Simulating the Time Dependent Schrödinger Equation on a Lattice

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Contents

1 Introduction

In this report, we present three algorithms/integrators to solve the time dependent Schrödinger equation: **Euler Integrator**, **Crank-Nicolson Integrator** and the **Strang Splitting Integrator**; discuss the evolution of the observables per timestep and give a visual animation for both 1D and 2D. The Modules that are constructed to solve the problem are the following:

Module Name	Summary
initialize_psi.py	Implements the Gaussian-wavepacket which will be propagated.
time_propagators.py	Implements time propagators, and tests their related properities (unitarity/energy conservation)
main.py	The main code and cli-based user interface
analyse.py	The module which is used to evaluate observables, norms etc. for each time step.
convergence_plot.py	Generate a convergence plot comparing all three propagators.

Table 1: Summary of python modules

The modules above also imports the modules that are constructed in TISE - Implementation, please see the related report to get more information about them. For an introduction on how to use the code, see 'README.md'

2 The Unit System

2.1 The Unitless Hamiltonian

As in the last project, before we start with simulations will have to entirely get rid of our units. For this we will take a look at the continuum Hamiltonian:

$$H = -\frac{\hbar^2}{2m}\sum_{i=1}^{d}\frac{\partial^2}{\partial x^2} + V_0\chi_{[0,\Delta x]}(x)$$

where

$$\chi_{[0,\Delta x]}(x) = \begin{cases} 1 & \text{if} \quad x \cdot e_1 \in [0, \Delta x] \\ 0 & \text{else} \end{cases}$$

Here Δx is the width of our potential barrier in x direction. In all other directions it spans out to infinity. V_0 is the hight of the potential barrier.
In the discretised case where $x \to an$ (a is the lattice spacing n is the lattice vector), our Hamiltonian does also change form a little.

$$H = -\frac{\hbar^2}{2m}\frac{1}{a^2}\sum_{i=1}^{d} D_i^2 + V_0\chi_{[0,\Delta x]}(an)$$

where

$$D_i^2\psi(an) = \psi(a(n+e_i)) + \psi(a(n-e_i)) - 2\psi(an)$$

Now we again want only dimensionless variables in our Hamiltonian. For length we will choose $aB = \Delta x$. One could now argue that V_0 is the natural energy unit in this problem. This however leads to problems when $V_0 = 0$. We will therefor choose as our reference energy: $E_0 = \frac{\hbar^2}{m(\Delta x)^2} = \frac{\hbar^2}{m(aB)^2}$ [1]. Finally, our unitless Hamiltonian looks like the following:

$$\hat{H} = \frac{H}{E_0} = -\frac{B^2}{2}\sum_{i=1}^{d} D_i^2 + \mu\chi_{[0,b]}(n)$$

where

$$\mu = \frac{m(aB)^2 V_0}{\hbar^2}$$

[1] Note that this is proportional to the kinetic energy of a free particle with wavelength $\lambda = \Delta x$

Additionally, this implies a natural choice for the units of t if we have a look at the unitary time propagator:

$$U_t = \exp\left\{-i\frac{Ht}{\hbar}\right\} = \exp\left\{-i\hat{H}\hat{t}\right\} \longrightarrow \hat{t} = t\frac{E_0}{\hbar}$$

And for the single time step we define $\frac{E_0}{\hbar}\tau = dt$. If not stated else, the total time T is given in units of $\frac{\hbar}{E_0}$ as well.

2.2 The discrete Wavepacket

A gaussian Wavepacket can be parametrized in the following way:

$$\psi(x) = A^{-1}\exp\left\{-\frac{(x-x_0)^2}{4\sigma^2} + ix\cdot k\right\}$$

Some simple calculations show that:

$$\begin{aligned} \langle x\rangle_\psi = x_0, \qquad & \langle p\rangle_\psi = \hbar k \\ Var(x)_\psi = \sigma^2, \qquad & Var(p)_\psi = \frac{\hbar^2}{4\sigma^2} \\ |A|^2 \quad = \quad & \int_{-\infty}^{\infty} \mathrm{d}x^d \exp\left\{-\frac{(x-x_0)^2}{2\sigma^2}\right\} \end{aligned}$$

Now let us consider the discrete version of ψ and express it in terms of unitless parameters:

$$\begin{aligned} \sigma = aB\frac{\sigma}{\Delta x} = aBs, \quad s = \frac{\sigma}{aB} \\ x - x_0 = an - a\frac{x_0}{a} = a(n-n_0), \quad n_0 = \frac{x_0}{a} \\ k = \frac{2\pi}{\Delta x}(\frac{\Delta x}{2\pi}k) = \frac{2\pi}{aB}\kappa, \quad \kappa = \frac{k}{aB/2\pi} \end{aligned}$$

Then our discrete wave function $\hat{\psi}(n)$ looks as the following:

$$\begin{aligned} \hat{\psi}(n) = \tilde{A}^{-1}\exp\left\{-\frac{(n-n_0)^2}{4(sB)^2} + i\frac{2\pi}{B}n\cdot\kappa\right\} \\ |\tilde{A}|^2 = \sum_{n\in\mathcal{L}}\exp\left\{-\frac{(n-n_0)^2}{2(sB)^2}\right\}^2 \end{aligned}$$

where $\mathcal{L}$ is the lattice.

2.3 Tunneling

For tunneling we will consider the the expected kinetic energy $\langle T\rangle_{free}$, which has the form of the wave function just defined.

$$\langle T\rangle_{free} = \frac{\langle p^2\rangle}{2m} = \frac{\hbar^2 k}{2m} = \frac{(\hbar 2\pi)^2}{2a^2B^2m}\kappa^2 = 2\pi^2 E_0\kappa^2$$

Tunneling now describes the case where $\langle T_1\rangle_{free} < V_0$ [3]. Now in our Unit system this means

$$\begin{aligned} 2\pi^2\kappa_1^2 < \mu \\ \implies \kappa_1 < \sqrt{\frac{\mu}{2\pi^2}} \end{aligned}$$

3 Tests of the Integrators

We wrote test codes which tests the unitarity and the energy conservation of Crank Nicolson integrator and the unitarity of the Strang Splitting integrator. As mentioned in the lecture, the unitarity is tested by verifying the conservation of the norm. The errors can be found as the following (per time step). The used values are: $N = 800$, $dt = 0.00001$, $B = 40$ $kap = \frac{B^2}{2}$, with randomly generated wave functions and potentials. The error is given as the maximum error of 100 tests with random potentials/(normalized) wave functions.

[3] We only need component in the direction normal to the surface of the barrier barrier, hence we only need T_1

```
Error in cn unitarity is:  9.900746889002221e-12
Error in ss unitarity is:  6.661338147750939e-16
Error in cn energy conservation and the smallest energy for random potential and wavefunction is:  (1.8046310401587107e-06, 367.71425362237164)
```

Figure 1: Tests of Integrators; Crank Nicolson(cn), Strang-Splitting(ss)

- The error in unitarity of the strang splitting integrator is in the magnitude 10^{-16} which can be considered as a numerical error of the algorithms that has been used and errors caused by the lattice discretisation.
- The error in Crank Nicolson unitarity is bigger than the Strang Splitting Integrator. This can be explained by the bigger numerical errors in the underlying Conjugate Gradient algorithm (Compared to the FFT which is used by Strang Splitting Integrator.)
- Again, for the conservation of energy, one must apply the Hamiltonian operator one more time to the evolved wave functions, which gives us a bigger error. Still if we compare this biggest error in energy after 100 iterations to the smallest actually calculated energy, there are still 8 orders of magnitude between them.

3.1 1D

For every following plot we used the following parameters (figures (5),(6)(7),(8)(9)(10). We chose that parameters so that we get a classically forbidden transition ($\langle T \rangle_{free} < V_0$):

$$
\begin{aligned}
&N = 1024, \quad B = 30, \quad \mu = 100.0, \\
&D = 1, \quad \text{tolerance of Conjugate Gradient} = 10 * 10^{-10}, \\
&\text{Recalculate iteration} = 100, \quad s = 1, \\
&k = [2, 25], \\
&n_0 = [-150], \quad dt = 0.001 \quad T = 2
\end{aligned}
$$

3.1.1 Observables

We plotted the evolution of the following observables for each time step:

- Total energy
- Kinetic Energy
- Potential Energy
- Expectation Value of the Position
- Uncertainty on the Position

3.1.2 Discussion

- We see that the Euler Integrator gives bad results in comparison to the others, which was expected since it is the most naive integrator we chose to use.
- ((5), (2)) For Strang-Splitting and the Crank-Nicolson Integrators, we can observe that the total energy is conserved. Energy conservation is actually not a property of the Strang-Splitting Integrator, but because of our choice of fine parameters ($\tau \to 0$), it gives the desired result. We can clearly see when the collision with potential barrier happens: It is the value where we have a peak for potential and a dip for the kinetic energy. After the collision, the wave is reflected/transmitted, and the potential energy is again converted to kinetic energy.
- ((7), (4)) We observe that the mean position begins from negative, increases until it hits the potential barrier (maximum of the mean position graph) and then propagates negatively (because most of it is reflected) as expected. The uncertainty after the collision with the barrier increases since the wave packet splits to two, a reflected and a transmitted part.
- ((6), (3)) For both of the integrators (CN and SS), the change of norm is considerably small (please notice the scalings of the graphs axes.). What is interesting here to notice is that the Strang Splitting Integrator actually preserves the norm far more better, which is an indication that this algorithm suffers less from the errors occuring from their respective underlying algorithms.(As discussed before in Tests in unitarity).

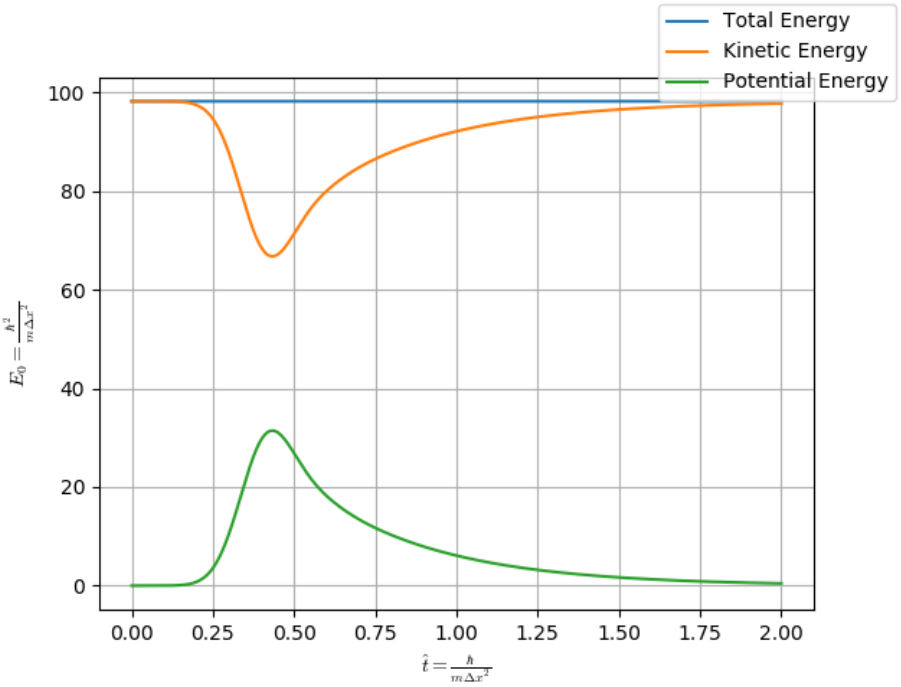

Figure 2: 1D - Energy graphs for Strang-Splitting Integrator.

- Overall the SS and CN integrators produce the same result for expectation values as $\tau \to 0$.
- ((11),(12),(13)) In order to show Euler Integrator can also produce the deserved plots, we fine tune the timestep to $\tau = 0.000005$. In these plots we can see the same behaviour of the energies and the position values again.

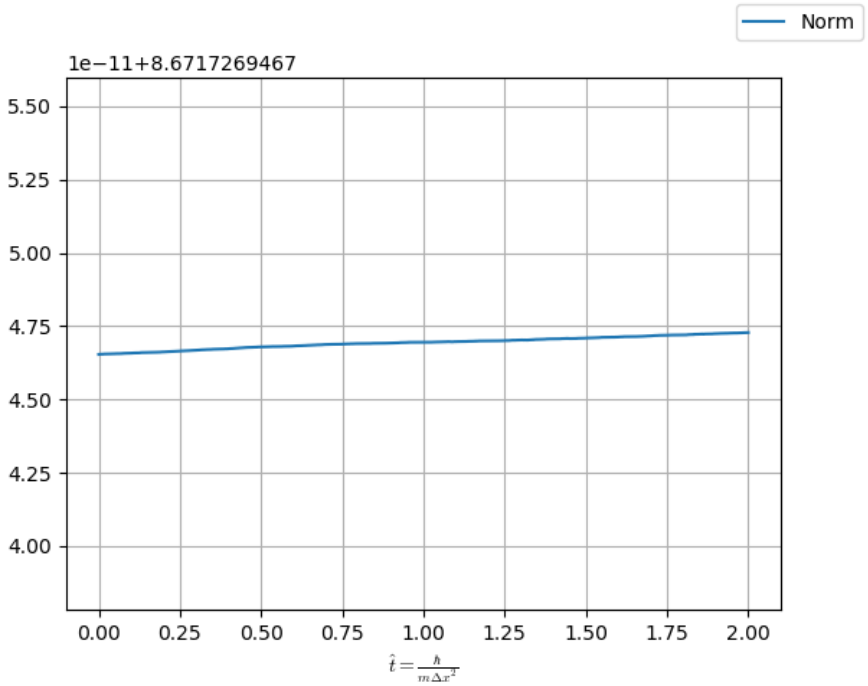

Figure 3: 1D-Evolution of the Norm of the Strang Splitting Integrator

3.2 2D

The Strang-Splitting Integrator is the most promising algorithm out of all three integrators we considered so far. Therefore, from now on, we will run our experiments only with this integrator.

3.2.1 Observables

The parameters we used can be found in the following:

$$
\begin{aligned}
&N = 256 \quad B = 30, \quad \mu = 51.0, \\
&D = 2, \quad \text{tolerance of Conjugate Gradient} = 10^{-9}, \\
&\text{Recalculate iteration} = 100, \quad s = 1, \\
&k = [1.59, 0.5], \\
&n_0 = [-150, -50], \quad dt = 0.005 \quad T = 1
\end{aligned}
$$

Again the parameters are chosen in a way that we consider the classically forbidden transmission.

3.2.2 Discussion

- ((14)) We observe now that the total energy is not conserved, which was an expected result of using Strang-Splitting Integrator. One could argue that the energy conservation can be recovered by $\tau \to 0$, as the 1D Example. What is important to notice is that we can clearly distinguish where the collision with the potential barrier happens, this is the place where kinetic energy has a dip and potential energy has a peak.
- ((15)) With the help of the norm plot one can clearly see that the norm is preserved, hence the unitarity.
- (16) In the position plot we see now 4 graphs instead of 2 since there are two dimensions now and we both have uncertainties and expected values of position in different dimensions. The time when the collusion occurs can be seen from the place of the maxima of the mean value of the x-coordinate. (Since after the maximum the wave gets reflected mostly and propagates in the negative x-direction. As mentioned before in 1D case, the uncertainity in the x-coordinate increases after the collision since the wave packet is divided into a reflected and a transmitted part.

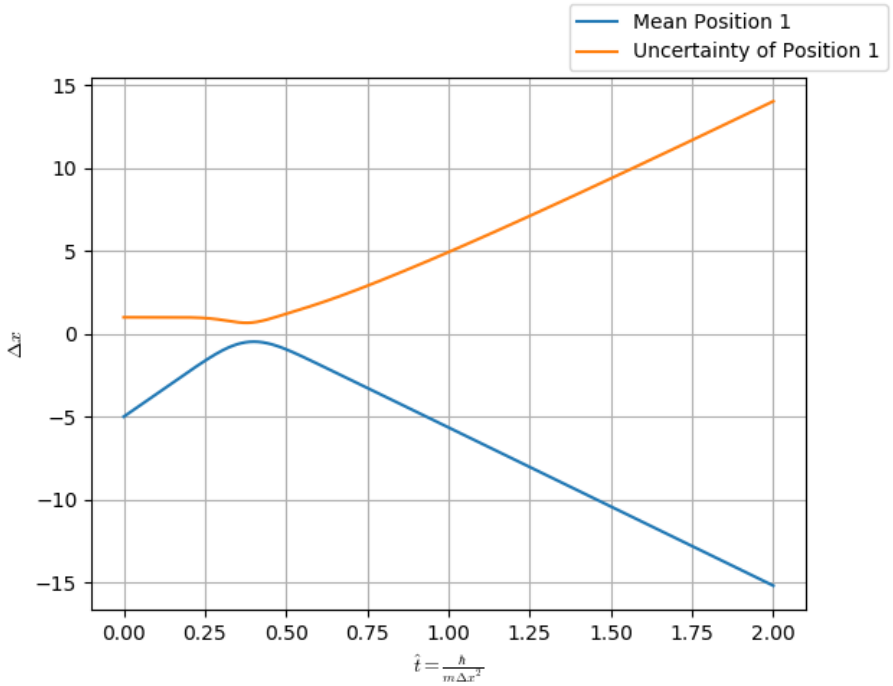

Figure 4: 1D-The Expectation Value and the Uncertainty of the Position for Strang splitting Integrator

3.2.3 Animations

The animations and the related parameter files can be seen in our git-repository, under the folder tdse. The parameter files can be found under tdse/input. In the GIF's there are two animation to be seen, a propagation in position space and a evolution in fourier space.

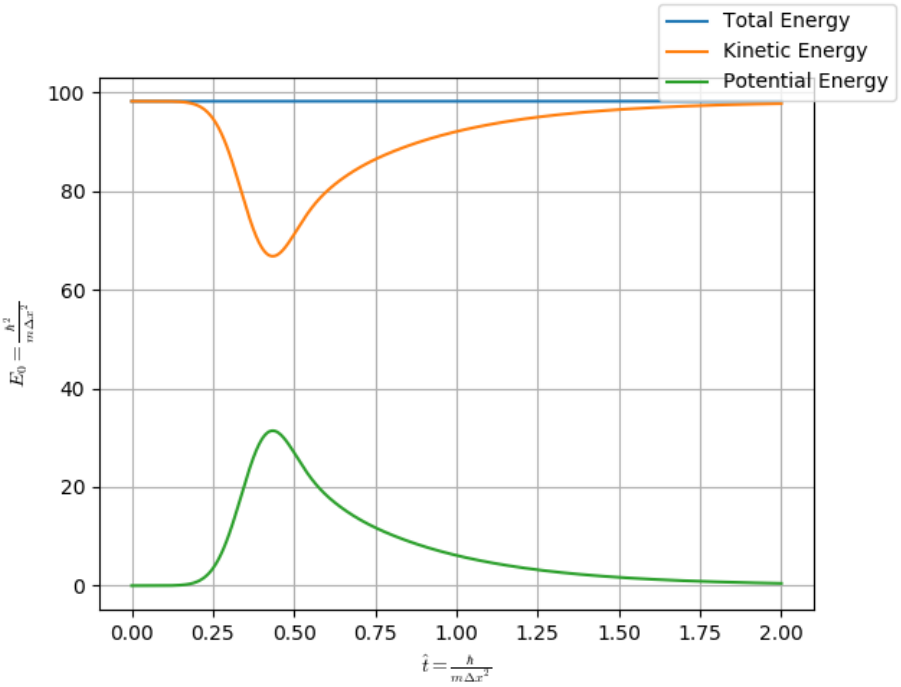

Figure 5: 1D-Energy graphs for Crank-Nicolson Integrator.

4 Convergence Test

For the convergence test we ran the 3 propagator for a total time of $\hat{T} = 0.1$ on with time steps τ between $3 * 10^{-3}$ and 10^{-5}. The simulation was done on a 1D Lattice with 513 Points, $B = 30$, $\mu = 100$.
As a measure of convergence we subtracted the expectation value of the position as calculated by the Strang Splitting Integrator $\langle x \rangle_{ss}$ at $\hat{t} = \hat{T}$ from the other two. We now would expect that the difference $\langle x \rangle_{eu/cn} - \langle x \rangle_{ss}$ goes to zero, faster in the case where we are using the Crank Nicolson Integrator. As is seen in 17 the Crank Nicolson does converge quite fast to the same result as the Strang Splitting and is already quite similar even for comparatively large $\hat{\tau}$. The Euler Integrator needs much smaller time steps to get similar levels of convergence. However at $\tau = 10^{-5}$ the difference $\langle x \rangle_{eu} - \langle x \rangle_{ss} \approx 2 * 10^{-4} \Delta x$, which is well below one Lattice spacing. The convergence also seems to speed up around $\tau = 10^{-4}$. This could be due to less error accumulation from previous steps.

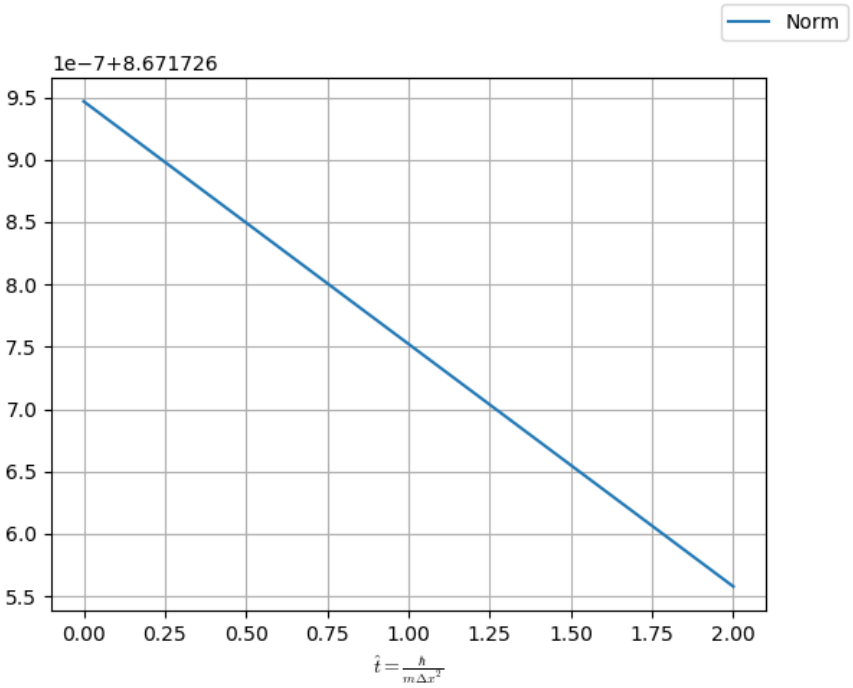

Figure 6: 1D-Evolution of the Norm for the Crank-Nicolson Integrator.

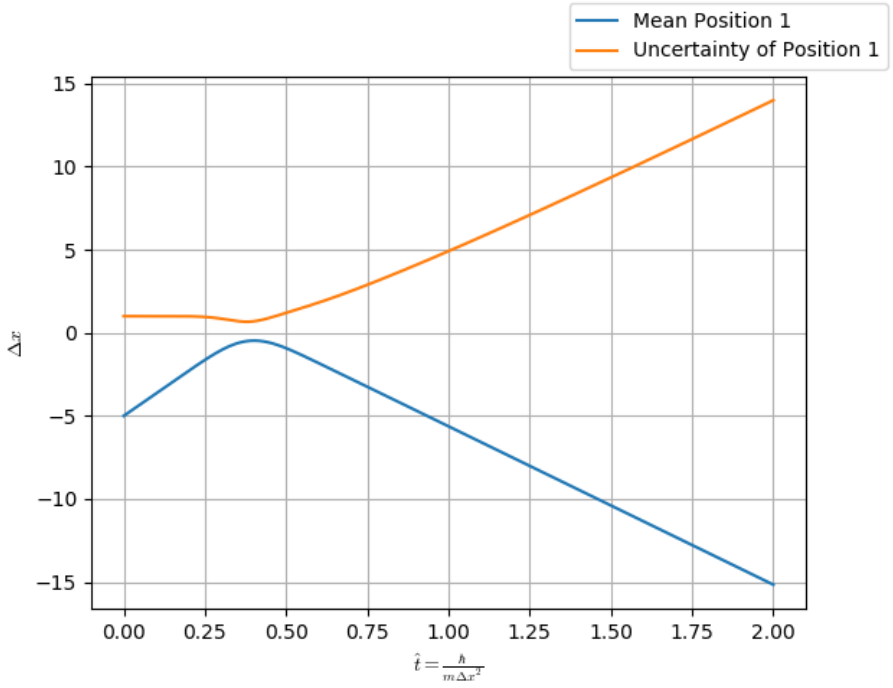

Figure 7: 1D-The Expectation Value and the Uncertainty of the Position for Crank-Nicolson Integrator

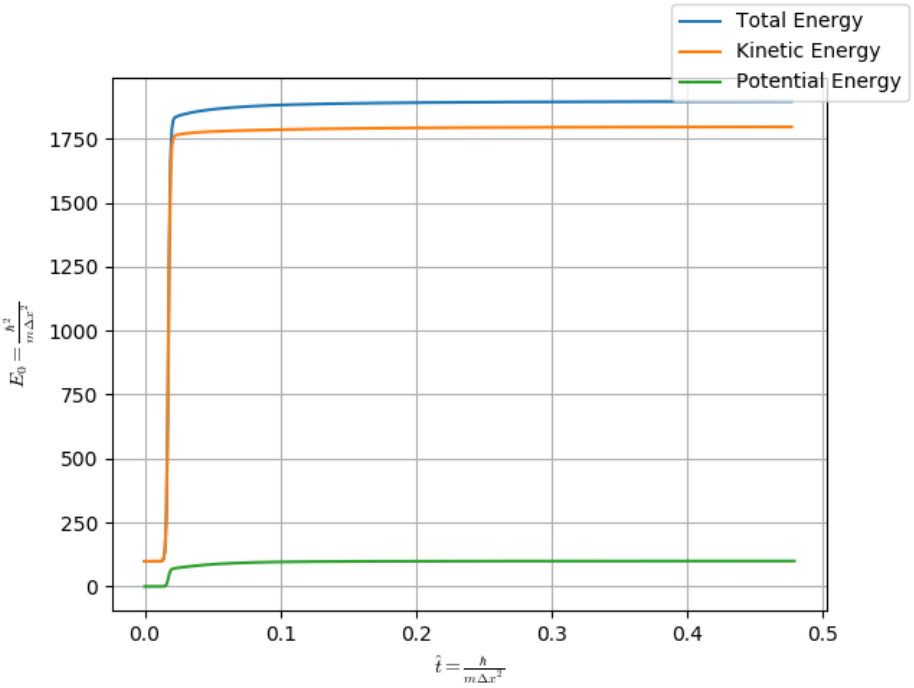

Figure 8: 1D-Energy Graphs for Euler Integrator

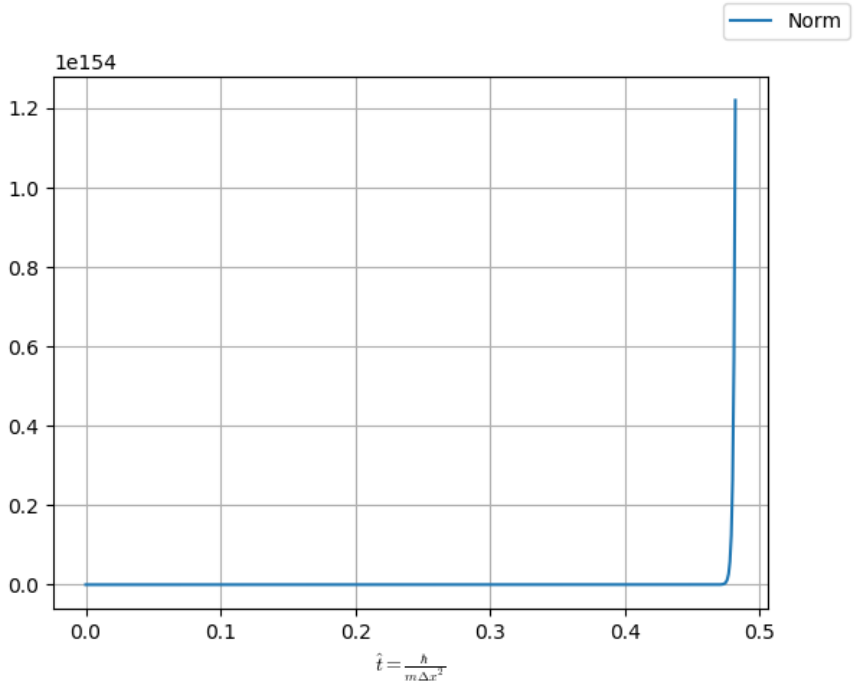

Figure 9: 1D-Norm Evolution for Euler Integrator

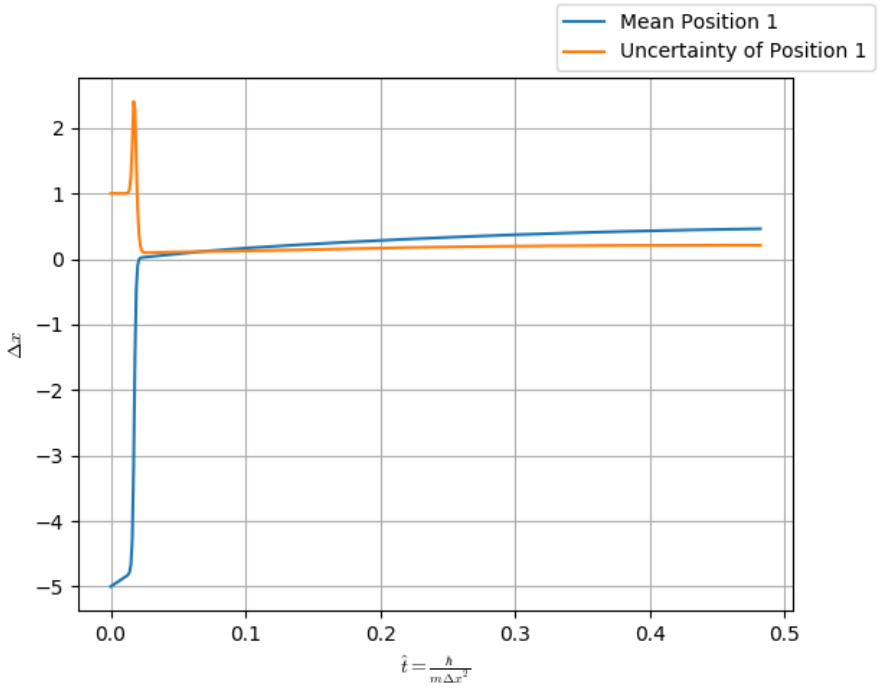

Figure 10: 1D-The Expectation Value and the Uncertainty of the Position for Euler Integrator

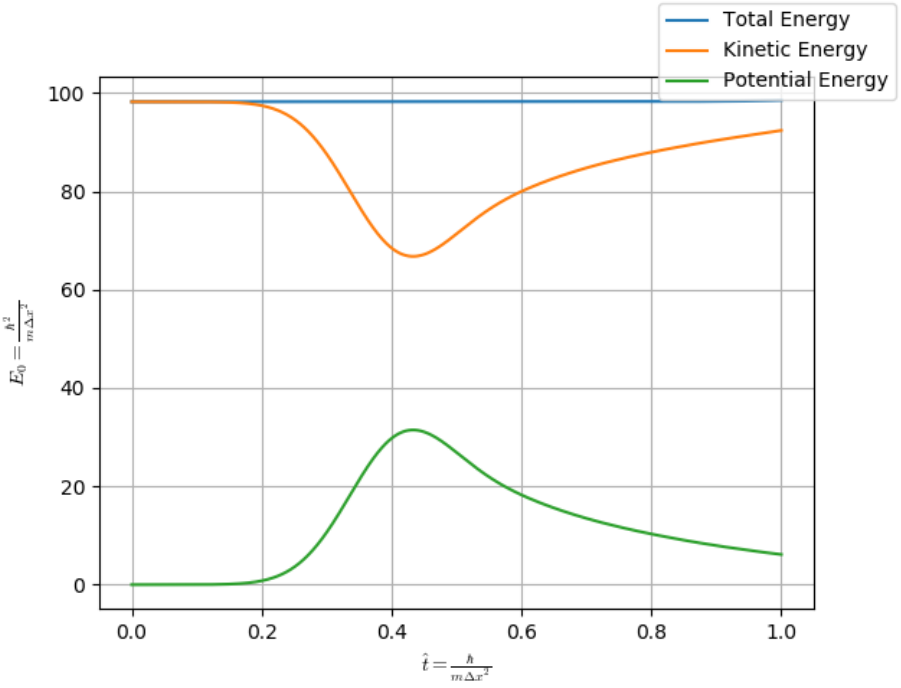

Figure 11: Energies of Euler Integrator for $\tau = 0.000005$

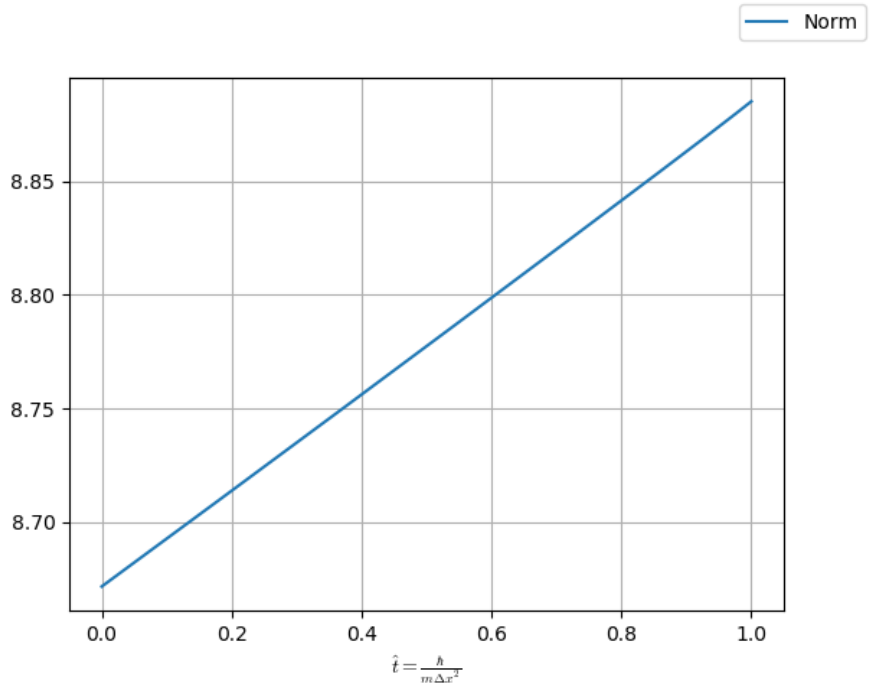

Figure 12: Norm of the Euler Integrator for $\tau = 0.000005$

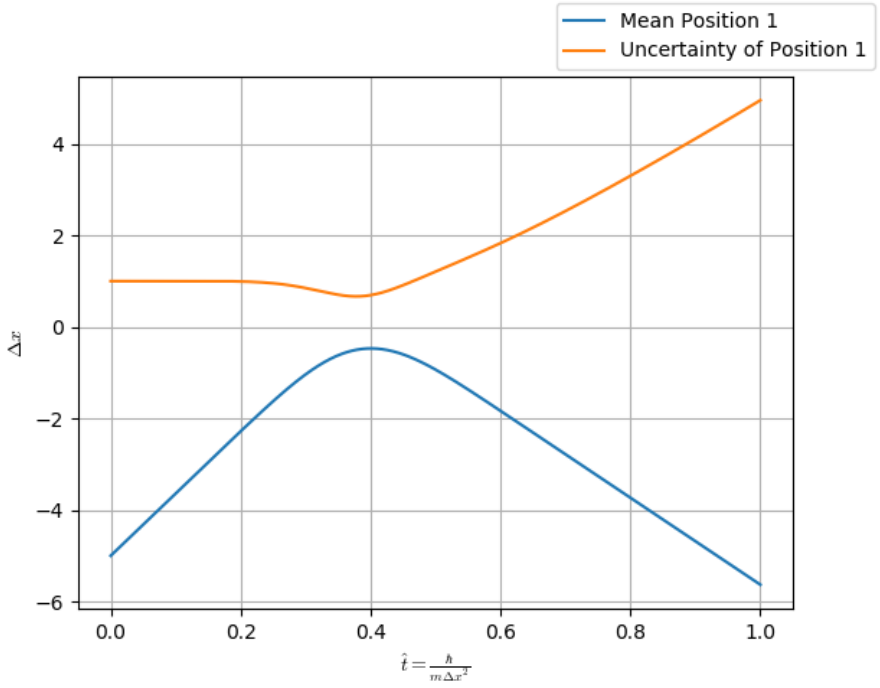

Figure 13: Mean Position/ Uncertainty of Position of Euler Integrator for $\tau = 0.000005$

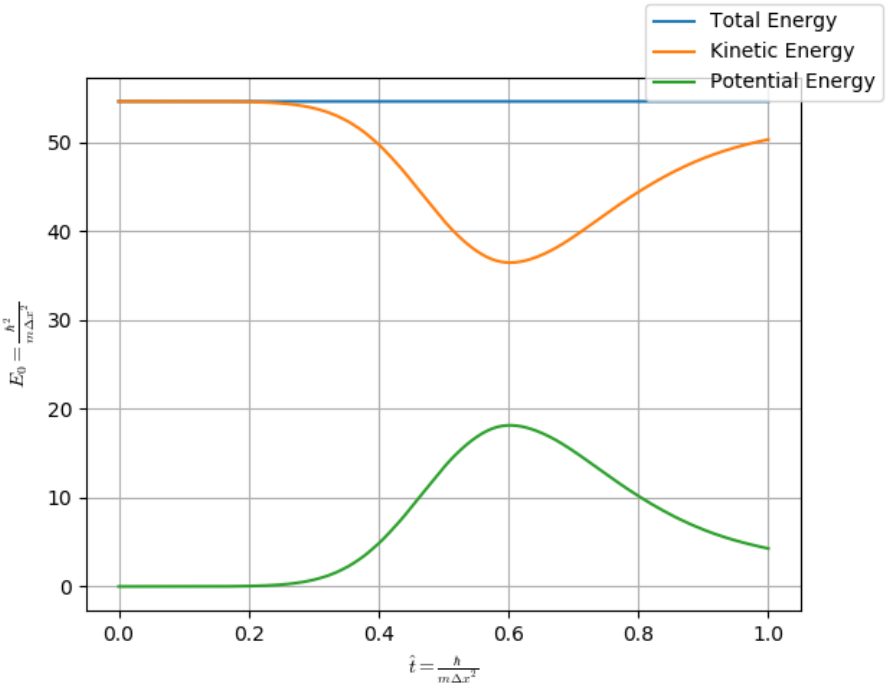

Figure 14: 2D - Energies for Strang Splitting

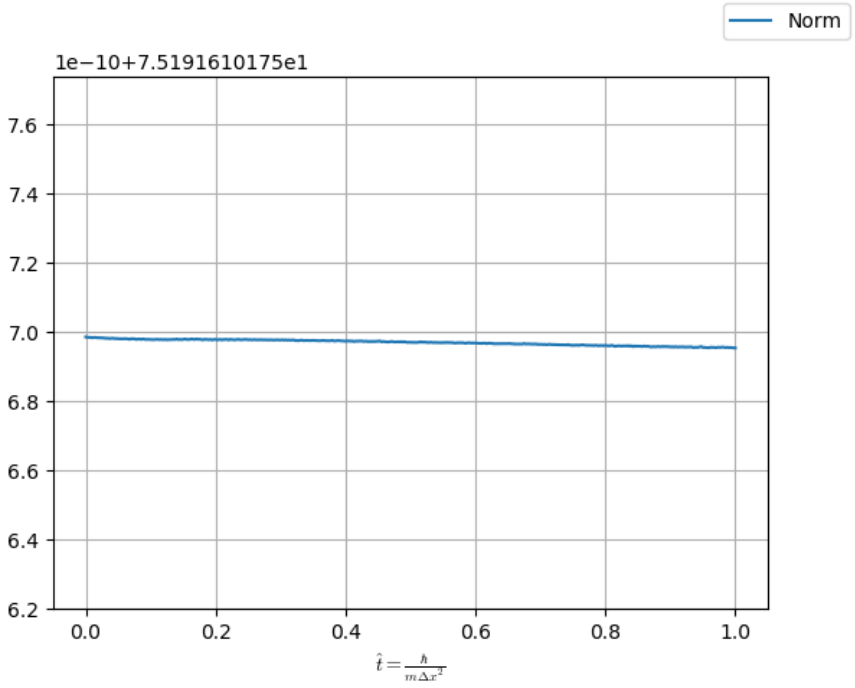

Figure 15: 2D - Norm for Strang Splitting

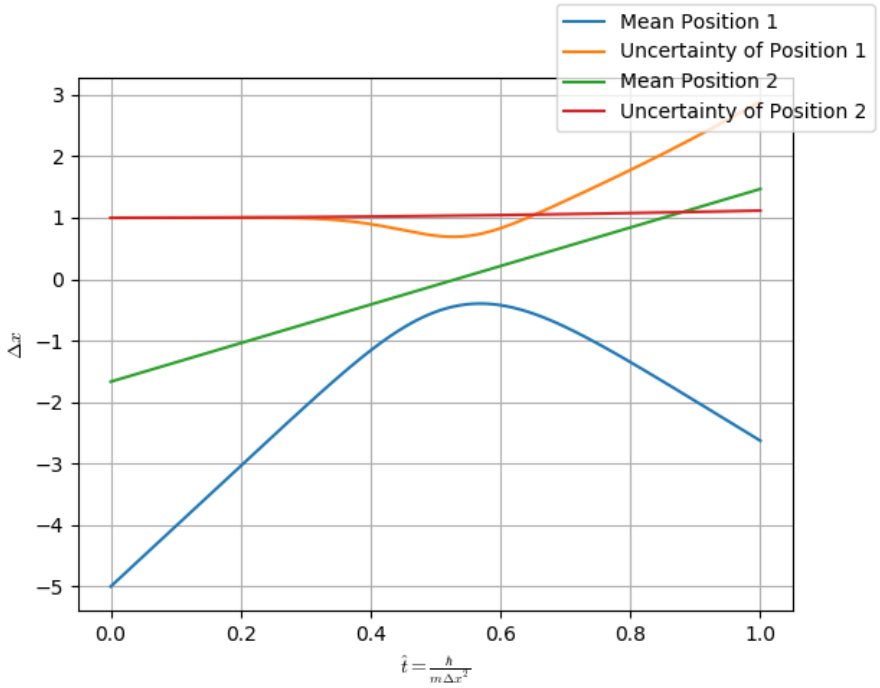

Figure 16: 2D- Mean Position and Uncertainty in Position for Strang Splitting

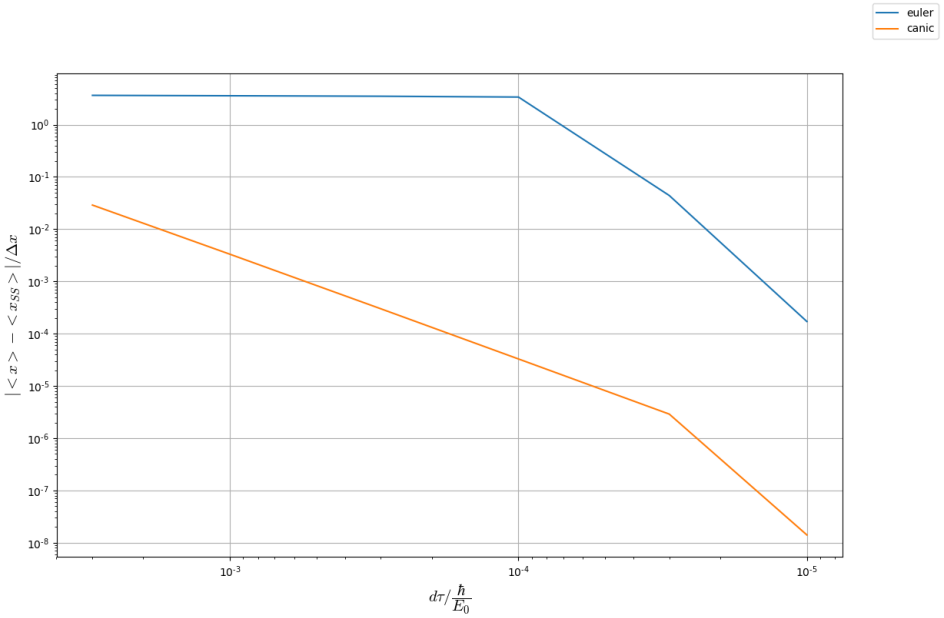

Figure 17: Convergence plot