Wave Packet Dynamics

Joar Svartholm - josv0150(josv0150@student.umu.se)

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Abstract

abstract

Numerical Methods in Physics
Supervisor:Claude Dion

Contents

1 Introduction

Quantum particles does not behave like ordinary particles. This is due to the fact that their motion cannot simply be determined by the position and velocity of the particle, that is, because their position is not well defined. According to the Heisenberg principle, it is impossible to determine the exact position and momentum of a particle at the same time. The position can however be modeled by a probability density, spanning all over space. This makes it possible only to find analytic solutions to the dynamics of a quantum particle for only a few sets of potentials and initial conditions. This is why numerical methods are of high importance when studiyng quantum effects. It is possible to model and simulate these by solving the time dependent Schrödinger equation (TDSE) numerically using high level algorithms. The complexity of this situation is that since the position is described by a probability density, a wavefunction, one must store and manipulate data from all over space in each time step in comparison to ordinary particles where only the position an momentum is needed. This makes the problem of solving TDSE non-trivial and only high performance computers able to finish the task within reasonable time.

In this report, TDSE will be solved for a free particle, a particle hitting a potential well and a potential barrier and the quantum effects that occur will be studied. In the end two different numerical methods of solving TDSE for the potential barrier will be compared in means of computational time.

2 Theory

The dynamics of a quantum particle is described by the time dependent Schrödinger equation

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\psi(x,t) = \hat{H}\psi(x,t) \tag{TDSE}$$

where $\hbar$ is planck's constant, ψ is the wavefunction of the particle, $i = \sqrt{-1}$ and $\hat{H}$ is the Hamiltonian

$$\hat{H} = \hat{T} + \hat{V} = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x), \tag{1}$$

the sum of the kinetic and potential operator. In this equation, m is the mass of the particle and $V(x)$ is the potential. The naive solution to Eq. (TDSE) is

$$\psi(x,t+\Delta t) \approx e^{-\frac{i\Delta t}{\hbar}\hat{H}}\psi(x,t) \tag{2}$$

for any small step size Δt. The problem with this naive solution is that taking the exponential of an operator is non-trivial.

2.1 Split operator method

One way to get around this is by noting that the kinetic operator includes a second derivative in position space but a a simple multiplication in momentum space. Namely that

$$e^{\frac{i\Delta t\hbar}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}}\psi(x,t) \longleftrightarrow e^{-\frac{i\Delta t}{2m\hbar}p^2}\psi(p,t)$$

This motivates the splitting of the hamilton operator into parts, taking the potential operator in position space and the kinetic operator in ordinary space. The final time stepping can thus be written as

$$\psi(x,t+\Delta t) = e^{-\frac{i\Delta t}{2\hbar}\hat{V}}\mathcal{F}^{-1}e^{-\frac{i\Delta t}{\hbar}\hat{T}_p}\mathcal{F}e^{-\frac{i\Delta t}{2\hbar}\hat{V}}\psi(x,t) \tag{3}$$

where $\hat{T}_p$ denotes the kinetic operator in momentum space and $\mathcal{F}$ and $\mathcal{F}^{-1}$ denotes the direct and inverse fourier transform to go from position space to momentum space and vice versa.

2.2 Second-order differencing

2.3 The free particle

In order to study the numerical algorithms for something more interesting it is good to first try them on something with a known solution. Consider the initial gaussian wavefunction with central wavenumber k_0 and width $2\sigma_0^2$

$$\psi(x,0) = \left(\frac{1}{\pi\sigma_0^2}\right)^{1/4} e^{ik_0x}e^{-(x-x_0)^2/2\sigma_0^2}. \tag{4}$$

The analytical solution to Eq. (TDSE) for this initial condition using $V(x) = 0$ yields

$$\psi(x,t) = \left(\frac{\sigma_0^2}{\pi}\right)^{1/4} \frac{e^{i\phi}}{(\sigma_0^2 + it)^{1/2}} e^{ik_0x} exp\left[-\frac{(x-x_0-k_0t)^2}{2\sigma_0^2+2it}\right] \tag{5}$$

where $\phi \equiv -\theta - k_0^2t/2$ and $\tan\theta = t/\sigma_0$.

2.4 The potential well

Changing the potential to

$$V(x) = \begin{cases} -V_0 & , |x| < a \\ 0 & , \text{else} \end{cases} \tag{6}$$

yields a more interesting case, with V_0 being a positive constant. Outside of the well the wave will propagate as a free particle (Eq. (5)) but when it hits the well it will either transmit through or reflect back. Since the wavefunction corresponds to a probability it can be shown that the probability of transmittance and reflectance will depend on the energy of the wave, and hence depend on the central wavenumber k_0. Namely that

$$T = \frac{1}{\left(1 + [V_0^2/4E(E+V_0)]\sin^2(2a\sqrt{2m(E+V_0)/\hbar^2})\right)}, \tag{7}$$

where $E = \hbar^2k_0^2/2m$ is the average energy of the particle, is the probability of the particle being transmitted through the well and similarly $R = 1 - T$ is the probability of reflectance. Looking at Eq. 7 on can see that it will resonate with the potential well and have maximum when

$$2a\sqrt{\frac{2m(E+V_0)}{\hbar^2}} = n\pi, \quad n = 1, 2, ... \tag{8}$$

This could be viewed as standing waves in the potential wave, making the well seem transparent to the wave packet.

2.5 The potential barrier

Changing the sign of V_0 in Eq. (6) yields a potential barrier. Now the intuitive solution would be that the the quantum particle would bounce on the barrier but in quantum mechanics, there is always a probability of transmittance, regardless of the energy of the particle. This is called tunneling. If the energy of the particle is less than the energy of the barrier, the transmission coefficient will be the same as Eq. (7) but with a change of sign from V_0 to $-V_0$. If the energy is larger than the barrier height, the transmission coefficient will be

$$T = \frac{1}{\left(1 + [V_0^2/4E(V_0 - E)] \sinh^2(2a\sqrt{2m(V_0 - E)/\hbar^2})\right)}. \tag{9}$$

The wavenumber corresponding to the energy of the potential barrier is $k_V = \sqrt{2mV_0/\hbar^2}$.

3 Results

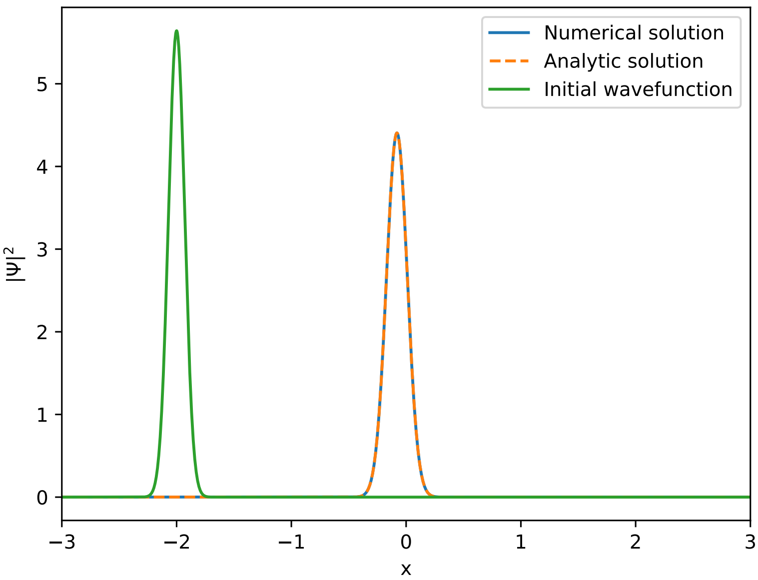

Figure 1: *Numerical and analytic solution of the time dependent schrödinger equation for a free particle.*

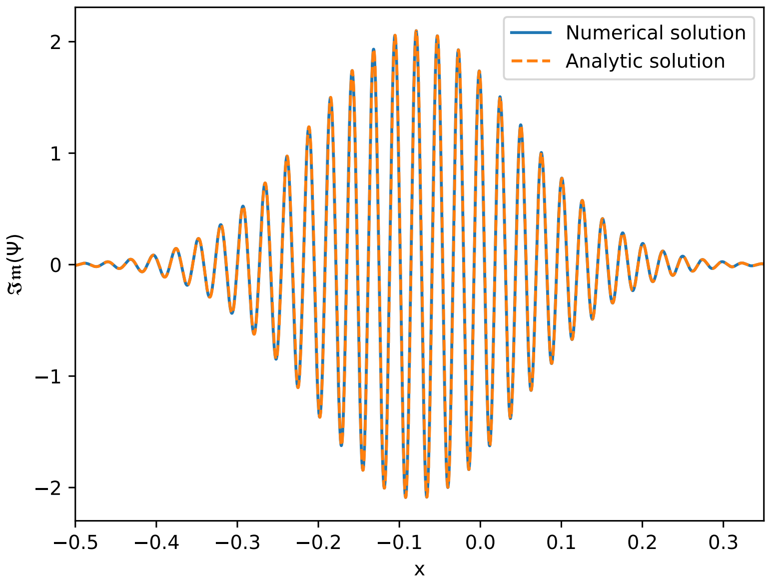

Figure 2: *Imaginary part of the solution in Fig. 1.*

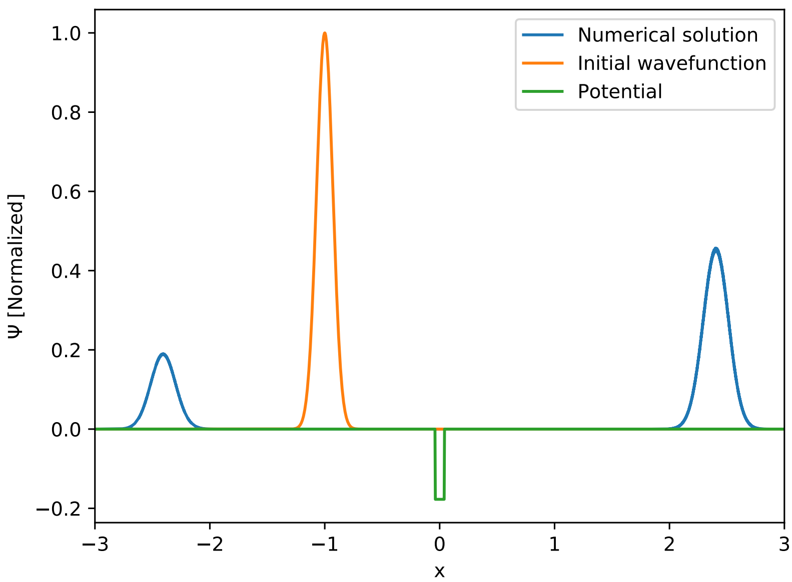

Figure 3: *Numerical solution of the time dependent schrödinger equation of the potential well.*

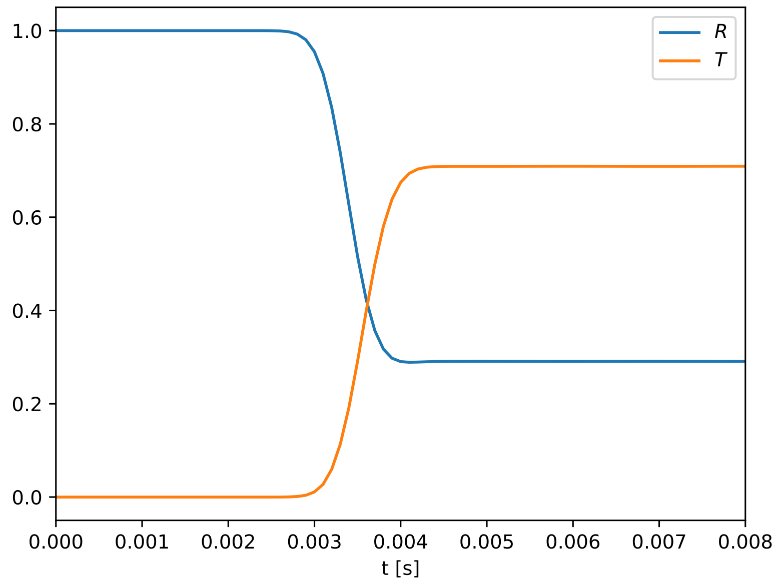

Figure 4: *Reflection and transmission coefficient of the particle in Fig. 3.*

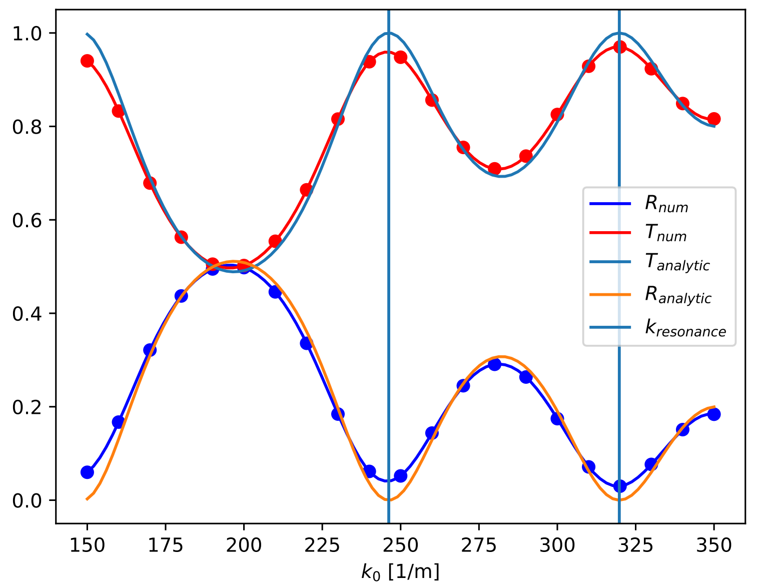

Figure 5: *Reflection and transmission coefficient for different center wave numbers used.*

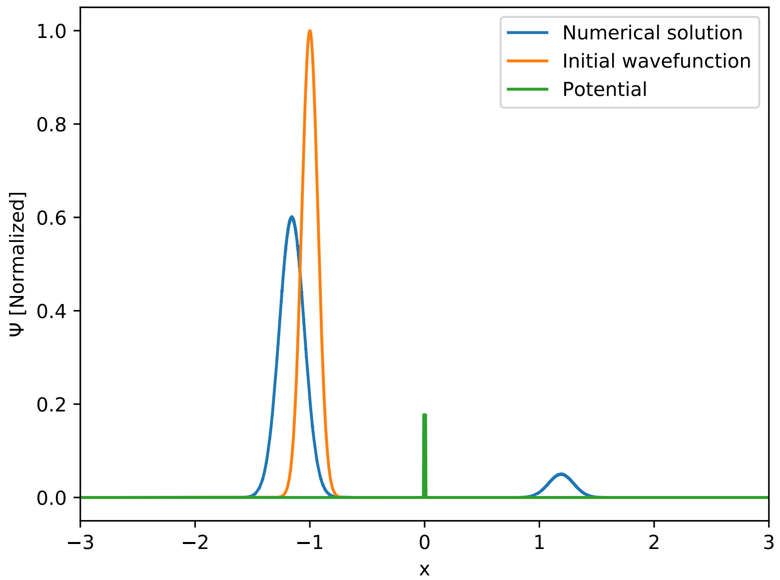

Figure 6: *Numerical solution of the time dependent schrödinger equation of the potential barrier.*

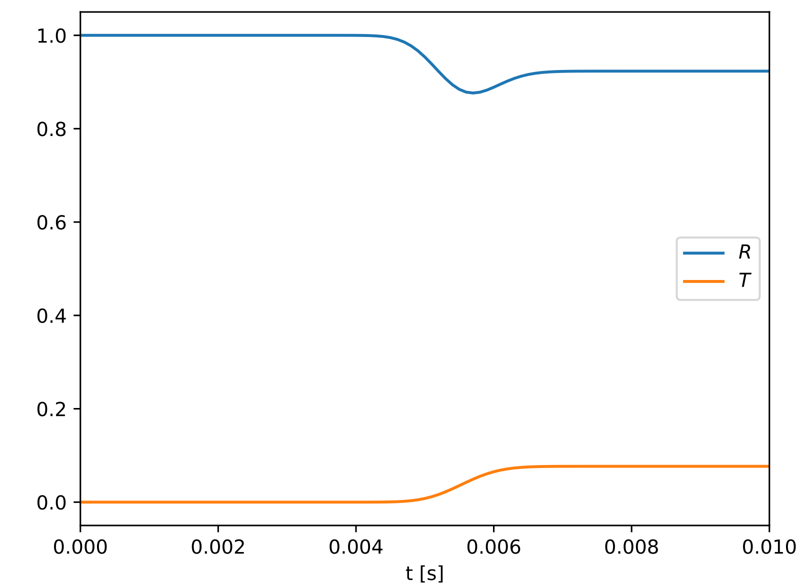

Figure 7: *Reflection and transmission coefficient for the particle in Fig. 6*

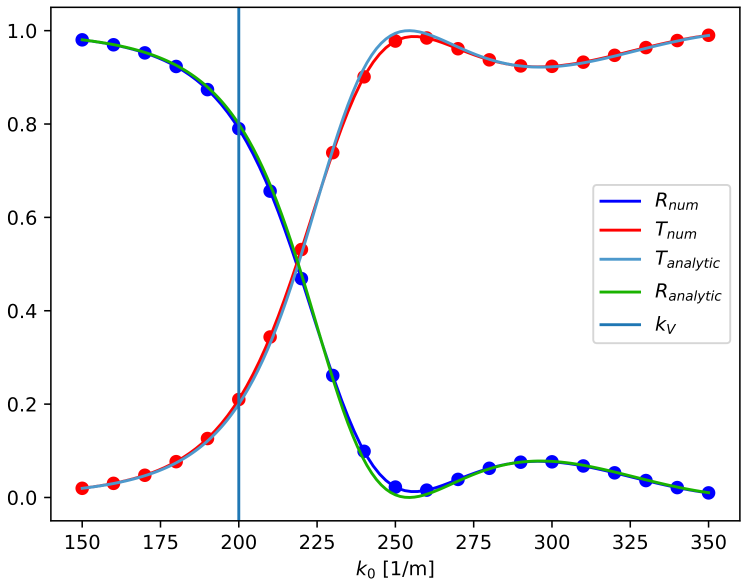

Figure 8: *Reflection and transmission coefficient for different center wavenumbers used. k_V is the wavenumber corresponding to the potential barrier height.*