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Chapter 3

Quantum dynamics

The picture of quantum mechanics that we have developed so far is purely kinematical: We know how to prepare quantum systems, know what quantum states and what observables are. We can keep track of the quantum state in a sequence of measurements of non-commuting observables. Still, an important ingredient is missing: Time evolution! We have tacitly assumed that all measurements are instantaneously performed, which may or may not be a valid approximation. In the first place, however, we would like to arrive at an understanding of how quantum theory captures time evolution and dynamics. This is what this chapter is dedicated to.

3.1 Basic quantum dynamics

3.1.1 Time evolution

The equation that governs time evolution is called the Schrödinger equation. It is actually quite simple: Once we are familiar with the Hamiltonian formalism of classical mechanics, we are almost there. We begin this chapter by stating the equation.

Schrödinger equation: State vectors of physical systems described by a Hamilton operator H evolve in time according to

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = H(t)|\psi(t)\rangle. \tag{3.1}$$

Here, we encounter for the first time the Hermitian Hamilton operator

$$H = H^\dagger, \tag{3.2}$$

taking essentially the same role as the Hamilton operator in classical mechanics. Frankly, it collects all there is to say about the nature of a physical system. It is clear from the above differential equation called Schroedinger equation that the norm of state vectors does not change in time,

$$\begin{aligned} i\hbar\frac{d}{dt}\langle\psi(t)|\psi(t)\rangle &= \left(i\hbar\frac{d}{dt}\langle\psi(t)\right)|\psi(t)\rangle + \langle\psi(t)|\left(i\hbar\frac{d}{dt}|\psi(t)\rangle\right) \\ &= -\langle\psi(t)|H(t)|\psi(t)\rangle + \langle\psi(t)|H(t)|\psi(t)\rangle = 0. \end{aligned} \tag{3.3}$$

Since the Schroedinger equation is also linear, its integration over the time interval $[t_0, t]$ must yield a unitary operator $U(t, t_0)$, such that

$$|\psi(t)\rangle = U(t, t_0)|\psi(t_0)\rangle. \tag{3.4}$$

Clearly, we have that

$$U(t_0, t_0) = \mathbb{1}. \tag{3.5}$$

Then, inserting Eq. (3.4) into the Schroedinger equation yields

$$i\hbar\frac{dU(t, t_0)}{dt}|\psi(t_0)\rangle = H(t)U(t, t_0)|\psi(t_0)\rangle. \tag{3.6}$$

Since this equation is true for all state vectors $|\psi(t_0)\rangle$, we find

$$i\hbar\frac{dU(t, t_0)}{dt} = H(t)U(t, t_0). \tag{3.7}$$

This differential equation, together with the initial condition Eq. (3.5) are equivalent to the integral equation

$$U(t, t_0) = \mathbb{1} - \frac{i}{\hbar}\int_{t_0}^{t} ds H(s)U(s, t_0). \tag{3.8}$$

One also finds a nice composition law (in fact, a group law):

$$U(t, t_0) = U(t, t_1)U(t_1, t_0), \tag{3.9}$$

for any $t \geq t_1 \geq t_0$. This is most intuitive: To evolve a state from t_0 to t is the same as first evolving it from t_0 to t_1 and then from t_1 to t. From this, we can also deduce

$$U(t_0, t)U(t, t_0) = \mathbb{1}, \tag{3.10}$$

for any two times t_0, t. Since $U(t_0, t)$ is unitary, we find the following:

Time evolution operator: Time evolution is governed by the time evolution operator satisfying

$$U(t, t_0) = U^{-1}(t_0, t) = U^{\dagger}(t_0, t), \tag{3.11}$$

$$U^{\dagger}(t, t_0)U(t, t_0) = \mathbb{1}, \tag{3.12}$$

$$U(t_0, t_0) = \mathbb{1}, \tag{3.13}$$

for any two times $t \geq t_0$.

In most important cases, the Hamilton operator does not explicitly depend on time, so

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = H|\psi(t)\rangle. \tag{3.14}$$

The time evolution operator then simply becomes

$$U(t,t_0) = e^{-i(t-t_0)H/\hbar}. \tag{3.15}$$

Here, we encounter the exponential of a matrix: This is to be read in the ordinary sense of a matrix function (so equivalently as the convergence exponential series or the exponential function applied to the eigenvalues of the matrix).

3.1.2 Schrödinger versus Heisenberg pictures

Since for an initial state vector $|\psi(t_0)\rangle$ we find the state vector at later times to be

$$|\psi(t)\rangle = U(t,t_0)|\psi(t_0)\rangle, \tag{3.16}$$

we can compute expectation values of observables A at time t as

$$\langle A\rangle(t) = \langle\psi(t)|A|\psi(t)\rangle = \left(\langle\psi(t_0)|U^\dagger(t,t_0)\right) A \left(U(t,t_0)|\psi(t_0)\rangle\right). \tag{3.17}$$

This "picture" is called Schroedinger picture, as we are deriving this from the Schroedinger equation. Of course, we are not forced to read the formula this way. Equivalently, we can think of this expression as

$$\langle A\rangle(t) = \langle\psi(t_0)|\Big(U^\dagger(t,t_0)AU(t,t_0)\Big)|\psi(t_0)\rangle. \tag{3.18}$$

This is the same expression, we have merely set different brackets. In this "picture", we view the observable as evolving in time, and the state vectors are being static. To make this manifest, we define

$$A(t) = U^\dagger(t,t_0)AU(t,t_0), \tag{3.19}$$

and interpret $A(t)$ as time-evolved observable. For historical reasons, this "picture" is called Heisenberg picture. This is not very deep, you might be tempted to say, it does not make any difference whatsoever whether we put the time evolution operator $U(t,t_0)$ to the state vector or to the observable! Yes, right. Still, it can be "psychologically inequivalent" to think of the two pictures as a slightly different description. Besides, there is an intermediate picture called interaction picture interpolating between the two pictures for interacting systems, which is very handy. Finally, in systems of quantum field theory that go beyond what we cover in this course, it can in many settings still make sense to think of a Heisenberg picture, while it is far from clear how to introduce a Schroedinger picture. So much for that.

3.1.3 Stationary states

This is a very important concept. Let us assume that $|\psi(t_0)\rangle$ is an eigenstate of H with eigenvalue E, so that

$$H|\psi(t_0)\rangle = E|\psi(t_0)\rangle. \tag{3.20}$$

Then time evolution is very simple to capture:

$$|\psi(t)\rangle = e^{-iE(t-t_0)/\hbar}|\psi(t_0)\rangle. \tag{3.21}$$

In other words, it is time independent, except from a global phase. Such state vectors are called *stationary*. In particular, if A is an observable,

$$\langle A\rangle(t) = \langle\psi(t)|A|\psi(t)\rangle = \langle\psi(0)|A|\psi(0)\rangle = \langle A\rangle(0), \tag{3.22}$$

so expectation values are left unchanged in time. We have assumed that the Hilbert space is finite-dimensional. If the Hilbert space is infinite-dimensional and H has spectral values which are not eigenvalues, then some mathematical subtleties arise, which we will postpone for a moment.

3.1.4 Wave mechanics

We now turn to how the Schroedinger equation acts in the position representation. In fact, this may be the even more famous formulation of the equation in the first place.

Schroedinger equation in the position representation:

$$i\hbar\frac{d}{dt}\psi(x,t) = H\psi(x,t). \tag{3.23}$$

What is H for a particle of mass m in one dimension moving in a potential $V:\mathbb{R}\to\mathbb{R}$?

$$H = -\frac{\hbar^2}{2m}\Delta + V(x,t). \tag{3.24}$$

This Hamiltonian, together with the above differential equation, gives rise to the familiar wave equation that governs the propagation of wave packets of particles in given potentials.

As a warm up, we show one property that we already anticipate: We look at a continuity equation. We consider again the particle density

$$\rho(x,t) = |\psi(x,t)|^2. \tag{3.25}$$

We know that this is the probability density to find the particle at the position x at time t. The time evolution of the density is governed by, omitting the dependencies of the functions in some instances,

$$\begin{aligned} \frac{d}{dt}\rho(x,t) &= \psi^*\psi + \psi^*\psi \\ &= \frac{1}{-i\hbar}(H\psi^*)\psi + \frac{1}{i\hbar}\psi^*(H\psi). \end{aligned} \tag{3.26}$$

Since the potential V is not even entering the equation here, we find

$$\frac{d}{dt}\rho(x,t) = \frac{\hbar}{2mi}\left((\nabla^2\psi^*)\psi - \psi^*(\nabla^2\psi)\right). \tag{3.27}$$

We define the current density as

$$j(x,t) = \frac{\hbar}{2mi}\left(\psi^*(\nabla\psi) - (\nabla\psi^*)\psi\right). \tag{3.28}$$

We hence arrive at the continuity equation

$$\frac{d}{dt}\rho(x,t) + \nabla j(x,t) = 0. \tag{3.29}$$

This is formally equivalent to a continuity equation of a fluid with density ρ.

3.2 Applications

3.2.1 Wave packets

How does a wave packet evolve in time? This is the question we will answer in this subsection. Let us first get a clear understanding what we mean by a wave packet.

Wave packet: We define a wave packet in the position representation to be

$$\psi(x,t) = \int \frac{dp}{2\pi\hbar}\phi(p)e^{\frac{i}{\hbar}\left(px - \frac{p^2}{2m}t\right)}, \tag{3.30}$$

where $\phi : \mathbb{R} \to \mathbb{C}$ is some normalized wave packet in the momentum representation.

This is nothing but a superposition of plane waves. A most important case is the Gaussian wave packet, where for a constant $A > 0$,

$$\phi(p) = Ae^{-(p-p_0)^2 w^2/\hbar^2}, \tag{3.31}$$

$p_0 \in \mathbb{R}$ defining the center of the wave packet in the momentum representation and w its width. Let us define the quantities

$$\alpha(t) = \frac{w^2}{\hbar^2} + i\frac{t}{2m\hbar}, \tag{3.32}$$

$$\beta = \frac{w^2 p_0}{\hbar^2} + i\frac{x}{2\hbar}, \tag{3.33}$$

$$\gamma = \frac{w^2 p_0^2}{\hbar^2}. \tag{3.34}$$

Then we get

$$\begin{aligned} \psi(x,t) &= \frac{A}{2\pi\hbar}\int dp \exp\Big(-\alpha\left(p-\beta/\alpha(t)\right)^2 + \beta^2/\alpha(t) - \gamma\Big) \\ &= \frac{A}{2\pi\hbar}\frac{\sqrt{\pi}}{\sqrt{\alpha(t)}}\exp\left(\frac{\beta^2}{\alpha(t)} - \gamma\right). \end{aligned} \tag{3.35}$$

Here, we have made use of the Gaussian integral

$$\int dy e^{-ay^2} = \frac{\sqrt{\pi}}{\sqrt{a}} \tag{3.36}$$

for any $a > 0$. Let us have a look at the particle density $\rho(x,t) = |\psi(x,t)|^2$. We get

$$\rho(x,t) = \left(\frac{A}{2\pi\hbar}\right)^2 \frac{\pi}{|\alpha(t)|}\exp\left(2\mathrm{re}\left(\frac{\beta^2 - \alpha(t)\gamma}{\alpha}\right)\right). \tag{3.37}$$

Let us now define

$$v = \frac{p_0}{m}, \tag{3.38}$$

$$\delta(t) = \frac{t\hbar}{2mw^2}. \tag{3.39}$$

In terms of these quantities, we get, up to normalization, which is not that interesting,

$$\rho(x,t) \sim \exp\left(-\frac{(x-vt)^2}{2w^2(1+\delta(t)^2)}.\right) \tag{3.40}$$

We can already guess what is going on here:

$$\langle X\rangle(t) = vt. \tag{3.41}$$

So the wave packet is propagating with a velocity of v, and the expectation values of the position operator evolve according to vt. This is just like a classical particle moving with the velocity of v. The width of the wave packet evolves as

$$(\Delta X)^2 = w^2(1+\delta^2(t)), \tag{3.42}$$

as a fairly straightforward calculation shows. This means that the wave packet is not only propagating. It is also "spreading", so becoming shallower in time. So the uncertainty in position will grow with time.