4. (Quantum Mechanics)

Find the differential and total cross sections of slow particles (small velocity) from a spherical delta potential $V(r) = V_0 \delta(r-a)$. You may use partial wave analysis.

Solution:

Solution by Audrey Farrell

I'm going to briefly walk through partial wave analysis in case you need a refresher, and because I need a refresher. There's a note where you would ideally start solving this problem for the comps. For spherically symmetric potentials V(r) the solutions to the Schrödinger equation are separable

$$\psi(r,\theta,\phi) = R(r)Y_l^m(\theta,\phi)$$

and the radial function u(r) = rR(r) is the solution the differential equation

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V(r) + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]u(r) = E\,u(r)$$

The third term in this equation is the centrifugal contribution.

Partial wave analysis splits the problem into three regions: the radiation region $(kr \gg 1)$, the intermediate region $(V \approx 0)$, and the scattering region. In the radiation region, both the potential and the centrifugal terms are negligible; in the intermediate region, the potential is negligible but the centrifugal term is not; in the scattering region all terms contribute significantly.

In the radiation region our radial equation simplifies to $(d_r^2 + k^2)u(r) \approx 0$, which has the familiar solution $u(r) = Ae^{ikr} + Be^{-ikr}$. The e^{-ikr} term represents *incoming* waves rather than scattered, so we take B = 0, and the radial equation at very large r is

$$R(r) \sim \frac{e^{ikr}}{r}$$
 in the radiation region

In the intermediate region our radial equation and general solution are

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + k^2\right]u(r) \approx 0 \to u(r) = Ar \, j_l(kr) + Br \, n_l(kr)$$

However spherical Bessel functions do not represent propagating waves, and we want to only look at *outgoing* waves. To represent the Bessel functions as outgoing and incoming waves, we use the spherical Hankel functions

$$h_l^{(1)}(x) \equiv j_l(x) + i n_l(x), \quad h_l^{(2)} \equiv j_l(x) - i n_l(x)$$

At large r, $h_l^{(1)}(kr) \sim e^{ikr}/r$ and $h_l^{(2)}(kr) \sim e^{-ikr}/r$, so we only take the $h_l^{(1)}$ term of the solution

 $R(r) \sim h_l^{(1)}(kr)$ outside the scattering region

Now we can write the wave function outside the scattering region $(V \approx 0)$ as

$$\psi(r,\theta,\phi) = A\left(e^{ikz} + \sum_{l,m} C_{lm} h_l^{(1)}(kr) Y_l^m(\theta,\phi)\right)$$

Since we're working with a spherically symmetric potential the wave function cannot be ϕ -dependent, so only m = 0 terms survive, and

$$Y_l^0(\theta) = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\theta)$$

The customary way of writing the partial wave expansion (that you should have written on your equation sheet) is

$$\psi(r,\theta) = A\left(e^{ikz} + k\sum_{l=0}^{\infty} i^{l+1}(2l+1) a_l h_l^{(1)}(kr) P_l(\cos\theta)\right)$$

For very large $r h_l^{(1)}(kr) \approx (-i)^{l+1} e^{ikr}/r$, so

$$\psi(r,\theta) \approx A\left(e^{ikz} + f(\theta)\frac{e^{ikr}}{r}\right), \text{ for } r \to \infty$$

where $f(\theta)$ is the scattering amplitude

$$f(\theta) = \sum_{l=0}^{\infty} (2l+1) a_l P_l(\cos \theta)$$

which is what we actually want to find in this problem since

$$\boxed{D(\theta) = \frac{d\sigma}{d\Omega} = |f(\theta)|^2} = \sum_{l,l'} (2l+1)(2l'+1) a_l^* a_{l'} P_l(\cos\theta) P_{l'}(\cos\theta) \to \sigma = 4\pi \sum_{l=0}^{\infty} (2l+1) |a_l|^2}$$

The last thing we need before actually starting the problem is an expression for e^{ikz} (the incoming plane wave) in spherical coordinates. This is given by *Rayleigh's formula*

$$e^{ikz} = \sum_{l=0}^{\infty} i^l \left(2l+1\right) j_l(kr) P_l(\cos\theta)$$

and our wave function outside the scattering region in spherical coordinates is

$$\psi(r,\theta) = A \sum_{l=0}^{\infty} i^l \left(sl+1\right) \left[j_l(kr+ik a_l h_l^{(1)}(kr)) \right] P_l(\cos\theta)$$

This is where you would ideally start solving this problem on the actual exam assuming you have the partial wave expansion written down on a reference sheet or memorized. I've boxed the key equations above needed to solve this problem.

The problem simmers down to determining the partial wave amplitudes a_l . To do so we need to solve the Schrödinger equation in the *scattering* region $(V(r) \neq 0)$ and match boundary conditions with the exterior solution.

Slow particles is your hint to take only the l = 0 term of the partial wave expansion right off the bat. Slow particles suggests low-energy scattering, and so $ka \ll 1$ where $k = \sqrt{2mE}/\hbar$. In this limit only the l = 0 term is significant.

For r < a we have V = 0 as well, so we can again take the general solution to the Schrödinger equation when V = 0

$$\psi(r,\theta,\phi) = \sum_{l,m} \left[A_{lm} j_l(kr) + B_{lm} n_l(kr) \right] Y_l^m(\theta,\phi), \quad l = 0 \to \psi_{int}(r) \approx B j_0(kr) = B \frac{\sin(kr)}{kr}$$

where we do not include the $n_0(kr)$ term in the wave function because it blows up at r = 0. This is the *interior* solution that we need to boundary match with our partial wave expansion (exterior solution) at r = a.

Keeping only

$$\psi_{ext}(r) \approx A \left[j_0(kr) + ik \, a_0 \, h_0^{(1)}(kr) \right] P_0(\cos \theta) = A \left[\frac{\sin(kr)}{kr} + ik \, a_0 \left(-i \frac{e^{ikr}}{kr} \right) \right]$$
$$= A \left[\frac{\sin(kr)}{kr} + a_0 \frac{e^{ikr}}{r} \right]$$

There are two boundary conditions on ψ : 1) ψ is *continuous* at r = a and 2) $\psi'(r) = \frac{\partial \psi}{\partial r}$ is *discontinuous* at r = a. The first is straightforward:

$$A\left[\frac{\sin(ka)}{ka} + a_0 \frac{e^{ika}}{a}\right] = B \frac{\sin(ka)}{ka} \tag{7}$$

The discontinuity in ψ' is found by integrating over the radial equation for u(r) with l = 0:

$$-\frac{\hbar^2}{2m}\int dr \,\frac{d^2u}{dr^2} + \int dr \,\alpha \,\delta(r-a)\,u(r) \to -\frac{\hbar^2}{2m}\Delta u' + \alpha u(a) = 0 \to \Delta u' = \frac{2m\alpha}{\hbar^2}\,u(a)$$

Since u(r) = rR(r), $u'(r) = R(r) + rR'(r) \rightarrow \Delta u' = \Delta R(a) + a\Delta R'(a) = \frac{2m\alpha}{\hbar^2}aR(a)$. It makes our lives easier to define the dimensionless constant

$$\beta \equiv \frac{2ma\alpha}{\hbar^2} \to \Delta \psi' = \frac{2m\alpha}{\hbar^2} \psi(a) = \frac{\beta}{a} \psi(a)$$

Now we can evaluate the boundary condition at r = a:

$$\left. \frac{d\psi_{ext}}{dr} \right|_{r=a} - \left. \frac{d\psi_{int}}{dr} \right|_{r=a} = \Delta \psi' = \frac{\beta}{a} \psi(a) \tag{8}$$

Taking the lefthand side of equation (8):

LHS =
$$\left(\frac{A}{ka}\left[k\cos(ka) + ik^2 a_0 e^{ika}\right] - \frac{A}{ka^2}\left[k\sin(ka) + k a_0 e^{ika}\right]\right) - \left(\frac{B}{a}\cos(ka) - \frac{B}{ka^2}\sin(ka)\right)$$

= $\frac{A}{ka}\left[k\cos(ka) + ik^2 a_0 e^{ika}\right] - \frac{B}{a}\cos(ka) - \frac{1}{a}\left(\frac{A}{ka}\left[k\sin(ka) + k a_0 e^{ika}\right] - \frac{B}{ka}\sin(ka)\right)$

The term in parentheses is zero by equation (7), so equation (2) becomes

$$A\left[\cos(ka) + ik\,a_0\,e^{ika}\right] = B\left[\cos(ka) + \frac{\beta}{ka}\sin(ka)\right]$$

Using (7) to write B in terms of A gives

$$A\left[\cos(ka) + ik a_0 e^{ika}\right] = A\left[\cot(ka) + \frac{\beta}{ka}\right] \left[\sin(ka) + k a_0 e^{ika}\right]$$
$$ik a_0 e^{ika} = \frac{\beta}{ka} \sin(ka) + k a_0 \cot(ka) e^{ika} + \frac{\beta}{a} a_0 e^{ika}$$
$$ik a_0 e^{ika} \left[1 + i \cot(ka) + i\frac{\beta}{ka}\right] = \frac{\beta}{ka} \sin(ka) \approx \frac{\beta}{ka} ka = \beta$$

Here we have taken advantage of the fact that $ka \ll 1$, so $\sin(ka) \approx ka$. We can also use this approximation for the left-hand side, taking $\cot(ka) = \frac{\cos(ka)}{\sin(ka)} \approx \frac{1}{ka}$ and $e^{ika} \approx (1 + ika)$

$$ik a_0(1+ika)\left[1+\frac{i}{ka}(1+\beta)\right] = ik a_0\left[1+\frac{i}{ka}(1+\beta)-(1+\beta)\right] = \beta$$

Because $ka \ll 1$, the second term dominates and we can solve for the partial scattering amplitude

$$ik a_0 \left[1 + \frac{i}{ka} (1+\beta) - (1+\beta) \right] \approx -\frac{a_0}{a} (1+\beta) = \beta \rightarrow \boxed{a_0 \approx -\frac{a\beta}{1+\beta}}$$

In the limit where l = 0 dominates, the scattering amplitude $f(\theta) \approx a_0$ and $\sigma = 4\pi D(\theta)$, and so

$$D(\theta) = |f(\theta)|^2 = \left(\frac{a\beta}{1+\beta}\right)^2 \to \sigma = 4\pi \left(\frac{a\beta}{1+\beta}\right)^2, \quad \beta \equiv \frac{2ma\alpha}{\hbar^2}$$