# Quantum scattering on a potential barrier

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## 1 Introduction

The aim of this work is to analyze transmission of a wave package on a potential barrier. Great thanks for DSc Tomasz Sowiński for his guidance in the project.

## 2 Wave function

The analysis of the transmission is made based on solving 1D time independent Schrodinger equation.

$$\left[\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\Psi(x,t) = i\hbar\frac{\partial}{\partial t}\Psi(x,t) \tag{1}$$

In the given problem Hamiltonian ($H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$) is time independent. Hence, the time independent Schrodinger equation can be used.

$$\Psi(x,t) = \phi(x)e^{-iEt/\hbar} \tag{2}$$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\phi(x) = E\phi(x) \tag{3}$$

where $E$ states for the energy of the wave.
Equation 3 has infinite number of solutions and corresponding energies. However we are looking for the general solution which is a linear combination of the mentioned solutions.

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n\phi(x)e^{-iEt/\hbar} \tag{4}$$

For every continuous function $\psi(x)$ its time evolution can be found with Eq. 4. Coefficients $c_n$ can be found with the formula:

$$c_n = \int_{x_{min}}^{x_{max}} \psi(x)\phi(x)^* dx \tag{5}$$

Knowing the time evolution $\Psi(x,t)$ of the initial function $\psi(x)$ the simulation can be conducted. The Hamiltonian can be represented in a form of a tridiagonal matrix. Which is:

$$H_{ij} = \left[\frac{1}{\Delta x^2} + V(x_i)\right]\delta_{ij} - \frac{1}{2\Delta x^2}\delta_{i,j\pm1} \tag{6}$$

Also the function $\psi(x)$ can be represented as a vector.

$$\boldsymbol{\psi(x)} = [\phi(x_1), \phi(x_2), \cdots \phi(x_n)] \tag{7}$$

Hence eq. 3 can be written in a matrix form

$$\boldsymbol{H\psi(x)} = \boldsymbol{E\psi(x)} \tag{8}$$

Finding eigenstates and eigenvalues of the Hamiltonian matrix $\boldsymbol{H}$ solutions ($\phi(x)$) and their energies are also found.

# 3 Simulation

The simulations are conducted for an initial wave of the Gaussian shape. For every timestep it is checked whether the wave package gets to the boundary, if so it is made zero and coefficients for expansion are recalculated. The visualization of the simulation is presented in the Fig. 1. The green rectangle states for the potential barrier and the blue curve for the wave function.

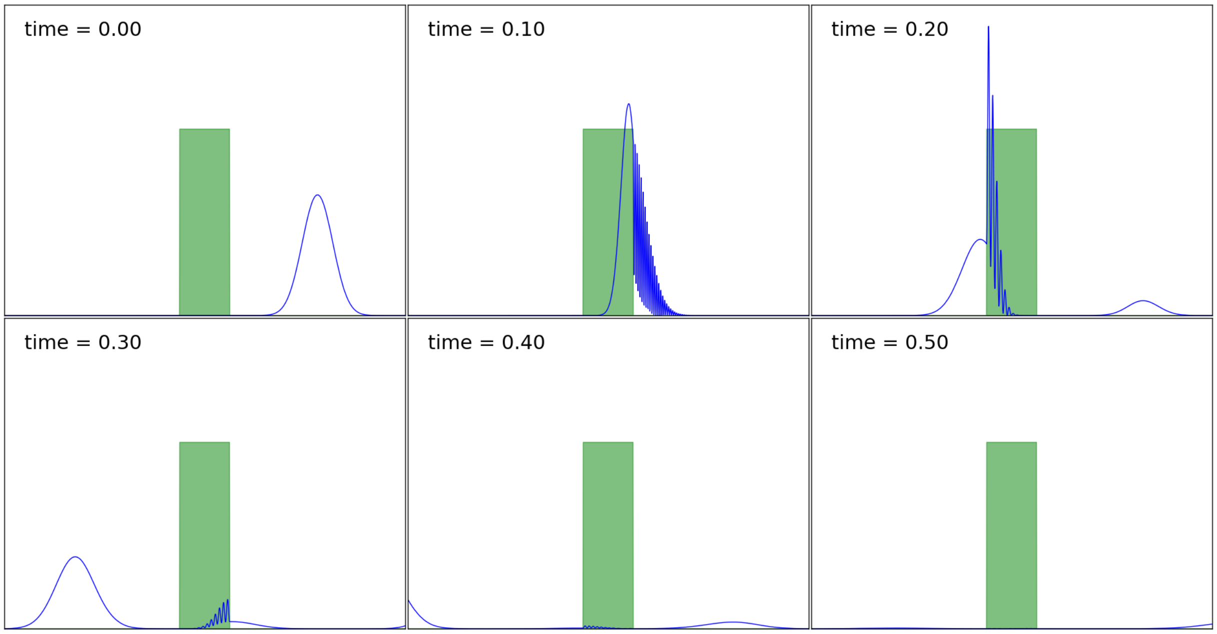


Figure 1: Visualization of the simulation.

# 4 Transmission analysis

Below there are a few example graphs with descriptions.

The Figure 2. shows scattering on a rectangular potential barrier as a function of particle's energy. The potential of the barrier is fixed and equals 1. Hence x-axis shows the relation between potential and particles energy. For energy smaller then 1, particle can still transmit through the barrier, even though it does not have enough energy to do so. This phenomenon is called quantum tunneling.

The Figure 3. shows scattering on a triangular barrier where the barrier's shape is an isosceles triangle.

The Figure 4. shows transmission as a function of barrier width. The energy equals 1.5. Interesting fact is that the transmission does not depend on barrier's width for bigger width values.

# References

[1] David J. Griffiths, *Introduction to Quantum Mechanics*, Prentice Hall, Inc. 1995

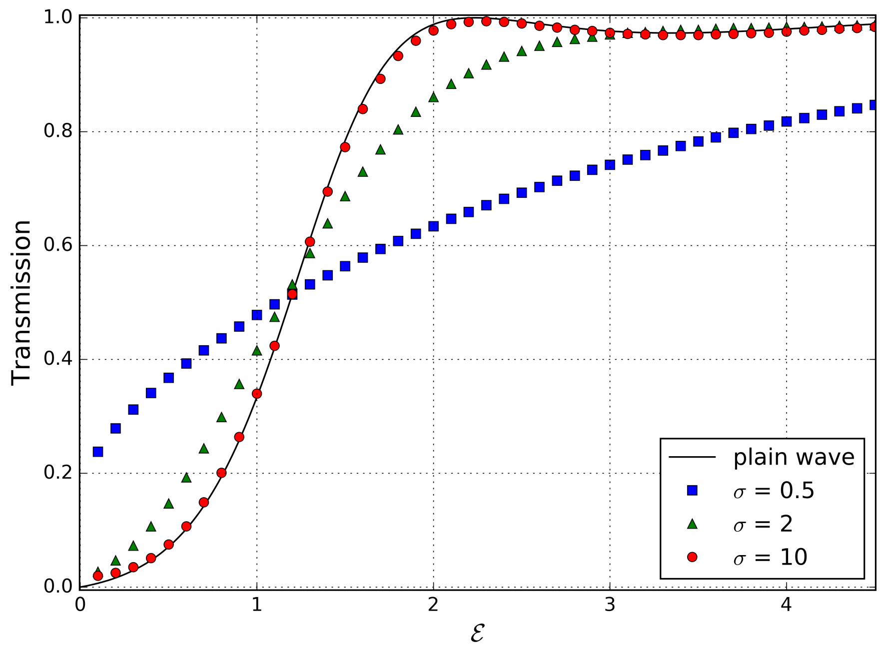


Figure 2: Scattering on a triangular potential barrier of width 4

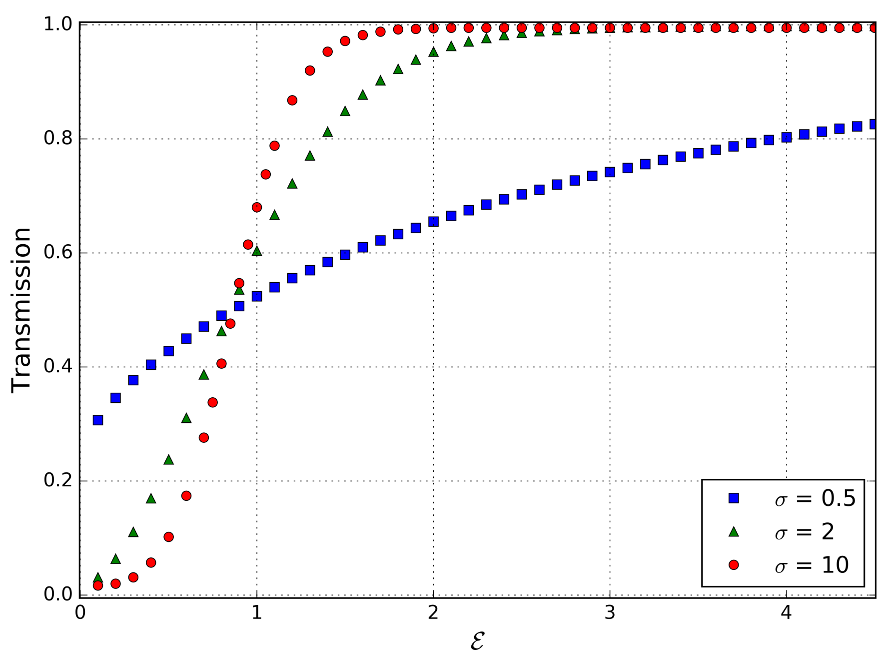


Figure 3: Scattering on a rectangular potential barrier of width 2

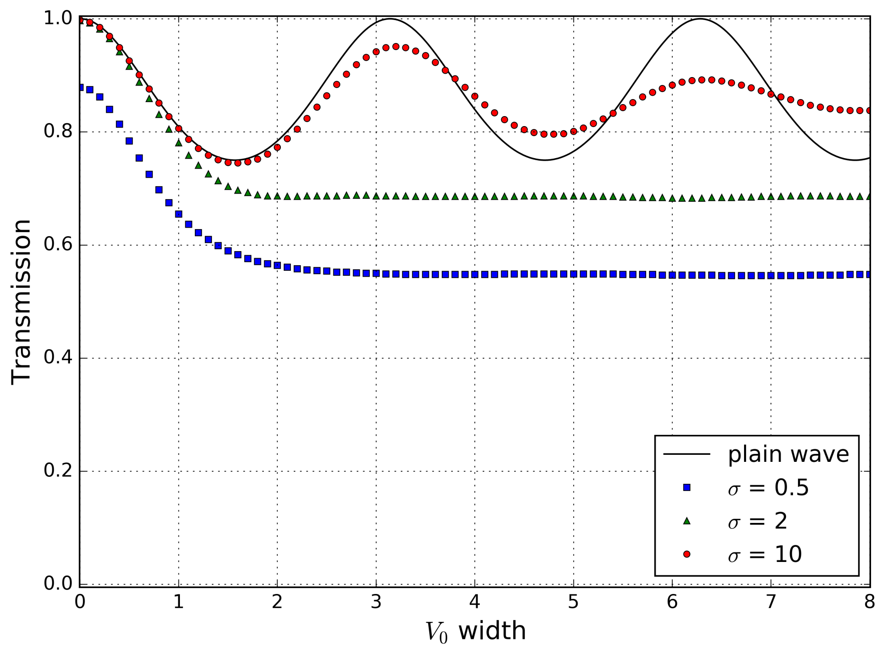


Figure 4: Scattering on a rectangular potential barrier of width energy 1.5