PHYS851 Quantum Mechanics I, Fall 2009
HOMEWORK ASSIGNMENT 7

1. **The continuity equation:** The probability that a particle of mass m lies on the interval $[a, b]$ at time t is

$$P(t|a,b) = \int_a^b dx\, |\psi(x,t)|^2 \tag{1}$$

Differentiate (1) and use the definition of the probability current, $j = -\frac{i\hbar}{2m}\left(\psi^* \frac{d}{dx}\psi - \psi \frac{d}{dx}\psi^*\right)$, to show that

$$\frac{d}{dt}P(t|a,b) = j(a,t) - j(b,t). \tag{2}$$

Next, take the limit as $b - a \to 0$ of both (1) and (2), and combine the results to derive the continuity equation: $\frac{d}{dx}j(x,t) = -\frac{d}{dt}\rho(x,t)$.

We start by differentiating Eq. (1),

$$\frac{d}{dt}P(t|a,b) = \int_a^b dx\, \left(\psi^*(x,t)\frac{d}{dt}\psi(x,t) + \psi(x,t)\frac{d}{dt}\psi^*(x,t)\right) \tag{3}$$

with $\frac{d}{dt}\psi(x,t) = i\frac{\hbar}{2M}\frac{d^2}{dx^2}\psi(x,t) - \frac{V(x)}{\hbar}\psi(x,t)$ this gives

$$\frac{d}{dt}P(t|a,b) = \frac{i\hbar}{2M}\int_z^b dx\, \left(\psi^*(x,t)\frac{d^2}{dx^2}\psi(x,t) - \psi(x,t)\frac{d^2}{dx^2}\psi^*(x,t)\right) \tag{4}$$

Integrating by parts gives

$$\begin{aligned}
\frac{d}{dt}P(t|a,b) &= \frac{i\hbar}{2M}\Bigg[\psi^*(x,t)\frac{d}{dx}\psi(x,t)\Big|_a^b - \int_a^b dx\,\frac{d}{dx}\psi^*(x,t)\frac{d}{dx}\psi(x,t) \\
&\quad - \psi(x,t)\frac{d}{dx}\psi^*(x,t)\Big|_a^b + \int_a^b dx\,\frac{d}{dx}\psi^*(x,t)\frac{d}{dx}\psi(x,t)\Bigg] \\
&= \frac{i\hbar}{2M}\left(\psi^*(x,t)\frac{d}{dx}\psi(x,t) - \psi(x,t)\frac{d}{dx}\psi^*(x,t)\right)\Bigg|_a^b \\
&= j(a,t) - j(b,t)
\end{aligned} \tag{5}$$

Taking the limit as $b - a \to 0$, we can then write the integral (area) as simply the height times the width:

$$\lim_{b-a\to 0} P(t|a,b) = |\psi(x,t)|^2(b-a) = \rho(x,t)(b-a) \tag{6}$$

where x is taken to be the point onto which a and b converge. This gives

$$\frac{d}{dt}\rho(x,t)(b-a) = j(a,t) - j(b,t). \tag{7}$$

dividing both sides by $b - a$ gives

$$\frac{d}{dt}\rho(x,t) = -\lim_{b-a\to 0}\frac{j(b,t) - j(a,t)}{b-a} = -\frac{d}{dx}j(x,t) \tag{8}$$

2. **Bound-states of a delta-well:** The inverted delta-potential is given by

$$V(x) = -g\,\delta(x), \tag{9}$$

where $g > 0$. For a particle of mass m, this potential supports a single bound-state for $E = E_b < 0$.

   (a) Based on dimensional analysis, estimate the energy, E_b, using the only available parameters, $\hbar$, m, and g.

   The only energy scale we can form from g, $\hbar$ and M is $E = \frac{mg^2}{\hbar^2} = \frac{\hbar^2}{Ma^2}$, where $a = \frac{\hbar^2}{mg}$ is the 'scattering length'. Thus we should expect the answer to be

$$E_b \sim -\frac{\hbar^2}{Ma^2} \tag{10}$$

   (b) Assume a solution of the form:

$$\psi_b(x) = c\,e^{-\frac{|x|}{\lambda}}, \tag{11}$$

   and use the delta-function boundary conditions at $x = 0$ to determine λ, as well as the the energy, E_b. You can then use normalization to determine c. What is $\langle X^2\rangle$ for this bound-state?

Calling $x < 0$ region 1, and $x > 0$ region 2, we have

$$\begin{aligned} \psi_1(x) &= ce^{\frac{x}{\lambda}} & (12)\\ \psi_2(x) &= ce^{-\frac{x}{\lambda}} & (13) \end{aligned}$$

The first boundary condition is

$$\psi_2(0) = \psi_1(0), \tag{14}$$

which is satisfied by construction. Integrating the energy eigenvalue equation from $x = -\epsilon$ to $x = \epsilon$ gives

$$\begin{aligned} \int_{-\epsilon}^{\epsilon} dx E\psi(x) &= -\frac{\hbar^2}{2M}\int_{-\epsilon}^{\epsilon} dx\,\frac{d^2}{dx^2}\psi(x) - \int_{-\epsilon}^{\epsilon} dx\, g\,\delta(x)\psi(x)\\ 2\epsilon E\psi(0) &= -\frac{\hbar^2}{2M}\left(\psi_2'(0) - \psi_1'(0)\right) - g\psi(0) & (15) \end{aligned}$$

Taking the limit $\epsilon \to 0$ then gives

$$\psi_2'(0) = \psi_1'(0) - \frac{2}{a}\psi(0) \tag{16}$$

With (12) and (13) the boundary conditions give

$$-\frac{c}{\lambda} = \frac{c}{\lambda} - \frac{2}{a}c \tag{17}$$

The solution is $\lambda = a$. For $x \neq 0$, the energy is purely Kinetic, so we can use $E_b\psi(x) = -\frac{\hbar^2}{2Ma^2}dx^2\psi(x)$ to find

$$E_b = -\frac{\hbar^2}{2Ma^2} \tag{18}$$

which is consistent with our estimation.
For normalization, we need

$$\begin{aligned}\int_{-\infty}^{\infty} dx\,|\psi(x)|^2 &= 1 \\ |c|^2 2\int_0^{\infty} dx\, e^{-\frac{2x}{a}} &= 1 \\ |c|^2 a &= 1\end{aligned} \tag{19}$$

so that

$$c = \frac{1}{\sqrt{a}} \tag{20}$$

As $\langle X\rangle = 0$ by symmetry, the variance will be given by $\Delta x = \sqrt{\langle X^2\rangle}$, where

$$\begin{aligned}\langle X^2\rangle &= \frac{1}{a}\int_0^{\infty} dx\, x^2 e^{-\frac{x}{a}} \\ &= a^2\int_0^{\infty} du\, u^2 e^{-u}\end{aligned} \tag{21}$$

We can solve this integral by integration by parts:

$$\begin{aligned}\langle X^2\rangle &= 2a^2\int_0^{\infty} ue^{-u} \\ &= 2a^2\int_0^{\infty} e^{-u} \\ &= 2a^2\end{aligned} \tag{22}$$

which would lead to $\Delta x = \sqrt{2}a$.

3. **Inverted delta scattering:** Consider a particle of mass m, subject to the inverted delta-potential, $V(x) = -g\,\delta(x)$, with $g > 0$. Only this time, consider an incoming particle with energy $E > 0$. What are the transmission and reflection probabilities, T, and R?

   Treating this like any other scattering problem, we define region 1 as $x < 0$ and region 2 as $x > 0$, then we let

$$\psi_1(x) = e^{ikx} + re^{-ikx} \tag{23}$$
$$\psi_2(x) = te^{ikx} \tag{24}$$

   The first boundary condition is

$$\psi_1(0) = \psi_2(0) \tag{25}$$

   which gives

$$1 + r = t \tag{26}$$

   The second boundary condition is the same as that in the previous problem:

$$\psi_2'(0) = \psi_1'(0) - \frac{2}{a}\psi(0) \tag{27}$$

   which gives

$$ik(1 - r) = ikt - \frac{2}{a}(1 + r) \tag{28}$$

   with $t = 1 + r$, this becomes

$$1 - r = \left(1 + \frac{2i}{ka}\right)(1 + r) \tag{29}$$

   solving for r then gives

$$r = -\frac{1}{1 - ika} \tag{30}$$

   Taking $g \to \infty$ corresponds to $a \to 0^-$, which gives $r \to -1$, which makes sense. Taking $g \to 0^+$ gives $a \to -\infty$, which gives $r \to 0$. So the answer seems reasonable.
   The reflection probability is then

$$R = \frac{1}{1 + (ka)^2} \tag{31}$$

   so that

$$T = 1 - R = \frac{(ka)^2}{1 + (ka)^2} \tag{32}$$

   which is exactly the same as the non-inverted delta scatterer.

4. **Combination of delta and step:** Consider a particle of mass m, whose potential energy is

$$V(x) = V_0 u(x) + g\delta(x), \tag{33}$$

where $u(x)$ is the unit step function and $V_0 > 0$.

(a) What are the two boundary conditions at $x = 0$ that $\psi(x)$ must satisfy?

The first boundary condition is continuity of ψ,

$$\psi_2(0) = \psi_1(0) \tag{34}$$

To find the second boundary condition, we integrate the energy eigenvalue equation from $-\epsilon$ to ϵ and take the limit $\epsilon \to 0$, which gives

$$\psi_2'(0) = \psi_1'(0) + \frac{2}{a}\psi(0) \tag{35}$$

(b) For an incident wave of the form e^{ikx}, use the 'plug and chug' approach to find the reflection and transmission amplitudes, r and t.

With the ansatz

$$\begin{aligned} \psi_1(x) &= e^{ikx} + re^{-ikx} && (36) \\ \psi_2(x) &= te^{iKx} && (37) \end{aligned}$$

where $K = \sqrt{k^2 - k_0^2}$, with $k_0^2 = 2MV_0/\hbar$, so that $K < k$.
Putting these into the boundary condition equations gives:

$$\begin{aligned} 1 + r &= t \\ ik(1 - r) &= iKt + \frac{2}{a}(1 + r) && (38) \end{aligned}$$

putting $t = 1 + r$ then gives

$$1 - r = \left(\frac{K}{k} - \frac{2i}{ka}\right)(1 + r) \tag{39}$$

which gives

$$r = -\frac{2 - i(k - K)a}{2 + i(k + K)a} \tag{40}$$

and then with $t = 1 + r$ we find

$$t = \frac{2ika}{2 + i(k + K)a} \tag{41}$$

in the limit $K \to k$ we should recover the solution to the previous problem, which clearly does work.

(c) Compute the reflection probability, R, and the transmission probability, T. What is the relationship between T and $|t|^2$?

$$R = |r|^2 = \frac{4 + (k - K)^2 a^2}{4 + (k + K)^2 a^2} \tag{42}$$

and

$$T = |t|^2 \frac{K}{k} = \frac{4kKa^2}{4 + (k + K)^2 a^2} \tag{43}$$

(d) Lastly, compute the transfer matrix for this potential at the discontinuity point, $x = 0$.

To compute the transfer matrix, we start from

$$\psi_1(x) = Ae^{ikx} + Be^{-ikx} \tag{44}$$
$$\psi_2(x) = Ce^{iKx} + De^{-iKx} \tag{45}$$

putting this in the boundary conditions gives

$$A + B = C + D \tag{46}$$
$$ik(A - B) = iK(C - D) - \frac{2}{a}(C + D) \tag{47}$$

In matrix form, this gives

$$\begin{pmatrix} 1 & 1 \\ ik & -ik \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ -\frac{2}{a} + iK & -\frac{2}{a} - iK \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix} \tag{48}$$

Solving for $(C, D)^T$ gives

$$\begin{aligned} \begin{pmatrix} C \\ D \end{pmatrix} &= \begin{pmatrix} 1 & 1 \\ -\frac{2}{a} + iK & -\frac{2}{a} - iK \end{pmatrix}^{-1} \begin{pmatrix} 1 & 1 \\ ik & -ik \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} \\ &= \frac{i}{2K} \begin{pmatrix} -\frac{2}{a} - K & -1 \\ \frac{2}{a} - K & 1 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ ik & -ik \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} \\ &= \frac{1}{2Ka} \begin{pmatrix} -2i + (k + K)a & -2i + (K - k)a \\ 2i - (K - k)a & 2i + (k + K)a \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} \end{aligned} \tag{49}$$

so we find

$$M_{step+\delta}(Ka, ka) = \frac{1}{2Ka} \begin{pmatrix} -2i + (k + K)a & -2i + (K - k)a \\ 2i - (K - k)a & 2i + (k + K)a \end{pmatrix} \tag{50}$$

For the case $g \to 0$ we have $a \to \infty$, which does give $M_{step}(k, K)$.
For the case $K \to k$, we can see that we will recover $M_\delta(ka)$.

(e) Compare your answer to the matrices

$$M_{\delta,step} = M_{step}(K,k)M_\delta(ka), \tag{51}$$

and

$$M_{step,\delta} = M_\delta(Ka)M_{step}(K,k), \tag{52}$$

where $K = \sqrt{k^2 - \frac{2mV_0}{\hbar^2}}$ and $a = \hbar^2/(Mg)$. Comment on your result.

With

$$M_\delta(ka) = \begin{pmatrix} 1 - \frac{i}{ka} & -\frac{i}{ka} \\ \frac{i}{ka} & 1 + \frac{i}{ka} \end{pmatrix} \tag{53}$$

and

$$M_{step}(K,k) = \frac{1}{2K}\begin{pmatrix} K-k & K-k \\ K-k & K+k \end{pmatrix} \tag{54}$$

we find

$$M_{\delta,step} = M_{step,\delta} = M_{step+\delta} \tag{55}$$

This shows that putting the delta to the left of the step and taking the limit as the separation goes to zero, and putting the delta to the right of the step and taking the separation to zero, both give the same result as putting the delta and the step at the same point.

5. **Delta function Fabry Perot Resonator:** Consider transmission of particles of mass m through two delta-function barriers, described by the potential

$$V(x) = g\delta(x) + g\delta(x-L), \tag{56}$$

where $g > 0$ and $L > 0$.

(a) First, compute the allowed k-values for an infinite square well of length L, where $k = \sqrt{2mE}/\hbar$.

For an infinite square well, the allowed k-values are $k_n = n\pi/L$ where $n = 1, 2, 3, \ldots$.

(b) Next, use the transfer-matrix approach to compute the full transfer matrix of the resonator.

$$\begin{aligned} M &= M_\delta(ka)M_f(kL)M_\delta(ka) \\ &= \begin{pmatrix} \Delta^2 e^{-i\theta/2} - (\Delta+i)^2 e^{i\theta/2} & -2i\Delta\left((\cos(\theta/2) + \Delta\sin(\theta/2)\right) \\ 2i\Delta\left(\cos(\theta/2) + \Delta\sin(\theta/2)\right) & \Delta^2 e^{i\theta/2} - (\Delta-i)^2 e^{-i\theta/2} \end{pmatrix} \end{aligned} \tag{57}$$

(c) Use the full transfer-matrix to compute the transmission probability, T, in terms of the dimensionless parameters $\theta = 2kL$ and $\Delta = 1/ka$, where $a = \hbar^2/(mg)$.

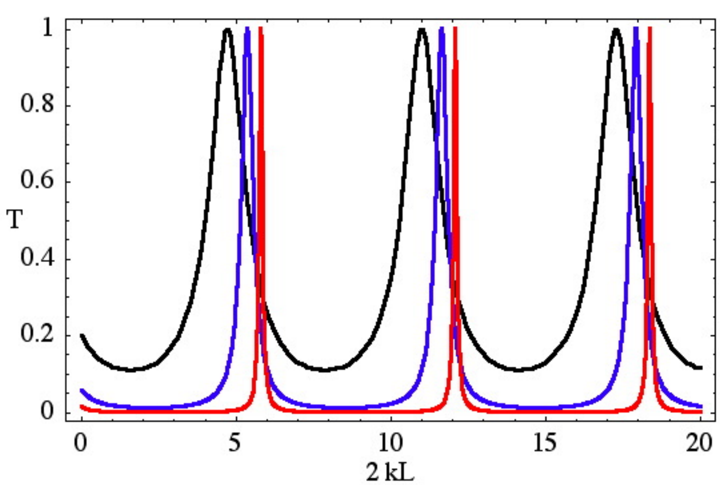
First we compute $R = |M_{21}/M_{22}|^2$, which gives

$$R = \frac{4\Delta^2\left(\cos(\theta/2) + \Delta\sin(\theta/2)\right)^2}{1 + 2\Delta^2(\Delta^2+1) - 2\Delta^2(\Delta^2-1)\cos\theta + 4\Delta^3\sin\theta} \tag{58}$$

$$T = 1 - R = \frac{1}{1 + 2\Delta^2(\Delta^2+1) - 2\Delta^2(\Delta^2-1)\cos\theta + 4\Delta^3\sin\theta} \tag{59}$$

(d) Make plots of T versus θ for $\Delta = 1$, $\Delta = 2$, and $\Delta = 4$. Compare the location of the transmission resonances on each plot to the locations of the allowed k-values from part (a).

Here is the plot of T versus $\theta = 2kL$. We see that as Δ increases, the resonances narrow, and approach the allowed k values from part (a).



6. Consider a particle of mass m incident on a square potential barrier of height $V_0 > 0$, and width W. Consider the case where the incident energy, E, is smaller than V_0.

   (a) Compute the probability to tunnel through the barrier, T, as function of the incident wave-vector, k.

   We can define the state just before the first step to be $(1, r)^T$, and the state just after the step to be $(A, B)^T$. Then just before the second step $(C, D)^T$, and just after the second step $(t, 0)^T$.
   The full transfer matrix for the step is then

$$\begin{aligned} M &= M_{step}(k, K) M_f(i\Gamma W) M_{step}(K, k) \\ &= \begin{pmatrix} \cosh(\gamma W) + i\frac{(k^2-\gamma^2)}{2k\gamma}\sinh(\gamma W) & -i\frac{(k^2+\gamma^2)}{2k\gamma}\sinh(\gamma W) \\ i\frac{(k^2+\gamma^2)}{2k\gamma}\sinh(\gamma W) & \cosh(\gamma W) - i\frac{(k^2-\gamma^2)}{2k\gamma}\sinh(\gamma W) \end{pmatrix} \end{aligned} \tag{60}$$

   We then find

$$T = |\det(M)/M_{2,2}|^2 = \frac{4k^2\gamma^2}{4k^2\gamma^2\cosh^2(\gamma W) + (k^2-\gamma^2)^2\sinh^2(\gamma W)} \tag{61}$$

   where $\gamma = \sqrt{2M(V_0 - E)}/\hbar$, and $k = \sqrt{2ME}/\hbar$

   (b) Write out the full form of the wavefunction of the particle in the tunneling region.

   To write the full form of the wavefunction, we first define $x = 0$ to be the location of the first step. Then we have

$$\psi_1(x) = e^{ikx} + re^{-ikx} \tag{62}$$
$$\psi_2(x) = Ae^{-\gamma x} + Be^{\gamma x} \tag{63}$$
$$\psi_3(x) = te^{ik(x-W)} \tag{64}$$

   where

$$r = \frac{(k^2+\gamma^2)\sinh(\gamma W)}{2ik\gamma\cosh(\gamma W) + (k^2-\gamma^2)\sinh(\gamma W)} \tag{65}$$

   to find t we use

$$t = \det(M)/M_{2,2} = \frac{2ik\gamma}{2ik\gamma\cosh(\gamma W) + (k^2-\gamma^2)\sinh(\gamma W)} \tag{66}$$

   to find A and B we use

$$\begin{pmatrix} A \\ B \end{pmatrix} = M_{step}(i\gamma, k)\begin{pmatrix} 1 \\ r \end{pmatrix} \tag{67}$$

   to find

$$A = \frac{e^{\gamma W}k(k+i\gamma)}{2ik\gamma\cosh(\gamma W) + (k^2-\gamma^2)\sinh(\gamma W)} \tag{68}$$

   and

$$B = -\frac{e^{-\gamma W}k(k-i\gamma)}{2ik\gamma\cosh(\gamma W) + (k^2-\gamma^2)\sinh(\gamma W)} \tag{69}$$

(c) Take limit as $W \to 0$ and $V_0 \to \infty$, while holding $V_0 W$ constant, and show that your answer agrees with the result for a delta-function potential, $V(x) = g\delta(x)$, with $g = V_0 W$.
For comparison with the delta function, we only need to look at the full transfer matrix. For $V_0 W = g$, we find that $\gamma W = \sqrt{2MV_0}\hbar W \to 0$. Expanding the cosh and sinh functions to leading order then gives

$$M = \begin{pmatrix} 1 - i\frac{\gamma^2 W}{2k} & -i\frac{\gamma^2 W}{2k} \\ i\frac{\gamma^2 W}{2k} & 1 + i\frac{\gamma^2 W}{2k} \end{pmatrix} \tag{70}$$

noting that

$$\frac{\gamma^2 W}{2k} = \frac{MV_0 W}{\hbar^2 k} = \frac{Mg}{\hbar^2 k} = \frac{1}{ka} \tag{71}$$

we have

$$M = \begin{pmatrix} 1 - \frac{i}{ka} & -\frac{i}{ka} \\ \frac{i}{ka} & 1 + \frac{i}{ka} \end{pmatrix} = M_\delta(ka) \tag{72}$$

which recovers the delta-function result.