PHYS-4601 Homework 7 Due 1 Nov 2018

This homework is due in the dropbox outside 2L26 by 10:59PM on the due date. You may alternately email a PDF (typed or black-and-white scanned) or give a hardcopy to Dr. Frey.

1. **Numerical Determination of Energy Eigenvalue** *related to Griffiths 2.51*

   Consider the potential

   $$V(x) = -\frac{\hbar^2 a^2}{m}\frac{1}{\sqrt{1+a^2x^2}} \ . \tag{1}$$

   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

   $$\frac{d^2\psi}{d\xi^2}(\xi) + \left(\frac{2}{\sqrt{1+\xi^2}} - \kappa^2\right)\psi(\xi) = 0 \ , \tag{2}$$

   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 $\kappa^2 = 2.0$, 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/sqrt(1+x^2)-2.00)*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. You should find a wavefunction with no nodes that blows up at large ξ.

   (c) By decreasing your chosen value of κ^2 to 1.0, 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? Attach a plot of your approximate ground state wavefunction.

   (d) Now find the first excited state, which should have exactly one node at $x = 0$. In other words, take initial conditions $\psi(0) = 0$, $\psi'(0) = 1$ (ignoring normalization). Then for $x > 0$, $\psi(x) > 0$ (going to zero at $x \to \infty$). Use the procedure above starting with $\kappa^2 = 1$ to find the first excited state energy (to three decimal places) and attach a plot of the wavefunction.

2. **Scattering and the Probability Current**

   We define the probability current $\vec{\jmath}(\vec{x}, t)$ as

   $$\vec{\jmath}(x,t) = \frac{i\hbar}{2m}\left(\Psi\vec{\nabla}\Psi^* - \Psi^*\vec{\nabla}\Psi\right) \tag{3}$$

   (in 1D, replace the gradient with $\partial\Psi/\partial x$).

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

$$\frac{\partial \rho}{\partial t} = -\vec{\nabla} \cdot \vec{\jmath}\,. \tag{4}$$

(This means that the change in probability within a region is equal to the net flow of probability into that region.) Consider an infinite square well potential ($V(x) = 0$ for $-a < x < a$, $V(x) = \infty$ for $|x| > a$). At time $t = 0$, the system is in state $|\Psi(0)\rangle = (|1\rangle + |2\rangle)/\sqrt{2}$, where $|1\rangle$ is the ground state and $|2\rangle$ is the first excited state. Find the $\Psi(x,t)$, probability density $\rho(x,t)$, and probability current $j(x,t)$, and verify that they obey the continuity equation.

(b) To understand reflection and transmission coefficients when the potential takes different values on either side of the barrier, we should think about conservation of probability. Specifically, write the wavefunction as $Ae^{ikx} + Be^{-ikx}$ to the far left and $Ce^{ik'x}$ to the far right. Show first that the probability current on the far left splits into an incident part ($j_{inc} \propto |A|^2$) and a reflected part ($j_{ref} \propto |B|^2$) and evaluate j_{inc}, j_{ref}. Then find the transmitted probability current j_{trans}. Finally, find the reflection and transmission coefficients $R = j_{ref}/j_{inc}, T = j_{trans}/j_{inc}$ in terms of A, B, C, k, k'.

(c) *from Griffiths 2.35* Consider a particle moving in a 1D potential

$$V(x) = \begin{cases} 0 & x < 0 \\ -V_0 & x \geq 0 \end{cases}\,. \tag{5}$$

Determine the reflection and transmission coefficients for a particle incoming from the left (negative x) with energy $E = V_0/3$. Use $R = j_{ref}/j_{inc}, T = j_{trans}/j_{inc}$ and verify that $R + T = 1$.

3. **Odd States of the Finite Square Well** *extended from Griffiths 2.29*

Consider the finite square well potential

$$V(x) = \begin{cases} 0 & \text{for } x < -a \\ -V_0 & \text{for } -a < x < a \\ 0 & \text{for } a < x \end{cases}\,, \tag{6}$$

as in class.

(a) Find the transcendental equation that determines the energy eigenvalues for bound states with *odd* wavefunctions. For a given V_0 and a, how many odd bound states are there?

(b) Mathematical software can find numerical values of the energy eigenstates even when a closed-form solution does not exist. To do so, first write your transcendental equation from part (a) in terms of dimensionless variables $z = \sqrt{2m(V_0 + E)}(a/\hbar)$ and $z_0 = \sqrt{2mV_0}(a/\hbar)$ in the form $f(z, z_0) = 0$. Then the Maple command `fsolve(f(z,3*Pi/4)=0,z=Pi/2)` finds the bound state energy for $V_0 = \hbar^2(3\pi/4)^2/2ma^2$ starting from an initial guess of $z = \pi/2$ for the solution. Find the energy in this case as a multiple of $\hbar^2/2ma^2$. Then find the 3 bound state energies for $V_0 = \hbar^2(11\pi/4)^2/2ma^2$ (you will want the three initial guesses $\pi/2, 3\pi/2, 5\pi/2$ for z). Attach a printout of your Maple worksheet. Give your answers to three decimal places.