

Phys Enph 479/879 Assignment #4: Time-Dependent Schrodinger Equation using the Space Discretized Leapfrog Technique

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This assignment discuss the Time Dependent Schrodinger equation and the effects of potential barriers on the wavepackets. The leapfrog integration method will be used with space discretization to simulate time-steps of the Schrodinger equation, simple animation will be used to visualise the behaviour of the particle within the system.

I. INTRODUCTION

A. Time Dependent Schrodinger Equation

Following the wave like properties exerted by particles at the beginning of the twentieth century. Edwin Schrodinger devised a mathematical equation describing the wave function or behaviour of particles systems, of which the eigenvalues of this equation were shown to correspond to the energy levels of the quantum mechanical system. This linear partial differential equation became known as the Schrodinger equation. We can numerically solve the Schrodinger equation using a space discretization leapfrog technique to describe the motion of a wave within a potential in one dimension.

II. THEORY AND EQUATIONS

A. Time Dependent Schrodinger Equation

The Time-Dependent Schrodinger Equation (TDSE) in one dimension in atomic units (a.u.), can be formulated as follows:

$$-\frac{1}{2} \frac{\partial^2 \psi(x, t)}{\partial x^2} + V(x, t)\psi(x, t) = i \frac{\partial \psi(x, t)}{\partial t}, \quad (1)$$

This can be broken up into a grid system, with the following space discretization conditions:

$$x_j = jh, \quad (2)$$

$$j = 0, 1, \dots, N, \quad (3)$$

$$\psi_j(t) = \psi(jh, t), \quad (4)$$

$$V_j(t) = V(jh, t), \psi_j(t) = R_j(t) + iI_j(t). \quad (5)$$

Where R and I represent the real and imaginary parts of the wave function. The full equations of motion for the real and imaginary parts of the wave function then become:

$$\frac{dR_j}{dt} = -\frac{1}{2h^2} I_{j-1} + \left(\frac{1}{h^2} + V_j\right) I_j - \frac{1}{2h^2} I_{j+1}, \quad (6)$$

$$\frac{dI_j}{dt} = \frac{1}{2h^2} R_{j-1} - \left(\frac{1}{h^2} + V_j\right) R_j + \frac{1}{2h^2} R_{j+1}. \quad (7)$$

B. Matrix Formulation

We can transform these equations into a more compact form using matrix algebra:

$$\mathbf{R} = \begin{bmatrix} R_0 \\ R_1 \\ \vdots \\ R_N \end{bmatrix}, \mathbf{I} = \begin{bmatrix} I_0 \\ I_1 \\ \vdots \\ I_N \end{bmatrix} \quad (8)$$

$$A = \begin{bmatrix} a_0 & b & & & \\ b & a_1 & b & & \\ & \ddots & \ddots & \ddots & \\ & & b & a_N & \end{bmatrix} \quad (9)$$

Where:

$$a_j = \frac{1}{h^2} + V_j, b = -\frac{1}{2h^2}.$$

This yeilds the following set equations of motion for the Time Dependent Schrodinger Equation in matrix form:

$$\frac{d\mathbf{R}}{dt} = A\mathbf{I}, \frac{d\mathbf{I}}{dt} = -A\mathbf{R}. \quad (10)$$

C. Leapfrog Method

Leapfrog Integration is the method that will be used to solve the Time-Dependent Schrodinger Equation, for a classical harmonic oscillator the algorithm solves the form:

$$\frac{dv}{dt} = -a(x), \frac{dx}{dt} = v, \quad (11)$$

This is the same form as our set of equations II.B.

A variation of the velocity Verlet integration method, the Leapfrog technique is a symplectic integrator meaning that it will conserve the energy of the system by preserving the area in phase space. Leapfrog is the second order method compared to Euler, but is stable for oscillatory motion for

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a constant time step. The algorithm for Leapfrog, to second order accuracy, is as follows:

$$R_{1/2} = R_0 + I_0 \frac{\Delta t}{2}, \quad (12a)$$

$$I_1 = I_0 + A R_{1/2} \Delta t, \quad (12b)$$

$$R_1 = R_{1/2} + A I_1 \frac{\Delta t}{2}. \quad (12c)$$

Due to the symplectic nature of the integrator energy is conserved within the system, General energy conservation then becomes:

$$\frac{d(\mathbf{R}^T \mathbf{R} + \mathbf{I}^T \mathbf{I})}{dt} = 0 \quad (13)$$

III. IMPLEMENTATION

A. Space Discretized Leapfrog

The first approach is to implement the space discretized leapfrog (SDLF) method to solve the Schrodinger equation in one dimension. Here the derivatives are obtained using a slicing technique, which exploits the tridiagonal form of the matrix. We determine a space grid of 1000 points ranging from $-10 \rightarrow 10$ in atomic units with a spatial step size (h) of 0.02. The wavepacket will then be simulated for two periods of the oscillator ($T = 2 \times 2\pi$ if $\omega_0 = 1$). This generates a total of roughly 63,200 steps. The potential used is the classic harmonic oscillator:

$$V(x) = \frac{1}{2}x^2. \quad (14)$$

In order to simulate the wavepacket initial conditions must be set for time ($t = 0$), the following Gaussian is chosen:

$$\psi(x, 0) = (\sigma\sqrt{\pi})^{-1/2} \exp\left(-\frac{(x - x_0)^2}{2\sigma^2} + ik_0x\right), \quad (15)$$

With the following parameters and periodic boundary conditions:

$$x_0 = -5, \quad (16)$$

$$\sigma = 0.5, \quad (17)$$

$$k_0 = 0, \quad (18)$$

$$\psi_{N+1} = \psi_0, \quad (19)$$

$$\psi_{-1} = \psi_N. \quad (20)$$

Using a simple animator the time evolution of the wavepacket can be studied and snapshots can be taken to show the solution at certain positions. A contour plot can be used to show the probability distribution of the wavepacket across all time steps.

B. Sparse Matrix Solution

The second method used is using the matrix form, using a sparse matrix. A sparse matrix is a type of matrix

which most of its elements are zero, like our A matrix for the Schrodinger equations, defined 9. Sparse matrices use specialised algorithms and data structures that take advantage of the density of zero elements to improve efficiency compared to regular matrices. However, in general matrix algebra is a laborious and computationally expensive task and we expect this approach to have a more significant run time compared to the slicing technique. We can test our theory easily and compare it for varying spatial grids of either 1000 points or 2000.

C. Virial Theorem

The Leapfrog method is symplectic in nature and so we expect the energy of the system to be constant throughout the duration of the simulation. We can test this by using the Virial theorem which is described as follows:

$$2\langle T \rangle = n\langle V \rangle. \quad (21)$$

Where $n = 2$ for the potential described earlier Vx^n . Here the angled brackets represent the expectation values of the operators for Kinetic energy (T) and the Potential (V):

$$\langle V \rangle = \int_{-\infty}^{\infty} \psi^*(x, t) V \psi(x, t) dx \quad (22)$$

$$\langle T \rangle = \frac{\hbar^2}{2m} \int_{-\infty}^{\infty} \left| \frac{\partial \psi}{\partial x} \right|^2 dx \quad (23)$$

D. Double-Wall Potential

The next problem will be to solve the double-wall potential problem, this potential has the form:

$$V = ax^4 - bx^2, \quad (24)$$

Here the constants will initially be chosen to be $a = 1, b = 2$. The problem uses the same Gaussian initial condition as before only now, the parameters have changed to the following:

$$x_0 = -\sqrt{2}, \quad (25)$$

$$\sigma = 0.5, \quad (26)$$

$$k_0 = 0. \quad (27)$$

The wavepacket will be analysed over several time periods, with a simple animation to show the evolution of the system in real time with the potential function superimposed on top of it. The probability density contour map can be produced again over four nominal periods to show the wavepacket at different positions at various times. We can also superimpose the positional expectation value on to the contour map to make sense of the data.

IV. CONCLUSIONS

A. Single-Wall Potential

As can be seen by the snapshots of the animation (5), the wavepacket tunnels to each side of the quadratic poten-

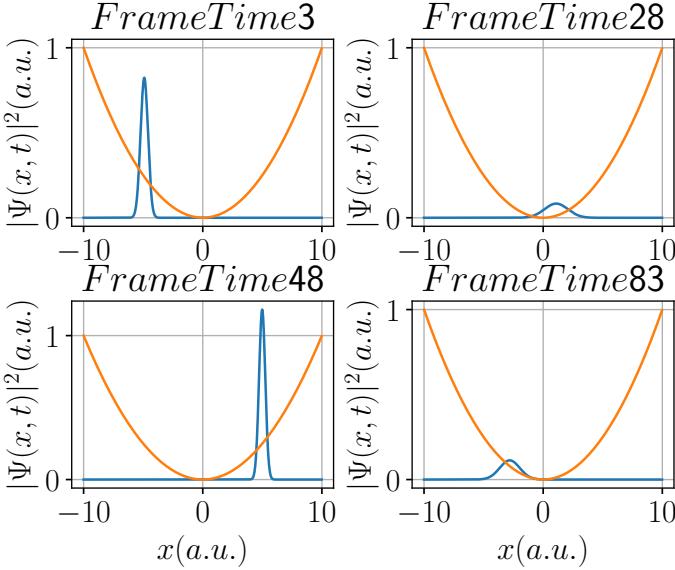


Figure 1. Slicing Technique animation snapshots at frames 3, 28, 48, 83

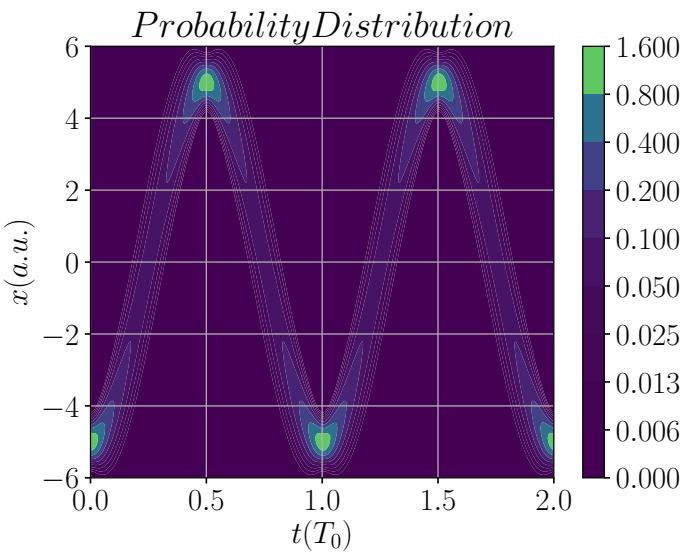


Figure 2. Probability density distribution for $V(x) = \frac{1}{2}x^2$.

tial, with its probability spreading out where the potential is at it's minimum. The probability distribution shows a heat-map of the most likely position of the particle as time progresses, it can clearly be seen that it follows a cyclic path over 2 time periods, with the most likely positions at either maximum limits.

B. Sparse Matrix Solver

Using the sparse matrix approach it was shown that it takes considerably more time to compute the solution, its also worth noting that its computationally expensive in terms of memory storage holding these huge matrices. Calculating the run times for 10 repetitions using for the first

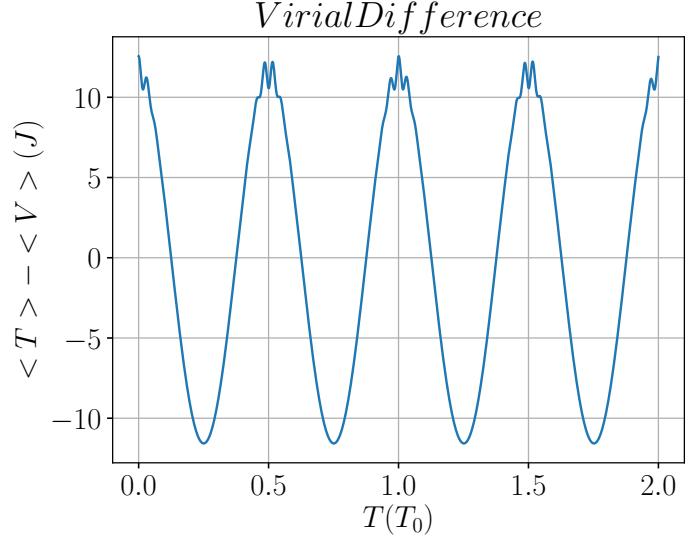


Figure 3. Difference between the expectation values for kinetic energy and potential energy.

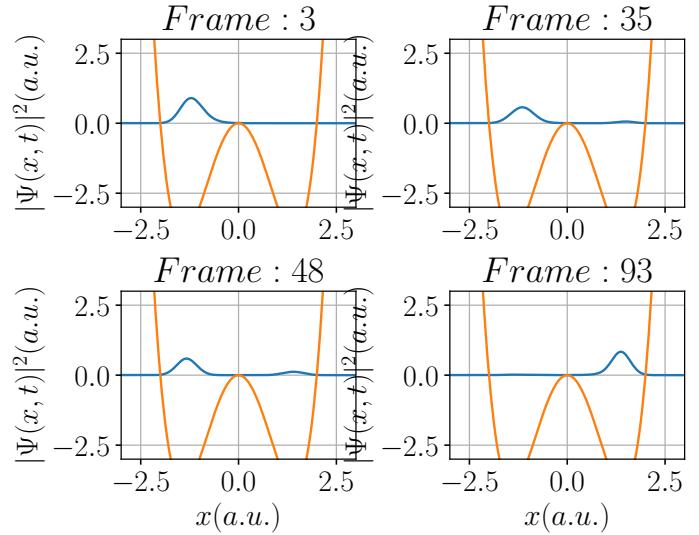


Figure 4. Snapshots at frames 3 , 35 ,48 ,93 for potential $V(x) = ax^4 - bx^2$, where $a = 1$ and $b = 4$.

set of initial conditions the sparse matrix approach took on average 140 seconds, compared to the slicing method which took 1.2 seconds this is much greater which shows that the slicing technique is the more viable option.

C. Virial

Graph 3 shows the differences between the expectation values for kinetic energy and potential energy, we say that Virial is satisfied when this value is equal to zero. It can be seen that this is the case at certain times but not always, the symplectic nature of the leapfrog method means that the energy of the system is conserved, I believe that this is the cause of the cyclic behaviour observed, oscillating around the point at which Virial's theorem is satisfied.

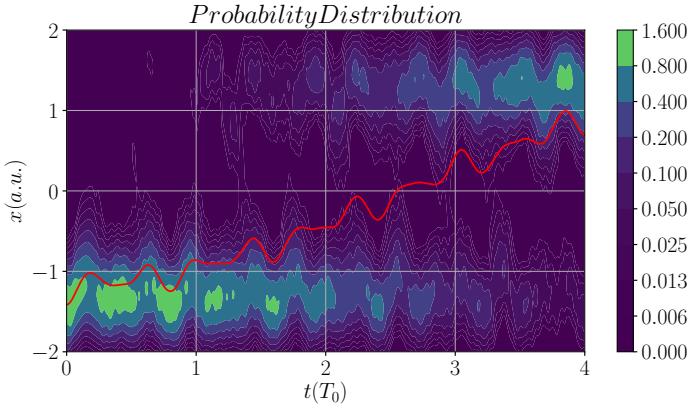


Figure 5. Probability distribution for potential $V(x) = ax^4 - bx^2$, where $a = 1$ and $b = 4$. Expectation value for the position has been superimposed.

D. Double-Wall Potential

For the potential of the form $V(x) = ax^4 - bx^2$ and initial condition described in equations 27, the wavepacket starts off in the left hand well or channel and as time pro-

gresses the probability declines here and increases in the right channel. This can be seen in the probability distribution as the expectation value for the position gradually shifts from one side to the other. Increasing the time shows that this behaviour is cyclic and the particle will alternate between each side of the well.

E. Parameter Tuning

Changing the potential parameters (a, b) has significant effects to the dynamics of the system. Increasing the potential barrier at a certain position decreases the probability of the particle occupying that space. Changing a alters the steepness of the potential, this causes the wavepacket to transition between each side of the well quicker since the area of low potential is narrowed giving the particle less space to fill. The particle's position also becomes more unpredictable with the probability density having multiple peaks at various positions. Tuning b causes the potential hole to become deeper and wider, this allows the particle more space to occupy and reduces the quantum tunnelling rate as the particle transitions into the opposite channel less frequently.