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:

Hamiltonian

$\Downarrow$

Equations of motion

$\Downarrow$

Differential equations

$\Downarrow$

Non-number-valued functions

$\Downarrow$

Number-valued functions

$\Downarrow$
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:

$$i\hbar \frac{d}{dt}\ \hat{x}_i^{(r)}(t) \ = \ [\hat{x}_i^{(r)}(t), \hat{H}]$$

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

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 nonzero 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.