Quantum dynamics simulations with a Crank-Nicolson method

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Abstract

The Schrödinger equation is a partial differential equation that governs the time-evolution of the wavefunction for a given potential and is of fundamental importance in quantum mechanics. The (non-relativistic) Schrödinger equation is solved numerically in one and two dimensions with the Crank-Nicolson method for a variety of potentials. The potentials used were chosen to mimic certain physical situations or to compare the simulation with analytical solutions.

Introduction

The (non-relativistic) Schrödinger equation for the wave-function $\Psi(x,t)$ of a particle in a time-dependent scalar potential $V(x,t)$ reads

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + \hat{V}(x,t)\right]\Psi(t),$$

where $\hbar$ is the quantum of action divided by 2π, m the mass of the particle and $\Psi(x,t)$ the wave function. Rescaling the units such that $\hbar = 2m = 1$ gives

$$i\frac{\partial}{\partial t}\Psi(t) = \hat{H}\Psi(t), \tag{1}$$

where the Hamiltonian $\hat{H}$ is given by

$$\hat{H} = -\nabla^2 + \hat{V} = \hat{T} + \hat{V}.$$

By solving equation 1 the time evolution of a system can be determined.

Crank-Nicolson method

We solve this partial differential equation numerically by using the Crank-Nicolson method (CNM). CNM is a finite difference method that is implicit in time and numerically stable [1].

The time derivative on the left hand side of equation 1 is approximated with a forward difference divided by the time step τ:

$$\frac{\partial}{\partial t}\Psi = \frac{\Delta_\tau[\Psi](t)}{\tau} + \mathcal{O}(\tau) = \frac{\Psi(t+\tau) - \Psi(t)}{\tau} + \mathcal{O}(\tau).$$

Equation 1 then becomes:

$$\Psi(t+\tau) - \Psi(t) = -i\tau\hat{H}\Psi(t).$$

Approximating the $\Psi(t)$ on the right hand side with $(\Psi(t+\tau) + \Psi(t))/2$, this equation can be rewritten as:

$$\left(\mathbb{1} + \frac{i\tau}{2}\hat{H}\right)\Psi(t+\tau) = \left(\mathbb{1} - \frac{i\tau}{2}\hat{H}\right)\Psi(t). \tag{2}$$

This is a system of linear equations of the form $\mathbf{Ax} = \mathbf{b}$. The wave function can be evaluated by solving this for $\mathbf{x}$.

When equation 2 is rewritten as:

$$\Psi(t+\tau) = \frac{\mathbb{1} - \frac{i\tau}{2}\hat{H}}{\mathbb{1} + \frac{i\tau}{2}\hat{H}}\Psi(t) \tag{3}$$

we note the close correspondence between the series expansion of this operator and the series expansion of the time evolution operator (when $\hat{H}$ is time-independent and up to second order in τ):

$$e^{-i\tau\hat{H}} = 1 - i\tau\hat{H} - \frac{\tau^2}{2}\hat{H}^2 + \frac{i\tau^3}{6}\hat{H}^3 + \mathcal{O}(\tau^4)$$
$$\frac{\mathbb{1} - \frac{i\tau}{2}\hat{H}}{\mathbb{1} + \frac{i\tau}{2}\hat{H}} = 1 - i\tau\hat{H} - \frac{\tau^2}{2}\hat{H}^2 + \frac{i\tau^3}{4}\hat{H}^3 + \mathcal{O}(\tau^4).$$

The operator in equation 3 is unitary as can be easily checked, which implies that the norm is preserved.

System of linear equations

In one dimension, the kinetic energy $\hat{T} = -\frac{\partial^2}{\partial x^2}$ is approximated with a central difference divided by a spatial step a:

$$\frac{\partial^2}{\partial x^2} \simeq \frac{\delta_a^2[\Psi](x)}{a^2} = \frac{\Psi(x+a) - 2\Psi(x) + \Psi(x-a)}{a^2}.$$

For $\hat{V} = 0$, the Hamiltonian matrix in the linear system shown in equation 2 then becomes an N by N tridiagonal matrix:

$$\hat{H} = \begin{pmatrix} 2 & -1 & \cdots & 0 \\ -1 & 2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & -1 \\ 0 & \cdots & -1 & 2 \end{pmatrix},$$

where N is the number of finite elements in one dimension. The $\Psi(x,t)$ vector lists all the finite elements of the wave function

$$\Psi(x,t) = \begin{pmatrix} \Psi(x_1,t) \\ \Psi(x_2,t) \\ \vdots \\ \Psi(x_N,t) \end{pmatrix}.$$

To add a potential to the system, the amplitudes of the potential are added to the corresponding diagonal elements of the Hamiltonian matrix. We solve this sparse linear system by using the iterative Biconjugate gradient stabilized method [1].

In the two dimensional case, the elements of the Ψ are also stored in a vector. This is done "row by row", where a row contains all the x-direction elements of one step the y-direction:

$$\Psi(x,y,t) = \begin{pmatrix} \Psi(x_1,y_1,t) \\ \Psi(x_2,y_1,t) \\ \vdots \\ \Psi(x_1,y_2,t) \\ \vdots \\ \Psi(x_N,y_N,t) \end{pmatrix}.$$

In this vector not all neighbouring vector elements are neighbouring elements in the domain. For example, the elements x_N, y_1 and x_1, y_2 are neighbours in the vector but not in the spatial domain. To take this into account, the Kronecker product between the N^2 by N^2 identity matrix and the old Hamiltonian is determined. For a $N = 2$ domain with $V = 0$ this becomes:

$$\hat{H} = \mathbb{1} \otimes \hat{H}_{\text{old}} = \begin{pmatrix} 2 & -1 & 0 & 0 \\ -1 & 2 & 0 & 0 \\ 0 & 0 & 2 & -1 \\ 0 & 0 & -1 & 2 \end{pmatrix},$$

There is also an additional spatial derivative in the y-direction. To incorporate this into the linear system, 2 is added to the diagonal elements of $\hat{H}$ and -1 is added to the N^{th} lower and upper diagonals. Note that using this method we are limited to square domains.

Results and discussion

We verified the simulation results by comparing them with physical or mathematical results known for certain potentials. The potentials analyzed are the infinite square well, barrier potential and harmonic oscillator potential. The infinite square well finds it physical realisation in studying the behaviour of electrons confined in a metal. The barrier potential can be used as a model for understanding quantum tunneling effects. The harmonic oscillator is an ubiquitous form for the potential, finding its use mostly in approximating complex potentials near their local minima. In two dimensions a double slit potential is used to simulate the quantum-mechanical effect of interference.

Stability of the infinite square well eigenstates

The eigenstates of the Hamiltonian have the property that they are, up to an unphysical global phase factor, invariant under time-translations. To check the stability and accuracy of the simulation, eigenstates of the Hamiltonian for the infinite square well are simulated in two dimensions. The deviation of the wave function with its initial state is then a measure for the accuracy and stability of the simulation. It might seem intuitive to define the deviation as the distance function that is naturally induced by the inner product on the Hilbert space. However, the projective nature of the Hilbert

[1] We use the bicgstab function from the Python module Scipy.

space in quantum mechanics should be taken into account, so that a more useful approach for the deviation D would be to define it as

$$D(t) = \int \mathrm{d}x \left(|\Psi(x,t)|^2 - |\Psi(x,0)|^2 \right)^2,$$

where the integral is over all space.

In figures 1, 2, 3 the eigenstate $\Psi(x,y,0) = \sin\left(\frac{3\pi x}{L}\right) \sin\left(\frac{2\pi y}{L}\right)$ is used as initial wavefunction for simulations with 500 time steps and $\tau = 1$ for $a = 1.0, 0.5$ and 0.2 respectively. It is noted that lowering the value of τ does not affect the deviation, since the system is close to equilibrium. The value of τ only starts to play a role when there are rapid changes in the wavefunction.

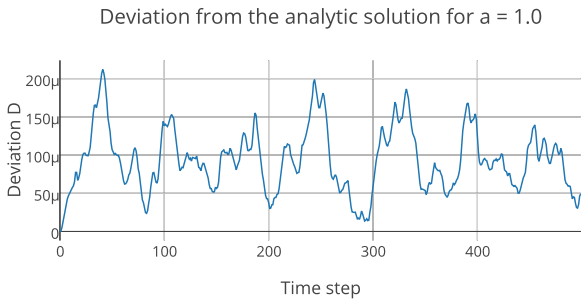

Figure 1: *Deviation for each timestep for* $a = 1.0$

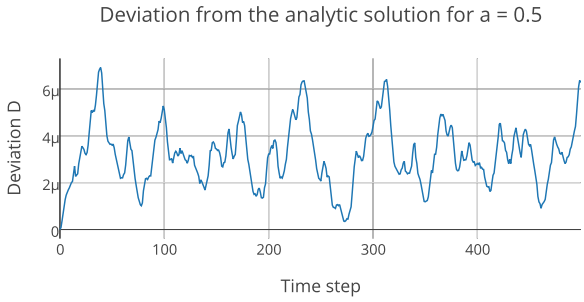

Figure 2: *Deviation for each timestep for* $a = 0.5$

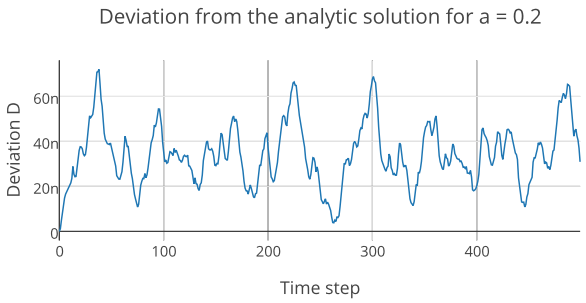

Figure 3: *Deviation for each timestep for* $a = 0.2$

The deviations are clearly dependent on the value chosen for a, but the running time is expected to be around $\mathcal{O}(a^2)$, so that a proper value of a should be chosen depending on the desired accuracy and running time of the simulation. The deviations occur primarily due to the fact that the analytic eigenstates of the Hamiltonian are not eigenstates of the discretized Hamiltonian[2]. The oscillations seen independent of a indicate that the analytic eigenstate and the eigenstate of the discretized Hamiltonian are relatively close with respect to the natural metric.

Unitarity of the simulation

Though the operator used in the CNM method is in theory unitary, finite precision in the storage of variables will cause the probability to be not conserved. For the following simulations the eigenstate from the previous section is simulated for 500 time steps with $\tau = 1$ and $a = 1.0, 0.5$ and 0.2 respectively (figure 4, 5 and 6).

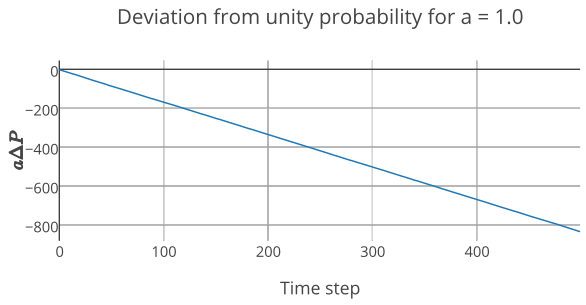

Figure 4: *Deviation from the norm for each timestep for* $a = 1.0$

[2]When the operator $(\mathbb{1} - \frac{i\tau}{2}\hat{H})/(\mathbb{1} + \frac{i\tau}{2}\hat{H})$ is explicitly calculated, it is possible to find approximate or exact eigenstates of the discretized Hamiltonian.

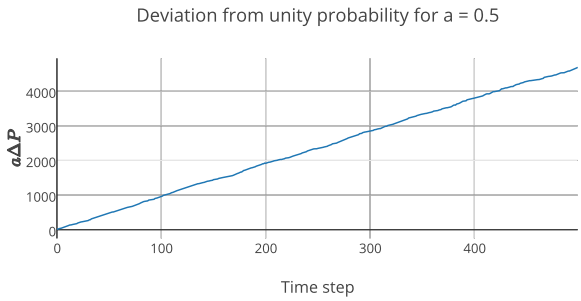

Figure 5: *Deviation from the norm for each timestep for* $a = 0.5$

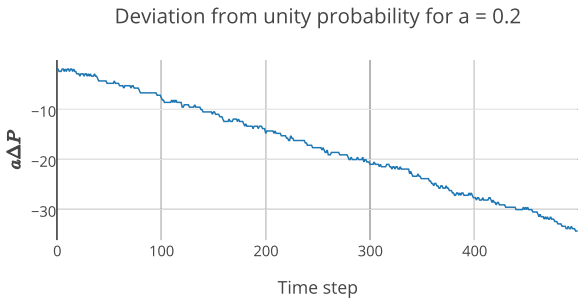

Figure 6: *Deviation from the norm for each timestep for* $a = 0.2$

The norm is seen to change linearly in time. It is clear that the total change is neglible, especially since the Schrödinger equation and the equations solved in CNM are linear. The sudden increase in the deviation for $a = 0.5$ in comparison to $a = 1.0$ and $a = 0.2$ could be attributed to the fact that the measure of how well a linear transformation conserves norm is not a simple function of its entries. If high precision in the absolute values of the probability is required, the wavefunctions can be renormalized after a certain amount of timesteps.

Transmission through a one-dimensional barrier potential

The simulated one-dimensional barrier potential has a value $V_0 > 0$ in the range $40 < x < 42.6$ and is zero elsewhere. Sending a Gaussian wave packet through the barrier can give rise to strictly quantum mechanical effects depending on the parameters of the wave packet and the barrier. In this case, the V_0 is changed while the rest of the parameters are kept constant. The transmission T can be calculated by integrating the probability distribution on one side of the barrier after a certain amount of tie steps.

Potential barrier in 1D

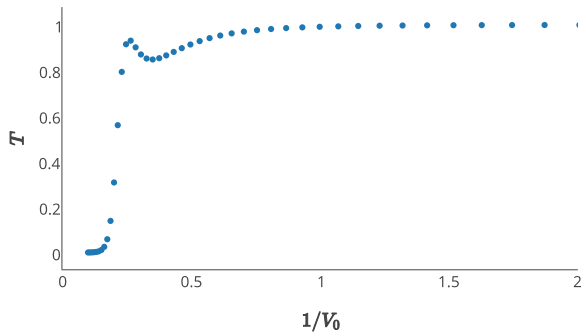

Figure 7: *Transmission through a potential barrier as a function of the barrier height.*

In figure 7 it can be seen that the particle tunnels partially through the barrier, even for high values of V_0. For low values of V_0 the transmission will be close to unity, as is expected. The small dip seen around $1/V_0 = 0.4$ is due to the wave packet resonating inside the potential barrier. This resonance effect is strongly dependent on the width of both the wave packet and the barrier.

Quantum harmonic oscillator potential

The harmonic oscillator potential is defined as $V(r) = \frac{1}{2}m\omega^2 r^2$, with r the distance from some point in space. It is known from the classical harmonic oscillator that a particle will oscillate with a certain frequency in space. This behaviour can also be seen in the quantum analog of the harmonic oscillator. A simulation was performed by giving an offsetted Gaussian wave packet with $\sigma_x = \sigma_y = 4.5$ a momentum in the positive x-direction in a harmonic potential with $\omega = 0.2$ on a domain of 40 by 40. Snapshots, evenly spread out over the duration of 150 time steps with $\tau = 0.5$ and $a = 0.5$, are shown in figure 8.

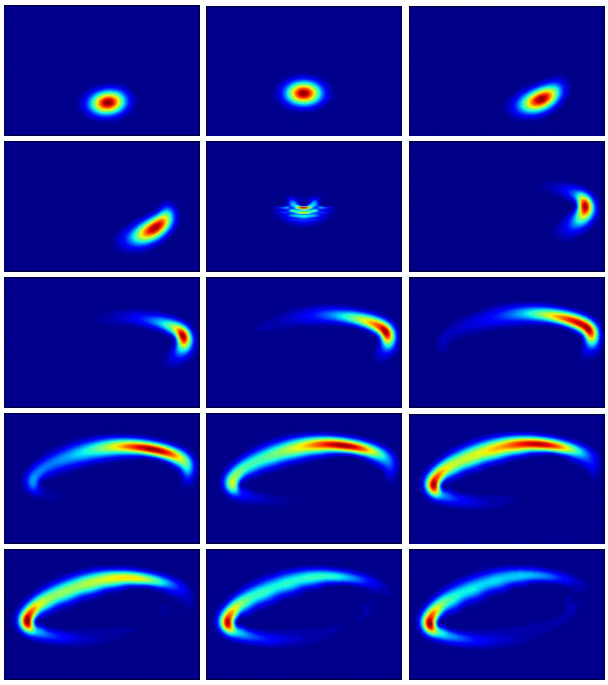

Figure 8: *Time-evolution of a moving Gaussian wave packet in a harmonic potential for 150 time steps. The snapshots are ordered from left to right and are equally distributed over time.*

Note that the spread in the wavefunction increases the closer the expectation value gets to the centre of the potential. This corresponds to the behaviour of the classical harmonic oscillator where the momentum is greatest as the particle moves through the centre, while the momentum is zero as it reaches its farthest point from the centre.

Double slit potential

A Gaussian wave packet with $\sigma_x = \sigma_y = 4.5$ is sent through a potential barrier with height $V_0 = 100$, with two regions of width 3 in the barrier where the potential is set to zero. The wavefunction will partially spread from these two slits and create an interference pattern on the other side. Twelve snapshots spread out evenly over 80 time steps with $\tau = 0.1$ and $a = 0.5$ are shown in figure 9. The simulation takes place on a domain of 40 by 40 units. [3]

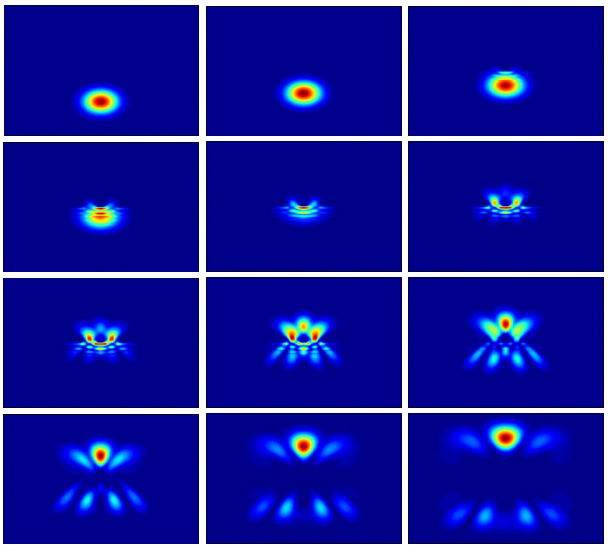

Figure 9: *Time-evolution of a Gaussian wave packet through a double slit for 80 time steps. The snapshots are ordered from left to right and are equally distributed over time.*

Figure 10 shows a cross-section along the x-axis at $y = 26.5$, $t = 60$, $\tau = 0.1$ of the probability distribution is seen figure 9. $t = 60$ corresponds rougly to the 9^{th} snapshot. The probability distribution is again normalized to find the conditional distribution.

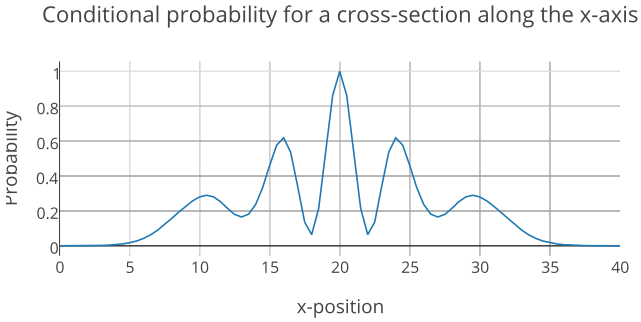

Figure 10: *Conditional probability distribution for $y = 26.5$ at $t = 60$.*

[3] Videos of these simulations can be viewed on: `https://github.com/dbouman1/iccp-assignment-3/tree/2D/videos`

Conclusion

The simulations performed agree very well with prior expected results, both from a physical and a mathematical point of view. The program could be improved in several places, however:

- Variable a and τ during the simulation. This would be beneficial for simulating systems with sudden jumps in the potential, like the double slit potential.
- Implementation of time-dependent potentials. This was not implemented since most known results in quantum mechanics are for time-independent potentials, making it hard to compare with known results.
- In the simulation the wavefunction is expressed in real space. By Fourier transforming it is possible to express the wavefunction in momentum space. Another possibility would then be to simulate the Wigner quasiprobability distribution in time, which is the quantum analog of a probability distribution in phase space.

References

[1] J. Crank and P. Nicolson. A practical method for numerical evaluation of solutions of partial differential equations of the heat-conduction type. *Advances in Computational Mathematics*, 6(1):207–226, 1996.