Quantum Mechanics II
HW 8

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Due: Nov. 11

1. Review of Lorentz transformation in relativistic notation

   A Lorentz boost from the unprimed inertial frame to the primed inertial frame, moving with velocity $\mathbf{v}$ relative to the original frame, can be written as

$$x_0' = \gamma\left(x_0 - \beta \cdot \mathbf{x}\right), \qquad \mathbf{x}' = \mathbf{x} + \frac{(\gamma-1)}{\beta^2}(\beta \cdot \mathbf{x})\beta - \gamma\beta x_0$$

   (a) Match the s-wave radial wavefunction at the delta function wall, and hence obtain an expression for $\tan\delta_0$, or $\sin\delta_0$, in terms of the momentum k and the parameters of the potential.

   (b) From this matching also find an expression for the amplitude A_0 of the s-wave radial wavefunction inside the cavity, relative to the amplitude of the s-wave radial wavefunction outside the cavity.

   (c) Plot $\delta_0(k)$, $\sigma_0(k)$, and $A_0(k)$ as functions of the dimensionless quantity kR, for $\Omega = 4$, and again for $\Omega = 10$.

   (d) Comment on the physical interpretation of the features of these plots.

   (a) For $r < R$, the solution to the radial Schrodinger equation is that of a free particle with regular behavior at the origin

$$R_l(r) = A_l j_l(kr)$$

   while for $r > R$ we again have a free particle but we include the Neumann function

$$R_l(r) = B_l j_l(kr) + C_l n_l(kr).$$

   At $r = R$, the wavefunction must be continuous

$$A_l j_l(kR) = B_l j_l(kR) + C_l n_l(kR).$$

   For the other boundary condition, the delta-function will specify what the discontinuity of the wavefunction is. Let us integrate the Schrodinger eq. with vanishing bounds around R

$$-\frac{\hbar^2}{2m}\int_{R-\epsilon}^{R+\epsilon} dr' \, \frac{d^2 u_l}{dr'^2} + \frac{\hbar^2}{2m}\int_{R-\epsilon}^{R+\epsilon} dr' \, \frac{\Omega}{R}\delta(r-R)u_l(r') = 0.$$

   The energy and centrifugal term vanish in the limit of $\epsilon \to 0$. From this equation we find

$$\left.\frac{du_l}{dr}\right|_{R_+} - \left.\frac{du_l}{dr}\right|_{R_-} = \frac{\Omega}{R}u(R)$$

   or

$$R\left.\frac{dR_l(r)}{dr}\right|_{R_+} + R_l(R_+) - R\left.\frac{dR_l(r)}{dr}\right|_{R_-} - R_l(R_-) = \frac{\Omega}{R}RR_l(R).$$

Using the continuity of the wavefunction this leads to

$$\left.\frac{dR_l}{dr}\right|_{R_+} - \left.\frac{dR_l}{dr}\right|_{R_-} = \frac{\Omega}{R} R_l(R).$$

or

$$A_l k j_l'(kR) - B_l k j_l'(kR) - C_l k n_l'(kR) = \frac{\Omega}{R}\left[B_l j_l(kR) + C_l n_l(kR)\right].$$

Ultimately, we want the relation between C and D to determine the phase shift. We can find this by first eliminating A_l and then solving for the ratio $\frac{C}{B}$

$$\frac{B_l j_l(kR) + C_l n_l(kR)}{j_l(kR)} j_l'(kR) - B_l j_l'(kR) - C_l n_l'(kR) = \frac{\Omega}{kR}\left[B_l j_l(kR) + C_l n_l(kR)\right].$$

We find

$$-\frac{C}{B} = \frac{\frac{\Omega}{kR} j_l(kR)}{\frac{\Omega}{kR} n_l(kR) + n_l'(kR) - n_l(kR)\frac{j_l'(kR)}{j_l(kR)}}.$$

At this point we diverge from the general l result and specifically restrict the problem to $l = 0$. We use the forms

$$j_0 = \frac{\sin(kr)}{kr}; \qquad n_0 = -\frac{\cos(kr)}{kr}$$

to simplify the ratio as

$$-\frac{C}{B} = \frac{\sin^2(kR)}{\frac{kR}{\Omega} - \cos(kR)\sin(kR)}.$$

Now if we take the wavefunction for $r > R$ at $r \to \infty$ we can show that it takes the form

$$R(r) = \frac{(B^2 + C^2)^{1/2}}{kr}\left[\sin\left(kr - \frac{(0)\pi}{2} + \delta_0\right)\right]$$

with

$$\tan\delta_0 = -\frac{C}{B}.$$

Hence we have found δ_0 in terms of the momentum and parameters of the potential

$$\tan\delta_0 = \frac{\sin^2(kR)}{\frac{kR}{\Omega} - \cos(kR)\sin(kR)}.$$

(b) In the same way that we arrived at the form of the asymptotic radial wavefunction for $r > R$, $r \to \infty$, we can take the solution of the free particle at the boundary $r = R$ and transform it in the same way:

$$\frac{1}{kR}\left[B\sin(kR) - C\cos(kR)\right] = \frac{(B^2 + C^2)^{1/2}}{kR}\left[\sin\left(kR + \delta_0\right)\right].$$

Now lets denote $D \equiv \sqrt{B^2 + C^2}$ and use this in our first boundary condition equation

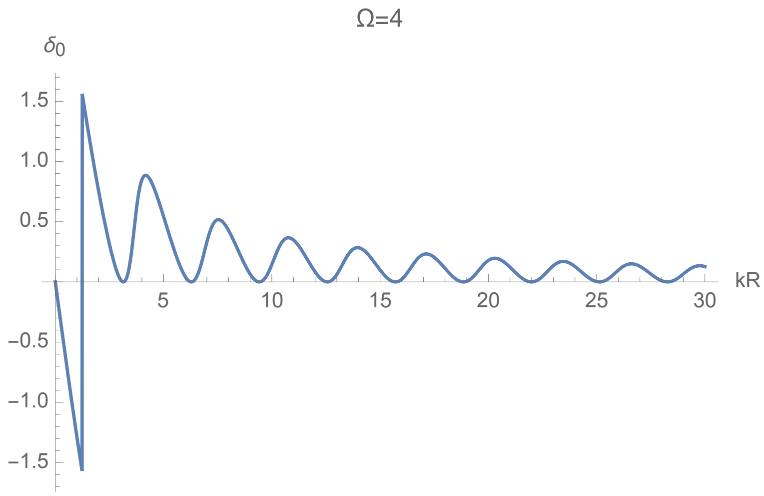
$$A\sin(kR) = D\sin\left(kR + \delta_0\right)$$

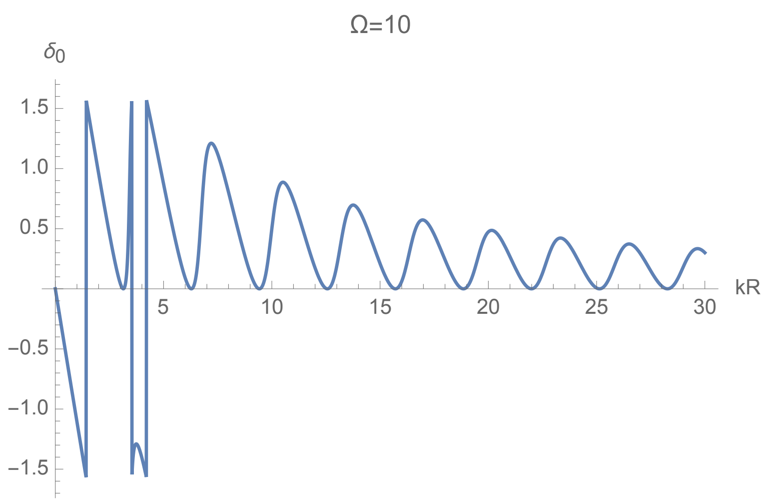
hence

$$\frac{A}{D} = \frac{\sin(kR + \delta_0)}{\sin(kR)}$$

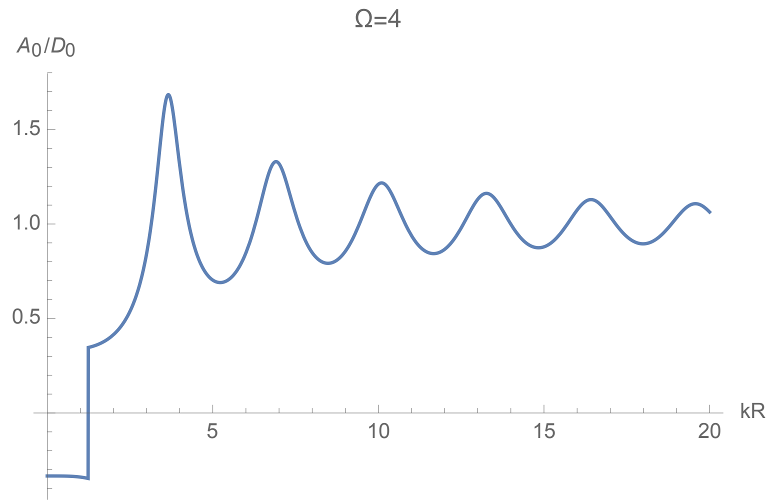
(c)

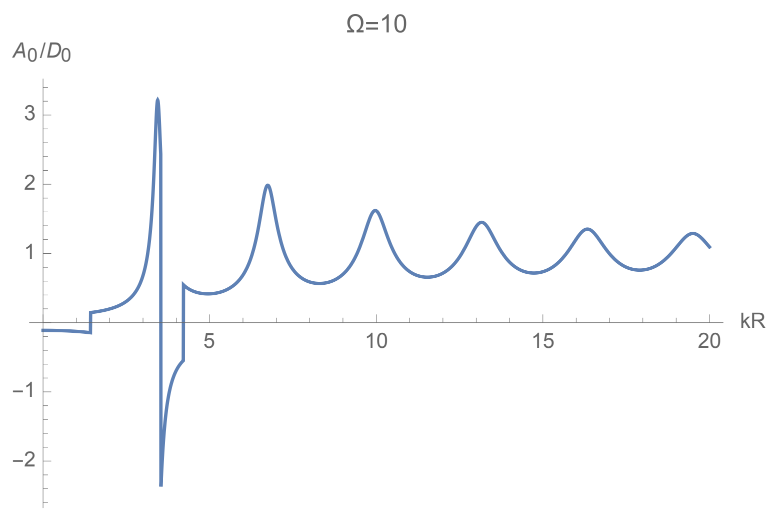
$$\boxed{\delta_0 = \tan^{-1}\left(\frac{\sin^2(kR)}{\frac{kR}{\Omega} - \cos(kR)\sin(kR)}\right)}$$



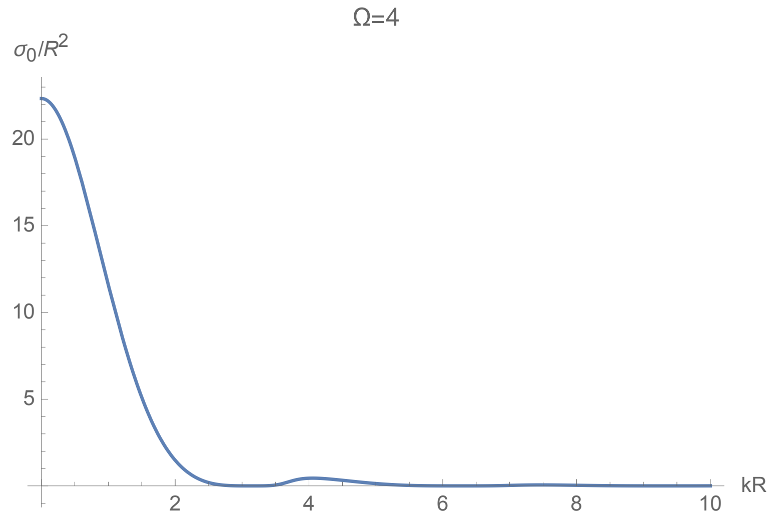


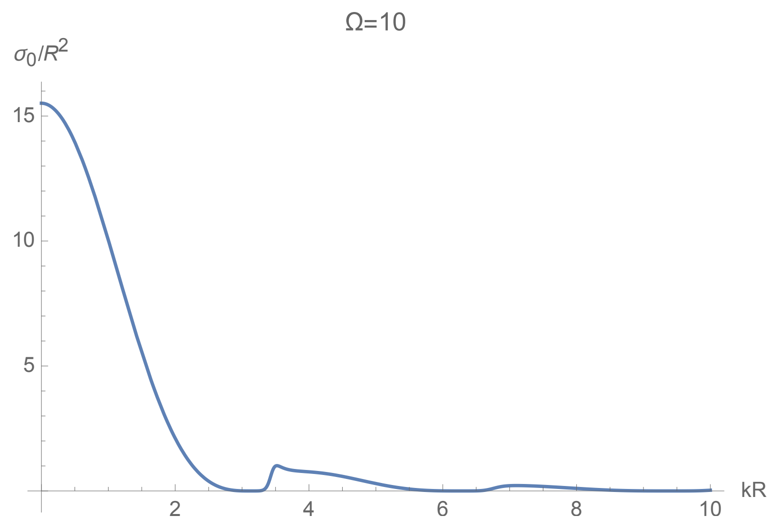
$$\boxed{\frac{A_0(k)}{D_0(k)} = \frac{\sin(kR+\delta_0)}{\sin(kR)}}$$





$$\boxed{\frac{\sigma_0}{R^2} = \frac{4\pi}{(kR)^2}\sin^2(\delta_0)}$$





(d) Both the amplitude and phase-shift have periodic maximums and minimums, which correspond to resonant energies of kR. The resonance is strongest at low energy - as we continue to increase the energy, the effect of resonance becomes weak and we can see that the relative amplitude inside the well equilibrates to the amplitude outside the well. Also, the s-wave cross section has the most significant contribution at low energy, which is what we expect - as we increase the energy, higher angular momentum terms are required. In addition, increasing the strength Ω of the potential increases the strength/effect of the resonance for the same given energy. This also shifts the σ_0 cross section energy dependence to larger values of kR.

2. Inverse square potential

Consider the scattering problem with a radial potential

$$V(r) = \frac{\alpha}{r^2}$$

(a) From the solution to the radial Schrodinger equation, write down an explicit expression for the phase shift δ_l. (Think about the form of the potential.)

(b) Show that in the large l limit

$$\delta_l \sim -\left(\frac{\pi m\alpha}{2\hbar^2 l}\right)$$

(c) What is the momentum dependence of the total cross section?

(a) With $V = 0$ the radial Schrodinger equation is

$$\left[\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2} + k^2\right] R(r).$$

With substitution $\rho = kr$ this becomes

$$\frac{d^2R}{d\rho^2} + \frac{2}{\rho}\frac{dR}{d\rho} + \left[1 - \frac{l(l+1)}{\rho^2}\right] R = 0$$

which is in fact the spherical Bessel differential equation whose solutions are the familiar $j_l(kr)$ and $n_l(kr)$. Of course, none of this is new.

Now add in the potential

$$\frac{d^2R}{d\rho^2} + \frac{2}{\rho}\frac{dR}{d\rho} + \left[1 - \frac{l(l+1)}{\rho^2} - \frac{(2m\alpha/\hbar^2)}{\rho^2}\right] R = 0.$$

With $s = \frac{2m\alpha}{\hbar^2}$ we can also write this as

$$\frac{d^2R}{d\rho^2} + \frac{2}{\rho}\frac{dR}{d\rho} + \left[1 - \frac{s + l(l+1)}{\rho^2}\right] R = 0$$

Using the fact that the spherical Bessel functions are not limited to integer values of the factor $l(l+1)$, this allows us to form a very similar differential equation whose solutions are in fact still spherical Bessel functions:

$$\frac{d^2R}{d\rho^2} + \frac{2}{\rho}\frac{dR}{d\rho} + \left[1 - \frac{\lambda(\lambda+1)}{\rho^2}\right] R = 0$$

where we have specifically defined

$$\lambda(\lambda+1) \equiv s + l(l+1).$$

Hence the solutions are

$$R_l(r) = j_\lambda(kr) + n_\lambda(kr)$$

with (solving the quadratic eq. for lambda)

$$\lambda = -\frac{1}{2} + \sqrt{\left(\frac{2l+1}{2}\right)^2 + s}.$$

The asymptotic form of the radial equation under the influence of the potential is

$$R_l(r) \underset{r\to\infty}{\longrightarrow} \frac{\sin\left(kr - \frac{\lambda\pi}{2}\right)}{kr}$$

while the general form in terms of the phase shift is

$$R_l(r) \underset{r\to\infty}{\longrightarrow} \frac{\sin\left(kr - \frac{l\pi}{2} + \delta_l\right)}{kr}.$$

To find δ_l we just have to match these

$$-\frac{\lambda\pi}{2} = -\frac{l\pi}{2} + \delta_l$$

so finally

$$\delta_l = \frac{\pi}{2}(l - \lambda) = \frac{\pi}{2}\left(l + \frac{1}{2} - \sqrt{\left(\frac{2l+1}{2}\right)^2 + \frac{2m\alpha}{\hbar^2}}\right).$$

(b) For large l we first have $l + \frac{1}{2} \approx l$ and thus

$$\delta_l \approx \frac{\pi}{2}\left(l - \sqrt{l^2 + s}\right).$$

Inputting the binomial expansion

$$\sqrt{l^2 + s} = l\sqrt{\frac{s}{l^2} + 1} \approx 1 + \frac{s}{2l^2}$$

we have

$$\delta_l \approx \frac{\pi}{2}\left(l - l\left(1 + \frac{s}{2l^2}\right)\right) = -\frac{\pi s}{4l}$$

and therefore

$$\delta_l \sim -\left(\frac{\pi m\alpha}{2\hbar^2 l}\right).$$

(c) With

$$\sigma_l = \frac{4\pi}{k^2}(2l+1)\sin^2\delta_l$$

the total cross section is

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

Interestingly, the phase shift does not depend on the energy. And so the momentum dependence is just $1/k^2$ as seen in

$$\sigma = \sum_{l=0}^{\infty}\sigma_l = \frac{1}{k^2}\sum_l f(l).$$

For large l, $f(l)$ decreases in magnitude and thus makes little contribution to the total cross section.

3. WKB Phase Shifts

Consider a radial potential $V(r)$ and define $U(r) = \frac{2m}{\hbar^2}V(r)$. The WKB expression for the phase shift is given by the difference between the WKB phases with and without the potential

$$\delta_l^{WKB}(k) = \int_{r'}^{\infty} dr\,\sqrt{k^2 - U(r) - \frac{l(l+1)}{r^2}} - \int_{r''}^{\infty} dr\,\sqrt{k^2 - \frac{l(l+1)}{r^2}}$$

Here r' and r'' are the relevant turning points with and without the potential.

(a) Consider the case of scattering from a hard sphere of radius a. For the energy regime where $kr > \frac{l(l+1)}{a^2}$, compute the WKB expression for the phase shift $\delta_l^{WKB(k)}$.

(b) For $l = 5$ and $l = 10$, plot the contribution to the cross section from the l^{th} partial wave, as a function of k with $k > \sqrt{\frac{l(l+1)}{a^2}}$, using the WKB expression found in the previous part, and compare it on the same plot with the exact expression.

(c) Comment on the differences between the WKB and exact plots in the previous part, and explain the origin of the discrepancy.

(a) As a hard sphere

$$V(r) = \begin{cases} \infty & \text{for} \quad r \leq a \\ 0 & \text{for} \quad r > a \end{cases}$$

For the particle under the potential influence, the turning point is simply a and the potential vanishes beyond a, so that we have

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

For the second integral, the turning point can be found as

$$k^2 = \frac{l(l+1)}{r^2}$$

or

$$r_0 = \sqrt{\frac{l(l+1)}{k^2}}.$$

Altogether then

$$\delta_l^{WKB} = \int_a^\infty dr' \sqrt{k^2 - \frac{l(l+1)}{r'^2}} - \int_{r_0}^\infty dr'' \sqrt{k^2 - \frac{l(l+1)}{r''^2}}.$$

Since we are in the energy regime $k^2 > \frac{l(l+1)}{a^2}$ this means $r_0 < a$ and we can write the phase shift as

$$\delta_l^{WKB} = -\int_{r_0}^a dr \sqrt{k^2 - \frac{l(l+1)}{r'^2}}.$$

Evaluating the integral we have

$$\delta_l^{WKB} = \frac{\pi}{2}\sqrt{l(l+1)} - \sqrt{(ka)^2 - l(l+1)} - l(l+1)\tan^{-1}\left(\frac{\sqrt{l(l+1)}}{\sqrt{(ka)^2 - l(l+1)}}\right)$$

(b) First let's compute the exact phase shift. For $r < a$, the wavefunction vanishes, while for $r > a$ it has the free particle form

$$R_l(r) = A_l j_l(kr) + B_l n_l(kr).$$

The boundary condition of continuity leads us to

$$R_l(a) = 0$$

or

$$-\frac{B_l}{A_l} = \frac{j_l(ka)}{n_l(ka)}.$$

As $r \to \infty$ the form is

$$R_l(r) \underset{r\to\infty}{\longrightarrow} \frac{(A^2+B^2)^{1/2}}{kr}\left[\sin\left(kr - \frac{l\pi}{2} + \tan^{-1}\left(\frac{-B_l}{A_l}\right)\right)\right]$$

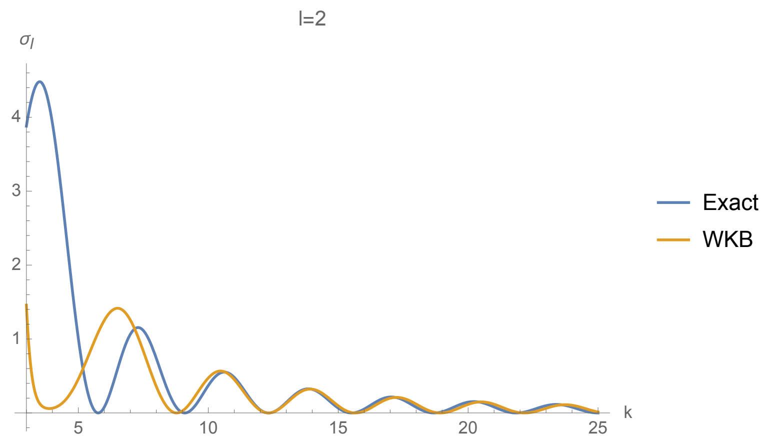
hence

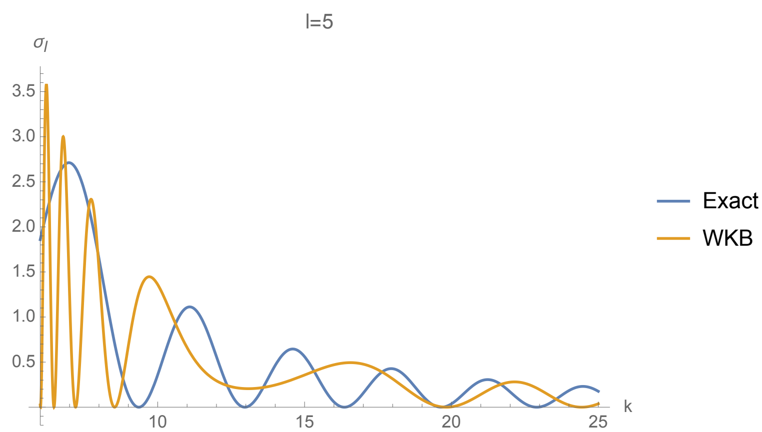
$$\delta_l = \tan^{-1}\left(\frac{-B_l}{A_l}\right) = \tan^{-1}\left(\frac{j_l(ka)}{n_l(ka)}\right).$$

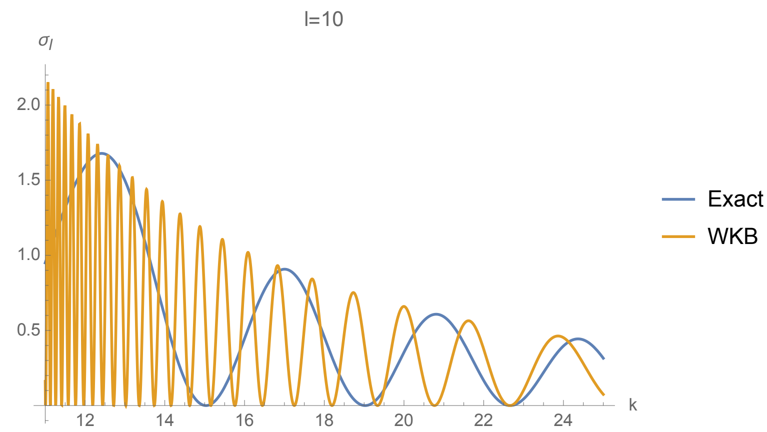
The l^{th} contribution to the total cross section is

$$\sigma_l = \frac{4\pi}{k^2}(2l+1)\sin^2\delta_l.$$

Both exactly and in the WKB approximation, we will plot σ_l as a function of k for $l = 2, 5, 10$. We set $a = 1$ and look at energies $(ka)^2 > l(l+1)$.







(c) The WKB approximation is good for energies in which the potential varies slowly in comparison to the wavelength of the particle $\lambda = 2\pi/k$ (this might be an oversimplification?). At the surface of the hard-sphere, the potential has a singular derivative and so the WKB fails to provide a reasonable approximation near $r = a$. Consequently, the phase shift absorbs this discrepancy.

As we increase l, the angular momentum barrier slope increases and again the WKB becomes less valid. At the same time, higher energies are needed to increase the distance between a and the angular momentum barrier, such that the phase shift can accumulate accurate contributions away from the spherical barrier at a. This is why we see the WKB being a good approximation at low values of l with high energy.