Numerical Schrödinger equation

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Abstract

This exercise is about solving the Shrödinger equation numerically and propagation of a Gaussian wave.

1. Normalizing the wave function

First of all we'll use a Gaussian wave packet as the wave function

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

where C is the normalization constant, t is the time, $x$is the position, x_s is the initial position, σ_x is the spatial width in x-direction, k_0 is the wave number and ω is the wave frequency. .The square of the absolute value of (1) then follows as

$$|\Psi(x,t)|^2 = C^2 e^{-\frac{(x-x_s)^2}{\sigma_x^2}}. \tag{2}$$

In order to normalize (2) the constant C has to be

$$C = \sqrt{\frac{1}{\int_0^L e^{-\frac{(x-x_s)^2}{\sigma_x^2}} dx}}. \tag{3}$$

When setting L, the total length, equal to 20, x_s to 5 and σ_x to 1.5 (3) becomes 0.613292.

Now it's possible to plot (2), the probability density for finding the particle at a position given by the wave packet, but before being able to plot (1) the wave number and frequency has to be set. The relation between them is

$$\omega = E/\hbar, \quad E = \frac{\hbar^2 k_0^2}{2m} \quad \Rightarrow \quad \omega = \frac{\hbar k_0^2}{2m}. \tag{4}$$

Choosing k_0 to be 20, m to be 1, and $\hbar$ to be 1 implies that ω has to be 200. The wave function and the probability density are plotted in figure 1 for t equal to zero.

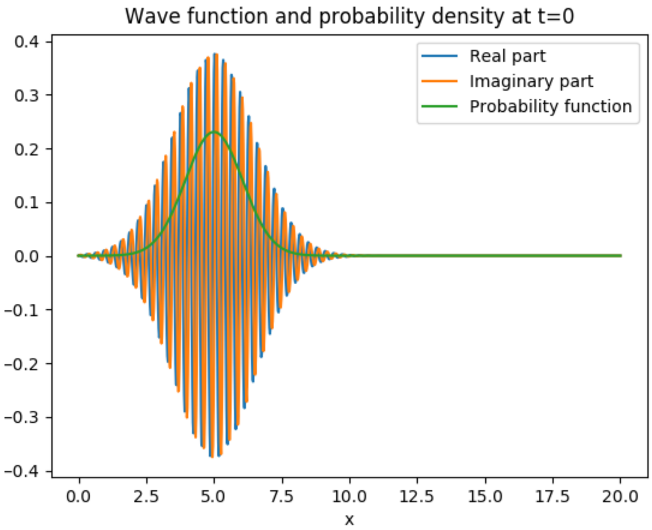


Figure 1: The plot presents the wave function from (1) and its possibility density for finding the particle at the given position, (2). The x-axis indicates the position, and the y-axis is dimensionless. The real part of the wave function is blue and the imaginary is yellow. The probability density is green.

2. Propagation of the wave function

The Schrödinger equation allows us to determine how the wave packet evolves over time

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = -\frac{\hbar}{2m}\Psi(x,t) + V(x)\Psi(x,t). \tag{5}$$

The wave function can be divided into a real and an imaginary part

$$\Psi(x,t) = \Psi_R(x,t) + i\Psi_I(x,t).$$

These two part have to be calculated separately, and by using central derivation (5) takes the form

$$\Psi_I(x,t+\frac{\Delta t}{2}) = \Psi_I(x,t-\frac{\Delta t}{2}) - \Delta t[\frac{V(x)}{\hbar}\Psi_R(x,t) - \frac{\hbar}{2m}\frac{\Psi_R(x+\Delta x,t)) - 2\Psi_R(x,t) + \Psi_R(x-\Delta x,t)}{(\Delta x)^2}],$$

$$\Psi_R(x,t+\Delta t) = \Psi_R(x,t) + \Delta t[\frac{V(x)}{\hbar}\Psi_I(x,t+\frac{\Delta t}{2}) - \frac{\hbar}{2m}\frac{\Psi_I(x+\Delta x,t+\frac{\Delta t}{2}) - 2\Psi_I(x,t+\frac{\Delta t}{2}) + \Psi_I(x-\Delta x,t+\frac{\Delta t}{2})}{(\Delta x)^2}$$

A matrix is then made with position horizontally and time vertically

$$\boldsymbol{\Psi(x,t)} = \begin{bmatrix} \Psi_R(0,0) & \Psi_R(1,0) & \dots & \Psi_R(N_x,0) \\ \Psi_I(0,1) & \Psi_I(1,1) & \dots & \Psi_I(N_x,1) \\ \Psi_R(0,2) & \Psi_R(1,2) & \dots & \Psi_R(N_x,2) \\ \vdots & \vdots & \ddots & \vdots \\ \Psi_I(0,N_t) & \Psi_I(1,N_t) & \dots & \Psi_I(N_x,N_t) \end{bmatrix}.$$

The grid has 1000 nodes, N_x resulting in 1000 elements for each row in the matrix. Furthermore the amount of time values, N_t, in each column is decided by

$$\frac{T}{N_t} = \Delta t = 0.3 * \frac{\hbar}{\frac{\hbar^2}{2m}\frac{1}{(\Delta x)^2} + V_{max}}, \quad \Delta x = \frac{L}{N_x - 1},$$

where Δ x is the step length, Δt is the time step and V_{max} is the height of the potential barrier. In order to propagate the wave a given distance the total time passed in order to propagate across half the grid, T, has to be determined. When the potential is zero over all within the constraints the total time is

$$T = \frac{L}{2v_g}, \quad v_g = \frac{\partial \omega}{\partial k}|_{k_0} = \frac{\hbar k_0}{m} \quad \Rightarrow \quad T = \frac{Lm}{2\hbar k_0} \tag{6}$$

The wave starts at x equal to 5, and shall propagate a distance of L equal to 20. From (6) this will then take 0.5 s. This is done with the spatial width, σ_x for first 0.5, then 1.0 and lastly 2.0.

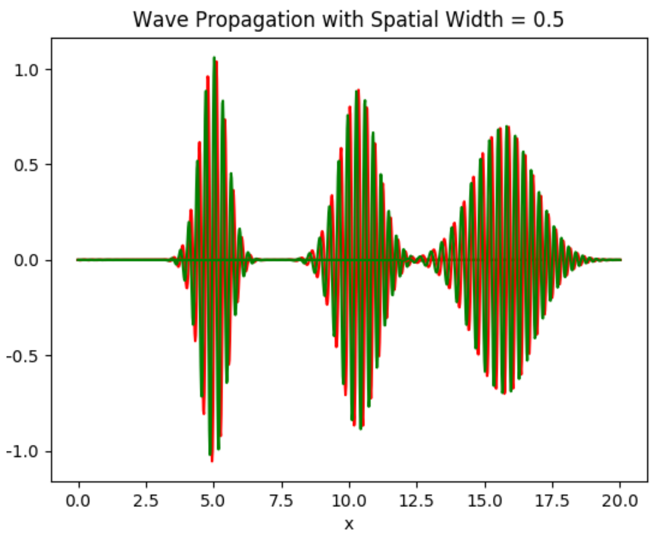


Figure 2: The wave packets presents the wave propagation over time from start position at 5, middle position at 10 and end position at 15. The displacement takes 0.50 s and has a spatial width of 0.5.

Now the probability density function (2) is again plotted, but this time both at the start time and the end time. The spatial widths used this time is 0.5 and 1.5. The

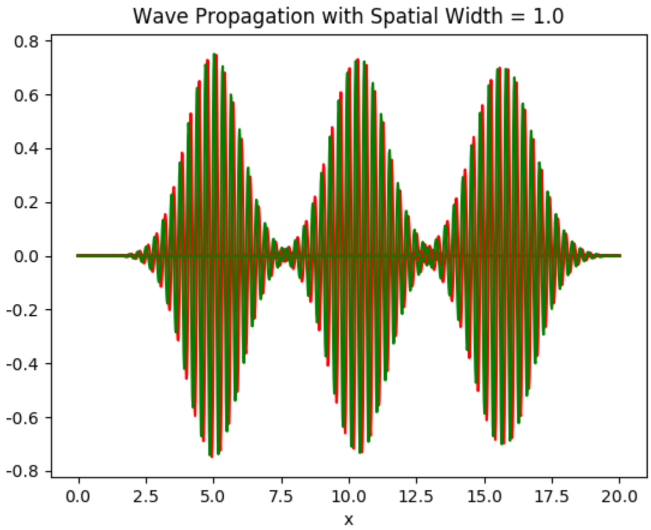
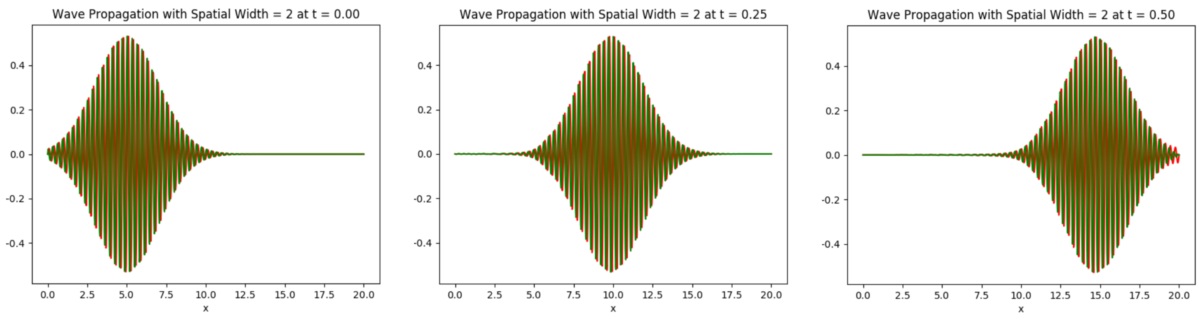


Figure 3: The wave packets presents the wave propagation over time from start position at 5, middle position at 10 and end position at 15. The displacement takes 0.50 s and has a spatial width of 1.0.



(a) Wave after 0 s.

(b) Wave after 0.25 s.

(c) Wave after 0.5 s.

Figure 4: The 3 sub figures presents the wave propagation over time from start position at 5 and end position at 15. The displacement takes 0.5 s and has a spatial width of 2.0.

probability density starts out rather sharp in figure 5 and ends a lot lower and wider, while in figure 6 where the spatial width is three times the size the probability density stays more constant throughout the propagation.

3. Transmission through a potential barrier

Next a potential barrier of a width l equal to a fiftieth of the total length and height equal to half the particle's initial energy is added

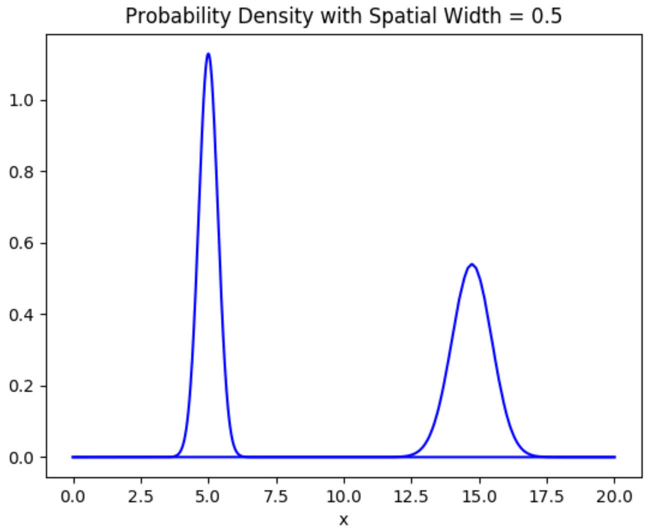


Figure 5: The 2 plots presents the probability density of finding particle at given position for start time and end time. The displacement takes 0.5 s and has a spatial width of 0.5.

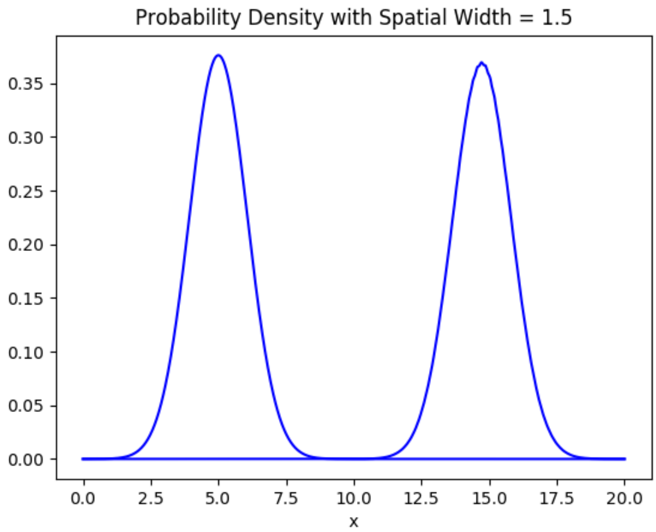


Figure 6: The 2 plots presents the probability density of finding particle at given position for start time and end time. The displacement takes 0.5 s and has a spatial width of 1.5.

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

The propagation now reflects a proportion of the wave when hitting the barrier as figure 7 presents. The spatial width for the rest of this exercise is set to 1.5.

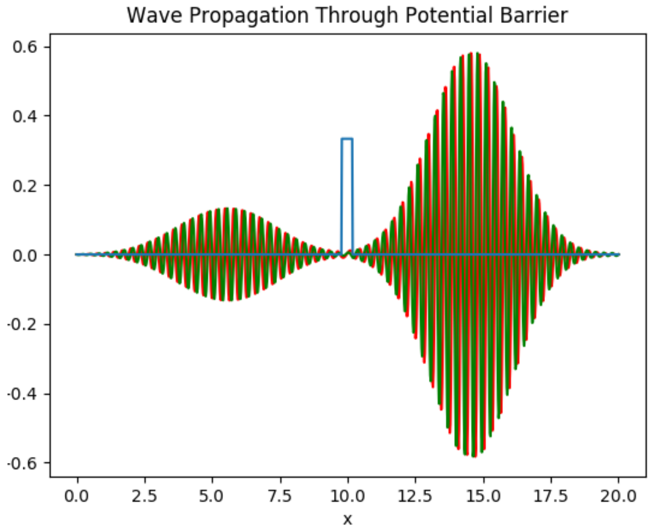


Figure 7: The plot presents the wave at end position 15. In the middle is a potential barrier with width equal to a fiftieth of the total length and height of half the initial energy of the particle. The wave on the left side has been reflected by the barrier and the wave on the right side has been transmitted.

When the wave is fully through the transmission and reflection it is possible to calculate the possibilities for each occurrence, $P(T)$ and $P(R)$. This is done my integrating over the square of the absolute value of the wave part of each either side

$$P(R) = \int_0^{\frac{L}{2}} |\Psi(x,t)|^2 dx, \quad P(T) = \int_{\frac{L}{2}}^{L} |\Psi(x,t)|^2 dx.$$

With the same initial conditions as for the free particle the probability of transmitting is 0.943 and the probability of reflecting is 0.0567.

4. Transmission and reflection probabilities as a function of barrier height

The procedure from previous section is repeated for 50 equally spaced heights of the potential barrier from 0 to $\frac{3}{2}E$. From figure 8 it seems like the probability of each occurrence is equal at about $0.9\frac{V_0}{E}$.

5. Transmission and reflection probabilities as a function of barrier width

Lastly the procedure from the previous section is repeated, but instead of varying the barrier height the width is now the variable. Setting the barrier height to $\frac{9}{10}E$, and the widths are equally spaced from 0 to $\frac{L}{20}$. Figure 9 shows that the transmission probability drops at a quick rate at the start from 1.0 to 0.4 where it evens out and stays almost to the end where it approaches 0.5. The reflection is of course 1 - the transmission probability.

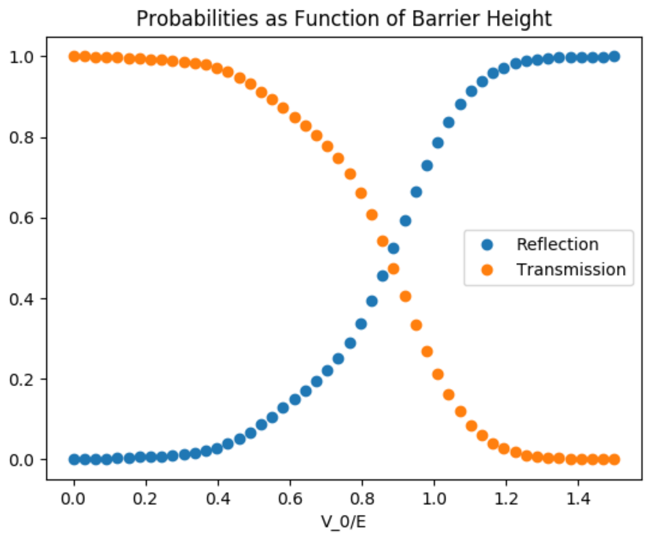


Figure 8: The plot presents how the probabilities of reflecting and transmitting varies with the barrier heights. The blue line is the reflection probability and the orange is the transmission probability. The x-axis is the height barrier divided by the initial energy.

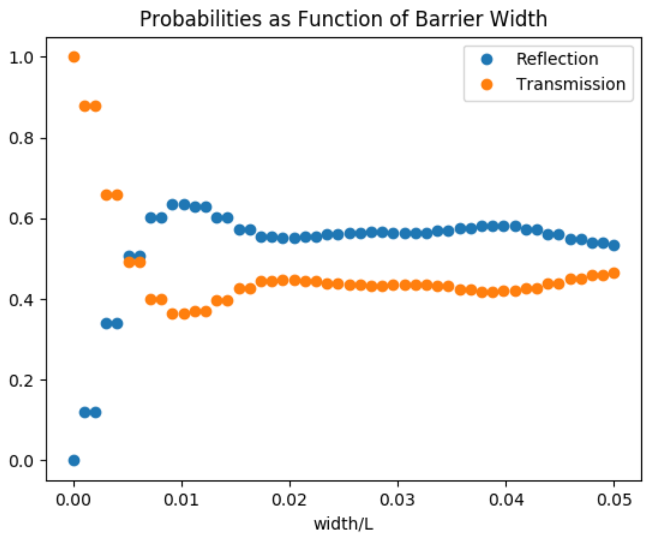


Figure 9: The plot presents how the probabilities of reflecting and transmitting varies with the barrier widths. The blue line is the reflection probability and the orange is the transmission probability.

6. Bibliography

Mathias Winkler, Numerical exercise in FY2045 Quantum Mechanics, NTNU, fall 2018.