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Wave Packet Dynamics

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Abstract

abstract

Numerical Methods in Physics
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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 two 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. Note that the potential operator is also split into two parts in order to make the operation unitary and thus reversible.

2.2 Second-order differencing

Another approach to this problem is to make a taylor expansion of the exponential. By doing this in one direction and again in the other and taking the difference yields the Second-order differencing method. Namely by subtracting

$$\begin{aligned}\psi(t+\Delta t) &= e^{-\frac{i\Delta t}{\hbar}\hat{H}}\psi(t)\\ \psi(t-\Delta t) &= e^{\frac{i\Delta t}{\hbar}\hat{H}}\psi(t)\end{aligned} \tag{4}$$

to get

$$\psi(t+\Delta t) - \psi(t-\Delta t) = (e^{-\frac{i\Delta t}{\hbar}\hat{H}} - e^{\frac{i\Delta t}{\hbar}\hat{H}})\psi(t). \tag{5}$$

By expanding the exponentials we get

$$\begin{aligned}e^{-\frac{i\Delta t}{\hbar}\hat{H}} &= 1 - \frac{i\Delta t}{\hbar}\hat{H} - \frac{\Delta t^2}{2\hbar^2}\hat{H}^2 + \frac{i\Delta t^3}{3!\hbar^3}\hat{H}^3 + \mathcal{O}(\Delta t^4)\\ e^{\frac{i\Delta t}{\hbar}\hat{H}} &= 1 + \frac{i\Delta t}{\hbar}\hat{H} - \frac{\Delta t^2}{2\hbar^2}\hat{H}^2 - \frac{i\Delta t^3}{3!\hbar^3}\hat{H}^3 + \mathcal{O}(\Delta t^4)\end{aligned} \tag{6}$$

which leads to

$$(e^{-\frac{i\Delta t}{\hbar}\hat{H}} - e^{\frac{i\Delta t}{\hbar}\hat{H}})\psi(t) = -\frac{2i\Delta t}{\hbar}\hat{H} + \mathcal{O}(\Delta t^3). \tag{7}$$

This means that the update scheme for this method can be written as

$$\psi(t+\Delta t) = -\frac{2i\Delta t}{\hbar}\hat{H}\psi(t) + \psi(t-\Delta t). \tag{8}$$

The man difficulty with this method is that two previous values are needed in order to start the sequence. A common solution to this is by taking one Euler step back in time in order to find ψ_{-1}. More about how this was implemented is found in the method section, Sec. 3.2.

2.3 The free particle

In order to study the numerical algorithms 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 $2\sigma_0^2$

$$\psi(x,0) = \left(\frac{1}{\pi\sigma_0^2}\right)^{1/4} e^{ik_0x}e^{-(x-x_0)^2/2\sigma_0^2}. \tag{9}$$

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

$$\psi(x,t) = \left(\frac{\sigma_0^2}{\pi}\right)^{1/4} \frac{e^{i\phi}}{(\sigma_0^2 + it)^{1/2}} e^{ik_0x} exp\left[-\frac{(x - x_0 - k_0t)^2}{2\sigma_0^2 + 2it}\right] \tag{10}$$

where $\phi \equiv -\theta - k_0^2t/2$ and $\tan\theta = t/\sigma_0$. By comparing this analytial solution to the one obtained by the numerical solution one can determine the validity and and stability of the numerical algorithm.

2.4 The potential well

Changing the potential to

$$V(x) = \begin{cases} -V_0 & , |x| < a \\ 0 & , \text{else} \end{cases} \tag{11}$$

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. (10)) 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

$$T = \frac{1}{\left(1 + [V_0^2/4E(E+V_0)]\sin^2(2a\sqrt{2m(E+V_0)/\hbar^2})\right)}, \tag{12}$$

where $E = \hbar^2k_0^2/2m$ is the average energy of the particle. Now T is the probability of the particle being transmitted through the well and similarly $R = 1 - T$ is the probability of reflectance. Looking at Eq. 12 on can see that it will resonate with the potential well and have maximum when

$$2a\sqrt{\frac{2m(E+V_0)}{\hbar^2}} = n\pi, \quad n = 1, 2, ... \tag{13}$$

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

2.5 The potential barrier

Changing the sign of V_0 in Eq. (11) 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. (12) 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

$$T = \frac{1}{\left(1 + [V_0^2/4E(V_0 - E)]\sinh^2(2a\sqrt{2m(V_0 - E)/\hbar^2})\right)}. \tag{14}$$

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

3 Method

In order to study the quantum particle using the methods in Sec. 2 the program called `wavepacket` was used [1]. First, the initial wavefunction was implemented together with a zero potential and the wave was simulated for $6.8 \cdot 10^{-3}$s using $k_0 = 200$ and the resulting wave was analyzed. Next, the potential was replaced with a potential well. For this case simulations was done for different inital wavenumbers from 250 to 350 in steps of 10 in order to find a relation of the reflection and transmission coefficients and thus be able to verify Eq. (12). The reflection and transmission coefficients was computed as

$$\begin{aligned} R &= \int_{-\infty}^{-a} |\psi(x,t)|^2 \mathrm{d}x \approx 0.5\psi(x=-8,t) + \sum_{i=1}^{x(i)<-a} \psi(x=-8+i\Delta x,t) + 0.5\psi(x=-a,t) \\ T &= \int_{a}^{\infty} |\psi(x,t)|^2 \mathrm{d}x \approx 0.5\psi(x=a,t) + \sum_{x(i)>a}^{x(i)<8} \psi(x=a+i\Delta x,t) + 0.5\psi(x=8,t) \end{aligned} \tag{15}$$

The final coefficients of each simulation was then used to plot R, T against the wavenumber.

The same study was then done with the potential changed to a barrier instead of a well.

As a final study the numerical algorithm was changed and the program `diffScheme` was used. The same results as with the potential barrier was produced and the two algorithms

was compared by the means of excecution time. In order to make a fair comparison both programs produced the same output and was set to the same simulated time in means of seconds.

3.1 wavepacket.c

The program `wavepacket` is a simulation program for quantum particles using the split-operator method described in Sec. 2.1. The program was used with different potentials yielding different executable files. There three potentials can be compiled using either of the commands

- `make freepart`
- `make potwell`
- `make barrier`

for the free particle, potential well and potential barrier correspondingly. The program uses `FFTW` in order to compute the fourier transforms so this library must be installed in order to compile the program correctly.

The simulations are then executed by adding and argument file containing the parameters (preferrably the template file in the appendix **??**) and an argument with the initial wavenumber. If the input file is found in a folder called `input_files` then a simulation for the potential well using $k_0 = 200$ could be excetuted using the line

```
./potwell input_files/pot_well_template.in 200
```

3.2 waveDiff.c

The program implementing the second-order differencing scheme is called `waveDiff` and can be compiled by the command `make diffScheme`. No external libraries was used in the implementation of this code. The same datatypes and general funcitons (e.g. the routine for reading parameters and printing results) as in `wavepacket` was used in order to be able to compare the computation times. A similar command can be used to execute a simulation using this program. Note however that the time step used must be about $5 \cdot 10^{-8}$ in order to achieve convergence.

4 Results

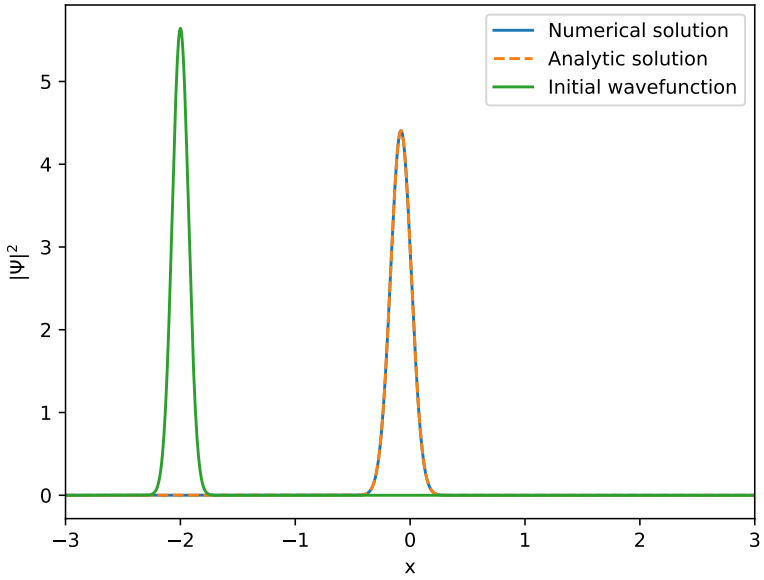

Figure 1: *Numerical and analytic solution of the time dependent schrödinger equation for a free particle.*

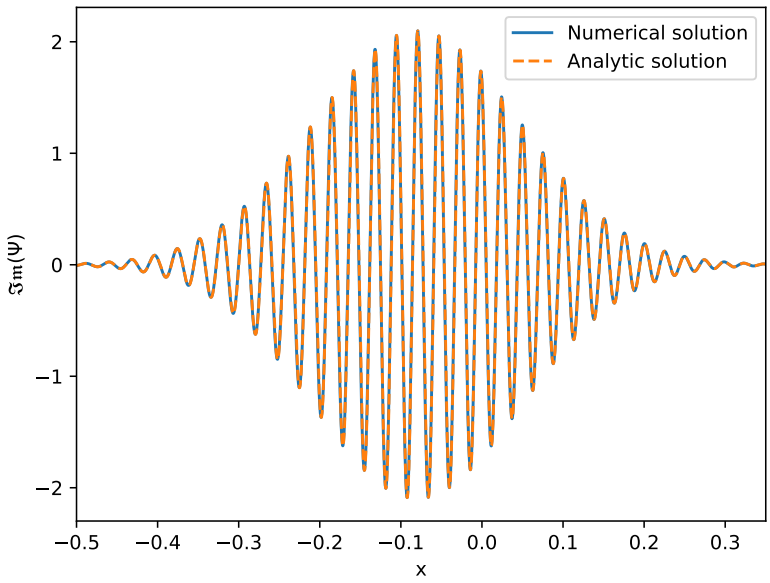

Figure 2: *Imaginary part of the solution in Fig. 1.*

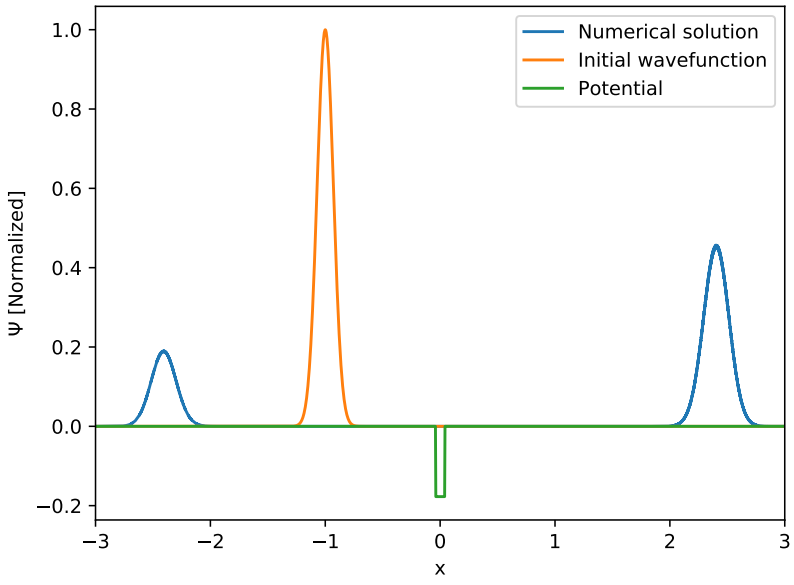

Figure 3: *Numerical solution of the time dependent schrödinger equation of the potential well.*

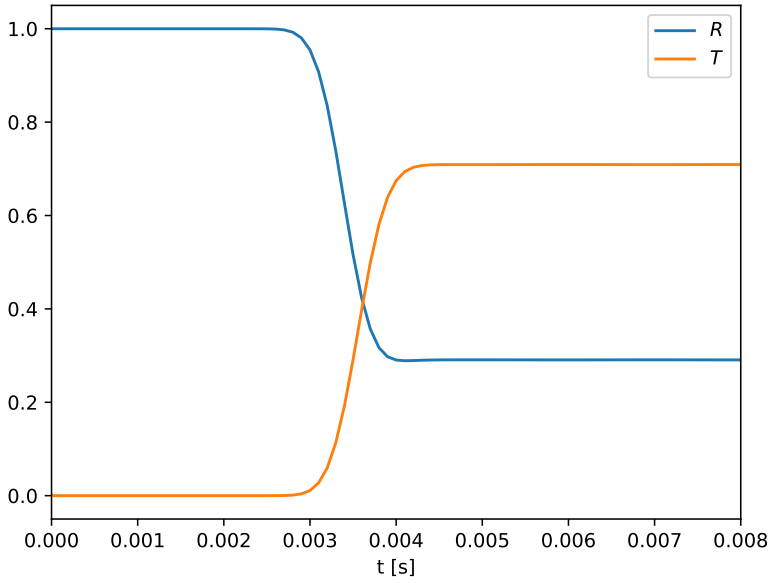

Figure 4: *Reflection and transmission coefficient of the particle in Fig. 3.*

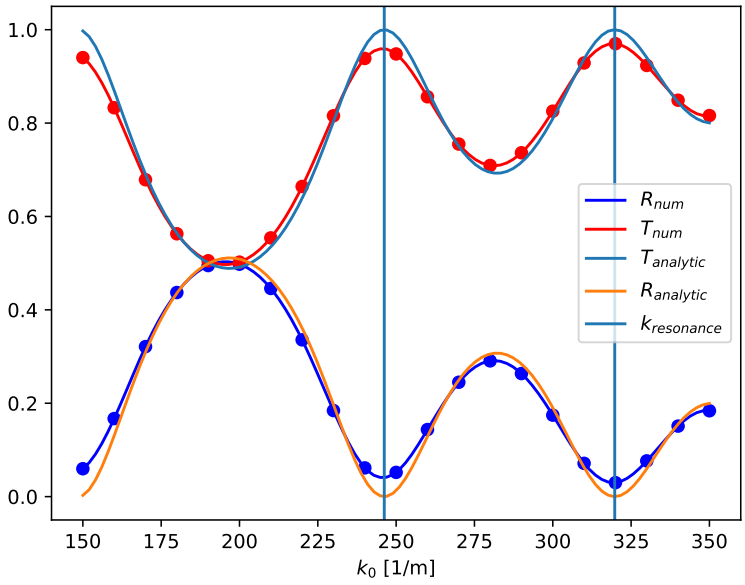

Figure 5: *Reflection and transmission coefficient for different center wave numbers used.*

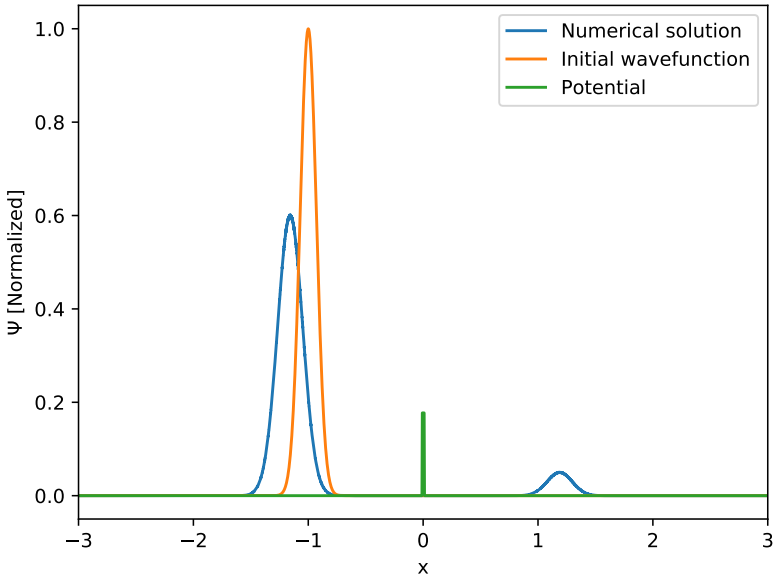

Figure 6: *Numerical solution of the time dependent schrödinger equation of the potential barrier.*

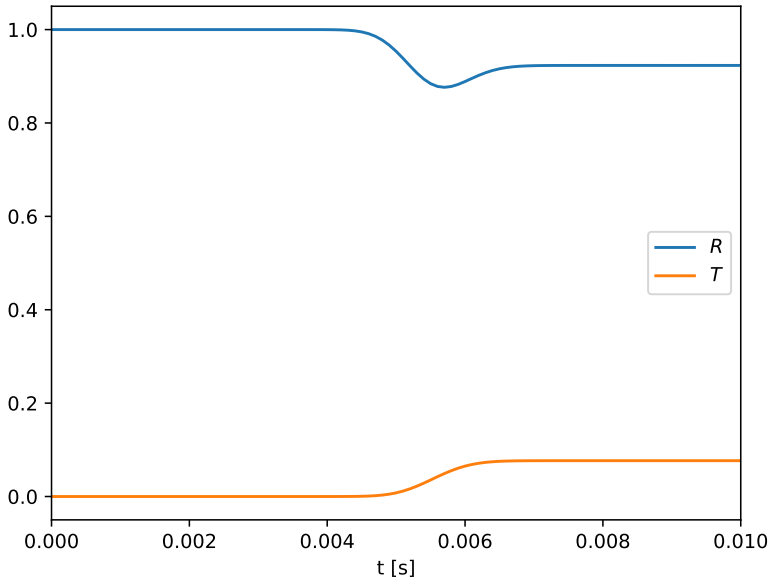

Figure 7: *Reflection and transmission coefficient for the particle in Fig. 6*

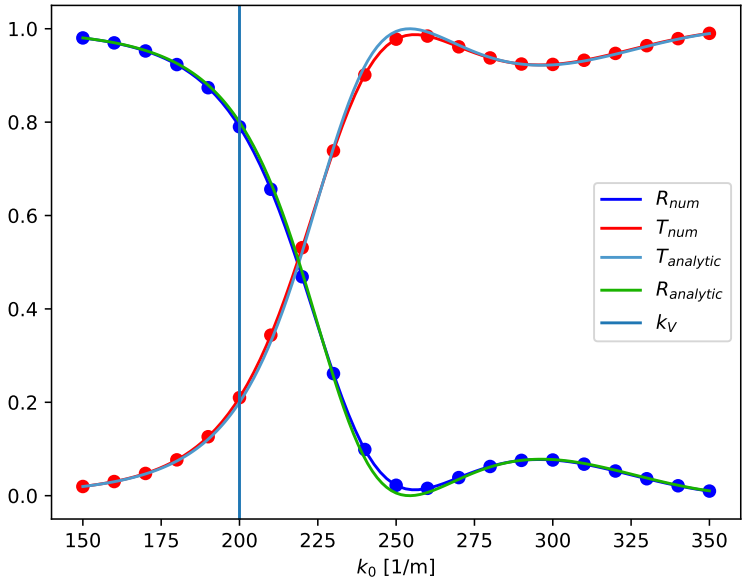

Figure 8: *Reflection and transmission coefficient for different center wavenumbers used. k_V is the wavenumber corresponding to the potential barrier height.*

References

[1] C. M. Dion, A. Hashemloo, and G. Rahali, Program for quantum wavepacket dynamics with time-dependent potentials, Comput. Phys. Commun. 185, 407 (2014).