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The Analysis of the Physical Quantity *N Grid*, *v*, and *dt* in Solving the Schrödinger Equation Using the Crank-Nicolson Method

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Abstract

Solving the Schrödinger equation may result in a wave function of a particle in a quantum system, which can afford the information with respect to the particle's behavior. The Schrödinger equation is useful for examining probability density and determining a wave function of free particles. This research focuses on solving the Schrödinger equation using the Crank-Nicolson method in free particles. The Crank-Nicolson method is a method of solving partial differential equations in the form of the Schrodinger equation, this method is very stable and accurate in giving numerical results. The result indicates that probability density and the form of the wave function of free particles are identified by varying the v, N grid, and dt. When dt = 1, v = 1, and v = 2, and the N grid remains at a score of 100, we acquire the same forms of the wave function and probability density. And yet, when dt = 2, v =2, and the N grid remains at a score of 100, the form of the wave function and probability density is constricted in one area. The N grid and dt are the two most affecting factors on the three variants. Using the Crank-Nicolson method, we can determine the wave function and probability for free particles by varying the value of N grid, dt.

Keywords: *Crack-Nicolson; Schrödinger equation; wave function*

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INTRODUCTION

Shangwha Yi [1] has made free particle wave functions as the solution of the Klein-Gordon equation. Bonda, et al. [2] stated that free particle cases are derived solely from the differentiation of the delta function. A particle's wave function contains a small fraction of an antiparticle's wave function [3]. The canonical quantization of a system of a free particle in a bounded value in space, a particle in a box containing a dissipative is carried out to the Dirac method [4]. Quantum mechanics remains an interesting topic to study. Experts study quantum mechanics when encountering the indication of classical mechanics' inability to explicate abundant experimental evidence as regards atomic size systems [5]. In the case of non-relativistic quantum mechanics, the main equation to be solved is the second-order differential equation or known as the Schrödinger equation [6-9]. Solving the Schrödinger equation may result in a wave function of a particle in a quantum system, which then confers the information concerning the particle's behavior [10-11]. The Schrödinger equation is useful to investigate energy measurement and the determination of a wave function for a free particle, a particle in a 1D box, a simple harmonic oscillator, and diverse studies of atoms and other quantum systems [12-13]. The focus of this study is the probability density of Gaussian form as a time function for a free particle. The current research trend concerns the study of the numerical method of the time-dependent Schrödinger equation using the general equation of the Crank-Nicholson approximation [14-15]. But no analysis has been done on the physical quantities N grid, v, and dt which are the most influential in determining the shape of the wave function and probability density. The purpose of this study is to analyze the physical quantities *N* grid, *v*, and *dt* which are the most influential in determining the shape of the wave function and probability density. The focus study is how to perform a simulation of the probability density of a function in relation to the Schrödinger equation, and what parameters are significant when the variation of *N* grid, *v*, and *dt* is made. This method is accurate and efficient for solving 1D Schrödinger equation. The idea is advocated by Dijk and Toyama, who developed an approximation to solve a time-dependent Schrödinger equation numerically [16]. However, they disregard quantification for free particles [17].

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relation to the Schrödinger equation, and what parameters are significant when the variation of *N* grid, *v*, and *dt* is made. This method is accurate and efficient for solving 1D Schrödinger equation. The idea is advocated by Dijk and Toyama, who developed an approximation to solve a time-dependent Schrödinger equation numerically [16]. However, they disregard quantification for free particles [17].

Comprehending quantum mechanics is not demanding and can be carried out by observing free particles for the Schrödinger equation concerned [18]. Free particles, addressed in this research, are particles with no style influences. The potentials are so weak that they can be neglected, and the particles move freely [19-20]. In this research, we are solving the Schrödinger equation using an efficient and effective numerical method to derive an accurate result. Also, in this research on free particles, we are studying what the density probability is when the position varies, what the waveform is, and how to solve a wave function that adheres to several types of wave equations that delineate classical waves. Meanwhile, standing waves will be explained in a more detailed way using the Crack-Nicholson method.

According to de Broglie, in regard to the wave nature of particles, only atomic or atomic nucleus size particles have nature as a wave, whereas the larger ones do not [21-22]. This phenomenon is brought about by a tiny Planck's constant. The free particles in this research are in atomic size, and accordingly, the nature of their waves is observable.

We use MATLAB to determine the numerical results as the program is equipped with some features, e.g., being competent in visualizing and simulating physical quantity in the free particles analyzed. Additionally, MATLAB has excellent numerical accuracy and an appealing color appearance [23-27]. Based on the background, the research examines how to solve the Schrödinger equation using the Crank-Nicholson method, how to perform a simulation of the probability density of a function in relation to the Schrödinger equation, and what parameters are significant when the variation of the *N* grid, *v*, and *dt* is made.

METHOD

The material used here is a set of laptops, in which MATLAB 2017B has been installed, to solve the Schrödinger equation. The method used is Crank-Nicholson, and the wave function ψ in the form of numerical iteration is [23]:

$$\psi_{j,n} = \psi\left(x_j, t_n\right) = \psi\left[x = \left(j-1\right)h, t = \left(n-1\right)\tau\right] \tag{1}$$

As such, the Schrödinger equation will be:

$$i\hbar \frac{\psi_{j,n+1} - \psi_{j,n}}{\tau} = -\frac{\hbar^2}{2m} \frac{\psi_{j+1,n} + \psi_{j-1,n} - 2\psi_{j,n}}{h^2} + V_j \psi_{j,n} \tag{2}$$

Where

$$V_j = V\left[x = \left(j-1\right)h\right] \tag{3}$$

Because the Hamiltonian operator is linear, Equation (2) will be:

$$i\hbar \frac{\psi_{j,n+1} - \psi_{j,n}}{\tau} = \sum_{k=1}^{N} \hat{H}_{jk} \psi_{k,n} \tag{4}$$

Matrix H_{jk} is the form of the iteration of the Hamiltonian operator, namely:

$$H_{jk} = -\frac{\hbar^2}{2m}\frac{\delta_{j,k+1} + \delta_{j,k-1} - 2\delta_{j,k}}{h^2} + V_j \delta_{j,k} \tag{5}$$

In a matrix form, the Schrödinger equation will be:

$$\psi_{n+1} = \left(1 - \frac{i\tau}{\hbar} H\right)\psi_n \tag{6}$$

Equation (6) is an explicit form in solving the Schrödinger equation. The Schrödinger equation can also be shown by applying the Hamiltonian operator to the wave function when n + 1, i.e. [28]:

$$\psi_{n+1} = \psi_n - \frac{i\tau}{\hbar}\hat{H}\psi_{n+1}$$

or

$$\left(1 + \frac{i\tau}{\hbar}\hat{H}\right)\psi_{n+1} = \psi_n$$

so

$$\psi_{n+1} = \left(1 + \frac{i\tau}{\hbar}\hat{H}\right)^{-1}\psi_n \tag{7}$$

The Crank-Nicholson method is very implicit and stable and has a fair accuracy effect in solving the Schrödinger equation, which is laid out as follows:

$$i\hbar\frac{\psi_{j,n+1} - \psi_{j,n}}{\tau} = \frac{1}{2}\sum_{k=1}^{N}\hat{H}_{jk}\left(\psi_{k,n+1} - \psi_{k,n}\right) \tag{8}$$

In a matrix notation, it can be written as:

$$\psi_{n+1} = \psi_n - \frac{i\tau}{2\hbar}\hat{H}\left(\psi_{n+1} - \psi_n\right) \tag{9}$$

and can be solved into:

$$\left(I + \frac{i\tau}{2\hbar}\hat{H}\right)\psi_{n+1} = \left(I - \frac{i\tau}{2\hbar}\hat{H}\right)\psi_n \tag{10}$$

so:

$$\psi_{n+1} = \left(I + \frac{i\tau}{2\hbar}\hat{H}\right)^{-1}\left(I - \frac{i\tau}{2\hbar}\hat{H}\right)\psi_n \tag{11}$$

Equation (11) is the solution to the Schrödinger equation using the Crank-Nicholson method, which is considered the best, fairly accurate, and most stable method.

Solving differential equations, including the Schrödinger equation, requires a preliminary condition that makes them solvable using numerical computation with a certain step size. In this condition, it is perceived that a free particle is in position x_0 with a wave packet and an average momentum $p_0 = \hbar k_0$ (k_0 is the wavenumber). If Gaussian wave packets are used, the initial wave will be:

$$\psi(x,t=0)=\frac{1}{\sqrt{\sigma_0\sqrt{\pi}}}e^{ik_0x}e^{-(x-x_0)^2/2\sigma_0^2} \tag{12}$$

This wave function is normalized so:

$$\int_{-\infty}^{\infty}|\psi|^2\,dx=1 \tag{13}$$

Considering the Heisenberg uncertainty principle $\Delta x\Delta p\leq\hbar/2$, the wave function in free space is:

$$\psi(x,t=0)=\frac{1}{\sqrt{\sigma_0\sqrt{\pi}}}\frac{\sigma_0}{\alpha}e^{ik_0(x-p_0t/2m)}e^{-(x-x_0-p_0t/2m)^2/2\sigma_0^2} \tag{14}$$

With $\alpha^2=\sigma_0^2+i\hbar t/m$, the probability density $P(x,t)=|\psi(x,t)|^2$ is:

$$P(x,t)=\frac{\sigma_0}{|\alpha|^2\sqrt{\pi}}\exp\left[-\left(\frac{\sigma_0}{\alpha}\right)^4\frac{(x-x_0-p_0t/m)^2}{\sigma_0^2}\right] \tag{15}$$

Equation (15) is stated in a Gaussian form as a time function. The maximum value of the Gaussian function can be expressed in the form of the expected value evaluation of the probability density function as:

$$\langle \mathrm{x}\rangle=\int xP(x,t)dx \tag{16}$$

In a time scale, a function moves as $\langle \mathrm{x}\rangle=x_0+p_0t/m$, a wave packet moves at a speed of p_0/m. The Gaussian function disperses in a time scale, and the standard deviation can be written as [24]:

$$\sigma(t)=\sigma_0\sqrt{\left(\frac{|\alpha|}{\sigma_0}\right)^4}=\sigma_0\sqrt{1+\frac{\hbar^2t^2}{m^2\sigma_0^4}} \tag{17}$$

RESULTS AND DISCUSSION

To elicit the result, the running program is performed by altering the variables v = 1.00, 1.75, and 2.00. The choosing of these numbers is based on how quickly the convergence is achieved, and seeing how far the free particle is located and the resulting probability density. Varying the v in the interval allows the wave function and probability density to be observed. Besides varying the v, varying N and dt is likewise called for to observe the wave function and probability density resulting. From the variation, the graphs of varied probability density and the forms of the wave function of free particles are then presented. The probability density of free particles can be presented in either 2D or 3D graphs. To investigate the form of the wave function and probability density, the following variation is made.

N = 50, dt = 3, and v = 1.75

By inputting N = 50, dt = 3, and v = 1.75, the wave function of free particles and probability density as seen as Figure 1.

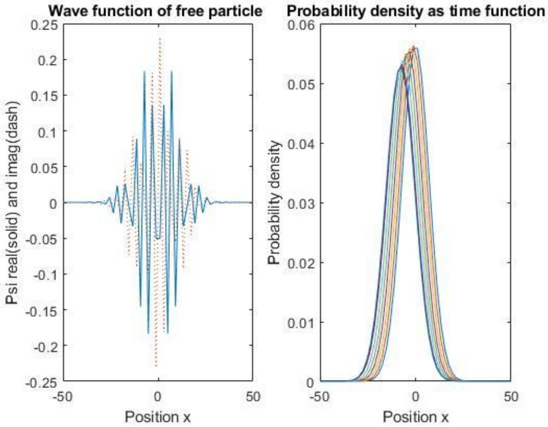

Figure 1. The form of the wave function of free particles and probability density if N = 50, dt = 3, and v = 1.75

Besides, the 3D graph of probability density is shown in Figure 2.

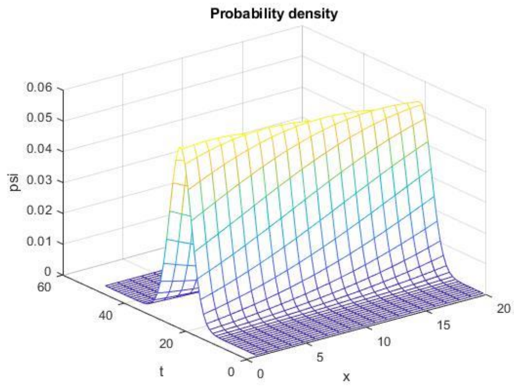

Figure 2. The 3D graph of probability density if N = 50, dt = 3, and v = 1.75

N = 30, dt = 1, v = 2

With N = 30, dt = 1, and v = 2, the form of the wave function of free particles and probability density are demonstrated in Figures 3 and 4.

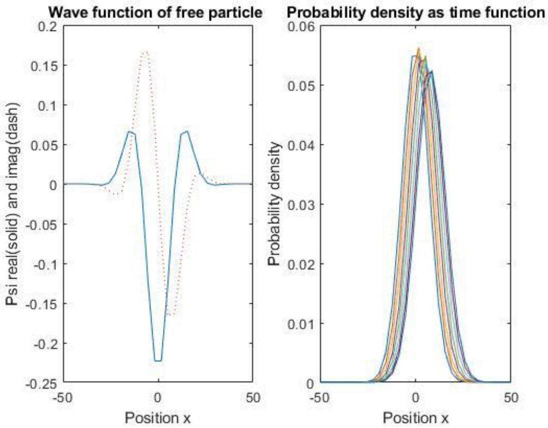

Figure 3. The wave function of free particles and probability density if $N = 30$, $dt = 1$, and $v = 2$

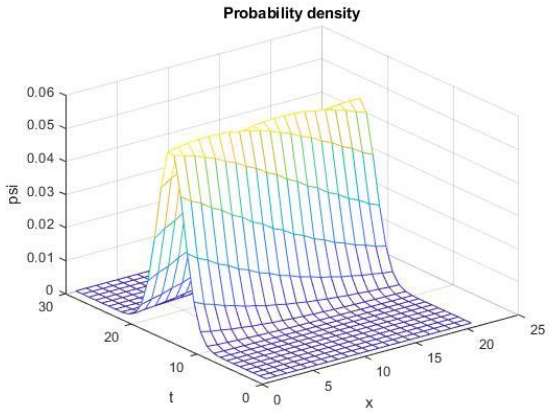

Figure 4. The 3D graph of probability density if $N = 30$, $dt = 1$, and $v = 2$

If $N = 100$, $dt = 1$, and $v = 2$:

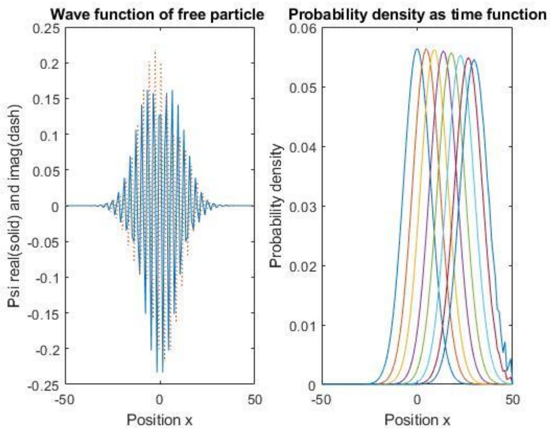

Figure 5. The wave function of free particles and probability density if $N = 100$, $dt = 1$, and $v = 2$

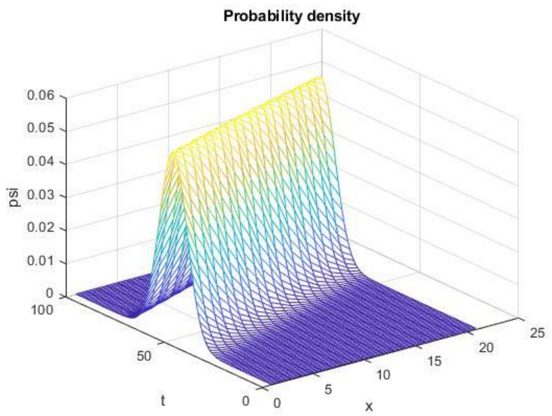

Figure 6. The 3D graph of probability density if $N = 100$, $dt = 1$, and $v = 2$

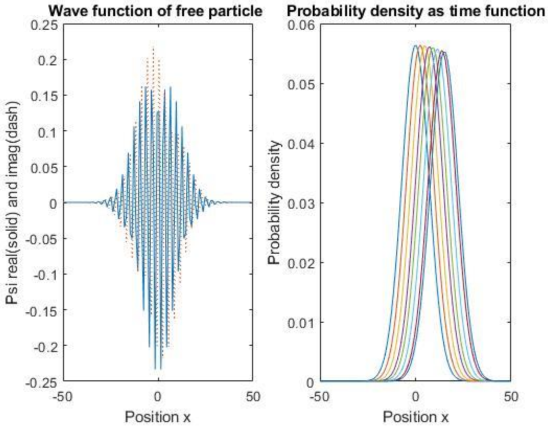

Figure 7. The wave function of free particles and probability density if $N = 100$, $dt = 2$, and $v = 2$

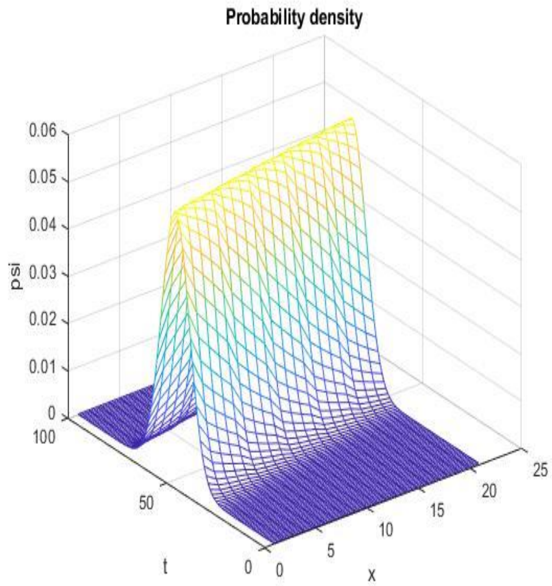

Figure 8. The 3D graph of probability density if $N = 100$, $dt = 2$, and $v = 2$

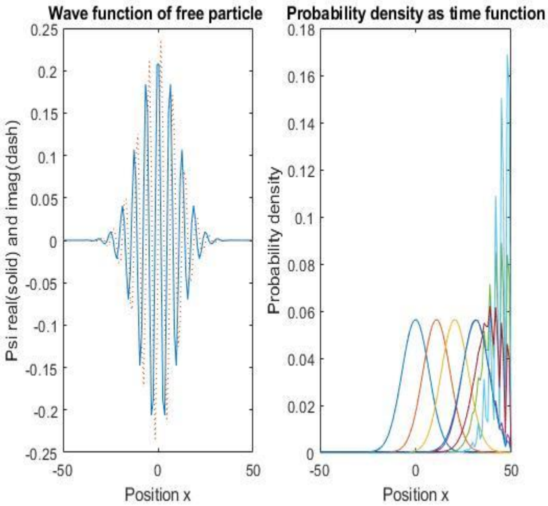

Figure 9. The wave function of free particles and probability density if $N = 100$, $dt = 2$, and $v = 1$

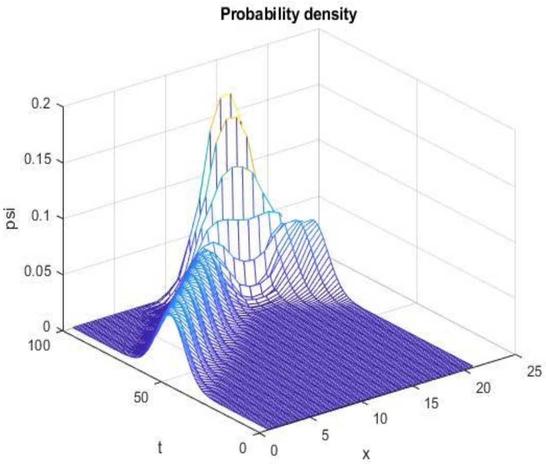

Figure 10. The 3D graph of probability density if $N = 100$, $dt = 2$, and $v = 1$

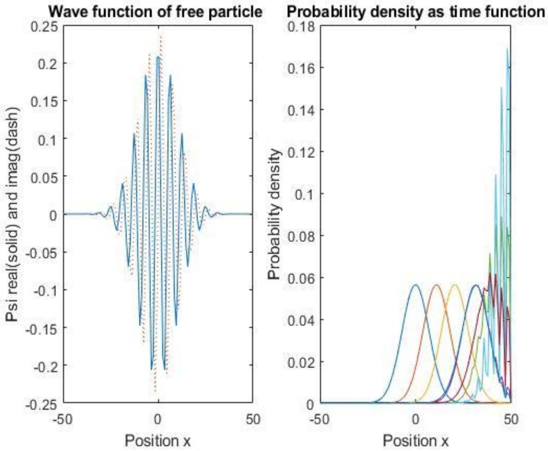

Figure 11. The wave function of free particles and probability density if $N = 100$, $dt = 1$, and $v = 1$

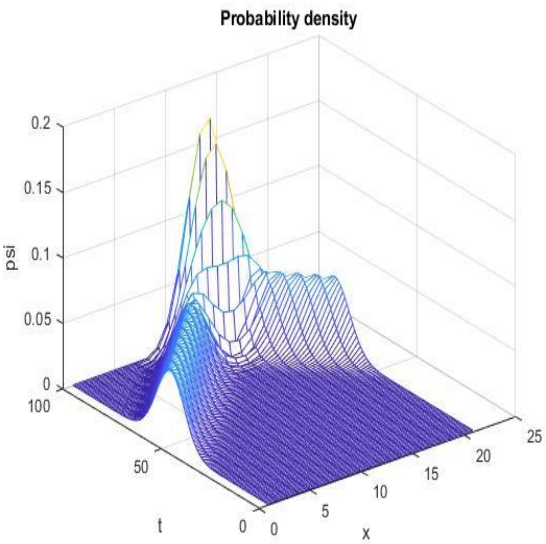

Figure 12. The 3D graph of probability density if $N = 100$, $dt = 1$, and $v = 1$

From the results of this study, it can be seen in the graph obtained in Figure 1 through

Figure 12. The graph was obtained by varying the values of *N*, *v* and *dt*. Variations in the values of *N* are 30, 50 and 100, while the values of *v* are 1.00, 1.75, 2.00 and the values of *dt* are 1 and 2.

The free particles examined here abide by de Broglie's hypothesis of waves, that particles possess wave-like properties with the momentum $p = h/\lambda$ and the wave number $k = 2\pi/\lambda$. The relationship between the two equations can be expressed as $p = \hbar k$. This equation constitutes the relationship between free particle momentum and de Broglie's wavenumber. If the momentum of a particle is $p = mv$, it can be substituted into the above equations and becomes $k_0 = \frac{mv}{h}$. The average wave number k_0 can be substituted into the list program to identify the form of the wave function and probability density resulted.

This research makes several variants to investigate the form of the wave function and probability density resulted. Probability density can be presented in a 3D form by inputting mesh (*p*-plot) in MATLAB. The more the *N* grids were added, the more constricted the form of the wave function resulted. This exhibits a larger possibility for finding particles in that area. *N* grid = 100 produces a better form of wave function than *N* grid = 30. The variation of *v* has an insignificant impact on the form of the wave function and probability density resulted because varying *v* means varying the wavenumber. In this research, with *v* varies at 1, 1.75, and 2 and *N* grid = 100, the form of the wave function and probability density resulted are slightly different. When *N* grid = 100, *dt* = 1, and *v* = 2, the form of the wave function and probability density are the same. And yet, when *N* grid = 100, *dt* = 1, and *v* = 2, the form of the wave function and probability density are constricted in only one area. On the three variants, the *N* grid and *dt* are the two most affecting factors. Studying the probability density always of a free particle can always be developed, as in Olga and Vladimir's research [29], probability representation of the quantum state. Crank-Nicolson method is good for solving partial differential equations [30], one of the numerical methods to solve a partial differential equation [31]. Crank–Nicolson difference scheme for the coupled nonlinear Schrödinger equations with the Riesz space fractional derivative [32]. Although the application of this method is not new, it can still be used in studies of different focuses, as in the literature described above. Thus, a discontinuous finite volume element method combined with the second order Crank–Nicolson method in time discretization is proposed to solve the coupled non-stationary Stokes–Darcy model [33]. A Crank–Nicolson difference scheme is first derived for solving the nonlinear time-space fractional Schrödinger equation [34].

The impact of this research in the field of quantum physics is the determination of that probability density and the shape of the free particle wave function by solving the Schrodinger equation using the Crank-Nicolson method, obtaining various graphic forms by varying the physical quantities that have been determined in this study. The limitation of this research is that it only varies certain physical quantities, especially for free particle systems. It is hoped that the next research can carry out on particles in one-dimensional, two-dimensional boxes and other quantum systems.

CONCLUSION

In performing the simulation of probability density and the wave function of free particles solved using the Schrödinger equation, the most contributive parameters are acquired when the variation of *N* grid, *v*, and *dt* is made. The more the *N* grids were added, the more constricted the wave function's form resulted. This exhibits a larger possibility for finding particles in that area. On the three variants, the *N* grid and the variation of *dt* are the two most affecting factors.

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AUTHOR CONTRIBUTIONS

Sri Purwaningsih designed the model and the computational framework, analysed the data and performed the calculations. Sri Purwaningsih wrote the manuscript with input from Ramacos Fardela.

DECLARATION OF COMPETING INTEREST

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

REFERENCES

[1] Shangwha Y. Klein-Gordon Equation and wave Function Free Particle in Rindler Space-Time, *International Journal of Advanced Reasearch in Physics Science*, 2020; **7**(9): 10-12. Available from: https://www.arcjournals.org/pdfs/ijarps/v7-i9/3.pdf.

[2] Bondar DI, Lompay RR, and Liu WK. Quantum Mechanics of a Free Particle from properties of the Dirac delta function, *American Journal Physics*, 2011; **79**: 392-394. DOI: https://doi.org/10.1119/1.3533715.

[3] Berger MS and Maziashvilli M. Free Particle wavefunction in light of the minimal-length deformed quantum mechanics and some of its phenomenological implication, *Physical Review D*, 2011; **84**: 044043. DOI: https://doi.org/10.1103/PhysRevD.84.044043.

[4] Saxon DS. *Elementary quantum mechanics*. US: Courier Corporation; 2013.

[5] Ajlouni AW, Joudeh B, and Salameh B. Particle in a box with dissipation, *Journal Applied Science*, 2007; **7**(9): 1314-1320. DOI: https://doi.og/10.3923/jas.2007.1314.1320.

[6] Olavo LSF. Foundations of quantum mechanics: non-relativistic theory. *Physica A: Statistical Mechanics and its Applications*. 1999; **262**(1-2): 197-214. DOI: https://doi.org/10.1016/S0378-4371(98)00395-1.

[7] Boonserm P and Visser M. Reformulating the Schrödinger equation as a Shabat–Zakharov system. *Journal of Mathematical Physics*. 2010; **51**(2): 022105. DOI: https://doi.org/10.1063/1.3282847.

[8] Kumar PR and Dong SH. A new quantization rule to the bound state problem in non-relativistic quantum mechanics. *Physics Letters A*. 2021; **417**: 127700. DOI: https://doi.org/10.1016/j.physleta.2021.127700.

[9] Poveda LA, de Peralta LG, Pittman J, and Poirier B. Non-relativistic Approach to Relativistic Quantum Mechanics: The Case of the Harmonic Oscillator. *Foundations of Physics*. 2022;

52(1): 29. DOI: https://doi.org/10.1007/s10701-022-00541-5.

[10] Guo X and Xu M. Some physical applications of fractional Schrödinger equation. *Journal of mathematical physics*. 2006; **47**(8): 082104. DOI: https://doi.org/10.1063/1.2235026.

[11] Dong J and Xu M. Some solutions to the space fractional Schrödinger equation using momentum representation method. *Journal of mathematical physics*. 2007; **48**(7): 072105. DOI: https://doi.org/10.1063/1.2749172.

[12] Han J, Zhang L, and Weinan E. Solving many-electron Schrödinger equation using deep neural networks. *Journal of Computational Physics*. 2019; **399**: 108929. DOI: https://doi.org/10.1016/j.jcp.2019.108929.

[13] Laskin N. Fractals and quantum mechanics. *Chaos: An Interdisciplinary Journal of Nonlinear Science*. 2000; **10**(4): 780-790. DOI: https://doi.org/10.1063/1.1050284.

[14] Owolabi KM and Atangana A. Numerical solution of fractional-in-space nonlinear Schrödinger equation with the Riesz fractional derivative. *The European Physical Journal Plus*. 2016; **131**(9): 335. DOI: https://doi.org/10.1140/epjp/i2016-16335-8.

[15] Nagel JR. A review and application of the finite-difference time-domain algorithm applied to the Schrodinger equation. *ACES Journal-Applied Computational Electromagnetics Society*. 2009; **24**(1): 1-8. Available from https://journals.riverpublishers.com/index.php/ACES/article/view/15873.

[16] van Dijk W, Toyama FM, Prins SJ, and Spyksma K. Analytic time-dependent solutions of the one-dimensional Schrödinger equation. *American Journal of Physics*. 2014; **82**(10): 955-961. DOI: https://doi.org/10.1119/1.4885376.

[17] van Dijk W and Toyama FM. Numerical solutions of the Schrödinger equation with source terms or time-dependent potentials. *Physical Review E*. 2014; **90**: 063309. DOI: https://doi.org/10.1103/PhysRevE.90.063309.

[18] Sellier JM, Nedjalkov M, and Dimov I. An introduction to applied quantum mechanics in the Wigner Monte Carlo formalism. *Physics Reports*. 2015; **577**: 1-34. DOI: https://doi.org/10.1016/j.physrep.2015.03.001.

[19] Pauli W. *General principles of quantum mechanics*. New York: Springer Science & Business Media; 2012.

[20] Blatt R and Roos CF. Quantum simulations with trapped ions. *Nature Physics*. 2012; **8**(4): 277-284. DOI: https://doi.org/10.1038/nphys2252.

[21] Weinberg S. The trouble with quantum mechanics. *The New York Review of Books*. 2017; **19**: 1-7. Available: http://quantum.phys.unm.edu/466-19/QuantumMechanicsWeinberg.pdf.

[22] Valentini A. Foundations of statistical mechanics and the status of the Born rule in de Broglie-Bohm pilot-wave theory. In *Statistical mechanics and scientific explanation: determinism, indeterminism and laws of nature*. 2020: pp. 423-477. DOI: https://doi.org/10.1142/9789811211720_0012.

[23] Rosique F, Navarro PJ, Fernandez C, and Padilla A. A systematic review of perception system and simulators for autonomous vehicles research. *Sensors*. 2009; **19**(3): 648. DOI: https://doi.org/10.3390/s19030648.

[24] Vesely FJ, Davenport F, McKay S, and Christian W. Computational Physics: An Introduction. *Computers in Physics*. 1996; **10**: 47. DOI: https://doi.org/10.1063/1.4822354.

[25] Horbatsch M. *Quantum Mechanics Using Maple*. New York: Springe; 1995. Available from: https://link.springer.com/content/pdf/bfm:978-3-642-79538-1/1.pdf.

[26] Amodio P, Brugnano L, and Iavernaro F. Analysis of Spectral Hamiltonian Boundary Value

Methods (SHBVMs) for the numerical solution of ODE problems. *Numerical Algorithms*. 2020; **83**(4): 1489-1508. DOI: https://doi.org/10.1007/s11075-019-00733-7.

[27] Moyer CA. Numerov extension of transparent boundary conditions for the Schrödinger equation in one dimension. *American Journal of Physics*. 2004; **72**(3): 351-358. DOI: https://doi.org/10.1119/1.1619141.

[28] Pang T. An introduction to computational physics. *American Journal of Physic*s. 1999; **67**(1): 94-95. DOI: https://doi.org/10.1119/1.19198.

[29] Olga VM and Vladimir IM, Probability Representation of Quantum State. *Entropy*. 2021; **23**(5): 549. DOI: https://doi.org/10.3390/e23050549.

[30] Fadugba SE, Edogbanya OH, and Zelibe SC. Crank-Nicolson methods for solving Parabolic Partial Differential Equations. *International Journal of Applied Mathematics and Modeling IJA2M*. 2013; **1**(3): 8-23.

[31] Fernandes N and Bhadkamkar R. An overview of a Crank-Nicolson to solve parabolic differential partial equation. *International Journal of Scientific and Engineering Research*. 2016; **7**(12): 1074-1078. Available from: https://www.ijser.org/onlineResearchPaperViewer.aspx?AN-OVERVIEW-OF-A-CRANK-NICOLSON-METHOD-TO-SOLVE-PARABOLIC-PARTIAL-DIFFERENTIAL-EQUATION.pdf.

[32] Wang D, Xiao A, and Yang W. Crank–Nicolson difference scheme for the coupled nonlinear Schrödinger equations with the Riesz space fractional derivative. *Journal of Computation Physics*. 2013; **242**. 670-681, DOI: https://doi.org/10.1016/j.jcp.2013.02.037.

[33] Li R, Gao Y, Yang W, and Chen Z. A Crank–Nicolson discontinuous finite volume element method for a coupled non-stationary Stokes–Darcy problem, *Journal of Computational and Applied Mathematics*. 2019; **353**(C): 86-112. DOI: https://doi.org/10.1016/j.cam.2018.12.025.

[34] Ran M and Zhang C. Linearized Crank–Nicolson scheme for the nonlinear time–space fractional Schrödinger equations, *Journal of Computational and Applied* Mathematics. 2019; **355**: 218-231, DOI: https://doi.org/10.1016/j.cam.2019.01.045.