Physics 5730/7730, Spring 2022 Homework #6

Due Monday April $25^{th}$

1. Solve the 1D time-dependent Schrödinger equation for a Gaussian pulse impacting a potential barrier. Use units in which $\hbar = 1$ and $m = 1$. The barrier should be a top-hat function centered at $x = 0$ and have a width of 1.0 (length units), and a height of 1,000 (energy units).

   The starting wave function is

   $$\psi_0 = \psi(t=0,x) = Ce^{-(x-x_0)^2/2\sigma^2}e^{ik(x-x_0)}$$

   where $x_0 = -3$; $k = 50$; $\sigma = 0.25$; and $C$ is a normalization constant for you to determine. It would be good for your program to output

   $$\text{integrated probability} = \int_{-\infty}^{+\infty} \psi_0^* \, \psi_0 \, dx$$

   to confirm that the total probability is unity.

   Your program should output a video of duration 0.2 (time units), showing the evolution of the wavefunction for $-5 < x < 5$ (length units). $\Delta x = \Delta t = 0.001$ should be an adequate grid spacing.

   Note that the boundary conditions are your choice, *e.g.* periodic, reflecting, or just ignore boundary effects (by making the domain big enough that edge effects don't appear in your animation).

   Submit your code **hw06a.py** along with an animation, **schro1d.mp4**.

2. Consider the 1D Laplace equation in spherical symmetry

   $$\begin{aligned} \nabla^2 V(r) = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)V(r) &= 4\pi\rho(r) \\ V''(r) + \frac{2}{r}V'(r) &= 4\pi\rho(r) \end{aligned}$$

   Replace $V'(r)$ and $V''(r)$ with their second order finite difference approximations. Apply Neuman boundary conditions at the origin

   $$\begin{aligned} \partial_r V &= 0 \quad r \to 0 \\ V_{-1} &= V_0 \end{aligned}$$

   and Robin conditions at the outer edge

   $$\begin{aligned} \partial_r(rV) &= 0 \quad r \to r_N \\ r_{N+1}V_{N+1} &= r_N V_N \end{aligned}$$

   to arrive at a matrix equation for $V$ of the form

   $$\mathbf{M} \cdot V(r) = 4\pi(\Delta r)^2\rho(r)$$

   Use *e.g.* **SciPy**'s **linalg.solve** to find $V(0 < r < 10)$ for a density $\rho(r < 1) = 1$; $\rho(r > 1) = 0$ and compare graphically with the analytic solution. Confirm second order convergence for your calculation.

Submit both your Python scripts and Schrödinger animation by 11:59 PM on Monday, April 25:

**submit p5730 hw06 hw06a.py schro1d.mp4 hw06b.py**