Numerical Exercise

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Introduction

In this exercise the goal was to study propagation of wave packets, numerical integration of the Schrödinger equation and some aspects of tunneling. The script is written in python using the numpy package.

The purpose of this exercise was to propagate an electron through a series of potentials of different widths and strengths and study the behavior of the wave packet through all the different potentials. Specifically we would study scattering by a barrier and tunneling.

The numerical solution started by looking at a plane wave multiplied by a Gaussian (1), thus making it possible to calculate the wave function as a sum of discrete stationary states (2).

$$\Psi(x,t) = Ce^{-\frac{(x-x_s)^2}{2\sigma_x^2}} e^{i(k_0 x - \omega t)} \tag{1}$$

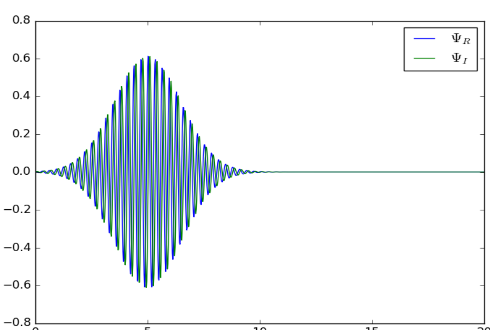
$$\Psi(x,t) = \sum_{n=0}^{N-1} c_n \psi_n(x) e^{\frac{iE_n t}{\hbar}} \tag{2}$$

Problem 1

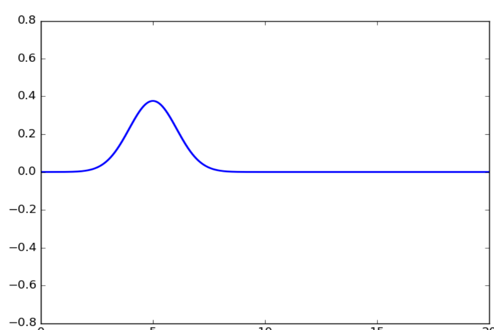
The calculated initial values for the real and imaginary parts of the wave function was $\Psi_R(0, \frac{\Delta t}{2}) = 2.799e-6$ and $\Psi_I(0,0) = 0$, and by integrating and solving (3) we found the normalization constant, C, to be equal to $(\frac{1}{\pi\sigma_x^2})^{\frac{1}{4}}$. The plots for the probability density and the real and imaginary parts of the wave function are shown in figure 1a and figure 1b.

$$\int_0^L |\Psi(x,t)|^2 = 1 \tag{3}$$

Figur 1



(a) Plot of Ψ_R og Ψ_I at $t = 0$

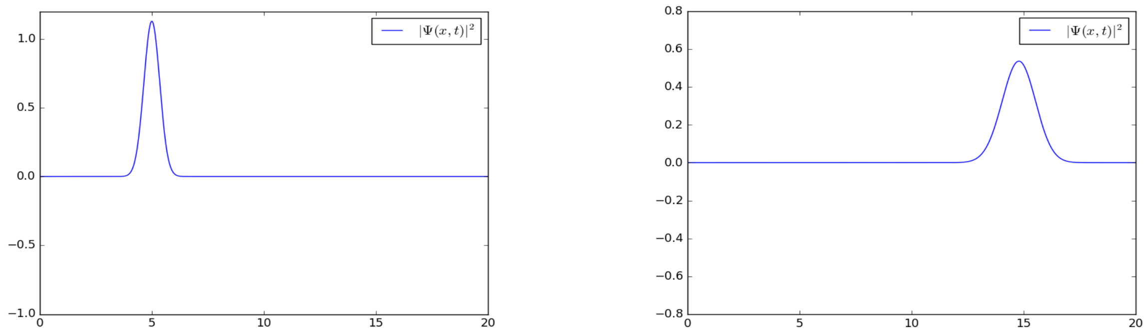


(b) Probability density $|\Psi(x,t)|^2$ at $t = 0$

Problem 2

By propagating the wave a distance $\frac{L}{2}$ from $x = 5$ to $x = 15$ we see that the dispersion of the wave increases as the wave propagates, which is shown in the plots in figure 2a, 2b, 3a and 3b. It shows also how the development of the dispersion is dependent on the value of σ_x. As shown in the figures, smaller values for σ_x makes the wave spread out more as it propagates.

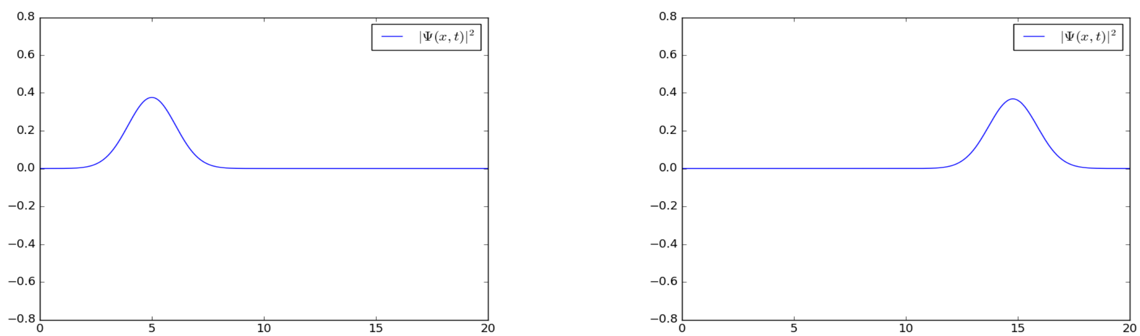
Figur 2: Wave packet with $\sigma_x = 0.5$



(a) $|\Psi(x,t)|^2$ centered at $x = 5$

(b) $|\Psi(x,t)|^2$ centered at $x = 15$

Figur 3: Wave packet with $\sigma_x = 1.5$



(a) $|\Psi(x,t)|^2$ centered at $x = 5$

(b) $|\Psi(x,t)|^2$ centered at $x = 15$

In the rest of the problems we set $\sigma_x = 1$.

Problem 3

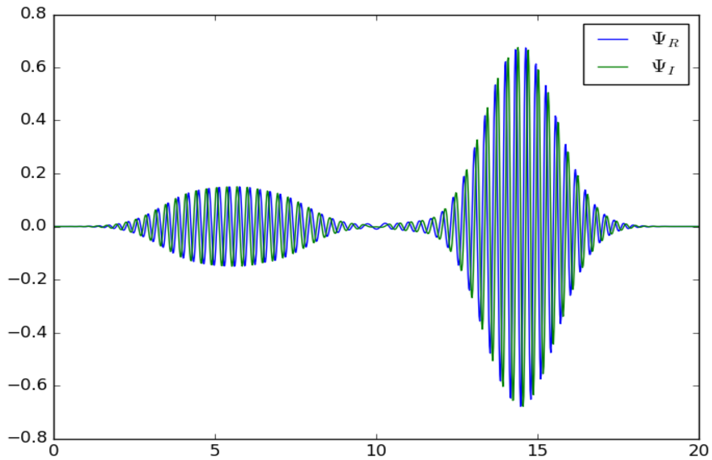
After introducing a potential barrier with width $l = \frac{L}{50}$ and height $V_0 = \frac{E}{2}$ we get a potential function given by:

$$V(x) = \begin{cases} \frac{E}{2} & \text{if } \frac{L}{2} - \frac{l}{2} < x < \frac{L}{2} + \frac{l}{2} \\ 0 & \text{otherwise} \end{cases}$$

After the wave has propagated through the potential it will be partially transmitted and partially reflected. Figure (4) shows the wave after passing through the potential.

The probabilities for reflection and transmission are found by calculating $\int_0^L |\Psi(x,t)|^2 dx$ and $\int_{\frac{L}{2}}^L |\Psi(x,t)|^2 dx$, respectively. The plot of the wave packet after propagating through the barrier is shown in figure 4.

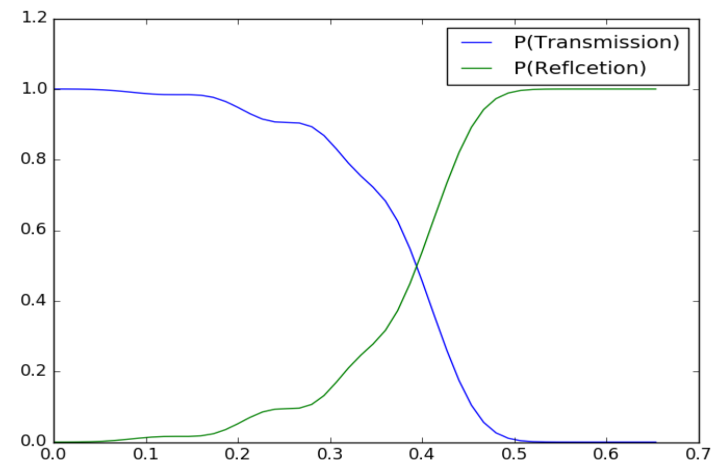
1. P(Transmission)=0.91923
2. P(Reflection)=0.08076



Figur 4: Plot of Ψ_R and Ψ_I after passing through the barrier

Problem 4

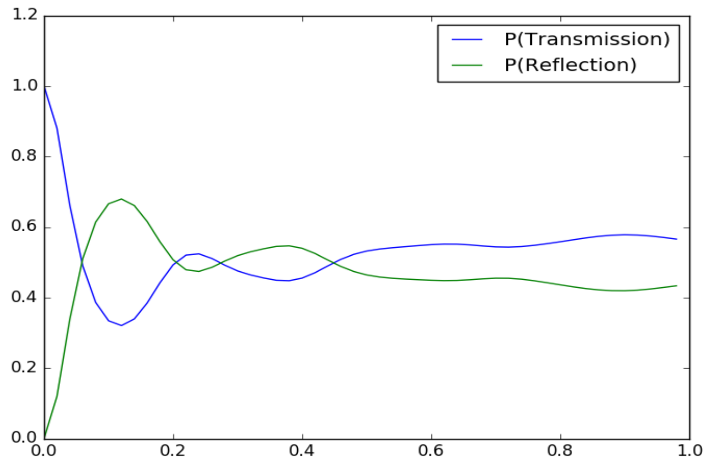
By using the same procedure as in problem 3, we calculated the probabilities for reflection and transmission for 50 different barrier heights spanning from $V_0 = 0E$ to $V_0 = \frac{3}{2}E$. In doing so we have plotted the probability of reflection and transmission as a function of E/V_0 as shown in figure 5.



Figur 5: Probability of reflection and transmission as a function of E/V_0

Problem 5

Doing the same as in Problem 4, however now for 50 different barrier widths spanning from 0 to $\frac{L}{20}$, we produce a plot of the probabilities as a function of barrier widths.



Figur 6: Probability of reflection and transmission as a function of barrier width