

Problem 1 – Chapter 3 # 3)

In the r -representation, the Schrödinger equation for a particle under the influence of a potential $V(\vec{r})$ is given by

$$i\hbar \frac{\partial}{\partial t} \Psi(\vec{r}, t) = \left[-\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r}) \right] \Psi(\vec{r}, t). \quad (1)$$

(a) By using the properties of the Fourier transform show that the Schrodinger equation in the p -representation can be written as

$$\left(i\hbar \frac{\partial}{\partial t} - \frac{\vec{p}^2}{2m} \right) \tilde{\Psi}(\vec{p}, t) = \frac{1}{(2\pi\hbar)^{3/2}} \int d^3\vec{p}' \tilde{V}(\vec{p} - \vec{p}') \tilde{\Psi}(\vec{p}', t), \quad (2)$$

where

$$\tilde{\Psi}(\vec{p}, t) = \int \frac{d^3\vec{r}}{(2\pi\hbar)^{3/2}} e^{-i\vec{p}\cdot\vec{r}/\hbar} \Psi(\vec{r}, t), \quad \tilde{V}(\vec{p}) = \int \frac{d^3\vec{r}}{(2\pi\hbar)^{3/2}} e^{-i\vec{p}\cdot\vec{r}/\hbar} V(\vec{r}). \quad (3)$$

Assume that $V(\vec{r})$ vanishes as $|\vec{r}| \rightarrow \infty$ fast enough for its Fourier transform to exist. Note that in the p -space Schrödinger equation as given above, the term with the potential reduces to a convolution product involving the Fourier transforms $\tilde{V}(\vec{p})$ and $\tilde{\Psi}(\vec{p}, t)$.

(b) Show that the p -space Schrödinger equation can also be written as

$$i\hbar \frac{\partial}{\partial t} \tilde{\Psi}(\vec{p}, t) = \left[\frac{\vec{p}^2}{2m} + V(i\hbar \vec{\nabla}_p) \right] \tilde{\Psi}(\vec{p}, t) \quad (4)$$

as given in the notes.

(a) We take the Fourier transform of the S.E.:

$$\int \frac{d^3\vec{r}}{(2\pi\hbar)^{3/2}} e^{-i\vec{p}\cdot\vec{r}/\hbar} \left\{ i\hbar \frac{\partial \Psi(\vec{r}, t)}{\partial t} - \left[-\frac{\hbar^2}{2m} \nabla^2 \Psi(\vec{r}, t) + V(\vec{r}) \Psi(\vec{r}, t) \right] \right\} = 0. \quad (5)$$

The first two terms are quite simple to determine. For the first, notice that there is not time-dependence in the integration except for the wave function, allowing us to pull it out of the integral, and for the second term, we can integrate by parts twice, giving

$$\frac{\partial \tilde{\Psi}(\vec{p}, t)}{\partial t} - \left[-\frac{\vec{p}^2}{2m} \tilde{\Psi}(\vec{p}, t) + \int \frac{d^3\vec{r}}{(2\pi\hbar)^{3/2}} e^{-i\vec{p}\cdot\vec{r}/\hbar} V(\vec{r}) \Psi(\vec{r}, t) \right] = 0. \quad (6)$$

All that remains now is to evaluate the last term, which is the Fourier transform of a product of functions. Note that we know that the fourier transform of a convolution of functions f and g is just the product of the individual fourier transforms of f and g . Because of the symmetric nature of the Fourier transform, we may expect that a similar result for the Fourier transform of a product of functions. Namely, the fourier transform

of this product is just a convolution in the conjugate space, which we now prove. Let $f, g \in L^2(\mathbb{R}^3)$. Thus,

$$\begin{aligned}
 & \int \frac{d^3\vec{r}}{(2\pi\hbar)^{3/2}} e^{-i\vec{p}\cdot\vec{r}/\hbar} f(\vec{r}) g(\vec{r}) \\
 &= \int \frac{d^3\vec{r}}{(2\pi\hbar)^{3/2}} e^{-i\vec{p}\cdot\vec{r}/\hbar} \left[\int \frac{d^3\vec{q}}{(2\pi\hbar)^{3/2}} e^{i\vec{q}\cdot\vec{r}/\hbar} \tilde{f}(\vec{q}) \right] \left[\int \frac{d^3\vec{l}}{(2\pi\hbar)^{3/2}} e^{i\vec{l}\cdot\vec{r}/\hbar} \tilde{g}(\vec{l}) \right] \\
 &= \int \frac{d^3\vec{q} d^3\vec{l}}{(2\pi\hbar)^{3/2}} \tilde{f}(\vec{q}) \tilde{g}(\vec{l}) \underbrace{\left[\int \frac{d^3\vec{r}}{(2\pi\hbar)^{3/2}} \frac{e^{i(\vec{q}+\vec{l}-\vec{p})\cdot\vec{r}/\hbar}}{(2\pi\hbar)^3} \right]}_{\delta^{(3)}(\vec{l}-[\vec{p}-\vec{q}])} \\
 &= \int \frac{d^3\vec{q}}{(2\pi\hbar)^{3/2}} \tilde{f}(\vec{q}) \tilde{g}(\vec{p}-\vec{q}) = \tilde{f} \star \tilde{g},
 \end{aligned} \tag{7}$$

which is the result we anticipated. Note that the convolution is commutative in f and g (i.e. $\tilde{f} \star \tilde{g} = \tilde{g} \star \tilde{f}$). Hence, we have

$$\boxed{\frac{\partial \tilde{\Psi}(\vec{p}, t)}{\partial t} = -\frac{\vec{p}^2}{2m} \tilde{\Psi}(\vec{p}, t) + \tilde{\Psi} \star \tilde{V}}. \tag{8}$$

Problem 2 – Chapter 4 # 2)

This problem deals with the solution of the S.E. in momentum space.

(a) Solve directly in momentum space for the bound-state energy and wave function in an attractive δ -function potential, given in coordinate space by $V(x) = -V_0\delta(x)$ with $V_0 > 0$.

(b) From the momentum space wave function so obtained, calculate the average kinetic energy of the particle. Repeat the calculation of this average kinetic energy but in coordinate space, using the wave function you derived in the previous problem. Note that the first derivative of the coordinate-space bound-state wave function is discontinuous at $x = 0$.

(a) If our potential $V(x) = -V_0\delta(x)$, then

$$\tilde{V}(p) = \int \frac{dx}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar} [-V_0\delta(x)] = -\frac{V_0}{\sqrt{2\pi\hbar}}. \tag{9}$$

Note that we could have repeated the process from part (a) on the time-independent S.E. to arrive at

$$\left[E - \frac{p^2}{2m} \right] \tilde{\psi}(p) = -\frac{V_0}{\sqrt{2\pi\hbar}} \int \frac{dp}{\sqrt{2\pi\hbar}} \tilde{\psi}(p). \tag{10}$$

Notice that the r.h.s is a constant with respect to p , meaning

$$\tilde{\psi}(p) = \frac{\mathcal{N}}{|E| + p^2/2m}, \tag{11}$$

where we have used the fact that $E < 0$ for a bound state. The energy E is determined using

$$\frac{V_0}{2\pi\hbar} \int_{-\infty}^{\infty} \frac{1}{|E| + p^2/2m} = 1 \Rightarrow \sqrt{\frac{2m}{|E|}} = \frac{2\hbar}{V_0} \quad (12)$$

$$E = -\frac{V_0^2}{4\hbar^2}(2m) = -\frac{mV_0^2}{2\hbar^2}. \quad (13)$$

Thus,

$$\tilde{\psi}(p) = \frac{\mathcal{N}}{p_0^2 + p^2}, \quad (14)$$

where we have defined $p_0^2 = 2mE$. Normalizing gives

$$\tilde{\psi}(p) = \sqrt{\frac{2p_0^3}{\pi}} \frac{1}{p_0^2 + p^2}, \quad (15)$$

which agrees with the result found in a previous homework where we explicitly took the Fourier transform of the coordinate space result.

(b) The average kinetic energy of a particle is given by

$$\langle T \rangle = \frac{1}{2m} \langle p^2 \rangle = \frac{1}{2m} \frac{2p_0^3}{\pi} \int_{-\infty}^{\infty} \frac{p^2}{(p_0^2 + p^2)^2} dp = \frac{p_0^3}{\pi m} \frac{\pi}{2p_0} = \frac{p_0^2}{2m} = E. \quad (16)$$

We can verify this result by repeating the calculation in coordinate space:

$$\begin{aligned} \langle T \rangle &= \frac{p_0}{\hbar} \int_{-\infty}^{\infty} e^{-p_0|x|/\hbar} \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} e^{-p_0|x|/\hbar} \right) dx \\ &= -\frac{p_0\hbar}{2m} \left[\int_{-\infty}^0 e^{p_0x/\hbar} \frac{d^2}{dx^2} e^{p_0x/\hbar} dx + \int_0^{\infty} e^{-p_0x/\hbar} \frac{d^2}{dx^2} e^{-p_0x/\hbar} dx \right] \\ &= -\frac{p_0\hbar}{m} \left(-\frac{p_0}{\hbar} \right)^2 \int_0^{\infty} e^{-2p_0x/\hbar} dx = \frac{p_0^3}{m\hbar} \frac{\hbar}{2p_0} = \frac{p_0^2}{2m} = E. \end{aligned} \quad (17)$$

Problem 3 – Chapter 5 # 4)

Consider a particle in one-dimension under the influence of the even potential given by

$$V(x) = \begin{cases} V_0 & |x| \leq a \\ 0 & |x| > a, \end{cases} \quad (18)$$

where $V_0 > 0$. Assume that the particle's energy E is in the range $0 < E < V_0$. Write the general solution as

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x < -a \\ Ce^{-\kappa x} + De^{\kappa x} & |x| < a \\ Fe^{ikx} + Ge^{-ikx} & x > a, \end{cases} \quad (19)$$

where $k = \sqrt{\epsilon}$, $\kappa = \sqrt{v_0 - \epsilon}$, $\epsilon = 2mE/\hbar^2$, and $v_0 = 2mV_0/\hbar^2$.

(a) By imposing the appropriate boundary conditions at $x = \pm a$, show that the coefficients A and B are related to the coefficients F and G in the following way

$$\begin{pmatrix} A \\ B \end{pmatrix} = \begin{bmatrix} (\cosh 2\kappa a + i(\alpha/2) \sinh 2\kappa a)e^{2ika} & i(\beta/2) \sinh 2\kappa a \\ -i(\beta/2) \sinh 2\kappa a & (\cosh 2\kappa a - i(\alpha/2) \sinh 2\kappa a)e^{-2ika} \end{bmatrix} \begin{pmatrix} F \\ G \end{pmatrix}, \quad (20)$$

where

$$\alpha = \frac{\kappa}{k} - \frac{k}{\kappa}, \quad \beta = \frac{\kappa}{k} + \frac{k}{\kappa}, \quad \beta^2 - \alpha^2 = 4. \quad (21)$$

(b) From the matrix relation obtained in part (a) above, show that the transmission coefficient T for a high and wide barrier with $\kappa a \gg 1$ is approximately given by

$$T \approx 16e^{-4\kappa a} \left(\frac{\kappa k}{k^2 + \kappa^2} \right)^2. \quad (22)$$

(c) Consider the case of a very narrow but very high barrier such that aV_0 is finite. Assume $V_0 \gg E$, $\kappa \gg k$, and $\kappa a \ll 1$, but $\kappa^2 a$ is finite. Show that the transmission coefficient under these conditions is the same as that obtained in the repulsive δ -function potential $V(x) = 2aV_0\delta(x)$, namely

$$T = \frac{\epsilon}{\epsilon + (2mV_0a/\hbar^2)^2}. \quad (23)$$

(a) The S.E. under this potential reads

$$\psi''(x) = \begin{cases} [v_0 - \epsilon]\psi(x) & |x| < a \\ -\epsilon\psi(x) & |x| > a, \end{cases} \quad (24)$$

where $v_0 = 2mV_0/\hbar^2$ and $\epsilon = 2mE/\hbar^2$. This has solution

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x < a \\ Ce^{-\kappa x} + De^{\kappa x} & |x| < a \\ Fe^{ikx} + Ge^{-ikx} & x > a, \end{cases} \quad (25)$$

where $k^2 = \epsilon$ and $\kappa^2 = v_0 - \epsilon$. We have the following boundary conditions

$$\psi(-a^-) = \psi(-a^+) \Rightarrow Ae^{-ika} + Be^{ika} = Ce^{\kappa a} + De^{-\kappa a} \quad (26)$$

$$\psi'(-a^-) = \psi'(-a^+) \Rightarrow ik(Ae^{-ika} - Be^{ika}) = \kappa(-Ce^{\kappa a} + De^{-\kappa a}) \quad (27)$$

$$\psi(a^-) = \psi(a^+) \Rightarrow Ce^{-\kappa a} + De^{\kappa a} = Fe^{ika} + Ge^{-ika} \quad (28)$$

$$\psi'(a^-) = \psi'(a^+) \Rightarrow \kappa(-Ce^{-\kappa a} + De^{\kappa a}) = ik(Fe^{ika} - Ge^{-ika}). \quad (29)$$

Let us solve for C and D in terms of A and B :

$$Ce^{-\kappa a} = \frac{e^{-ika}(\kappa - ik)}{2\kappa e^{2\kappa a}}A + \frac{e^{ika}(\kappa + ik)}{2\kappa e^{2\kappa a}}B \quad (30)$$

$$De^{\kappa a} = \frac{e^{-ika}(\kappa + ik)}{2\kappa e^{-2\kappa a}}A + \frac{e^{ika}(\kappa - ik)}{2\kappa e^{-2\kappa a}}B. \quad (31)$$

The last two equations from the BCs are then

$$\frac{e^{-ika}}{2\kappa} \left[\frac{\kappa - ik}{e^{2\kappa a}} + \frac{\kappa + ik}{e^{-2\kappa a}} \right] A + \frac{e^{ika}}{2\kappa} \left[\frac{\kappa - ik}{e^{-2\kappa a}} + \frac{\kappa + ik}{e^{2\kappa a}} \right] B = Fe^{ika} + Ge^{-ika} \quad (32)$$

$$\frac{e^{-ika}}{2} \left[\frac{-\kappa + ik}{e^{2\kappa a}} + \frac{\kappa + ik}{e^{-2\kappa a}} \right] A + \frac{e^{ika}}{2} \left[\frac{\kappa - ik}{e^{-2\kappa a}} - \frac{\kappa + ik}{e^{2\kappa a}} \right] B = ik(Fe^{ika} - Ge^{-ika}). \quad (33)$$

Observe that these equations reduce to

$$e^{-ika} \left[\cosh(2\kappa a) + i \frac{k}{\kappa} \sinh(2\kappa a) \right] A + e^{ika} \left[\cosh(2\kappa a) - i \frac{k}{\kappa} \sinh(2\kappa a) \right] B = Fe^{ika} + Ge^{-ika} \quad (34)$$

$$e^{-ika} \left[\cosh(2\kappa a) - i \frac{\kappa}{k} \sinh(2\kappa a) \right] A - e^{ika} \left[\cosh(2\kappa a) + i \frac{\kappa}{k} \sinh(2\kappa a) \right] B = Fe^{ika} - Ge^{-ika}. \quad (35)$$

Solving for F and G gives

$$F = \left[\cosh(2\kappa a) - i(\alpha/2) \sinh(2\kappa a) \right] e^{-2ika} A - i(\beta/2) \sinh(2\kappa a) B \quad (36)$$

$$G = i(\beta/2) \sinh(2\kappa a) A + \left[\cosh(2\kappa a) + i(\alpha/2) \sinh(2\kappa a) \right] e^{2ika} B, \quad (37)$$

and rewriting in matrix form

$$\begin{pmatrix} F \\ G \end{pmatrix} = \begin{bmatrix} \left(\cosh(2\kappa a) - i(\alpha/2) \sinh(2\kappa a) \right) e^{-2ika} & -i(\beta/2) \sinh(2\kappa a) \\ i(\beta/2) \sinh(2\kappa a) & \left(\cosh(2\kappa a) + i(\alpha/2) \sinh(2\kappa a) \right) e^{2ika} \end{bmatrix} \begin{pmatrix} A \\ B \end{pmatrix}. \quad (38)$$

Notice that the matrix on the r.h.s is unitary¹, meaning we can write

$$\begin{pmatrix} A \\ B \end{pmatrix} = \begin{bmatrix} \left(\cosh(2\kappa a) + i(\alpha/2) \sinh(2\kappa a) \right) e^{2ika} & i(\beta/2) \sinh(2\kappa a) \\ -i(\beta/2) \sinh(2\kappa a) & \left(\cosh(2\kappa a) - i(\alpha/2) \sinh(2\kappa a) \right) e^{-2ika} \end{bmatrix} \begin{pmatrix} F \\ G \end{pmatrix}. \quad (39)$$

(b) The transmission coefficient (in the limit $\kappa a \gg 1$ – noting that $\cosh x \approx \sinh x \approx e^x/2$ when $x \gg 1$) is given by

$$\begin{aligned} T &= \left| \frac{1}{\cosh(2\kappa a) + i(\alpha/2) \sinh(2\kappa a)} e^{2ika} \right|^2 \approx 16e^{-4\kappa a} \frac{1}{4 + \alpha^2} \\ &= 16e^{-4\kappa a} \left[4 + \left(\frac{\kappa - k}{k\kappa} \right)^2 \right]^{-1} = 16e^{-4\kappa a} \left(\frac{\kappa k}{k + k} \right)^2. \end{aligned} \quad (40)$$

Note that this implies that the probability of transmission for such a potential is exponentially suppressed.

(c) If we now consider the case where our square barrier approaches a delta barrier ($a \rightarrow 0$, $v_0 \rightarrow \infty$, $2aV_0 = \text{constant}$), the transmission coefficient becomes

$$\begin{aligned} T &= \frac{1}{\cosh^2(2\kappa a) + (\alpha/2)^2 \sinh^2(2\kappa a)} = \frac{1}{\cosh^2(2\sqrt{\kappa^2 a} \sqrt{a}) + \frac{\alpha^2}{4} \sinh^2(2\sqrt{\kappa^2 a} \sqrt{a})} \\ &= \frac{1}{1 + \frac{\kappa^2}{4k^2} (4\kappa^2 a^2) + \dots} \approx \frac{\epsilon}{\epsilon + v_0^2 a^2} = \frac{\epsilon}{\epsilon + (2mV_0 a / \hbar^2)^2}, \end{aligned} \quad (41)$$

which is the result we expected.

Problem 4 – Chapter 5 # 5)

Consider a particle of mass m under the action of a potential given by

$$V(x) = \frac{\hbar^2}{2m} [v_0 \theta(-x) - w_0 \delta(x)], \quad (42)$$

where $\theta(z)$ is the Heaviside step function.

(a) Show that the presence of the potential step of height v_0 does not alter the boundary conditions that the wave function and its first derivative must satisfy at $x = 0$. Is there a bound state? If there is, what is its energy?

¹Justification: (1) Without resorting to wave packets, notice that taking $x \rightarrow -x$, we have $A^* = G$ and $B^* = F$, meaning $|F|^2 + |G|^2 = |B^*|^2 + |A^*|^2 = |A|^2 + |B|^2$. (2) Using wave packets, we would see that $j(-\infty) = j(\infty)$, where j is the probability current density. Thus, $|A|^2 + |B|^2 = |F|^2 + |G|^2$. (3) One could also just do the algebra, but noticing that the scattering matrix is indeed unitary without some other physical intuition/rationale would certainly be some divine inspiration.

- (b) Assume $\epsilon > v_0$. Calculate the reflection and transmission coefficients. What are these coefficients in the limit $\epsilon \gg v_0, w_0$?
- (c) Now, assume $0 < \epsilon < v_0$. Calculate the reflection and transmission coefficients in this case. Explain why you could have anticipated the result. Compute the time delay associated with the reflected wave packet in this case.