Physics 827 Problem Set 6 Due Friday 11/13/2009

6.1) Consider the two delta-function potential,

$$V(x) \;=\; va\delta(x+a) \;+\; va\delta(x-a)$$

where $v < 0$.
(a) Find the transcendental equation that determines the ground state (Use the parity of the ground state wave function to choose the form of the wave function in the region $(-a,\, a)$ intelligently.) Is there always a bound state?
(b) Repeat part (a) for the first excited state or odd parity states in general.
(c) When $|v| \;>>\; \hbar^2/(ma^2)$ find the even and odd parity energies and the splitting between them. Compare with the discussion for the double well in class. (10 points)

We have

$$V(x) \;=\; va\,(\,\delta(x-a) \;+\; \delta(x+a)\,)\,. \tag{1}$$

For the even solution we write down the wave functions in the three regions (defined as I for $x \leq -a$, III for $x \geq a$ and II for the region between a and $-a$:

$$\psi_I(x) \;=\; Ae^{\kappa x}\;,\quad \psi_{II}(x) \;=\; B\cosh(\kappa x) \;\;\text{and}\;\; \psi_{III}(x) \;=\; Ae^{-\kappa x} \tag{2}$$

where $\kappa \;=\; \sqrt{2m \mid E \mid /\hbar^2}$. We use the boundary conditions at $x = a$ to obtain

$$Ae^{-\kappa a} \;=\; B\cosh(\kappa a) \tag{3}$$

$$-\kappa Ae^{-\kappa a} \;-\; \kappa B\sinh(\kappa a) \;=\; \frac{2mav}{\hbar^2}\,Ae^{-\kappa a} \tag{4}$$

Dividing one equation by the other we find

$$\kappa\,\tanh(\kappa a) \;=\; -\kappa \;-\; \frac{2mav}{\hbar^2}\,.$$

This implies that

$$\kappa\,[1+\tanh(\kappa a)] \;=\; -\,\frac{2mav}{\hbar^2}\,. \tag{5}$$

Note that the right-hand side is positive since $v < 0$. We write

$$1+\tanh x \;=\; 1 \;+\; \frac{1-e^{-2x}}{1+e^{-2x}} \;=\; \frac{2}{1+e^{-2x}}\,.$$

Equation (5) becomes

$$1 \;+\; e^{-2\kappa a} \;=\; \kappa a \times \frac{\hbar^2}{ma^2|v|}\,. \tag{6}$$

Note that the left-hand side decays montonically from 1 at $\kappa = 0$ to 0 at infinity. The right-hand side is linear in κ and increasing from 0 at $\kappa = 0$. Thus there will always be one and only one intersection and thence, only one even bound state solution.

For the odd parity solution we have

$$\begin{aligned} Ae^{-\kappa a} &= B\sinh(\kappa a) && (7) \\ -\kappa Ae^{-\kappa a} - \kappa B\cosh(\kappa a) &= \frac{2mav}{\hbar^2} Ae^{-\kappa a} && (8) \end{aligned}$$

Dividing one equation by the other we find

$$\kappa \coth(\kappa a) = -\kappa - \frac{2mav}{\hbar^2}\,.$$

This implies that

$$\kappa\left[1 + \coth(\kappa a)\right] = -\frac{2mav}{\hbar^2}\,. \qquad (9)$$

Note that the right-hand side is positive since $v < 0$. We write

$$1 + \coth x = 1 + \frac{1 + e^{-2x}}{1 - e^{-2x}} = \frac{2}{1 - e^{-2x}}\,.$$

Equation (9) becomes

$$1 - e^{-2\kappa a} = \kappa a \times \frac{\hbar^2}{ma^2|v|}\,. \qquad (10)$$

Note that the left-hand side vanishes at $\kappa = 0$ and increases linearly with slope 2 as a function of κa. The right-hand side is linear and increasing with slope $\hbar^2/(ma^2|v|)$. Thus there will be an odd bound state solution if

$$|v| > \frac{\hbar^2}{2ma^2}$$

What happens if equality holds?

(c) The ground state energy is determined by

$$\kappa a = \frac{ma^2 v}{\hbar^2}\left(1 + e^{-2\kappa a}\right)\,.$$

We can solve this iteratively: first set $\kappa a = \frac{ma^2v}{\hbar^2}$; next substitute this into the right-hand side to obtain

$$\kappa a \approx \frac{ma^2|v|}{\hbar^2}\left(1 + e^{-2ma^2|v|/\hbar^2}\right)\,.$$

This is a good approximation since $ma^2|v|/\hbar^2$ is large the correction is exponentially small. The ground state energy is

$$E_g \;=\; -\frac{\hbar^2\kappa^2}{2m} \;\approx\; -\frac{ma^2v^2}{2\hbar^2}\,\Big(1\,+\,2e^{-2ma^2|v|/\hbar^2}\Big)\;.$$

Since $ma^2|v|/\hbar^2$ is large the odd first excited state exists and we can solve for κa similarly and obtain

$$\kappa a \;\approx\; \frac{ma^2|v|}{\hbar^2}\,\Big(1\,-\,e^{-2ma^2|v|/\hbar^2}\Big)\;.$$

The first excited state energy is

$$E_e \;=\; -\frac{\hbar^2\kappa^2}{2m} \;\approx\; -\frac{ma^2v^2}{2\hbar^2}\,\Big(1\,-\,2e^{-2ma^2|v|/\hbar^2}\Big)\;.$$

The difference has the expected form for tunneling splitting:

$$E_e - E_g \;\approx\; \frac{2ma^2v^2}{\hbar^2}\,\times\,e^{-2ma^2|v|/\hbar^2}\,.$$

Please check if this corresponds to your WKB intuition.

6.2) For the infinite potential well compute and plot the probability of finding a momentum value between p_0 and p_0+dp for the ground state and the first excited state. Please use Mathematica or Tables to do the integrals. (6 points)

Use

```
f0[a_, k_] =
 Integrate[(1/Sqrt[2 Pi]) Exp[I k x] Cos[Pi x/a] Sqrt[2/a], {x, -a/2,
   a/2}, Assumptions -> {Im[k] == 0, a \[Element] Reals}]
   f1[a_, k_] =
 Integrate[(1/Sqrt[2 Pi]) Exp[I k x] Sin[2 Pi x/a] Sqrt[2/a], {x, -a/
    2, a/2}, Assumptions -> {Im[k] == 0, a \[Element] Reals}]
```

to do the integrals in k-space to obtain $\psi_g(k)$ for the $g$round state and $\psi_e(k)$ for the first $e$xcited sate We compute the squared modulus of $\psi(k)$ to obtain $P(k)$ the probability density. Note that $P(p) = P(k)/\hbar$. We have

$$\psi_g(k) \;=\; \frac{\sqrt{2\pi a}\,\cos(ka/2)}{\pi^2 - k^2a^2}$$

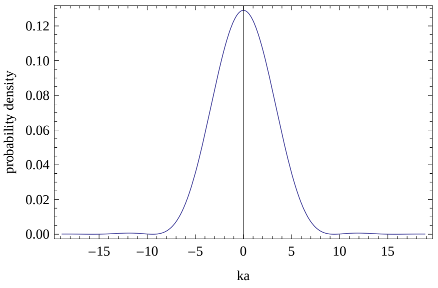

Figure 1: Ground state momentum distribution

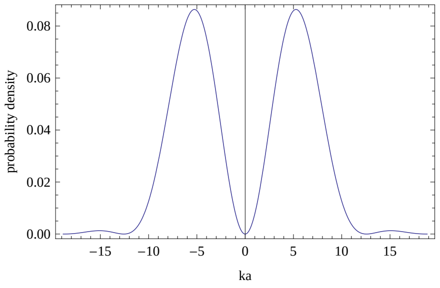

Figure 2: Momentum distribution of the first excited state

$$\psi_e(k) \;=\; i\,\frac{4\sqrt{\pi a}\,\sin(ka/2)}{4\pi^2 - k^2a^2}$$

The probability densities are given by

$$P_g(p) \;=\; \frac{2\pi a}{\hbar}\,\frac{\cos^2\left(\frac{pa}{2\hbar}\right)}{\left(\frac{p^2a^2}{\hbar^2} - \pi^2\right)^2}$$

$$P_e(p) \;=\; \frac{16\pi a}{\hbar}\,\frac{\sin^2\left(\frac{pa}{2\hbar}\right)}{\left(\frac{p^2a^2}{\hbar^2} - 4\pi^2\right)^2}$$

6.3) This is easy and done in class. Please do it yourselves: Exercises 5.3.3. and 5.3.4 on page 167. (4 points)

6.4) The first part is easy. For $E > V_0$ the incident wave is e^{ikx}, the reflected wave is re^{-ikx} and the transmitted wave is te^{iqx} where $\hbar^2q^2/(2m) \equiv E - V_0$ and $\hbar^2k^2/(2m) \equiv E$. The boundary conditions yield

$$1 + r \;=\; t\,.$$

$$ik\,(1-r) \;=\; iqt$$

Adding we have $\boxed{t \;=\; \frac{2k}{k+q}}$. Substituting into the first equation $\boxed{r \;=\; \frac{k-q}{k+q}}$. The reflection coefficient is given by $R \;=\; |r|^2 \;=\; \left(\frac{k-q}{k+q}\right)^2$. The transmission coefficient is obtained by computing the ratio of the currents:

$$T \;=\; \frac{|t|^2\,\frac{\hbar q}{m}}{1\frac{\hbar k}{m}} \;=\; |t|^2\,\frac{q}{k} \;=\; \frac{4kq}{(k+q)^2}\,.$$

The sum is clearly unity. You can do the incidence from the right similarly and check that the roles of k and q are interchanged. The incident wave is e^{-iqx}, the reflected wave is $r'e^{iqx}$ for $x > 0$ and the transmitted wave is $t'e^{-ikx}$ for $x < 0$ The boundary conditions yield

$$1 + r' = t' .$$

$$-iq\,(1 - r') = -ikt'$$

Adding we have $\boxed{t = \frac{2q}{k+q}}$. Substituting into the first equation $\boxed{r' = \frac{q-k}{k+q}}$. Note that $r' = -r$. The reflection and transmission coefficients are the same.

Very few appear to have done the second part correctly. It is non-trivial. We use two general properties of the time-independent Schrödinger equation. If ψ is a solution ψ^* is a solution and since the equation is linear the superposition principle holds. Thus we are given one solution (call it ψ_1)

$$e^{ikx} + re^{-ikx} \quad |Unknownpotential| \quad te^{ikx}$$

and therefore its complex conjugate ψ_1^*

$$e^{-ikx} + r^*e^{ikx} \quad |Unknownpotential| \quad t^*e^{-ikx}$$

is also a solution. The idea is to find a superposition of these two solutions that will yield the other given solution ψ_2:

$$\tau e^{-ikx} \quad |Unknownpotential| \quad e^{-ikx} + \rho e^{ikx}$$

It is clear how to do this since we want the right-moving wave to be absent in the leftmost region, i.e., we want to make the coefficient of e^{ikx} vanish. Clearly $\psi_1 - \frac{1}{r^*}\psi_1^*$ will do this. This superposition yields the solution

$$\left(r - \frac{1}{r^*}\right) e^{-ikx} \quad |Unknownpotential| \quad te^{ikx} - \frac{t^*}{r^*}e^{-ikx}$$

This is the same configuration as ψ_2 except for the normalization. We divide by $-t^*/r^*$ so that the incident amplitude is 1. Thus we obtain

$$\frac{r - \frac{1}{r^*}}{-\frac{t^*}{r^*}} e^{-ikx} \quad |Unknownpotential| \quad e^{-ikx} - \frac{t}{t^*}r^*e^{ikx}$$

Compare with ψ_2 to obtain

$$\rho = -\frac{t}{t^*}r^* .$$

$$\tau = \frac{r - \frac{1}{r^*}}{-\frac{t^*}{r^*}} = \frac{1 - rr^*}{t^*} = t\,.$$

Thus the transmission amplitude is the same both ways while the reflection amplitude is changed by a phase factor. This is true for any smooth, real potential: I find this amazing! Note also that if all the amplitudes are real $\rho = -r$.

6.5) We will use the WKB formula without paying attention to the prefactor:

$$T \sim e^{-2\int_{x_1}^{x_2} dx \sqrt{2m(V(x)-E)}/\hbar}$$

In our case the turning points are given by

$$V_0 \frac{a^2 - x_t^2}{a^2} = E \quad \Rightarrow \quad x_t = \pm\, a \sqrt{\frac{V_0 - E}{V_0}}\,.$$

We simplify the integrand by substituting for E from the above expression (this is a useful trick):

$$V(x) - E = V_0 \frac{a^2 - x^2}{a^2} - V_0 \frac{a^2 - x_t^2}{a^2} = \frac{V_0}{a^2}\,(x_t^2 - x^2)\,.$$

The integral to be performed is

$$\int_{-x_t}^{x_t} dx \sqrt{\frac{2mV_0}{\hbar^2}}\,\frac{1}{a}\sqrt{x_t^2 - x^2} = \sqrt{\frac{2mV_0}{\hbar^2}}\,\frac{1}{a}\int_{-x_t}^{x_t} dx\,\sqrt{x_t^2 - x^2}$$

The integral is easy to do with or without Mathematica and we have

$$\int_{-x_t}^{x_t} dx\,\sqrt{x_t^2 - x^2} = \pi \frac{x_t^2}{2}\,.$$

Assembling all the terms together we obtain

$$e^{-\pi\, a \sqrt{\frac{2mV_0}{\hbar^2}\,\frac{V_0 - E}{V_0}}}\,.$$

For comparison with the square barrier result we can rewrite this as

$$e^{-\left[4\,a\sqrt{\frac{2m(V_0-E)}{\hbar^2}}\right] \times \left[\frac{\pi}{4}\sqrt{\frac{V_0-E}{V_0}}\right]}\,.$$

Let us evaluate the extra factor at $E = 3V_0/4$ for tunneling at a quarter of the barrier height below the maximum. We find $\pi/8 \approx 0.4$. Thus if the tunneling probability for the rectangular barrier is 10^{-10} for the circular barrier the number is 10^{-4}, considerably smaller.