Chapter 3

Motion of a pointlike particle with a single degree of freedom

3.1 Continuous observables

In this chapter, we study basic quantum physics of the simplest mechanical system: translational motion of a pointlike particle with a single degree of freedom. In classical mechanics, this motion is described by two canonical variables, position and momentum. Accordingly, in our quantum treatment, we introduce two observable operators: position $\hat{x}$ and momentum $\hat{p}$.

In a Hilbert space of finite dimension, we expect (see Ex. 1.76) the set of eigenstates of any physical observable to form an orthonormal basis. However, in the present case this rule can be applied only partially. This is because, although the *geometric* space containing the particle is one-dimensional, the associated *Hilbert* space is of infinite dimension: for example, there are infinitely many position eigenstates $|x\rangle$, and all these eigenstates are incompatible[1]. Furthermore, position eigenstates form a *continuum*: for every real value of x there exists an associated eigenstate $|x\rangle$. The same is true for the momentum observable.

The continuous nature of these observables implies that most mathematical rules (state and operator decomposition, normalization, basis conversion, etc.) derived for finite-dimension Hilbert spaces have to be modified: summation must be replaced by integration. This is our task for this section. In order to reproduce these rules in the form that closely resembles those for the discrete case, we need to define a special normalization convention for continuous observable eigenstates. Instead of normalizing these states to one, as we would do in the discrete case [*cf.* Eq. (1.8)], we write:

$$\langle x|\, x'\rangle = \delta(x - x'); \tag{3.1}$$

$$\langle p|\, p'\rangle = \delta(p - p'). \tag{3.2}$$

This appears strange at first. According to Eq. (3.1), the inner product of the position eigenstate $|x\rangle$ with itself is $\langle x|\, x\rangle = \delta(0)$, so this state has infinite norm. The same applies to momentum eigenstates. How is this consistent with the First postulate of quantum mechanics, which says that all physical states must have norm 1? We answer this question by saying that *continuous-observable eigenstates are unphysical*: it is impossible to set a particle at an absolutely precise location or make it move at an absolutely precise velocity. Therefore, the First postulate does not apply to these states; they are just a mathematical abstraction[2]. This notwithstanding, all physically realistic

[1] One may argue that one can also introduce continuous observables in finite-dimensional Hilbert spaces: for example, the polarization angle of a photon can take on any value from 0 to 180°. However, this would not be an observable in the quantum mechanical sense, because the relevant eigenstates are not orthogonal: a photon polarized at 45° is a superposition of the 0° and 90° polarization states. On the other hand, a particle located at $x = 4\text{m}$ is not a superposition of the $|x = 3\text{m}\rangle$ and $|x = 5\text{m}\rangle$ position eigenstates. A particle's position is a valid observable while a photon's polarization angle is not.

[2] To treat this matter more rigorously, one introduces a special construction called *rigged Hilbert space*.

states, which have some uncertainty both in the position and momentum, do have norm one in accordance with the First postulate.

Any quantum states $|\psi\rangle$ can be decomposed into the basis associated with a continuous-variable observable according to

$$|\psi\rangle = \int_{-\infty}^{+\infty} \psi(x)\,|x\rangle\,dx. \tag{3.3}$$

This equation replaces Eq. (1.1) for the decomposition of a state into a discrete basis. The function $\psi(x)$ is called the *wavefunction* of the state $|\psi\rangle$ in the x-basis (-representation) and is the continuous-observable analog of the column representation of a vector in a Hilbert space of a finite dimension. Taking the adjoint of both sides of Eq. (3.3),

$$\langle\psi| = \int_{-\infty}^{+\infty} \psi^*(x)\,\langle x|\,dx. \tag{3.4}$$

we also find that the wavefunction of $\langle\psi|$ is $\psi^*(x)$.

Exercise 3.1 Show that we can construct the following continuous analogues to important discrete-case relations:

a) Instead of Eq. (1.11), we can write

$$\psi(x) = \langle x|\,\psi\rangle\,; \tag{3.5}$$

b) Instead of Eq. (1.31), we can write

$$\int_{-\infty}^{+\infty} |x\rangle\langle x|\,dx = \hat{\mathbf{1}}; \tag{3.6}$$

c) Instead of Eq. (1.9), we can write

$$\langle\psi_1|\,\psi_2\rangle = \int_{-\infty}^{+\infty} \psi_1^*(x)\psi_2(x)dx; \tag{3.7}$$

Exercise 3.2 Show that, if the normalization rule were, as in the finite-dimensional case, $\langle x|\,x'\rangle = \begin{cases} 1 \text{ if } x{=}x' \\ 0 \text{ if } x{\neq}x' \end{cases}$, the above relations would be invalid.

Exercise 3.3 Show that, for physical states,

$$\int_{-\infty}^{+\infty} |\psi(x)|^2 \mathrm{d}x = 1. \tag{3.8}$$

Exercise 3.4 Calculate the normalization factor A for the states with the following wavefunctions:

a) a "top-hat function"

$$\psi_{\mathrm{top-hat}}(x) = \begin{cases} 0 \text{ if } x < a \text{ or } x > b; \\ A \text{ if } a \leq x \leq b; \end{cases} \tag{3.9}$$

b) a Gaussian wavefunction

$$\psi_{\mathrm{Gauss}}(x) = Ae^{-\frac{x^2}{2d^2}}. \tag{3.10}$$

Exercise 3.5 Find the wavefunction of the state of definite position $|x_0\rangle$ in the position basis.

As in the discrete case, operators associated with continuous observables are given by

$$\hat{x} = \int_{-\infty}^{+\infty} x\,|x\rangle\,\langle x|\,dx. \tag{3.11}$$

The operator functions are naturally defined as

$$f(\hat{x}) = \int_{-\infty}^{+\infty} f(x) \, |x\rangle \, \langle x| \, dx. \tag{3.12}$$

For an arbitrary operator $\hat{A}$, the two-dimensional function

$$A(x, x') = \langle x| \, \hat{A} \, |x'\rangle \, , \tag{3.13}$$

is referred to as the operator's *matrix element*.

As we see below and similarly to the discrete-variable case, the information about the matrix element $\langle x| \, \hat{A} \, |x'\rangle$ for all x and x' is sufficient to reconstruct the operator. More generally, we can perform operations with states and operators represented by one- and two-dimensional functions, respectively, just as we operate with matrices in the discrete case, only replacing summation with integration.

Exercise 3.6 Show that $\hat{x} \, |x\rangle = x \, |x\rangle$.

Exercise 3.7 Prove that:

a) any operator $\hat{A}$ can be written as

$$\hat{A} = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} A(x, x') \, |x\rangle\langle x'| \, dx \, dx'; \tag{3.14}$$

b) if the operator is a function of $\hat{x}$,

$$\langle \psi| \, f(\hat{x}) \, |\psi\rangle = \int_{-\infty}^{+\infty} \psi^*(x) f(x) \psi(x) dx; \tag{3.15}$$

c) for any operator $\hat{A}$, and any two states $|\psi\rangle$, $|\phi\rangle$

$$\langle \phi| \, \hat{A} \, |\psi\rangle = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \phi^*(x) A(x, x') \psi(x') dx \, dx'; \tag{3.16}$$

d) the wavefunction of the state $\hat{A} \, |\psi\rangle$ is

$$\left\langle x \right| \hat{A} \left| \, \psi \right\rangle = \int_{-\infty}^{+\infty} A(x, x') \psi(x') dx'; \tag{3.17}$$

e) the wavefunction of the state $\langle \psi| \, \hat{A}$ is

$$\left\langle \psi \right| \hat{A} \left| \, x \right\rangle = \int_{-\infty}^{+\infty} \psi^*(x') A(x', x) dx'; \tag{3.18}$$

f) matrix elements of an operator $\hat{A}$ and its adjoint $\hat{A}^\dagger$ are related as

$$(A^\dagger)(x, x') = A^*(x', x); \tag{3.19}$$

g) the product of operators $\hat{A}$ and $\hat{B}$ can be written in terms of their "matrices" as

$$\left\langle x \right| \hat{A}\hat{B} \left| \, x' \right\rangle = \int_{-\infty}^{+\infty} A(x, x'') B(x'', x') dx''. \tag{3.20}$$

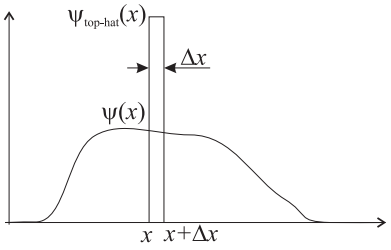


Figure 3.1: Approximate measurement of the position by projecting state $|\psi\rangle$ onto a state with a "top-hat" wavefunction.

Let us now reformulate the Second postulate of quantum mechanics for measurements in continuous-variable bases. Suppose observable $\hat{x}$ is measured in quantum state $|\psi\rangle$ with wavefunction $\langle x|\ \psi\rangle = \psi(x)$. Acting similarly to the discrete case, we assign value $\mathrm{pr}_x = |\psi(x)|^2$ as the probability to observe a particular value of x. A subtlety arises, though, because if we associate this (or any other finite) probability value to each *specific* x out of the continuum, the total probability to detect *any* x will be infinite. This is not surprising because, as we discussed earlier, eigenstates of the position operator are unphysical, and so is a projection measurement involving these states. It is even theoretically not feasible to realize a *perfectly* precise measurement of the position observable.

As an alternative, let us model the measurement of x project state $|\psi\rangle$ onto the state with a "top-hat" wavefunction (3.9) that takes a constant, non-zero value in the interval between x and $x + \Delta x$, where Δx is arbitrarily small (Fig. 3.1). We find in the first order approximation

$$\langle\psi|\ \psi_{\mathrm{top-hat}}\rangle = \frac{1}{\sqrt{\Delta x}} \int_x^{x+\Delta x} \psi(x)\mathrm{d}x \approx \sqrt{\Delta x}\psi(x) \tag{3.21}$$

and hence the probability to detect state $|\psi_{\mathrm{top-hat}}\rangle$ in state $|\psi\rangle$ equals

$$\mathrm{pr}_x \Delta x = |\langle\psi|\ \psi_{\mathrm{top-hat}}\rangle|^2 = |\psi(x)|^2 \Delta x. \tag{3.22}$$

Of course, not all apparata that measure the particle's position involve projection onto the top-hat function. However, the above result is universally applicable: the probability to detect a particle in state $|\psi\rangle$ within a small interval $[x, x + \Delta x]$ is given by Eq. (3.22). Accordingly, the quantity $\mathrm{pr}_x = |\psi(x)|^2$ has the meaning of the *probability density* associated with the state at position x.

If we apply Eq. (3.22) to find the probability to detect *any* value of x between $-\infty$ to $+\infty$, we find unity in accordance with Eq. (3.8). This is not surprising: the particle can with certainty be found *somewhere*, even though its precise position is not known.

Upon which state $|\psi\rangle$ will project after the measurement? The self-suggesting answer $|x\rangle$ is, as we discussed, unphysical. Yet it is useful as an approximation for many theoretical applications, as long as we do not forget to take the normalization issue into account. The more physically realistic answer will depend on the specifics of the measurement apparatus; generally, one would obtain some superposition or statistical mixture of multiple position eigenstates within a certain narrow interval. For example, in the case studied above, the answer is $|\psi_{\mathrm{top-hat}}\rangle$.

Closely related to measurements is the notion of the expectation value. Definition 1.26 can be reformulated for the continuous domain as follows: the expectation value associated with a measurement of a random continuous variable x with probability density pr_x is given by

$$\langle x\rangle = \int_{-\infty}^{+\infty} x\mathrm{pr}_x \mathrm{d}x. \tag{3.23}$$

Under this definition, the expression (1.36) for the quantum expectation value remains the same. I invite the reader to verify this independently in the following exercise.

Exercise 3.8 Show that the expectation value of a continuous observable $\hat{x}$ [defined as $\langle x\rangle = \int_{-\infty}^{+\infty} x\,\mathrm{pr}(x)\,dx$] in a state $|\psi\rangle$ is given by $\langle x\rangle = \langle\psi|\,\hat{x}\,|\psi\rangle$.

Exercise 3.9 Show that the eigenstates of a Hermitian operator corresponding to different eigenvalues are orthogonal[3].

Table 3.1: Comparative summary of rules for operating with discrete-and continuous-variable bases

	discrete basis $\{\|v_i\rangle\}$	continuous basis $\{\|x\rangle\}$
orthonormality	$\langle v_i\|\ v_j\rangle = \delta_{ij}$	$\langle x\|\ x'\rangle = \delta(x-x')$
decomposition	$\|\psi\rangle = \sum_i \psi_i\,\|v_i\rangle$	$\|\psi\rangle = \int_{-\infty}^{+\infty} \psi(x)\,\|x\rangle$
of a state	$\psi_i = \langle v_i\|\ \psi\rangle$	$\psi(x) = \langle x\|\ \psi\rangle$
second postulate	$\mathrm{pr}_i = \|\langle v_i\|\ \psi\rangle\|^2$ (probability)	$\mathrm{pr}_x = \|\langle x\|\ \psi\rangle\|^2$ (probability density)
decomposition	$A_{ij} = \left\langle v_i\right\vert \hat{A}\left\vert v_j\right\rangle$	$A(x,x') = \left\langle x\right\vert \hat{A}\left\vert x'\right\rangle$
of an operator	$\hat{A} = \sum_{i,j} A_{ij}\,\|v_i\rangle\langle v_j\|$	$\hat{A} = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} A(x,x')\,\|x\rangle\langle x'\|\,dxdx'$
decomposition of $\hat{\mathbf{1}}$	$\hat{\mathbf{1}} = \sum_i \|v_i\rangle\langle v_i\|$	$\hat{\mathbf{1}} = \int_{-\infty}^{+\infty} \|x\rangle\langle x\|\,dx$
product of operators	$(AB)_{ij} = \sum_k A_{ik}B_{kj}$	$(AB)(x,x') = \int_{-\infty}^{+\infty} A(x,x'')B(x'',x)dx'$

3.2 De Broglie wave

In the previous section, we studied the general mathematical machinery for handling the basis of the Hilbert space formed by the eigenstates of a continuous observable. Now it is time to bring some physics into the picture. We begin by postulating the relation between the position and momentum eigenstates:

$$\langle x|\ p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{i\frac{px}{\hbar}}. \tag{3.24}$$

Relation (3.24) states that the wavefunction of the state with definite momentum is an infinite wave of wavelength

$$\lambda_{dB} = 2\pi\hbar/p, \tag{3.25}$$

which is known as the *de Broglie wave*. It manifests one of the central concepts of quantum mechanics — *wave-particle duality*, i.e. the property of all quantum matter to exhibit both particle and wave features.

The de Broglie wave cannot be derived from the quantum mechanics postulates we studied so far. Rather, it is a generalization of a multitude of experimental observations and theoretical insights. The historical path towards the de Broglie wave can be briefly outlined as follows.

In 1900, Max Planck explained the experimentally observed spectrum of blackbody radiation by introducing the quantum of light, now known as the photon[4]. He found that a good agreement between theory and experiment can be obtained if one assumes that the energy of the photon is proportional to the frequency ω of the light wave. The proportionality coefficient, $\hbar$, became known as the Planck constant.

Subsequently, in 1913, Niels Bohr has used the Planck constant in developing his model of the atom, according to which, the electron's orbital is stable if its angular momentum equals an integer number of $\hbar$. Based on this assumption one can calculate the spectrum of optical transitions of the hydrogen atom, which exhibits very good agreement with the experiment. Similarly to Planck's

[3]This appears to follow from Ex. 1.76. However, the statement of that Exercise was proven for a Hilbert space of a finite dimension. In the present Chapter, the dimensions are infinite.

[4]The term *photon* has been introduced much later, in 1926, by the physical chemist Gilbert Lewis.

theory of light, Bohr's model was empirical: it seemed to explain experimental results, but the physics behind it remained a mystery.

The next major step towards the discovery of the de Broglie wave was made in 1923 by Arthur Holly Compton, who provided theoretical explanation of diffraction of X rays on free electrons. In Compton's theory, photons were treated as ultrarelativistic particles, whose energy follows the famous Einstein's relation $E = mc^2$. Since we also have $E = \hbar\omega$ due to Planck, we can calculate the mass of the photon, $m = \hbar\omega/c^2$, and its momentum[5], $p = mc = \hbar\omega/c$. Expressing the electromagnetic wave frequency in terms of the wavelength, $\omega = 2\pi c/\lambda$, we find $p = 2\pi\hbar/\lambda$ [*cf.* Eq. (3.25)]. The collision between a photon and an electron can then be treated using the laws of momentum and energy conservation, and an experimentally verifiable dependence of the wavelength of the scattered waves as a function of the scattering angle can be obtained. Again, this dependence showed excellent agreement with the experiment.

Louis De Broglie in his 1924 PhD thesis hypothesized that Compton's theory did not have to be limited to light particles. In fact, *any* particle that is moving with a certain momentum can be associated with a wave with the wavelength given by Eq. (3.25). Under this assumption, one can reinterpret Bohr's rule as a standing wave condition: the electron's model is stable if its circumference fits an integer number n of de Brolie waves:

$$2\pi r = n\lambda_{dB}, \tag{3.26}$$

where r is the radius of the orbit[6]. Substituting expression (3.25) into Eq. (3.26), we find $pr = n\hbar$. This is equivalent to Bohr's condition, because the electron's angular momentum is the product of its momentum and the orbit's radius.

The hypothesis of de Broglie was quickly confirmed by experiment. In 1927 at Bell Labs, Clinton Davisson and Lester Germer observed diffraction of a flux of electrons on the crystalline lattice of nickel and measured the associated wavelength, which turned out to be in agreement with de Broglie's calculations.

We now proceed to derive some of the main consequences of the relationship between the position and momentum eigenstates defined by the de Broglie wave.

Exercise 3.10 Estimate the de Broglie wavelength for

a) a car;

b) air molecules at the room temperature;

c) electrons in an electron microscope with a kinetic energy of 100 keV;

d) rubidium atoms in a Bose-Einstein condensate ate a temperature of 100 nanokelvin.

Exercise 3.11 Show that, according to the property (3.24), the position and momentum eigenstates can be expressed through each other as follows:

$$|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} e^{i\frac{px}{\hbar}} |x\rangle \, \mathrm{d}x; \tag{3.27}$$

$$|x\rangle = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} e^{-i\frac{px}{\hbar}} |p\rangle \, \mathrm{d}p. \tag{3.28}$$

Exercise 3.12 Relying on the relation $\langle x|\, x'\rangle = \delta(x - x')$, show explicitly that Eq. (3.24) is consistent with the orthonormality condition $\langle p|\, p'\rangle = \delta(p - p')$.
Hint: use Eq. (3.7).

[5] The relation $p = E/c$ between the momentum and energy of the photon is consistent with the expression for the radiation pressure, which, according to Maxwell's theory, equals the intensity of that radiation divided by the speed of light. Radiation pressure has been experimentally observed by Peter Lebedev in 1900.

[6] "Smearing" of the wave function was not known at that time.

As we discussed earlier, the convention to normalize continuous-variable eigenstates to a delta function is mathematically convenient, but unphysical. For this reason, it is not correct to interpret the square absolute value of the de Broglie wave, $\langle x|\ p\rangle = 1/2\pi\hbar$, as a probability density in the sense defined in Sec. 3.1. Actually, the deBroglie wave has infinite extent in space, and thus the probability to detect the particle within any final interval is infinitesimal.

The *wavevector* of the de Broglie wave is

$$k = \frac{2\pi}{\lambda_{dB}} = \frac{p}{\hbar}. \tag{3.29}$$

Sometimes it is convenient to handle momentum eigenstates $|p\rangle$ in the physically equivalent form of wavevector eigenstates $|k = p/\hbar\rangle$, because then we need not worry about the Planck constant in the exponent.

A minor subtlety associated with wavevector eigenstates is their normalization. The de Broglie wavefunction for these states is given by

$$\langle x|\ k\rangle = \frac{1}{\sqrt{2\pi}} e^{ikx}, \tag{3.30}$$

i.e. there is no factor of $\sqrt{\hbar}$ in the denominator, in contrast to Eq. (3.24). Indeed, recalculating Ex. 3.12 with Eq. (3.30), we obtain $\langle k|\ k'\rangle = \delta(k - k')$ as we would expect from eigenstates of a continuous observable. Accordingly,

$$|k\rangle = \sqrt{\hbar}\,|p\rangle\,. \tag{3.31}$$

We see that two physically equivalent states, $|p\rangle$ and $|k\rangle$, have a different norm. This is another consequence of the unphysical character of normalization for continuous observable eigenstates.

3.3 Position and momentum representations

This section is dedicated to converting the representations of various states and operators between the position and momentum bases. As in the discrete case, the primary tool for such conversion is the method of "inserting the identity operator", i.e. utilizing the fact that the operator

$$\hat{\mathbf{1}} = \int_{-\infty}^{+\infty} |x\rangle\langle x|\,\mathrm{d}x = \int_{-\infty}^{+\infty} |p\rangle\langle p|\,\mathrm{d}p \tag{3.32}$$

can be inserted into any inner product expression.

Exercise 3.13 Find the explicit formulae for converting between the position $\psi(x)$ and momentum $\tilde{\psi}(p)$ representations of a given quantum state $|\psi\rangle$.

Answer:

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \tilde{\psi}(p) e^{i\frac{px}{\hbar}} dp; \tag{3.33a}$$

$$\tilde{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \psi(x) e^{-i\frac{px}{\hbar}} dx \tag{3.33b}$$

For reference, we also write these formulae in the *wavevector* representation:

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \tilde{\psi}(k) e^{ikx} dk; \tag{3.34}$$

$$\tilde{\psi}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \psi(x) e^{-ikx} dx. \tag{3.35}$$

As we see, conversion between the position and wavevector representations and back is simply the direct and inverse Fourier transformation, respectively.

In this course, we will always use a tilde [e.g. $\tilde{\psi}(p)$ or $\tilde{\psi}(k)$] to denote wavefunctions in the momentum or wavevector representations. Comparing Eqs. (3.33b) and (3.35) we find the relation between these two representations:

$$\tilde{\psi}(p) = \frac{\tilde{\psi}(k)}{\sqrt{\hbar}} \tag{3.36}$$

for $p = k\hbar$.

Exercise 3.14 Consider a function $V(\hat{x})$ of the position operator. Write the matrix element of this operator in the momentum basis.
Answer:

$$V(p', p'') = \langle p'| V(\hat{x}) |p''\rangle = \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} e^{\frac{i}{\hbar}x(p''-p')} V(x) dx. \tag{3.37}$$

Exercise 3.15 Find the momentum representation of the position operator function $V(\hat{x}) = V_0\delta(x)$.
Answer: Constant $V_0/(2\pi\hbar)$.

Exercise 3.16 For a normalized Gaussian wavefunction

$$\psi(x) = \frac{1}{(\pi d^2)^{1/4}} e^{i\frac{p_0 x}{\hbar}} e^{-\frac{(x-a)^2}{2d^2}}, \tag{3.38}$$

a) calculate the corresponding wavefunction in the momentum basis. Verify normalization. (**Hint:** use the standard rules for the Fourier transformation);

b) calculate the expectation values of the position and momentum.

Answer:

$$\tilde{\psi}(k) = \left(\frac{d^2}{\pi}\right)^{1/4} e^{-i(k-k_0)a} e^{-(k-k_0)^2 d^2/2}, \tag{3.39}$$

where $k_0 = p_0/\hbar$. $\langle x\rangle = a$, $\langle p\rangle = p_0$.

Exercise 3.17 Show that the matrix element $\langle x| \hat{p} |x'\rangle$ of the momentum in the position representation is given by

$$\langle x| \hat{p} |x'\rangle = -i\hbar \frac{d}{dx}\delta(x - x') = i\hbar \frac{d}{dx'}\delta(x - x') \tag{3.40}$$

Exercise 3.18 Show that, for an arbitrary state $|\psi\rangle$,

$$\langle x| \hat{p} |\psi\rangle = -i\hbar \frac{d}{dx} \langle x| \psi\rangle = -i\hbar \frac{d}{dx}\psi(x). \tag{3.41}$$

Exercise 3.19 Show that $\langle x| \hat{p}^2 |\psi\rangle = -\hbar^2 d^2\psi(x)/dx^2$.

Equation (3.41) is an important relation demonstrating the action of the momentum operator upon a quantum state in the position basis. If state $|\psi\rangle$ has wavefunction $\psi(x)$ in the position basis, state $\hat{p}|\psi\rangle$ has wavefunction $-i\hbar \mathrm{d}\psi(x)/\mathrm{d}x$.

Exercise 3.20 Obtain the analogues of the two expressions above for the position operator in the momentum representation.

a) Show that the matrix element is

$$\langle p| \hat{x} |p'\rangle = i\hbar \frac{d}{dp}\delta(p - p') \tag{3.42}$$

b) Show that, for an arbitrary state $|\psi\rangle$,

$$\langle p| \hat{x} |\psi\rangle = i\hbar \frac{d}{dp}\tilde{\psi}(p). \tag{3.43}$$

An important operator in one-dimensional quantum mechanics is the *position displacement operator*, which translates the wavefunction in the position basis by a certain distance. As we see below, this operator is given by $e^{-i\hat{p}x_0/\hbar}$, where x_0 is the displacement distance (Fig. 3.2). The momentum displacement operator is defined similarly and given by $e^{ip_0x/\hbar}\psi(x)$, p_0 being the displacement momentum.

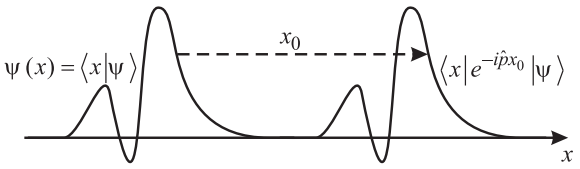


Figure 3.2: Effect of the position displacement operator on a wavefunction.

Exercise 3.21 Show that

a)
$$e^{-i\hat{p}x_0/\hbar}|x\rangle = |x + x_0\rangle\,; \tag{3.44}$$

b) if the wavefunction of state $|\psi\rangle$ is $\psi(x)$, then the wavefunction of state $e^{-i\hat{p}x_0/\hbar}|\psi\rangle$ is $\psi(x-x_0)$;

c) application of the position displacement operator to a state adds x_0 to the mean position value, but does not change the mean momentum value;

d) application of the position displacement operator to a state does not change the position and momentum uncertainties.

Exercise 3.22 Show that the momentum displacement operator $e^{ip_0\hat{x}\hbar}$ has similar properties with respect to the momentum as does the position displacement operator with respect to the position.

Exercise 3.23 Do the position and momentum displacement operators commute?

Exercise 3.24 Show that for a real wave function $\psi(x)$, $\mathrm{pr}(p) = \mathrm{pr}(-p)$. Show that the expectation value of the momentum observable is zero.

Now that we have practiced switching between the position and momentum bases, we are ready to introduce the uncertainty relation between these observables. As we know from Sec. 1.14, the uncertainty relation of any two observables is determined by their commutator.

Exercise 3.25 Show that, for any state $|\psi\rangle$,

a)
$$\langle x|\,\hat{x}\hat{p}|\,\psi\rangle = -i\hbar x\frac{\mathrm{d}}{\mathrm{d}x}\psi(x); \tag{3.45}$$

b)
$$\langle x|\,\hat{p}\hat{x}|\,\psi\rangle = -i\hbar x\frac{\mathrm{d}}{\mathrm{d}x}\psi(x) - i\hbar\psi(x); \tag{3.46}$$

c)
$$[\hat{x},\hat{p}] = i\hbar. \tag{3.47}$$

Exercise 3.26 Show that the Heisenberg uncertainty principle for the position and momentum operators has the form
$$\langle\Delta x^2\rangle\langle\Delta p^2\rangle \geq \frac{\hbar^2}{4}. \tag{3.48}$$

Exercise 3.27 For a Gaussian wavefunction,

$$\psi_{\text{Gauss}}(x) = \frac{1}{\pi^{1/4}\sqrt{d}} e^{-\frac{x^2}{2d^2}}, \tag{3.49}$$

calculate $\langle \Delta x^2 \rangle$, $\langle \Delta p^2 \rangle$ and verify the uncertainty principle.
Hint:

$$\int_{-\infty}^{+\infty} x^2 e^{-x^2} dx = \sqrt{\pi}/2 \tag{3.50}$$

Answer: $\langle \Delta x^2 \rangle = d^2/2$, $\langle \Delta p^2 \rangle = \hbar^2/2d^2$.

We have thus obtained the uncertainty principle in its original form, as defined by Werner Heisenberg in 1927: simultaneous, precise measurement of a particle's position and momentum is not possible. From the last example above we see that the position-momentum uncertainty can be interpreted as a consequence of one of the properties of the Fourier transformation: if the wavefunction in the position basis becomes "narrower", its Fourier transform, i.e. the wavefunction in the momentum basis, becomes "wider". A reduction in the position uncertainty of a state entails an increase in the momentum uncertainty, and vice versa.

Now let us reproduce in its original form another research masterpiece, the 1935 Einstein-Podolsky-Rosen paradox.

Exercise 3.28 Suppose each of the two observers, Alice and Bob, holds a one-dimensional pointlike particle. The two particles are prepared in entangled state $|\Psi_{AB}\rangle$ whose wavefunction is

$$\Psi(x_A, x_B) = \delta(x_A - x_B) \tag{3.51}$$

a) Express the state of the two particles in the momentum representation. Neglect normalization.

b) Suppose Alice performs a measurement of her particle's position and obtains some result x_0. Onto which state will Bob's particle project?

c) Suppose Alice instead performs a measurement of her particle's momentum and obtains some result p_0. Onto which state will Bob's particle project?

Answer: a)$\tilde{\Psi}(p_A, p_B) = \delta(p_A + p_B)$; b)$|x_0\rangle$; c)$|-p_0\rangle$.

Here is how Einstein, Podolsky and Rosen describe this paradoxical situation:
...either one or the other, but not both simultaneously, of the quantities P and Q can be predicted, they are not simultaneously real. This makes the reality of P and Q depend upon the progress of the measurement carried out on the first system, which does not disturb the second system in any way. No reasonable definition of reality could be expected to permit that.[7]

In other words, by choosing to measure in the position or momentum basis, Alice can create one of two mutually incompatible physical realities associated with Bob's particle: either a state with a certain position and uncertain momentum or the other way around. This appears unphysical because the physical reality at Bob's location is changed through a remote action by Alice without any interaction.

3.4 The free space potential

For the remainder of this chapter, we will solve the Schrödinger equation for the motion of a pointlike particle in a field of some conservative force. In classical physics, this motion is determined by the Hamiltonian, i.e. the sum of the kinetic and potential energies expressed as a function of the particle's position and momentum. The quantum expression for the Hamiltonian is identical to classical except that the canonical observables are written as operators:

$$\hat{H} = V(\hat{x}) + \frac{\hat{p}^2}{2m}. \tag{3.52}$$

[7] Einstein, Podolsky and Rosen use symbols Q and P for the position and momentum observables, respectively.

Here m ia the particle's mass, $\hat{p}^2/2m$ is the kinetic energy operator and $V(\hat{x})$ is the potential energy operator, which is the function of the position operator. Our goal is to solve the Schrödinger equation associated with this Hamiltonian.

Because both canonical observables can be expressed in the position basis (see Ex. 3.19), it is also convenient to write the Schrödinger equation in this basis — that is, take the inner product of $\langle x|$ with both sides of Eq. (1.76).

Exercise 3.29 Show that in the x-basis, the Schrödinger equation (1.76) takes the form

$$\frac{d\psi(x,t)}{dt} = -\frac{i}{\hbar}\left[V(x) - \frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right]\psi(x,t). \tag{3.53}$$

We have thus rewritten the Schrödinger equation, describing the quantum evolution of an abstract object — the quantum state — as something much more concrete: a partial differential equation. Let us now solve this equation for the simplest case, $V(x) \equiv 0$ (the *free space* evolution). Under this condition, any eigenstate $|p\rangle$ of the momentum operator with eigenvalue p is also an eigenstate of the Hamiltonian (3.52) with the eigenvalue $E = p^2/2m$.

Exercise 3.30 Show that the wavefunction describing the evolution of state $|p\rangle$ under Hamiltonian (3.52) with $V(x) \equiv 0$ is given by

$$\psi_p(x,t) = \frac{1}{\sqrt{2\pi\hbar}} e^{i\frac{p}{\hbar}x - i\frac{p^2}{2m\hbar}t}. \tag{3.54}$$

Find the phase velocity of this wave.

According to the above, the time-dependent behavior of the wavefunction of the momentum eigenstate is similar to that of a traveling wave of wavevector $k = p/m$ and angular frequency

$$\omega = p^2/2m\hbar = \hbar k^2/2m. \tag{3.55}$$

The evolution of this wave consists of translation with the *phase velocity* $v_{ph} = \lambda_{dB}/T = \omega/k = p/2m$, where $T = 2\pi/\omega$ is the period associated with the wave motion.

Note that the phase velocity is different from the value p/m expected classically. The explanation is that in the momentum eigenstate, the position is completely uncertain and the probability of finding the particle anywhere in space is the same, $\mathrm{pr}_x \propto |\psi_p(x,t)|^2 = 1/2\pi\hbar$. This probability does not change with time. Accordingly, the phase velocity of the de Broglie wave does not have any direct correspondence to the motion of matter[8].

In order to understand how the Schrödinger evolution translates into motion, we have to study a state whose wavefunction is to some extent localized in space (we use the term *wavepacket* for such wavefunctions). For example, let us investigate the Gaussian wavepacket with a nonzero mean momentum.

Exercise 3.31 Consider a wavefunction that at the moment $t = 0$ has a Gaussian form (3.38) with $a = 0$.

a) Find the corresponding wavefunction $\tilde{\psi}(k,0)$ in the wavevector representation. Find its evolution $\tilde{\psi}(k,t)$ under the free space Hamiltonian.

[8] In fact, the phase velocity of the de Broglie wave is a matter of convention rather than physics. If we assume a constant potential $V(x) = V_0$ and calculate the Hamiltonian eigenstate with energy $E + V_0$, its time-dependent wavefunction will be of the form

$$\psi_p(x,t) = \frac{1}{\sqrt{2\pi\hbar}} e^{i\frac{p}{\hbar}x - i\frac{E+V_0}{\hbar}t}.$$

The spatial behavior of this wavefunction is the same as that in Eq. (3.54), because the energy is related to the momentum according to $E = p^2/2m$. But the time evolution will be faster because the frequency of the wave now equals $(E+V_0)\hbar$ rather than $E/\hbar$. Accordingly, the wavefunction, which describes the physical setting that is identical to that of a free particle of energy E, will have a different phase velocity.

b) Find the wavefunction $\psi(x,t)$ in the position basis.
Hint: express $k = k_0 + \delta k$. Perform the inverse Fourier transformation with respect to δk and then use Eqs. (C.24) and (C.25) for the Fourier transformation of a shifted function.

c) Find the mean value of the position $\langle x \rangle$ and its variance $\langle \Delta x^2 \rangle$ as functions of time. Compare the velocity of the wavepacket with that expected classically and the phase velocity of the de Broglie wave.
Answer: $\langle x \rangle = (p_0/m)t$, $\langle \Delta x^2 \rangle = \frac{d^2}{2}\left(1 + \frac{\hbar^2 t^2}{m^2 d^4}\right)$

We see that the evolution of the Gaussian wavepacket consists of three features: (1) multiplication by an overall phase factor (which has no physical consequences), (2) translation with the effective velocity $v_{gr} = p_0/m$ and (3) spreading in space. As we see below, the spreading is a secondary effect that can often be neglected. Aside from that spreading, the shape of the Gaussian wavepacket remains the same; it travels as a single unit, reproducing the classical motion of a pointlike particle.

Exercise 3.32 a) Show that if p_0 greatly exceeds the momentum uncertainty of the initial wavepacket, the distance traveled by the center of the wavepacket during time t is much greater than the length over which it spreads.

b) Estimate the time required by a wavepacket associated with a single electron with the position uncertainty on the scale of 1 Å, to spread over a length of 1 mm.

It is instructive to draw an analogy with wave optics. In its many aspects, the evolution of the wavepacket resembles that of a short laser pulse. Such a pulse can be decomposed, by means of the Fourier transform, into a set of plane waves with different frequencies. If the pulse propagates in vacuum, such that all its plane wave components travel with the same phase velocity (c), the group velocity of the wavepacket is also c and the wavepacket does not spread. But if the pulse enters a refractive medium in which the phase velocity depends on the wavelength (i.e. *dispersion* is present), then the wavepacket motion will be determined by its *group velocity*,

$$v_{gr} = \mathrm{d}\omega/\mathrm{d}k, \tag{3.56}$$

and the wavepacket may experience spreading. This is exactly what we observe with our matter wavepacket.

Exercise 3.33 Apply expression (3.56) to Eq. (3.55) to show that the group velocity of a matter wavepacket with a mean momentum p_0 and momentum uncertainty $\Delta p \ll p_0$ equals $v_{gr} \approx p_0/m$.

Classical features associated with the motion of wavepackets can be revealed in an even more general form by way of the following calculations.

Exercise 3.34 Show that for any arbitrary state $|\psi\rangle$ that evolves in accordance with the Schrödinger equation and any arbitrary operator $\hat{A}$,

$$\frac{d\left\langle \hat{A} \right\rangle}{dt} = \frac{i}{\hbar}\left\langle [\hat{H}, \hat{A}] \right\rangle, \tag{3.57}$$

where averaging is meant in the quantum-mechanical sense, i.e. $\left\langle \hat{A} \right\rangle = \langle\psi| \hat{A} |\psi\rangle$.

Exercise 3.35 For the Schrödinger evolution of a state of a pointlike particle, show that

a)
$$\langle \dot{\hat{x}} \rangle = \langle \hat{p} \rangle / m. \tag{3.58}$$

b)
$$\frac{d\langle \hat{p} \rangle}{dt} = \int_{-\infty}^{+\infty} \psi(x)\psi^*(x)\left(-\frac{dV(x)}{dx}\right) dx = -\left\langle \psi \left| \frac{d\hat{V}}{dx} \right| \psi \right\rangle, \tag{3.59}$$

where $V(x)$ is the potential as a function of the position.

Relation (3.59) is known as the *Ehrenfest theorem*. In order to understand its meaning, let us remember that, in classical mechanics, we associate a potential energy with a conservative force field by means of the following expression (here specialized to one-dimensional motion):

$$U(x_1) - U(x_2) = \int_{x_1}^{x_2} F(x)\mathrm{d}x. \tag{3.60}$$

Using the Newton-Leibniz axiom, we can rewrite it as

$$F(x) = -\frac{dV(x)}{dx}. \tag{3.61}$$

But the right-hand side of the above equation is identical to that entering Eq. (3.59). In other words, Eq. (3.59) tells us that the time derivative of the particle's mean momentum equals the mean force acting on that particle. But this is simply the second Newton's law!

3.5 Multidimensional motion and probability flux

Exercise 3.36 Recalling that $\mathrm{pr}(x) = \psi(x)\psi^*(x)$, derive the following equation:

$$\frac{d\mathrm{pr}(x)}{dt} = -\frac{dj}{dx}, \tag{3.62}$$

where

$$j = -i\frac{\hbar}{2m}\left(\psi^*\frac{d\psi}{dx} - \psi\frac{d\psi^*}{dx}\right). \tag{3.63}$$

Definition 3.1 The quantity j in the above equation is the *probability current density* indicating the flow of the probability density per unit time. Eq. (3.62) is called the *continuity equation*.

Note 3.1 The continuity equation, whose multidimensional form is $\frac{d\mathrm{pr}(x)}{dt} = -\vec{\nabla}\cdot\vec{j}$ governs the flow of any conserved quantity and is present in many fields of physics, for example, electro- and hydrodynamics.

Exercise 3.37 If the wavefunction can be made real through multiplying by an overall phase factor, the probability flow vanishes.

Exercise 3.38 Show that the probability density current for the de Broglie wave is proportional to its momentum.

Exercise 3.39 Verify the continuity equation explicitly for a spreading Gaussian wavepacket at rest (Ex. 3.31).

Exercise 3.40 Consider a wavefunction which is a superposition of two wavepackets, one defined by Eq. (3.38) and one being its mirror image around the point $x = 0$. Assume $p_0 = 0$ and $a \gg d$, i.e. the two wavepackets have almost no spatial overlap.

a) What is the correct normalization factor?

b) Find the corresponding probability density $\mathrm{pr}(p)$ in the momentum space.

c)* Using the result of Exercise 3.31, find the probability density in the position space after a very long time t. Discuss the analogy with two-slit diffraction in optics.

Exercise 3.41 Derive, for a three-dimensional geometric space,

a) the Schrödinger equation in the x-basis;

b) the quantum-mechanical continuity equation.

3.6 Time-independent Schrödinger equation

Frequently, our goal is to find the energy eigenstates, i.e. such states $|\psi\rangle$ that $\hat{H}|\psi\rangle = E|\psi\rangle$. This equation is referred to as the *time-independent Schrödinger equation*. In the x-basis, it takes the form (*cf.* Eq. (3.29)):

$$\left[V(x) - \frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right]\psi(x) = E\psi(x) \tag{3.64}$$

This is a second-order ordinary differential equation, which can be readily solved, particularly if the potential is a "nice" function of the position. For example, let us find the solution for a constant potential.

Exercise 3.42 Find the general solutions to Eq. (3.64) for $V(x) = V_0$. Consider the cases (a) $E > V_0$ (b) $E < V_0$.
Answer: (a) $Ae^{ikx} + Be^{-ikx}$; (b) $Ae^{kx} + Be^{-kx}$ where $k = \sqrt{2m|E - V_0|}/\hbar$ and A, B are random coefficients.

We see that the solutions are fundamentally different for the energies above and below the potential level. In the former case, we obtain an oscillatory solution akin to the de Broglie wave. In the latter case, the solutions are exponentially growing or falling as a function of the position. If the potential is constant for all positions, such a solution will blow up at $x \to \pm\infty$ — a behavior which implies infinite probabilities and thus cannot occur in a physical state (or even in an approximation thereof). Hence there are no Hamiltonian eigenstates with eigenvalues below the potential energy level. However, situations where the energy is lower than the potential for a *part* of the position axis are possible, as is the case, for example, with quantum tunneling.

Before we proceed to finding the energy eigenwavefunctions for specific potentials, let us derive a few general properties of these wavefunctions that will assist us in this task.

Exercise 3.43 Show that, if $\psi(x)$ is a solution of the time-independent Schrödinger equation, then both $\psi(x)$ and $\mathrm{d}\psi(x)/\mathrm{d}x$ must be continuous if both the potential $V(x)$ and the wavefunction are finite for all x.

This result will turn out extremely useful for many problems in which the potential is given by a piecewise function, i.e. a set of different elementary functions each defined on its own interval of positions. It is relatively easy to find the solution for each interval, but then these solutions must be "stitched together" to form a physically meaningful wavefunction. Exercise 3.43 provides us with the guideline for this "stithcing".

Exercise 3.44 Consider set S_E consisting of all Hamiltonian eigenstates with energy eigenvalue E. Show that:

a) There exists a spanning set of S_E which consists only of states with real wavefunctions — so any element of S_E can be written as a linear combination of energy eigenstates with the same energy eigenvalue and real wavefunctions;

b) if $V(x)$ is an even function of the position, ehere exists a spanning set of S_E consisting only of states with wavefunctions that are either even or odd.

Exercise 3.44 simplifies our search for solutions of the time-independent Schrödinger equation. In particular, it is sufficient to only look for wavefunctions that are real. Then we are guaranteed not to "miss" any solution that cannot be written as a linear combination of those solutions that we have found.

For example, the de Broglie wave

$$\psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}}e^{i\frac{px}{\hbar}}, \tag{3.65}$$

associated with momentum eigenstate $|p\rangle$, is a solution of the time-independent Schrödinger equation with energy eigenvalue $E = p^2/2m$. The same is true for the wavefunction

$$\psi_{-p}(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{-i\frac{px}{\hbar}}, \tag{3.66}$$

which is the de Broglie wave for momentum eigenstate $|-p\rangle$. But then the real wavefunctions

$$\psi_{p,+}(x) = \frac{\psi_p(x) + \psi_{-p}(x)}{2} = \frac{1}{\sqrt{2\pi\hbar}} \cos\frac{px}{\hbar} \tag{3.67}$$

and

$$\psi_{p,-}(x) = \frac{\psi_p(x) - \psi_{-p}(x)}{2i} = \frac{1}{\sqrt{2\pi\hbar}} \sin\frac{px}{\hbar} \tag{3.68}$$

also represent energy eigenstates with the same eigenvalue. The de Broglie wavefunctions (3.65) and (3.66) — and hence can any other wavefunction corresponding to the same energy — can be written as linear combinations of these real wavefunctions.

3.7 Bound states

Bound states are characterized by a wavefunction that tends to zero at $|x| \to \pm\infty$, so the particle exhibits some degree of localization. This property is typical for energy eigenstates in well-shaped potentials, i.e. such fields in which the particle is attracted towards a certain location or a set of locations. Physical examples include a pea inside a glass, a ball on a spring (harmonic oscillator) or an electron within an atom. For this type of potentials, we usually take advantage of Ex. 3.44(a) and look for solutions of the time-independent Schrödinger equation in the real domain.

Exercise 3.45 Consider a potential $V(x)$ that approaches a particular value V_0 at $|x| \to \pm\infty$. Show that an energy eigenstate is bound if and only if its energy does not exceed V_0.

As we shall see in the examples below, the boundary conditions imposed on the behavior of the wavefunction at $|x| \to \pm\infty$ can be satisfied only for specific, discrete values of the energy. In other words, a well-shaped potential features a *discrete* or *quantized* spectrum of energy eigenvalues.

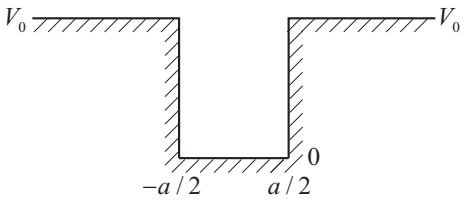


Figure 3.3: Potential for Ex. 3.69

Exercise 3.46 Find the energy eigenvalues and eigenwavefunctions for the *finite square well* potential:

$$V(x) = \begin{cases} V_0 \text{ for } |x| > a/2 \\ 0 \text{ for } |x| \le a/2 \end{cases} \tag{3.69}$$

a) Write the general solution for each region where the potential is constant. Eliminate unphysical terms that grow at infinity.

b) Apply the statement of Ex. 3.43 to "stitch" these results together. Derive the transcendental equation defining the energy eigenvalues.

Hint: use the result of Ex. 3.44(b).
Answer: Even wavefunctions:

$$\tan\theta = \sqrt{(\theta_0/\theta)^2 - 1}; \tag{3.70a}$$

odd wavefunctions:

$$\cot\theta = -\sqrt{(\theta_0/\theta)^2 - 1}, \tag{3.70b}$$

where

$$\theta = \sqrt{2mE}a/2\hbar; \quad \theta_0 = \sqrt{2mV_0}a/2\hbar. \tag{3.71}$$

c) Solve the equation for the energy eigenvalues graphically.

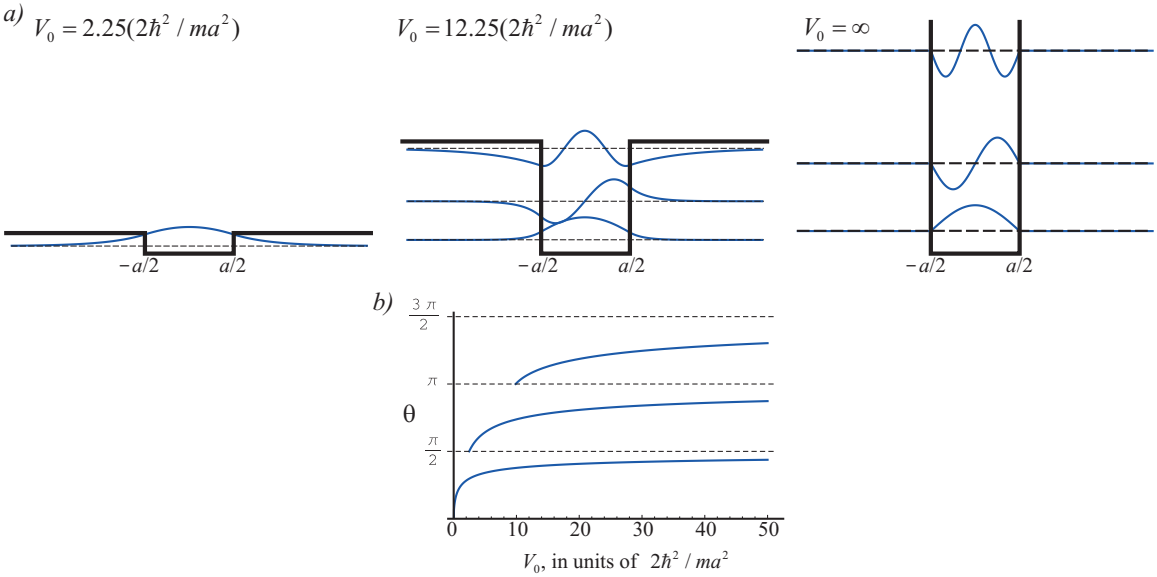


Figure 3.4: Solution for Ex. 3.69. a) Wavefunctions for the lowest energy eigenstates with different well depths. The well on the left supports only one bound state; the well in the middle, three bound states, the well on the right supports infinitely many. The zero of each wavefunction corresponds to the associated energy eigenvalue. b) Three lowest energy solutions of the transcendental equations (3.70) as a function of the well depth. At least one bound state exists for all V_0; the existence of further bound states is conditional on V_0 exceeding certain threshold values.

It is instructive to plot the wavefunctions for a few lowest energy eigenstates of potential (3.69). As we can see in , the wavefunction extends outside the box, so there is a finite probability to find the particle in the region where the potential is higher than the particle's energy. This is, of course, an expressly nonclassical phenomenon. The deeper the well, the smaller the part of the wavefunction outside the well, and hence the probability to find the particle in that region. In the limit $V_0 \to \infty$, this probability tends to zero. In this case, the problem permits an analytic solution, as we see in the following Exercise.

As expected from Ex. 3.42, we see exponential decay outside the well and oscillatory behavior inside. For each subsequent energy eigenstate, the number of times the wavefunction crosses the x axis increments by one. The increasing number of crossings is associated with a faster oscillation, a higher wavevector, and hence a higher energy value. Accordingly, for each number of crossings there exists a certain minimum potential, below which the bound state no longer exist [Fig. 3.4(b)]. A well of a finite depth can thus support only a finite number of bound states. However, no matter how shallow the well, it does support at least one bound state [Fig. 3.4(b)].

Exercise 3.47 Find the energy eigenvalues and bound stationary states for Ex. 3.46 in the case $V_0 \to \infty$ (the potential referred to as the *potential box*).
Answer: A discrete energy spectrum with

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2ma^2}; \tag{3.72}$$

$$\begin{aligned} \psi_n(x) &= \left\{ \begin{array}{l} \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right), \quad \text{even } n \\ \sqrt{\frac{2}{a}} \cos\left(\frac{n\pi x}{a}\right), \quad \text{odd } n. \end{array} \right\}, \quad -a/2 \leq x \leq a/2; \\ \psi_n(x) &= 0, \quad |x| > a/2. \end{aligned} \tag{3.73}$$

These wavefunctions are displayed in Fig. 3.4(a), right panel.

The above wavefunctions exhibit a number of interesting features:

- $\psi(x) = 0$ outside the box;
- $\mathrm{d}\psi(x)/\mathrm{d}x$ exhibits discontinuities at $x = \pm a/2$;
- $\psi(x)$ is continuous for all position values.

In order to better understand them, let us rewrite the time-independent Schrödinger equation (3.64) as follows:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = [E - V(x)]\psi(x). \tag{3.74}$$

Outside the box, $V(x) = \infty$. Therefore, if $\psi(x)$ is nonzero, the right-hand side of the above equation becomes infinite, and so does $\mathrm{d}^2\psi(x)/\mathrm{d}x^2$ over a continuous interval of positions. This is not possible for any regular function.

The infinite value of the potential outside the box also implies that the conditions of Ex. 3.43 are not fulfilled, so neither the wavefunction nor its derivative have to be continuous at $x = \pm a/2$. In the present case, we observe that the wavefunction is continuous but the derivative is not. Intuitively this can be understood as follows. A discontinuity in $\mathrm{d}\psi(x)/\mathrm{d}x$ implies that the right-hand side of Eq. (3.74) is singular, i.e. it takes on infinite values — which is exactly what we have in our problem. But if the wavefunction itself is not continuous, the potential must exhibit singularity of the second order — i.e. be a derivative of a function that is already singular. Such potentials are extremely exotic and do not occur within the scope of basic quantum mechanics. Therefore, in solving the time-independent Schrödinger equation in the position basis, it is generally safe to assume that the wavefunction behaves continuously.

Exercise 3.48 For the eigenstates of the previous problem, find the uncertainties of the position and momentum and verify the uncertainty principle.

Exercise 3.49 Consider the state $\psi(x) = \left\{ \begin{smallmatrix} Ax \text{ for } |x|<a/2 \\ 0 \text{ for } |x|\geq a/2 \end{smallmatrix} \right.$ ($A = 2\sqrt{3}/a^{3/2}$ being the norm) in the potential of the previous problem. Find the energy spectrum of this state, i.e. the probabilities $\mathrm{pr}(E_n)$ to measure each energy eigenvalue. Show that these probabilities sum up to 1. (**Hint:** $\sum 1/n^2 = \pi^2/6$.)

Exercise 3.50 For the finite well potential (3.69):

a) Find analytically the approximate corrections to the first two energy levels of an infinitely deep potential well (Ex. 3.47) when it is replaced by a finite well with a $V_0 \gg E_1$, where E_1 is given by Eq. (3.72).

b) Find numerically all energy eigenvalues for $k_0 a = 10$. How many energy levels are there altogether? Is your result for $n = 1, 2$ consistent with the result of part (a)?

c) What is the minimum depth that is required in order for the well to contain a given number N of bound eigenstates?

Exercise 3.51 Find the transcendental equation for the energy eigenvalues associated with the bound stationary states of the potential

$$V(x) = \begin{cases} +\infty \text{ for } x \leq 0; \\ 0 \text{ for } 0 < x \leq a; \\ V_0 \text{ for } x > a. \end{cases}$$

Compare your result with that of Ex. 3.69.

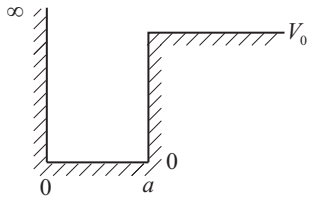


Figure 3.5: Potential for Ex. 3.51

Exercise 3.52 Solve the time-independent Schrödinger equation for the finite well potential (3.69) anlytically in the limit of an infinitely deep and narrow potential well: $a \to 0$, $V_0 = W_0/a$, with $W_0 = \text{const}$. How many bound states can this well contain?

Exercise 3.53 Find the energy eigenvalues and the bound stationary states of the potential $V(x) = -W_0\delta(x)$

a) (a) using the position basis; (b) using the momentum basis.

Verify the consistency of your solutions with one another and with the result of Ex. finitewellEx2
Hint:

$$\int_{-\infty}^{+\infty} \frac{1}{1+x^2}dx = \pi; \quad \int_{-\infty}^{+\infty} \frac{1}{(1+x^2)^2}dx = \pi/2 \tag{3.75}$$

Answer: Single eigenstate with $E = -W_0^2 m/2\hbar^2$. Wavefunctions:

$$\psi(x) = \sqrt{k_0} \begin{cases} e^{-k_0 x} \text{ at } x > 0 \\ e^{k_0 x} \text{ at } x \leq 0 \end{cases};$$

$$\tilde{\psi}(k) = \frac{2k_0^{3/2}}{\sqrt{2\pi}(k_0^2 + k^2)},$$

where $k_0 = \sqrt{-2mE}/\hbar = W_0 m/\hbar^2$.

Exercise 3.54 A particle is in the bound state of the potential $V(x) = -W_0\delta(x)$. The potential suddenly changes to $V(x) = -2W_0\delta(x)$. Find the probability that the particle will remain in a bound state.

Exercise 3.55 Investigate the bound states of the potential $V(x) = -W_0\delta(x-a) - W_0\delta(x+a)$.

a) Find the transcendental equation for the energy eigenvalues (consider both the even and odd case).

b) Show that in the limit $a \to \infty$ this equation becomes identical to that for a single well.

c) Find the first order correction to the solution of the transcendental equation for the case of a being very large ($k_0 a \gg 1$), but not infinite.

Exercise 3.56 Under the conditions of the previous problem (distant wells), suppose the particle at the moment $t = 0$ is localized at the first well (i.e. its wavefunction is that of Ex. 3.53 centered at $x = a$). What is the probability of finding it in the second well as a function of time?

Exercise 3.57* (Kronig-Penney solid state model). Find allowed ranges (zones) of energy eigenvalues for a particle in a periodic potential field

a)

$$V(x) = \sum_{n=-\infty}^{\infty} \frac{\hbar^2 k_0}{m} \delta(x - na); \tag{3.76}$$

b)

$$V(x) = -\sum_{n=-\infty}^{\infty} \frac{\hbar^2 k_0}{m} \delta(x - na). \tag{3.77}$$

Consider both limiting cases $k_0 a \gg 1$ and $k_0 a \ll 1$.

Exercise 3.58* Show that bound energy eigenstates states of a pointlike particle with a single degree of freedom cannot be degenerate.

3.8 Unbound states

Unbound wavefunctions take finite, nonzero values at infinity. In contrast to bound states, stationary unbound states possess the following properties.

- Their energy exceeds the value of the potential at $x \to -\infty$ or $x \to +\infty$ or both.
- They are not normalizable.
- Their associated energy eigenvalues form a continuous spectrum.
- They can be degenerate: more than one linearly independent wavefunctions may correspond to a specific energy eigenvalue.

The most straightforward example of the unbound state is the momentum eigenstate $|p\rangle$ in free space. The associated energy eigenvalue, $E = p^2/2m$, exceeds the potential $V(x) = 0$ at infinity. Since there exists a momentum eigenstate $|p\rangle$, where $p = \sqrt{2mE}$, for every energy value, these values form a continuum. For every energy value, states $|\pm p\rangle$ are degenerate.

Let us now study the unbound energy eigenstates that correspond to more complicated potential energy functions.

Exercise 3.59 (the single-step potential). Find the eigenstates of the Hamiltonian

$$V(x) = \begin{cases} 0 \text{ for } x \leq 0 \\ V_0 \text{ for } x > 0 \end{cases} \tag{3.78}$$

(Fig. 3.6) corresponding to a given energy $E > V_0$. Show that, for every value of E, there exist two linearly independent solutions. Choose the solutions that correspond to the following physical situations: (1) a wave approaching the step only from the left and (2) a wave approaching only from the right.

Answer (in the notation of Fig. 3.6). First solution ($D = 0$):

$$B = A\frac{k_0 - k_1}{k_0 + k_1}; \quad C = A\frac{2k_0}{k_0 + k_1}, \tag{3.79a}$$

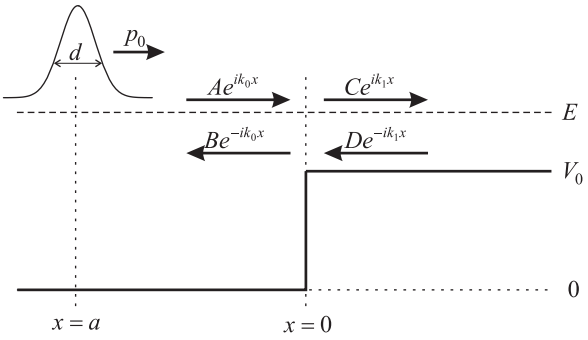


Figure 3.6: Notation for the de Broglie component waves in a single-step potential (Ex. 3.59 and 3.62)

and (2) an initial de Broglie wave approaching from the right ($A = 0$)

$$B = D\frac{2k_1}{k_0 + k_1}; \quad C = D\frac{k_1 - k_0}{k_0 + k_1}. \tag{3.79b}$$

Now let us try and relate our calculation to the intuitive physical picture of a material particle encountering a potential step. Making this connection may be difficult because the energy eigenstate is time independent, whereas the collision of a particle with a step, as we intuitively imagine it, is an intrinsically time-dependent phenomenon.

Some intuitive connection can be drawn in we recall that even stationary states experience quantum evolution, which consists of the time-dependent phase factor $e^{-iEt/\hbar}$. Accordingly, the de Broglie waves associated with amplitudes A and C (we will call them the A- and C-waves, respectively) move to the right while the B-wave is moving to the left.

This situation resembles a continuous laser beam which propagates from air into glass, experiencing partial reflection in accordance with the Fresnel equations. Similarly to the situation with the quantum particle, the reflection is not an instantaneous event but a stationary process which comprises motion of the electromagnetic waves in space and time. In fact, if we compare the Fresnel equations for the field amplitudes with Eqs. (3.79), and take into account that the optical wavevector is proportional to the index of refraction, we will find these two sets of equations completely identical!

An interesting feature of the result (3.79) is that the amplitude C of the transmitted de Broglie wave is higher than the amplitude A of the incident one. The particle appears more likely to be found behind the step than within the same interval in front of it. Doesn't that contradict the law of conservation of matter?

We can gain some insight for answering this question by looking at optical waves again. According to Fresnel equations, the amplitude of the light wave inside glass is also higher than that in the air. However, this does not conflict with the law of energy conservation because the wave inside the glass travels at a lower speed. Accordingly, the flux of energy (Poynting vector) carried by the transmitted wave is lower than that of the incident wave.

A similar argument can be drawn in the case of a quantum particle. It is not the probability density associated with the wavefunction that determines the conservation of matter but rather the probability density *current* studied in Sec. 3.5. As we learned in Ex. 3.38, this current is proportional not only to the squared absolute value of the de Broglie wave amplitude, but also to its momentum. If we take this into account, we will observe that the conservation of matter is perfectly sustained.

Exercise 3.60 Find the probability density currents for each wave in Eqs. (3.79a) and (3.79b). Find the reflection and transmission coefficients for these currents and show that their sum is one. What is the behavior of these coefficients for $E \to V_0$ and $E \to \infty$?

Exercise 3.61 Solve Ex. 3.59 for energies below V_0. Verify that the reflection coefficient is one.

An even better overview of the quantum reflection of a particle on a potential step can be obtained if we combine multiple de Broglie waves into a Gaussian wavepacket and then study its evolution in a way that is similar to Ex. 3.31, but in the potential given by Eq. (3.78).

Exercise 3.62 Find the evolution of a Gaussian packet initially described by Eq. (3.38) with a positive p_0 and negative a in the single-step potential field (Fig. 3.6). Assume that

- $|a| \gg d$ so the wavepacket is at first entirely to the left of the step;
- $d^2 \gg \hbar t/m$ so spreading of the wavepacket (Ex. 3.31) can be neglected;
- the initial average energy of the particle $E = p_0^2/2m$ is greater than V_0;
- the rms momentum uncertainty of the wavepacket $\hbar/2d$ is small compared to the average momentum $\hbar k_1 = \sqrt{2m(E_0 - V_0)}$ behind the step.

As we see, upon encountering the step the initial wavepacket splits. A part of the wavepacket continues to propagate past the step with a lower group velocity, and another part reflects off the step and begins to propagate in the backward direction.

As the final comment about the potential step problem let us note that the fact that the particle has a probability to bounce off a potential step that is lower than the particle's energy or even negative (as in the case described by Eq. (3.79b)) is expressly quantum. Any classical particle will simply "fly above" the potential step, reducing or increasing the speed but never reversing the direction of its motion.

Even more nonclassical is the effect of *quantum tunneling*, which we study next.

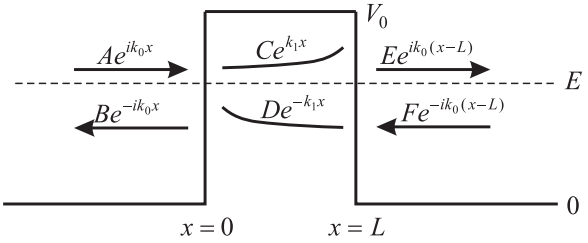


Figure 3.7: Tunnelling through a barrier (Ex. 3.63)

Exercise 3.63 Consider the potential in Fig. 3.7, i.e.

$$V(x) = \begin{cases} 0 \text{ for } x \leq 0 \text{ or } x > L \\ V_0 \text{ for } 0 < x \leq L \end{cases} \tag{3.80}$$

a) What is the degeneracy of energy levels?

b) Find the solution of the time-independent Schrödinger equation corresponding to a de Broglie wave entering from the left and $0 < E < V_0$.

c) Find the transmission and reflection coefficients for the probability current. Is their sum equal to one?

d) Investigate the boundary cases $E \to 0$ and $E \to V_0$.

Answer.

$$T = \left|\frac{E}{A}\right|^2 = \frac{4k_0^2k_1^2}{4k_0^2k_1^2 + (k_1^2 + k_0^2)^2 \sinh(k_1L)}; \tag{3.81a}$$

$$R = \left|\frac{B}{A}\right|^2 = \frac{(k_1^2 + k_0^2)^2 \sinh(k_1L)}{4k_0^2k_1^2 + (k_1^2 + k_0^2)^2 \sinh(k_1L)}. \tag{3.81b}$$

We observe that a particle encountering a finite potential barrier which is higher than the particle's kinetic energy has a finite probability of "tunnelling" through this barrier. This phenomenon has, of course, no analogy in classical physics.

Exercise 3.64 Repeat Ex. 3.63 for $E > V_0$. Is the sum of the reflection and transmission coefficients equal to one in this case?

Exercise 3.65 Calculate the reflection and transmission for scattering on a delta-potential $V(x) = W_0\delta(x)$. Compare your results with those obtained from Eqs. (3.81) for an infinitely thin and high rectangular potential barrier ($L \to 0$, $V_0 = W_0/L$).

Exercise 3.66* Perform numerical investigations of the propagation of a Gaussian wavepacket in a potential shown in Fig. 3.7. Make simplifying assumptions as necessary. What time does it take the wavepacket to penetrate the barrier?

Solving the previous exercise, we find that the wavepacket spends no time inside the barrier. The tunnelling occurs *instantaneously*: the transmitted wavepacket emerges behind the barrier simultaneously with the initial wavepacket being absorbed. This can be traced back to the fact that the C- and D-waves have a constant phase, so the complex argument $\mathrm{Arg}\psi(x)$ of the wavefunction at points $x = 0$ and $x = L$ is the same. Schrödinger evolution of a de Broglie wave is equivalent to a phase shift, and the lack thereof translates into a zero delay between the incident and transmitted waves, resulting in an infinite group velocity.

In Chapter 2 we already encountered a quantum phenomenon that appeared to enable faster-than-light communication, but, after careful analysis, found this to be only an illusion. The same can be said about the present situation, although the reason is different. Let us ask ourselves: at what moment does an observer behind the barrier learn that the particle is entering the barrier? Is it when a half of the wavepacket has emerged from the barrier, three-fourths or nine-tenths?

The correct answer is, much earlier than that. From complex analysis, we know that the Gaussian function is *analytic*: any fragment of this function allows one to reconstruct its behavior in the entire complex plane. Therefore, any observer anywhere in space is aware of the presence of the particle with a Gaussian wavefunction, and can predict its evolution, from the initial moment of our analysis. With this in mind, it makes no sense to talk about instant communication.

What if we instead tried a different wavefunction, for example, of the top-hat shape (3.9), which takes on nonzero values only within a finite spatial region? The problem with such wavefunctions is that, in contrast to the Gaussian case, their decompositions into the momentum basis are not narrow: for example, the Fourier transform of the top-hat function is the sinc function. For such functions, we cannot apply the approximations used to calculate the evolution of Gaussian functions (see Ex. 3.62) — for example, because they have significant components corresponding to energies above the barrier. This tremendously complicates the calculations; however, if the analysis is perform thoroughly, it will exclude any possibility of superluminal propagation.

3.9 Harmonic oscillator

3.9.1 Annihilation and creation operators

The harmonic oscillator is a physical system of primary importance. Its applications extend far beyond the motion of simple mechanical systems. For example, the quantum description of light, not limited by the single-photon subspace studied in Chapters 1 and 2, is identical to that of the harmonic oscillator. Other applications include solid state physics, molecular spectroscopy and even atomic physics.

Figure 3.8(a) displays a classical harmonic oscillator — a "ball on a spring". The oscillation frequency ω is related to the spring constant k in accordance with $k = m\omega^2$. Because the potential energy of the spring is $U = kx^2/2$, its full Hamiltonian is given by

$$H = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2} \tag{3.82}$$

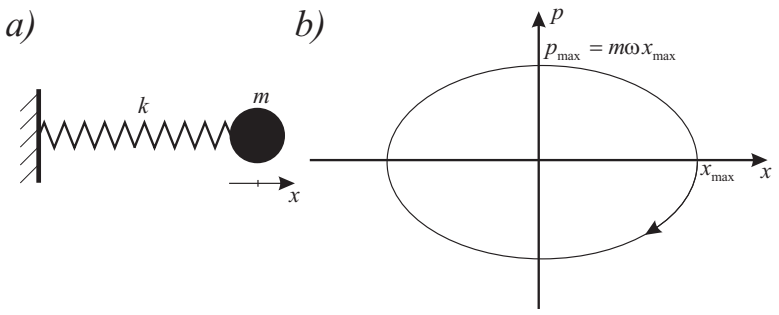


Figure 3.8: A classical harmonic oscillator. a) The physical model; b) motion in the phase space.

The trajectory is elliptical with the half-axes $p_{max} = m\omega x_{max}$.

The harmonic oscillator is a typical potential well. Therefore its energy eigenstates are bound and nondegenerate (see Ex. 3.58). It is possible to find the wavefunctions of these states by solving the time-independent Schrödinger equation (3.64) in the position basis. However, because the harmonic oscillator is such an important physical system, we choose to develop its quantum theory in a more general fashion. We begin by rescaling the position and momentum observables so they are more convenient to operate with.

Exercise 3.67 Rescale the position and momentum observables, i.e. define new observables ($X = Ax, P = Bp$) with proportionality constants A and B such that (a) in the new variables (X, P) the phase space trajectory is circular [$P_{max} = X_{max}$, see Fig. 3.8(b)] and (b) for corresponding quantum operators, $[\hat{X}, \hat{P}] = i$.
Answer:

$$\hat{X} = \hat{x}\sqrt{\frac{m\omega}{\hbar}}; \quad \hat{P} = \frac{p}{\sqrt{m\omega\hbar}} \tag{3.83}$$

Exercise 3.68 Show that the rescaled observables $\hat{X}$ and $\hat{P}$ are dimensionless.

Exercise 3.69 If a certain quantum state has wavefunctions $\psi(x) = \langle x|\ \psi\rangle$ and $\tilde{\psi}(p) = \langle p|\ \psi\rangle$, what are the corresponding wavefunctions $\psi(X) = \langle X|\ \psi\rangle$ and $\tilde{\psi}(P) = \langle P|\ \psi\rangle$ in the rescaled variables? Write the relations analogous to (3.33) for converting wavefunctions between $\hat{X}$- and $\hat{P}$- bases.

Exercise 3.70 Show that

$$\langle X|\,\hat{P}\,|\psi\rangle = -i\frac{d}{dX}\psi(X); \quad \langle P|\,\hat{X}\,|\psi\rangle = i\frac{d}{dP}\psi(P). \tag{3.84}$$

Exercise 3.71 Write the Hamiltonian in terms of $\hat{X}$ and $\hat{P}$
Answer:

$$\hat{H} = \frac{1}{2}\hbar\omega\left(\hat{X}^2 + \hat{P}^2\right). \tag{3.85}$$

We now proceed to defining and studying the properties of the two operators which, as we shall see in the next subscection, enact transitions between adjacent energy eigenstates.

Definition 3.2 The *annihilation* operator is defined as follows:

$$\hat{a} = \frac{1}{\sqrt{2}}\left(\hat{X} + i\hat{P}\right); \tag{3.86}$$

The operator $\hat{a}^\dagger$ is called the *creation* operator.

Exercise 3.72 Show that:

a) the creation operator is

$$\hat{a}^\dagger = \frac{1}{\sqrt{2}}\left(\hat{X} - i\hat{P}\right); \tag{3.87}$$

b) the creation and annihilation operators are not Hermitian;

c) their commutator is

$$[\hat{a}, \hat{a}^\dagger] = 1; \tag{3.88}$$

d) position and momentum can be expressed as

$$\hat{X} = \frac{1}{\sqrt{2}}\left(\hat{a} + \hat{a}^\dagger\right); \quad \hat{P} = \frac{1}{i\sqrt{2}}\left(\hat{a} - \hat{a}^\dagger\right); \tag{3.89}$$

e) the hamiltonian can be written as

$$\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right); \tag{3.90}$$

f) the commutators

$$[\hat{a}, \hat{a}^\dagger\hat{a}] = \hat{a}; \quad [\hat{a}^\dagger, \hat{a}^\dagger\hat{a}] = -\hat{a}^\dagger. \tag{3.91}$$

3.9.2 Fock states

Our next goal is to find eigenvalues and eigenstates of the Hamiltonian. Because of Eq. (3.90), they are also eigenstates of operator $\hat{n} = \hat{a}^\dagger\hat{a}$.

Exercise 3.73 Suppose some state $|n\rangle$ is an eigenstate of the operator $\hat{a}^\dagger\hat{a}$ with eigenvalue n:

$$\hat{a}^\dagger\hat{a}\,|n\rangle = n\,|n\rangle \tag{3.92}$$

Show that

a) the state $\hat{a}\,|n\rangle$ is also an eigenstate of $\hat{a}^\dagger\hat{a}$ with eigenvalue $n-1$;

b) the state $\hat{a}^\dagger\,|n\rangle$ is also an eigenstate of $\hat{a}^\dagger\hat{a}$ with eigenvalue $n+1$.

Hint: Use Eq. (3.91).

As we know, energy spectra of bound states are nondegenerate, i.e. for each value of n there exists no more than a single energy eigenstate $|n\rangle$. Therefore Ex. 3.73 shows that the states $\hat{a}\,|n\rangle$ and $\hat{a}^\dagger\,|n\rangle$ are proportional to states $|n-1\rangle$ and $|n+1\rangle$, respectively. The proportionality coefficient can be found from the requirement that the energy eigenstates must be normalized.

Exercise 3.74 Show that

a)

$$\hat{a}\,|n\rangle = \sqrt{n}\,|n-1\rangle; \tag{3.93a}$$

b)

$$\hat{a}^\dagger\,|n\rangle = \sqrt{n+1}\,|n+1\rangle; \tag{3.93b}$$

Hint: use $\langle n|\,\hat{a}^\dagger\hat{a}\,|n\rangle = n$.

We found that, if state $|n\rangle$ with energy $\hbar\omega(n+1/2)$ exists as a physical state (i.e. is a normalized element of the Hilbert space), so does the state $|n-1\rangle$ with energy $\hbar\omega(n-1/2)$. Similarly, states $|n-2\rangle$, $|n-3\rangle$, and so on must also exist. Continuing this chain for sufficiently many steps, we will end up with energy eigenstates with negative energy values.

How can we resolve this contradiction? The only way is to assume that n *must be nonnegative integer* so the chain is broken at $n=0$, in which case

$$\hat{a}\,|0\rangle = |\text{zero}\rangle\,. \tag{3.94}$$

Then (provided that the state $|n=0\rangle$ exists), energy eigenstates form an infinite set with equidistant eigenvalues $\hbar\omega(n+1/2)$.

Definition 3.3 Energy eigenstates of a harmonic oscillator are called *Fock* or *number* states. The state $|0\rangle$ is called the *vacuum state*.

Exercise 3.75 Express $|n\rangle$ through $|0\rangle$.
Answer:

$$|n\rangle = \frac{\left(\hat{a}^\dagger\right)^n}{\sqrt{n!}}\,|0\rangle \tag{3.95}$$

Exercise 3.76 Calculate the wavefunction of the vacuum state in the position and momentum representations.
Hint: use Eqs. (3.84), (3.86) and (3.94).
Answer:

$$\psi_0(X) = \frac{1}{\pi^{1/4}}e^{-X^2/2}; \quad \tilde{\psi}_0(P) = \frac{1}{\pi^{1/4}}e^{-P^2/2}. \tag{3.96}$$

Note that the above wavefunctions are unique up to an arbitrary overall phase factor. For the vacuum state, by convention, we choose this factor so as to obtain a real and positive definite wavefunction in the position basis. It then automatically follows that the wavefunction in the momentum basis is also real and positive. Furthermore, as we shall see below, this convention ensures that the wavefunctions of all other Fock states are also real.

By having explicitly found the wavefunction of the vacuum states, we have proven its existence, and thus, automatically, the existence of all other Fock states — because these states are obtained from the vacuum state by applying the creation operator.

Now the physical meaning of the eigenvalue n of operator $\hat{n}$ becomes also clear: this is the number of *excitation quanta* in the harmonic oscillator. The number of such quanta is always integer and, because energy levels are equidistant, all of them have the same energy, $\hbar\omega$. In this way, the excitation quanta in a harmonic oscillator resemble particles and, in many cases, they do behave like particles. Among the examples are photons in an optical pulse phonons in a vibrational mode of a solid state.

Exercise 3.77 a) By applying Eq. (3.95), calculate the wavefunctions of Fock states $|1\rangle$ and $|2\rangle$.

b) Show that the wavefunction of an arbitrary Fock state $|n\rangle$ is given by

$$\psi_n(X) = \frac{H_n(X)}{\pi^{1/4}\sqrt{2^n n!}}e^{-X^2/2}, \tag{3.97}$$

where $H_n(X)$ are the Hermite polynomials,

$$H_n(X) = (-1)^n e^{x^2/2}\frac{\mathrm{d}^n}{\mathrm{d}X^n}e^{-x^2/2}. \tag{3.98}$$

As we have proven in Ex. 1.76, eigenstates of a Hermitian operator form a basis of the relevant Hilbert space. Since the proof was made for Hilbert spaces of finite dimensions, one should generally be careful applying that result to infinite-dimensional spaces, such as those studied in this chapter. For example, all the eigenstates of the infinite potential box (Ex. 3.47) have wavefunctions that

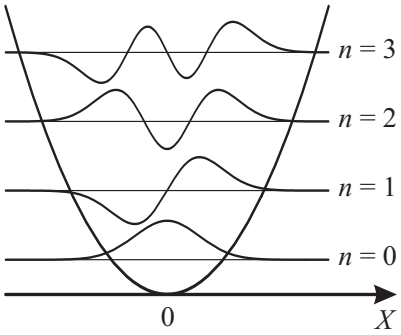


Figure 3.9: Wavefunctions of the first three energy levels of a harmonic oscillator.

vanish outside the box, so they do not span the space of all possible wavefunctions. On the other hand, these wavefunctions do span the space of all quantum states that are localized within the box, i.e. are *physically allowed* under this potential. Even more complicated is the situation with a finite well (Ex. 3.69), whose energy eigenstates combine a discrete (for $E < V_0$) and continuous (for $E \geq V_0$) spectra.

The situation with the Harmonic oscillator is convenient in this respect because, on the one hand, there are no quantum states that are not physically allowed and, on the other hand, the entire energy spectrum is discrete. As a result, the Fock states do form an orthonormal basis in the Hilbert space. This statement also follows from mathematical properties of the Hermite functions (3.97), which are known to form a basis in the Hilbert space of all normalizable functions defined on the real axis.

It is instructive to compare the wavefunctions of the Fock states with those of energy eigenstates of the finite potential well (shown in Fig. 3.4). In both cases, the wavefunctions exhibit oscillatory behavior inside the well and exponentially fall off outside. The difference is that the energy levels are equidistant for the harmonic oscillator, but not equidistant for the rectangular well. Also, each eigenwavefunction of the well is defined in a piecewise fashion [see Eqs. (8.19) and (8.28)] while for the harmonic oscillator potential it is a single elementary function.

Exercise 3.78 For an arbitrary $|n\rangle$, calculate $\langle X\rangle$, $\langle \Delta X^2\rangle$, $\langle P\rangle$, $\langle \Delta P^2\rangle$ and verify the uncertainty principle.
Hint: Rather than integrating the wavefunctions, it is more convenient to employ Eqs. (3.89) and (3.93).

Note 3.2 The vacuum state is the only minimum-uncertainty Fock state.

Exercise 3.79 Find the evolution of the state $\alpha\,|0\rangle + \beta\,|1\rangle$; calculate the time dependence of $\langle X\rangle$, $\langle P\rangle$ and plot the trajectory in the phase space.
Answer (for real α, β):

$$\langle X\rangle = \sqrt{2}\alpha\beta(\cos\omega t); \langle P\rangle = -\sqrt{2}\alpha\beta(\sin\omega t).$$

This last result is remarkable. The Fock states themselves are stationary and thus exhibit no time variation of the mean position and momentum. But in their linear combinations, the mean position and momentum oscillate similarly to those of a classical harmonic oscillator. Of course, this behavior is still very dissimilar to classical: the mean values of the position and momentum are microscopic, and their scale is compatible to that of their own uncertainties. In the next subsection we will study those states whose behavior under Schrödinger evolution resembles classical much more significantly.

3.9.3 Coherent states

The coherent state is the closest quantum approximation of the classical picture of the harmonic oscillator motion. As we shall see, in this state the mean position and momentum vary as functions of

time in the same way as do those of a classical ball on a spring. The amplitude of this oscillation can be arbitrarily high, but the position and momentum uncertainties remain as low as in the vacuum state. Because of their classical-like behavior, coherent states frequently occur in nature, not only in mechanical oscillators, but also in other "incarnations" of the harmonic oscillator. For example, the quantum state of light in a laser pulse is also a coherent state.

Definition 3.4 The *coherent state* $|\alpha\rangle$ is an eigenstate of the annihilation operator with eigenvalue α:

$$\hat{a}\,|\alpha\rangle = \alpha\,|\alpha\rangle\,. \tag{3.99}$$

The quantity $|\alpha|$ is called the *amplitude*, $\operatorname{Arg}\alpha$ the *phase* of the coherent state.

Exercise 3.80 For a coherent state $|\alpha\rangle$, show that its wavefunctions in the position and momentum bases are given by

$$\psi_\alpha(X) = \frac{1}{\pi^{1/4}} e^{-i\frac{P_\alpha X_\alpha}{2}} e^{iP_\alpha X} e^{-\frac{(X-X_\alpha)^2}{2}}; \tag{3.100}$$

$$\tilde{\psi}_\alpha(P) = \frac{1}{\pi^{1/4}} e^{i\frac{P_\alpha X_\alpha}{2}} e^{-iX_\alpha P} e^{-\frac{(P-P_\alpha)^2}{2}}, \tag{3.101}$$

where

$$X_\alpha = \sqrt{2}\mathrm{Re}\,\alpha; \quad P_\alpha = \sqrt{2}\mathrm{Im}\,\alpha. \tag{3.102}$$

The overall phase factors $e^{\pm iP_\alpha X_\alpha/2}$ are included into Eqs. (3.100) and Eq. (3.101) as a matter of convention in order to make these two equations (which are obtained from one another by means of a direct or inverse Fourier transform) look similar. We will see shortly that this convention is in fact pretty useful.

By comparing Eq. (3.100) with Eq. (3.38) we observe that the coherent state wavefunction is a Gaussian wavepacket centered at $\sqrt{2}\mathrm{Re}\alpha$. Aside from a linearly varying phase factor and the shift of the center, the shape of the wavefunction is identical to that of the vacuum state. This is not surprising given that, according to the above definition, the vacuum state *is* a coherent state with zero amplitude. In fact, one can show the following:

Exercise 3.81 Show that the coherent state can be obtained from the vacuum state by applying displacement operators

$$\begin{aligned} |\alpha\rangle &= e^{-iP_\alpha X_\alpha/2} e^{iP_\alpha \hat{X}} e^{-iX_\alpha \hat{P}}\,|0\rangle \\ &= e^{iP_\alpha X_\alpha/2} e^{-iX_\alpha \hat{P}} e^{iP_\alpha \hat{X}}\,|0\rangle\,. \end{aligned} \tag{3.103}$$

Exercise 3.82 Show that the expectation values of the position and momentum in coherent state $|\alpha\rangle$ are

$$\langle X\rangle = \sqrt{2}\mathrm{Re}\,\alpha; \quad \langle P\rangle = \sqrt{2}\mathrm{Im}\,\alpha. \tag{3.104}$$

Show that the uncertainties of these observables equal

$$\left\langle \Delta X^2 \right\rangle = \left\langle \Delta P^2 \right\rangle = \frac{1}{2}. \tag{3.105}$$

One can picture the coherent state in the phase space as a circle positioned at points $(\sqrt{2}\,\mathrm{Re}\,\alpha, \sqrt{2}\,\mathrm{Im}\,\alpha)$ (Fig. 3.10). The radius of the circle, $1/\sqrt{2}$, symbolically represents the standard deviation of the position and momentum, which are independent of the coherent amplitude[9]. In all coherent states, similarly to the vacuum state, the position-momentum uncertainty product takes the minimum possible value.

Now let us find the Schrödinger evolution of the coherent state in time. To this end, we decompose the coherent state into energy eigenstates and apply the evolution operator to each of these states.

[9] In fact, this circle has more than just a symbolic value. The behavior of uncertainties in the phase space is described by the so-called *Wigner function*, which is the analog of the classical phase-space probability density.

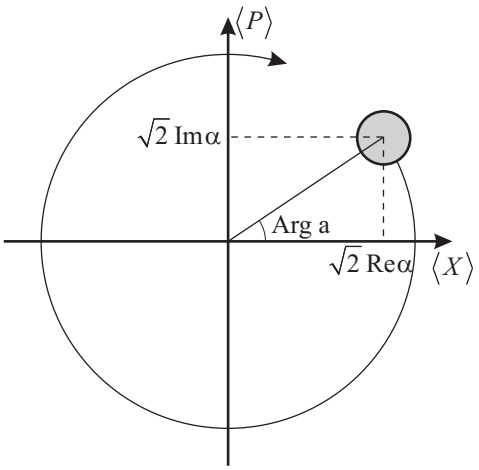


Figure 3.10: The phase space picture and evolution of the position and momentum observables in the coherent state.

Exercise 3.83* Show that the coherent state can be written as

$$|\alpha\rangle = e^{-|\alpha|^2/2} e^{\alpha \hat{a}^\dagger} e^{-\alpha^* \hat{a}} |0\rangle . \tag{3.106}$$

Show that Eq. (3.106) can be simplified as follows:

$$|\alpha\rangle = e^{-|\alpha|^2/2} e^{\alpha \hat{a}^\dagger} |0\rangle . \tag{3.107}$$

Hint: use Eq. (3.103) and the Baker-Hausdorff-Campbell formula (1.70).

Exercise 3.84 Find the decomposition of the coherent state into the number basis (make sure your answer is properly normalized).
Answer:

$$|\alpha\rangle = e^{-|\alpha|^2/2} \sum_n \frac{\alpha^n}{\sqrt{n!}} |n\rangle . \tag{3.108}$$

Now the role of the convention for the overall phase in Eqs. (3.100) and (3.100) becomes clear. With this convention, the decomposition (3.108) of the coherent state in to the Fock basis takes an extremely simple form.

If one performs an energy measurement on a coherent state, one will find, in accordance with Eq. (3.108), that that the probability to project onto a particular Fock state is given by:

$$\mathrm{pr}_n = |\langle n|\ \alpha\rangle|^2 = e^{-|\alpha|^2} \frac{|\alpha|^{2n}}{n!}. \tag{3.109}$$

This probability distribution is very well known in mathematical statistics. It is the so-called *Poisson distribution*, which expresses the probability of a number of events to occur within a given period of time if these events occur with a known average rate and independently of each other. Let us distract ourselves from pure quantum physics for a few minutes and study the properties of this distribution.

Exercise 3.85 Find $\langle n\rangle$, $\langle \Delta n^2\rangle$ for a coherent state.
Answer: $\langle n\rangle = \langle \Delta n^2\rangle = |\alpha|^2$.

For example, in a certain city, 25 babies are born per day on average. The exact number of babies that are born on each day varies: sometimes there are exactly 25, sometimes (for example)

22, and sometimes 32. The probability that a specific number n of babies are born on some specific day is then given by Eq. (3.109) with $\langle n \rangle = |\alpha|^2 = 25$. The mean square uncertainty in the number of babies equals $\sqrt{\langle \Delta n^2 \rangle} = \sqrt{\langle n \rangle} = 5$, i.e. on a typical day it is much more likely to see 20 or 30 babies rather than 10 or 40 (Fig. 3.11).

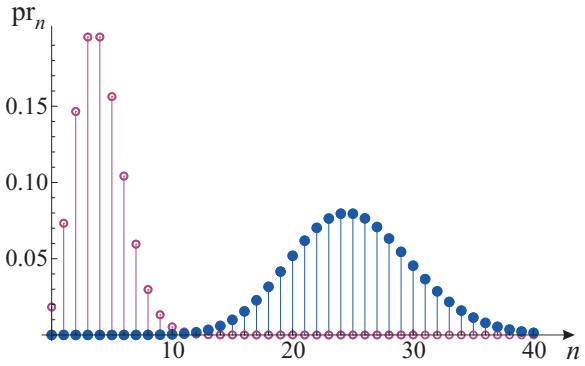


Figure 3.11: the Poisson distribution with $\langle n \rangle = 4$ (empty circles) and $\langle n \rangle = 25$ (filled circles).

Although the absolute uncertainty of n increases with $\langle n \rangle$, the *relative* uncertainty $\sqrt{\langle \Delta n^2 \rangle}/\langle n \rangle$ decreases. In our example above, the relative uncertainty is $5/25 = 20\%$. But in a smaller town, where $\langle n \rangle = 4$, the relative uncertainty is as high as $2/4 = 50\%$.

Returning to the quantum oscillator, the higher the amplitude of the coherent state, the lower is the relative uncertainty in the number of excitation quanta within that state. For example, if we measure the energies of laser pulses (which are in the coherent state), the observed value will vary from pulse to pulse — the phenomenon known as the *shot noise*. For a higher intensity laser beam, with a higher average pulse energy, the relative magnitude of the shot noise will decrease. The more macroscopic the coherent state becomes, the less significant are its quantum features.

Exercise 3.86 A laser of wavelength $\lambda = 800$ nm emits pulses with a repetition rate $f = 100$ MHz. The average power of the laser is $P = 1$ Watt. Calculate

a) the mean energy of each laser pulse;

b) the mean number of photons in each pulse;

c) the relative uncertainty in the energy of the pulses due to the shot noise.

How will the answer in part (c) change if the average laser power is $P' = 1$ μW?

Exercise 3.87 Show that $\langle \alpha |\, \alpha' \rangle = e^{-|\alpha|^2/2 - |\alpha'|^2/2 + \alpha'^* \alpha}$.

In regards to the last exercise, one may ask how come the coherent states associated with different α's are not orthogonal. Didn't we prove in Ex. 1.76 that eigenstates of an operator form an orthonormal basis? The answer is that the statement of Ex. 1.76 only applies to Hermitian operator — and the annihilation operator is not Hermitian. Coherent states do form a spanning set, but they are not orthogonal.

Exercise 3.88 Do eigenstates of the creation operator exist and if so, what is their decomposition into the number basis?

Exercise 3.89 Show that the action of the evolution operator $\exp(i\hat{H}t/\hbar)$ upon the state $\hat{\alpha}$ is given by

$$\exp(-i\hat{H}t/\hbar)\,|\alpha\rangle = e^{-i\omega t/2}\,\left|e^{-i\omega t}\alpha\right\rangle . \tag{3.110}$$

This result is remarkable. Neglecting the overall quantum phase factor $e^{-i\omega t/2}$, a coherent state evolves into another coherent state with the same amplitude, but different phase. Note the distinction between the *quantum* phase factor outside the ket in Eq. (3.110) (which does not reflect in any measurement results) and the *coherent* phase factor $e^{-i\omega t}$ inside the ket, which indicates a different eigenvalue of the annihilation operator and hence a physically different quantum state.

The role of the coherent phase is evident from Fig. 3.10. The Hamiltonian evolution of the coherent state entails linear growth of the phase and hence the circular motion of the expectation values in the phase space. Assuming α real, we find:

$$\begin{aligned} \langle X \rangle &= \sqrt{2}\mathrm{Re}(e^{-i\omega t}\alpha) = \sqrt{2}\alpha\cos\omega t; \\ \langle P \rangle &= \sqrt{2}\mathrm{Im}(e^{-i\omega t}\alpha) = \sqrt{2}\alpha\sin\omega t. \end{aligned} \tag{3.111}$$

Aside from a microscopic uncertainty, the behavior of the position and momentum observables in the coherent state is identical to classical.

Exercise 3.90 Are coherent states stationary?