PHYS-4601 Homework 6 Due 18 Oct 2012

This homework is due in the dropbox outside 2L26 by 11:59PM on the due date. If you wish to turn it in ahead of time, you may email a PDF or give a hardcopy to Dr. Frey.

1. **Proofs About Stationary States**

   (a) *Rephrasing Griffiths 2.1(b)* Consider the spatial part of a stationary state $\psi(\vec{x})$ (that is, $\Psi(\vec{x},t) = \psi(\vec{x})e^{-iEt/\hbar}$). Show that $\psi(\vec{x})$ can be chosen real as follows. Argue that, for any ψ that solves the time-independent Schrödinger equation, so does ψ^*. Use that to show that the real and imaginary parts of ψ are also solutions with the same energy. Finally, argue that normalizability of ψ implies normalizability of its real and imaginary parts.

   (b) *Griffiths 2.2 rephrased* Suppose that the energy E of a stationary state in one dimension is less than the minimum value of the potential. Use the time-independent Schrödinger equation to show that the second derivative of the wavefunction always has the same sign as the wavefunction. Then use that fact to argue qualitatively that such a wavefunction cannot be normalized, proving by contradiction that E must be greater than the minimum value of the potential.

2. **The Probability Current and the Transmission Coefficient**

   Consider a conserved quantity Q (this could be electric charge or total probability in quantum mechanics) with a density ρ and current $\vec{\jmath}$. These quantities satisfy the *continuity equation*

$$\frac{\partial \rho}{\partial t} = -\vec{\nabla}\cdot\vec{\jmath}\,. \tag{1}$$

   Remember that the divergence represents the lines of $\vec{\jmath}$ heading out through a surrounding surface (think of the divergence theorem and Gauss's law in electromagnetism). So this just says that that the change in the charge in a small volume is equal to the amount of charge flowing out through the surface surrounding the volume.

   (a) Consider the probability density $\rho = |\Psi(x,t)|^2$. Use the Schrödinger equation to show that the probability current

$$\vec{\jmath}(x,t) = \frac{i\hbar}{2m}\left(\Psi\vec{\nabla}\Psi^* - \Psi^*\vec{\nabla}\Psi\right) \tag{2}$$

   satisfies the continuity equation.

   Suppose that we have a potential barrier or well in 1D with incoming wave $\Psi_{in} = Ae^{ikx-i\omega t}$, reflected wave $\Psi_{ref} = Be^{-ikx-i\omega t}$, and transmitted wave $\Psi_{trans} = Ce^{ik'x-i\omega t}$. The total wavefunction to the left of the potential barrier/well is $\Psi_{in}+\Psi_{ref}$ and is just Ψ_{trans} to the right. Generally, if the potential is different on the different sides of the barrier/well, $k' \neq k$.

   (b) Show that the probability current to the left of the barrier is $\vec{\jmath}_{in}+\vec{\jmath}_{ref}$ (the currents of Ψ_{in}, Ψ_{ref} respectively).

   (c) Since the magnitude of the probability currents determine the probability carried off in the reflected and transmitted waves, we should define the reflection and transmission coefficients as

$$R = \left|\frac{\vec{\jmath}_{ref}}{\vec{\jmath}_{in}}\right|\ ,\quad T = \left|\frac{\vec{\jmath}_{trans}}{\vec{\jmath}_{in}}\right|\ . \tag{3}$$

   Find R and T in terms of the variables A, B, C, k, k'.

3. **Numerical Determination of Energy Eigenvalue** *some combination of Griffiths 2.54 and 2.51*

   Consider the potential

$$V(x) = -\frac{\hbar^2 a^2}{m}\text{sech}^2(ax) \ . \tag{4}$$

   Find the ground state energy using the numerical "wag the dog" method with Maple, as follows:

   (a) Show that the Schrödinger equation for a bound state can be written in terms of dimensionless variables as

$$\frac{d^2\psi}{d\xi^2}(\xi) + \left(2\,\text{sech}^2(\xi) - \kappa^2\right)\psi(\xi) = 0 \ , \tag{5}$$

   where κ is a positive constant.

   (b) The ground state should be an even function, so if we ignore normalization, we can choose initial conditions $\psi(0) = 1$, $\psi'(0) = 0$. Starting with $\kappa^2 = 0.99$, enter the Schrödinger equation and initial conditions into Maple and solve the ODE numerically over the range $\xi = 0 - 10$. Then plot the solution. You may find the following Maple code helpful (note that we rename variables for ease of typing):

```
with(plots):
schr := diff(u(x),x$2)+(2*sech(x)^2-0.99)*u(x) = 0
init1 := u(0) = 1
init2 := (D(u))(0) = 0
psi := dsolve({init1, init2, schr}, numeric, range = 0 .. 10)
psiplot := odeplot(psi)
display(psiplot)
```

   Attach a printout of your code with results.

   (c) What happens to the wavefunction as ξ gets large? By increasing your chosen value of κ^2 to 1.01, you should be able to get the "tail" of the wavefunction to flip over. Since the correct wavefunction should go to zero at large ξ, this means you have bracketed the correct eigenvalue for κ^2. Choose successively closer together values of κ^2 to find the eigenvalue down to three decimal places. What's the ground state energy?

   (d) This potential is exactly solvable, and the (unnormalized) ground state wavefunction is $\psi(x) = \text{sech}(ax)$. Plot both your numerical wavefunction and the exact one together on one plot and attach a hardcopy of your code and plot.

   (e) Now suppose we cut the potential in half to $V(x) = -(\hbar^2 a^2/2m)\text{sech}^2(ax)$. Using the same method, find the ground state energy. Numerically determined quantities should be good to three decimal places. Attach a plot of your unnormalized ground state wavefunction in the same dimensionless variables as above.