Quantum Mechanics 3 - Class Exercise 2

9.11.2022

Reflection and Transmission Coefficients

Consider an arbitrary potential $V(x)$ which vanishes at $x \to \pm\infty$. Let us assume that a wave-function propagates to the right with momentum k and scatters off the potential[1] [2],

$$\psi_R(x) = \begin{cases} e^{ikx} + re^{-ikx} & x \to -\infty \\ te^{ikx} & x \to \infty \end{cases}. \tag{1}$$

We define the reflection and transmission coefficients as

$$R \equiv \frac{|j_r|}{|j_i|} = \left| \frac{\frac{\hbar}{m}\,\mathrm{Im}\left\{\psi_r^* \frac{\partial}{\partial x}\psi_r\right\}}{\frac{\hbar}{m}\,\mathrm{Im}\left\{\psi_i^* \frac{\partial}{\partial x}\psi_i\right\}} \right| = |r|^2 \tag{2}$$

$$T \equiv \frac{|j_t|}{|j_i|} = \left| \frac{\frac{\hbar}{m}\,\mathrm{Im}\left\{\psi_t^* \frac{\partial}{\partial x}\psi_t\right\}}{\frac{\hbar}{m}\,\mathrm{Im}\left\{\psi_i^* \frac{\partial}{\partial x}\psi_i\right\}} \right| = |t|^2, \tag{3}$$

where j is the probability density current and $\psi_i = e^{ikx}$, $\psi_r = re^{-ikx}$, $\psi_t = te^{ikx}$. Note that due to probability conservation, $|j_i| = |j_r| + |j_t|$ and

$$R + T = |r|^2 + |t|^2 = 1. \tag{4}$$

Question 1

In general, where the potential isn't symmetric, we would have different coefficients r', t' for a wave-function that propagates to the left,

$$\psi_L(x) = \begin{cases} t'e^{-ikx} & x \to -\infty \\ e^{-ikx} + r'e^{ikx} & x \to \infty \end{cases}. \tag{5}$$

Interestingly, the reflection and transmission coefficients do not depend on the side from which the wave-function scatters off the potential, i.e. $R' = R$, $T' = T$. Prove that!

[1] This wave-function should be multiplied by a factor of $L^{-1/2}$, where L is the size of the system. Yet, we omit this factor from our calculations in the name of brevity.

[2] Note that elastic scattering was assumed here as the momentum of the wave-function k does not change due to the interaction with the potential.

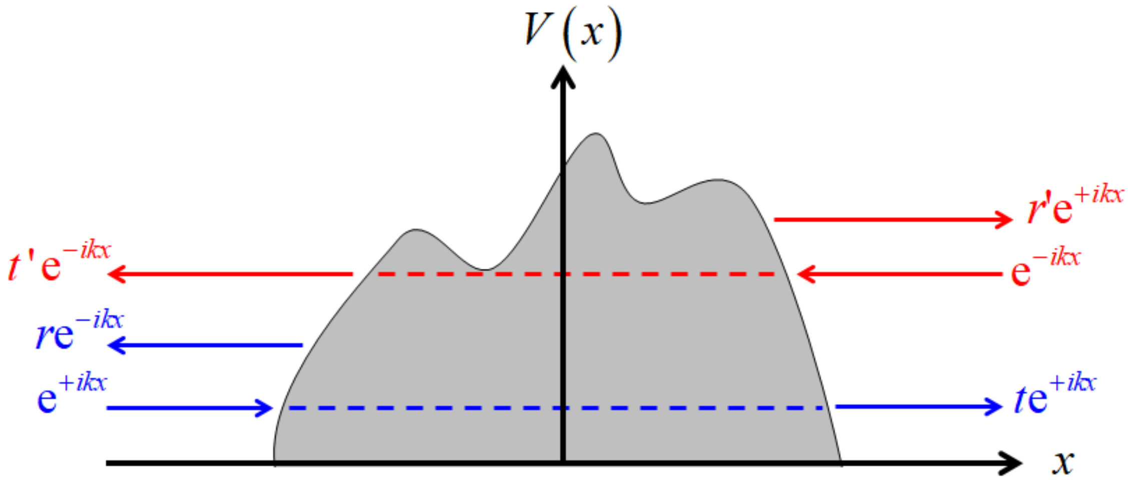

Figure 1: Free wave-function hits a potential of arbitrary shape (not necessarily symmetric). Part of the wave-function is reflected and part of it is transmitted to the other side through tunneling. In blue: $\psi_R(x)$. In red: $\psi_L(x)$.

Solution

Far away from the potential, at $x \to \pm\infty$, the free wave-function ψ_R is an eigen-state of the Hamiltonian with energy $\hbar^2 k^2/2m$ and it satisfies the time-independent Schrödinger equation. Since this equation is linear and has no imaginary coefficients that multiply ψ_R, then $(\psi_R^* - r^*\psi_R)/t^*$ is also a solution. But:

$$\frac{\psi_R^* - r^*\psi_R}{t^*} = \begin{cases} \frac{r^*-r^*}{t^*}e^{ikx} + \frac{1-|r|^2}{t^*}e^{-ikx} & x \to -\infty \\ e^{-ikx} - r^*\frac{t}{t^*}e^{ikx} & x \to \infty \end{cases} = \begin{cases} te^{-ikx} & x \to -\infty \\ e^{-ikx} - r^*\frac{t}{t^*}e^{ikx} & x \to \infty \end{cases}, \tag{6}$$

where in the last step we used Eq. (4). This has the exact form of ψ_L with

$$\boxed{\begin{array}{ccc} t' = t & \Longrightarrow & T' = T \\ r' = -r^*\dfrac{t}{t^*} & \Longrightarrow & R' = R \end{array}}. \tag{7}$$

The S-Matrix

Note that we can write Eqs. (1) and (5) in matrix notation:

$$\begin{bmatrix} \psi_R \\ \psi_L \end{bmatrix} = \begin{bmatrix} I_R \\ I_L \end{bmatrix} + S \begin{bmatrix} O_R \\ O_L \end{bmatrix}, \tag{8}$$

where

$$\begin{bmatrix} I_R \\ I_L \end{bmatrix} \equiv \begin{bmatrix} e^{ikx} & \text{at } x \to -\infty \\ e^{-ikx} & \text{at } x \to \infty \end{bmatrix}, \qquad \begin{bmatrix} O_R \\ O_L \end{bmatrix} \equiv \begin{bmatrix} e^{ikx} & \text{at } x \to \infty \\ e^{-ikx} & \text{at } x \to -\infty \end{bmatrix}, \qquad S \equiv \begin{bmatrix} t & r \\ r' & t' \end{bmatrix}. \tag{9}$$

Question 2

Show that S is unitary.

Solution

We compute

$$SS^{\dagger}=\begin{bmatrix} t & r \\ r' & t' \end{bmatrix}\begin{bmatrix} t^{*} & r'^{*} \\ r^{*} & t'^{*} \end{bmatrix}=\begin{bmatrix} \left|t\right|^{2}+\left|r\right|^{2} & tr'^{*}+rt'^{*} \\ t^{*}r'+t'r^{*} & \left|t'\right|^{2}+\left|r'\right|^{2} \end{bmatrix}=\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \tag{10}$$

where in the last step we used Eqs. (4) and (7).

Question 3

Find the S matrix for the potential

$$V\left(x\right)=V_{0}\left[\delta\left(x-a\right)+\delta\left(x+a\right)\right], \tag{11}$$

and find quasi-bound states for large V_0. What is the lifetime of these states?

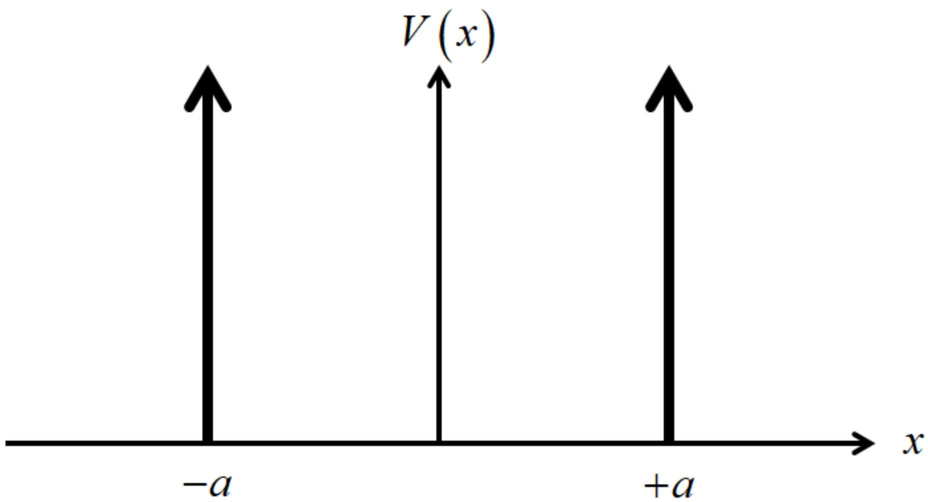

Figure 2: The double delta potential.

Solution

Since the potential is symmetric, it is clear that $r'=r$ ($t'=t$ always happens as we proved in Eq. (7)) and

$$\psi_{L}\left(x\right)=\psi_{R}\left(-x\right). \tag{12}$$

Moreover, as a consequence of this symmetry, the Hamiltonian commutes with the parity operator, $[\hat{H},\hat{P}]=0$, and $\hat{H}$ and $\hat{P}$ share the same eigen-states. Notice that

$$\begin{aligned} P\psi_{L}\left(x\right)&=\psi_{L}\left(-x\right)=\psi_{R}\left(x\right)\\ P\psi_{R}\left(x\right)&=\psi_{R}\left(-x\right)=\psi_{L}\left(x\right). \end{aligned} \tag{13}$$

Therefore, if we define

$$\begin{aligned}\psi_+(x) &\equiv \psi_L(x) + \psi_R(x) \\ \psi_-(x) &\equiv \psi_L(x) - \psi_R(x),\end{aligned} \tag{14}$$

then it is easy to see that these are parity eigen-states:

$$\begin{aligned}P\psi_+(x) = P\psi_L(x) + P\psi_R(x) = \psi_R(x) + \psi_L(x) = +\psi_+(x) \\ P\psi_-(x) = P\psi_L(x) - P\psi_R(x) = \psi_R(x) - \psi_L(x) = -\psi_-(x),\end{aligned} \tag{15}$$

and therefore $\psi_+(x)$, $\psi_-(x)$ are also the eigen-states of the Hamiltonian.

We can write Eq. (14) in the form of matrix notation:

$$\begin{bmatrix}\psi_+ \\ \psi_-\end{bmatrix} = M\begin{bmatrix}\psi_R \\ \psi_L\end{bmatrix}, \qquad M = \begin{bmatrix}1 & 1 \\ -1 & 1\end{bmatrix}. \tag{16}$$

Thus, according to Eq. (8),

$$\begin{bmatrix}\psi_+ \\ \psi_-\end{bmatrix} = M\begin{bmatrix}\psi_R \\ \psi_L\end{bmatrix} = M\begin{bmatrix}I_R \\ I_L\end{bmatrix} + MSM^{-1}M\begin{bmatrix}O_R \\ O_L\end{bmatrix} = \begin{bmatrix}I_+ \\ I_-\end{bmatrix} + \underbrace{MSM^{-1}}_{S_P}\begin{bmatrix}O_+ \\ O_-\end{bmatrix}. \tag{17}$$

Let's calculate S_P explicitly.

$$S_P = MSM^{-1} = \begin{bmatrix}1 & 1 \\ -1 & 1\end{bmatrix}\begin{bmatrix}t & r \\ r & t\end{bmatrix}\begin{bmatrix}1/2 & -1/2 \\ 1/2 & 1/2\end{bmatrix} = \begin{bmatrix}t+r & 0 \\ 0 & t-r\end{bmatrix} \equiv \begin{bmatrix}S_{++} & 0 \\ 0 & S_{--}\end{bmatrix}. \tag{18}$$

Thus, Eqs. (17) and (18) allow us to calculate $\psi_\pm(x)$ at $|x| > a$ where the potential vanishes,

$$\begin{cases}\psi_+(x) &= \quad \mathrm{e}^{-ik|x|} + S_{++}\mathrm{e}^{ik|x|} \\ \psi_-(x) &= \quad \mathrm{sgn}(x)\cdot\left(\mathrm{e}^{-ik|x|} + S_{--}\mathrm{e}^{ik|x|}\right)\end{cases}, \qquad |x| > a. \tag{19}$$

How $\psi_\pm(x)$ look like within the potential barriers? In this region, we are looking for solutions of Schrödinger equation with energy $E = \hbar^2k^2/2m$ and zero potential. The solutions are combinations of $\mathrm{e}^{\pm ikx}$, but $\psi_\pm(x)$ have definite parity so

$$\begin{cases}\psi_+(x) &= \quad A\cos(kx) \\ \psi_-(x) &= \quad B\sin(kx)\end{cases}, \qquad |x| < a. \tag{20}$$

We can find the coefficients A and B by requiring the wave-functions to be continuous at $x = \pm a$. This yields

$$A\cos(ka) = \mathrm{e}^{-ika} + S_{++}\mathrm{e}^{ika} \tag{21}$$

$$B\sin(ka) = \mathrm{e}^{-ika} + S_{--}\mathrm{e}^{ika}. \tag{22}$$

In order to find S_{++}, S_{--} we can integrate Schrödinger equation in the vicinity of $x = a$.

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_\pm(x) + V_0\left[\delta(x-a) + \delta(x+a)\right]\psi_\pm(x) = E\psi_\pm(x) \tag{23}$$

$$\Longrightarrow -\frac{\hbar^2}{2m}\left[\psi'_\pm\left(a^+\right) - \psi'_\pm\left(a^-\right)\right] + V_0\psi_\pm(a) = 0 \tag{24}$$

After doing the boring algebra (which I'm sure you are all capable of) we get:

$$S_{++} = \mathrm{e}^{-2ika} \frac{i\hbar^2 k \mathrm{e}^{+ika} + 2mV_0 \cos(ka)}{i\hbar^2 k \mathrm{e}^{-ika} - 2mV_0 \cos(ka)} \tag{25}$$

$$S_{--} = \mathrm{e}^{-2ika} \frac{i\hbar^2 k \mathrm{e}^{+ika} + 2mV_0 \sin(ka)}{i\hbar^2 k \mathrm{e}^{-ika} - 2mV_0 \sin(ka)}. \tag{26}$$

As a quick sanity check, we note that the magnitude of both S_{++} and S_{--} is unity. This is required due to the unitarity of S_P. We can therefore write

$$S_{++} = \mathrm{e}^{2i\delta_+(k)}, \qquad S_{--} = \mathrm{e}^{2i\delta_-(k)}. \tag{27}$$

$\delta_\pm(k)$ are called *phase shifts* (you will learn more about these later in the course).

Let us suppose first that $V_0 \to \infty$. If $k \neq \frac{\pi}{2a}(2n+1)$ (where $n \in \mathbb{N}$) the V_0 term is dominant in the numerator and denominator of Eq. (25), and $S_{++} = -\mathrm{e}^{-2ika}$. Likewise, we conclude $S_{--} = -\mathrm{e}^{-2ika}$ if $k \neq \frac{\pi}{2a}(2n)$. What is the reflection coefficient in that case?

$$r = \frac{S_{++} - S_{--}}{2} = 0, \qquad \text{for } k \neq \frac{\pi n}{2a},\ V_0 \to \infty \tag{28}$$

This result implies that we cannot sense the potential if the incoming particles don't have the "correct" value of k (in 3D, the cross section of the target would vanish for such particles). What happens if $k = \pi n/2a$? We end up with bound states between the potential barriers! Particles with eigen-energies

$$E = \frac{\hbar^2 k^2}{2m} = \frac{\pi^2 n^2}{8ma^2} \tag{29}$$

are doomed to remain in their prison for eternity.

Notice that the special k values of the bound states correspond to poles of the S matrix. For instance, let us examine the denominator of S_{++} (Eq. 25).

$$i\hbar^2 k \mathrm{e}^{-ika} = 2mV_0 \cos(ka) = mV_0 \left(\mathrm{e}^{ika} + \mathrm{e}^{-ika}\right)$$

$$\implies \mathrm{e}^{2ika} + 1 = \frac{i\hbar^2 k}{mV_0} \xrightarrow[V_0 \to \infty]{} 0 \tag{30}$$

$$\implies \mathrm{e}^{2ika} = -1$$

$$\implies k = \frac{\pi}{2a}(2n+1) \qquad n \in \mathbb{N}. \tag{31}$$

Similarly, the poles of S_{--} correspond to $k = \frac{\pi}{2a}(2n)$. This is an example to a general connection between the poles of the S matrix and the bound states of the system.

What happens if V_0 is large but finite? We return to Eq. (30), but this time we take the logarithm of both sides and approximate $\ln(1-x) \approx -x - x^2/2$.

$$2ika = \ln\left(\frac{i\hbar^2 k}{mV_0} - 1\right) = 2\pi i n + \pi i + \ln\left(1 - \frac{i\hbar^2 k}{mV_0}\right) \approx 2\pi i\left(n + \frac{1}{2}\right) - \frac{i\hbar^2 k}{mV_0} - \frac{1}{2}\left(\frac{i\hbar^2 k}{mV_0}\right)^2 \tag{32}$$

$$\implies k = \underbrace{\frac{\pi}{2a}(2n+1)}_{k_n} - \frac{\hbar^2 k}{2mV_0 a} - i\frac{\hbar^4 k^2}{4m^2 V_0^2 a}. \tag{33}$$

As before, taking $V_0 \to \infty$ will retrieve the bound states (Eq. 31). But now we want to find the poles of the S matrix for a finite V_0. Therefore, we plug Eq. (33) in itself, but we omit all $\mathcal{O}\left(V_0^{-3}\right)$ terms.

$$\begin{aligned} k &= k_n - \frac{\hbar^2}{2mV_0 a}\left(k_n - \frac{\hbar^2(k_n + \dots)}{2mV_0 a} + \dots\right) - i\frac{\hbar^4 (k_n + \dots)^2}{4m^2 V_0^2 a} \\ &= k_n - \frac{\hbar^2 k_n}{2mV_0 a} + \frac{\hbar^4 k_n}{4m^2 V_0^2 a^2} - i\frac{\hbar^4 k_n^2}{4m^2 V_0^2 a} + \mathcal{O}\left(V_0^{-3}\right). \end{aligned} \tag{34}$$

The particle's energy is given by

$$E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 k_n^2}{2m} - \frac{\hbar^4 k_n^2}{2m^2 V_0 a} + \frac{3\hbar^6 k_n^2}{8m^3 V_0^2 a^2} - i\frac{\hbar^6 k_n^3}{4m^3 V_0^2 a} + \mathcal{O}\left(V_0^{-3}\right). \tag{35}$$

These states evolve in time according to

$$\mathrm{e}^{-iEt/\hbar} = \mathrm{e}^{-i\,\mathrm{Re}\{E\}t/\hbar}\mathrm{e}^{\mathrm{Im}\{E\}t/\hbar} = \mathrm{e}^{-i\,\mathrm{Re}\{E\}t/\hbar}\mathrm{e}^{-t/2\tau}, \tag{36}$$

where we identified the states lifetime[3],

$$\boxed{\tau = -\frac{\hbar}{2\,\mathrm{Im}\{E\}} = \frac{2m^3 V_0^2 a}{\hbar^5 k_n^3} = \frac{16m^3 V_0^2 a^4}{\pi^3 \hbar^5 (2n+1)^3}}. \tag{37}$$

τ is the resonance lifetime — eventually these states decay because they tunnel out of the delta barriers (which is impossible when $V_0 \to \infty$). Such states are called *quasi-bound states*.

[3]There are additional lifetimes that correspond to the poles of S_{--}. Their expression is the same except $2n+1 \to 2n$.