Visualization of Schrodinger Equations Polar Wave Functions for Non-Central Coulombic Rosen Morse Potential in ExcitationState $n_r = 2$ and l = 1

Cecilia Yanuarief

Physics Department, Faculty of Science and Technology, UIN Sunan Kalijaga Jl. Marsda Adisucipto No. 1 Yogyakarta 55281, Indonesia. Tel. + 62-274-540971, Fax. + 62-274-519739 Email : cecilia.yanuarief@uin-suka.ac.id

Abstract. Research has been conducted which shows the quantization visualization of hydrogen atom orbitals angular space in Rosen Morse potential system interference when the electrons are excited in the state of $n_r = 2$ and l = 1 through the polar function analysis of the Schrödinger Potential of Non-Central Coloumbic Rosen Morse. The polar Schrödinger equation is solved using the Romanovski polynomial method to obtain the polar wave function. To show the accuracy of the analysis, the polar wave function spectrum is visualized with Matlab-based computer programming.

Keywords: Non-central coulombic rosen morse, Romanovski polynomi

INTRODUCTION

Quantum mechanics has long been known as a "basic science" for examining the symptoms and various properties of microscopic systems. Its utilization not only succeeded in expanding and deepening understanding of natural events in the laboratory, but also resulted in widespread technological advances, and indirectly influenced the quality and style of human life. The development of quantum mechanics is rooted in the basic concepts of quantum theory which include both discrete and irregular expectations. Quantum theory is proven to be able to explain quantum phenomena from macroscopic systems such as superconductivity and superfluidity which have the potential for important applications. In the process of learning quantum physics, especially quantum mechanics always involves complex equations and the solution requires analysis and high thinking. Examples of problems that are quite complicated are the completion of the wave function of the Schrödinger equation (Greiner and Muller, 2004). The Schrödinger equation is obtained starting from the wave function of the free-moving particle. The expansion of the Schrödinger equation for the special case of free particles to the general case with a particle which experiences arbitrary force that changes with space and time is a possibility that can be pursued. But there is no one exact way that proves that expansion is true. All you can do is take the postulate that the Schrödinger equation applies to various physical situations and compares the results with the experimental results. If the results are suitable, the postulate must be discarded and another approach must be explored. In other words, the Schrödinger equation cannot be derived from the

first principle, but the Schrödinger equation itself is the first principle.

The Schrödinger equation has produced very precise predictions of the experimental results obtained and it must be admitted that the Schrödinger equation states a successful postulate concerning certain aspects of the physical world. It should be noted that the Schrödinger equation is not the addition of many postulates needed to provide the physical workings, because Newton's second law of motion which in classical mechanics is seen as a postulate can be derived from the Schrödinger equation. Research on the completion of the wave function in the Schrödinger equation is a very important research in modern physics. Various methods that have been developed include the Super Symmetry method (Compean and Kirchbach. 2008), the Nikiforov-Uvarov method (Ikot et al., 2011), and the Romanovski polynomial method (Alvarenz and Castillo, 2009). Based on these facts, a research was conducted to solve the complexity of completing the wave function of the Schrödinger equation by using the Romanovski polynomial method. As a distinguishing feature of this article is the system studied is the movement of electrons in the first excitation state with $n_r = 2$ and l = 1 which is disturbed by the non-central potential of Rosen Morse which is the main candidate as an effective potential in Quantum Chromodynamic (QCD) (Compean and Kirchbach, 2006), so that the Schrödinger equation model used uses a combination of two non-central potentials, namely the potential of non-central Coulomb and potential of non-central Rosen Morse (Flugge, 1971).

MATERIALS AND METHODS

Romanovski Polynomial

The second order hypergeometric equation is stated as follows,

$$\sigma(x)\frac{d^2y_n(x)}{dx^2} + \tau(x)\frac{dy_n(x)}{dx} + \lambda_n y_n(x) = 0 \quad , \quad (1)$$

$$\sigma(x) = ax^2 + bx + c \qquad , \quad \tau = dx + e \qquad , \quad (2a)$$

with Romanovski parameters,

$$a = 1$$
, $b = 0$, $c = 1$, $d = 2(1 - p)$, dan $e = q$,

$$p > 0, y_n(x) = D_n^{(p,q)}(x), p > n$$
 (2b)

So, the second-order hypergeometric equation is filled by Romanovski polynomials, namely,

$$(1+x^2)\frac{d^2D_n^{(p,q)}(x)}{dx^2} + (2x(1-p)+q)\frac{dD_n^{(p,q)}(x)}{dx} - \{n(n-1)+2n(1-p)\}D_n^{(p,q)}(x) = 0$$
(3)

The Schrödinger equation can be reduced to a second-order differential equation expressed in the form of equation (3) by doing the appropriate variable substitution. The method used is to substitute the wave function of the Schrödinger equation with the Romanovki wave function, that is,

$$g(x) = (1+x^2)^{\frac{\beta}{2}} e^{\frac{-\alpha}{2} \tan^{-1}x} D_n^{(p,q)}(x)$$
(4)

with,

$$D_n^{(p,q)}(x) = \frac{1}{w(x)} \frac{d^n}{dx^n} ((1+x^2)^n w(x))$$
(5)

Equation (5) is a Romanovski polynomial, where w (x) is a weighting factor that can be determined using Pearson differential equations, namely,

$$\frac{d}{dx}(\sigma(x)w(x)) = \tau(x)w(x) \quad . \tag{6}$$

By substituting equations (2a) and (2b) into equation (6), it is obtained,

$$w(x) = \exp\left(\int \frac{(d-2a)x + (e-b)}{ax^2 + bx + c} dx\right) ,$$

$$w(x) = \exp\left(\int \frac{-2px + q}{1 + x^2} dx\right) ,$$

$$w(x) = \exp\left[-p\ln(1 + x^2) + q\tan^{-1}x\right] ,$$

$$w(x) = (1 + x^2)^{-p} e^{q \tan^{-1}(x)}$$
(7)

Determining Polar Wave Functions with Romanovski Polynomials

Non-central potential which is a combination of Coulomb potential and Rosen Morse's non-central potential,

$$V(r,\theta) = \frac{-e^2}{r} + \frac{\hbar^2}{2mr^2} \left(\frac{\nu(\nu+1)}{\sin^2\theta} - 2\mu\cot\theta \right)$$
(8)

with, $\nu > 0$, $\mu > 0$. The Schrodinger 3 Dimension equation for non-central potential is written as follows,

$$-\frac{\hbar^{2}}{2m}\left\{\frac{1}{r^{2}}\frac{\partial}{\partial r}\left(r^{2}\frac{\partial}{\partial r}\right) + \frac{1}{r^{2}sin\theta}\frac{\partial}{\partial\theta}\left(sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^{2}sin^{2}\theta}\frac{\partial^{2}}{\partial\varphi^{2}}\right)\psi(r,\theta,\varphi) ,$$

$$+\left\{\frac{-e^{2}}{r} + \frac{\hbar^{2}}{2mr^{2}}\left(\frac{v(v+1)}{sin^{2}\theta} - 2\mu \cot\theta\right)\right\}\psi(r,\theta,\varphi) = E\psi(r,\theta,\varphi)$$
(9)

from equation (9) is obtained,

$$\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{2mr^2}{\hbar^2}\frac{e^2}{r} + \frac{2mr^2}{\hbar^2}E = \lambda$$
(10a)

$$-\frac{1}{Psin\theta}\frac{\partial}{\partial\theta}\left(sin\theta\frac{\partial}{\partial\theta}\right) - \frac{1}{\phi sin^{2}\theta}\frac{\partial^{2}}{\partial\varphi^{2}} + \left(\frac{\nu(\nu+1)}{sin^{2}\theta} - 2\mu cot\theta\right) = \lambda$$
(10b)

With λ is the spatial constant with the value $\lambda = 1$ (1 + 1) for the motion of the hydrographic atom in the Coulomb potential. Whereas the completion of the wave equation in the azimuth part is obtained from equation (10b), that is,

$$p = A_m e^{im\varphi} \quad , \tag{11}$$

with A_m is the normalization constant and $m = \pm 1, \pm 2, \pm 3, \pm 4, \dots$

Completion of the Polar Part of the Schrodinger Equation

Obtained from equation (10b), the polar part of the Schrodinger equation is,

$$\frac{\partial^2 P(\theta)}{\partial \theta^2} + \cot\theta \frac{\partial P(\theta)}{\partial \theta} - \left(\frac{v(v+1) + m^2}{\sin^2\theta} - 2\mu\cot\theta\right) P(\theta) + \lambda P(\theta) = 0$$
(12)

with the substitution of the variable $\cot \theta = x$ in equation (11), obtained,

$$(1+x^2)\frac{\partial^2 P}{\partial x^2} + x\frac{\partial P}{\partial x} - \left\{ (v(v+1)+m^2) - \frac{2\mu x}{(1+x^2)} - \frac{\lambda}{(1+x^2)} \right\} P = 0$$
(13)

By comparing equations (13) and (4), a general solution is obtained,

$$P(\theta) = g_{n_l}(x) = (1+x^2)^{\frac{\beta}{2}} e^{\frac{-\alpha}{2}tan^{-1}x} R_{n_l}^{(-\beta,-\alpha)}(x)$$
(14)

 $-\infty < x < \infty$.

If equation (14) is substituted into equations (5) and (3), it is obtained,

$$(1+x^2)\frac{\partial^2 R}{\partial x^2} + \{x(2\beta+1) - \alpha\}\frac{\partial R}{\partial x} - \{v(v+1) + m^2 - \beta^2 - \beta + \beta\}R = 0$$
(15)

Equation (15) is then compared with equation (3), obtained,

$$\alpha_{n_l} = \frac{2\mu}{\beta - \frac{1}{2}} = -\frac{2\mu}{\sqrt{\nu(\nu + 1) + m^2} + n_l + \frac{1}{2}}$$
(16)

$$\beta_{n_l} = -\sqrt{\nu(\nu+1) + m^2} - n_l \quad , \tag{17}$$

$$l + \frac{1}{2} = \sqrt{\left(\sqrt{\nu(\nu+1) + m^2} + n_l + \frac{1}{2}\right)^2 - \frac{\mu^2}{\left(\sqrt{\nu(\nu+1) + m^2} + n_l + \frac{1}{2}\right)^2}} \qquad (18)$$

From equations (16), (17) and (18), the polar wave function can be obtained through equation (14), so that a general equation is obtained,

$$w^{(-\beta,-\alpha)} = (1+x^2)^{\beta_{n_l}} \cdot e^{-\alpha_{n_l} \tan^{-1} x} \quad , \tag{19}$$

$$R_{n_l}^{(-\beta,-\alpha)} = \frac{1}{(1+x^2)^{\beta_{n_l}} \cdot e^{-\alpha_{n_l}\tan^{-1}x}} \frac{d^{n_l}}{dx^{n_l}} \Big[(1+x^2)^{n_l+\beta_{n_l}} \cdot e^{-\alpha_{n_l}\tan^{-1}x} \Big]$$
(20)

$$P_l^m = g(x) = (1+x^2)^{\frac{\beta_{n_l}}{2}} \cdot e^{-\frac{\alpha_{n_l}}{2}\tan^{-1}x} \cdot R_{n_l}^{(-\beta,-\alpha)}$$
(25)

(a)

RESULTS AND DISCUSSION

Table 1. Polar wave functions coulombic non-central potential Schrodinger rosen morse excitation State $n_{\tau} = 2$ and l = 1.

No.	n _r	n_l	m	ν	μ	l	P_l^m
1.	2	0	±1	0	0	1	$\sqrt{\sin^2 \theta}$
2.	2	0	± 1	1	1	1,69	$\sqrt{\sin^{3,463}\theta}$
3.	2	0	± 1	2	2	2,58	$\sqrt{\sin^{5,292}\theta}$



Figure 1. (a) Visualization of electron excited $(n_{\pm} = 2 \text{ and } l = 1)$ polar wave function undisturbed by non-central Rosen Morse potential $(P_{\pm}^{\pm 1} = \sqrt{\sin^2 \theta})$; (b) Amplitude of electron excited $(n_{\pm} = 2 \text{ and } l = 1)$ polar wave function undisturbed by non-central Rosen Morse potential $(P_{\pm}^{\pm 1} = \sqrt{\sin^2 \theta})$.

Pml*sin(theta)*sin(phi)



Figure 2. (a) Visualization of electron excited $(n_r = 2 \text{ and } l = 1)$ polar wave function disturbed by non-central Rosen Morse potential $(P_{1,\theta\theta}^{\pm 1} = \sqrt{\sin^{2,4\theta\Xi} \theta})$; (b) Amplitude of electron excited $(n_r = 2 \text{ and } l = 1)$ polar wave function disturbed by non-central Rosen Morse potential $(P_{1,\theta\theta}^{\pm 1} = \sqrt{\sin^{2,4\theta\Xi} \theta})$.



Figure 3. (a) Visualization of electron excited $(n_r = 2 \text{ and } l = 1)$ polar wave function disturbed by non-central Rosen Morse potential $(P_{z,zz}^{\pm 1} = \sqrt{\sin^{5,646} \theta})$; (b) Amplitude of electron excited $(n_r = 2 \text{ and } l = 1)$ polar wave function disturbed by non-central Rosen Morse potential $(P_{z,zz}^{\pm 1} = \sqrt{\sin^{5,646} \theta})$.

The system potential in the Schrodinger equation actually limits the motion of particles under the potential influence. If the potential of the system is zero, then a particle in the system will be free or referred to as free particles (Beiser, 1992). In the case of electron motion in the Hydrogen Atom system, electrons move around the atomic nucleus, which means that the electron is in a potential influence that limits its motion. The motion potential of electrons in the hydrogen atom is Coulomb potential. This Coulomb potential causes electrons to move around the atomic nucleus. Rotating electrons around the atomic nucleus can experience excitation to higher energy levels, for example from basic energy levels to value $n_r = 1$ towards first level energy with value $n_r = 2$. When viewed from equation (18), the quantum number of the orbital l which physically affects the shape of the electron orbit, is influenced by the value of \boldsymbol{v} and $\boldsymbol{\mu}$. If viewed from equations (16) and (17), the value of \boldsymbol{v} and μ affect the values of α_{n_l} and β_{n_l} where both of them are coefficients of hamiltonian intruders where when $\alpha_{n_1} > 0$ and/or $\beta_{n_1} > 0$, illustrates the existence of "problems" in the system, and when $\alpha_{n_l} = \beta_{n_l} = 0$ illustrates that the system is not interrupted assuming changes in the values of α_{n_l} and β_{n_l} change continuously, so that eigenfunctions and eigen energy disturbed changes subtly into eigenfunctions and eigen energy is not disturbed.

If viewed from equations (8) and (21) which are general equations of polar wave functions, for values $v = \mu = 0$, Rosen Morse's potential is zero which means the wave function does not get interference from Rosen Morse potential, the wave function is only affected by Coulomb potential alone. Visualization of electron motion space when excited at the first level energy under the influence of Coulomb potential can be seen in Figure 1 which shows the visualization of the motion of electrons with values $v = \mu = 0$, which means that electrons are only affected by Coulomb's potential or do not get interference from potential noncentral Rosen Morse. But for $\nu > 0$ and $\mu > 0$, the wave function is interrupted by Rosen Morse potential with the form of interference as shown in Figure 2 and 3. The disturbance form \boldsymbol{v} and $\boldsymbol{\mu}$ values can be explained by equation (18) where the value of \boldsymbol{v} and $\boldsymbol{\mu}$ affect the value of the l orbital quantum number which affects the shape of the electron orbit. The greater the value of \boldsymbol{v} and $\boldsymbol{\mu}$, the greater the interference from the non-central potential system of Rosen Morse against the Coulomb potential. With the existence of potential non-central interference, Rosen Morse generally limits the movement of electrons when rotating around the atomic nucleus, quantitatively, the physical changes are shown in Figures 2 and 3, when the electrons are excited at the first level energy, the amplitude of the electron polar wave function is increasingly decreases with increasing v and μ .

CONCLUSIONS

From the description above, visualizing the polar wave function of the non-central Schrödinger potential of Coulombic Rosen Morse in excitation state $n_r = 2$ and l = 1 can be done with matlab-based programming by first determining the general equation of the polar wave function using Romanovski polynomials and special equations of polar wave functions by substituting a quantum number the potential value is undisturbed and potentially disturbed into the general equation of the polar wave function.

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REFERENCES

- Alvarenz-Castillo. D.E. 2009. *Exactly Solvable Potentials and Romanovski Polynomials in Quantum Mechanics*. Physics Thesis of Autonomous University of San Luis Potosi, Mexico.
- Beiser, A.1992. Konsep Fisika Modern (3rd Edition). Jakarta: Erlangga.
- Compean. C.B. and Kirchbach. M. 2006. The Trigonometric Rosen-Morse Potential as a Prime Candidate for an Effective QCD Potential. Av. Manuel Nava No. 6, S.L.P. 78290, México (Abstr.)
- Compean. C.B. and Kirchbach. 2008. The Trigonometric Rosen-Morse Potential in the Supersymmetric Quantum Mechanics and its Exact Solutions. Av. Manuel Nava 6, San Luis Potos'1, S.L.P. 78290, M'exico: 12.
- Flugge, S. 1971. Practical Quantum Mechanics II. New York: Springer.
- Greiner, W and B. Muller. 2004. Quantum Mechanics: Symmetries. Berlin-Heidelberg: Springer. 2nd rev. ed.
- Ikot et al. 2011. Analytical Solutions of Schrödinger Equation with Two-Dimensional Harmonic Potential in Cartesian and Polar Coordinates Via Nikiforov-UvarovMethod.JVR. 65-76.