of identical systems has strange consequences for the way that identical systems combine to form larger systems.

Namely, remember that, when two systems A and B with Hilbert spaces $\mathcal{H}^{(A)}$ and $\mathcal{H}^{(A)}$ are combined then the combined system AB possesses the Hilbert space $\mathcal{H}^{(AB)} = \mathcal{H}^{(A)} \otimes \mathcal{H}^{(B)}$. While this is true, system AB is actually not able to use all of this Hilbert space if systems A and B are indistinguishable. Namely, if we combine two copies of the same system, A, say two protons or two Hydrogen atoms, then $\mathcal{H}^{(AA)} \neq \mathcal{H}^{(A)} \otimes \mathcal{H}^{(A)}$. To see this, we need to study the swapping of two subsystems.

16.1 Swapping identical subsystems

Let's assume that we measure an observable $\hat{Q}$ in both of two identical subsystems. We obtain two measurement values, say q_n and q_m. Now let us clarify which state $|\Omega_{after}\rangle$ the system will collapse into. Is it the state $|q_n\rangle|q_m\rangle$? Or, why not the state $|q_m\rangle|q_n\rangle$? Or, since we cannot tell one subsystem from the other is it perhaps a linear combination of the two? From the indistinguishability of the two subsystems, we know that the state $|\Omega_{after}\rangle$ after the collapse must be a state which remains unchanged when we swap the two subsystems, up to a phase $e^{i\alpha}$ with $\alpha \in [0, 2\pi)$ that does not change the normalization. So we should have that:

$$\text{swap}(|\Omega_{after}\rangle) = e^{i\alpha}|\Omega_{after}\rangle \tag{16.1}$$

It will turn out that the value of α will matter! So what value can or should α take? To find out, let us consider the swapping of two subsystems more closely.

Proposition: The swap of two subsystems amounts to a rotation by 2π.

To prove this, it would be necessary to study the properties of the rotation group. For now, to get some intuition, here is a simple experiment that you can do. Two people hold a belt, one person at each end, so that the belt hangs down to form a U shape, without any twists or rotations in the belt. Now the two people trade their places, while carefully parallel transporting their end of the belt without changing the orientation in space of their end of the belt. The two ends of the belt thereby end up trading places and the belt ends up hanging down to form a U shape again. Now, however, the belt will have a twist in it. One of the two belt holders should then carefully rotate her end of the belt until the belt no longer has a twist, while keeping track of the amount of rotation that she implements. The accumulated angle is 2π, confirming that two objects trading places amounts in this sense to a full rotation. This argument goes back to A. Broyles and R. Feynman.

Definition: (Bosons) A rotation by 2π would normally be expected to lead to the exact same vector as before the rotation. Given that a swap amounts to a rotation by 2π we would, therefore, expect that α above is 0. This is the case for a certain type of identical systems. That's the type of identical systems called bosonic. Examples of bosonic elementary particles are photons, gluons, W and Z particles, the Higgs and the inflaton particle species.

Definition: (Fermions) Rotations by 2π do not always lead back to the exact same vector. Instead, we may pick up a minus sign! In this case, in Eq.16.1, we have that $e^{i\alpha} = -1$, i.e., $\alpha = \pi$. In this case, we have to perform an additional rotation by 2π to undo that minus sign and, therefore, to recover the exact same vector. A simple example in which only a 4π rotation leads back to the starting point is this: Stretch out your arm horizontally, palm up as if holding a serving plate. Now, while always keeping your palm horizontal, rotate your palm counter clockwise by 2π. Your arm will be twisted, i.e., you are not in the same position is the one you started in. Now continue the counter-clockwise rotation, while still keeping your palm horizontal, for another 2π rotation. After this 4π rotation, your arms should be back in the initial position (or terribly twisted if things went wrong). Identical quantum systems for which only a 4π rotations reaches back to the same state vector, are called fermionic. Examples of fermionic elementary particle species are electrons, quarks and neutrinos.

Remark: Given the way that minus signs propagate, any system that consists of any number of bosons and n fermions is a boson if n is even and it is a fermion if n is odd.

Definition: (Anyons) In a $3+1$ dimensional spacetime, and in all higher-dimensional spacetimes, the study of the rotation group shows that the eigenvalues of the swapping operation can only be $+1$ and -1, i.e., there can only be bosons and fermions. However, in effectively lower-dimensional systems, such as effectively two-dimensional layers in condensed matter systems, the rotation group shows that essentially any value of α might occur! This means that there could be effective degrees of freedom, called anyons, that behave neither as bosons nor as fermions. Anyons have been discussed, for example, in the context of graphene, the quantum Hall effect and in layered high temperature superconductors such as YBCO.

16.2 Examples of composite boson and fermion systems

For a concrete example, let us now combine two identical boson systems. For simplicity, we will assume that each subsystem has a 2-dimensional Hilbert space $\mathcal{H}^{(A)}$ which is spanned by two orthonormal vectors $|a_1\rangle$ and $|a_2\rangle$. Therefore, in the Hilbert space $\mathcal{H}^{(A)} \otimes \mathcal{H}^{(A)}$ we have that these four vectors form an orthonormal basis:

$$|a_1\rangle|a_1\rangle, \quad |a_1\rangle|a_2\rangle, \quad |a_2\rangle|a_1\rangle, \quad |a_2\rangle|a_2\rangle \tag{16.2}$$

However, as mentioned before, the Hilbert space of the combined system, $\mathcal{H}^{(AA)} \neq \mathcal{H}^{(A)} \otimes \mathcal{H}^{(A)}$. This is because, in the case of identical bosonic systems, all states $|\Omega\rangle \in \mathcal{H}^{(AA)}$ of the combined system AA must obey Eq.16.1 with $\alpha = 0$, i.e.:

$$\text{swap}(|\Omega_{after}\rangle) = |\Omega_{after}\rangle \tag{16.3}$$

Not all vectors in $\mathcal{H}^{(A)} \otimes \mathcal{H}^{(A)}$ obey this condition. In particular, the vector $|\psi\rangle := |a_1\rangle|a_2\rangle - |a_2\rangle|a_1\rangle$ does not obey the condition Eq.16.3 because it obeys:

$$\begin{aligned} \text{swap}(|\psi\rangle) &= \text{swap}(|a_1\rangle|a_2\rangle - |a_2\rangle|a_1\rangle) && (16.4)\\ &= |a_2\rangle|a_1\rangle - |a_1\rangle|a_2\rangle && (16.5)\\ &= -|\psi\rangle && (16.6) \end{aligned}$$

Therefore, the one-dimensional vector space spanned by the vector $|\psi\rangle$ is a sub vector space of $\mathcal{H}^{(A)} \otimes \mathcal{H}^{(A)}$ which is not contained in the actual Hilbert space of the combined system, $\mathcal{H}^{(AA)}$.

So what about the remaining three dimensions of $\mathcal{H}^{(A)} \otimes \mathcal{H}^{(A)}$, do they obey the bosonic condition Eq.16.3? Yes, they do, as we can see by noticing that these three orthonormal vectors obey the condition Eq.16.1 with the bosonic value $\alpha = 0$:

$$|a_1\rangle|a_1\rangle, \quad |a_2\rangle|a_2\rangle, \quad \frac{1}{\sqrt{2}}\left(|a_1\rangle|a_2\rangle + |a_2\rangle|a_1\rangle\right) \tag{16.7}$$

We conclude that the Hilbert space $\mathcal{H}^{(AA)}$ that we obtain by combining these two copies of a bosonic system is 3-dimensional and is spanned by the basis vectors given in Eq.16.7.

Now similarly, let us consider two copies of a fermionic system A that is also two-dimensional and has orthonormal basis vectors $|a_1\rangle$ and $|a_2\rangle$. The Hilbert space $\mathcal{H}^{(AA)}$ of the combined system now consists of all those vectors in $\mathcal{H}^{(A)} \otimes \mathcal{H}^{(A)}$ which obey Eq.16.1 with the fermionic value for α namely $\alpha = \pi$. As we saw in Eqs.16.4-16.6, there is only one dimension in $\mathcal{H}^{(A)} \otimes \mathcal{H}^{(A)}$ that obeys this anti-symmetry condition and it is spanned by the vector $|\psi\rangle$. We conclude that the Hilbert space $\mathcal{H}^{(AA)}$ of such a composite fermionic system is only one-dimensional.

In general, the Hilbert space of a composite system whose subsystems are identical fermions is given by the subspace of antisymmetric vectors in $\mathcal{H}^{(A)} \otimes \mathcal{H}^{(A)}$:

$$\mathcal{H}^{(AA)} = \text{Antisym}\left(\mathcal{H}^{(A)} \otimes \mathcal{H}^{(A)}\right) \tag{16.8}$$

Similarly, the Hilbert space of a composite system whose subsystems are identical bosons is given by the subspace of symmetric vectors in $\mathcal{H}^{(A)} \otimes \mathcal{H}^{(A)}$:

$$\mathcal{H}^{(AA)} = \text{Sym}\left(\mathcal{H}^{(A)} \otimes \mathcal{H}^{(A)}\right) \tag{16.9}$$

16.3 Bose statistics versus Fermi statistics

We are now ready to observe a major difference between systems of two identical bosons and systems of two identical fermions, namely that identical bosons prefer to be in the same state while identical fermions cannot be in the same state. That identical fermionic subsystems cannot be in the same state is clear because that state could not be antisymmetric as required by Eq.16.1 for fermions. To see in which sense bosons prefer to be in the same state, let us consider a composite system consisting of two identical bosonic systems as above, i.e., with each subsystem having a two-dimensional Hilbert space $\mathcal{H}^{(A)}$ and the combined system possessing the three-dimensional Hilbert space $\mathcal{H}^{(AA)}$ spanned by the three vectors given in Eq.16.7. Let us now assume that the combined system AA is in thermal equilibrium with a heat bath of some temperature T. This means that our system AA is in a mixed state of a particular kind, namely a thermal state. Recall that the state $\hat{\rho}$ of a system with Hamiltonian $\hat{H}$ in equilibrium with a heat bath of temperature T, is given by:

$$\hat{\rho} = \frac{e^{-\frac{1}{kT}\hat{H}}}{\text{Tr}(e^{-\frac{1}{kT}\hat{H}})} \tag{16.10}$$

Here, k is the Boltzmann constant. Let us assume that the total Hamiltonian of system AA is given by $\hat{H}^{(AA)} = \hat{H}^{(A)} \otimes 1 + 1 \otimes \hat{H}^{(A)}$ and we start with the simple case where $\hat{H}^{(A)}|a_j\rangle = E_c|a_j\rangle$, where $j \in \{1, 2\}$ and E_c is some fixed real value. In this case, all three vectors in Eq.16.7 are eigenvectors of the full Hamiltonian with eigenvalue $2E_c$.

This means that in this basis the Hamiltonian is a 3×3 diagonal matrix with each diagonal entry taking the value $2E_c$. As a consequence, the thermal state's density matrix is also diagonal and its entries are $1/3, 1/3, 1/3$. We can conclude that each of the three basis vectors of Eq.16.7 is found with equal probability. In the first two of the three states of Eq.16.7 the bosons are in the same state and in only in the third state they are in different states. We conclude that the identical bosons are with probability $2/3$ in the same state and only with probability $1/3$ in different states.

For comparison, if the two subsystems were not identical, system AA would have the usual fully four-dimensional Hilbert space spanned by the basis vectors given in Eq.16.2, all of these basis vectors having the same energy and therefore all being equally likely. Since in two of the basis vectors, namely $|a_1\rangle|a_1\rangle$ and $|a_2\rangle|a_2\rangle$ the subsystems are in the same state and in two basis vectors, namely $|a_1\rangle|a_2\rangle$ and $|a_2\rangle|a_1\rangle$ they are in different states, the probability for non-identical subsystems to be in the same state or not is 50:50. There is then no preference. The preference of identical bosonic systems for being in the same state is ultimately responsible for a number of important phenomena such as lasers, superconductivity and more generally for Bose Einstein condensates. Conversely, the inability for identical fermions to be in the same state leads to the phenomenon of Fermi pressure which explains how neutron stars hold up against gravity and which also explains why electrons about a highly charged nucleus fill up the lowest available energy levels.

Exercise 16.1 *In the example of two identical bosonic subsystems just above, assume now that* $\hat{H}^{(A)}|a_j\rangle = E_j|a_j\rangle$ *with* $E_1 = 0$ *and* $E_2 = E > 0$*. a) Calculate the thermal density matrix of the system AA. In particular, what are the probabilities for the three basis states of Eq.16.7 as a function of the temperature? b) Determine the temperature dependence of the preference of bosons to be in the same state: Does this preference here increase or decrease as the temperature either goes to zero or to infinity?*

Chapter 17

Feynman quantum mechanics

We discussed the various pictures of the time evolution. Each makes the same predictions for observables

$$\bar{f}(t) = \langle\psi|\hat{U}^\dagger(t)\hat{f}\hat{U}(t)|\psi\rangle \tag{17.1}$$

and they differ merely in how they bracket this expression. For example, in the Schrodinger picture, the states are time dependent, i.e., we bracket this way:

$$\bar{f}(t) = \left(\langle\psi|\hat{U}^\dagger(t)\right)\hat{f}\left(\hat{U}(t)|\psi\rangle\right) \tag{17.2}$$

and in the Heisenberg picture the observables are time dependent, i.e., we bracket:

$$\bar{f}(t) = \langle\psi|\left(\hat{U}^\dagger(t)\hat{f}\hat{U}(t)\right)|\psi\rangle \tag{17.3}$$

Correspondingly, we either solve the Scvhrödinger equation to obtain the time dependence of the Schroedinger states or we solve the Heisenberg equations to obtain the time dependence of the Heisenberg operators.

In the Feynman picture, we do not bracket at all. Instead, in the Feynman picture, we calculate the time-dependent time evolution operator $\hat{U}(t)$ itself. Normally, this means solving its equation of motion:

$$i\hbar\frac{d}{dt}\hat{U}(t) = \hat{H}_S(t)\hat{U}(t) \tag{17.4}$$

and $\hat{U}(t_0) = 1$. Equivalently, in the position representation, the time evolution operator is the Green's function

$$G(x,x',t) := \langle x|\hat{U}(t)|x'\rangle \tag{17.5}$$

and it obeys:

$$i\hbar\frac{d}{dt}G(x,x',t) = \hat{H}_s(\hat{x}.,\hat{p}.t)G(x,x',t) \tag{17.6}$$

along with $G(x, x', 0) = \delta(x - x')$. While all this is quite unremarkable so far, Feynman famously found an entirely new way to calculate the Green's function and time evolution operators in general. Feynman's method does not involve solving a differential equation at all. Instead, Feynman showed how to calculated the Green's function by evaluating a so-called path integral instead. The path integral can then serve as the foundation of quantum theory. From this perspective, quantum theory arises from the Lagrangian formalism of classical mechanics, instead of the Hamiltonian formalism that we pursued so far. Feynman's picture provides deep new insights. In particular, Feynman showed that quantum theory can be understood as a new probability theory, namely a probability theory that applies whenever a system is undisturbed and therefore unobserved.

17.1 Basic rules of probabilities

Let us begin by reviewing the basic rules of ordinary probability theory. First, there is the rule of alternatives. For example, if either event A_1 or event A_2 or some other event can happen, then:

$$\text{prob}(A_1 \text{ or } A_2) = \text{prob}(A_1) + \text{prob}(A_2) \tag{17.7}$$

Second, there is the rule of conditionals. For example, assume that event B can happen only if event A has happened. Then:

$$\text{prob}(A \text{ and } B) = \text{prob}(A)\ \text{prob}(B \text{ if } A) \tag{17.8}$$

For example, let us consider a box that is filled with Helium gas. At time t_0, an emitter emits a Neon[1] atom at some fixed position x_e in the box. From then onward, the Ne atom will be kicked around by the He atoms, due to their thermal motion. This means that the Ne atom will travel on a random walk through the box. It also means that the location of the Ne atom is frequently being measured to some accuracy by the He atoms, even if we personally do not know where the Ne atom is. Then, at some later time, t, an apparatus that is specialized on detecting Ne atoms is checking if the Ne atom happens to be at the location of the detector, x_d, at some fixed place[2] in the box. Now assume that t' is an intermediary time:

$$t_0 < t' < t \tag{17.9}$$

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[1] We are choosing Helium and Neon because they do not form molecules.

[2] Of course, the locations x_e and x_d would have to be of finite size in practice and also in theory because position eigenvectors are nonnormalizable, but we know how to handle this and we will therefore here neglect this subtlety for simplicity of the notation.

Then, according to the basic rules of probability above, the probability for the Ne atom to make it from the emitter at (x_e, t_0) to the detector at (x_d, t) obeys this equation:

$$\text{prob}[(x_e,t_0) \to (x_d,t)] = \int_{box} \text{prob}[(x_e,t_0) \to (x',t')]\ \text{prob}[(x',t') \to (x_d,t)]\ d^3x' \tag{17.10}$$

Conditionals multiply and alternatives, which are here a continuum of positions x', add, i.e., here the alternatives are to be integrated.

17.2 The rules of probability amplitudes

Let us now consider the situation where there is no He gas and also no other particles, such as photons, that could interact with the Ne atom. The Ne atom therefore propagates freely in the box and its path is not observed in any way.

Now in quantum mechanics we have:

$$\text{prob}[(x_e,t_0) \to (x_d,t)] = |G(x_d,x_e,t,t_0)|^2 = |\langle x_d|\hat{U}(t,t_0)|x_e\rangle|^2 \tag{17.11}$$

To see this, let us remember that the observable that tests if a particle such as a Ne atom is at position[3] x_d is:

$$\hat{Q} = |x_d\rangle\langle x_d| \tag{17.12}$$

The measurement apparatus of $\hat{Q}$ returns a 1 if the Ne is detected and it returns a 0 if it is not detected. Therefore, in an ensemble of experiments:

$$\bar{Q}(t) = \text{prob}[\text{particle is at } x_d \text{ at } t] \tag{17.13}$$

Therefore,

$$\begin{aligned}
\bar{Q}(t) &= \text{prob}[(x_e,t_0) \to (x_d,t)] && (17.14)\\
&= \langle x_e|\hat{U}^\dagger(t,t_0)\hat{Q}\hat{U}(t,t_0)|x_e\rangle && (17.15)\\
&= \langle x_e|\hat{U}^\dagger(t,t_0)|x_d\rangle\langle x_d|\hat{U}(t,t_0)|x_e\rangle && (17.16)\\
&= |\langle x_d|\hat{U}(t,t_0)|x_e\rangle|^2 && (17.17)\\
&= |G(x_d,x_e,t,t_0)|^2 && (17.18)
\end{aligned}$$

which proves Eq.17.11. This means that the Greens function is the so-called probability amplitude for the Ne atom to propagate from (x_e, t_0) to (x_d, t):

$$\text{probamp}[(x_e,t_0) \to (x_d,t)] = G(x_d,x_e,t,t_0) = \langle x_d|\hat{U}(t,t_0)|x_e\rangle \tag{17.19}$$

As always for probability amplitudes, its squared modulus is the probability.

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[3] We should use $\hat{Q} = \int_V |x\rangle\langle x|\ d^3x$ where V is a small volume around x_d but we omit this subtlety for notational simplicity.

Now let us again consider an intermediary time, t', i.e., $t_0 < t' < t$. For the time evolution operator, we always have:

$$\hat{U}(t, t_0) = \hat{U}(t, t')\hat{U}(t', t_0) \tag{17.20}$$

For example, for constant H:

$$e^{\frac{1}{i\hbar}(t-t_0)\hat{H}} = e^{\frac{1}{i\hbar}(t-t')\hat{H}} e^{\frac{1}{i\hbar}(t'-t_0)\hat{H}} \tag{17.21}$$

Therefore, inserting a resolution of the identity, the probability amplitudes obey

$$\begin{aligned} \langle x_d|\hat{U}(t,t_0)|x_e\rangle &= \langle x_d|\hat{U}(t,t')\hat{U}(t',t_0)|x_e\rangle && (17.22)\\ &= \int_{box} \langle x_d|\hat{U}(t,t')|x'\rangle\langle x'|\hat{U}(t',t_0)|x_e\rangle \; d^3x' && (17.23)\end{aligned}$$

which means:

$$\text{probamp}[(x_e, t_0) \to (x_d, t)] = \tag{17.24}$$

$$\int_{box} \text{probamp}[(x_e, t_0) \to (x', t')] \; \text{probamp}[(x', t') \to (x_d, t)] \; d^3x' \tag{17.25}$$

Comparing this equation with Eq.17.10, we now see that they are structurally the same equation. We conclude, therefore, that during undisturbed and therefore unobserved evolution, the probability amplitudes obey the rules that probabilities obey in the observed case: For unobserved alternatives, the probability amplitudes add. For unobserved conditionals, the probability amplitudes multiply.

Crucially, this implies that unobserved dynamics does not obey the rules of probabilities. In general, if Eq.17.25 holds then Eq.17.10 does not hold. Mathematically, this is because probability amplitudes are complex numbers and it matters, therefore, whether we first add them and then take the modulus squared (to obtain the probability), or whether we first take the moduli squared and then add them. In general: $|c_1 + c_2|^2 \neq |c_1|^2 + |c_2|^2$.

17.3 The path integral

In Eq.17.23, we can introduce an arbitrary number, N, of intermediate times

$$t_0 < t_1 < t_2 < ... < t_N < t \tag{17.26}$$

by further factoring the time evolution operator and using for each a resolution of the identity. We obtain:

$$\begin{aligned} \text{probamp}[(x_e, t_0) \to (x_d, t)] = \int_{box} \cdots \int_{box} & \text{probamp}[(x_e, t_0) \to (x_1, t_1)] && (17.27)\\ & \cdot \text{probamp}[(x_1, t_1) \to (x_2, t_2)] \\ & ... \\ & \cdot \text{probamp}[(x_N, t_N) \to (x_d, t)] \; d^3x_1 ... d^3x_N \end{aligned}$$

Here, the product rule for conditional probability amplitudes means that each of the terms in the integrand is a probability amplitude for the path that the Ne atom goes through specified points along the way from (x_e, t_0) to (x_d, t):

$$\text{probamp}[(x_e, t_0) \to (x_1, t_1) \to ...(x_N, t_N) \to (x_d, t)] =$$

$$\text{probamp}[(x_e, t_0) \to (x_1, t_1)]\text{probamp}[(x_1, t_1) \to (x_2, t_2)] \cdots \text{probamp}[(x_N, t_N) \to (x_d, t)]$$

We obtain:

$$G(x_d, x_e, t, t_0) = \text{probamp}[(x_e, t_0) \to (x_d, t)] \tag{17.28}$$

$$= \int_{box} \cdots \int_{box} \text{probamp}[(x_e, t_0) \to (x_1, t_1) \to ...(x_N, t_N) \to (x_d, t)]\ d^3x_1...d^3x_N$$

We now let $N \to \infty$ so that the time interval $[t_0, t]$ is subdivided into infinitesimally small intervals. We can then write the Green's function as a sum over all paths, a so-called path integral:

$$G(x_d, x_e, t, t_0) = \int_{allpaths} \text{probamp}[path]\ D[x(t)] \tag{17.29}$$

The key insight of Feynman was that for any given path $x(t)$ that a particle may take from (x_e, t_0) to (x_d, t) there exists an efficient way to calculate the probability amplitude of that path. In fact, as Feynman showed, this probability amplitude can be calculated without any tools from quantum mechanics. For this reason, Feynman's path integral, along with his prescription for calculating the probability amplitudes of paths can be viewed to be a new complete formulation of quantum mechanics.

17.4 How the path integral avoids noncommutative operators

Before we go into the derivation, here is already the gist of why Feynman's method succeeds. First, the technical difficulties of quantum mechanical calculations mostly stem from the noncommutativity of the operators, such as the $\hat{x}$ and $\hat{p}$ operators and the Hamiltonian. If they were commutative, we would have, for example, for the time evolution operator:

$$\hat{U}(t, t_0) = e^{\frac{(t-t_0)}{i\hbar}\left(\frac{\hat{p}^2}{2m} + V(\hat{x})\right)} \tag{17.30}$$

$$= e^{\frac{(t-t_0)}{i\hbar}\frac{\hat{p}^2}{2m}}\ e^{\frac{(t-t_0)}{i\hbar}V(\hat{x})} \tag{17.31}$$

We could then easily calculate the Green's function:

$$G(x_d, x_e, t, t_0) = \langle x_d | e^{\frac{(t-t_0)}{i\hbar}\left(\frac{\hat{p}^2}{2m} + V(\hat{x})\right)} | x_e \rangle \tag{17.32}$$

$$= \langle x_d| e^{\frac{(t-t_0)}{i\hbar}\frac{\hat{p}^2}{2m}}\ e^{\frac{(t-t_0)}{i\hbar}V(\hat{x})}|x_e\rangle \tag{17.33}$$

$$= \langle x_d| e^{\frac{(t-t_0)}{i\hbar}\frac{\hat{p}^2}{2m}}\ e^{\frac{(t-t_0)}{i\hbar}V(x_e)}|x_e\rangle \tag{17.34}$$

$$= \langle x_d| e^{\frac{(t-t_0)}{i\hbar}\frac{\hat{p}^2}{2m}}|x_e\rangle\ e^{\frac{(t-t_0)}{i\hbar}V(x_e)} \tag{17.35}$$

$$= \int \langle x_d|p\rangle\langle p| e^{\frac{(t-t_0)}{i\hbar}\frac{\hat{p}^2}{2m}}|x_e\rangle\ e^{\frac{(t-t_0)}{i\hbar}V(x_e)}\ d^3p \tag{17.36}$$

$$= \int \langle x_d|p\rangle\langle p| e^{\frac{(t-t_0)}{i\hbar}\frac{p^2}{2m}}|x_e\rangle\ e^{\frac{(t-t_0)}{i\hbar}V(x_e)}\ d^3p \tag{17.37}$$

$$= \int \langle x_d|p\rangle\langle p|x_e\rangle\ e^{\frac{(t-t_0)}{i\hbar}\frac{p^2}{2m}}\ e^{\frac{(t-t_0)}{i\hbar}V(x_e)}\ d^3p \tag{17.38}$$

$$= \int \frac{e^{ip(x_d-x_e)}}{(2\pi\hbar)^3}\ e^{\frac{(t-t_0)}{i\hbar}\frac{p^2}{2m}}\ e^{\frac{(t-t_0)}{i\hbar}V(x_e)}\ d^3p \tag{17.39}$$

The problem of obtaining a Green's function would be reduced to just a Fourier transform. But of course, the steps from Eq.17.30 to Eq.17.31 and correspondingly from Eq.17.32 to Eq.17.33 are incorrect because the operators $\hat{x}$ and $\hat{p}$ do not commute. Here is, however, where the path integral comes in: In the path integral we break the time evolution into many successive tiny time intervals. Crucially, as a time interval Δt tends to zero, we do have, with better and better accuracy:

$$\hat{U}(t,t_0) = e^{\frac{\Delta t}{i\hbar}\left(\frac{\hat{p}^2}{2m}+V(\hat{x})\right)} \tag{17.40}$$

$$\approx e^{\frac{\Delta t}{i\hbar}\frac{\hat{p}^2}{2m}}\ e^{\frac{\Delta t}{i\hbar}V(\hat{x})} \tag{17.41}$$

This is expressed in the Trotter product formula.

17.5 A useful tool: Trotterization

In order to calculate the probability amplitude for a path, we will use a useful mathematical tool, the Trotter product formula.

To this end, let us assume that $\hat{A}$ and $\hat{B}$ are self-adjoint operators that do not commute: $[\hat{A},\hat{B}]\neq 0$. Then we have that

$$e^{i(\hat{A}+\hat{B})} \neq e^{i\hat{A}}e^{i\hat{B}} \tag{17.42}$$

However, since $\hat{C} := \hat{A}+\hat{B}$ commutes with itself, we have

$$e^{i(\hat{A}+\hat{B})} = e^{\frac{i}{2}(\hat{A}+\hat{B})}e^{\frac{i}{2}(\hat{A}+\hat{B})} \tag{17.43}$$

and more generally:

$$e^{i(\hat{A}+\hat{B})} = \left(e^{\frac{i}{N}(\hat{A}+\hat{B})}\right)^N \tag{17.44}$$

Expanding the exponential, we have:

$$e^{\frac{i}{N}(\hat{A}+\hat{B})} = 1 + \frac{i}{N}(\hat{A}+\hat{B}) + O(1/N^2) \tag{17.45}$$

Silimarly:

$$e^{\frac{i}{N}\hat{A}} = 1 + \frac{i}{N}\hat{A} + O(1/N^2) \tag{17.46}$$

and

$$e^{\frac{i}{N}\hat{B}} = 1 + \frac{i}{N}\hat{B} + O(1/N^2) \tag{17.47}$$

and, therefore:

$$\begin{aligned} e^{\frac{i}{N}\hat{A}}e^{\frac{i}{N}\hat{B}} &= (1 + \frac{i}{N}\hat{A} + O(1/N^2))(1 + \frac{i}{N}\hat{B} + O(1/N^2)) \qquad (17.48) \\ &= 1 + \frac{i}{N}(\hat{A}+\hat{B}) + O(1/N^2) \qquad (17.49) \end{aligned}$$

For large N, Eq.17.49 with Eq.17.45 shows that $e^{\frac{i}{N}(\hat{A}+\hat{B})}$ and $e^{\frac{i}{N}\hat{A}}e^{\frac{i}{N}\hat{B}}$ agree to first order in $1/N$:

$$e^{\frac{i}{N}(\hat{A}+\hat{B})} = e^{\frac{i}{N}\hat{A}}e^{\frac{i}{N}\hat{B}} + O(1/N^2) \tag{17.50}$$

Finally, in Eq.17.44, in the limit $N \to \infty$, the term that is first order in $1/N$ dominates and one obtains the Trotter product formula:

$$e^{i(\hat{A}+\hat{B})} = \lim_{N\to\infty}\left(e^{\frac{i}{N}\hat{A}}e^{\frac{i}{N}\hat{B}}\right)^N \tag{17.51}$$

17.6 The probability amplitudes for paths

We can now apply the Trotter product expansion to the time evolution operator:

$$\hat{U}(t,t_e) = e^{\frac{t-t_0}{i\hbar}\left(\frac{\hat{p}^2}{2m}+V(\hat{x})\right)} \tag{17.52}$$

Here,

$$i\hat{A} = \frac{t-t_0}{i\hbar}\frac{\hat{p}^2}{2m}, \qquad i\hat{B} = \frac{t-t_0}{i\hbar}V(\hat{x}) \tag{17.53}$$

so that the Trotter formula yields:

$$\begin{aligned} \hat{U}(t,t_e) &= \lim_{N\to\infty}\left(e^{\frac{t-t_0}{N}\frac{1}{i\hbar}\frac{\hat{p}^2}{2m}}\; e^{\frac{t-t_0}{N}\frac{1}{i\hbar}V(\hat{x})}\right)^N \qquad (17.54) \\ &= \lim_{N\to\infty}\left(e^{\frac{\Delta t}{i\hbar}\frac{\hat{p}^2}{2m}}\; e^{\frac{\Delta t}{i\hbar}V(\hat{x})}\right)^N \qquad (17.55) \end{aligned}$$

We therefore obtain for the Green's function:

$$\begin{aligned}
&G(x_d,x_e,t,t_0) = \langle x_d|\hat{U}(t,t_0)|x_e\rangle \qquad (17.56)\\
&= \lim_{N\to\infty} \langle x_d| \left(e^{\frac{\Delta t}{i\hbar}\frac{\hat{p}^2}{2m}}\ e^{\frac{\Delta t}{i\hbar}V(\hat{x})}\right)^{N+1} |x_e\rangle \qquad \text{with} \qquad \Delta t = (t-t_0)/(N+1)\\
&= \lim_{N\to\infty} \langle x_d| e^{\frac{\Delta t}{i\hbar}\frac{\hat{p}^2}{2m}}\ e^{\frac{\Delta t}{i\hbar}V(\hat{x})} \cdot \ldots \cdot e^{\frac{\Delta t}{i\hbar}\frac{\hat{p}^2}{2m}}\ e^{\frac{\Delta t}{i\hbar}V(\hat{x})}|x_e\rangle\\
&= \lim_{N\to\infty} \int \ldots \int \langle x_d| e^{\frac{\Delta t}{i\hbar}\frac{\hat{p}^2}{2m}}\ e^{\frac{\Delta t}{i\hbar}V(\hat{x})}|x_N\rangle\langle x_N|\ldots|x_1\rangle\langle x_1|e^{\frac{\Delta t}{i\hbar}\frac{\hat{p}^2}{2m}}\ e^{\frac{\Delta t}{i\hbar}V(\hat{x})}|x_e\rangle d^3x_N..d^3x_1\\
&= \lim_{N\to\infty} \int \ldots \int \langle x_d| e^{\frac{\Delta t}{i\hbar}\frac{\hat{p}^2}{2m}}\ e^{\frac{\Delta t}{i\hbar}V(x_N)}|x_N\rangle\langle x_N|\ldots|x_1\rangle\langle x_1|e^{\frac{\Delta t}{i\hbar}\frac{\hat{p}^2}{2m}}\ e^{\frac{\Delta t}{i\hbar}V(x_e)}|x_e\rangle d^3x_N..d^3x_1\\
&= \lim_{N\to\infty} \int \ldots \int \langle x_d| e^{\frac{\Delta t}{i\hbar}\frac{\hat{p}^2}{2m}}|x_N\rangle\langle x_N|\ldots|x_1\rangle\langle x_1|e^{\frac{\Delta t}{i\hbar}\frac{\hat{p}^2}{2m}}|x_e\rangle e^{\sum_{j=0}^N \frac{\Delta t}{i\hbar}V(x_j)} d^3x_N..d^3x_1\\
&= \lim_{N\to\infty} \int \ldots \int \langle x_d| e^{\frac{\Delta t}{i\hbar}\frac{\hat{p}^2}{2m}}|p_N\rangle\langle p_N|x_N\rangle\ldots\langle x_1|p_1\rangle\langle p_1|e^{\frac{\Delta t}{i\hbar}\frac{\hat{p}^2}{2m}}|x_e\rangle e^{\sum_{j=0}^N \frac{\Delta t}{i\hbar}V(x_j)} d^3x_N..d^3x_1\\
&= \lim_{N\to\infty} \int \ldots \int \langle x_d| e^{\frac{\Delta t}{i\hbar}\frac{p_N^2}{2m}}|p_N\rangle\langle p_N|x_N\rangle\ldots\langle x_1|p_1\rangle\langle p_1|e^{\frac{\Delta t}{i\hbar}\frac{p_1^2}{2m}}|x_e\rangle e^{\sum_{j=0}^N \frac{\Delta t}{i\hbar}V(x_j)} d^3x_N d^3p_N..d^3x_1 d^3p_1\\
&= \lim_{N\to\infty} \int \ldots \int \langle x_d|p_N\rangle\langle p_N|x_N\rangle\ldots\langle x_1|p_1\rangle\langle p_1|x_e\rangle e^{\sum_{k=1}^N \frac{\Delta t}{i\hbar}\frac{p_k^2}{2m}} e^{\sum_{j=0}^N \frac{\Delta t}{i\hbar}V(x_j)} d^3x_N d^3p_N..d^3x_1 d^3p_1\\
&= \lim_{N\to\infty} \int \ldots \int \frac{e^{i\frac{(p_N(x_d-x_N)+\ldots+p_1(x_1-x_e))}{\hbar}}}{(2\pi\hbar)^{3N/2}} e^{\sum_{k=1}^N \frac{\Delta t}{i\hbar}\frac{p_k^2}{2m}} e^{\sum_{j=0}^N \frac{\Delta t}{i\hbar}V(x_j)} d^3x_N d^3p_N..d^3x_1 d^3p_1\\
&= \lim_{N\to\infty} \int \ldots \int \frac{1}{(2\pi\hbar)^{3N/2}} e^{\sum_{k=1}^N \left(i\frac{p_k(x_k-x_{k-1})}{\hbar}+\frac{\Delta t}{i\hbar}\frac{p_k^2}{2m}\right)} e^{\sum_{j=0}^N \frac{\Delta t}{i\hbar}V(x_j)} d^3x_N d^3p_N..d^3x_1 d^3p_1
\end{aligned} \qquad (17.57)$$

We now use a completion of the squares:

$$\int_{-\infty}^{\infty} e^{i(ap+bp^2)}dp = \int_{-\infty}^{\infty} e^{ib(p+\frac{a}{2b})^2-i\frac{a^2}{4b}}dp \qquad (17.58)$$

$$= e^{i\frac{a^2}{4b}}\int_{-\infty}^{\infty} e^{ib\tilde{p}^2}d\tilde{p} \quad \text{with} \quad \tilde{p} := p + a/2b \qquad (17.59)$$

$$= \mu\ e^{-i\frac{a^2}{4b}} \qquad (17.60)$$

Here, $\mu = \int_{-\infty}^{\infty} e^{ib\tilde{p}^2}d\tilde{p}$ is divergent but takes the finite value $\sqrt{\pi/\mathrm{Im}(b)}$ if we temporarily give b an arbitrarily small positive imaginary part to ensure convergence. To carry out each of the momentum integrals above, we define:

$$a := \frac{x_j - x_{j-1}}{\hbar}, \qquad b := -\frac{\Delta t}{2m\hbar}, \quad \text{i.e.,} \quad \frac{a^2}{4b} = -\frac{(x_j-x_{j-1})^2 m}{2\hbar\Delta t} \qquad (17.61)$$

Notice that since b does not depend on the x_i, neither does μ. Therefore, all factors of μ can be pulled in front of the path integral. We obtain for the path integral:

$$G(x_d,x_e,t,t_0) \qquad (17.62)$$

$$= \lim_{N\to\infty} \int ... \int \frac{1}{(2\pi\hbar)^{3N/2}} e^{\sum_{k=1}^{N}\left(i\frac{p_k(x_k - x_{k-1})}{\hbar} + \frac{\Delta t}{i\hbar}\frac{p_k^2}{2m}\right)} e^{\sum_{j=0}^{N}\frac{\Delta t}{i\hbar}V(x_j)} d^3x_N d^3p_N..d^3x_1 d^3p_1$$

$$= \lim_{N\to\infty}\left(\frac{\mu}{2\pi\hbar}\right)^N \int ... \int e^{\frac{i}{\hbar}\sum_{j=1}^{N}\left(\frac{m}{2}\left(\frac{x_j - x_{j-1}}{\Delta t}\right)^2 - V(x_j)\right)\Delta t} d^3x_1...d^3x_N \tag{17.63}$$

$$= \nu \int_{\text{all paths}} e^{\frac{i}{\hbar}S[x(t)]} D[x(t)] \tag{17.64}$$

Here, ν is a normalization constant and we defined the so-called action, S, of a path through the Lagrangian

$$S[x(t)] := \int_{t_0}^{t} L(x(t))\ dt \tag{17.65}$$

with the Lagrangian being defined through:

$$L(x(t)) := \frac{1}{2}m\left(\frac{dx}{dt}\right)^2 - V(x(t)) \tag{17.66}$$

In conclusion, the Green's function can, therefore, be calculated, in principle, through the path integral,

$$G(x_d, x_e, t, t_0) = \nu \int_{\text{all paths}} e^{\frac{i}{\hbar}S[x(t)]} D[x(t)] \tag{17.67}$$

with the probability amplitude for a particle, such as our Ne atom, to travel on a path $x(t)$ given by

$$\text{probamp[path } x(t)] = e^{\frac{i}{\hbar}S[x(t)]} \tag{17.68}$$

Remark: In the path integral, we are to integrate over "all" paths from (x_e, t_0) to (x_d, t). It is a major problem to make this set of paths well-defined as the derivation did not involve any smoothness condition. Fortunately, it is usually not necessary to calculate a path integral by going to back to its definition. The situation is similar to that of ordinary integrals. We rarely need to integrate a function by taking the Riemann sum limit. Instead, we use manipulation rules for integrals such as integration by part of the substitution rule. The path integral is a powerful method in quantum theory because, similarly, rules of integration by part and substitution can successfully be applied to the path integral.

17.7 Relationship to classical mechanics

At the beginning of this course, we discussed that classical mechanics needed to be formulated on a higher level of abstraction, namely on the level of Hamiltonians, in order to be able to see how it relates to quantum mechanics.

Feynman's formulation of quantum mechanics offers a new perspective on how classical and quantum mechanics are related. Feynman's path integral relates closely to the so-called Lagrangian formulation of classical mechanics. The Lagrangian formulation of classical mechanics is on the same level as the Hamiltonian formulation since both provide a means to derive the equations of motion.

Let us briefly recall the Lagrangian formulation of the classical mechanics of a point particle. Here, every path that the particle may take is assigned its action $S[x(t)]$, as in Eqs.17.65,17.66. The paths that particles do take, according to classical mechanics, are those for which the action does not change to first order in changing the path.

$$\frac{\delta S}{\delta x(t)} = 0, \quad \text{i.e.,} \quad \frac{\partial L}{\partial x(t)} - \frac{d}{dt}\frac{\partial L}{\partial \dot{x}(t)} = 0 \tag{17.69}$$

Since the derivative vanishes we have a critical point and we may call this the principle of critical action. It is often called the principle of least action but this name is misleading. For example, the relativistic motion of a point particle in curved spacetime follows a principle of maximum action in the sense of maximum proper time along the path. The action need not be minimal or maximal but only needs to be critical. To see this, let us reconsider the path integral:

$$G(x_d, x_e, t, t_0) = \nu \int_{\text{all paths}} e^{\frac{i}{\hbar}S[x(t)]} D[x(t)] \tag{17.70}$$

Its integrand consists of only phase functions and they tend to be highly oscillatory. On can show that for oscillatory integrals such as these, the main contribution to the path integral comes from integrands (i.e., here from paths) in which the phases are stationary, i.e., for which Eq.17.69 holds, i.e., which are close to the trajectories that classical mechanics predicts. Quantum mechanical phenomena are due to higher order contributions to the path integral, i.e., contributions that arise from paths, so-called quantum fluctuations, that are some distance away from the classical trajectory. Feynman's path integral shows that what matters to obtain classical mechanics is only that the action is stationary or 'critical', i.e., that the action does not change to first order in changes of the path.

Feynman's approach to quantum theory also works for the quantum theory of fields, where it is usually preferred over the operator approach because it is manifestly covariant and because Feynman's framework is more suitable for perturbative calculations by naturally leading to the formalism of Feynman graphs.

Chapter 18

The gauge principle

18.1 A level of abstraction above Hamiltonians and Lagrangians

The gauge principle is one level of abstraction higher than the level of Hamiltonians and Lagrangians. This is because it allows us to derive improved Hamiltonians of Lagrangians. Namely, given the Hamiltonian of a simple system, such as that of a free electron, the gauge principle allows us to derive a new Hamiltonian which describes the electron interacting with a force field.

The electromagnetic force was already known long before the discovery of the gauge principle around the 1940s. However, once it was understood that electromagnetism could be obtained from the gauge principle, the gauge principle was then very useful for the development of the Hamiltonians of other force fields, namely those of the so-called weak interaction, which explains, for example, radioactive decay, and the so-called strong interaction which describes, for example, what holds protons and neutrons together. Even gravity can be described as a gauge theory.

18.2 The simplest example of the gauge principle

We will now start with a free electron and then use the gauge principle to arrive at the conclusion that it would be natural for there to exist magnetic fields in nature. In particular, the gauge principle also shows us exactly how the Hamiltonian that includes the magnetic field should look.

The gauge principle begins with the observation that all expectation values and, therefore, all predictions of quantum mechanics stay the same when the vector that describes the state of a system is multiplied with phase:

$$|\psi\rangle \to e^{i\alpha}|\psi\rangle \tag{18.1}$$

In the position representation, this is the statement that all predictions stay the same under

$$\psi(x) \to e^{i\alpha}\psi(x) \tag{18.2}$$

Abstractly, this is because:

$$\langle\psi|\hat{f}(\hat{x},\hat{p})|\psi\rangle = \langle\psi|e^{-i\alpha}\hat{f}(\hat{x},\hat{p})e^{i\alpha}|\psi\rangle \tag{18.3}$$

In the position representation this reads:

$$\int_{\mathbb{R}} \psi(x)^*\hat{f}(\hat{x}.,\hat{p}.)\psi(x)\ d^3x = \int_{\mathbb{R}} \psi(x)^* e^{-i\alpha}\hat{f}(\hat{x}.,\hat{p}.)e^{i\alpha}\psi(x)\ d^3x \tag{18.4}$$

To keep the notation uncluttered, we here did not write indices on the position and momentum operators, but we allow all three position and all three momentum operators to occur. Hence, we integrate over all three spatial directions.

The above transformations are called gauge transformations that are global because α has the same value everywhere, i.e., globally. What, however, if we try so-called local gauge transformations, i.e., if we allow the gauge function $\alpha(x)$ to be position dependent? In this case, the predictions do generally change because we have:

$$\int_{\mathbb{R}} \psi(x)^*\hat{f}(\hat{x}.,\hat{p}.)\psi(x)\ d^3x \neq \int_{\mathbb{R}} \psi(x)^* e^{-i\alpha(x)}\hat{f}(\hat{x}.,\hat{p}.)e^{i\alpha(x)}\psi(x)\ d^3x \tag{18.5}$$

For example, if we choose $\hat{f} = \hat{p}_j$ and recalling that $\hat{p}_j.\psi(x) = -i\hbar\frac{d}{dx_j}\psi(x)$, we find:

$$\begin{aligned}
\int_{\mathbb{R}} \psi(x)^*\left(-i\hbar\frac{d}{dx_j}\right)\psi(x)\ d^3x \ \ &\neq \ \ \int_{\mathbb{R}} \psi(x)^* e^{-i\alpha(x)}\left(-i\hbar\frac{d}{dx_j}\right)e^{i\alpha(x)}\psi(x)\ d^3x \\
&= \int_{\mathbb{R}} \psi(x)^*\cancel{e^{-i\alpha(x)}}\,\cancel{e^{i\alpha(x)}}\left(-i\hbar\frac{d}{dx_j}\psi(x)\right)\ d^3x \\
&\quad + \int_{\mathbb{R}} \psi(x)^* e^{-i\alpha(x)}\left(-i\hbar\frac{d}{dx_j}e^{i\alpha(x)}\right)\psi(x)\ d^3x
\end{aligned}$$

We see that the problem is that the momentum operators $\hat{p}_j.$ can no longer be commuted past $e^{i\alpha(x)}$ if α depends on the position x. Instead, the product rule of the derivatives in the operators $\hat{p}_j.$ causes extra terms to arise which contain derivatives of $\alpha(x)$. The gauge principle is a method to fix this so that also under gauge transformations that are local all predictions stay the same.

To this end, the strategy is to define afresh what we mean by momentum operators and what we mean by a local gauge transformation. First, we define new canonical momentum operators, $\hat{\mathbf{p}}_{\mathbf{i}}$ for $i = 1, 2, 3$, that act on position wave functions as follows:

$$\hat{\mathbf{p}}_{\mathbf{i}}.\psi(x) := \left(-i\hbar\ \frac{d}{dx_i} + A_i(x)\right)\psi(x) \tag{18.6}$$

Here, we introduced a new vector-valued function $A(x)$. For now, the sole role of $A(x)$ will be to absorb these extra terms that arise from the product rule. We now define what we mean by a local gauge transformation. First, it transforms the wave function via:

$$\psi(x) \to \tilde{\psi}(x) := e^{i\alpha(x)}\psi(x) \tag{18.7}$$

Secondly, the gauge transformation is defined to transform also the new function $A_i(\hat{x})$, namely via:

$$A_i(x) \to \tilde{A}_i(x) := A_i(x) - \hbar\frac{\partial\alpha(x)}{\partial x^i} \tag{18.8}$$

This then means that a gauge transformation also affects the new momentum operators, because they contain $A_i(x)$:

$$\hat{\mathbf{p}}_\mathbf{i} \to \tilde{\hat{\mathbf{p}}}_\mathbf{i} := \hat{\mathbf{p}}_\mathbf{i} - \hbar\frac{\partial\alpha(x)}{\partial x^i} \tag{18.9}$$

Now, with this definition of the canonical momenta and this definition of what a gauge transformation of the $\psi(x)$ and the $A(x)$ is, every prediction $\int \psi(x)^* \hat{f}(\hat{x}., \hat{\mathbf{p}}.)\psi(x)\ d^3x$ yields the same value before and after a local gauge transformation as defined by Eqs.18.7-18.9. Here, $\hat{f}(\hat{x}., \hat{\mathbf{p}}.)$ is allowed to contain all three position and all three momentum operators (which of course transform under a local gauge transformation).

To see this, let us work out the special case of the prediction of a momentum expectation value, i.e., the special case where the observable is $\hat{f} = \hat{\mathbf{p}}_i$. The general case for arbitrary observables $\hat{f}$ follows easily. First, we assume given a position wave function $\psi(x)$ and a field $A(x)$. Then, the expectation value of the observable $\bar{f} = \bar{\mathbf{p}}_i$ is:

$$\begin{aligned} \bar{\mathbf{p}}_i &= \int \psi(x)^* \hat{\mathbf{p}}_i \psi(x)\ d^3x & (18.10)\\ &= \int \psi(x)^* \left(-i\hbar\frac{\partial}{\partial x_i} + A_i(x)\right)\psi(x)\ d^3x & (18.11)\\ &= \int \psi(x)^* \left(-i\hbar\frac{\partial}{\partial x_i}\psi(x)\right) + \psi(x)^* A_i(x)\psi(x)\ d^3x & (18.12)\end{aligned}$$

Now, let us assume we have chosen an arbitrary $\alpha(x)$ and perform the corresponding gauge transformations Eqs.18.7,18.8. We obtain that the momentum expectation value is unchanged, i.e., that $\tilde{\bar{\mathbf{p}}}_i = \bar{\mathbf{p}}_i$:

$$\begin{aligned} \tilde{\bar{\mathbf{p}}}_i &= \int \tilde{\psi}(x)^* \tilde{\hat{\mathbf{p}}}_i \tilde{\psi}(x)\ d^3x & (18.13)\\ &= \int \tilde{\psi}(x)^* \left(-i\hbar\frac{\partial}{\partial x_i} + \tilde{A}_i(x)\right)\tilde{\psi}(x)\ d^3x & (18.14)\\ &= \int \psi(x)^* e^{-i\alpha(x)} \left(-i\hbar\frac{\partial}{\partial x_i} + A_i(x) - \hbar\frac{\partial\alpha(x)}{\partial x_j}\right) e^{i\alpha(x)}\psi(x)\ d^3x & \end{aligned}$$

$$= \int \psi(x)^* \left(-i\hbar\frac{\partial}{\partial x_i}\psi(x)\right) + \psi(x)^* A_i(x)\psi(x)\ d^3x \tag{18.15}$$

$$= \bar{\mathbf{p}}_i \tag{18.16}$$

This shows that under a local gauge transformation in this sense, all expectation values and therefore all predictions stay the same. To achieve this, we had to switch to a new so-called canonical momentum operator that required the introduction of a new function $A_i(x)$. We can make $A_i(x)$ take many different values by simply gauging it along with $\psi(x)$. Since the values of $A_i(x)$ are, therefore gauge dependent, $A_i(x)$ cannot be observable. However, it turns out that there is a part of $A_i(x)$ which does not change under gauge transformations and that part is observable.

18.3 The gauge principle predicts new fields and their Hamiltonian

To see which part of $A_i(x)$ is gauge invariant, let us remember that curl of a gradient field vanishes: A gradient field is a vector field for which there exists a scalar field Λ such that:

$$V(x) = \nabla\Lambda(x) = \left(\frac{\partial\Lambda(x)}{\partial x_1}, \frac{\partial\Lambda(x)}{\partial x_2}, \frac{\partial\Lambda(x)}{\partial x_3}\right) \tag{18.17}$$

The curl of a vector field W (in three dimensions) is the vector field:

$$\begin{aligned} C(x) &= \nabla \times W(x) \qquad (18.18) \\ &= \left(\frac{\partial W_2(x)}{\partial x_3} - \frac{\partial W_3(x)}{\partial x_2}, \frac{\partial W_3(x)}{\partial x_1} - \frac{\partial W_1(x)}{\partial x_3}, \frac{\partial W_1(x)}{\partial x_2} - \frac{\partial W_2(x)}{\partial x_1}\right) \end{aligned}$$

From this, given that

$$\frac{\partial}{\partial x_i}\frac{\partial}{\partial x_j} = \frac{\partial}{\partial x_j}\frac{\partial}{\partial x_i} \tag{18.19}$$

it is straightforward to check that for any gradient field $V(x)$, its curl vanishes:

$$\nabla \times V(x) = \nabla \times \nabla\Lambda(x) = 0 \tag{18.20}$$

Coming back to the topic of gauge transformations, Eq.18.8 shows that a gauge transformation affects the field $A(x)$ by adding to it a gradient field:

$$A(x) \to \tilde{A}(x) := A(x) - \hbar\nabla\alpha(x) \tag{18.21}$$

We can now conclude that the curl of the field $A(x)$,

$$B(x) := \nabla A(x) \tag{18.22}$$

is unaffected by the gauge transformations. $B(x)$ is indeed an observable physical field, namely the magnetic field. One can derive also the electric field from the gauge principle, namely by requiring local gauge invariance for gauge functions $\alpha(x,t)$ that depend arbitrarily not only on space but also on time.

So why then is the gauge principle on a level of abstraction that is one level higher than the level of Hamiltonians? In which sense does the gauge principle allow us to *derive* fundamental Hamiltonians?

To see how, let us reconsider the case of the Hamiltonian of just a free particle, $\hat{H} = \sum_{i=1}^{3} \hat{p}_i^2/2m$. Then, imposing the gauge principle led us to introduce the new $A_i(x)$ field and the Hamiltonian then becomes $\hat{H} = \sum_{i=1}^{3} \hat{\mathbf{p}}_{\mathbf{i}}^2/2m$. Now the particle's Hamiltonian describes not just the free evolution anymore but also the particle's interaction with the new field $A_i(x)$, or actually with it observable part, the magnetic field $B(x)$.

Further we are then led to ask what the free Hamiltonian H_A for the field $\vec{A}(x)$ should be. That Hamiltonian has to a scalar and gauge invariant. The simplest possibility[1] that fits both requirements is $H_A = \nu B(x) \cdot B(x)$. The constant ν is to be determined by comparing predictions to experiments.

What is important here is that the gauge principle predicted that there should be a new field, $A(x)$, that only its curl $B(x)$ can be observable, and it predicted the form of the Hamiltonian of the new field. Does the gauge principle also predict an interaction Hamiltonian that describes how the electron interacts with the new field? Yes, remember that we such a term already: The term $\hat{\mathbf{p}}^2/2m$ now includes the A field through Eq.18.6, thereby coupling the electron to the electromagnetic field.

The significance of the gauge principle is that it can be further generalized covariantly to wave functions and fields that are not number but vector-valued. These are so-called isospinor fields $\psi_i(x,t)$ with n components, i.e., $i = 1, 2, ...n$. For $n = 2$ and $n = 3$ respectively one use the gauge principle to predict fields that turn out to carry the electroweak and the strong force, and whose quanta are the the W and Z bosons and of the gluons respectively. After quantizing these new fields one arrives at what is called the current standard model of particle physics. Even Einstein gravity is somewhat similarly derivable from a local gauge principle. In the case of gravity, the local gauge transformations are local Lorentz transformations or in some formulations even local Poincaré transformations. It has not been possible so far to conclusively quantize gravity, however. Given that gravity is not just any force but is a property of spacetime itself, it is being speculated that what is really required is not merely a quantization of gravity. It could be that quantum theory itself needs to be adapted to general relativity. For the future, a key challenge will be to determine the role that the gauge principle plays in the fundamental theory of gravity that is still to be developed. Is there a way to see how the gauge principle arises from a more fundamental principle, i.e., how can we take another step up in the hierarchy of levels of abstraction?

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[1] If we also included the time-dependent gauge principle we would also obtain the electric field with its Hamiltonian, E^2.