FY2045 - Numerical Exercise

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1 Introduction

With the following, we aim to answer the numerical exercise given in the course FY2045 at NTNU, fall 2018. We will solve the *time-dependent Schrödinger equation* numerically in python, and thereby investigate propagation of wave packets and scattering through potential barriers.

We will only study time-invariant potentials. As such, we have chosen to solve the Schrödinger equation by expanding the initial state in terms of the energy eigenstates of the given potential (solving the *time independent equation*).[1] In other words, we have expressed the wave function as

$$\Psi(x,t) = \sum_n c_n \psi_n(x) e^{\frac{\imath E_n t}{\hbar}}, \tag{1}$$

where ψ_n and E_n are the eigenstates and eigenvalues (associated energies) respectively in the well potential. The energy eigenstates ψ_n are found by solving the time-independent equation,

$$\hat{H}\psi_n(x) = E_n \psi_n(x), \tag{2}$$

where $\hat{H}$ is now a matrix and ψ is an array. The coefficients c_n are given as the projection of the state Ψ on to the eigenstates, i.e

$$c_n = \langle \psi_n, \Psi(x,0)\rangle = \int_{\text{space}} \psi_n^* \Psi(x,0) \mathrm{d}x, \tag{3}$$

which can be approximated by the standard inner (dot) product for array vectors.

Throughout this exercise, we will assume the waves to be in initial states given by a normalised Gauss wave, namely

$$\Psi(x,0) = (2\pi\sigma^2)^{-\frac{1}{4}} e^{-\frac{(x-\langle x\rangle_0)^2}{4\sigma^2}} e^{\frac{\imath p_0 x}{\hbar}}, \tag{4}$$

where $p_0 = \hbar k_0$ is the initial momentum,[2] and the initial expectation value $\langle x\rangle_0$ is selected to be in $x = 5$. We will also select $L = 20$ units to be the range of x, and the wave number to always be $k = k_0 = 20$.

2 Answers to the posed problems

2.1 Problem 1: Initial state

First off, we simply want to create an initial state. We use eq. (4) with $\sigma = 0.75$ to calculate the state, and we show some representations of it in fig. 1.

[1] This is not the method showcased in the exercise sheet, but it is equally valid in time-independent potentials.
[2] As in the work sheet, we use atomic units. We set $m_e = 1$ and $\hbar = 1$ and let the other units be in relation to these.

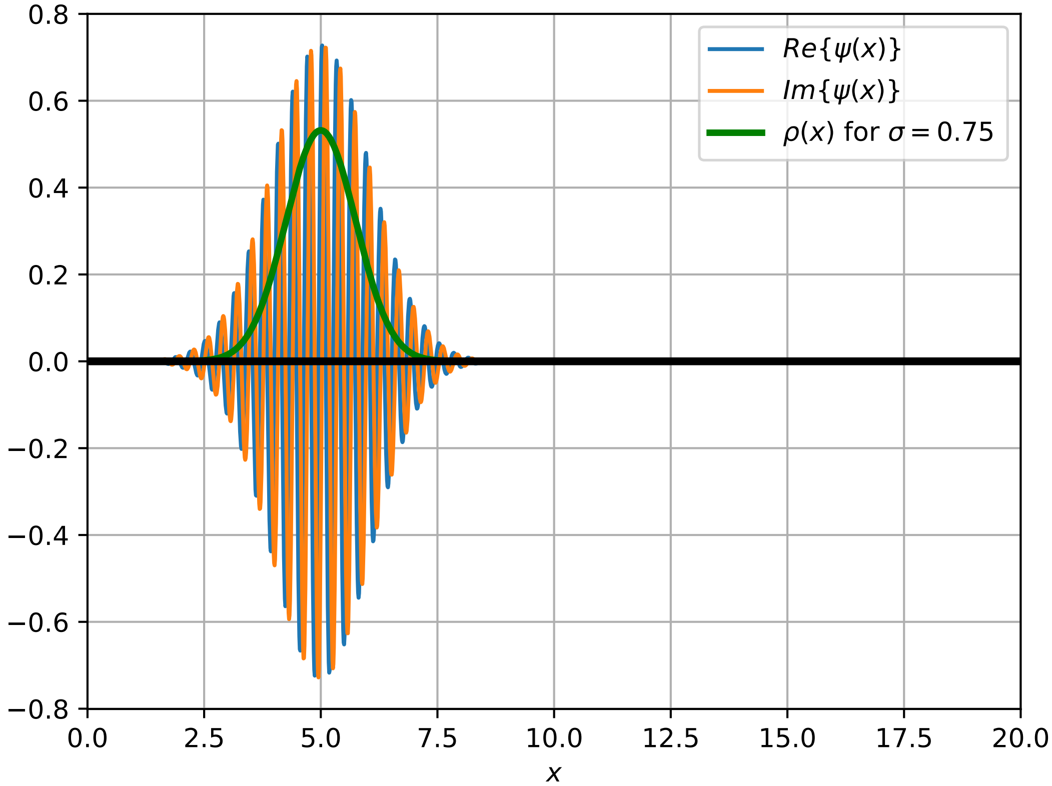

Figure 1: The real and imaginary parts of the starting state $\Psi_0 = \Psi(x, 0)$, and the corresponding probability density $\rho(x) = |\Psi_0|^2$. This state is a Gauss wave centred at $\langle x \rangle = 5$.

2.2 Problem 2: Wave packet propagation

We now want to investigate the propagation of such starting states. We let the wave packet propagate from $\langle x \rangle = 5$ to $\langle x \rangle = 15$. Using Ehrenfest's theorem, we treat the expected position value classically. Thereby, translating $\langle x \rangle$ a distance of 10 units takes a time $T = 10/v_g$, where v_g is the group velocity given by

$$v_g = \left(\frac{\partial \omega}{\partial k}\right)_{k=k_0} = \left(\frac{\partial}{\partial k}\frac{E}{\hbar}\right)_{k=k_0} = \left(\frac{\partial}{\partial k}\frac{p^2}{2m\hbar}\right)_{k=k_0} = \frac{\hbar}{2m}\left(\frac{\partial}{\partial k}k^2\right)_{k=k_0} = \frac{\hbar k_0}{m}. \tag{5}$$

Inserting the T that corresponds to this, and choosing two representative values for σ, $\sigma_1 = 0.5$ and $\sigma_2 = 1.0$, we solve eq. (2) and express Ψ as in eq. (1). The resulting probability densities' development over time can be seen in fig. 2. In this plot, we notice that the wave packets have altered their shape slightly after being propagated. This is known as *dispersion*, and it can be understood by considering that the phase velocity of a wave is frequency-dependent.[3] The initial state is a linear combination of harmonic waves with *different* frequencies,[4] so the observed result is no surprise.

Until now, we have chosen the time discretisation and spatial discretisation to be $\Delta t = 0.01$ and $\Delta x = 0.01$. In atomic units, we have $T = 5$, so within good margin, $\Delta t < T$. As we have used a different method than described in the exercise text, altering Δt does not have any influence on the observed state in $t = T$. This is because in our case, all the numerical heavy lifting is contained to finding the eigenvalues of the $\hat{H}$-matrix, which is discretised in x. Altering Δt also did not impact computing time.

[3] Phase velocity is given by $\omega/k = \lambda/T$.

[4] In fact, the Fourier series of a Gauss wave function has infinitely many non-zero terms.

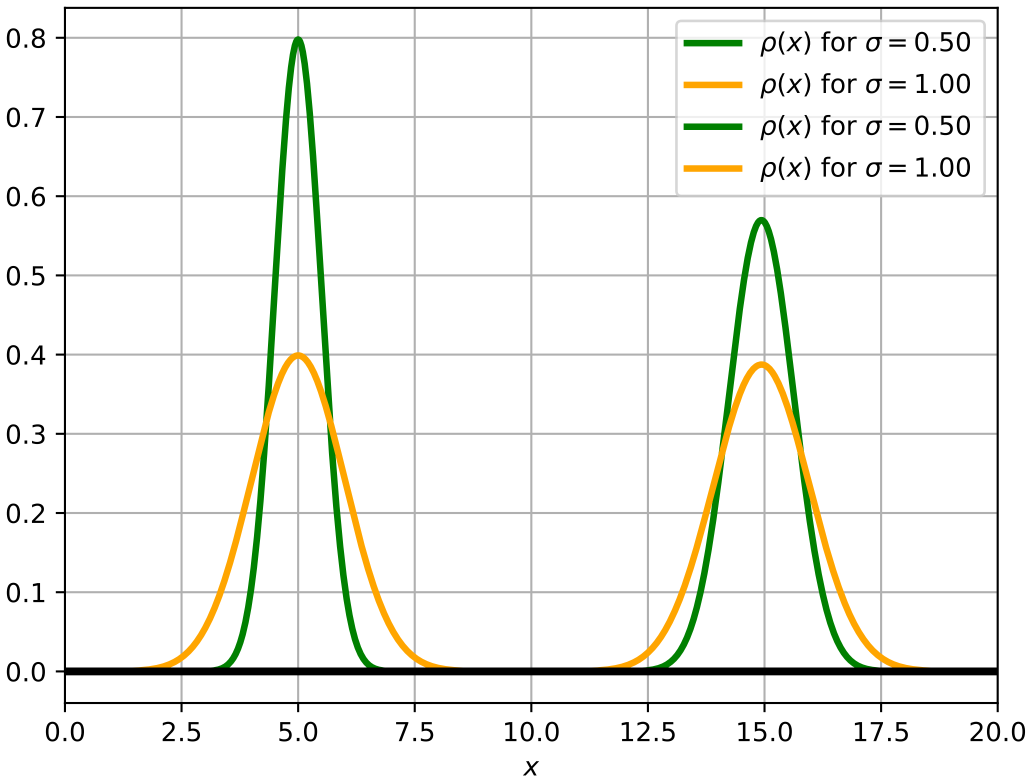

Figure 2: Two different starting states seen in $\langle x \rangle = 5$, and their corresponding states after being propagated to $\langle x \rangle = 15$. We note that dispersion has taken place.

We try to alter Δx instead. Choosing Δx to be as large as 0.1 did not really change the resulting final wave away from its previously dispersed form. However, it really seemed to halt the propagation. Testing for different Δx, we notice that $\Delta x \to 0 \implies \langle x \rangle \to 15$, which is the theoretical value. Larger values (such as $\Delta x = 0.01$), yields $\langle x \rangle$ to become smaller and smaller (thus farther and farther from the theoretical value).

We determine that the previous plots with $\Delta x = 0.01$ are satisfactory, and continue to use this value.

2.3 Problem 3: Wave packet scattering

We now impose a potential barrier for the wave packet (with energy $E = p^2/2m$) to overcome. More specifically, rather than setting $V = V(x) = 0$, we insert a potential barrier with width $l = L/50$ and height $V_0 = E/2$ in the middle of the box such that

$$V(x) = \begin{cases} \frac{E}{2} & \text{if } |x - L/2| < l/2 \\ 0 & \text{if } |x - L/2| \geq l/2 \end{cases} . \tag{6}$$

After the wave packet has hit V, we observe what we refer to as *scattering*. Similar to a wave packet on a rope that consists of two concatenated strings with different mass densities, one part of the wave will *transmit*[5] through the barrier and the other part will *reflect* off the barrier. Whether a particle will

[5] Also called *quantum tunnelling*.

transmit or not is uncertain, but we can examine the *scattering probabilities*

$$P(\text{particle is transmitted}) \equiv \tau \tag{7}$$

$$P(\text{particle is reflected}) \equiv R. \tag{8}$$

We calculate τ by summing up the norm of $\Psi(x, T)$(that is, $\langle x \rangle \approx 15$) on the right-hand side of the barrier,

$$\tau = \int_{L/2}^{L} |\Psi(x, t = T)|^2 \mathrm{d}x. \tag{9}$$

Considering transmission and reflection are the only possibilities, it follows that $R = 1 - \tau$.

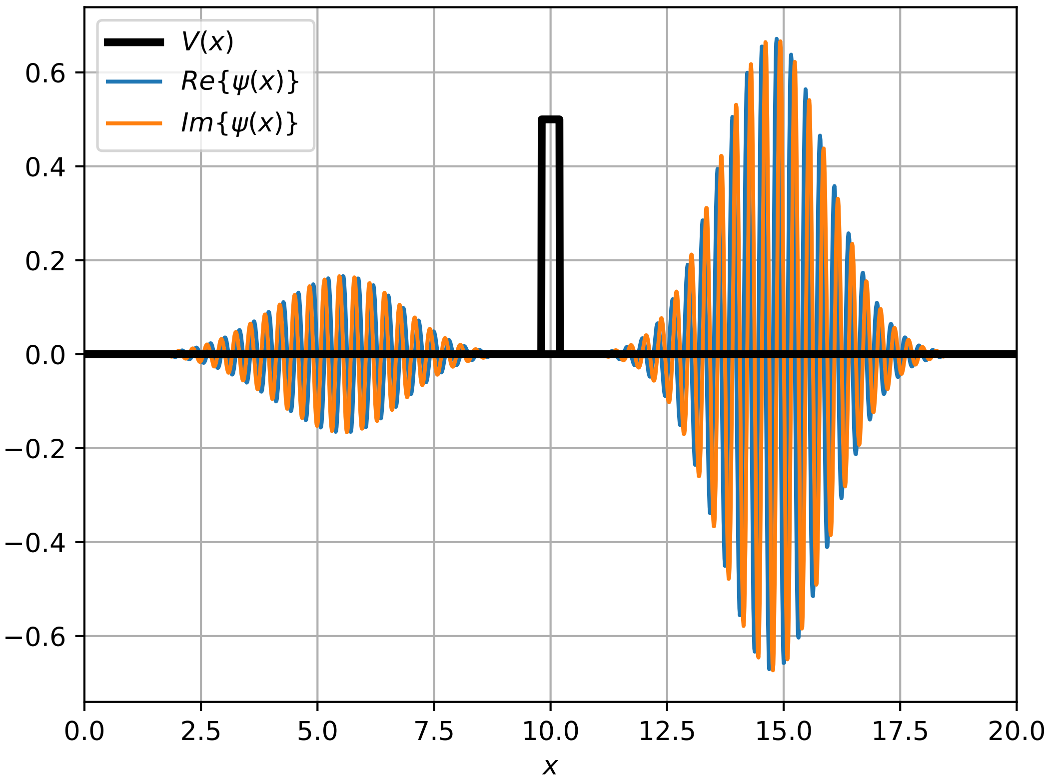

Figure 3: The state after scattering on the potential $V(x) = E/2$. Note that $V(x)$ is scaled down here to fit inside the plot. The part of Ψ to the right of V is transmitted, and the part to the left is reflected.

Using the same initial state as in section 2.1, we let the wave packet propagate over the barrier given in eq. (6). The resulting state is shown in fig. 3. In this case, we found that $\tau = 0.934$ by using eq. (9). Thus, 93.4% of the wave is transmitted and the remaining 6.6% is reflected.

2.4 Problem 4: Scattering on different barrier heights

Keeping the width l the same, we now let the barrier height vary from $V_0 = 0$ to $V_0 = 3E/2$, and calculate τ and R for these different cases. The plot of this is given in fig. 4. We observe that $\tau = 1$ for $V_0 = 0$ (no barrier at all), and $\tau \to 0$ for very tall barriers. No surprises here.

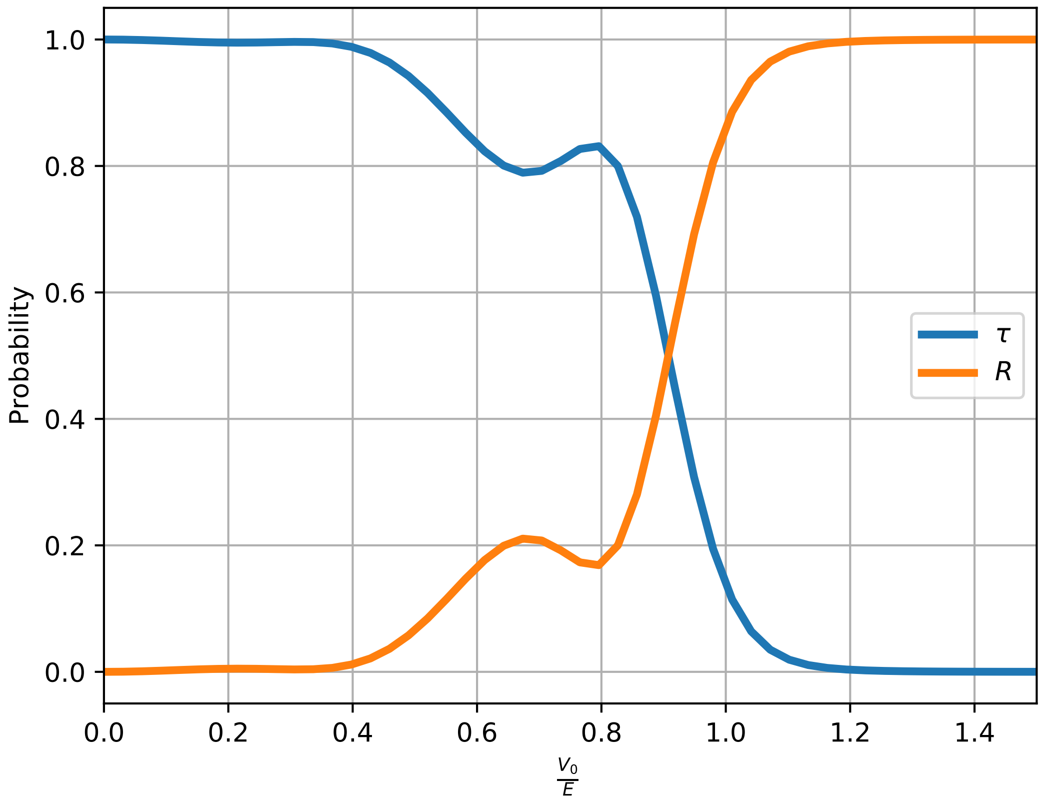

Figure 4: Probabilities of transmission, τ, and reflection, R, for different barrier heights. The barrier width is $l = L/50$.

2.5 Problem 5: Scattering on different barrier widths

Now keeping the barrier height at $V_0 = 9E/10$, we plot τ and R for barrier widths varying from $l = 0$ to $l = L/20$ in fig. 5.

Unsurprisingly, no barrier width gives $\tau = 1$, but unlike the previous case, it is not obvious from the figure what happens for large l. A extended numerical calculation could maybe be run here.

3 Closing words

3.1 Bonus problems

For the sake of time, we did not solve the bonus problems. However, we present some ideas about how we *could*[6] have solved them with a base in the code we have written so far.

Periodic boundary conditions could *probably* be implemented in the definition of $\hat{H}$, by adding matrix elements of 1 in the top-right and bottom-left hand corners. These correspond to how the Ψ-components in the far edges in our defined area interact with each other, and inserting this value would imply we want $\Psi(0) = \Psi(L)$.

Arbitrarily shaped potentials would pose no larger challenge than to write the potential as a function $(V(x))$ in python, and the exactly repeating the procedure from section 2.3.

[6]Meaning none of this is tested. I'm just writing down possible solutions as I come up with them right now.

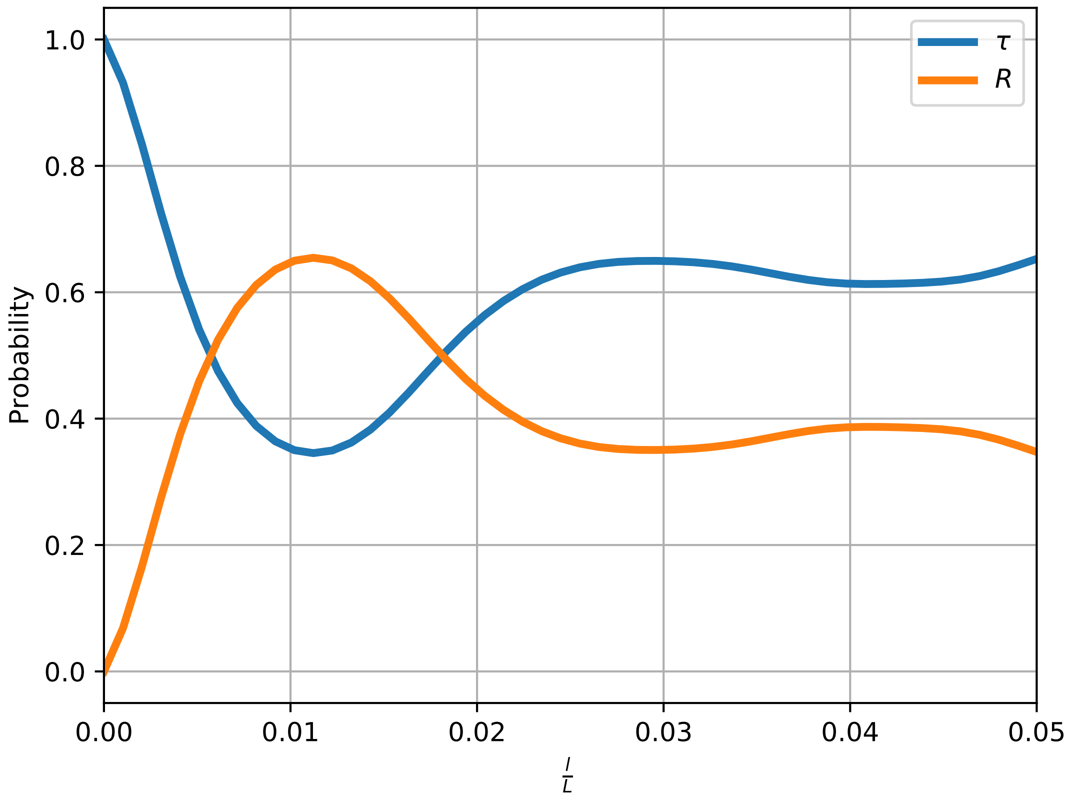

Figure 5: Probabilities of transmission, τ, and reflection, R, for different barrier widths. The barrier height is $V_0 = 9E/10$.

3.2 Summary

Using numerical analysis, we have seen the Schrödinger equation in action. After defining a particle as a wave packet, we have demonstrated dispersion in wave packet propagation and scattering on (rectangular) barriers. We found that a incoming particle is more likely to be reflected from a large barrier. Also, we have found that some proportion of particles will be reflected by small barriers, and some proportion will transmit through large barriers. Classically, we would expect transmission and reflection to be determined solely by comparing V and E, but the quantum world proves to be different yet again.