Wave Function Simulation

Zoltán Simon

Advisors: Dr. Balázs Csébfalvi

October 22, 2023

Abstract

In quantum mechanics, the wave function describes the state of a physical system. In the non-relativistic case, the time evolution of the wave function is described by the time-dependent Schrödinger equation. In 1982, D Kosloff and R Kosloff proposed a method [2] to solve the time-dependent Schrödinger equation efficiently using Fourier transformation. In 2020, Géza István Márk published a paper [1] describing a computer program for the interactive solution of the time-dependent and stationary two-dimensional (2D) Schrödinger equation. Some details of quantum phenomena are only observable by calculating with all three spatial dimensions. We found it worth stepping out from the two-dimensional plane and investigating these phenomena in three dimensions. We implemented the said method for the three-dimensional case to simulate the time evolution of the wave function. We used our implementation to simulate typical quantum phenomena using wave packet dynamics. First, we tried the method on analytically describable cases, such as the simulation of the double-slit experiment, then we investigated the operation of flash memory. We used raytraced volumetric visualization to render the resulting probability density. In our work, we introduce the basics of wave packet dynamics in quantum mechanics. We describe the method in use in detail and showcase our simulation results.
For further information and animations please visite
https://zoltansimon.info/src/content/research/wavepacketsim.html

Kivonat

A kvantummechanikában a hullámfüggvény írja le egy fizikai rendszer állapotát. Nemrelativisztikus esetben a hullámfüggvény időbeli fejlődését az időfüggő Schrödinger-egyenlet határozza meg. 1982-ben D Kosloff és R Kosloff közölt egy módszert [2] az időfüggő Schrödinger-egyenlet hatékony megoldására Fourier-transzformáció felhasználásával. 2020-ban Márk Géza István cikkében [1] bemutatott egy interaktív számítógépes programot az időfüggő és a stacionárius kétdimenziós Schrödinger-egyenlet megoldására. A kvantumos jelenségek bizonyos részletei csak mindhárom térdimenzióval számolva figyelhetők meg. Érdemesnek tartottuk a síkból kilépve, térben is megvizsgálni ezeket a jelenségeket. Munkánkban háromdimenziós esetre implementáltuk az említett módszert, hogy szimuláljuk a hullámfüggvény időbeli fejlődését. Hullámcsomagdinamikát használva kipróbáltuk több jellegzetes kvantumos jelenség szimulációját. A módszert először analitikusan kezelhető esetekre teszteltük, például a kétréses kísérlet szimulációjára, ezután megvizsgáltuk a flash

memória cella működését. A szimuláció kimeneteként előálló valószínűségi sűrűséget sugárkövetéses térfogati megjelenítéssel ábrázoltuk. Dolgozatunkban ismertetjük a kvantummechanikai hullámcsomag-dinamika alapjait. Részletesen leírjuk a használt eljárást, és bemutatjuk a szimulációnk eredményeit.
További információ és animációk találhatóak a
https://zoltansimon.info/src/content/research/wavepacketsim.html webcímen.

1 Introduction

Quantum mechanics (QM) describes the behaviour of physical systems [3]. It is a common view that while Albert Einstein's General Relativity (GR) [4] provides a model that accurately describes the laws of nature governing large scale phenomena, quantum theory is the best for small things. Although humanity has not yet accepted a single theory that would be capable of modelling both the small and the large thus bridging the gap between QM and GR, there are many features of both mentioned theories that require effort to master. In this writing we discuss a numeric approximation of the solution of one of QM-s fundamental equations, the Schrödinger equation. In non-relativistic QM the time dependent Schrödinger equation [5] governs the time evolution of the wave function $\psi(\vec{r};t)$, where $\vec{r}$ is the position vector and t is the time. This equation can be written in the form 1.

$$i\frac{\delta}{\delta t}\psi(\vec{r};t) = H\psi(\vec{r};t) \tag{1}$$

Here i is the complex unit, $\frac{\delta}{\delta t}$ is the partial differential operator with respect to time and H is the H is the Hamiltonian operator. Consequently the properties of the physical system are encoded in the Hamiltonian. If the potential is conservative, then $H = K + V$ is true, where K is the kinetic energy operator and V is the operator corresponding to the potential energy. For local potentials the V operation simply stands for a multiplication with the $V(\vec{r})$ position dependent potential value. Generally solving equation 1 analytically is not possible except for a few special cases such as the Hydrogen atom.

Géza I. Márk [1] presents a method to approximate the solution of the Schrödinger equation. In his article he provides detailed description of separate methods for both the time dependent and the time independent equation's approximation. In the focus of their article is an implementation called Web-Schrödinger. This program is capable of approximating both the time dependent and the time independent equation for 2D spaces. In our work we have only dealt with the time dependent version. On the flip side, we implemented the method in 3D.

2 Used method

The time dependent Schrödinger equation as written in 1, is a linear partial differential equation. The H operator and a given $\psi(\vec{r};t_0)$ initial state fully determines the $\psi(vecr;t)$ wave function. Formal solution of equation 1 can be given in the form of equation 2.

$$\psi(\vec{r};t) = U\psi(\vec{r},t_0) \qquad U = e^{-iH(t-t_0)} \tag{2}$$

Here U is the time development operator. The exponent containing H can not be trivially factored. We can use an approximation described in equation 3.

$$e^{-i(K+V)\delta t} \approx e^{-iK\delta t/2}e^{-iV\delta t}e^{-iK\delta t/2} \tag{3}$$

The error of this approximation is $O\left[(\delta t)^3\right]$. We have to consider this when designing the time resolution of the simulation. The evolution operator is now split into three consecutive steps. These are a free propagation

for time $\delta t/2$, a potential only propagation for δt and another free propagation for $\delta t/2$. Since the effect of V is a multiplication with $V(\vec{r})$ we can write the potential propagator as a multiplication with $e^{-iV(\vec{r})\delta t}$. The effect of the free propagator is simple when applied in the k momentum space. In this case it is simply a multiplication with $e^{i|k|^2\delta t/4}$. To use this formula we have to convert from real space to momentum space and backward. To do this we must calculate the Fourier transform of the wave function. On the computer this is approximated by calculating the Discrete Fourier Transform (DFT). DFT can be implemented with an algorithmic complexity of $O\left[n\,log(n)\right]$ with the Fast Fourier Transform (FFT) algorithm. This method utilises the symmetries naturally occurring while calculating the DFT by definition. Namely that you can reuse some values by pairing the odd and even indexed members of the input vector.

Given a ψ_n current state, the next state occurring after δt time can be obtained by executing the following steps.

1. $\psi_n^{(1)} := FFT^{-1}\left[P_{kinetic}(\delta t/2)\ FFT(\psi_n)\right]$
2. $\psi_n^{(2)} := P_{potential}(\delta t)\ \psi_n^{(1)}$
3. $\psi_{n+1} := FFT^{-1}\left[P_{kinetic}(\delta t/2)\ FFT(\psi_n^{(2)})\right]$

Here $P_{kinetic}(\delta t/2)$ is the previously discussed free propagator applied by multiplying with $e^{i|k|^2\delta t/4}$, and $P_{potential}(\delta t)$ is the potential propagator applied by multiplying with $e^{-iV(\vec{r})\delta t}$.

To obtain a convergent and aliasing free simulation one must choose small enough δx, δy grid resolution that is smaller than the *de Broglie* wavelength of the simulated system.

The output of the simulation is the probability density function of the simulated volume. This can be obtained by calculating the square of the absolute value of the wave function for each position as seen in equation 4.

$$p(\vec{r};t) = |\psi(\vec{r},t)|^2 \tag{4}$$

3 Our implementation

We have created our own implemented the method described in section 2. Our program is written in Python 3.8 programming language [6]. For the mathematical operations we used the NumPy library [7]. NumPy enabled us to easily handle large data structures such as the large 3D arrays containing complex numbers. It also comes with an FFT implementation that is capable of transforming multidimensional inputs.

For now we have simplified the initialisation of the wave function. Although there is a description of the method used by Géza I. Márk in his article, we choose to not use it. Rather we initialised the wave function with a heuristic distribution. This did not seem to cause real problems or rather artifacts introduced by this choice where marginal. We simulated the time development of the system for 1000 time steps. The resulting probability density function was visualized used the Plotly Python library [**?**]. This allows the generation of 3D isosurface plots.

First we did not use any potential barriers. This resulted in unrealistic interference patterns as seen in figure 1. This was the direct result of the way the used DFT transformation handles larger than zero values near the borders of the simulated volume.

To solve this problem we introduced a large potential barrier on each side of the simulated cube. This wedged the probability density into the middle of the cube, where the potential remained zero.

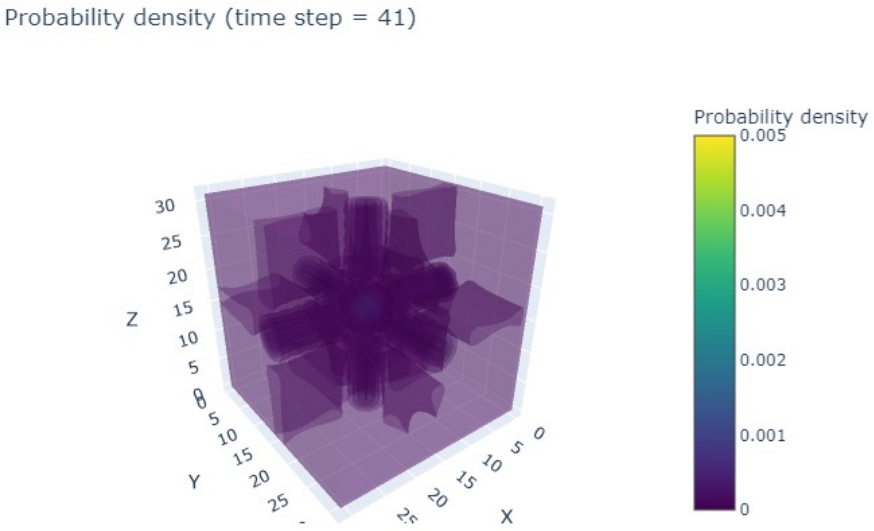

Figure 1. Unrealistic interference patterns as a result of DFT.

4 Results

In this section we describe the results of the simulation with the potential barrier. In the first few time steps the distribution filled the zero potential volume. Right after filling the zero potential area, small amount of probability density penetrated deeper into the larger potential sections of the simulated volume. This can be observed in figure 2. We speculate that this is the result of high initial momentum of the distribution. The high energy resulted in quantum tunnelling-like behaviour, where the wave was able to defeat the potential obstacle to some degree. The amount of penetration could be related to the fact that the potential barrier increases linearly towards the edge of simulated volume. We also considered the possibility of the penetration being simply an artifact that is the result of the heuristic initial wave.

After the previously described initial phase the wave function filled the middle part of the simulated volume where the potential was zero and began interfering with itself. When the wave first filled the zero potential cube, it was seemingly homogenous observing only the probability density. Shortly after nodes with higher probability density emerged from the homogenous volume. These nodes where arranged in a grid-like pattern. This can be observed in figure 3.

The nodes transformed into a series of different patterns. These patterns showed periodicity. This behaviour is similar to the phenomena called quantum revival [8].

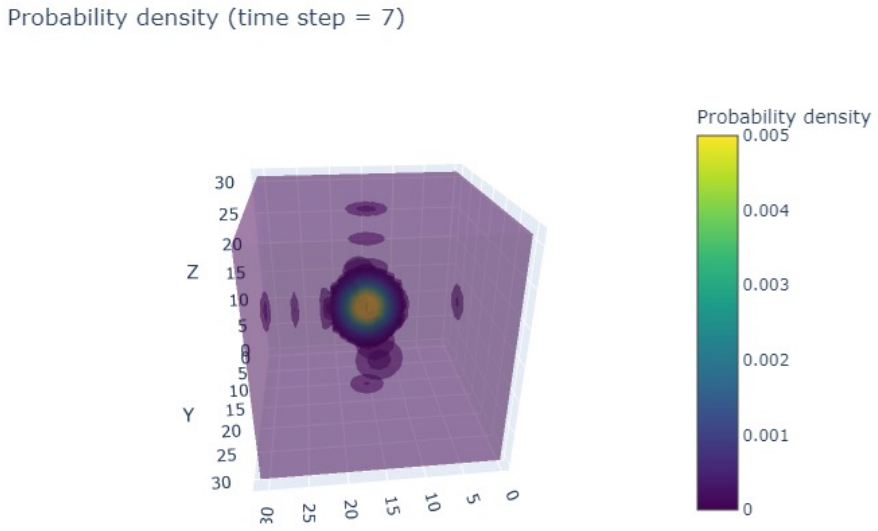

Figure 2. Wave penetrating the linearly increasing potential barrier at an early stage of the simulation

5 Discussion

Seeing all the images generated by our implementation, it is safe to say that the described method has a lot of potential when it comes to simulating and visualizing quantum wave functions.

To measure the stability of the simulation we integrated the probability density over the simulated volume to check the deviation from the awaited $P = 1$. This test resulted in fairly low additive error of magnitude $\approx 10^{-13}$ even after 1000 time steps.

In order to maintain the convergence of the numeric approximation described in section 2 we have to choose small enough time steps. To battle the $O\left[(\delta t)^3\right]$ error of the approximated time development operator we used the formula 5 published in [1] multiplied by a heuristically chosen 0.1.

$$\delta t < \frac{4}{\pi} \frac{(\delta x,\, \delta y)^2}{D} \tag{5}$$

Here D stand for the number of dimensions simulated. In our case this is equal to 3.

The time required to run the simulation for all the 1000 frames took multiple hours. Partially this is due to the slow plotting of the used isosurface visualisation. The bottleneck of core algorithm are the multiple FFT runs.

In the future we want to further develop the method. We plan on experimenting with advanced wave function setups. We are going to implement a custom ray tracer to create nicer visualizations of the simulation results.

We will explore the possibilities of using this method to simulate atomic structures and more advanced molecules.

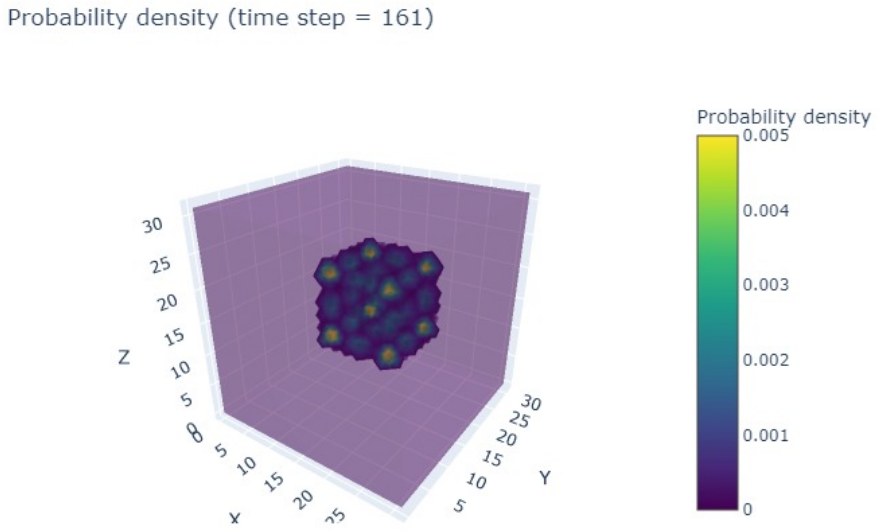

Figure 3. Wave forming pattern of high probability density nodes

6 Acknowledgement

I would like to thank my advisor, Dr. Balázs Csébfalvi, who has always been very supportive! This work would also not be possible without the advise of Dr. János Asbóth, who suggested to look into the work of Dr. Géza I. Márk. Finally I am very grateful for Dr. Géza I. Márk's work in the field of wave function simulation.

References

[1] G. I. Márk, "Web-schrödinger: Program for the interactive solution of the time dependent and stationary two dimensional (2d) schrödinger equation," 2020. [Online]. Available: https://doi.org/10.48550/arXiv.2004.10046

[2] D. Kosloff and R. Kosloff, "A fourier method solution for the time dependent schrödinger equation as a tool in molecular dynamics," *Journal of Computational Physics*, vol. 52, no. 1, pp. 35–53, 1983. [Online]. Available: https://www.sciencedirect.com/science/article/pii/0021999183900153

[3] F. Schwabl, *Quantum mechanics*. Springer Science & Business Media, 2007.

[4] R. M. Wald, *General relativity*. University of Chicago press, 2010.

[5] E. Schrödinger, "An undulatory theory of the mechanics of atoms and molecules," *Phys. Rev.*, vol. 28, pp. 1049–1070, Dec 1926. [Online]. Available: https://link.aps.org/doi/10.1103/PhysRev.28.1049

[6] P. S. Foundation. (2023) Python. [Online]. Available: https://www.python.org/

[7] . N. A. rights reserved. (2023) NumPy. [Online]. Available: https://numpy.org/

[8] D. F. Styer, "Quantum revivals versus classical periodicity in the infinite square well," *American Journal of Physics*, vol. 69, no. 1, pp. 56–62, 2001.