Assignment 4 — PDEs: The Schrodinger Equation, again.

This assignment problem builds upon the code you developed in Workshop X to investigate quantum tunnelling. Consider the Schrodinger equation

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = \hat{H}\psi(x,t) \qquad\qquad \hat{H} = \hat{T} + \hat{V} = -\tfrac{\hbar^2}{2m}\tfrac{\partial^2}{\partial x^2} + V(x) \tag{1}$$

for a particle in a double well potential

$$V(x) = -V_0\left\{\exp\left[-\frac{(x-a)^2}{\sigma^2}\right] + \exp\left[-\frac{(x+a)^2}{\sigma^2}\right]\right\}. \tag{2}$$

....

† **Questions are *optional*:** † = [**+1 bonus mark**]
+1 bonus mark for: code formatting / program structure
+1 bonus mark for: clear and concise answers / report layout / figure quality.

Part A

1. [**4 marks**] Defining appropriate parameters for length x_0, and time t_0, show the equation of motion takes the form

$$i\partial_t\psi = \left[-\tfrac{1}{2}\partial_x^2 - V_0\left(e^{-(x-a)^2} + e^{-(x+a)^2}\right)\right]\psi, \tag{3}$$

where all quantities are now dimensionless. Give an alternative example that would be suitable for the potential Eq. (2) (there are several), and briefly explain how the form would change.

2. [**4 marks**] Use imaginary time evolution, $t \to it$, to calculate the groundstate of the potential numerically, and plot $|\psi(x)|^2$ and $V(x)$ on the same graph. Do this for

   a) $a = 2$, $V_0 = 1.5$

   b) $a = 2$, $V_0 = 1.5$, but when only the left well is active.

3. [**4 marks**] The split operator method you applied in the workshop can be improved by a simple modification of splitting one of the operators*:

$$\exp\left[-i(\hat{T}+\hat{V})\delta t\right] \approx \exp\left[-i\hat{V}\delta t/2\right]\exp\left[-i\hat{T}\delta t\right]\exp\left[-i\hat{V}\delta t/2\right] + \mathcal{O}(\delta t)^3. \tag{4}$$

   a) In our implementation, why is it more computationally efficient to split $\hat{V}$ instead of $\hat{T}$? Could the program have been constructed in a way that it would be better to do the opposite?

   b) Can you see a way Eq. (4) could be further optimized for computational speed? Explain. [Hint: consider two successive time steps applied to the wavefunction]

*This can be shown from the Baker-Cambell-Hausdorf formula: for any two non-commuting operators X and Y the product of their exponentials is $e^{X\delta t}e^{Y\delta t} = e^{(X+Y)\delta t + [X,Y]\delta t^2/2 + \dots}$.

Part B

4. **[8 marks]** Suppose initially only the left well is active and a particle sits in the groundstate of the well at $x = -a$, with $a \geq 1$. The right well is then instantly turned on at $t = 0$.

a) Upgrade the algorithm to use Eq. (4).

†b) Implement the optimization in you identified in Q3. b) above.

c) Simulate the dynamics of this system, and plot the probability of finding the particle in the left well vs. time

$$P_L(t) = \int_{x<0} dx\, |\psi(x,t)|^2, \tag{5}$$

for a few combinations of a and V_0. Comment.

d) Compare how well Eq. (4) conserves energy $\langle \hat{H} \rangle$ against the ordinary split operator method for a few values of Δt. Tabulate or plot the result.

††e) Use $P_L(t)$ to calculate the tunnelling frequency vs. a (for fixed V_0).

f) Investigate the same tunneling scenario for the *nonlinear* schrodinger equation*

$$i\partial_t \psi = [-\tfrac{1}{2}\partial_x^2 + U(x)]\psi, \qquad\qquad U(x) = V(x) + g|\psi(x,t)|^2. \tag{6}$$

Explore the effect of nonlinear interactions on the tunnelling for $V_0 = 1.5$, $a = 2$, and $0 \leq g \leq 1$, and report your findings.

*This equation describes (under certain assumptions) a gas of interacting atoms collectively described by the wavefunction $\psi(x,t)$; the particle interaction strength g depends on the type of atom and the number of particles, and the effective potential $U(x)$ depends on the density of particles through $|\psi(x,t)|^2$.