HW #3 Solutions (221B)

1) Marble

The phase shifts $\tan\delta_l = -\frac{j_l(ka)}{n_l(ka)}$ were derived in the lectures notes. To study their behavior, we will need various relations of the spherical bessel functions, most of which can be found in your favorite QM textbook. All can be found in Gradshteyn and Ryzhik (G&R), *Table of Integrals, Series, and Products*, which lives behind the desk in the physics library. There's a party on every page. (Please do not confuse G&R with their namesakes GNR, i.e. Guns 'n' Roses, who also sponsor worthy parties.) Note that Prof. Murayama's definition of spherical bessel functions are related to those in G&R and those in Mathematica by

$$j_l(z) = \sqrt{\frac{\pi}{2z}} J_{l+\frac{1}{2}}(z), \qquad n_l(z) = -\sqrt{\frac{\pi}{2z}} N_{l+\frac{1}{2}}(z). \tag{1}$$

a)

This is an excercise in massaging spherical bessel and trig. functions.

$$-\frac{j_l(ka)}{n_l(ka)} = \tan\delta_l = -i\frac{e^{i\delta_l} - e^{-i\delta_l}}{e^{i\delta_l} + e^{-i\delta_l}} = -i\frac{e^{2i\delta_l} - 1}{e^{2i\delta_l} + 1}.$$

Algebra then gives

$$e^{2i\delta_l} = \frac{n_l(ka) - ij_l(ka)}{n_l(ka) + ij_l(ka)} = \frac{h_l^{(-)}(ka)}{h_l^{(+)}(ka)}.$$

Note that Prof. Murayama's n_l differs from that given in most quantum mechanical textbooks by a sign (the same minus sign as in eqn. [1]), and his Hankle functions $h_l^{(\pm)}$ differ by factors of i.

b)

Here we make use of the small-argument expansion of the spherical bessel functions. Remembering Prof. Murayama's definitions of j_l, n_l,

$$j_l(z) \to \frac{(z)^l}{(2l+1)!!}, \qquad n_l(z) \to \frac{(2l-1)!!}{(z)^{l+1}} \qquad \text{as } z \to 0.$$

This is the first term in the general series expansion for $J_\nu(z)$ given on p. 970 of the most recent G&R, and it is sufficient for this problem. For small

ka all the phase shifts tend to zero, so that

$$\delta_l \approx \tan\delta_l = -\frac{j_l(ka)}{n_l(ka)} \approx -\frac{(ka)^l}{(2l+1)!!}\frac{(ka)^{l+1}}{(2l-1)!!} = -\frac{(ka)^{2l+1}}{(2l+1)!!(2l-1)!!}.$$

Since factorials increase much faster than logs, the factorials in the denominator actually play a larger role in damping the large-l δ_l's than the $(ka)^{2l+1}$ (for fixed ka).

c)

In this and the next part, we are trying to demonstrate by explicit calculation the semi-classical argument that for $l \gtrsim ka$, the particle cannot penetrate the potential barrier to the region of potential; only the exponential tail of the wavefunction leaks into the scatterer, so the partial wave cross sections σ_l should be strongly damped.

By simple algebra,

$$\tan^2\delta_l = -\frac{j_l^2(ka)}{n_l^2(ka)} \implies \sin^2\delta_l = \frac{j_l^2(ka)}{j_l^2(ka)+n_l^2(ka)},$$

so that

$$\sigma_l = \frac{4\pi}{k^2}(2l+1)\frac{j_l^2(ka)}{j_l^2(ka)+n_l^2(ka)}. \tag{2}$$

The mathematica computations for sample l values can be found in the separate notebook file.

d)

Since we are interested in values $l \gtrsim ka$, we cannot use the asymptotic expansions

$$j_l(z) \to \frac{\sin(z-l\pi/2)}{z}, \qquad n_l(z) \to \frac{\cos(z-l\pi/2)}{z} \qquad \text{as } |z| \to \infty, \tag{3}$$

because $l \gtrsim ka$ presupposes finite ka. (We will use these expressions in part (e).) Instead we need an expansion good for large but finite $ka \lesssim l$. G&R p. 974 offers such an expression. They look a little bit nasty, but since we are only interested in leading behvior in ka/l, we only need consider the exponential factors out front. In G&R notation,

$$J_\nu(\frac{\nu}{\cosh\alpha}) \sim \frac{e^{\nu\tanh\alpha-\nu\alpha}}{\sqrt{2\nu\pi\tanh\alpha}}, \qquad N_\nu(\frac{\nu}{\cosh\alpha}) \sim -\frac{e^{\nu\alpha-\nu\tanh\alpha}}{\sqrt{\frac{\pi}{2}\nu\tanh\alpha}}.$$

In our notation, $\nu = l + \frac{1}{2}$; and for large l/ka we have $(l+\frac{1}{2})/ka \approx \cosh\alpha \approx e^\alpha/2$, $\alpha \approx \log{(2l+1)}/ka$, $\tanh\alpha \approx 1 - 2e^{-2\alpha} \approx 1 - \frac{(ka)^2}{(2l+1)^2} \approx 1$; so that in our notation these relations become

$$j_l(ka) \sim \sqrt{\frac{\pi}{2ka}} \frac{e^{(l+\frac{1}{2})-(l+\frac{1}{2})\log{(2l+1)}/ka}}{\sqrt{(2l+1)\pi}} = \sqrt{\frac{1}{2(2l+1)ka}} e^{-(l+\frac{1}{2})(\log{(2l+1)}/ka-1)},$$

$$n_l(ka) \sim \sqrt{\frac{\pi}{2ka}} \frac{e^{(l+\frac{1}{2})\log{(2l+1)}/ka-(l+\frac{1}{2})}}{\sqrt{\frac{(l+\frac{1}{2})\pi}{2}}} = \sqrt{\frac{2}{(2l+1)ka}} e^{+(l+\frac{1}{2})(\log{(2l+1)}/ka-1)}.$$

For large l, n_l clearly dominates over j_l, so that after rewriting the exponentials,

$$\sigma_l \approx \frac{4\pi}{k^2}(2l+1)\frac{j_l^2(ka)}{n_l^2(ka)} \sim \frac{\pi}{k^2}(2l+1)\left(\frac{eka}{2l+1}\right)^{2l+1} \qquad (l \gtrsim ka).$$

This approximation presupposes l somewhat larger than ka and becomes increasingly valid as $l \gg ka$. For $l \gtrsim ka$, the σ_l are exponentially damped in l, which matches the behavior found in part (c).

e)

The analysis of parts (c) and (d) tells us that the partial cross sections for $l \gtrsim ka$ make negligible contribution to the total cross section, so to good approximation we can cutoff the sum over partial waves at $l = ka$:

$$\sigma \approx \sum_{l=0}^{ka} \sigma_l.$$

Now that $l < ka$ for all l of interest, we can use the large-ka aymptotic expansions in equation [3]. Plugging into equation [2] and approximating further by sending $\sum \to \int$,

$$\sigma \approx \sum_{l=0}^{ka} \sigma_l \approx \frac{4\pi}{k^2}\int_0^{ka} dl\,(2l+1)\sin^2{(ka - l\pi/2)}.$$

For large ka, the $\sin^2$ term oscillates rapidly, and being multiplied by the slow linear function $(2l+1)$, effectively contributes a factor equal to its average value of $1/2$. The main error comes from counting incomplete cycles of the $\sin^2$ function and decreases linearly as ka increases. Thus

$$\sigma \approx \frac{4\pi}{k^2}\int_0^{ka} dl\,\frac{2l+1}{2} \approx 2\pi a^2.$$

2) Moat

For the potential

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

we are asked to consider certain scattering and bound S-wave states. For macroscopic a, $\gamma < 0$, this potential has physical interpretation as castle defense. In the microscopic with $\gamma > 0$ this potential imitates some gross features of a nucleus: An incoming α particle faces a repulsive electric barrier but can be trapped on the interior by the strong nuclear force. The nucleus then is unstable to α decay, the α tunneling out through the potential barrier.

a)

This is the particle in a box. The radial part of the free wavefunction finite at the origin is $R_0 \propto j_0(kr)$. (The problem asks only for S-waves.) The wavefunction must vanish at the infinite potential wall at $r = a$, requiring $j_0(ka) = 0$. Then

$$0 = j_0(ka) = \frac{\sin ka}{ka} \implies ka = n\pi.$$

This is the same condition as for poles in the scattering amplitudes with $\gamma \to \infty$.

b)

In this part we are asked to find conditions on γ such that a bound state can exist about $r = a$. This is the 1-d bound state problem for the delta-function potential; we seek an ordinary bound state, distinguished from the metastable bound states in the scattering problem by having a purely imaginary k (or real negative E.)

The program is that of HW #1: Find a free-particle wave function and match the discontinuity in derivatives at $r = a$ to the strength of the delta function. We need our wavefunction to be finite at the origin and to decay to zero as $r \to \infty$. Thus

$$R_0 = \begin{cases} j_0(i\kappa r) = \frac{\sinh \kappa r}{\kappa r}, & r < a \\ Bh_0^{(+)}(i\kappa r) = B' \frac{e^{-\kappa r}}{\kappa r}, & r > a, \end{cases}$$

where κ is real > 0, defined by $E = -\frac{\hbar^2\kappa^2}{2m}$, and $B' = iB$ are constants. We require E real < 0 for a bound state.

At $r = a$ continuity of R_0 forces $B' = e^{\kappa a}\sinh\kappa a$. Integrating the Schrodinger equation over $(a-\epsilon, a+\epsilon)$ as $\epsilon \to 0$ requires additionally that

$$-\frac{\hbar^2}{2m}\Big(-B'\frac{\kappa e^{-\kappa a}}{\kappa a} - B'\frac{e^{-\kappa a}}{\kappa a^2} - \frac{\kappa\cosh\kappa a}{\kappa a} + \frac{\sinh\kappa a}{\kappa a^2}\Big) + \frac{\gamma\sinh\kappa a}{\kappa a} = 0,$$

or

$$-\frac{2m\gamma}{\hbar^2\kappa} = 1 + \coth\kappa a.$$

For given γ, a bound state will exist if this equation has a solution for κ real > 0. (You should check that you can find this same condition by looking for poles in the scattering amplitude for $k = i\kappa$ purely imaginary.) Such solutions will only exist for γ sufficiently negative. By playing around with graphical solutions in Mathematica, I find that a solution and hence a bound state exists when $\frac{-2m\gamma a}{\hbar^2} > 1$.

Analytically you can see this by noting that as $\kappa \to \infty$,

$$-\frac{2m\gamma a}{\hbar^2}\frac{1}{\kappa a} < 1 + \coth\kappa a$$

regardless of γ. Then look at small κ. If for some κ we find

$$-\frac{2m\gamma a}{\hbar^2}\frac{1}{\kappa a} > 1 + \coth\kappa a,$$

the functions must have crossed, i.e. we have a solution. As stated above, this will happend when $\frac{-2m\gamma a}{\hbar^2} := 1 + \varepsilon > 1$. This is because at small κ, $1 + \coth\kappa a \sim 1 + 1/\kappa a > 1/\kappa a$ when $\varepsilon = 0$, but $1 + 1/\kappa a < (1+\varepsilon)/\kappa a$ for $\varepsilon > 0$ and some sufficiently small κ.

c)

The analysis here repeats the above, except that we take $E = \frac{\hbar^2 k^2}{2m} > 0$ for a scattering solution. The radial wavefunction finite at the origin goes as

$$R_0 = \begin{cases} \frac{\sin kr}{kr}, & r < a \\ B\frac{\sin(kr+\delta_0)}{kr}, & r > a, \end{cases}$$

Imposing the same boundary conditions at $r = a$ as in part (b), we find the condition

$$-\frac{2m\gamma}{\hbar^2 k} = -\cot(ka + \delta_0) + \cot ka.$$

Now it's just an algebra problem to find

$$e^{2i\delta_0} = \frac{1 + \frac{2m\gamma}{\hbar^2 k} e^{-ika} \sin ka}{1 + \frac{2m\gamma}{\hbar^2 k} e^{ika} \sin ka}.$$

In the limit $\gamma \to 0$, $\cot(ka + \delta_0) = \cot ka$ implies $\delta_0 = 0$, no scattering. In the limit $\gamma \to \infty$, $\cot ka$ is finite, and we must have $\cot(ka + \delta_0)$ infinite, i.e. $\delta_0 = -ka$, the hard sphere result.