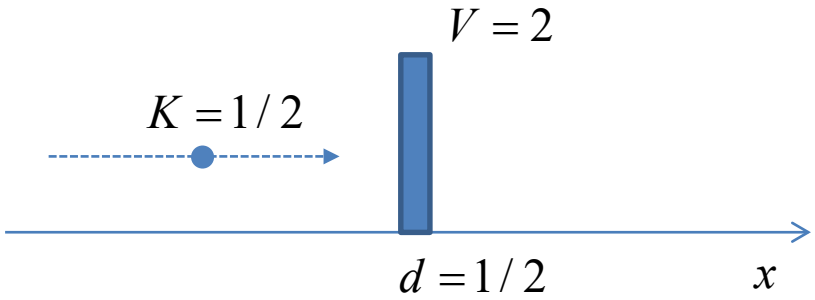
Computational Physics – Exercise 8: Time-dependent Schrödinger equation

Kristel Michielsen
Institute for Advanced Simulation
Jülich Supercomputing Centre
Forschungszentrum Jülich
k.michielsen@fz-juelich.de
http://www.fz-juelich.de/ias/jsc/qip

Exercise

- Task: Solve the time-dependent Schrödinger equation for a particle impinging on a potential barrier → tunneling
- Kinetic energy K is less than the potential barrier V ➔ in classical mechanics, the particle has no chance to appear on the right hand side of the barrier
  - In quantum theory it has!



Exercise

- Solve the TDSE

$$i\hbar\frac{\partial}{\partial t}\Phi(x,t)=\left(-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial x^2}+V(x)\right)\Phi(x,t)$$

  by means of the product formula approach with the initial value of the wave function

$$\Phi(x,t=0)=(2\pi\sigma^2)^{-1/4}e^{iq(x-x_0)}e^{-(x-x_0)^2/4\sigma^2}$$

  a Gaussian wave packet centered around x_0 with a width σ and wave vector q

- Use units such that $M=\hbar=1$

Exercise

- Set

$$0 \le x \le 100$$

$$\sigma = 3 \quad , \quad x_0 = 20 \quad , \quad q = 1$$

$$V(x) = \begin{cases} 0 & \text{no barrier} \\ \begin{cases} 2 & 50 \le x \le 50.5 \\ 0 & \text{otherwise} \end{cases} & \text{barrier} \end{cases}$$

$$\Delta = 0.1 \quad , \quad L = 1001 \quad , \quad \tau = 0.001 \quad , \quad m = 50000 \quad , \quad \text{discretization}$$

- Center of wave packet will move from $x = 20$ to about $x = 70$

Exercise

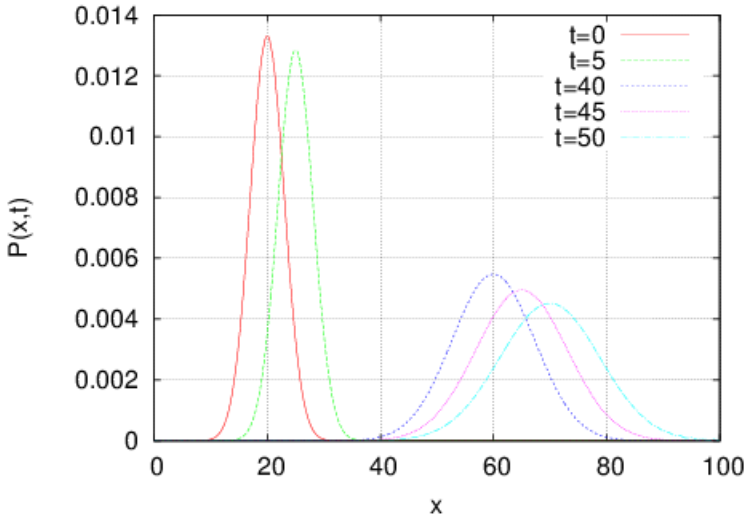
- Show snapshots of the probability distribution
- Explain why the center of the wave packet that tunnels through the barrier seems to have gained speed

Exercise

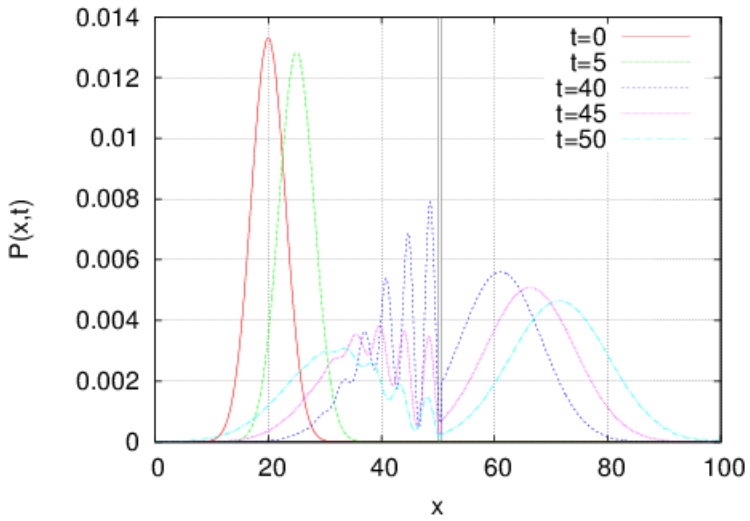
- Important “details”:
  - Plot the probability $P(x,t) = \Phi^*(x,t)\Phi(x,t) = \left|\Phi(x,t)\right|^2$ not the wave function
  - The part of the wave that “tunnels” through the barrier has very little probability
    - Compute the total probability for $x > 50.5$ at the times at which snapshots are taken.
      Normalize the probabilities $P(x > 50.5, t)$ by the maximum of the total probability for $x > 50.5$

Exercise

- No potential barrier



- Potential barrier



The wave packet that tunnels through the barrier moves faster than the wave packet that moves in free space!

Report

Ms. Vrinda Mehta v.mehta@fz-juelich.de
Dr. Madita Willsch m.willsch@fz-juelich.de
Dr. Fengping Jin f.jin@fz-juelich.de

- Filename: Please follow the instructions of the tutors
- Content of the report:
  - Names + matricle numbers + e-mail addresses + title
  - Introduction: describe briefly the problem you are modeling and simulating (write in complete sentences)
  - Simulation model and method: describe briefly the model and simulation method (write in complete sentences)
  - Simulation results: show figures (use grids, with figure captions !) depicting the simulation results. Give a brief description of the results (write in complete sentences)
  - Discussion: summarize your findings
  - Appendix: Include the listing of the program

Due date: 10 AM, July 2, 2043