CompPhys project

1. Crank-Nicolson method

The Crank–Nicolson method is a numerical technique used to solve partial differential equations, that combines both the explicit and implicit time-stepping schemes. It is second-order accurate in both time and space and is unconditionally stable. For the Schrodinger equation, we obtain it by taking the average of the simple finite difference scheme:

$$\psi_i^{p+1} = \psi_i^p - \frac{j\Delta t}{\hbar}\left(-\frac{\hbar^2}{2m\Delta x^2}(\psi_{i+1}^p + \psi_{i-1}^p - 2\psi_i^p) + V_i\psi_i^p\right)$$

(conditionally stable)
and the implicit scheme:

$$\psi_i^{p+1} = \psi_i^p - \frac{j\Delta t}{\hbar}\left(-\frac{\hbar^2}{2m\Delta x^2}(\psi_{i+1}^{p+1} + \psi_{i-1}^{p+1} - 2\psi_i^{p+1}) + V_i\psi_i^{p+1}\right)$$

(unconditionally stable but diffusive)
where p – timestep, i – spatial index.
The result is a matrix equation of type:

$$\mathbf{A}\psi^{p+1} = \mathbf{B}\psi^p$$

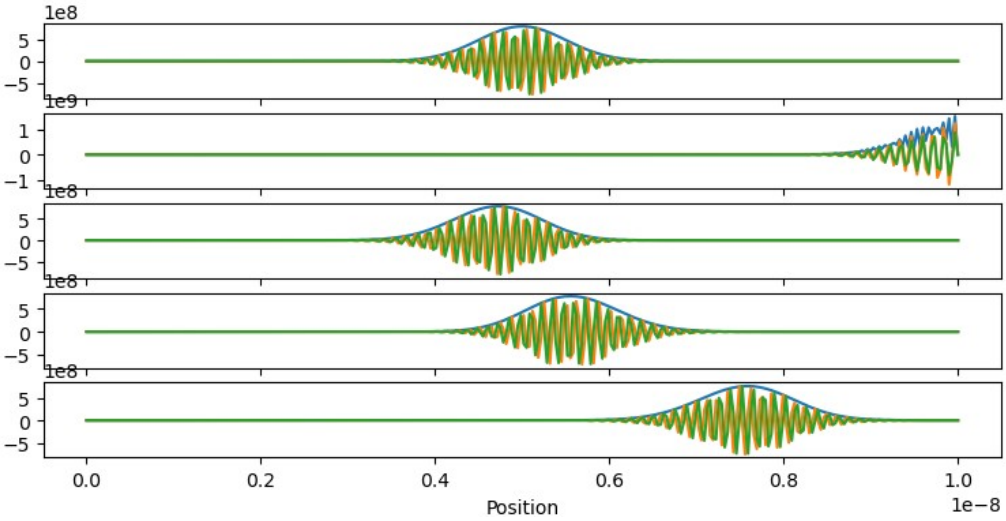
Crank-Nicolson method is characterized by low diffusion and unconditional stability.

Implicit method – unknown value for a given timestep depends on other unknown values at the same time step.
Unconditionally stable – numerically stable for any size of timestep, if it was conditionally stable, timestep would need to satisfy some amplification factor condition so the error would not pile up and blow up after some time.
Diffusive – has a tendency to artificially smooth out sharp features of the solution, could make e.g. wave packets spread out faster.

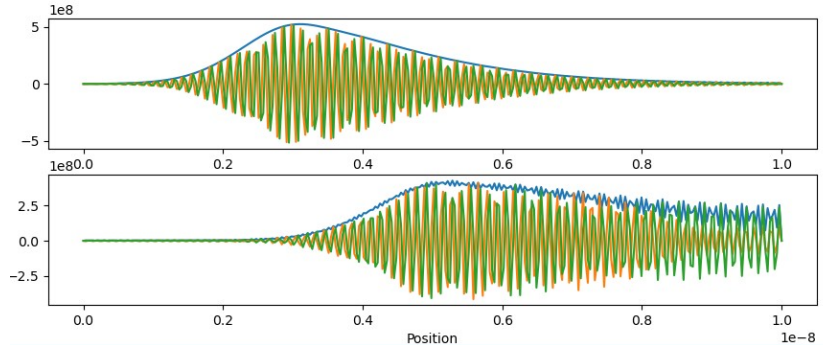
2. Infinite potential well – gaussian packet

Initial wave function of form:

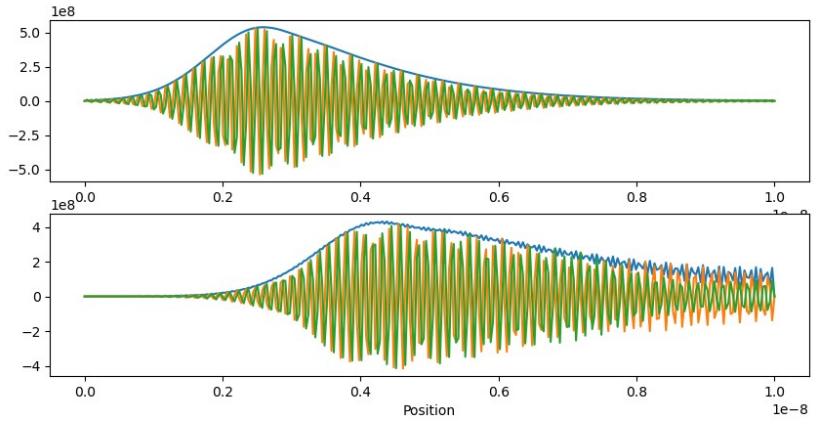
$$\psi(x, t = 0) \sim \frac{1}{\sigma\sqrt{2\pi}} e^{-(x-x_0)^2/2\sigma^2} e^{j\kappa x}$$




Modulus (blue color), real part (green) and imaginary part (orange) of the wave functions at different times. From top to bottom: time step 0, 1500, 3000, 6000, 8000; time step length: 1e-18 s; 300 spatial steps. We observe the wave packet bouncing from one wall to the other. At step 1500 we can see the moment of the packet touching the wall, the modulus becomes deformed when interacting with the potential. Modulus seems to be conserved for all times, as expected.




Same configuration, time steps 50 0000 and 90 000. We observe that for longer times, the packet becomes ‘washed out’ – the modulus decreases, the width increases.

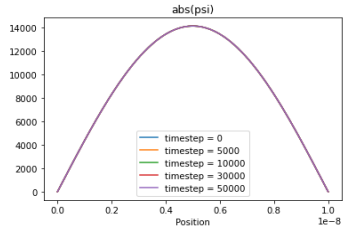


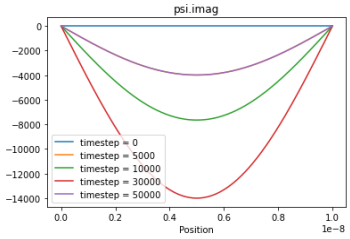

Time steps 500 000 and 900 000 for time step length 1e-19 s (equivalent to previous time values but with smaller time step). We observe that the wave function is less ‘washed out’ – better precision for smaller time step.

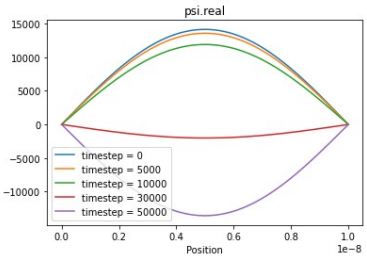
3. Infinite well – eigenstates

Wave function of type:

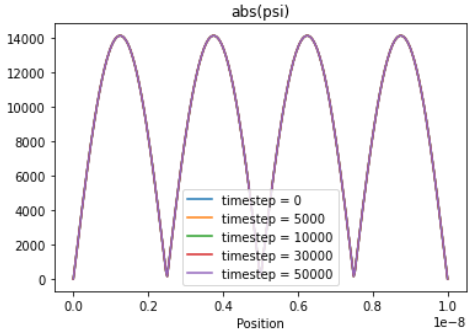
$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right), \quad n = 1, 2, 3, \ldots$$

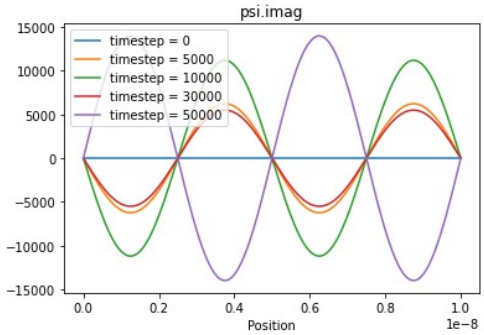


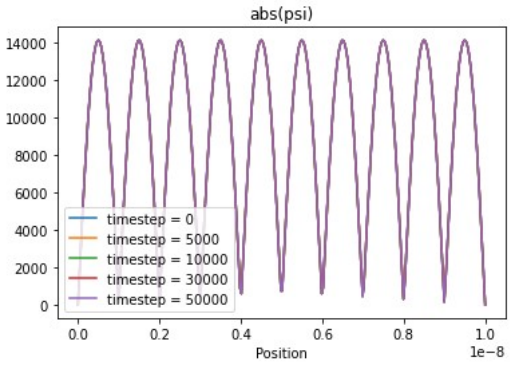



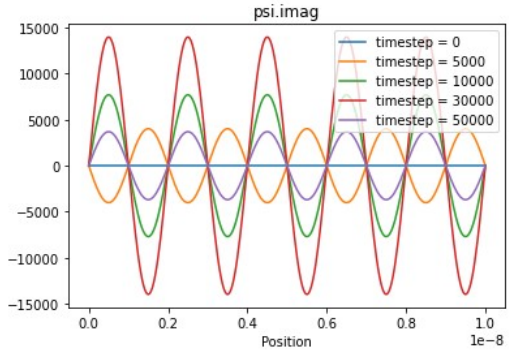

n=1, L=1e-8, del_t=1e-17
Modulus conserved in time, imaginary part oscillates with time



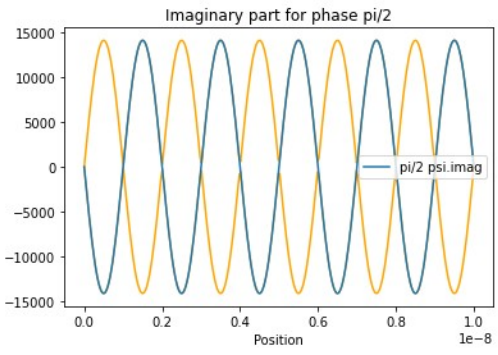



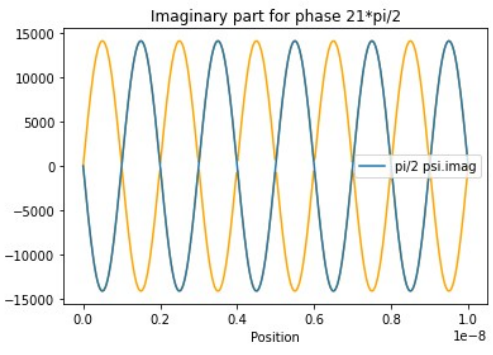

n=4



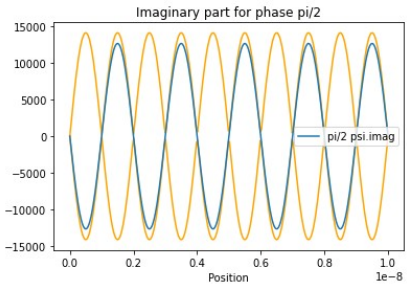




del_t=1e-18, n=10
Modulus conserved, imaginary part oscillates, for bigger times the correct solution.
But doesn't it oscillate faster/slower than expected?



A thing to test was also whether the oscillations of the imaginary and real part happen at the same speed as expected. We calculated the time needed for phase change of pi/2 using the energy of the function, and checked how the imaginary part compares to the modulus (should be equal to modulus) in the first oscillation and for more oscillations. Here example of 21st oscillation, we deduce the speed of oscillations is actually the same as expected.




Precision lowers for t=1e-15, mostly because timestep starts being comparable to oscillation period.

4. Step potential

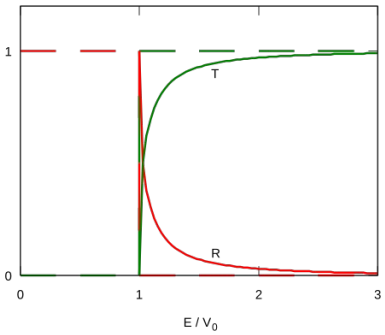
As the wave function, we take again a gaussian packet:

$$\psi(x, t = 0) \sim \frac{1}{\sigma\sqrt{2\pi}} e^{-(x-x_0)^2/2\sigma^2} e^{j\kappa x}$$

kappa = 5e10, sigma=1e-9,
in the first quarter of the space (0-N/4) and let it propagate. Step potential at N/2.
Transmission and reflection factors:

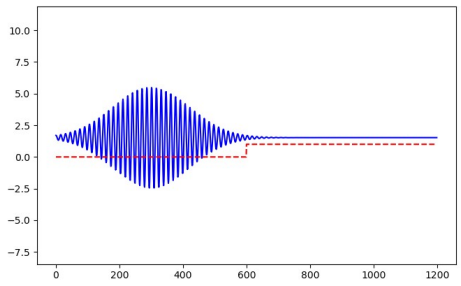
$$\sqrt{T} = \frac{2\sqrt{k_1 k_2}}{k_1 + k_2}$$
$$\sqrt{R} = \frac{k_1 - k_2}{k_1 + k_2}$$

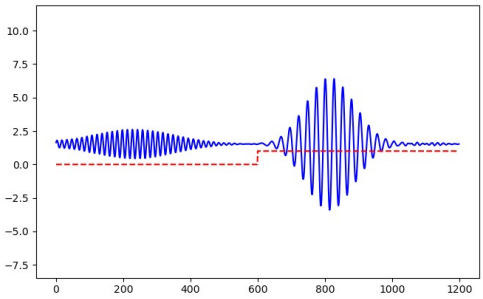
$$k_1 = \sqrt{2mE/\hbar^2},$$
$$k_2 = \sqrt{2m(E - V_0)/\hbar^2}$$




Reflection and transmission probability at a Heaviside-step potential. Dashed: classical result. Solid lines: quantum mechanics. For E < V0 the classical and quantum problem give the same result.

P = 20000 # number of time steps
N = 1200 # number of space steps
L = 1e-8 # total space size,
E = 1.52e-17, V=1e-17
del_t = 1e-19:

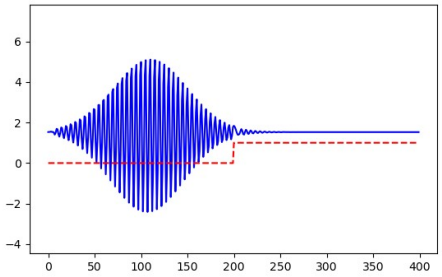


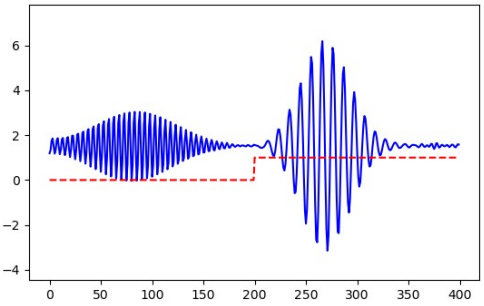




Simulated R:  0.0758028653249095
Simulated T:  0.9038975953183477
Theoretical R:  0.0676712951646093
Theoretical T:  0.9323287048353905

del_t=1e-17:
Simulated R:  0.07656896605757814
Simulated T:  0.9211495831612297
Theoretical R:  0.0676712951646093
Theoretical T:  0.9323287048353905

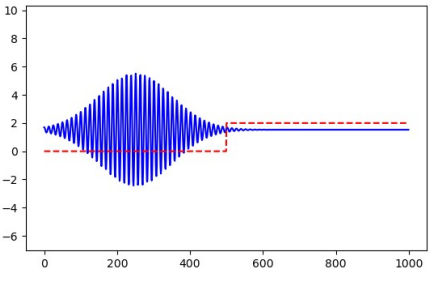
del_t=1e-18, P=2000, N=800:
Simulated R:  0.08549823210525395
Simulated T:  0.9020853642004021
Theoretical R:  0.0676712951646093
Theoretical T:  0.9323287048353905

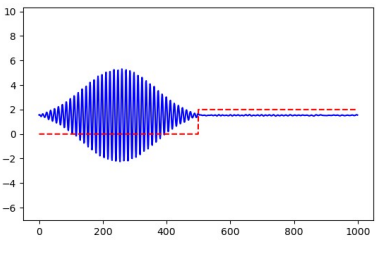



^^^ N=400:
Simulated R:  0.1651778391290107
Simulated T:  0.8239903945781211
Theoretical R:  0.0676712951646093
Theoretical T:  0.9323287048353905

For smaller timesteps, pretty small difference in T, R results, even as timestep approaching the time needed to go over the potential. Big difference for decresing number of timesteps.



Basically full reflection for V=2e-17, bigger than E – as expected.

5. Conclusions:

- The Crank–Nicolson method proves to be a highly effective and stable numerical technique for solving the time-dependent Schrödinger equation, balancing accuracy and computational cost.

- Simulations of a Gaussian wave packet in an infinite potential well show expected behavior: reflection at the walls and conservation of modulus over time. At long times or with large time steps, numerical diffusion becomes noticeable, emphasizing the importance of time step size.

- Simulations of stationary eigenstates confirm stability and correctness of phase evolution. The method captures expected oscillation frequencies, although precision decreases when the time step approaches the oscillation period.

- For a step potential, both transmission and reflection probabilities closely match theoretical predictions, with deviations mostly influenced by spatial and temporal discretization. Finer grids and smaller time steps yield results closer to quantum mechanical expectations.

- Overall, the method allows for detailed quantum simulations across various potentials. However, care must be taken with discretization parameters to maintain both precision and efficiency.

6. What could be next?

- Multiparticle systems: for non-interacting particles, the wavefunction would be simply a product of two wavefunctions for a single particle

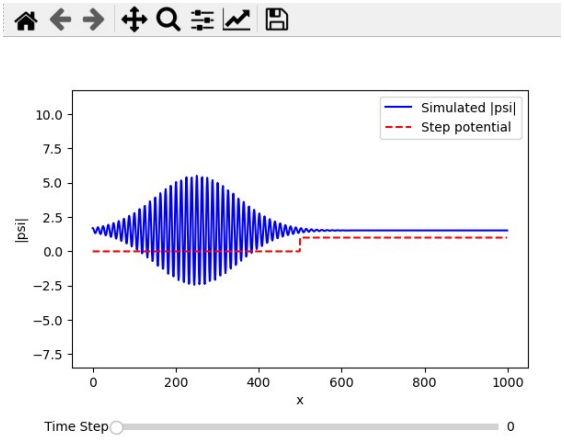
$$\psi(x_1, x_2) = \psi_{n_1}(x_1)\psi_{n_2}(x_2)$$

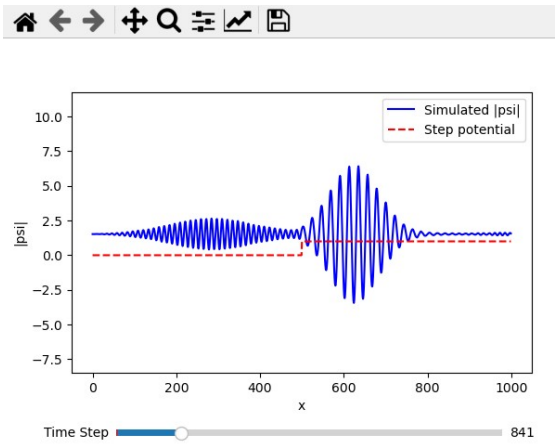
- Symmetric, antisymmetric function for bosons/fermions:

$$\psi(x_1, x_2) = \frac{1}{\sqrt{2}} \left[\psi_{n_1}(x_1)\psi_{n_2}(x_2) \pm \psi_{n_1}(x_2)\psi_{n_2}(x_1)\right]$$

- For charged particles:

$$\hat{H} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2}\right) + \frac{1}{|x_1 - x_2|}$$


Simulated |psi|
Step potential
|psi|
x
Time Step
0


Simulated |psi|
Step potential
|psi|
x
Time Step
841