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. Remark: I recommend that you do not just copy and paste from some place like Wikipedia. Best 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:

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

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

$$\{\hat{x}_i, \hat{p}_j\} = \delta_{i,j} \tag{3.16}$$
$$\{\hat{x}_i, \hat{x}_j\} = 0 \tag{3.17}$$
$$\{\hat{p}_i, \hat{p}_j\} = 0 \tag{3.18}$$

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

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:

Hamiltonian

$\Downarrow$

Equations of motion

$\Downarrow$

Differential equations

$\Downarrow$

Non-number-valued functions

$\Downarrow$

Number-valued functions