HW #3 Solutions (221B)

1) The δ-Shell Potential

The potential

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

we are asked to consider certain scattering and quasi-bound S-wave states. 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)

Writing the $l = 0$ radial Schrödinger equation (SE) for $rR_0(r)$ with the potential above, taking the $\gamma \to \infty$ limit, we simply get a particle in a box for $r < a$. The wavefunction (rR_0) must vanish at the origin giving $rR_0 \propto \sin kr$. The wavefunction must also vanish at the infinite potential wall at $r = a$, requiring

$$\sin(ka) = 0 \implies ka = n\pi.$$

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

b)

The wavefunction rR_0 obeys the free 1D SE for $r \neq a$ (with the boundary condition that rR_0 vanishes at the origin). We proceed by following the regular prescription to finding the phase shift. We write a wavefunction that behaves like a 'shifted free planewave' as $r \to \infty$, and find the phase shift by comparing this form with the solution to the SE. In this case, since the potential vanishes beyond $r = a$ we can let the asymptotic behavior of the shifted planewave extend as close to the origin as $r = a$, and match to the solution of the SE inside the shell.. We can write the wavefunction as

$$rR_0 = \begin{cases} \sin(kr) & \text{for } x < a \\ B\sin(kr+\delta_0) & \text{for } x > a \end{cases}.$$

We now demand the appropriate matching between the interior and the exterior of the shell i.e. we demand continuity at $r = a$

$$\sin(ka) = Asin(ka+\delta_0) \tag{1}$$

and we demand the regular kink in the wavefunction due to the delta function $(rR_0)'|_{a^-}^{a^+} = \frac{m\gamma}{\hbar^2} rR_0\big|_{r=a}$

$$Ak\cos(ka + \delta_0) - k\cos(ka) = \frac{m\gamma}{\hbar^2}\sin(ka) \tag{2}$$

Using equations (1) and (2) we can eliminate A and go through the algebra to solve for δ_0 and get

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

c)

In the limit $\gamma \to 0$, $e^{2i\delta_0} = 1$ implies $\delta_0 = 0$, no scattering. In the limit $\gamma \to \infty$, $e^{2i\delta_0} = e^{-2ika}$, i.e. $\delta_0 = -ka$, the hard sphere result.

d) See Mathematica notebook.

e)

Picking up from equation (53) in the lecture notes (Scattering theory III) we need to solve

$$2ika = \log\left(1 - 2i\frac{\hbar^2 k}{2m\gamma}\right) + 2in\pi \tag{3}$$

for the location of the poles in the S-matrix. If γ^{-1} is small we can expand the log

$$\log\left(1 - 2i\frac{\hbar^2 k}{2m\gamma}\right) = -2i\frac{\hbar^2 k}{2m\gamma} - \frac{1}{2}\left(2i\frac{\hbar^2 k}{2m\gamma}\right)^2 + O(\gamma^{-3}). \tag{4}$$

Many of you went on to plug this expansion in eq. (3) and compared real and imaginary parts on both side. This yields the correct result, of course. But, I think there is a shorterer way to the solution, as follows. Lets start with $O(\gamma^{-1})$, taking only the first two terms in the expansion. This gives a simple equation for k

$$2ika = -2i\frac{\hbar^2 k}{2m\gamma} + 2in\pi + O(\gamma^{-2})$$
$$\implies k_{pole} = \frac{n\pi}{a + \frac{\hbar^2}{2m\gamma}} + O(\gamma^{-2})$$

Obviously, taking only the first two terms in the log expansion was not enough. We got a real result for k_{pole}, and we expect an imaginary part as well. Even tough the leading imaginary part of k_{pole} is $O(\gamma^{-2})$ it has a dramatic effect on the physics, as we show in the next part. Therefore $O(\gamma^{-2})$ cannot be neglected in the imaginary part of k_{pole}. However, the $O(\gamma^{-2})$ contribution to the real part of k_{pole} can be ignored since its effect on the behavior of our solution is small.

Proceeding to the next order of the expansion (4) gives the desired imaginary part. The equation now reads

$$\left(a + \frac{\hbar^2}{2m\gamma}\right) k = n\pi - i\left(\frac{\hbar^2 k}{2m\gamma}\right)^2 + O(\gamma^{-3}).$$

Since the added piece already contains γ^{-2} we can plug the zeroth order solution we already have $k = n\pi/a$ instead of the k on the right hand side above. Doing this and solving for k, dropping the $O(\gamma^{-3})$ that arises, we get

$$k_{pole} = \frac{n\pi}{a + \frac{\hbar^2}{2m\gamma}} - i\left(\frac{\hbar^2}{2m\gamma}\right)^2 \frac{(n\pi)^2}{a^3} + O(\gamma^{-2})$$

where the $O(\gamma^{-2})$ term is now real. We learn that it is often good to do expansions of tis kind step by step, dropping higher order terms as we encounter them.

f) See Mathematica notebook.

g)

This was the hard part of the problem set. See part 5 of the lecture notes 'Scattering Theory III' for a convincing analysis of this problem.

2) WKB Scattering

a)

In using the WKB method, we are using an approximation, and we must adjust our formalism to maintain consistency within this approximation. In particular, the phase *shifts* are by definition the difference in the phase between scattered and unscattered waves, the latter being the wavefunction for zero potential. There's nothing subtle or duplicitous going on here; we just have to be internally consistent: necessarily $\delta_l \to 0$ as $V \to 0$.

After expanding in angular momentum eigenstates, the Schrodinger equation reduces to the one-dimensional form

$$\chi_l'' + \Big(k^2 - U(r) - \frac{l(l+1)}{r^2}\Big)\chi_l = 0,$$

where as usual $\chi_l = rR_l$, $E = \frac{\hbar^2 k^2}{2m}$ and $U(r) = \frac{2m}{\hbar^2}V(r)$. The one-dimensional WKB results apply to this problem, considering an effective potential $V_{eff} = U(r) - \frac{l(l+1)}{r^2}$.

At sufficiently large r, where both the centrifugal barrier and the well-behaved potential V decay to zero, a particle scattering in the potential V_{eff} will be in a classically allowed region. For the purposes of this problem, we can take the WKB-approximate solution in this regime to be

$$\chi_l(R) \approx \frac{1}{\sqrt{p(R)}}\cos\Big(\frac{1}{\hbar}\int_{r'}^{R} p(r)\,dr\Big), \tag{5}$$

where $p(r) = \hbar\sqrt{k^2 - U(r) - \frac{l(l+1)}{r^2}}$ is the classical momentum, and r' is the classical turning point defined by $p(r) = 0$. There are some subtleties here, but we can arrive at the right conclusion about the phase shift without being too careful. First, equation (5) looks like it comes from matching the exponentially damped solution to the left of the barrier, except there is a $-\pi/4$ missing. In fact, since we have the boundary condition $\chi_l \to 0$ at the origin, there will be both exponentially damped and exponentially increasing parts in the classically forbidden region, and our matching should take this into account. Ignoring all but the exponential factors,

$$\mathrm{Ai}(-u) - \mathrm{Bi}(-u) \sim e^{-\frac{2}{3}|u|^{3/2}} - e^{+\frac{2}{3}|u|^{3/2}}$$

matches to

$$\cos\big(\frac{2}{3}u^{3/2} - \frac{\pi}{4}\big) - \sin\big(\frac{2}{3}u^{3/2} - \frac{\pi}{4}\big) = \sqrt{2}\cos\big(\frac{2}{3}u^{3/2}\big),$$

which gives equation (5). As long as the $U = 0$ and $U \neq 0$ matchings are the same, it doesn't matter what constant phase is in (5) as far as the phase shift is concerned. But say the potential U is sufficiently attractive. It is possible that the classical turning point is the origin, which would change the form of the $U \neq 0$ WKB solution relative to the $U = 0$ case. As long as we forbid such potentials, the matching will be the same for both $U \neq 0$ and $U = 0$, and then we can simplify our lives by working with (5).

When $U = 0$, we have the asymptotic form

$$\chi_l(R) \to \frac{1}{2i\hbar k}\left(e^{i\int_{r''}^{R}\sqrt{k^2-\frac{l(l+1)}{r^2}}\,dr} + e^{-i\int_{r''}^{R}\sqrt{k^2-\frac{l(l+1)}{r^2}}\,dr}\right) \qquad (R\to\infty), \tag{6}$$

You can identify a sum of ingoing and outgoing (roughly) spherical waves, but this asymptotic behavior is different from that of the exact result

$$\chi_l \to \frac{1}{2i\hbar k}(e^{ikr} - (-1)^l e^{-ikr}).$$

For $U \neq 0$ WKB yields

$$\begin{aligned}\chi_l(R) &\to \frac{1}{2i\hbar k}\left(e^{i\int_{r'}^{R}\sqrt{k^2-U(r)-\frac{l(l+1)}{r^2}}\,dr} + e^{-i\int_{r'}^{R}\sqrt{k^2-U(r)-\frac{l(l+1)}{r^2}}\,dr}\right)\\ &= \frac{\text{phase}}{2i\hbar k}\left(e^{2i\int_{r'}^{R}\sqrt{k^2-U(r)-\frac{l(l+1)}{r^2}}\,dr-2i\int_{r''}^{R}\sqrt{k^2-\frac{l(l+1)}{r^2}}\,dr}e^{+i\int_{r''}^{R}\sqrt{k^2-\frac{l(l+1)}{r^2}}\,dr}\right.\\ &\qquad\left.-e^{-i\int_{r''}^{R}\sqrt{k^2-\frac{l(l+1)}{r^2}}\,dr}\right) \qquad (R\to\infty),\end{aligned} \tag{7}$$

after pulling out an overall phase. Comparing equation (7) with equation (6) in analogy with the exact treatment, we can read off the phase shift from (7),

$$e^{2i\delta_l} = e^{2i\int_{r'}^{R}\sqrt{k^2-U(r)-\frac{l(l+1)}{r^2}}\,dr-2i\int_{r''}^{R}\sqrt{k^2-\frac{l(l+1)}{r^2}}\,dr} \qquad (R\to\infty).$$

b)

For the hard sphere, the turning point

$$r' = \begin{cases} a & k^2 > \frac{l(l+1)}{a^2} \\ \sqrt{\frac{l(l+1)}{k^2}} & k^2 < \frac{l(l+1)}{a^2}. \end{cases}$$

If the energy is large enough, the particle penetrates into the region of potential and is reflected by the hard sphere; otherwise it is reflected by the centrifugal barrier. The turning point $r'' = \sqrt{\frac{l(l+1)}{k^2}}$ always.

Case 1, $k^2 < \frac{l(l+1)}{a^2}$: In this case the particle does not have enough energy to surmount the centrifugal barrier. It never reaches the region of potential and so classically should not be scattered. Indeed, since $r' = r'' > a$,

$$\delta_l = \lim_{R\to 0}\int_{r''}^{R}\sqrt{k^2-\frac{l(l+1)}{r^2}} - \int_{r''}^{R}\sqrt{k^2-\frac{l(l+1)}{r^2}} = 0.$$

The WKB approximation is qualitatively right—scattering should be suppressed—but it's not perfect. We saw in lecture that for small momenta, $\delta_l \propto k^{2l+1}$

The exponential tail of the wavefunction leaks into the classically forbidden region to the potential, and so there is some scattering, even though it is small for large l, small ka. WKB misses this essentially quantum mechanical behavior. As energy gets large, we expect WKB to give better results....

Case 2, $k^2 > \frac{l(l+1)}{a^2}$: Now $r' = a$, the particle reaches the potential.

$$\delta_l = \lim_{R\to 0} \int_a^R \sqrt{k^2 - \frac{l(l+1)}{r^2}} - \int_{\sqrt{\frac{l(l+1)}{k^2}}}^R \sqrt{k^2 - \frac{l(l+1)}{r^2}}$$

$$= \int_a^{\sqrt{\frac{l(l+1)}{k^2}}} \sqrt{k^2 - \frac{l(l+1)}{r^2}}.$$

To integrate, substitute

$$r = \sqrt{\frac{l(l+1)}{k^2}} \sec\theta,$$

whence the integral

$$\int_a^{r''} \frac{k}{r}\sqrt{r^2 - \frac{l(l+1)}{k^2}} \to \int \sqrt{l(l+1)} \tan^2\theta \, d\theta = \sqrt{l(l+1)}(\tan\theta - \theta).$$

At the upper and lower limits of integration $\tan\theta$ is 0 and $\sqrt{\frac{k^2a^2}{l(l+1)} - 1}$, respectively, so that

$$\delta_l = -\sqrt{k^2a^2 - l(l+1)} + \sqrt{l(l+1)} \arctan \sqrt{\frac{k^2a^2 - l(l+1)}{l(l+1)}}.$$

We can easily see that this result agrees with the exact result we got for $l = 0, \delta_l = -ka$. For higher l, by plotting $\sigma_l \propto \sin^2\delta_l$, as some of you did, we can see that WKB only gives the general shape of the correct cross section for high momenta, and is shifted from the exact solution by a phase. For example, the following notebook compares the two for $l = 10$.

Set $a = 1$.

```
In[2]:= j[l_, z_] := Sqrt[π/(2 z)] BesselJ[l + 1/2, z]; n[l_, z_] := -Sqrt[π/(2 z)] BesselY[l + 1/2, z]
```

$$j[l\_, z\_] := \sqrt{\frac{\pi}{2z}}\,\text{BesselJ}\left[l + \frac{1}{2}, z\right];\ n[l\_, z\_] := -\sqrt{\frac{\pi}{2z}}\,\text{BesselY}\left[l + \frac{1}{2}, z\right]$$

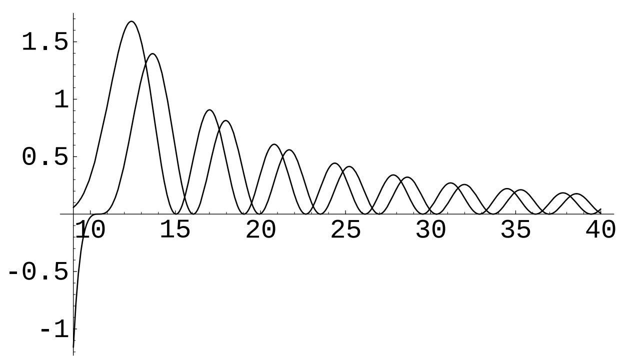
In[60]:=

$$\text{sigmaexact}[l\_, k\_] := \frac{4\pi}{k^2}(2l+1)\frac{j[l,k]^2}{j[l,k]^2 + n[l,k]^2}$$

In[83]:=

$$\text{sigmaWKB}[l\_, k\_] := \frac{4\pi}{k^2}(2l+1)\,\text{Sin}\left[-\sqrt{k^2 - l(l+1)} + \sqrt{l(l+1)}\,\text{ArcTan}\left[\sqrt{\frac{k^2 - l(l+1)}{l(l+1)}}\right]\right]\text{^}2$$

```
In[84]:= Plot[{sigmaexact[10, k], sigmaWKB[10, k]}, {k, 9, 40}]
```



Out[84]= - Graphics -