Contents

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* (or "Hamiltonian")

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

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,

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

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, for static Hamiltonians 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

$$
\begin{aligned}
U(t, t_0) &= U^{-1}(t_0, t) = U^{\dagger}(t_0, t), & (3.11) \\
U^{\dagger}(t, t_0)U(t, t_0) &= \mathbb{1}, & (3.12) \\
U(t_0, t_0) &= \mathbb{1}, & (3.13)
\end{aligned}
$$

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

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

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,

$$\langle A \rangle(t) = \langle \psi(t)|A|\psi(t)\rangle = \langle \psi(t_0)|A|\psi(t_0)\rangle = \langle A \rangle(t_0), \tag{3.22}$$

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. We summarize:

Time-independent Schroedinger equation: The time independent Schroedinger equation is the eigenvalue equation

$$H|\psi\rangle = E|\psi\rangle. \tag{3.23}$$

The solutions $|\psi\rangle$ are called stationary state vectors.

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:

$$i\hbar\frac{d}{dt}\psi(x,t) = H\psi(x,t). \tag{3.24}$$

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

$$H = -\frac{\hbar^2}{2m}\Delta + V(x,t). \tag{3.25}$$

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

$$\rho(x,t) = |\psi(x,t)|^2. \tag{3.26}$$

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,

$$\begin{aligned}\frac{d}{dt}\rho(x,t) &= \left(\frac{d}{dt}\psi^*\right)\psi + \psi^*\left(\frac{d}{dt}\psi\right) \\ &= \frac{1}{-i\hbar}(H\psi^*)\psi + \frac{1}{i\hbar}\psi^*(H\psi).\end{aligned} \tag{3.27}$$

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

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

We define the current density as

$$j(x,t) = \frac{\hbar}{2mi}\left(\psi^*(\nabla\psi) - (\nabla\psi^*)\psi\right). \tag{3.29}$$

We hence arrive at the continuity equation

$$\frac{d}{dt}\rho(x,t) + \nabla j(x,t) = 0. \tag{3.30}$$

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

$$\psi(x,t) = \int \frac{dp}{2\pi\hbar}\phi(p)e^{\frac{i}{\hbar}\left(px - \frac{p^2}{2m}t\right)}, \tag{3.31}$$

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 $A > 0$,

$$\phi(p) = Ae^{-(p-p_0)^2 w^2/\hbar^2}, \tag{3.32}$$

$p_0 \in \mathbb{R}$ defining the center of the wave packet in the momentum representation and w its width. We now consider the time evolution of such a wave packet. For this, we choose the potential to be vanishing,

$$V = 0, \tag{3.33}$$

such that we only have the kinetic term.

Let us define the quantities

$$a(t) = \frac{w^2}{\hbar^2} + i\frac{t}{2m\hbar}, \tag{3.34}$$

$$b = \frac{w^2 p_0}{\hbar^2} + i\frac{x}{2\hbar}, \tag{3.35}$$

$$c = \frac{w^2 p_0^2}{\hbar^2}. \tag{3.36}$$

These quantities do not have any direct physical significance, we merely introduce them here for simplicity of notation. Then we get

$$\psi(x,t) = \frac{A}{2\pi\hbar} \int dp \exp\left(-a\left(p - b/a(t)\right)^2 + b^2/a(t) - c\right)$$

$$= \frac{A}{2\pi\hbar} \frac{\sqrt{\pi}}{\sqrt{a(t)}} \exp\left(\frac{b^2}{a(t)} - c\right). \tag{3.37}$$

Here, we have made use of the Gaussian integral

$$\int dy e^{-dy^2} = \frac{\sqrt{\pi}}{\sqrt{d}} \tag{3.38}$$

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

$$\rho(x,t) = \left(\frac{A}{2\pi\hbar}\right)^2 \frac{\pi}{|a(t)|} \exp\left(2\mathrm{re}\left(\frac{b^2 - a(t)c}{a}\right)\right). \tag{3.39}$$

Let us now define

$$v = \frac{p_0}{m}, \tag{3.40}$$

$$d(t) = \frac{t\hbar}{2mw^2}. \tag{3.41}$$

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

$$\rho(x,t) \sim \exp\left(-\frac{(x-vt)^2}{2w^2(1+d(t)^2)}\right) \tag{3.42}$$

We can already guess what is going on here:

$$\langle X \rangle(t) = vt. \tag{3.43}$$

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

$$(\Delta X)^2 = w^2(1 + d^2(t)), \tag{3.44}$$

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.

3.2.2 The algebraic solution of the quantum harmonic oscillator

One of the most important quantum systems is the harmonic oscillator. There seem to be two reasons for this. The first one is related to the fact that harmonic oscillators appear for good reasons in numerous situations as a very good approximation of the actual physical situation. Frankly, harmonic oscillators are ubiquitous in physics. They describe the motion of particles such as atoms or ions in harmonic potentials, appear in condensed-matter physics, in quantum field theory, and many other subfields of quantum theory. At the basis of this is the insight that whenever interactions are small, to a good approximation the resulting system can be approximated by a harmonic oscillator.

The second reason is that it can be solved analytically, in a very elegant fashion. And here, one has to acknowledge the observation that theoretical physics is only indirectly about nature. It is about models of systems appearing in nature. And hence, models that can be solved in all their beauty in a closed form come in very handy. A decent proportion of theoretical physics is not done because it captures nature so well, but because it can be done. And there is a point in that: Exactly solvable models can be very illustrative and educational, it can be that many features of the fully-fletched situation are already visible. Hence, it should not be a surprise that the harmonic oscillator is ubiquitous in quantum theory, to say the least.

The classical harmonic oscillator of mass m and frequency ω is associated with the Hamilton operator

$$H = \frac{1}{2m}p^2 + \frac{m\omega^2}{2}x^2. \tag{3.45}$$

The quantum mechanical Hamiltonian in fact takes the identical form, merely the numbers reflecting position and momentum are replaced by the position and momentum operators, respectively,

$$H = \frac{1}{2m}P^2 + \frac{m\omega^2}{2}X^2. \tag{3.46}$$

As a side remark, the map from a classical Hamiltonian to a quantum one is sometimes called "quantisation", but we should keep in mind that this procedure can only here applied in such an unambiguous fashion. As a warm up, we also formulate the time-independent Schroedinger equation in the position representation

$$\left(-\frac{\hbar^2}{2m}\frac{d}{dx^2} + \frac{m\omega^2}{2}x^2 \right)\psi(x) = E\psi(x). \tag{3.47}$$

We can also define the characteristic length of the harmonic oscillator as

$$x_0 = \sqrt{\frac{\hbar}{\omega m}}. \tag{3.48}$$

We will now formulate what is called the algebraic solution of the quantum harmonic oscillator. For that, define the operator

$$a = \frac{\omega m x + ip}{\sqrt{2\omega m\hbar}}. \tag{3.49}$$

In terms of this operator and its Hermitian conjugate, the position and momentum operators become

$$X = \left(\frac{\hbar}{2\omega m} \right)^{1/2}(a + a^\dagger), \tag{3.50}$$

$$P = -i\left(\frac{\hbar\omega m}{2} \right)^{1/2}(a - a^\dagger). \tag{3.51}$$

The commutation relations then become

$$[a, a^\dagger] = 1. \tag{3.52}$$

Inserting this operator into the Hamilton operator, we get

$$H = \frac{1}{2}\hbar\omega(a^\dagger a + aa^\dagger), \tag{3.53}$$

which is the following:

Hamiltonian of the harmonic oscillator: The Hamiltonian of the quantum harmonic oscillator is given by

$$H = \hbar\omega\left(a^\dagger a + \frac{1}{2} \right), \tag{3.54}$$

where $[a, a^\dagger] = 1$.

The operator

$$N = a^\dagger a \tag{3.55}$$

is also called *number operator*, for reasons that will become clear in a second. Since the Hamiltonian H is different from the number operator merely by an additive and multiplicative constant, we can for simplicity of notation also look at the eigenvectors and eigenvalues of the number operator. Its commutation relations are given by

$$[N, a] = -a, \tag{3.56}$$
$$[N, a^\dagger] = a^\dagger. \tag{3.57}$$

To start with, N is a so-called positive operator, which means that it is Hermitian and none of its eigenvalues is negative. This is easy to see. Denote with $|0\rangle$ the eigenvector of the smallest eigenvalue λ_0. Then

$$\begin{aligned} \lambda_0 &= \langle 0|N|0\rangle \\ &= \langle 0|a^\dagger a|0\rangle = (\langle 0|a\rangle (a|0\rangle)) \geq 0, \end{aligned} \tag{3.58}$$

and hence

$$\lambda_0 \geq 0. \tag{3.59}$$

In many books, shockingly, it is argued that this necessarily means that the smallest eigenvalue must be zero. This is true, but for different reasons than commonly stated.

Let us denote with $|\nu\rangle$ an eigenvector with eigenvalue ν, so

$$N|\nu\rangle = \nu|\nu\rangle. \tag{3.60}$$

We already know that $\nu \geq 0$. The point is that due to the commutation relations, we have

$$Na|\nu\rangle = (aN - a)|\nu\rangle = (\nu - 1)a|\nu\rangle, \tag{3.61}$$
$$Na^\dagger|\nu\rangle = (a^\dagger N + a^\dagger)|\nu\rangle = (\nu + 1)a^\dagger|\nu\rangle, \tag{3.62}$$
$$\tag{3.63}$$

So as long as $\nu \neq 0$, we see that $a|\nu\rangle$ is again an eigenvector of N, just with eigenvalue $\nu - 1$ instead of ν. Similarly, $a^\dagger|\nu\rangle$ is an eigenvalue of N with eigenvalue $\nu + 1$. Starting from ν, the possible eigenvalues are therefore

$$\{\nu + k : k \in \mathbb{Z}\}. \tag{3.64}$$

But since we know that $\mu \geq 0$, we know that the possible eigenvalues must be all integers (otherwise one immediately finds eigenvalues smaller than zero, which must not be the case). That is to say, the eigenvalues of the number operator are just the positive integers and zero ($\lambda_0 = 0$). We also find the eigenvectors, and this is now worth a box:

Eigenvalues and eigenvectors of the number operator: The eigenvalues of the number operator are the positive integers including zero, and the respective normalized eigenvectors are

$$|n\rangle = \frac{1}{\sqrt{n!}}(a^\dagger)^n|0\rangle. \tag{3.65}$$

They satisfy $\langle k|n\rangle = d_{k,n}$.

Let us take a deep breath at this point. We have come a long way, and know the eigenvalues and eigenvectors of the number operator and hence also of the quantum harmonic oscillator. We have achieved this without diving into the specifics of the Hamiltonian. In fact, all we have used are the commutation relations of the operators a and N! Such an approach is referred to as an algebraic approach. Since the operators a and $a^\dagger$ lower and raise the eigenvalues by one, respectively, they are also called annihilation operators and creation operators. This may not be a very nice word, but this is how these bosonic operators are usually called.

Annihilation and creation operators: The annihilation operator a and the creation operator $a^\dagger$ satisfy

$$\begin{aligned} a|n\rangle &= \sqrt{n}|n-1\rangle, & (3.66)\\ a^\dagger|n\rangle &= \sqrt{n+1}|n+1\rangle, & (3.67)\\ N|n\rangle &= n|n\rangle, & (3.68) \end{aligned}$$

for non-negative integers n.

Having said all that, we also know the eigenvalues of the quantum harmonic oscillator: They are given by

$$\left\{\hbar\omega\left(n+\frac{1}{2}\right) : n \in \mathbb{N}_0\right\}. \tag{3.69}$$

We can also at this point come back to our original problem, the one of time evolution. If the initial state vector of the system is given by

$$|\psi(t_0)\rangle = \sum_{n=0}^{\infty} a_n|n\rangle, \tag{3.70}$$

then – following Eq. (3.21) – the state vector at later times $t \geq t_0$ is given by

$$|\psi(t_t)\rangle = \sum_{n=0}^{\infty} a_n e^{-i(t-t_0)\omega\left(n+\frac{1}{2}\right)}|n\rangle. \tag{3.71}$$

3.2.3 Wave functions of the quantum harmonic oscillator

We will now become a bit dirtier and actually compute the wave functions of the eigenvectors. Of course, we can do so by simply solving the above time-independent Schroedinger equation as a differential equation. We can also solve this problem in a slightly more elegant way, which we are about to do now: Let us denote the wave functions, so the position representations by

$$\langle x|n\rangle = \psi_n(x). \tag{3.72}$$

We know that in the position representation (again we do not distinguish between an operator and its representation)

$$a = \frac{1}{\sqrt{2}} \left(\frac{x}{x_0} + x_0 \frac{d}{dx} \right). \tag{3.73}$$

From $a|0\rangle = 0$, we find

$$\left(\frac{x}{x_0^2} + \frac{d}{dx} \right) \psi_0(x) = 0. \tag{3.74}$$

The solution of this is a Gaussian,

$$\psi_0(x) \sim \exp\left(-\frac{1}{2} \left(\frac{x}{x_0} \right)^2 \right), \tag{3.75}$$

so with proper normalization

$$\psi_0(x) = (\sqrt{\pi} x_0)^{-1/2} \exp\left(-\frac{1}{2} \left(\frac{x}{x_0} \right)^2 \right). \tag{3.76}$$

This means that the wave function of the state vector with the lowest energy, the *ground state vector*, is a Gaussian wavepacket. But we can say more. From Eq. (3.65) we find that

$$\psi_n(x) = \frac{1}{\sqrt{n!}} \frac{1}{2^{n/2}} \left(x - \frac{d}{dx} \right)^2 \psi_0(x). \tag{3.77}$$

Therefore, we can use the identity

$$x - \frac{d}{dx} = e^{-x^2/2} \frac{d}{dx} e^{-x^2/2}. \tag{3.78}$$

In this way, we arrive at a Gaussian function, multiplied by a polynomial in x, for each n. These polynomials have been given a name, given their enormous importance. There are many ways of defining them, for example using the above identity. We are now in the position to formulate the wave functions of the quantum harmonic oscillator:

Wave functions of the eigenvectors of the quantum harmonic oscillator:
They are given by

$$\psi_n(x) = (2^n n! \sqrt{\pi} x_0)^{-1/2} \exp\left(-\frac{1}{2}\left(\frac{x}{x_0}\right)^2\right) H_n\left(\frac{x}{x_0}\right), \qquad (3.79)$$

for non-negative integers n.

For completeness, we name the first five Hermite polynomials. The first one, H_0, should not surprise us at this point:

$$
\begin{aligned}
H_0(x) &= 1, & (3.80) \\
H_1(x) &= 2x, & (3.81) \\
H_2(x) &= 4x^2 - 2, & (3.82) \\
H_3(x) &= 8x^3 - 12x, & (3.83) \\
H_4(x) &= 16x^4 - 48x^2 + 12, & (3.84) \\
H_5(x) &= 32x^5 - 160x^3 + 120x. & (3.85)
\end{aligned}
$$

Note that H_n is a polynomial of degree n.

3.2.4   Coherent states

We will finally, as a bit of an exercise, look at properties of the so-called *coherent states*. Their state vectors are eigenvectors the annihilation operators a. Let us write, for complex $\alpha \in \mathbb{C}$,

$$a|\alpha\rangle = \alpha|\alpha\rangle. \qquad (3.86)$$

Let us now express this in terms of the eigenvectors of the harmonic oscillator,

$$|\alpha\rangle = \sum_{n=0}^{\infty} c_n|n\rangle. \qquad (3.87)$$

Then we find

$$c_n\sqrt{n} = \alpha c_{n-1} \qquad (3.88)$$

for $n = 1, 2, \ldots$. Thus

$$c_n = \frac{\alpha^n}{\sqrt{n!}} c_0, \qquad (3.89)$$

and with the appropriate normalization, we find the following:

Coherent states: The state vectors of coherent states are for $\alpha \in \mathbb{C}$ given by

$$|\alpha\rangle = \exp\left(-\frac{1}{2}|\alpha|^2\right) \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}}|n\rangle. \qquad (3.90)$$

Using the above definitions, we find that another equivalent way of writing this is

$$|\alpha\rangle = \exp\left(-\frac{1}{2}|\alpha|^2\right) e^{\alpha a^\dagger}|0\rangle. \qquad (3.91)$$

How do the wave functions of coherent states look like? They are given by

$$\langle x|\alpha\rangle = \sqrt{\frac{\alpha}{\sqrt{\pi}}} \exp\left(-\frac{1}{2}(|\alpha|^2 - \alpha^2)\right) \exp\left(-\frac{1}{2}(\alpha x - \sqrt{2}x)^2\right). \qquad (3.92)$$

In fact, these wave functions are "minimum uncertainty wave functions": They just so satisfy the Heisenberg uncertainty inequality with equality. In other words, they are at the same time as narrow in position and momentum as the uncertainty relation allows them to be.

Time evolution of coherent states is also quite simple: For a quantum harmonic oscillator with frequency ω we have that if we prepare a quantum system initially in $|\alpha\rangle$ for some $\alpha \in \mathbb{C}$, then the state vector at later times is given by

$$|\psi(t)\rangle = e^{-i\omega t/2}|\alpha e^{-i\omega t}\rangle. \qquad (3.93)$$

So the property of being a minimum uncertainty state is preserved under time evolution.

3.2.5 Ehrenfest's theorem

We know that, for a particle in one dimension in a time-independent potential V, so a system with Hamiltonian

$$H = \frac{1}{2m}P^2 + V(x), \qquad (3.94)$$

the expectation values of the position and momentum operators are

$$\frac{d}{dt}\langle X\rangle(t) = \frac{1}{m}\langle P\rangle(t), \qquad (3.95)$$

$$\frac{d}{dt}\langle P\rangle(t) = -\langle (V')(X)\rangle. \qquad (3.96)$$

This latter term can also be interpreted as a "force",

$$K(X) = -V'(X). \qquad (3.97)$$

That is to say, one arrives at an equation of motion

$$m\frac{d^2}{dt^2}\langle X\rangle(t) = \langle K(X)\rangle(t). \tag{3.98}$$

This equation is sometimes called *Ehrenfest's theorem*. So the equations of mo-
tion for the expectation value of the position operator fulfills an equation of
motion that resembles the classical equation of motion. But there is a major
difference: The right hand side does not depend on $\langle X\rangle$ only, but is the ex-
pectation value of $K(X)$. If V is harmonic, so a quadratic polynomial, then
indeed

$$\langle K(X)\rangle = K(\langle X\rangle). \tag{3.99}$$

Therefore, for harmonic oscillators and for free particles with $V = 0$, one has

$$m\frac{d^2}{dt^2}\langle X\rangle(t) = K(\langle X\rangle(t)). \tag{3.100}$$

Then it is precisely true that the expectation values follow the classical equa-
tions of motion. This again highlights the particular status of harmonic poten-
tials.

3.2.6   Potential wells

In this section, we would like to discuss the problem of particles scattering at a
potential well, defined by the stationary potential

$$V(x) = \begin{cases} 0 & x \in (-\infty, -a), \\ -V_0 & x \in [-a, a], \\ 0 & x \in (a, \infty), \end{cases} \tag{3.101}$$

for $a, V_0 > 0$. We have already discussed the bound state wave functions, so
we will consider now the wave functions with $E > 0$. The wave numbers we
encounter are

$$k = \sqrt{2mE}/\hbar \tag{3.102}$$

outside the well and

$$q = \sqrt{2m(E + V_0)}/\hbar \tag{3.103}$$

inside.

   We make the ansatz for the wave function to the left of the potential well,
so for $x < -a$:

$$\psi(x) = \psi_{\text{in}}(x) + \psi_{\text{out}}(x), \tag{3.104}$$

where

$$\psi_{\text{in}}(x) = Ae^{ikx}, \tag{3.105}$$

with some constant $A > 0$, and

$$\psi_{\text{out}}(x) = AS(E)\frac{i}{2}\left(\frac{q}{k} - \frac{k}{q}\right)\sin(2qa)e^{-ikx} \tag{3.106}$$

where $S : \mathbb{R}^+ \to \mathbb{R}$ a function that captures the transmission as a function of the energy E, and —S(E)— is usually referred to as the *transmission coefficient*, In the inner of the potential well, $|x| \leq a$,

$$\psi_{\text{inner}}(x) = Ce^{-iqx} + De^{iqx}, \tag{3.107}$$

with suitable constants $C, D \in \mathbb{C}$. To the right of the potential well, for $x > a$, we have a transmitted wave,

$$\psi_{\text{right}}(x) = AS(E)e^{ikx}. \tag{3.108}$$

With the same reasoning as before, we find for the transmission coefficient

$$|S(E)| = \left| \frac{e^{-2ika}}{\cos(2qa) - (i/2)((q/k) + (k/q)\sin(2qa)} \right|, \tag{3.109}$$

so

$$|S(E)| = \frac{1}{1 + (1/4)((q/k) - (k/q))^2 \sin^2(2qa)}, \tag{3.110}$$

with

$$\left(\frac{q}{k} - \frac{k}{q} \right)^2 = \left(\frac{\sqrt{E + V_0}}{\sqrt{E}} - \frac{\sqrt{E}}{\sqrt{E + V_0}} \right)^2 = \frac{V_0^2}{E(E + V_0)}. \tag{3.111}$$

So this gives

$$|S(E)|^2 = \left(1 + \frac{\sin^2(2qa)}{4(E/V_0)(1 + (E/V_0))} \right)^{-1}. \tag{3.112}$$

What are the properties of $|S(E)|$? It is not difficult to see that it takes the value 1 for

$$2qa = n\pi, \ n \in \mathbb{N}. \tag{3.113}$$

For wave packets with exactly this energy (E can be computed from q), the potential is fully transmittant: The wave packet just goes through and is not reflected at all. This is an exact expression. Local minima are – as an approximate expression – close to $2qa(2n + 1)\pi/2$. For these values, a significant fraction of the wave packet is reflected, and this even though the wave packet had positive energy. Probably unsurprisingly,

$$\lim_{E \to \infty} |S(E)| = 1, \tag{3.114}$$

so for large energies, all will be transmitted. The maxima of the transmission coefficient are called *resonances*. Intuitively, one may argue as follows: The wave packet is coming in from the left and alters its amplitude and wave vector when entering the potential region. A part of it is reflected at $x = a$. At $4aq = 2\pi n$ for $n \in \mathbb{N}$, the incoming and the reflected wave are in phase, whereas the wave reflected at $-a$ will encounter a phase jump of π. Therefore, the waves reflected at a and $-a$ will always be out of phase and will interfere destructively. For large values of V_0, the resonances become sharper and sharper.