Computer simulations of 1D tunneling of a Gaussian wave packet

Aboubakr El Mahdaoui *

*Delft, University of Technology

The time evolution of a Gassian wave packet has been simulated using the split-operator scheme through a 1D rectangular barrier. The split-operator scheme allows for the evaluation of the time evolution using diagonal operators exclusively. Results show the effect of tunneling through a higher potential barrier as expected in quantum mechanics.

Introduction

The time evolution of a wavefunction is governed by the time dependent Schrödinger equation:

$$|\psi(t)\rangle = e^{-it\hat{H}/\hbar}|\psi(0)\rangle \qquad [1]$$

With $\hat{H}$ the hamiltonian, $|\psi(t)$ the wavefunction at time t. This can also be calculated as a product where t is a number of timesteps Δt, $t = n\Delta t$:

$$|\psi(t)\rangle = \prod_{i=1}^{n} e^{-i\Delta t\hat{H}/\hbar}|\psi(0)\rangle \qquad [2]$$

In this way each next timestep the wavefunction can be evaluated using the previous one:

$$|\psi(t+\Delta t)\rangle \approx e^{-i\Delta t\hat{H}/\hbar}|\psi(t)\rangle \qquad [3]$$

Split operator scheme

The hamiltonian of a wavefuntion with a kinetic energy K and a potential V can be written as:

$$\hat{H} = \hat{K} + \hat{V} \qquad [4]$$

With $\hat{K} = \frac{\hat{p}^2}{2m}$. Now we can rewrite and approximate eq. 3:

$$|\psi(t+\Delta t)\rangle = e^{-i\Delta t(\hat{K}+\hat{V})/\hbar}|\psi(t)\rangle \qquad [5]$$
$$\approx e^{-i\Delta t\hat{p}^2/2m\hbar}e^{-i\Delta t\hat{V}/\hbar}|\psi(t)\rangle \qquad [6]$$

Here, the operator with $\hat{V}$ is diagonal in real space and the operator with $\hat{p}$ is diagonal in momentum space. One way to evaluate the next timestep could be to evaluate the potential part, use the Fourier Transform to transform the result to momentum space and then apply the momentum part of the operator and inverse Fourier Transform again to get the wavefunction of the next time step in real space.

Results & Discussion

In this section we will provide the results of the simulations performed for a normalized Gaussian wavepacket with normalization constant A of the form:

$$\psi(x) = A\exp^{\frac{-x^2}{2\alpha^2}}\exp^{ikx} \qquad [7]$$

As can be seen in Fig. 2 the flow of the wavepacket clearly shows tunneling through a much larger potential barrier. Periodic boundary conditions are applied to show interference effects as well. It would be interesting to expand this model for higher dimensions and simulate quantum effects there as well.

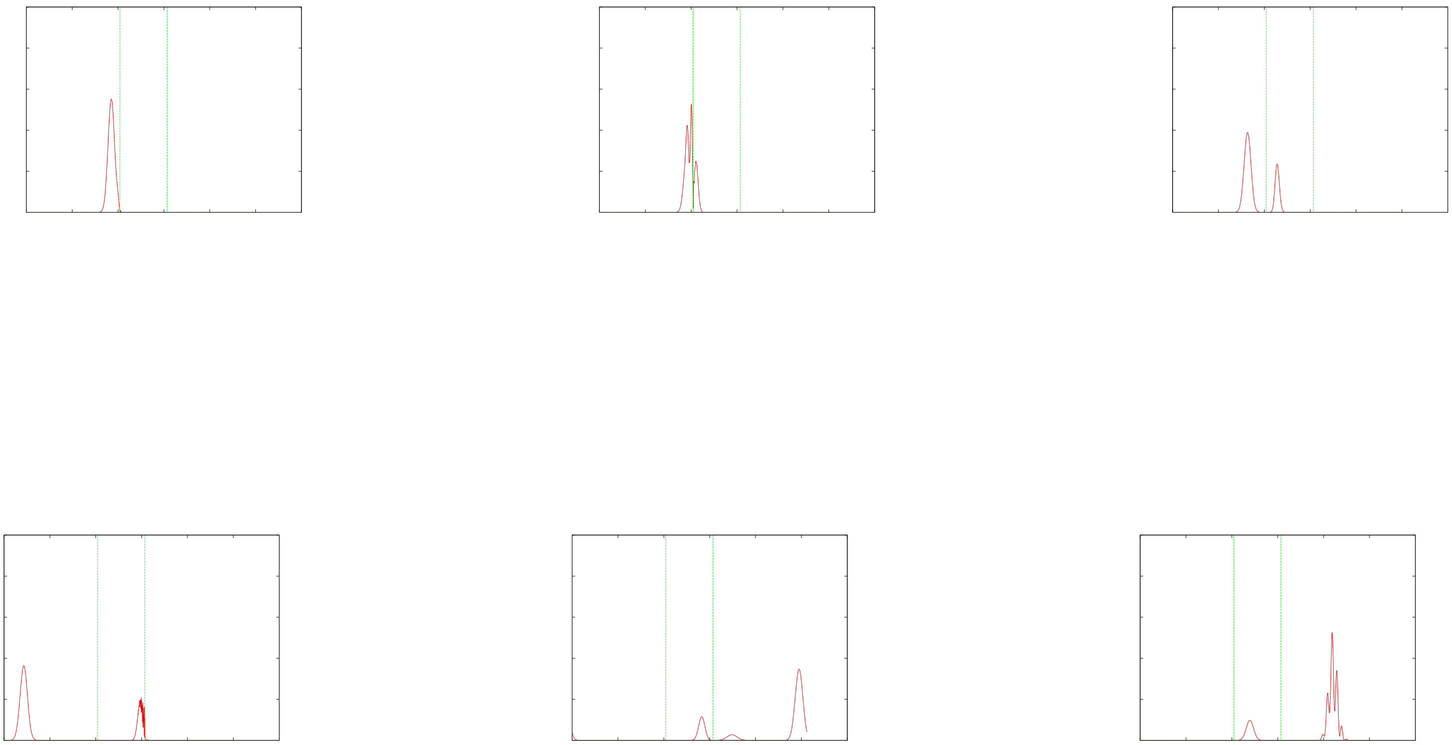

Fig. 2: A right moving Gaussian wave packet tunneling through a potential barrier and interfering with itsself as periodic boundary conditions are applied

1. D. J. Griffiths, Introduction to Quantum Mechanics, (2005).
2. J. M. Thijssen, Computational Physics, Cambridge University Press, 2nd ed. (2007)