HW #4 Solutions (221B)

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

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

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

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

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 subtlties here, but we can arrive at the right conclusion about the phase shift without being too careful. First, equation (1) 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,

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

matches to

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

which gives equation (1). As long as the $U = 0$ and $U \neq 0$ matchings are the same, it doesn't matter what constant phase is in (1) 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 (1).

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

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

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

$$\begin{aligned}
\chi_l(R) &\to \frac{1}{2i\hbar k}\left(e^{i\int_{r'}^{R}\sqrt{k^2 - U(r) - \frac{l(l+1)}{r^2}}\,dr} + e^{-i\int_{r'}^{R}\sqrt{k^2 - U(r) - \frac{l(l+1)}{r^2}}\,dr}\right) \\
&= \frac{\text{phase}}{2i\hbar k}\left(e^{2i\int_{r'}^{R}\sqrt{k^2 - U(r) - \frac{l(l+1)}{r^2}}\,dr - 2i\int_{r''}^{R}\sqrt{k^2 - \frac{l(l+1)}{r^2}}\,dr}\, e^{+i\int_{r''}^{R}\sqrt{k^2 - \frac{l(l+1)}{r^2}}\,dr}\right. \\
&\qquad \left. -e^{-i\int_{r''}^{R}\sqrt{k^2 - \frac{l(l+1)}{r^2}}\,dr}\right) \qquad (R \to \infty),
\end{aligned}$$
(3)

after pulling out an overall phase. Comparing equation (3) with equation (2) in analogy with the exact treatment, we can read off the phase shift from (3),

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

b)

The usual validity criterion, as discussed in the lecture notes, applies here.

c)

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 found in HW #3 that for small momenta,

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

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 $\tan \theta = 0, \sqrt{\frac{k^2 a^2}{l(l+1)} - 1}$, respectively, so that

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

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Last week we took the limit $ka \gg l$ of the exact phase shifts using the asymptotic expressions for the spherical bessel functions, giving

$$\tan \delta_l = -\frac{j_l(ka)}{n_l(ka)} \approx -\tan\left(ka - \frac{l\pi}{2}\right),$$

so that $\delta_l \approx -ka + \frac{l\pi}{2}$. With our WKB result, $ka \to \infty$ sends the arctan to $\pi/2$,

$$\delta_l \approx -ka + \frac{1}{2}\frac{l(l+1)}{k^2 a^2} + \sqrt{l(l+1)}\frac{\pi}{2} \approx -ka + \frac{\sqrt{l(l+1)}\pi}{2} \qquad (ka \gg l).$$

This is the same as the asymptotic approximation up to a phase $\approx \pi/4$ which comes from $\frac{\sqrt{l(l+1)}\pi}{2} \approx \frac{l\pi}{2} + \frac{\pi}{4}$. For $l = 0$ WKB reproduces the exact result, $\delta_l = -ka$.

As many of you did, we can plot the exact and WKB cross sections as functions of k. While their shapes match closely, the WKB result is shifted outward by the aforementioned phase $\approx \pi/4$. I take $l = 10$ in this example:
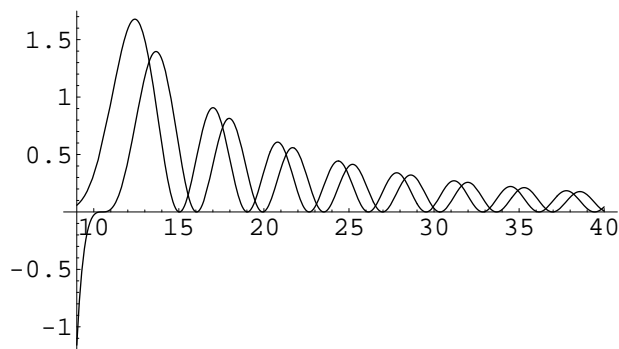
Set $a = 1$.

$In[2]:=$ **j[l_, z_] :=** $\sqrt{\dfrac{\pi}{2\,z}}$ **BesselJ**$\left[l + \dfrac{1}{2},\, z\right];$ **n[l_, z_] :=** $-\sqrt{\dfrac{\pi}{2\,z}}$ **BesselY**$\left[l + \dfrac{1}{2},\, z\right]$

$In[60]:=$ **sigmaexact[l_, k_] :=** $\dfrac{4\,\pi}{k^2}$ **(2 l + 1)** $\dfrac{\text{j[l, k]}^2}{\text{j[l, k]}^2 + \text{n[l, k]}^2}$

$In[83]:=$ **sigmaWKB[l_, k_] :=**

$\dfrac{4\,\pi}{k^2}$ **(2 l + 1) Sin**$\left[-\sqrt{k^2 - l\,(l+1)} + \sqrt{l\,(l+1)}\ \text{ArcTan}\left[\sqrt{\dfrac{k^2 - l\,(l+1)}{l\,(l+1)}}\,\right]\right]$ **^2**

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

$Out[84]=$ ‑ Graphics ‑

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