Numerical Solution of 1D Schrödinger equation for a Gaussian wave packet

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Contents

1 Introduction and remarks

The next simulations have been done using an algorithm, which can be found in the file 'algorithm.py', very similar to the one stated in the guide, although it has some minor changes to the one in the guide to accelerate the calculus of the solutions. Files 'Question{n from 1 to 4}.py' include some specific methods to make the requested plots and some cool animations. 'Main.py' is a one threaded not very robust GUI (Graphical User Interface), that serves to dynamically explore more solutions to this 1-D wave equation and see specific plots related to them that are not included in this report.
All packets have been simulated, except when explicitly stated otherwise, with the next values.

Parameter	Value
t	0.005
t_{final}	50
x	0.05
x_{min}	-60
x_{max}	60
k_0	1
σ_0	2
x_0	-10
L	2
V_0	2
M	10
N	10000

Table 1: Parameter values to used to simulate the wave packet

Note that the value of N is significantly higher than the recommended in the guide. This change was partially made to assure the stability of the solution, which is higher than 99.99% for each state, and mostly just for fun, they look very impressive.

2 Question 1

Produce a sequence of plots (or make a movie!) showing the probability density for the electron at least for the following times:

$$t = 0, 500\Delta t, 1000\Delta t, 1500\Delta t and 2000\Delta t$$

Overlay these plots with another showing the potential so that you can see the relative position of barrier and packet. Rescale all plots so that you can easily see the effect of the barrier on the wave function. Compare your results with Fig. 2. If the agreement is good, you can then proceed to solve the next items!

Below, you can see in Figure 1 the graphical representation of the packet with the conditions of Table 1 at different times. Note that the potential has a value of $2V$.

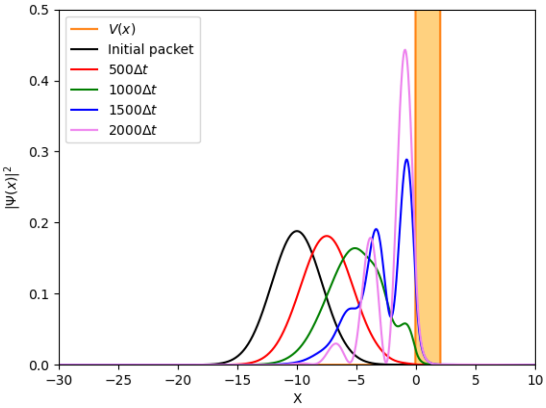

Figure 1: A Gaussian packet advances towards a finite square barrier of 2 volts. Both reflection and quantum tunneling are apparent from the shape of the wave function ahead and beyond of the barrier at later times.

From it, we can clearly see how the packet approaches the wall and collides with it, bouncing back in its most entirety. The reflection and quantum tunneling of the packet become much more apparent when increasing the value of k_0:

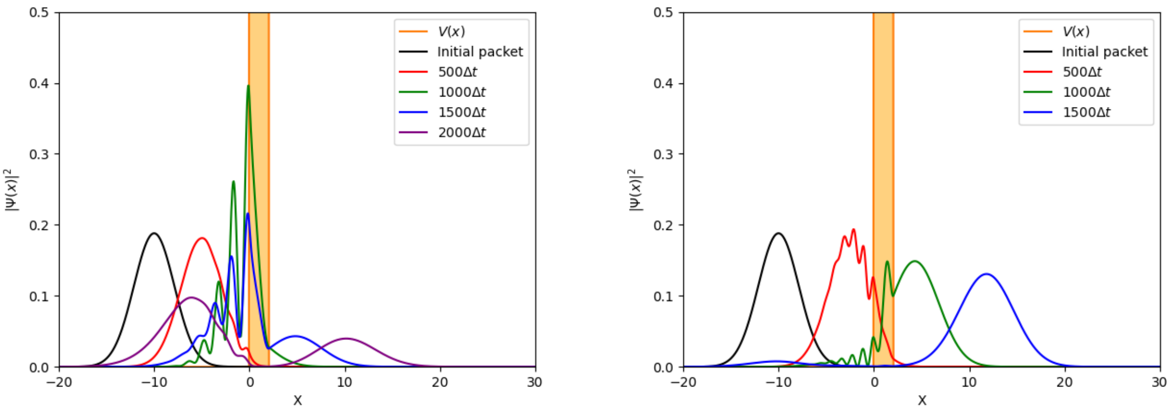

Figure 2: **Left:** Gaussian packet with $k_0 = 2$. **Right:** Gaussian packet with $k_0 = 3$

Here we see that the wave packet with $k_0 = 2$ struggles much less to pass the wall as its energy is higher, which, as it is explained in the next questions, is around 2.06 J. However, the packet with $k_0 = 3$ passes through the wall without problems. This is due to its higher energy, of about 4.56 J, so with this packet it is more interesting to check the reflection than the transmission.

3 Question 2

Calculate the probability T of finding the electron beyond the barrier as a function of time for the previous run. You can estimate it via the same sum as in Eq. 23, but restricting the sum to the mesh

positions to the right of the end of the barrier. Produce a plot showing the time dependence of the estimated transmission probability T and find its asymptotic value as shown in Fig. 3.

The next figures represent the transmitted part of the wave function and the estimated transmission probability T:

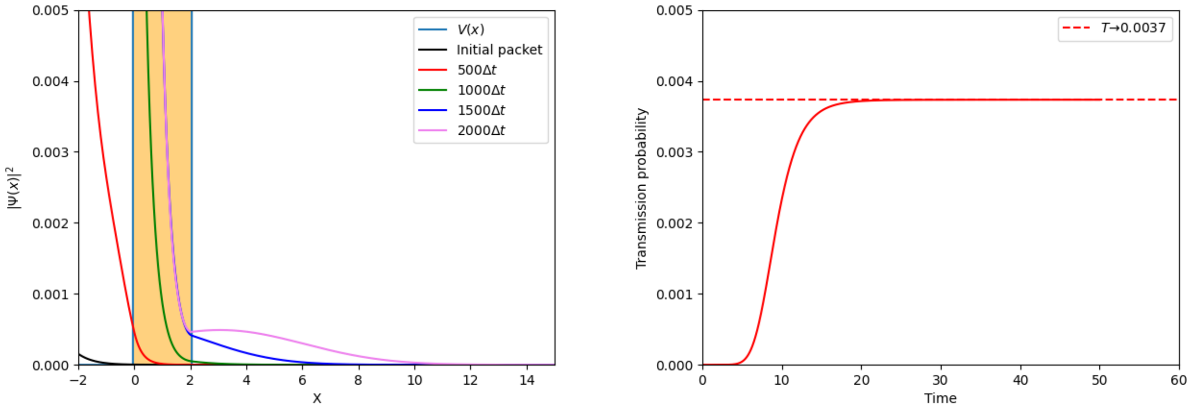

Figure 3: **Left:**: Zoom-in of the transmission region beyond the barrier. **Right:** Resulting transmission probability T(t) with asymptotic value at 0.003734 shown with a dashed line.

4 Question 3

Study the dependence of the (asymptotic) transmission probability on k_0.- For this study, you need to carry out a series of simulations for various values of k_0, varying from 0.5 to 8. All other parameters remain with the same values collected in Table 1. Use at least fifteen different values for k_0.
The following plots show the transmission probabilities of the same wave packet with different k_0 varying from 0.5 to 8.

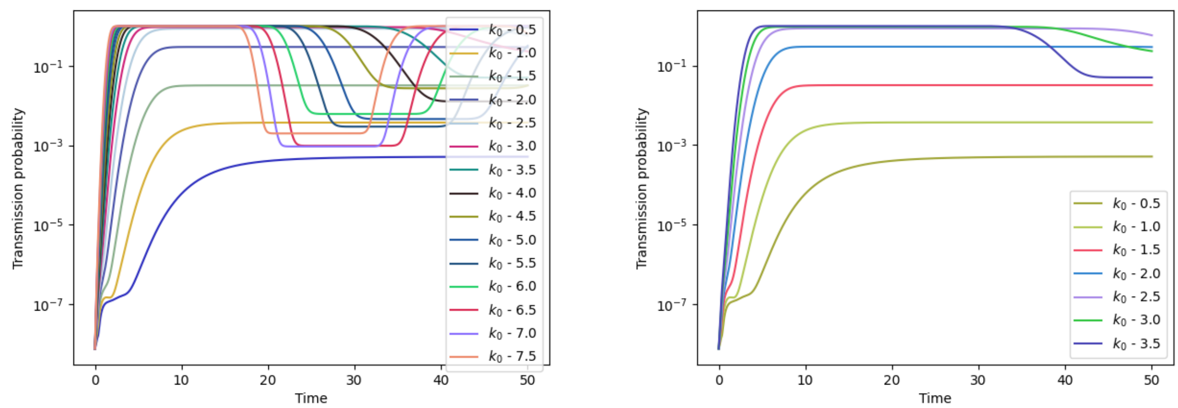

Figure 4: **Left:**: Transmission probabilities as a function of time for various values of k_0. **Right:** Transmission probabilities as a function of time for half of the k_0 values of the left figure.
Remark: The colors have been randomly generated :(

By the way, can you explain why, at the largest values of k_0, a drop in the transmission probability is observed? Help: Remember that we are estimating it as the integral of the wave function beyond the barrier! Why is the drop not observed for the lower k_0? Would it be also observed if we wait for a longer time?

These drops occur because the boundaries of the problem are not taken into account in the estimated transmission probability. As we have finite boundaries, in this case the wave packet is confined in [-60,60] it can bounce back and traverse again the wall in the opposite direction. This is much more apparent in waves with higher k_0 because they have a much higher energy, so they move much quicker and go through the wall as a hot knife through butter. If we wait enough time, even the packets with low k_0 values would also experiment this consequence numerous times.

5 Question 4

Study the dependence of the (asymptotic) transmission probability on the energy E0. Plot the values of the transmission probabilities obtained in the previous section as a function of $E_0 = (k_0^2 + 1/(2\sigma_0^2))/2$. The plot should look like Fig. 5, You should also throw in the theoretical formula (derived in class!) for the transmission coefficient as a function of the energy of a plane wave with energy E, that in atomic units is:

$$x = \begin{cases} \left[1 + \frac{V_0^2}{4E(V_0-E)} sinh^2\left(L\sqrt{2(V_0-E)}\right)\right]^{-1} & E < V_0 \\ \left[1 + \frac{V_0^2}{4E(E-V_0)} sinh^2\left(L\sqrt{2(E-V_0)}\right)\right]^{-1} & E > V_0 \end{cases}$$

The oscillations on the transmission coefficient for the theoretical formula are clear in the plot, with the maxima showing where resonant transmission takes place. For the wave packet case, can you observe any oscillations? Are they as clear as the one for the plane wave solution? If not, argue a possible reason. Can you propose how to change the parameters of our simulation to reproduce the oscillations of the theoretical formula?

This last graph shows the transmission probabilities of a planar wave with energy E_0:

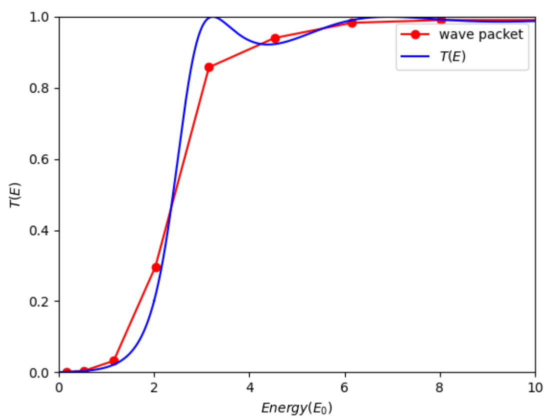

Figure 5: Transmission probabilities as a function of the expected energy E0. In blue, the theoretical transmission coefficient for a plane wave of the same energy is shown.

Concerning the last questions, a planar wave presents resonance, that is, only at some energies the transmission coefficient will be 1, but a wave packet is made of infinitely many planar waves, each with its own resonance, which will generally not coincide, that is why in this case we do not observe such clear oscillations. A way to reproduce more accurately the oscillations, would be to increase the value of σ_0, consequently increasing the standard error of the position and lowering the deviation of the velocity, thus the energy too.

6 Bibliography

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