

PHYS 661 - Quantum Mechanics II
Modern Quantum Mechanics by *J. J. Sakurai*
Student: **Ralph Razzouk**

Homework 5

Problem 1 - 1D δ -potential Revisited

Consider a 1D potential well $U(x) = -\alpha\delta(x)$ where $\alpha > 0$ so there is a bound state. The ground state of this system is a bound level with wave function $\psi_0(x) = \sqrt{\kappa}e^{-\kappa|x|}$ and energy $E_0^{(0)} = -\frac{\hbar^2\kappa^2}{2m}$, where $\kappa = m\alpha/\hbar^2$.

- (a) Show that the continuous spectrum wave functions are $\psi_{+,k}(x) = \frac{1}{\sqrt{\pi}} \cos(k|x| + \frac{\varphi_k}{2})$ and $\psi_{-,k} = \frac{1}{\sqrt{\pi}} \sin(kx)$, both with energy $E_k^{(0)} = \frac{\hbar^2 k^2}{2m}$. (The subscript \pm denotes spatial parity eigenvalues.) Find the phase φ_k .
- (b) Show that the continuous spectrum states are δ -normalized, $\int_{-\infty}^{\infty} dx \psi_{a,k}(x) \psi_{b,k'}(x) = \delta_{ab} \delta(k - k')$. Show that they are orthogonal to the bound state ψ_0 . (Note that it is enough to consider $k, k' > 0$ since the states with $k < 0$ are not linearly independent.) You can use the helpful identity $\int_0^{\infty} dx e^{i(k-k')x} = i \frac{1}{k-k'} + \pi \delta(k - k')$.
- (c) By using a scattering wave function of the form

$$\psi_k(x) = \begin{cases} e^{ikx} + r e^{-ikx} & x < 0, \\ t e^{ikx} & x > 0, \end{cases}$$

find the transmission coefficient $D = |t|^2$ of the scattering state. Express D in terms of the energy of the scattering state.

Solution. (a) Let's verify these wave functions by checking if they satisfy the Schrödinger equation with the delta potential:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} - \alpha\delta(x)\psi = E\psi$$

For the even parity state $\psi_{+,k}$, we need to check that it satisfies the free Schrödinger equation away from $x = 0$ as well as having a discontinuity in its derivative at $x = 0$, matching the delta function potential.

- For $x \neq 0$, $\psi_{+,k}$ clearly satisfies

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = \frac{\hbar^2 k^2}{2m} \psi = E_k^{(0)} \psi.$$

- At $x = 0$, integrating the Schrödinger equation from $-\epsilon$ to ϵ and taking $\epsilon \rightarrow 0$, we get

$$-\frac{\hbar^2}{2m} [\psi'(\epsilon) - \psi'(-\epsilon)] = -\alpha\psi(0).$$

Evaluating the derivatives and using $\psi_{+,k}(0) = \frac{1}{\sqrt{\pi}} \cos(\frac{\varphi_k}{2})$, we get

$$\frac{\hbar^2 k}{\sqrt{\pi} m} \sin\left(\frac{\varphi_k}{2}\right) = \frac{\alpha}{\sqrt{\pi}} \cos\left(\frac{\varphi_k}{2}\right).$$

This gives us

$$\tan\left(\frac{\varphi_k}{2}\right) = \frac{m\alpha}{\hbar^2 k} = \frac{\kappa}{k}.$$

Therefore, $\varphi_k = 2 \arctan\left(\frac{\kappa}{k}\right)$. The odd parity state $\psi_{-,k}$ automatically satisfies the delta potential condition since it vanishes at $x = 0$.

(b) For the normalization, let's consider each case.

- For $\psi_{+,k}$ with $\psi_{+,k'}$, we have

$$\begin{aligned} \int_{-\infty}^{\infty} \psi_{+,k}(x) \psi_{+,k'}(x) dx &= \frac{2}{\pi} \int_0^{\infty} \cos\left(kx + \frac{\varphi_k}{2}\right) \cos\left(k'x + \frac{\varphi_{k'}}{2}\right) dx \\ &= \delta(k - k'). \end{aligned}$$

- For $\psi_{-,k}$ with $\psi_{-,k'}$, we have

$$\begin{aligned} \int_{-\infty}^{\infty} \psi_{-,k}(x) \psi_{-,k'}(x) dx &= \frac{1}{\pi} \int_{-\infty}^{\infty} \sin(kx) \sin(k'x) dx \\ &= \delta(k - k'). \end{aligned}$$

The cross terms between $\psi_{+,k}$ and $\psi_{-,k'}$ vanish due to odd/even parity.

For orthogonality with the bound state, we have

$$\begin{aligned} \int_{-\infty}^{\infty} \psi_0(x) \psi_{+,k}(x) dx &= 2\sqrt{\frac{\kappa}{\pi}} \int_0^{\infty} e^{-\kappa x} \cos\left(kx + \frac{\varphi_k}{2}\right) dx = 0 \\ \int_{-\infty}^{\infty} \psi_0(x) \psi_{-,k}(x) dx &= 0 \text{ (by parity)} \end{aligned}$$

(c) For the scattering state, we need to match the wave functions at $x = 0$ and match the discontinuity in derivatives at $x = 0$ due to the delta function.

At $x = 0$, we have $1 + r = t$ due to continuity and $ik(t - (1 - r)) = -\frac{m\alpha}{\hbar^2}t$ due to discontinuity. Solving, we get

$$r = \frac{-i\kappa}{k + i\kappa}, \quad t = \frac{k}{k + i\kappa}.$$

Therefore, the transmission coefficient is

$$D = |t|^2 = \frac{k^2}{k^2 + \kappa^2} = \frac{E}{E + |E_0^{(0)}|},$$

where we've expressed it in terms of the energy $E = \frac{\hbar^2 k^2}{2m}$ and the bound state energy $E_0^{(0)} = -\frac{\hbar^2 \kappa^2}{2m}$. ■

Problem 2 - Scattering Time-delay

Consider 1D scattering with a Gaussian wave packet so that the incident wave from the left is $\psi_{\text{inc}}(x, t) = \int_0^\infty dk e^{-\frac{1}{2}(k-k_0)^2/\Delta k^2} e^{-ikx} e^{-iE_k t/\hbar}$ for $x > a$ and the reflected wave is assumed to be $\psi_{\text{refl}}(x, t) = \int_0^\infty dk e^{-\frac{1}{2}(k-k_0)^2/\Delta k^2} e^{2i\delta(k)} e^{ikx} e^{-iE_k t/\hbar}$ for $x > a$. We denote $E_k = \hbar^2 k^2/(2m)$.

- Show that in the absence of scattering, the reflected wave packet peak at time t is at position $x = v_0 t$ where v_0 is the mean velocity. You can assume Δk is small.
- Calculate the peak position in the presence of scattering and show that now the peak is at $x = v_0(t - \Delta t)$, where $\Delta t = 2\hbar \left[\frac{d\delta(E)}{dE} \right]_{E=E_{k_0}}$.
- Calculate the time-delay for the example $V = \alpha\delta(x - a)$ that we discussed in the lecture. In the limit of large barrier, find the time delay for a wave packet that has k_0 such that 1. $|E_{k_0} - E_n| \gg \Gamma_n$, and 2. $E_{k_0} = E_n$. Comment on your findings.

Solution. (a) Let's analyze the incident wave packet first. Without scattering ($\delta(k) = 0$), the wave packet is

$$\psi_{\text{inc}}(x, t) = \int_0^\infty dk \exp \left[-\frac{(k - k_0)^2}{2\Delta k^2} - ikx - i\frac{\hbar k^2}{2m}t \right].$$

For small Δk , we can expand around k_0 to get

$$k^2 \approx k_0^2 + 2k_0(k - k_0).$$

This gives:

$$\begin{aligned} \psi_{\text{inc}}(x, t) &\approx \exp \left[-i\frac{\hbar k_0^2}{2m}t \right] \int_0^\infty dk \exp \left[-\frac{(k - k_0)^2}{2\Delta k^2} - ikx - i\frac{\hbar k_0}{m}(k - k_0)t \right] \\ &= \exp \left[-i\frac{\hbar k_0^2}{2m}t \right] \exp \left[-ik_0x - \frac{\Delta k^2}{2} \left(x + \frac{\hbar k_0}{m}t \right)^2 \right]. \end{aligned}$$

The peak of the wave packet occurs where the exponent is maximum, which is at

$$x + \frac{\hbar k_0}{m}t = 0.$$

Therefore, $x = v_0 t$ where $v_0 = \frac{\hbar k_0}{m}$ is the mean velocity.

- (b) With scattering, the phase shift $\delta(k)$ adds to the phase. The reflected wave becomes:

$$\psi_{\text{refl}}(x, t) = \int_0^\infty dk \exp \left[-\frac{(k - k_0)^2}{2\Delta k^2} + 2i\delta(k) + ikx - i\frac{\hbar k^2}{2m}t \right].$$

We can expand $\delta(k)$ around k_0 to get

$$\delta(k) \approx \delta(k_0) + \left. \frac{d\delta}{dk} \right|_{k_0} (k - k_0).$$

Using the same approximation for k^2 and completing the square in the exponent, the peak position now satisfies

$$x + \frac{\hbar k_0}{m}t + 2 \left. \frac{d\delta}{dk} \right|_{k_0} = 0.$$

Therefore

$$x = v_0(t - \Delta t),$$

where

$$\Delta t = 2 \left. \frac{d\delta}{dk} \right|_{k_0} = 2\hbar \left. \frac{d\delta}{dE} \right|_{E_{k_0}}.$$

(c) For $V = \alpha\delta(x - a)$, we found in lectures that

$$\delta(k) = -\arctan\left(\frac{m\alpha}{\hbar^2 k}\right).$$

Thus

$$\begin{aligned}\frac{d\delta}{dE} &= -\frac{m}{\hbar^2 k} \frac{1}{1 + \left(\frac{m\alpha}{\hbar^2 k}\right)^2} \frac{d}{dk} \left(\frac{m\alpha}{\hbar^2 k}\right) \frac{dk}{dE} \\ &= \frac{m^2 \alpha}{(\hbar^2 k^2 + m^2 \alpha^2) E}.\end{aligned}$$

- When $|E_{k_0} - E_n| \gg \Gamma_n$, we're far from resonance, so

$$\Delta t \approx \frac{2m^2 \alpha}{(\hbar^2 k_0^2 + m^2 \alpha^2) E_{k_0}}.$$

For a large barrier ($\alpha \rightarrow \infty$), $\Delta t \rightarrow 0$.

- At resonance, $E_{k_0} = E_n$, and the time delay reaches its maximum value

$$\Delta t \approx \frac{2m}{E_n \Gamma_n}.$$

Far from resonance, particles spend little time near the barrier. At resonance, particles are temporarily trapped in quasi-bound states, leading to significant time delays. This is analogous to classical resonance where energy is stored temporarily in the system. The time delay at resonance is inversely proportional to the width Γ_n , showing that narrower resonances lead to longer delays. ■

Problem 3 - Born Approximation

By using the Born approximation, find the scattering amplitude and total scattering cross section for the following 3D central potentials. For the total cross section, you can assume low energy and give leading $E \rightarrow 0$ behavior.

(a) $V(r) = \alpha\delta(r - a)$

(b) $V(r) = \begin{cases} V_0 & r < a \\ 0 & r > a \end{cases}$

Solution. (a) Consider the integral form of Schrödinger's equation

$$\psi_{\mathbf{k}}(\mathbf{r}) = \psi_{\mathbf{k}}^{(0)}(\mathbf{r}) + \frac{2m}{\hbar^2} \int \frac{d^3\mathbf{r}'}{4\pi} \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} V(\mathbf{r}') \psi_{\mathbf{k}}(\mathbf{r}')$$

with first order iterative solution given by

$$\psi_{\mathbf{k}}(\mathbf{r}) = \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{(2\pi)^{\frac{3}{2}}} + \frac{m}{2\pi\hbar^2} \int \frac{d^3\mathbf{r}' e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} V(\mathbf{r}') \frac{e^{i\mathbf{k}\cdot\mathbf{r}'}}{(2\pi)^{\frac{3}{2}}} + \mathcal{O}(v^2).$$

Since we have placed the detectors far away from the scattering center, we can apply the approximation

$$\begin{aligned} |\mathbf{r}-\mathbf{r}'| &= (\mathbf{r}^2 + \mathbf{r}'^2 - 2\mathbf{r}\cdot\mathbf{r}')^{\frac{1}{2}} \\ &= r \left(1 + \frac{\mathbf{r}'^2}{r^2} - \frac{2\mathbf{r}\cdot\mathbf{r}'}{r} \right)^{\frac{1}{2}} \\ &\approx r \left(1 - \frac{\mathbf{r}\cdot\mathbf{r}'}{r^2} \right). \end{aligned}$$

Thus,

$$\begin{aligned} \psi_{\mathbf{k}}(\mathbf{r}) &= \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{(2\pi)^{\frac{3}{2}}} + \frac{m}{2\pi\hbar^2} \int \frac{d^3\mathbf{r}' e^{ikr \left(1 - \frac{\mathbf{r}\cdot\mathbf{r}'}{r^2} \right)}}{r \left(1 - \frac{\mathbf{r}\cdot\mathbf{r}'}{r^2} \right)} V(\mathbf{r}') \frac{e^{i\mathbf{k}\cdot\mathbf{r}'}}{(2\pi)^{\frac{3}{2}}} \\ &= \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{(2\pi)^{\frac{3}{2}}} + \frac{e^{ikr}}{r} \frac{m}{2\pi\hbar^2} \int \frac{d^3\mathbf{r}' 4 e^{-ik\hat{\mathbf{r}}\cdot\mathbf{r}'} V(\mathbf{r}') e^{i\mathbf{k}\cdot\mathbf{r}'}}{(2\pi)^{\frac{3}{2}} (1 - \frac{\mathbf{r}\cdot\mathbf{r}'}{r^2})} \\ &\approx \frac{1}{(2\pi)^{\frac{3}{2}}} \left(e^{i\mathbf{k}\cdot\mathbf{r}} + \frac{e^{ikr}}{r} \frac{(2\pi)^{\frac{1}{2}} m}{\hbar^2} \int \frac{d^3\mathbf{r}'}{(2\pi)^{\frac{3}{2}}} e^{-ik\hat{\mathbf{r}}\cdot\mathbf{r}'} V(\mathbf{r}') e^{i\mathbf{k}\cdot\mathbf{r}'} \right). \end{aligned}$$

From the ansatz

$$\Psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} + \frac{e^{ikr}}{r} f_{\mathbf{k}}|\tilde{r}|,$$

we immediately read the scattering amplitude as

$$f_{\mathbf{k}}(\hat{r}) = \frac{m}{2\pi\hbar^2} \int d^3\mathbf{r}' e^{-ik\hat{\mathbf{r}}\cdot\mathbf{r}'} V(\mathbf{r}') e^{i\mathbf{k}\cdot\mathbf{r}'}.$$

(a) Let $V(\mathbf{r}) = \alpha\delta(r - a)$, then, we can write

$$\begin{aligned} f_{\mathbf{u}}(\hat{r}) &= \frac{m\alpha}{2\pi\hbar^2} \int_0^\infty dr' r'^2 \delta(r' - a) \int_0^{2\pi} d\phi' \int_{-1}^{+1} d(\cos(\theta)) e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}'} \\ &= \frac{m\alpha}{\hbar^2} \int_0^\infty dr' r'^2 \delta(r' - a) \left(\frac{e^{-i|\mathbf{k}-\mathbf{k}'|r'} - e^{+i|\mathbf{k}-\mathbf{k}'|r'}}{-i|\mathbf{k}-\mathbf{k}'|r'} \right) \\ &= 2m \int_0^\infty \frac{dr' r'}{|\mathbf{k}-\mathbf{k}'|} \sin(|\mathbf{k}-\mathbf{k}'| r') \alpha\delta(r' - a) \\ &= \frac{2ma\alpha}{\hbar^2 |\mathbf{k}-\mathbf{k}'|} \sin(|\mathbf{k}-\mathbf{k}'| a). \end{aligned}$$

Let $\theta = \arccos(\hat{k} \cdot \hat{r})$, we write

$$\begin{aligned}\mathcal{F}_{\mathbf{u}}|\theta| &= \sin\left(a\left(2k^2 - 2k^2 \cos(\theta)\right)^{\frac{1}{2}}\right) \cdot \frac{2ma\alpha}{F^2\left(2k^2 - 2k^2 \cos(\theta)\right)^{\frac{1}{2}}} \\ &= \sin\left(2ak \sin\left(\frac{\theta}{2}\right)\right) \cdot \frac{m\alpha a}{F^2 k \sin\left(\frac{\theta}{2}\right)}.\end{aligned}$$

Thus, the differential cross section is

$$\frac{d\sigma}{d\Omega} = \frac{m^2 \alpha^2 a^2}{\hbar^4 k^2} \sin^2\left(2ak \sin\left(\frac{\theta}{2}\right)\right) \csc^2\left(\frac{\theta}{2}\right).$$

Integrating over the solid angle, we get

$$\sigma = \left(\frac{m\alpha a}{\hbar^2 k}\right)^2 \int_0^{2\pi} d\phi \int_0^\pi \sin(\theta) \csc^2\left(\frac{\theta}{2}\right) \sin^2\left(2ak \sin\left(\frac{\theta}{2}\right)\right) d\theta.$$

We may now consider low energy approximation, for which $ka \ll 1$, such that we obtain

$$\begin{aligned}\sigma &\underset{E \rightarrow 0}{\approx} 2\pi \left(\frac{m\alpha a}{\hbar^2 k}\right)^2 \int_0^\pi \sin(\theta) \csc^2\left(\frac{\theta}{2}\right) \left(4a^2 k^2 \sin^2\left(\frac{\theta}{2}\right)\right) d\theta \\ &= \frac{16\pi m^2 \alpha^2 a^4}{\hbar^4}\end{aligned}$$

for $V(\mathbf{r}) = \alpha\delta(r - a)$, $ka \ll 1$.

(b) Let

$$V(r) = \begin{cases} V_0 & r < a, \\ 0 & r > a. \end{cases}$$

Then

$$\begin{aligned}f_{\mathbf{k}}(\hat{r}) &= \frac{m}{2\pi\hbar^2} \int d^3r' e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}'} \theta(a-r) V_0 \\ &= \frac{2m}{\hbar^2} \int_0^a \frac{dr' r' \sin(r'|\mathbf{k}-\mathbf{k}'|)}{|\mathbf{k}-\mathbf{k}'|} V_0 \\ &= \frac{2mV_0}{\hbar^2 |\mathbf{k}-\mathbf{k}'|} \int_0^a dr' r' \sin(r'|\mathbf{k}-\mathbf{k}'|) \\ &= \frac{2mV_0}{\hbar^2 |\mathbf{k}-\mathbf{k}'|^3} [\sin(|\mathbf{k}-\mathbf{k}'|a) - a|\mathbf{k}-\mathbf{k}'| \cos(a|\mathbf{k}-\mathbf{k}'|)] \\ &= \frac{mV_0}{4\hbar^2 k^3 \sin^3\left(\frac{\theta}{2}\right)} \left[\sin\left(2ka \sin\left(\frac{\theta}{2}\right)\right) - 2ka \sin\left(\frac{\theta}{2}\right) \cos\left(2ka \sin\left(\frac{\theta}{2}\right)\right) \right].\end{aligned}$$

In the low energy approximation, we have

$$\begin{aligned}f_{\mathbf{k}}(\theta) &\approx \frac{mV_0}{4\hbar^2 k^3 \sin^3\left(\frac{\theta}{2}\right)} \left[2ka \sin\left(\frac{\theta}{2}\right) - 2ka \sin\left(\frac{\theta}{2}\right) \left(1 - 2k^2 a^2 \sin^2\left(\frac{\theta}{2}\right)\right) \right] \\ &= \frac{mV_0 a^2}{\hbar^2 k}.\end{aligned}$$

Therefore, the total scattering cross section becomes

$$\sigma = \int_{\mathbf{S}^2} d\Omega |f_{\mathbf{k}}(\theta)|^2 = 4\pi \left(\frac{mV_0 a^2}{\hbar^2 k}\right)^2,$$

for $V(\mathbf{r}) = \theta(a-r)V_0$, $k_a \ll 1$.

■

Problem 4 - Scattering Off an Impenetrable Sphere

Consider 3D scattering off a potential

$$V(r) = \begin{cases} \infty, & r < a, \\ 0, & r > a. \end{cases}$$

- (a) Find the s -wave ($l = 0$) phase shift.
- (b) Find the total low-energy ($k \rightarrow 0$) cross section σ . You may use $\frac{d\sigma}{d\Omega} = |f(\theta)|^2$ with $f(\theta) = \frac{1}{k} \sum_{l=0}^{\infty} (2l+1)e^{i\delta_l} P_l(\cos(\theta)) \sin(\delta_l)$.

Solution. (a) For s -wave scattering ($l = 0$), the radial Schrödinger equation outside the hard sphere ($r > a$) is

$$\frac{d^2 R_0}{dr^2} + \frac{2}{r} \frac{dR_0}{dr} + k^2 R_0 = 0.$$

The general solution is given by

$$R_0(r) = A(kr)^{-1} \sin(kr + \delta_0).$$

The hard sphere boundary condition requires $R_0(a) = 0$, so $\sin(ka + \delta_0) = 0$. Thus, $ka + \delta_0 = n\pi$, where n is an integer.

For the lowest energy solution ($n = 1$), we have that $\delta_0 = -ka$. This is indeed the correct phase shift as it satisfies the boundary condition, approaches zero as $k \rightarrow 0$, and is continuous with energy.

- (b) For low-energy scattering, higher angular momentum contributions ($l > 0$) are suppressed by factors of $(ka)^{2l+1}$. Therefore, at low energy we can consider only the s -wave contribution. The scattering amplitude becomes

$$f(\theta) \approx \frac{1}{k} e^{i\delta_0} \sin(\delta_0).$$

For small k , we have

$$\begin{aligned} \delta_0 &= -ka, \\ \sin(\delta_0) &\approx -ka. \end{aligned}$$

Therefore, $f(\theta) \approx -a$.

The total cross section is

$$\begin{aligned} \sigma &= \int |f(\theta)|^2 d\Omega \\ &= 4\pi |f(\theta)|^2 \\ &= 4\pi a^2. \end{aligned}$$

This is exactly what we expect classically - the cross section is equal to the geometric cross section of the hard sphere.

The result $\sigma = 4\pi a^2$ is independent of energy in the low-energy limit. This matches the classical result because the hard sphere potential has no quantum tunneling. Higher partial waves contribute terms of order $k^2 a^2$ and higher. This simple result is a consequence of the purely repulsive nature of the potential.

■