# 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

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

for a particle in a double well potential

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

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† Questions are optional — [**1 bonus mark**]

## Part A

1. [**5 marks**] Choosing the well width $\sigma$ as a reference unit, define appropriate dimensionless parameters for length $x_0$, time $t_0$, and energy $E_0$, and express the equation in dimensionless a form. Give an alternative example that would be suitable for this potential (there are several).

2. [**5 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 axes. Do this for

   a) $\tilde{a} = 2$, $\tilde{V}_0 = 1$

   b) $\tilde{a} = 2$, $\tilde{V}_0 = 1$, but when only the left well is active.

   † c) For case b), show the potential can be approximated as $V(x) \approx -V_0 + \frac{1}{2}m\omega^2(x+a)^2$, with $\omega = \omega(V_0)$. Compare graphically $|\psi(x)|^2$ for the exact groundstate and the harmonic approximation.

3. [**5 marks**] The split operator method you applied in the workshop can be improved by a simple modification of splitting one of the operators*:

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

   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. (3) could be further optimized for computational speed? Explain. [Hint: consider two successive time steps applied to the wavefunction]

   c) Compare how this method conserves energy $\langle\hat{H}\rangle$ against the ordinary split operator method for a few values of $\Delta t$. Tabulate or plot the result.

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*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. **[5 marks]** Suppose initially only the left well is active and a particle sits in the groundstate of the single well. The right well is then instantly turned on at $t = 0$ at some distance $a$.

a) Simulate the dynamics, and plot the probability of finding the particle in the left well

$$P_L(t) = \int_{x<0} dx \, |\psi(x,t)|^2. \tag{4}$$

b) You should find in a) the particle will oscillate between the two sites. Use $P_L(t)$ to calculate the tunnelling frequency vs. $\tilde{a}$.

c) If many particles are in the trap, their interactions (under certain assumptions) can be included through an effective *nonlinear* potential that depends on the local "density" of the particles:

$$U(x) = V(x) + g|\psi(x,t)|^2, \tag{5}$$

with the interaction strength $g$ proportional to the number of particles. Explore the effect of nonlinear interactions on the tunnelling for $a = 2$, and $0 \leq g \leq 2$, and report your findings.