# Chapter 6

# Wave Mechanics (Part B)

This is the second part of Wave Mechanics where we study simple one-dimensional problems that admit bound states or scattering states or both.

## 6.1 Bound States

We now analyze a series of Hamiltonians that illustrate some of the general properties of wave functions we have derived above, as well as show some remarkable properties of the quantum world. We first consider a few examples of systems with bound states, thus studying eigenstates of the Hamiltonian with energies $E < V(\pm\infty)$. As we have discussed previously, these are also physical states, since they can be normalized. We will consider scattering states in a separate section.

### 6.1.1 Particle in a box

The first system we study here consists of a particle inside a one-dimensional box with hard walls, that prevent the particle from escaping. We can model this situation with a symmetric potential

$$V(x) = \begin{cases} 0, & -\frac{L}{2} \leq x \leq \frac{L}{2}, \\ \infty, & \text{otherwise}, \end{cases} \tag{6.1.1}$$

where we have called $L$ the linear size of the box, as also shown in Fig. 6.1. Since the potential is infinite at $x \to \pm\infty$, we expect to find only physically valid, bound states, as also found for the harmonic-oscillator case.
Outside the box we must have $|\Psi(x)|^2 = 0$, since we have assumed that the potential is infinite and the particle is not found outside. Inside the box the potential energy is zero, thus the time-independent Schrödinger equation reads

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} = E\Psi, \tag{6.1.2}$$

which can also be written

$$\frac{\partial^2\Psi}{\partial x^2} = -k^2\Psi, \tag{6.1.3}$$

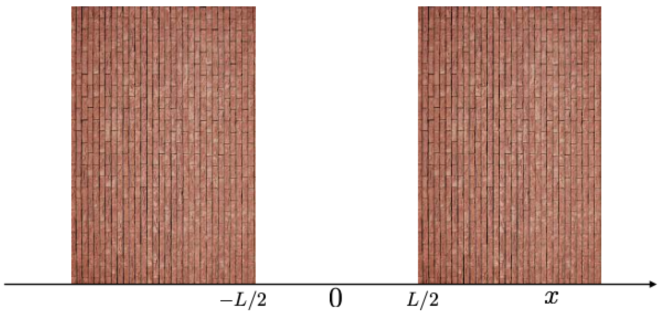


Figure 6.1: Potential of a particle in a box with hard walls. The potential energy is taken to be infinite beyond the limits $0 \leq x \leq L$.

where we have introduced $k = \sqrt{2mE}/\hbar$. From the general bound derived in the previous section, the energy must be $E \geq 0$ (here $V_{\text{min}} = 0$). It follows that $k$ is real and $k \geq 0$; the solution to differential Eq. (6.1.3) is

$$\Psi(x) = A \sin kx + B \cos kx, \tag{6.1.4}$$

where $A$ and $B$ are two constants to be determined. From the discussion on the parity operator, we know that the eigenfunctions are of two types in this symmetric potential, namely

$$\Psi_+(x) = B \cos k_+ x, \tag{6.1.5}$$

$$\Psi_-(x) = A \sin k_- x. \tag{6.1.6}$$

where $E^\pm = \hbar^2 k_\pm^2/2m$ are the energies of, respectively, even and odd states. We now fix the free constants by imposing appropriate boundary conditions and the normalization of the wave function. Specifically, continuity of the wave function implies

$$\Psi_\pm\Big(-L/2\Big) = 0, \tag{6.1.7}$$

$$\Psi_\pm\Big(L/2\Big) = 0. \tag{6.1.8}$$

These conditions yield

$$B \cos\Big(k_+ L/2\Big) = 0, \tag{6.1.9}$$

$$A \sin\Big(k_- L/2\Big) = 0, \tag{6.1.10}$$

which are satisfied if

$$k_+ \frac{L}{2} = \left(n_+ + \tfrac{1}{2}\right)\pi, \tag{6.1.11}$$

$$k_- \frac{L}{2} = n_- \pi, \tag{6.1.12}$$

thus

$$
\begin{aligned}
k_- &= \frac{2n_-\pi}{L}, && (6.1.13)\\
&= \left(0,\ \tfrac{2\pi}{L},\ \tfrac{4\pi}{L}, \dots\right), && (6.1.14)\\
k_+ &= \frac{(2n_+ + 1)\pi}{L}, && (6.1.15)\\
&= \left(\tfrac{\pi}{L},\ \tfrac{3\pi}{L}, \dots\right). && (6.1.16)
\end{aligned}
$$

The solution with $n_- = 0$ can be discarded, since it corresponds to a null wave function. Overall, the allowed values of $k$ are therefore

$$
\begin{aligned}
k_n &= \frac{n\pi}{L}, && (6.1.17)\\
n &= 1, 2, \dots, && (6.1.18)
\end{aligned}
$$

yielding a discrete spectrum. With even/odd $n$ we recover, respectively, spatially odd and even wave functions. This quantization of $k$ implies the quantization of energies, which we label with the integer index $n$:

$$
\begin{aligned}
E_n &= \frac{\hbar^2 k_n^2}{2m}, && (6.1.19)\\
&= \frac{\hbar^2\pi^2}{2mL^2}\, n^2. && (6.1.20)
\end{aligned}
$$

Thus a quantum particle in a box can take only discrete energy values, in radical contrast with the classical case. In order to determine the normalization constants, we need to impose the normalization condition, $\langle\Psi^-|\Psi^-\rangle = 1$. For the odd states:

$$
\begin{aligned}
\langle\Psi^-|\Psi^-\rangle &= \int_{-\infty}^{\infty} dx\, |\Psi_\pm(x)|^2 && (6.1.21)\\
&= 2\int_0^{L/2} dx\, |\Psi_\pm(x)|^2 && (6.1.22)\\
&= 2A^2 \int_0^{L/2} dx\, \sin^2(kx) && (6.1.23)\\
&= A^2 \int_0^{L/2} dx\, [1 - \cos(2kx)] && (6.1.24)\\
&= A^2 \int_0^{kL} \frac{dx'}{2k}\, [1 - \cos x'] \quad (x' = 2kx) && (6.1.25)\\
&= \frac{A^2}{2k}\, [x' - \sin x']_0^{kL} && (6.1.26)\\
&= \frac{A^2}{2k}\, (kL) && (6.1.27)\\
&= A^2 \frac{L}{2} && (6.1.28)\\
&= 1. && (6.1.29)
\end{aligned}
$$

Hence $A = \sqrt{2/L}$. A similar procedure gives $B = \sqrt{2/L}$ for the even solutions. In summary, the eigenfunctions of the Hamiltonian are

$$\Psi_n(x) = \begin{cases} \sqrt{\dfrac{2}{L}}\cos(n\pi x), & n \text{ odd}, \\ \sqrt{\dfrac{2}{L}}\sin(n\pi x), & n \text{ even}, \end{cases} \tag{6.1.30}$$

These states vanish at the edges of the box and have $n-1$ nodes (points where the wave-function vanishes inside the box), as illustrated in Fig. 6.2.

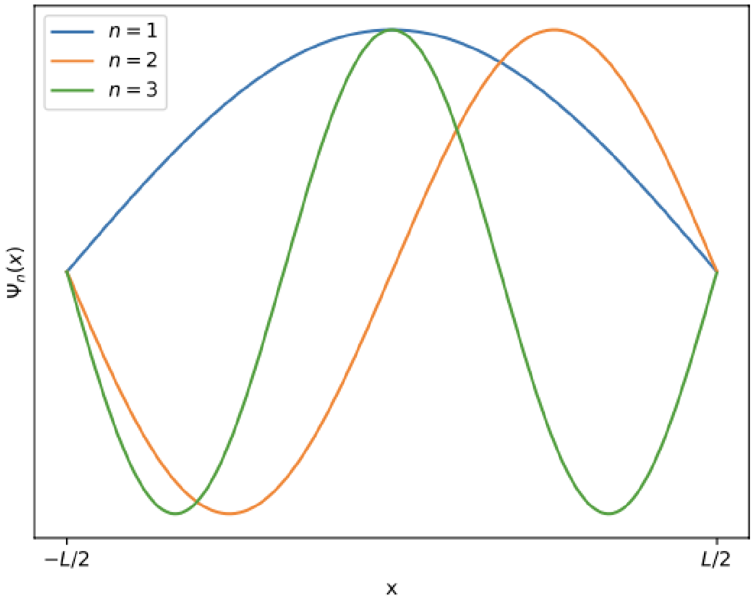


Figure 6.2: Energy eigenstates of a particle in a box with hard walls. The wave function is shown for $0 \leq x \leq L$; it vanishes elsewhere.

From the general theory we also know that a solution of the time-dependent Schrödinger equation can be written as a linear superposition of these basis states (since the Hamiltonian is time independent), thus

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n(t)\,\Psi_n(x), \tag{6.1.31}$$

where the time-dependent coefficients $c_n(t)$ are determined by the initial conditions,

$$c_n(t) = \langle \Psi_n | \Psi(t=0) \rangle\, e^{-iE_n t/\hbar}, \tag{6.1.32}$$

and the initial amplitudes $\langle \Psi_n | \Psi(t=0) \rangle$ are obtained with the usual inner-product rules introduced earlier. For instance, if the initial state is known to be an even function in position space, $\Psi(x,0) = \Psi(-x,0)$, only the even $n$ coefficients are non-zero and

$$\langle \Psi_n | \Psi(t=0) \rangle = \int_{-\infty}^{\infty} dx\, \Psi_n(x)\, \Psi(x,0) \tag{6.1.33}$$

$$= \sqrt{\frac{2}{L}} \int_{-L/2}^{L/2} dx\, \cos\!\left(n\pi \tfrac{x}{L}\right) \Psi(x,0). \tag{6.1.34}$$

### 6.1.2 Finite potential well

We now generalize the previous case and consider a finite potential well, described by

$$V(x) = \begin{cases} V_0, & x < -\dfrac{L}{2}, \\ 0, & -\dfrac{L}{2} \le x \le \dfrac{L}{2}, \\ V_0, & x > \dfrac{L}{2}, \end{cases} \tag{6.1.35}$$

so that three distinct spatial regions (I, II, III) exist, as sketched in Fig. 6.3.

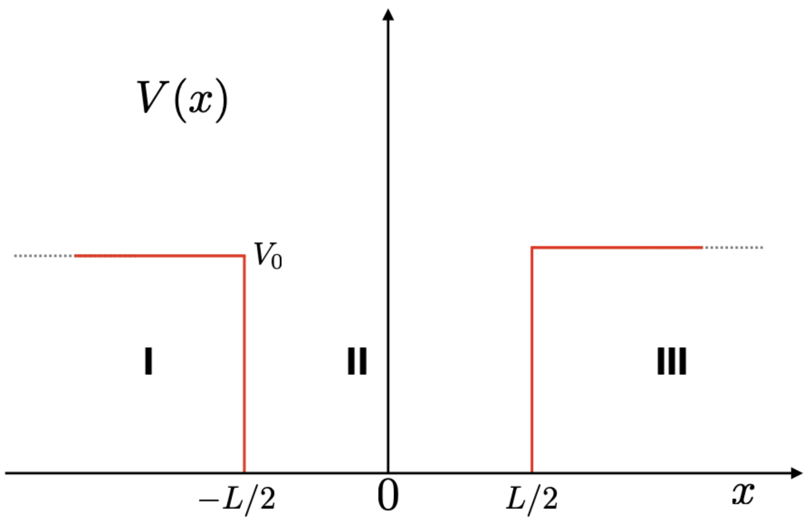


Figure 6.3: Potential of a particle in a finite well. The potential energy vanishes inside the box (region II) and equals $V_0$ outside $-\frac{L}{2} \le x \le \frac{L}{2}$ (regions I and III).

We concentrate on bound-state solutions, i.e. $E < V_0$. The Schrödinger equation in the three regions reads

$$\begin{cases} \Psi''(x) + k^2 \Psi(x) = 0, & |x| \le \dfrac{L}{2}, \\ \Psi''(x) - \rho^2 \Psi(x) = 0, & |x| > \dfrac{L}{2}, \end{cases} \tag{6.1.36}$$

where we have defined

$$k = \sqrt{2mE}/\hbar, \tag{6.1.37}$$

$$\rho = \sqrt{2m(V_0 - E)}/\hbar. \tag{6.1.38}$$

The solutions in the three regions are therefore

$$\Psi(x) = \begin{cases} N_I e^{\rho x}, & x < -\dfrac{L}{2}, \\ N_{II}\cos(kx) + N'_{II}\sin(kx), & -\dfrac{L}{2} \le x \le \dfrac{L}{2}, \\ N_{III} e^{-\rho x}, & x > \dfrac{L}{2}, \end{cases} \tag{6.1.39}$$

where we have discarded the non-normalisable exponentials in regions I and II. Because the potential is everywhere finite, continuity of $\Psi$ and of its derivative imposes the four conditions

$$\begin{cases} \Psi_I\big(-L/2\big) = \Psi_{II}\big(-L/2\big) \\ \Psi'_I\big(-L/2\big) = \Psi'_{II}\big(-L/2\big) \\ \Psi_{II}\big(L/2\big) = \Psi_{III}\big(L/2\big) \\ \Psi'_{II}\big(L/2\big) = \Psi'_{III}\big(L/2\big) \end{cases} \tag{6.1.40}$$

**Even solutions**

We first consider the even case,

$$\Psi(x) = \Psi(-x), \tag{6.1.41}$$

which implies $N_{III} = N_I$ and $N'_{II} = 0$. Equations (6.1.40) reduce to

$$\begin{cases} N_I e^{-\rho L/2} = N_{II}\cos(kL/2) \\ N_I\rho\, e^{-\rho L/2} = N_{II}k\sin(kL/2) \end{cases} \tag{6.1.42}$$

which yield the transcendental relation

$$\frac{\rho}{k} = \tan\!\left(\frac{kL}{2}\right). \tag{6.1.43}$$

Recalling

$$k = \sqrt{2mE}\,/\hbar, \tag{6.1.44}$$

$$\rho = \sqrt{2m(V_0 - E)}\,/\hbar, \tag{6.1.45}$$

we observe

$$\rho^2 + k^2 = \frac{2m}{\hbar^2}\Big[E^2 + (V_0 - E)^2 + 2(V_0 - E)E\Big] = \frac{2m}{\hbar^2}V_0^2 = k_0^2, \tag{6.1.46}$$

where $k_0 = V_0\sqrt{2m}/\hbar$. Since $\rho/k > 0$, Eq. (6.1.43) can be recast as

$$\frac{\rho^2}{k^2} = \tan^2\!\left(\frac{kL}{2}\right), \tag{6.1.47}$$

$$\frac{k_0^2}{k^2} - 1 = \frac{1}{\cos^2(kL/2)} - 1, \tag{6.1.48}$$

so the allowed $k$ values satisfy

$$\left|\frac{k}{k_0}\right| = \left|\cos\!\left(\frac{kL}{2}\right)\right|, \tag{6.1.49}$$

$$\tan\!\left(\frac{kL}{2}\right) > 0. \tag{6.1.50}$$

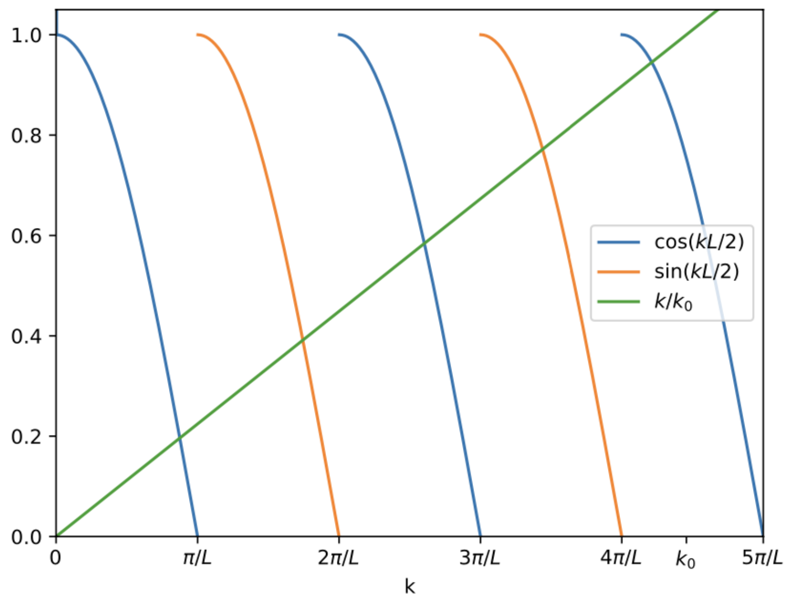


Figure 6.4: Graphical solution of the non-linear equations (6.1.49) (blue) and (6.1.53) (orange). Intersections with the straight line $k/k_0$ (green) give the allowed $k$-values. In this example there are three even solutions and two odd solutions.

### Odd solutions

For odd parity one has

$$\Psi(x) = -\Psi(-x). \tag{6.1.51}$$

For odd parity, $\Psi(x) = -\Psi(-x)$, Eqs. (6.1.40) become

$$\begin{cases} N_I e^{-\rho L/2} = -\,N_{II} \sin(kL/2) \\ N_I \rho\, e^{-\rho L/2} = N_{II} k \cos(kL/2) \end{cases} \tag{6.1.52}$$

and the transcendental condition to be satisfied is

$$\left|\frac{k}{k_0}\right| = \left|\sin(kL/2)\right|, \tag{6.1.53}$$

$$\tan\Big(kL/2\Big) < 0. \tag{6.1.54}$$

The non-linear equations (6.1.49) and (6.1.53) can be solved numerically. Graphically, each solution corresponds to an intersection of the straight line $k/k_0$ with the trigonometric curves $\cos(kL/2)$ (even) and $\sin(kL/2)$ (odd). Figure 6.4 illustrates a case where three even and two odd bound states exist.

Example wave functions for the even solutions are displayed in Fig. 6.5. Note that each bound-state wave function has finite support in the classically forbidden regions $|x| > L/2$; the exponential tails reflect the finite probability of finding the particle outside the well. Classically a particle with $E < V_0$ cannot escape, whereas quantum mechanically it can tunnel through the barrier.

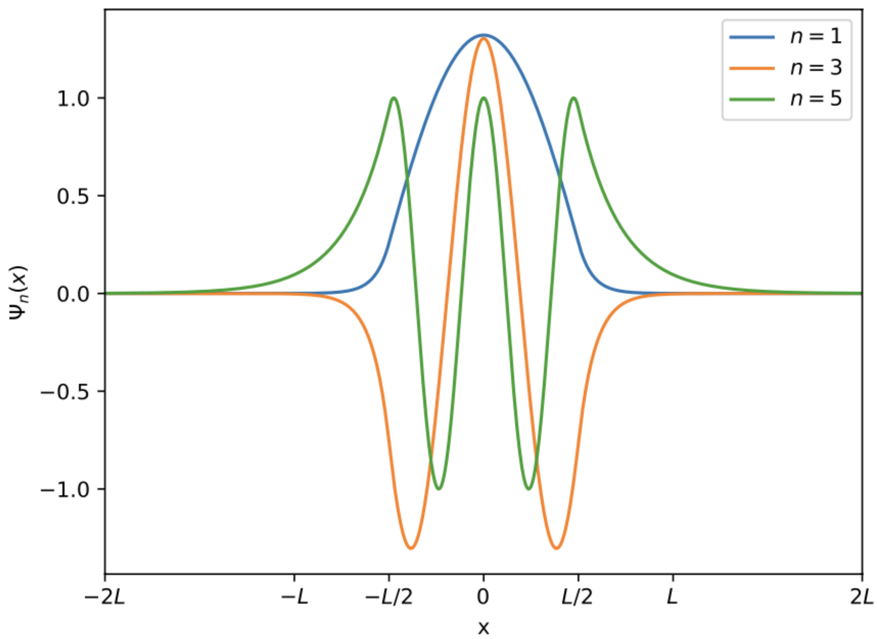


Figure 6.5: Example of spatially even stationary states for the finite-well potential. The three curves correspond to the same value of $V_0$ used in Fig. 6.4.

### 6.1.3 Delta potential

$$V(x) = -\alpha\,\delta(x), \tag{6.1.55}$$

with $\alpha > 0$ the time-independent Schrödinger equation for the delta well is

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x)}{\partial x^2} - \alpha\,\delta(x)\Psi(x) = E\Psi(x). \tag{6.1.56}$$

We restrict to bound states, hence $E < 0$. For $x \neq 0$ the potential is zero, so the solutions are exponential. Defining $\rho = \sqrt{2m|E|}/\hbar$,

$$\Psi_<(x) = A\,e^{-\rho x} + B\,e^{\rho x}, \qquad x < 0, \tag{6.1.57}$$

$$\Psi_>(x) = F\,e^{-\rho x}, \qquad x > 0, \tag{6.1.58}$$

where normalisability forces $A = 0$ (otherwise $\Psi \to \infty$ as $x \to -\infty$). Continuity at $x = 0$ gives $B = F$.
Next we apply the derivative–discontinuity condition obtained by integrating Eq. (6.1.56) across an infinitesimal interval around $x = 0$:

$$\Psi'(0^+) - \Psi'(0^-) = \frac{2m}{\hbar^2}\int_{-\epsilon}^{+\epsilon} V(x)\Psi(x)\,dx = -\frac{2m\alpha}{\hbar^2}\Psi(0). \tag{6.1.59}$$

Using Eqs. (6.1.57)–(6.1.58):

$$\Psi'(0^+) = -\rho B, \qquad \Psi'(0^-) = +\rho B,$$

so Eq. (6.1.59) becomes

$$-2\rho B = -\frac{2m\alpha}{\hbar^2}\,B, \tag{6.1.60}$$

and therefore

$$\rho = \frac{m\alpha}{\hbar^2}. \tag{6.1.61}$$

Finally, using $\rho = \sqrt{2m|E|}/\hbar$ we find the single bound-state energy

$$E = -\frac{m\alpha^2}{2\hbar^2}. \tag{6.1.62}$$

The corresponding normalised wave function is

$$\Psi(x) = \sqrt{\rho}\,e^{-\rho|x|}, \qquad \rho = \frac{m\alpha}{\hbar^2}. \tag{6.1.63}$$

Using (6.1.61) fixes the energy through the only admissible value of $\rho$:

$$\rho = \alpha\frac{m}{\hbar^2}, \tag{6.1.64}$$

$$E = -\frac{m\alpha^2}{2\hbar^2}. \tag{6.1.65}$$

Hence this potential admits only a single bound state. With the constant $B$ determined by normalization, the wave function is

$$\Psi(x) = \sqrt{\frac{m\alpha}{\hbar}}\,e^{-\alpha m|x|/\hbar^2}. \tag{6.1.66}$$

## 6.2 Scattering states

We now analyze solutions of the Schrödinger equation that are not normalizable, yet play an important role in understanding quantum dynamics.

### 6.2.1 Wave packets

Consider the Hamiltonian of a free particle

$$\hat{H} = \frac{\hat{p}^2}{2m}, \tag{6.2.1}$$

whose eigenstates are the momentum eigenkets with energies $p^2/2m$:

$$\hat{H}\,|p\rangle = \frac{p^2}{2m}\,|p\rangle\,, \tag{6.2.2}$$

where

$$\langle x|p\rangle = \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}}. \tag{6.2.3}$$

The difficulty with these eigenstates is that they solve the time-independent Schrödinger equation but are not square-normalizable, and therefore are not physical states. However, we have seen that a generic solution of the time-dependent Schrödinger equation for a time-independent Hamiltonian is

$$|\Psi(t)\rangle = e^{-i\hat{H}t/\hbar}\,|\Psi(0)\rangle\,. \tag{6.2.4}$$

For the free-particle Hamiltonian the time evolution is particularly simple in momentum representation:

$$\langle p|\Psi(t)\rangle = \int dp'\ \langle p|p'\rangle\ e^{-i\hat{H}t/\hbar}\ \langle p'|\Psi(0)\rangle \tag{6.2.5}$$

$$= \int dp'\, e^{-ip'^2t/2m\hbar}\,\delta(p-p')\ \langle p'|\Psi(0)\rangle \tag{6.2.6}$$

$$= e^{-ip^2t/2m\hbar}\ \langle p|\Psi(0)\rangle\,. \tag{6.2.7}$$

In coordinate representation the expressions are more involved but follow directly from the momentum eigenkets in the $x$-basis. Using $\langle x|p\rangle = e^{ipx/\hbar}/\sqrt{2\pi\hbar}$ we have

$$\langle x|\Psi(t)\rangle = \int dp\ \langle x|p\rangle\ \langle p|\Psi(t)\rangle \tag{6.2.8}$$

$$= \int dp\,\frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}}\,e^{-ip^2t/2m\hbar}\ \langle p|\Psi(0)\rangle \tag{6.2.9}$$

$$= \int dp\,\frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}}\,e^{-ip^2t/2m\hbar}\int dx'\ \langle p|x'\rangle\ \Psi(x',0) \tag{6.2.10}$$

$$= \frac{1}{2\pi\hbar}\int dx'\ \Psi(x',0)\int dp\,e^{ip(x-x')/\hbar}\,e^{-ip^2t/2m\hbar} \tag{6.2.11}$$

$$= \sqrt{\frac{m}{2\pi\hbar t}}\ e^{-i\pi/4}\int dx'\ \Psi(x',0)\ \exp\Big[\,i\frac{m(x-x')^2}{2\hbar t}\Big]. \tag{6.2.12}$$

Thus in real space the initial wave function is convolved with the time-dependent kernel $\exp[im(x-x')^2/2\hbar t]$. If the initial state is normalized then it remains normalized at all later times; the non-normalizable kets $\langle x|p\rangle$ merely serve as a mathematical tool for constructing the solution.

### 6.2.2 Group velocity

The evolving free-particle wave packet depends on the specific initial momentum-space amplitude $\Phi(p) = \langle p|\Psi(0)\rangle$:

$$\Psi(x,t) = \int dp\, \frac{e^{i\left(px - \frac{p^2}{2m}t\right)/\hbar}}{\sqrt{2\pi\hbar}}\, \Phi(p). \tag{6.2.13}$$

Assume $\Phi(p)$ is a smooth function sharply peaked around $\bar{p}$ with width $\Delta p$. Expanding the energy $E(p) = p^2/2m$ about $\bar{p}$ we obtain

$$\begin{aligned} E(p) &= \frac{p^2}{2m} && (6.2.14)\\ &\simeq \frac{\bar{p}^2}{2m} + \frac{\bar{p}}{m}(p-\bar{p}) + O\big(\Delta p^2\big) && (6.2.15)\\ &= E(\bar{p}) + E'(\bar{p})(p-\bar{p}) + O\big(\Delta p^2\big), && (6.2.16) \end{aligned}$$

where $E'(\bar{p}) = \bar{p}/m$. Substituting (6.2.16) into (6.2.13) and writing $p = s + \bar{p}$ gives

$$\begin{aligned} \Psi(x,t) &\simeq \frac{e^{-iE(\bar{p})t/\hbar}}{\sqrt{2\pi\hbar}} \int dp\, e^{i\left(px - E'(\bar{p})(p-\bar{p})t\right)/\hbar}\, \Phi(p) && (6.2.17)\\ &= \frac{e^{-iE(\bar{p})t/\hbar}}{\sqrt{2\pi\hbar}} \int ds\, e^{i\left((s+\bar{p})x - E'(\bar{p})st\right)/\hbar}\, \Phi(s+\bar{p}) && (6.2.18)\\ &= \frac{e^{i\left(E'(\bar{p})\bar{p} - E(\bar{p})\right)t/\hbar}}{\sqrt{2\pi\hbar}} \int ds\, e^{i(s+\bar{p})\left(x - E'(\bar{p})t\right)/\hbar}\, \Phi(s+\bar{p}) && (6.2.19)\\ &= \frac{e^{i\left(E'(\bar{p})\bar{p} - E(\bar{p})\right)t/\hbar}}{\sqrt{2\pi\hbar}} \int dp\, e^{ip\left(x - E'(\bar{p})t\right)/\hbar}\, \Phi(p) && (6.2.20)\\ &= e^{-i\left(E(\bar{p}) - E'(\bar{p})\bar{p}\right)t/\hbar}\, \Psi\big(x - E'(\bar{p})t, 0\big). && (6.2.21) \end{aligned}$$

This expression is particularly interesting because it tells us that the form of the time-evolved wave packed (apart from a phase factor) is approximately equal to the initial state but in the moving frame $x'(t) = x - E'(\bar{p})t$. The packet's peak therefore moves with velocity

$$\begin{aligned} v_{\mathrm{g}} &= E'(\bar{p}) && (6.2.22)\\ &= \frac{\bar{p}}{m}, && (6.2.23) \end{aligned}$$

called the group velocity; it coincides with the classical velocity of a free particle whose momentum is $\bar{p}$. The approximation leading to Eqs. (6.2.22)–(6.2.23) remains valid provided quadratic corrections to the energy are negligible, i.e.

$$\Delta p^2 \frac{t}{m\hbar} \ll 1, \tag{6.2.24}$$

thus for time scales given by the inverse of the momentum spread of the initial state

$$t \ll \frac{m\hbar}{\Delta p^2}. \tag{6.2.25}$$

### 6.2.3 Step potential

Next we analyze the step potential

$$V(x) = \begin{cases} 0, & x < 0, \\ V_0, & x > 0, \end{cases} \tag{6.2.26}$$

which supports only scattering states. We consider the two cases $E > V_0$ and $E < V_0$. In both, the stationary-state solutions extend to $x \to -\infty$ and are non-normalizable; nonetheless they form a useful basis for constructing physical (normalizable) wave packets, exactly as for the free particle. Before addressing dynamics we first detail those stationary states.

#### Stationary states for $E > V_0$

Define

$$k_1 = \sqrt{2mE}/\hbar, \tag{6.2.27}$$

$$k_2 = \sqrt{2m(E - V_0)}/\hbar. \tag{6.2.28}$$

In both spatial regions the time-independent Schrödinger equation takes the form

$$\Psi''_<(x) + k_1^2 \Psi_<(x) = 0, \qquad x < 0, \tag{6.2.29}$$

$$\Psi''_>(x) + k_2^2 \Psi_>(x) = 0, \qquad x > 0, \tag{6.2.30}$$

so the general solutions read

$$\Psi_<(x) = Ae^{ik_1 x} + Be^{-ik_1 x}, \tag{6.2.31}$$

$$\Psi_>(x) = Ce^{ik_2 x} + De^{-ik_2 x}. \tag{6.2.32}$$

We have four constants $(A, B, C, D)$ to fix (aside from the energy $E$). Physically we are interested in an initial wave packet incident from the left ($x = -\infty$) with positive momentum, i.e. travelling toward the step at $x = 0$. Therefore we keep only left-to-right propagation in region II by setting $D = 0$. Continuity of the wave function at $x = 0$ then yields

$$A + B = C. \tag{6.2.33}$$

The continuity of the derivative at $x = 0$ gives

$$ik_1 A - ik_1 B = ik_2 C, \tag{6.2.34}$$

and combining Eqs. (6.2.33) and (6.2.34) we obtain

$$\frac{B}{A} = \frac{k_1 - k_2}{k_1 + k_2}, \tag{6.2.35}$$

$$\frac{C}{A} = \frac{2k_1}{k_1 + k_2}. \tag{6.2.36}$$

Further insight comes from the probability current

$$J(x,t) = \frac{i\hbar}{2m}\Big[(\partial_x\Psi^*)\Psi - \Psi^*\partial_x\Psi\Big] \tag{6.2.37}$$

$$= \frac{\hbar}{m}\,\mathrm{Im}\Big[\Psi^*\,\partial_x\Psi\Big]. \tag{6.2.38}$$

For the left region ($x < 0$),

$$J_<(x,t) = \frac{\hbar}{m}\,\mathrm{Im}\Big[(A^*e^{-ik_1x} + B^*e^{ik_1x})(ik_1Ae^{ik_1x} - ik_1Be^{-ik_1x})\Big] \tag{6.2.39}$$

$$= \frac{\hbar k_1}{m}\big(|A|^2 - |B|^2\big), \tag{6.2.40}$$

while to the right of the step ($x > 0$)

$$J_>(x,t) = \frac{\hbar k_2}{m}\,|C|^2. \tag{6.2.41}$$

Because the stationary states satisfy the continuity equation $\partial_x J + \partial_t|\Psi|^2 = 0$, the current is time independent. Using Eqs. (6.2.35)–(6.2.36) one finds

$$J_< = \frac{\hbar k_1}{m}|A|^2\left(1 - \left|\frac{B}{A}\right|^2\right) \tag{6.2.42}$$

$$= \frac{\hbar k_1}{m}|A|^2\left(1 - \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2\right) \tag{6.2.43}$$

$$= \frac{\hbar k_1}{m}|A|^2\left(\frac{4k_1k_2}{(k_1 + k_2)^2}\right), \tag{6.2.44}$$

and

$$J_> = \frac{\hbar k_2}{m}\,|A|^2\left(\frac{2k_1}{k_1 + k_2}\right)^2. \tag{6.2.45}$$

thus $J_< = J_>$. It is convenient to decompose the left current into its incoming ($J_A$), reflected ($J_B$), and transmitted ($J_C$) parts, and to define the <u>reflection</u> and <u>transmission</u> coefficients

$$R \equiv \frac{J_B}{J_A} = \frac{|B|^2}{|A|^2} = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2 \le 1, \tag{6.2.46}$$

$$T \equiv \frac{J_C}{J_A} = \frac{k_2|C|^2}{k_1|A|^2} = \frac{4k_1k_2}{(k_1 + k_2)^2} \le 1. \tag{6.2.47}$$

Note that, in general, $R$ and $T$ are defined as <u>ratios of probability currents</u>, not merely of amplitudes. As expected,

$$R + T = 1. \tag{6.2.48}$$

### Stationary states for $E < V_0$

For $E < V_0$ we replace the transmitted wave vector by the decay constant

$$\rho_2 = \sqrt{2m(V_0 - E)}/\hbar, \tag{6.2.49}$$

so that

$$\Psi_<(x) = Ae^{ik_1x} + Be^{-ik_1x}, \qquad x < 0, \tag{6.2.50}$$
$$\Psi_>(x) = Ce^{\rho_2x} + De^{-\rho_2x}, \qquad x > 0. \tag{6.2.51}$$

Normalizability requires $C = 0$ (the solution must decay for $x \to +\infty$). Continuity at $x = 0$ yields

$$\frac{B}{A} = \frac{k_1 - i\rho_2}{k_1 + i\rho_2}, \tag{6.2.52}$$
$$\frac{D}{A} = \frac{2k_1}{k_1 + i\rho_2}. \tag{6.2.53}$$

To evaluate the reflection coefficient we re-express the first ratio:

$$\frac{B}{A} = \frac{i(k_1 - i\rho_2)}{i(k_1 + i\rho_2)} \tag{6.2.54}$$
$$= -\frac{\rho_2 - ik_1}{\rho_2 + ik_1} \tag{6.2.55}$$
$$= \frac{(\rho_2^2 + k_1^2)e^{i\delta(E)}}{(\rho_2^2 + k_1^2)e^{-i\delta(E)}} \tag{6.2.56}$$
$$= -e^{2i\delta(E)}, \tag{6.2.57}$$

with

$$\delta(E) = \arctan\frac{k_1}{\rho_2} \tag{6.2.58}$$
$$= \arctan\sqrt{\frac{E}{V_0 - E}}\ . \tag{6.2.59}$$

Notice that in this case the reflection coefficient is

$$R = \left|\frac{B}{A}\right|^2 \tag{6.2.60}$$
$$= \left|-e^{i\delta(E)}\right|^2 \tag{6.2.61}$$
$$= 1. \tag{6.2.62}$$

A unit reflection coefficient means no probability current is transmitted, though it does not imply the probability of finding a particle beyond the barrier is strictly zero. Since on the right we have a normalizable exponential tail, the current there vanishes:

$$J_> = \frac{\hbar}{m}\,\mathrm{Im}\Big[\Psi_>^*\,\Psi_>'\Big] \tag{6.2.63}$$
$$= -\frac{\hbar}{m}|D|^2\,\mathrm{Im}\Big[\rho_2 e^{-2\rho_2x}\Big] \tag{6.2.64}$$
$$= 0. \tag{6.2.65}$$

Hence $J_< = J_A - J_B = 0$ as well, so that

$$J_A = J_B, \qquad J_C = 0. \tag{6.2.66}$$

### 6.2.4 Wave packets

We can now form physical solutions of the time-dependent Schrödinger equation, considering the time evolution of an initial wave function $|\Psi(0)\rangle$, which in momentum space we denote by $\Phi(p) = \langle p|\Psi(0)\rangle$. We assume $\Phi(p)$ is sharply peaked around a certain value $\bar{p}$ (one may think, for instance, of a Gaussian wave packet in momentum space with mean $\bar{p}$; the precise functional form is not essential, provided the wave function is peaked near $\bar{p}$ and suppressed elsewhere). Our analysis will focus on the two cases in which the initial state is non-vanishing only for $p < p_0$ or for $p > p_0$, where $p_0$ is the characteristic momentum associated with the barrier.

$$p_0 = \sqrt{2mV_0}, \tag{6.2.67}$$

$$k_0 = \frac{\sqrt{2mV_0}}{\hbar}. \tag{6.2.68}$$

$\boldsymbol{\bar{p} > p_0}$

In general

$$\Psi(x,t) = \int_0^\infty dE\, e^{-iEt/\hbar} \, \langle E|\Psi(0)\rangle \, \langle x|E\rangle \,, \tag{6.2.69}$$

but, since the initial state has no support for $E < E_0$, we may write

$$\Psi(x,t) = \begin{cases} \int_{E_0}^\infty dE \left(Ae^{ik_1x} + Be^{-ik_1x}\right) e^{-iE(k_1)t/\hbar} \, \langle E|\Psi(0)\rangle \,, & x < 0, \\ \int_{E_0}^\infty dE \left(Ce^{ik_2x}\right) e^{-iE(k_2)t/\hbar} \, \langle E|\Psi(0)\rangle \,, & x > 0, \end{cases} \tag{6.2.70}$$

and changing the integration variable from energy to wavenumber we obtain

$$\Psi(x,t) = \begin{cases} \frac{\hbar^2}{m} \int_{k_0}^\infty dk_1\, k_1 \Big(Ae^{ik_1x} + Be^{-ik_1x}\Big) e^{-iE(k_1)t/\hbar} \Phi(k_1), & x < 0, \\ \frac{\hbar^2}{m} \int_{k_0}^\infty dk_2\, k_2\, Ce^{ik_2x}\, e^{-iE(k_2)t/\hbar} \Phi(k_2), & x > 0, \end{cases} \tag{6.2.71}$$

which we decompose into three contributions (incoming, reflected and transmitted):

$$\Psi(x,t) \propto \begin{cases} \Psi_{\rm inc}(x,t) + \Psi_{\rm ref}(x,t), & x < 0, \\ \Psi_{\rm tran}(x,t), & x > 0, \end{cases} \tag{6.2.72}$$

with

$$\Psi_{\rm inc}(x,t) = \int_{k_0}^\infty dk_1\, \tilde{A}(k_1) e^{ik_1x}\, e^{-iE(k_1)t/\hbar} \Phi(k_1), \tag{6.2.73}$$

$$\Psi_{\rm ref}(x,t) = \int_{k_0}^\infty dk_1\, \tilde{B}(k_1) e^{-ik_1x}\, e^{-iE(k_1)t/\hbar} \Phi(k_1), \tag{6.2.74}$$

$$\Psi_{\rm tran}(x,t) = \int_{k_0}^\infty dk_2\, \tilde{C}(k_2) e^{ik_2x}\, e^{-iE(k_2)t/\hbar} \Phi(k_2), \tag{6.2.75}$$

where $\tilde{A}(k), \tilde{B}(k), \tilde{C}(k)$ are smooth functions of momentum. The first term represents an incoming wave packet whose group velocity, in the limit where $\Phi(p)$ is sharply peaked around the momentum $\bar{p}$, is obtained exactly as before; the packet maximum propagates according to

$$x = \frac{\bar{p}}{m}\,t, \tag{6.2.76}$$

with constant speed $\bar{p}/m$. Note, however, that $\Psi_{\text{inc}}(x,t)$ is defined only for $x < 0$; hence this relation is meaningful only for $t < 0$.
For $\Psi_{\text{ref}}(x,t)$ one has $\Psi_{\text{ref}}(-x,t)$ in the same functional form as previously analysed for wave packets, implying that

$$x = -\frac{\bar{p}}{m}\,t, \tag{6.2.77}$$

which now requires $t > 0$; the term indeed corresponds to a packet that originates at the barrier at $t = 0$ and propagates backward after reflection.
Finally, since $k_2^2 + k_0^2 = k_1^2$ we have for the transmitted component

$$v_{\text{trans}} = \partial_{k_2} E(k_2)\Big|_{\bar{k}_2} \tag{6.2.78}$$
$$= \frac{\hbar k_2(\bar{p})}{m} \tag{6.2.79}$$
$$= \frac{\sqrt{\bar{p}^2 - p_0^2}}{m}. \tag{6.2.80}$$

This solution is valid for $x > 0$ and $t > 0$; it therefore coexists with the reflected wave, which travels in the opposite direction, while the transmitted packet propagates with the positive velocity $\sqrt{\bar{p}^2 - p_0^2}/m$.
In conclusion, the incoming wave packet is partially reflected (with the same speed, in modulus, as the incident packet) and the transmitted component continues beyond the barrier with a reduced velocity.

### $\bar{p} < p_0$

In the last case we take initial states with $\Phi(p > p_0) = 0$, so only eigenstates with $E < V_0$ (i.e. evanescent solutions) participate. The time-dependent solution in momentum space is then built exclusively from the stationary states derived for $E < V_0$.
For $E < V_0$ we restrict attention to the region $x < 0$, where our previous approximate methods still apply. There we have

$$\Psi(x,t) \propto \left\{ \int_0^{k_0} dk_1\, k_1 \left( e^{ik_1 x} - e^{2i\delta(E)} e^{-ik_1 x} \right) e^{-iE(k_1)t/\hbar} \Phi(k_1) \right\}_{x<0}, \tag{6.2.81}$$

so that

$$\Psi_{\text{inc}}(x,t) = \int_0^{k_0} dk_1\, k_1 e^{ik_1 x} e^{-iE(k_1)t/\hbar} \Phi(k_1), \tag{6.2.82}$$
$$\Psi_{\text{ref}}(x,t) = -\int_0^{k_0} dk_1\, k_1 e^{2i\delta(E)} e^{-ik_1 x} e^{-iE(k_1)t/\hbar} \Phi(k_1). \tag{6.2.83}$$

The most important difference with respect to the previous case is that the coefficient of the reflected wave ($B$ in the preceding section) is no longer real; instead it is a pure phase, $B/A = -e^{2i\delta(E)}$. Consequently the earlier analysis of the wave-packet velocity must be modified, because one must expand $\delta\big(E(k)\big)$ about $p_0$ in addition to expanding the energy:

$$2\delta(E) - k_1 x - \frac{E(k_1)t}{\hbar} \simeq \text{const} + 2\partial_{k_1}\delta(E)\Big|_{\bar{k}} k_1 - k_1 x - \frac{E'(\bar{k})t}{\hbar}, \tag{6.2.84}$$

equivalent to the transformation

$$x \;\longrightarrow\; -x + 2\partial_{k_1}\delta(E)\Big|_{\bar{k}} = \; -x + \Delta_x. \tag{6.2.85}$$

Recalling

$$\delta(E) = \arctan\sqrt{\frac{E}{V_0 - E}}, \tag{6.2.86}$$

we have

$$\partial_{k_1}\delta(E) = \partial_E\delta(E)\,\frac{k_1^2}{m}, \tag{6.2.87}$$

$$\partial_E\delta(E) = \frac{1}{2}\sqrt{\frac{1}{E(V_0 - E)}} \geq 0. \tag{6.2.88}$$

Hence

$$\Delta_x = 2\partial_E\delta(E)\Big|_{\bar{p}}\frac{\bar{p}}{m} \tag{6.2.89}$$

$$= \Delta_t\,\frac{\bar{p}}{m} \tag{6.2.90}$$

$$= \frac{p_0}{m}\sqrt{\frac{1}{E(V_0 - \bar{E})}}, \tag{6.2.91}$$

where $\bar{E} = \bar{p}^2/2m$. This yields the peak displacement of the reflected wave packet:

$$-x + \Delta_x = \frac{\bar{p}}{m}\,t, \tag{6.2.92}$$

$$x = -\frac{\bar{p}}{m}(t - \Delta_t). \tag{6.2.93}$$

Thus the reflected packet moves back with the same speed as the incoming one, but after a time delay $\Delta_t > 0$.

## 6.3 References and Further Reading

A general discussion of Schrödinger's formulation of wave mechanics can be found in Sakurai's Modern Quantum Mechanics (Chapter 2, Secs. 2.4–2.5), although that treatment omits some of the introductory details covered in these notes. Cohen-Tannoudji's text provides a comprehensive study of one-dimensional problems, including both bound and scattering states; see in particular Chapter 1 (complements H1 and J1 are recommended).