SINTECHCOM: Science, Technology and Communication Journal
Vol. 3, No. 1, October 2022, pp. 19-24, DOI: 10.59190/stc.v3i1.221

Schrödinger's equation as a Hamiltonian system

Suhaivi Hamdan*, Erwin Amiruddin
Department of Physics, Universitas Riau, Pekanbaru 28293, Indonesia

ABSTRACT

This article describes the concept of the time-dependent Schrödinger equation (TDSE) as a review to add a detailed understanding of the steps to formulate TDSE which can be seen from the classical mechanic's concept as a mechanical wave function. In this article, a comprehensive approach to the concepts of momentum and energy in particles will be described using operators working on wave functions. The results show that the use of momentum and energy operators can show that TDSE is a Hamiltonian system.

ARTICLE INFO

Article history:

Received Sep 17, 2022
Revised Oct 12, 2022
Accepted Oct 20, 2022

Keywords:

Energy
Hamiltonian System
Momentum
Time-Dependent Schrödinger Equation

* **Corresponding Author**
E-mail address: suhaivi@gmail.com

1. INTRODUCTION

The time-dependent Schrödinger equation (TDSE) plays a very important role in the development of modern physics, especially quantum mechanics, logically it can be analogous to the laws of classical physics [1-5]. The Schrödinger equation is a wave function that is used to provide information about the waveform of a particle [6-10].

The Schrödinger equation explains that the behavior of free particles such as electrons has certain energy levels that are discrete [11-15]. If the wave function can represent the motion of electrons, then the wave energy or the energy of the electrons that represent it must be the same [16-21]. An electron has a total energy consisting of kinetic and potential energy where the potential energy is a function of the x position so that the total energy of the electron as a particle is [22]:

$$E = \frac{p^2}{2m} + E_p \tag{1}$$

In a general coordinate system, the total energy of a function representing the energy of a particle can be defined by the momentum p, position x, and time t as a Hamiltonian system as in the following equation [23]:

$$H(x,p,t) = \frac{p^2}{2m} + E_p(x,t) \tag{2}$$

The Schrödinger equation is a wave equation that is derived directly from the mechanical wave function by approaching the momentum and energy of the particle. In this article, we will comprehensively describe the approach to the concepts of momentum and energy in particles using operators working on wave functions.

2. RESEARCH METHODS

According to Ward (2006), the wave function for a free particle moves with a certain momentum and energy where the state of this particle is related to Planck's quantization principle [24]. Particle momentum has a relationship with wavelength and applies the frequency and wavelength relationship to energy and momentum using angular frequency and wave number as in the following equation [25]:

$$E = hv = \hbar\omega \tag{3}$$

and

$$p = \frac{E}{c} = \frac{h}{\lambda} = \hbar k \tag{4}$$

In the case of a particle moving freely in the positive x-axis direction with momentum $p_x > x$ where $p_x > 0$. In the case of a traveling wave function moving according to the motion of the free particle this is a plane waveform as in the following equation [26]:

$$\psi(x,t) = Ae^{i(k_x x - \omega t)} \tag{5}$$

by substituting Equation (3) and Equation (4) into Equation (5), the wave function of Equation (5) can be simplified to:

$$\psi(x,t) = Ae^{i\frac{(p_x x - Et)}{\hbar}} \tag{6}$$

This wave function is a mechanical wave function that can be used to formulate the Schrödinger equation. The energy of a free particle in classical mechanics which is related to the concept of momentum is:

$$E = \frac{{p_x}^2}{2m} \tag{7}$$

from Equation (7) can be derived the equation of motion of the free particle, namely:

$$\hat{E}\psi(r,t) = \frac{1}{2m}\hat{p}^2\psi(x,t) \tag{8}$$

This wave function can be used to formulate the Schrödinger equation by operating this function by differentiating position and time as follows:

$$-i\hbar\frac{\partial}{\partial x}\psi(x,t) = p_x\psi(x,t) \tag{9}$$

According to Briggs and Rost (2001), operation $-i\hbar(\partial/\partial x)$ expresses the momentum p_x of the wave function, then the second form of differentiation with respect to time is [27]:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = E\psi(x,t) \tag{10}$$

where the $i\hbar(\partial/\partial t)$ operation states the energy value E of the wave function. According to Sarma (2011) Equation (9) and Equation (10) is an eigen equation that shows the operators $-i\hbar(\partial/\partial x)$ and $i\hbar(\partial/\partial t)$ which are the values of momentum and energy [28] so that the momentum and energy operators can be defined as follows:

$$\hat{p}_x = -\hbar\frac{\partial}{\partial x} \tag{11}$$

and

$$\hat{E} = i\hbar\frac{\partial}{\partial t} \tag{12}$$

The momentum and energy operators obtained from the plane wave function must be suitable for free particles under general conditions and must be the same for different variables [29].

3. RESULTS AND DISCUSSIONS

The procedure for obtaining the Schrödinger equation for free particles in one-dimensional space using the free particle wave function given by Equation (8) can be simplified by applying Hamilton's principle as in the following equation [26, 30]:

$$H = T + V \tag{13}$$

Hamilton's equations can be derived using the canonical transformation equations for spatial coordinates and canonical momentum for an *n*-dimensional classical mechanical system as follows:

$$E = \frac{{p_x}^2}{2m} \tag{14}$$

if the wave function in Equation (6) is differentiated twice with respect to x then we get:

$$\frac{\partial^2}{\partial x^2}\psi(x,t) = \left[-\frac{{p_x}^2}{\hbar^2}\right]\psi(x,t) \tag{15}$$

then the wave function in Equation (6) is reduced to t then we get:

$$\frac{\partial}{\partial t}\psi(x,t) = \left[\frac{iE}{\hbar}\right]\psi(x,t) \tag{16}$$

by using the relationship in Equation (14) then Equation (15) and Equation (16) can be simplified to:

$$\frac{\partial}{\partial t}\psi(x,t) = \left[\frac{i\hbar}{2m}\right]\left[-\frac{i{p_x}^2}{2m\hbar}\psi(x,t)\right] \tag{17}$$

then by substituting Equation (15) into Equation (17) we get:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) \tag{18}$$

In general, the three-dimensional coordinate system of equations of motion for free particles can be expressed using Laplacian ∇^2 so that Equation (18) can be written as:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\nabla^2\psi(r,t) \tag{19}$$

on a freely moving particle in a system with a certain potential $V(r,t)$ so that Equation (19) becomes:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\nabla^2\psi(r,t) + V(r,t)\psi(r,t) \tag{20}$$

by using Equation (20) in the classical variable form of the wave function in Equation (15) which is a two-times differential with respect to x so that the equation of motion of the free particle can be written as:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hat{p}^2}{2m}\psi(r,t) + V(r,t)\psi(r,t) \tag{21}$$

by writing the Hamiltonian equation in Equation (21) in the form of a Hamiltonian operator such as:

$$\hat{H} = \hat{T} + \hat{V} \tag{22}$$

where $\hat{T} = \hat{p}^2/2m$ so that Equation (21) can be simplified to:

$$\hat{E}\psi(x,t) = \left[\frac{\hat{p}^2}{2m} + V(r,t)\right]\psi(r,t) \tag{23}$$

then divide Equation (23) by the wave function $\psi(r,t)$, so that Equation (23) becomes a simpler form, namely:

$$\hat{E} = \frac{\hat{p}^2}{2m} + V(r,t) = \hat{T} + \hat{V} \tag{24}$$

or

$$\hat{H}(r,p,t) = \frac{\hat{p}^2}{2m} + V(r,t) \tag{25}$$

from Equation (25) where TDSE satisfies the principle of Hamilton's system in classical mechanics as a function of position, momentum, and time.

4. CONCLUSION

In deriving TDSE, it can be done by using a mathematical approach and the concepts of momentum and energy operators to obtain a wave equation or a partial differential equation. Furthermore, TDSE can be reduced to classical mechanics as a principle of the Hamiltonian system, so that TDSE can be written in a simplified form of the Hamiltonian system $\hat{H} = \hat{T} + \hat{V}$ as a function of position, momentum, and time.

REFERENCES

[1] Nelson, E. (1966). Derivation of the Schrödinger equation from Newtonian mechanics. *Physical Review*, **150**(4), 1079.

[2] Amini, K., Chacón, A., Eckart, S., Fetić, B., & Kübel, M. (2021). Quantum interference and imaging using intense laser fields. *The European Physical Journal D*, **75**(10), 1–22.

[3] Hamdan, S. & Amiruddin, E. (2022). Decomposition and estimation of gauge transformation for Chern-Simons-Antoniadis-Savvidy forms. *Science, Technology and Communication Journal*, **2**(3), 73–78.

[4] Yattaqi, E., Gemawati, S., & Hasbiyati, I. (2021). On left fq-derivations of B-algebras. *Science, Technology and Communication Journal*, **2**(1), 1–8.

[5] Baker, L. A., Marchetti, B., Karsili, T. N., Stavros, V. G., & Ashfold, M. N. (2017). Photoprotection: extending lessons learned from studying natural sunscreens to the design of artificial sunscreen constituents. *Chemical Society Reviews*, **46**(12), 3770–3791.

[6] Tozar, A., Tasbozan, O., & Kurt, A. (2021). Optical soliton solutions for the (1+ 1)-dimensional resonant nonlinear Schröndinger’s equation arising in optical fibers. *Optical and Quantum Electronics*, **53**(6), 316.

[7] Shen, Y. X., Peng, Y. G., Cai, F., Huang, K., Zhao, D. G., Qiu, C. W., Zheng, H., & Zhu, X. F. (2019). Ultrasonic super-oscillation wave-packets with an acoustic meta-lens. *Nature Communications*, **10**(1), 3411.

[8] Purwaningsih, S. & Fardela, R. (2022). The Analysis of the Physical Quantity N Grid, v, and dt in Solving the Schrödinger Equation Using the Crank-Nicolson Method. *Jurnal Penelitian Fisika dan Aplikasinya (JPFA)*, **12**(1), 1–13.

[9] Tozar, A., Tasbozan, O., & Kurt, A. (2021). Optical soliton solutions for the (1+ 1)-dimensional resonant nonlinear Schröndinger’s equation arising in optical fibers. *Optical and Quantum Electronics*, **53**(6), 316.

[10] Gu, Y., Chen, B., Ye, F., & Aminakbari, N. (2022). Soliton solutions of nonlinear Schrödinger equation with the variable coefficients under the influence of Woods–Saxon potential. *Results in Physics*, **42**, 105979.
[11] Zhang, X., Yang, B., Wei, C., & Luo, M. (2021). Bounded solution structure of Schrödinger equation in the presence of the minimal length and its effect: Bound states in the continuum are universal. *Communications in Nonlinear Science and Numerical Simulation*, **96**, 105694.
[12] Nakatsuji, H., Nakashima, H., & Kurokawa, Y. I. (2018). Solving the Schrödinger equation of atoms and molecules: Chemical-formula theory, free-complement chemical-formula theory, and intermediate variational theory. *The Journal of Chemical Physics*, **149**(11).
[13] Wang, H. Y. (2020). New results by low momentum approximation from relativistic quantum mechanics equations and suggestion of experiments. *Journal of Physics Communications*, **4**(12), 125004.
[14] Nakatsuji, H., Nakashima, H., & Kurokawa, Y. I. (2018). Solving the Schrödinger equation of atoms and molecules: Chemical-formula theory, free-complement chemical-formula theory, and intermediate variational theory. *The Journal of Chemical Physics*, **149**(11).
[15] Wang, H. Y. (2020). New results by low momentum approximation from relativistic quantum mechanics equations and suggestion of experiments. *Journal of Physics Communications*, **4**(12), 125004.
[16] Bliokh, K. Y., Ivanov, I. P., Guzzinati, G., Clark, L., Van Boxem, R., Béché, A., Juchtmans, R., Alonso, M. A., Schattschneider, P., Nori, F., & Verbeeck, J. (2017). Theory and applications of free-electron vortex states. *Physics Reports*, **690**, 1–70.
[17] Weinberg, S. (2017). The trouble with quantum mechanics. *The New York Review of Books*, **19**, 1–7.
[18] Ghosh, S., Verma, P., Cramer, C. J., Gagliardi, L., & Truhlar, D. G. (2018). Combining wave function methods with density functional theory for excited states. *Chemical reviews*, **118**(15), 7249–7292.
[19] Gagliardi, L., Truhlar, D. G., Li Manni, G., Carlson, R. K., Hoyer, C. E., & Bao, J. L. (2017). Multiconfiguration pair-density functional theory: A new way to treat strongly correlated systems. *Accounts of chemical research*, **50**(1), 66–73.
[20] Zhang, X., Yang, B., Wei, C., & Luo, M. (2021). Quantization method and Schrödinger equation of fractional time and their weak effects on Hamiltonian: phase transitions of energy and wave functions. *Communications in Nonlinear Science and Numerical Simulation*, **93**, 105531.
[21] Zhang, X., Yang, B., Wei, C., & Luo, M. (2021). Bounded solution structure of Schrödinger equation in the presence of the minimal length and its effect: Bound states in the continuum are universal. *Communications in Nonlinear Science and Numerical Simulation*, **96**, 105694.
[22] Curchod, B. F., & Martínez, T. J. (2018). Ab initio nonadiabatic quantum molecular dynamics. *Chemical Reviews*, **118**(7), 3305–3336.
[23] Kolodrubetz, M., Sels, D., Mehta, P., & Polkovnikov, A. (2017). Geometry and non-adiabatic response in quantum and classical systems. *Physics Reports*, **697**, 1–87.
[24] Ward, D. W. & Volkmer, S. M. (2006). How to derive the schrodinger equation *American Journal of Physics*, 1–12.
[25] Nouredine, Z. (2009). *Quantum mechanics concept and applications second edition*. John Wiley and Sons: Jacksonville State University USA.
[26] Barde, N. P., Patil, S. D., Kokne, P. M., & Bardapurkar, P. P. (2015). Deriving time dependent Schrödinger equation from Wave-Mechanics, Schrödinger time independent equation, Classical and Hamilton-Jacobi equations. *Leonardo Electronic Journal of Practices and Technologies*, **14**(26), 31–48.
[27] Briggs, J. S. & Rost, J. M. (2001). On the derivation of the time-dependent equation of Schrödinger. *Foundations of Physics*, **31**, 693–712.
[28] Sarma, P. R. (2011). Direct derivation of Schrödinger equation from Hamilton-Jacobi equation using uncertainty principle. *Rom. J. Phys*, **56**, 1053–1056.

[29] Griffiths, D. J. (2009). *Introduction to quantum mechanics second edition*. Person Prentice Hall: New Jersey USA.
[30] Kovalchuk, V. & Slawianowski, J. J. (2008). Hamiltonian systems inspired by the Schrödinger equation. *SIGMA. Symmetry, Integrability and Geometry: Methods and Applications*, **4**, 046.