Quantum Physics III (8.06) Spring 2006
Solution Set 10

May 12, 2006

1. **Scattering from a Reflectionless Potential (10 points)**

(a) **(2 points)** Plugging $\psi_0(x) = A\text{sech}(ax)$ into the Schrodinger equation, one finds that it is an eigenstate with energy $E_0 = -\frac{\hbar^2 a^2}{2m}$. Since $E < 0$ and the potential goes zero as $x \to \pm\infty$, this is a bound state.

(b) **(3 points)** We now consider the wave function

$$\psi(x) = (k/a + i \tanh(ax))e^{ikx} \tag{1}$$

Since

$$\frac{\partial^2 \psi}{\partial x^2} = -k^2\psi - 2ak\text{sech}^2(ax)e^{ikx} - 2ia^2 e^{ikx}\tanh(ax)\text{sech}^2(ax) = -(k^2 + 2a^2\text{sech}^2(ax))\psi,$$

we find

$$\begin{aligned} H\psi &= -\frac{\hbar^2}{2m}\left[-k^2\psi - 2a^2\text{sech}^2(ax)\psi\right] - \frac{\hbar^2 a^2}{m}\text{sech}^2(ax)\psi \\ &= \frac{\hbar^2 k^2}{2m}\psi. \end{aligned}$$

This is true for any (real) k, so we have a continuum of scattering states ψ_k.

(c) **(3 points)** In order to study scattering, we ask what happens to a plane wave sent in from $x = -\infty$. When the particle interacts with the potential, some of the wave will be transmitted and some reflected, so that asymptotically the solution should reduce to $\psi(x \to -\infty) = e^{ikx} + Re^{-ikx}$ on the left and $\psi(x \to \infty) = Te^{ikx}$ on the right.

Now, look at solution (1). Since $\lim_{x\to\infty} \tanh(ax) = 1$, we find

$$\psi(x \to \infty) = \frac{k + ia}{a}e^{ikx} \tag{2}$$

As $x \to -\infty$ we find that

$$\psi(x \to -\infty) = \frac{k - ia}{a}e^{ikx} \tag{3}$$

Since there is no term proportional to e^{-ikx} in (3), R must be zero. As a consistency check, we now show $|T| = 1$. To find T we take the ratio of the coefficients before e^{ikx} in (2) and (3) (since (3) is not normalized in the standard form)

$$T = \frac{k + ia}{k - ia} = 1.$$

From this expression we see that $|T| = 1$— which we must have by flux conservation, as there is no reflected wave.

(d) **(2 points)** As we can see from part (c), $T(k)$ has a pole at $k = ia$. In terms of energy, the location of the pole is at the bound state energy, $E_0 = -\frac{\hbar^2 a^2}{2m}$.

2. **Simple Properties of Cross Sections (15 points)**

(a) **(2 points)** The incident flux is

$$\vec{S}_i = \frac{\hbar k}{m}\hat{z},$$

while the scattered flux is (to leading order in $1/r$)

$$\vec{S}_s = \frac{\hbar k}{m}\frac{|f|^2}{r^2}\hat{r}.$$

(b) **(2 points)** Using part (a),

$$\frac{d\sigma}{d\Omega}d\Omega = \lim_{r\to\infty}\frac{S_s\cdot\hat{r}}{|S_i|}dA = \frac{|f|^2}{r^2}r^2 d\Omega,$$

and therefore $\frac{d\sigma}{d\Omega} = |f|^2$.

(c) **(11 points)** From conservation of probability, we must have $\int \nabla\cdot S_{total} = 0$, and therefore $\int S_{total}\cdot dA = 0$, with the integral is taken over the boundary of space. Now, $S_{total} = S_i + S_s + S_{int}$, where

$$\begin{aligned} S_{int} &= \frac{\hbar}{2mi}\left[e^{-ikz}\nabla\frac{f}{r}e^{ikr} + e^{-ikr}\frac{f^*}{r}\nabla e^{ikz} - c.c.\right] \\ &= \frac{\hbar k}{m}\frac{1}{r}\mathrm{Re}\left[f e^{ik(r-z)}\right](\hat{z}+\hat{r}). \end{aligned}$$

Let's consider $\int S_{total}\cdot dA = 0$ term by term. The first term we consider is $\int S_{int}\cdot dA$. The easiest coordinate system to use is cylindrical coordinates, in which we take the boundary of space to be two planes at $z = \pm\infty$. (You can check that the contribution to the integral from $\rho\to\infty$ is sub leading.) We have, then,

$$\begin{aligned} \int S_{int}\cdot dA &= \frac{\hbar k}{m}\int d\phi\,\rho d\rho\,\frac{1}{r}\mathrm{Re}\left[f e^{ik(r-z)}\right](\hat{z}+\hat{r})\cdot\hat{z} \\ &\simeq \frac{\hbar k}{m}\int d\phi\,\rho d\rho\,\frac{1}{z}\mathrm{Re}\left[f(\theta=0)e^{ik\rho^2/2z}\right](\hat{z}\pm\hat{z})\cdot\hat{z}, \end{aligned}$$

where in the second line I have used the approximations

$$\begin{aligned} \hat{r} &\simeq \pm\hat{z}, \\ r &= |z| + \frac{\rho^2}{2|z|} + \ldots, \\ \theta &\simeq 0. \end{aligned}$$

Because at $z = -\infty$, $\hat{z} = -\hat{r}$, there is no contribution from the plane at $z = -\infty$. The plane at $z = \infty$ contributes

$$\begin{aligned} \int S_{int}\cdot dA &= \frac{4\pi\hbar k}{mz}\int \rho d\rho\,\mathrm{Re}\left[f(\theta=0)e^{ik\rho^2/2z}\right] \\ &= \frac{4\pi\hbar k}{m}\int da\,\mathrm{Re}\left[f(\theta=0)e^{ika}\right] \\ &= \frac{4\pi\hbar k}{m}\lim_{\alpha\to 0}\int da\,e^{-\alpha a}\left[\mathrm{Re}f(\theta=0)\cos(ka) - \mathrm{Im}f(\theta=0)\sin(ka)\right] \\ &= -\frac{4\pi\hbar}{m}\mathrm{Im}f(\theta=0). \end{aligned}$$

The other two terms are simpler, as $\int \nabla \cdot S_i = 0$ and

$$\int S_s \cdot dA = \frac{\hbar k}{m} \int d\Omega |f|^2.$$

Conservation of flux then tells us

$$\int |f|^2 d\Omega = \frac{4\pi}{k} \mathrm{Im} f(0).$$

3. **Born Approximations for Scattering from Yukawa and Coulomb Potentials (15 points)**

(a) **(6 points)** The Yukawa potential is spherically symmetric, so $f(\theta) = -\frac{2m}{\hbar^2 \kappa} \int_0^\infty dr\, r V(r) \sin \kappa r$, where $\kappa = |\vec{k} - \vec{k'}|$. The integral we need to perform is

$$\begin{aligned} \int dr\, e^{-\mu r} \sin \kappa r &= \frac{1}{2i} \left[\frac{e^{-(\mu+i\kappa)r}}{\mu + i\kappa} - \frac{e^{-(\mu-i\kappa)r}}{\mu - i\kappa} \right] \\ &= \frac{\kappa}{\mu^2 + \kappa^2}. \end{aligned}$$

Using this,

$$f(\theta) = -\frac{2m\beta}{\hbar^2(\mu^2 + \kappa^2)}.$$

From this we find

$$\frac{d\sigma}{d\Omega} = \left(\frac{2m\beta}{\hbar^2(\mu^2 + \kappa^2)} \right)^2.$$

The total cross-section is

$$\sigma = \int |f|^2 d\Omega = \left(\frac{2m\beta}{\hbar^2} \right)^2 \int \sin\theta d\theta d\phi \frac{1}{(\mu^2 + 4k^2 \sin^2 \frac{\theta}{2})^2}.$$

To evaluate the θ integral, make the variable change $a = 4k^2 \sin^2(\theta/2)/\mu^2$. Then the θ integral becomes $\frac{1}{2\mu^2 k^2} \int_0^{4k^2/\mu^2} \frac{da}{(1+a)^2} = \frac{2}{\mu^2(\mu^2 + 4k^2)}$, and

$$\sigma = \frac{4\pi}{\mu^2 + 4k^2} \left(\frac{2m\beta}{\hbar^2 \mu} \right)^2 = \frac{4\pi}{\hbar^2 \mu^2 + 8mE} \left(\frac{2m\beta}{\hbar \mu} \right)^2.$$

(b) **(2 points)** Putting $\beta = Q_1 Q_2$ and $\mu = 0$, we find

$$\frac{d\sigma}{d\Omega} = \left(\frac{2m Q_1 Q_2}{2\hbar^2 k^2 (1 - \cos\theta)} \right)^2 = \left(\frac{Q_1 Q_2}{4E} \right)^2 \frac{1}{\sin^4 \theta/2},$$

which is precisely the Rutherford cross-section.

(c) **(2 points)** To prevent confusion, I will use the symbol T for thickness. Since the number of particles scattered per unit solid angle per unit time per scatterer is $\frac{d\sigma}{d\Omega} \frac{d^2 N}{dt dA}$, and the number density of scatterers is n, the number of particles scattered into unit solid angle per unit time is $\int dA\, T n \frac{d\sigma}{d\Omega} \frac{d^2 N}{dt dA} = \frac{d\sigma}{d\Omega} \frac{dN}{dt} n T$. This is independent of beam area and beam uniformity, as desired. The key point here is that the factors of area cancel *independently* for each area element, so non uniformity of the beam is not an issue.

(d) **(3 points)** With the numbers

$$\begin{aligned} Q_1 &= 2e & Q_2 &= 79e & \theta &= \frac{\pi}{2} \\ T &= 10^{-6}m & d\Omega &= 10^{-4}\text{rads}^2 & E &= 8 \ \text{MeV} \\ n &= \rho_{Au}/m_{Au} = 5.9 \times 10^{28}\text{atoms}/m^3, \end{aligned}$$

we find that the number of scattered alpha particles seen in the detector per second is 3.7.

(e) **(2 points)** The number of particles detected in the detector depends on θ as

$$\frac{1}{\sin^4 \frac{\theta}{2}} \sin\theta \qquad (4)$$

where the second factor $\sin\theta$ comes from the solid angle. The quantity in (4) takes on the following values:

$$\begin{array}{rl} 3009 & \theta = 10^o \\ 33 & \theta = 45^o \\ 0.97 & \theta = 135^o \\ 0.18 & \theta = 170^o. \end{array}$$

When we took $\theta = 90^o$ and therefore $\frac{\sin\theta}{\sin^4\theta/2} = 4$, we found that there were 3.7 particles per second scattered into the detector. Using this, the number of particles observed per second in the detector at the various angular locations are

$$\begin{array}{rl} 2784 & \theta = 10^o \\ 30.5 & \theta = 45^o \\ 0.9 & \theta = 135^o \\ 0.16 & \theta = 170^o. \end{array}$$

Note that the observed number of particles shoots up very sharply near $\theta = 0$.

4. **The Size of Nuclei (10 points)**

(a) **(4 points)** Using the charge distribution $\rho(r) = \frac{3Z}{4\pi R^3}$ for $r \leq R$ and 0 otherwise, we find

$$\int r^2 dr \, \sin\theta d\theta \, d\phi \, e^{iqr\cos\theta}\rho(r) = \frac{3Z}{R^3 q^2}\left[\frac{1}{q}\sin qR - R\cos qR\right],$$

and therefore

$$f = \frac{6mZe^2}{\hbar^2 q^2 (qR)^3}(\sin qR - qR\cos qR).$$

The scattering cross-section is

$$\frac{d\sigma}{d\Omega} = |f|^2 = \left(\frac{6mZe^2}{\hbar^2 q^2 (qR)^3}\right)^2 (\sin qR - qR\cos qR)^2.$$

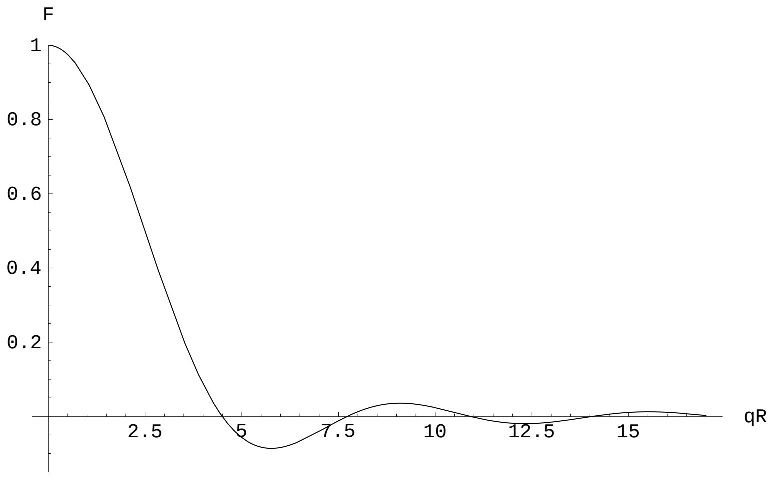

Figure 1: The form factor $F(qR)$.

(b) **(3 points)** For a point particle, $\rho(x) = Z\delta^3(r)$, so the scattering amplitude is $f_0 = 2me^2Z/(\hbar^2 q^2)$. We define the form factor

$$F(qR) = \frac{f}{f_0} = \frac{3}{(qR)^3}(\sin qR - qR\cos qR).$$

We plot this function in figure 1.

(c) **(3 points)** As θ goes from 0 to π, q goes from 0 to $2E/(\hbar c)$. In the relativistic regime, $qR = \frac{2ER}{\hbar c}\sin\theta/2$, so if $E/(\hbar c) \ll 1/R$, then $qR \ll 1$. In this regime,

$$\begin{aligned} F(qR) &= \frac{3}{(qR)^3}\left(qR - \frac{(qR)^3}{6} + \ldots - \left(qR - \frac{(qR)^3}{2} + \ldots\right)\right) \\ &\simeq 1. \end{aligned}$$

Since the form factor is unity, this means that in this regime there is no difference between the scattering from a point particle and an object of size $R \ll \hbar c/E$.

If $R = (2-7)\times 10^{-15}m$, then we need $E \simeq \hbar c/(2-7)\times 10^{-15}m = 30 - 100$ MeV in order to resolve the finite size of the nucleus.

THE PROBLEMS BELOW SHOULD NOT BE HANDED IN. THEY WILL NOT BE GRADED. THEY ARE INTENDED AS A STUDY GUIDE TO HELP YOU UNDERSTAND SCATTERING THEORY AND THE GROVER ALGORITHM. SOLUTIONS WILL BE PROVIDED.

5. **The Born Approximation in One Dimension (15 points)**

(a) **(6 points)** We need to show that $\psi(x) = \psi_0(x) - \frac{im}{\hbar^2 k}\int_{-\infty}^{\infty} e^{ik|x-x_0|}V(x_0)\psi(x_0)dx_0$ satisfies the Schrodinger equation with eigenvalue $\frac{\hbar^2k^2}{2m}$. Now,

$$\frac{\partial^2}{\partial x^2}e^{ik|x-y|} = \left[2ik\delta(x-y) - k^2\right]e^{ik|x-y|},$$

so

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi = \frac{\hbar^2k^2}{2m}\left(\psi_0 - \frac{im}{\hbar^2k^2}\int dy\, e^{ik|x-y|}V(y)\psi(y)\right) - \psi(x)V(x).$$

It is therefore easy to see that

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x) = \frac{\hbar^2k^2}{2m}\psi(x).$$

(b) **(5 points)** Using $\psi_0(x) \simeq Ae^{ikx}$, the first Born approximation becomes

$$\psi(x) \simeq Ae^{ikx} - \frac{Aim}{\hbar^2 k}\int dy\, e^{ik|x-y|}V(y)e^{iky}.$$

We want to find the reflection coefficient, which as Griffiths defines it is $R = |\text{reflected wave}|^2/|\text{incident wave}|^2$ (since this problem comes from Griffiths, we will use his definitions for R and T in this problem). The reflected wave is the component of ψ that behaves like e^{-ikx} at $x \to -\infty$. Now, as $x \to -\infty$, $|x-y| = y-x$, and thus the coefficient of the reflected wave is $-\frac{Aim}{\hbar^2k}\int dy\, e^{2iky}V(y)$. The incident wave is the component of ψ that behaves like e^{ikx} at $x \to -\infty$, and the coefficient of this piece of ψ is A. Therefore,

$$R = \left|\frac{m}{\hbar^2k}\int dy\, e^{2iky}V(y)\right|^2. \tag{5}$$

(c) **(4 points)** First, we set $V(x) = -\alpha\delta(x)$. In this case, the integral in equation (5) becomes $-\int dy\, e^{2iky}\alpha\delta(y) = -\alpha$. The reflection coefficient is therefore $R = \frac{m^2\alpha^2}{\hbar^4k^2} = \frac{m\alpha^2}{2\hbar^2E}$. From this, we find the first Born approximation to the transmission coefficient,

$$T = 1 - R = 1 - \frac{m\alpha^2}{2\hbar^2E}.$$

The exact answers are, defining $w = \frac{m\alpha^2}{2\hbar^2E}$,

$$R_{exact} = \frac{w}{w+1}, \qquad T_{exact} = \frac{1}{1+w},$$

so the first Born approximation has found the first term in an expansion of R_{exact}, T_{exact} in small w. Small w means that the strength of the potential (measured by α) is small compared to the energy of the particle, and so this means that the Born approximation is good in the weak scattering regime.

Second, we set $V(x) = -V_0$ when $|x| < a$ and 0 otherwise. In this case, the integral of (5) is $-V_0 \int_{-a}^{a} dy\, e^{2iky} = -\frac{V_0 \sin(2ka)}{k}$. The reflection coefficient is then $R = \left(\frac{m}{\hbar^2 k^2} V_0 \sin(2ka)\right)^2$, and the transmission coefficient is

$$T = 1 - R = 1 - \left(\frac{V_0}{2E} \sin(2ka)\right)^2 .$$

The exact answer is

$$T_{exact} = \left(1 + \frac{V_0^2}{4E(E+V_0)} \sin^2(2ka)\right)^{-1} \simeq 1 - \left(\frac{V_0}{2E} \sin(2ka)\right)^2$$

where the approximation holds when $V_0/E \ll 1$, that is, in the weak scattering regime. Again, we have found the first term in the weak scattering expansion of the exact answer.

6. **Scattering from a Small Crystal (8 points)**

(a) **(4 points)** In the first Born approximation, the scattering amplitude is given by the formula $f(\theta, \phi) = -\frac{m}{2\pi\hbar^2} \sum_i \int d^3r\, e^{-iq\cdot r} v(r - X_i)$. In order to proceed further, we Fourier expand the scattering potential of the single atom, $v(x) = \int (2\pi)^{-3} d^3k\, e^{ik\cdot x} v_k$. Plugging this in, we find

$$f(\theta, \phi) = -\frac{m}{2\pi\hbar^2} \sum_i \int (2\pi)^{-3} d^3k\, v_k e^{ik\cdot X_i} \int d^3r\, e^{-i(q-k)\cdot r}.$$

The integral over r yields a delta function, $\int d^3r\, e^{-i(q-k)\cdot r} = (2\pi)^3 \delta^3(q-k)$, which makes the integration over k trivial, so that

$$f(\theta, \phi) = -\frac{m}{2\pi\hbar^2} v_q \left(\sum_i e^{-iq\cdot X_i}\right).$$

The differential cross-section is given by

$$\frac{d\sigma}{d\Omega} = \left(\frac{m}{2\pi\hbar^2}\right)^2 |v_q|^2 \left|\sum_i e^{-iq\cdot X_i}\right|^2 .$$

Note that the last factor contains all the information about the crystal structure, in the form of the sum over atom positions X_i, while the factor $|v_q|^2$contains all the information about the individual atom potential.

(b) **(4 points)** Consider scattering from two atoms, separated by a distance $\vec{d}$. Let the incoming momentum be $\vec{k}$, while the outgoing momentum is $\vec{k}'$. Constructive interference will occur when $d \cdot (k - k') = d \cdot q = 2\pi n$, for some integer n. Taking the entire crystal into account, constructive interference will occur when $X_i \cdot q = 2\pi n$, for all X_i. (This is simply a fancy way of defining a Bragg plane.) Now, if the scattered wave satisfies the condition $X_i \cdot q = 2\pi n$, then $e^{-iq\cdot X_i} = 1$, so that $\frac{d\sigma}{d\Omega} \propto N^2$, where N is the number of atoms in the crystal; otherwise, generically, the interference between scattered wave will lead to $\frac{d\sigma}{d\Omega} \simeq 0$. Thus, scattering amplitudes are only large when the Bragg condition is satisfied.

7. **Partial Waves (10 points)**

(a) **(1 point)** Since the first term in $f(\theta)$ is independent of θ, and the second term is proportional to $\cos\theta$, the partial waves that are active are $\ell = 0$ and $\ell = 1$.

(b) **(3 points)** Recalling the expansion $f(\theta) = \sum_\ell (2\ell+1) P_\ell(\cos\theta) f_\ell$, we identify

$$\begin{aligned} f_0 &= \frac{1}{k} \frac{\Gamma k}{k_0 - k - ik\Gamma} \\ &= \frac{1}{k} \frac{\sin\delta_0}{\cos\delta_0 - i\sin\delta_0}, \end{aligned}$$

and therefore

$$\sin\delta_0 = \frac{\Gamma k}{\sqrt{(k_0-k)^2 + (\Gamma k)^2}}.$$

As $k \to 0$, $\sin\delta_0 \simeq \delta_0 \simeq (\Gamma/k_0)k$. This goes like k, as we expect.

For $\ell = 1$, we have

$$\begin{aligned} f_1 &= \frac{1}{k} e^{2i\beta k^3} \sin(2\beta k^3) \\ &= \frac{1}{k} \sin\delta_1 e^{i\delta_1}, \end{aligned}$$

and therefore

$$\delta_1 = 2\beta k^3.$$

This goes to 0 as k^3, again as we expect.

(c) **(1 point)** The differential cross-section is

$$\begin{aligned} \frac{d\sigma}{d\Omega} &= |f_0 + 3\cos\theta f_1|^2 \\ &= \frac{1}{k^2} \frac{(\Gamma k)^2}{(k_0-k)^2 + (\Gamma k)^2} + \frac{9}{k^2} \cos^2\theta \sin^2(2\beta k^3) \\ &\quad - \frac{6\cos\theta}{k^2} \frac{\Gamma k \sin(2\beta k^3)}{(k_0-k)^2 + (\Gamma k)^2} \left((k_0 - k)\cos(2\beta k^3) - \Gamma k \sin(2\beta k^3) \right). \end{aligned}$$

(d) **(1 point)** The partial wave cross-sections are

$$\begin{aligned} \sigma_0 &= \frac{4\pi}{k^2} \frac{(\Gamma k)^2}{(k_0-k)^2 + (\Gamma k)^2} \\ \sigma_1 &= \frac{4\pi}{k^2} \sin^2(2\beta k^3). \end{aligned}$$

(e) **(2 points)** If $\beta k_0^3 \ll 1$, and $k \simeq k_0$, then $\sigma_1 \ll \sigma_0$, and we can approximate $\sigma_{total} \simeq \sigma_0$. In other words,

$$\sigma_{total} \simeq \frac{4\pi\Gamma^2}{(k_0-k)^2 + (\Gamma k)^2}.$$

(f) **(2 points)** we should find $\sigma_1 + \sigma_0 = \frac{4\pi}{k} \mathrm{Im} f(\theta = 0)$. We calculate

$$\mathrm{Im} f(0) = \frac{1}{k} \left[\frac{(\Gamma k)^2}{(k_0-k)^2 + (\Gamma k)^2} + 3\sin^2(2\beta k^3) \right].$$

On the other hand, the total cross-section is

$$\sigma_1 + \sigma_0 = \frac{4\pi}{k^2}\left[\frac{(\Gamma k)^2}{(k_0-k)^2+(\Gamma k)^2} + 3\sin^2(2\beta k^3)\right]$$

We conclude that the optical theorem is satisfied.

8. **Combining Born and Partial Waves (6 points)**

(a) **(no points)** We recall from the previous problem set that the scattering amplitude for the Yukawa potential is $f_Y(\theta) = -\frac{2m\beta}{\hbar^2(\mu^2+\kappa^2)}$, where $\kappa = 2k\sin(\theta/2)$.

(b) **(4 points)** We need to subtract the quantity $\bar{f} = \frac{1}{4\pi}\int \sin\theta\, d\theta d\phi f_Y(\theta) = -\frac{m\beta}{\hbar^2\mu^2}\int \frac{\sin\theta d\theta}{1+\frac{4k^2}{\mu^2}\sin^2\frac{\theta}{2}}$. Making the variable substitution $a = \frac{4k^2}{\mu^2}\sin^2\frac{\theta}{2}$, we find

$$\bar{f} = -\frac{m\beta}{2\hbar^2 k^2}\ln\left(\frac{4k^2+\mu^2}{\mu^2}\right).$$

Therefore, the modified scattering amplitude is

$$f_{mod} = -\frac{2m\beta}{\hbar^2}\left[\frac{1}{\mu^2+4k^2\sin^2\frac{\theta}{2}} - \frac{1}{4k^2}\ln\left(\frac{4k^2+\mu^2}{\mu^2}\right)\right].$$

(c) **(2 points)** Adding back in an unknown s-wave contribution, the scattering amplitude is now

$$f(\theta) = \frac{1}{2ik}(e^{2i\delta_0}-1) - \frac{2m\beta}{\hbar^2}\left[\frac{1}{\mu^2+4k^2\sin^2\frac{\theta}{2}} - \frac{1}{4k^2}\ln\left(\frac{4k^2+\mu^2}{\mu^2}\right)\right].$$

This leads to the differential cross-section

$$\begin{aligned}\frac{d\sigma}{d\Omega} &= \frac{\sin^2\delta_0}{k^2} - \frac{\sin(2\delta_0)}{k}\frac{2m\beta}{\hbar^2}\left[\frac{1}{\mu^2+4k^2\sin^2\frac{\theta}{2}} - \frac{1}{4k^2}\ln\left(\frac{4k^2+\mu^2}{\mu^2}\right)\right] \\ &\quad + \left(\frac{2m\beta}{\hbar^2}\right)^2\left[\frac{1}{\mu^2+4k^2\sin^2\frac{\theta}{2}} - \frac{1}{4k^2}\ln\left(\frac{4k^2+\mu^2}{\mu^2}\right)\right]^2.\end{aligned}$$

9. **Scattering from a δ-shell (13 points)**

(a) **(1 point)** With $r < R$, the potential vanishes, so the solution is simply the free solution. We have the boundary condition that $u(r) = 0$ at $r = 0$, which determines $u(r) = A\sin(kr)$.

(b) **(2 points)** From integrating the Schrodinger equation, we have the equation

$$\left.\frac{\partial u}{\partial r}\right|_{R-\epsilon}^{R+\epsilon} = \frac{\lambda}{R}u(R),$$

or in other words

$$\left.\frac{u'}{u}\right|_{R+\epsilon} - \left.\frac{u'}{u}\right|_{R-\epsilon} = \frac{\lambda}{R}.$$

Using our solution for $u(r)$, this becomes

$$\cot(kR+\delta) - \cot(kR) = \frac{\lambda}{kR}. \qquad (6)$$

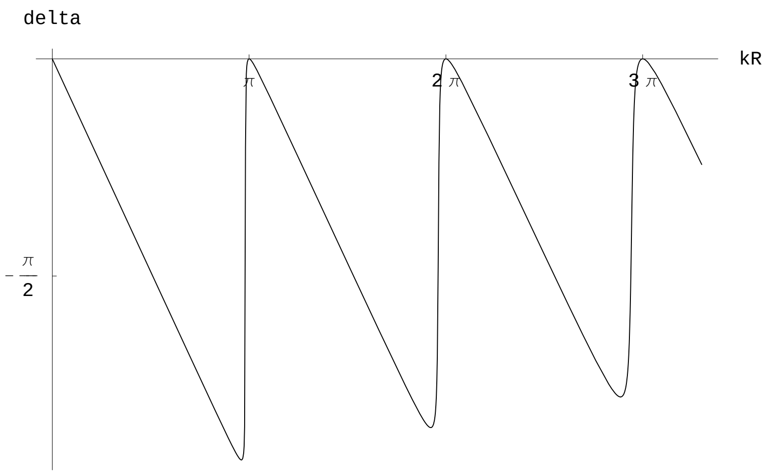

Figure 2: The phase shift δ.

(c) **(2 points)** We know that $\delta \to 0$ as $k \to 0$, so that we can take both $kR \ll 1$ and $kR + \delta \ll 1$. In this case, the result of part (b) becomes

$$\frac{1}{kR+\delta} - \frac{1}{kR} = \frac{\lambda}{kR},$$

or

$$\delta = kR\left(-\frac{\lambda}{1+\lambda}\right).$$

Using $\lim_{k\to 0}\delta = -ka$, this determines

$$a = R\left(\frac{\lambda}{\lambda+1}\right).$$

Notice that, when $\lambda \gg 1$, $a \simeq R$.

(d) **(8 points)** We plot δ as a function of kR in figure 1. We can understand this plot as follows. Consider equation (6). There are three regimes: first, when $\cot(kR+\delta) \gg 1$; second, when $\cot(kR+\delta) = 0$; third, when $\cot(kR+\delta) \ll -1$.

In the second case, we have $\frac{\lambda}{kR} + \cot(kR) = 0$, which is possible when $kR = \pi - \epsilon$, where ϵ is a calculable small quantity. Also, if $\cot(kR+\delta) = 0$, then $kR + \delta = \frac{\pi}{2}$. Combining these, we find $\delta = -\frac{\pi}{2} + \epsilon$.

In the first case, we now know that $kR \in [0, \pi - \epsilon]$. The condition that $\cot(kR+\delta) > 0$ then tells us $-kR < \delta < \frac{\pi}{2} - kR$. Moreover, for most values of kR, we will have $\cot(kR) \ll \frac{\lambda}{kR}$, so that we expect in general $\delta \sim -kR$. (This is the same physics as the result of part (c) above that for small k, $\delta \simeq -kR$.)

In the third case, $kR \in [\pi - \epsilon, \pi]$. The condition that $\cot(kR+\delta) < 0$ now tells us that $\frac{\pi}{2} - kR < \delta < \pi - kR$, or $-\frac{\pi}{2} + \epsilon < \delta < \epsilon$. Note also that if $kR = \pi$, then $\delta = 0$.

Putting all of this together, we arrive at figure 1. The first half of the rapid increase by π occurs when the phase shift makes the transition from the $\delta \sim -kR$ regime to $\delta = -\frac{\pi}{2} + \epsilon$; the

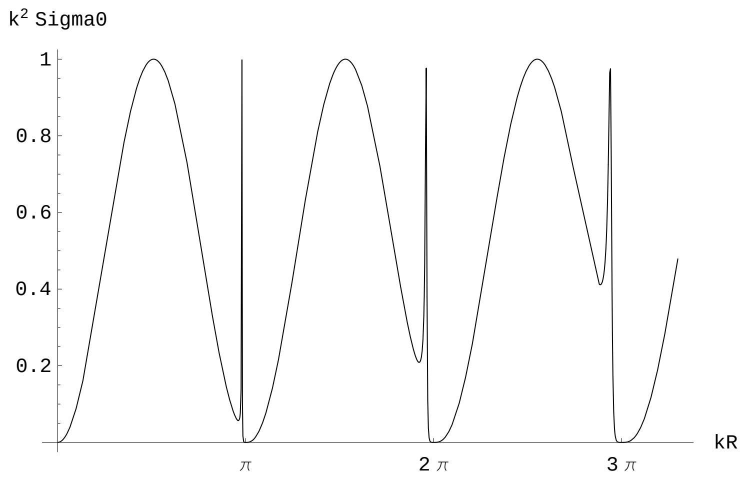

Figure 3: The s-wave cross-section.

second half of the rapid increase occurs when δ increases from the value at resonance to $\delta = 0$ at $kR = \pi$. The function $\delta(k)$ is not quite periodic, because the term $\frac{\lambda}{kR}$ is not periodic. As kR increases, this term becomes less important, and therefore the regions where δ increases rapidly become larger.

The s-wave cross-section is $\sigma_0 = \frac{4\pi}{k^2} \sin^2 \delta$, and is plotted in figure 2. The corresponding quantity for hard sphere scattering is $\sigma_0^{HS} = \frac{4\pi^2}{k^2} \sin^2(kR)$. But as we showed, $\delta \simeq -kR$, except near $n\pi$ (or for $kR > \lambda$, a regime we are not considering). Therefore, $\sigma_0 \simeq \sigma_0^{HS}$, except near $kR = n\pi$, where an infinitely deep square well has bound states.

The resonances, visible as spikes in the cross-section in figure 2, therefore correspond to bound states (strictly speaking, quasi-bound states) of the potential.

10. **Ramsauer-Townsend Effect (6 points)**

(a) **(3 points)** We get the s-wave phase shift directly from the Schrodinger equation. When $r \leq a$, we have

$$u'' + \left(k^2 + 2mV_0\hbar^2\right) u \equiv u'' + \kappa^2 u = 0.$$

The solution for this which is appropriate for the boundary condition at $r = 0$ is $u = A\sin(\kappa r)$.

When $r > a$, the Schrodinger equation is $u'' + k^2 u = 0$, and the solution is $u = B\sin(kr + \delta)$. Asking that the wave function be continuous at $r = a$ yields the condition

$$\frac{\kappa a}{\tan(\kappa a)} = \frac{ka}{\tan(ka + \delta)}.$$

In order for the cross-section to vanish as $k \to 0$, we need $\lim_{k\to 0} \delta = 0$. When $k = 0$, then $\kappa a = \gamma$, and the condition above becomes

$$\frac{\gamma}{\tan \gamma} = 1.$$

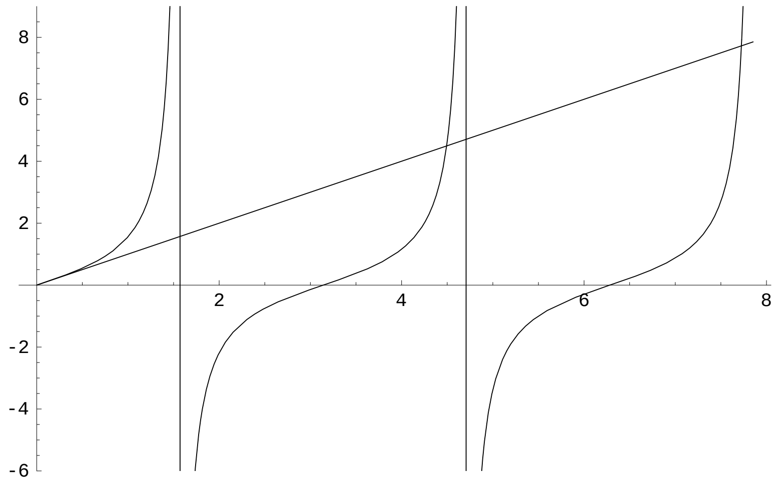

Figure 4: Graphical solution to $\gamma = \tan\gamma$.

To solve this graphically, see figure 3. The points of intersection are the solutions. The first two solutions are $\gamma = 4.4934$ and $\gamma = 7.7253$.

(b) **(3 points)** For a bound state, $E < 0$, and the wave function must fall off outside the well as $u = Be^{-kr}$. Redefining $\kappa^2 = \frac{2mV_0}{\hbar^2} - k^2$, the solution inside the well is still $u = A\sin(\kappa r)$. The continuity condition is now

$$\frac{\kappa a}{\tan(\kappa a)} = -ka.$$

When $k = 0$, at threshold, this condition becomes $\gamma/\tan\gamma = 0$. This is solved by $\gamma = (2n+1)\pi/2$. From figure 3, it is clear that $(2n+1)\pi/2 > \gamma_n$, where γ_n is the n^{th} solution to $\gamma = \tan\gamma$. Since $\gamma \propto \sqrt{V_0}$, we conclude that a square well that displays an exact Ramsauer-Townsend effect must be made slightly deeper to have a bound state at threshold.

11. **Scattering in the Semi-classical Approximation (4 points)**

The WKB approximation gives the wave function to be $u(k,r) \simeq \frac{A}{\sqrt{p}} \sin \frac{1}{\hbar} \int_0^r p(r)dr$, where $p = \sqrt{2m(E-V)}$, and $E = \frac{\hbar^2 k^2}{2m}$. We have determined the phase of the wave function by asking that $u(r=0) = 0$.

Asymptotically, this wave function becomes $u(r \to \infty, k) = \frac{A}{\sqrt{k}} \sin \frac{1}{\hbar} \int_0^{r\to\infty} p(r)dr$, or

$$u(r \to \infty, k) = \sin\left[kr + \int_0^\infty dr \left(\sqrt{k^2 - \frac{2mV}{\hbar^2}} - k\right)\right].$$

(We have dropped the factor $\frac{A}{\sqrt{k}}$ as it limits to a constant.) We therefore conclude

$$\delta(k) = \int_0^\infty dr \left(\sqrt{k^2 - \frac{2mV}{\hbar^2}} - k\right).$$

12. **A Semiclassical Analysis of Resonant Scattering (13 points)**

(a) **(1 point)** In the classically allowed region, the WKB wave function is $u(r) = \frac{A}{\sqrt{p}} \sin \frac{1}{\hbar} \int_0^r p(r)dr$.

(b) **(3 points)** For generic values of E, the wave function in the forbidden region $a < r < b$ will contain both exponentially growing and exponentially falling terms. Therefore,

$$\frac{|A_{outside}|}{|A_{inside}|} \simeq e^{\frac{1}{\hbar} \int_a^b dr \sqrt{2m(V-E)}} \gg 1.$$

(c) **(4 points)** For values of E close to (quasi-) bound states of the potential, the coefficient of the exponentially growing term in the forbidden region will vanish. A quick glance at the connection formulae tells us that the condition for this to happen is

$$\cos\left(\frac{1}{\hbar}\int_0^a drp(r) - \frac{\pi}{4}\right) = 0,$$

or

$$\int_0^a dr\, \sqrt{2m(E-V)} = \left(n + \frac{3}{4}\right)\pi\hbar$$

for $n = 0, 1, 2, \ldots$. At these special values of E, since the wave function dies off exponentially as it travels through the barrier, $|A_{inside}| \gg |A_{outside}|$.

(d) **(5 points)** Qualitatively, we expect the phase shift δ to increase by π as we go through a resonance. We can indeed see this in the semiclassical approximation: at resonance, the forbidden region wave function is proportional to a dying exponential only, so in the classically allowed region $r > b$, the wave function goes like $u(r) \propto \sin\left(\frac{1}{\hbar}\int drp(r) - \frac{3\pi}{4}\right)$. On the other hand, when the forbidden region wave function is proportional to a growing exponential only, the wave function in the classically allowed region $r > b$ goes like $u(r) \propto \sin\left(\frac{1}{\hbar}\int drp(r) - \frac{\pi}{4}\right)$. Thus, δ goes through a net shift of π as it cycles through a quasibound state, as the phase must increase from that determined by a growing exponential to that determined by a dying exponential at the resonance, and then back to that determined by a growing exponential. This seems like a net phase shift of 2π until we recall that in the WKB approximation, the overall sign of the wave function is not determined; so we really have a phase shift of π. Because the phase shift increases by π, it must at some point in this evolution pass through the value $(2n+1)\pi/2$. This leads to a peak in the cross-section, given by $\sin^2\delta$, at the location of the resonance.

13. **The Grover Algorithm**

(a) Consider the unitary transformation that maps the state $|0\rangle$ into the state $\frac{1}{\sqrt{2}}(|1\rangle + |0\rangle)$. This is a 45^orotation on the two-dimensional Hilbert space spanned by $|0\rangle$ and $|1\rangle$, and is represented by the matrix $V = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}$. Now we need to extend this to a matrix acting on the full, 8-dimensional Hilbert space. The rotation of spin three by 45^o rotates $|0\rangle$ into $\frac{1}{\sqrt{2}}(|0\rangle + |4\rangle)$, $|1\rangle$ into $\frac{1}{\sqrt{2}}(|1\rangle + |5\rangle)$, and so on. The matrix representing this action on the full Hilbert space is

$$V_3 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

Similarly, V_2 rotates the second spin by the same angle and therefore connects $|0\rangle$ and $\frac{1}{\sqrt{2}}(|0\rangle + |2\rangle)$, etc., and has the matrix representation

$$V_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \end{pmatrix},$$

while V_1 rotates the first spin by the same angle and has the representation

$$V_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \end{pmatrix}.$$

¿From these, we can calculate $U_{initialize} = V_3V_2V_1$ (notice that the order of the three V_i does not matter, as the matrices commute). This yields

$$U_{initialize} = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \\ 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix}.$$

This matrix is unitary and maps $|0\rangle$ into $|s\rangle$, by construction.

(b) The operator $(-1)^f$ has the matrix representation $(-1)^f = \text{Diag}[1,1,1,-1,1,1,1,1]$.

(c) The matrix elements of U_s are $(U_s)_{rn} = \langle r|\,(2|s\rangle\langle s| - 1)\,|n\rangle = \frac{1}{4} - \delta_{rn}$. Explicitly, this is

$$U_s = \frac{1}{4}\begin{pmatrix} -3 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & -3 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & -3 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & -3 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & -3 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & -3 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & -3 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & -3 \end{pmatrix}.$$

(d) Let $|out_k\rangle = \left(U_s(-1)^f\right)^k |s\rangle$. For the lowest values of k, this is

$$\begin{aligned} |out_0\rangle &= |s\rangle \\ |out_1\rangle &= \frac{1}{\sqrt{8}}\frac{1}{2}(1,1,1,5,1,1,1,1) \\ |out_2\rangle &= \frac{1}{\sqrt{8}}\frac{1}{4}(-1,-1,-1,11,-1,-1,-1,-1) \\ |out_3\rangle &= \frac{1}{\sqrt{8}}\frac{1}{8}(-7,-7,-7,13,-7,-7,-7,-7) \end{aligned}$$

The probability of obtaining $|3\rangle$ in a measurement is

$$P_3 = \begin{cases} .125 & k=0 \\ .781 & k=1 \\ .945 & k=2 \\ .330 & k=3 \end{cases}$$

Thus $k = 2$ is the optimal choice for finding the outcome $|3\rangle$.