Bound State Solutions and Energy Spectrum of the Schrödinger Equation for Core-Shell Polystyrene/Silver Nanoparticle with Born-Mayer Potential Using Nikiforov-Uvarov Method

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Abstract

In this paper, the Born-Mayer potential is used to describe the core-shell polystyrene nanoparticle and the Schrodinger equation for this nanoparticle is solved rigorously using the Nikiforov-Uvarov (NU) method to obtain the exact bound state solutions and energy spectrum. This is achieved by inserting the Born-Mayer potential into the Time Independent Schrödinger Equation (TISE), obtaining the radial part and solving, exactly, for the expectation values of the energy spectrum and the corresponding eigenfunctions applying the Nikiforov Uvarov (NU) method. The eigenvalue expression obtained is similar to earlier work on Soliton solution in nonlinear lattice with the nearest neighbor Born-Mayer interaction.

Keywords: Polystyrene; Nanoparticles; Nikiforov Uvarov; Core-shell; Born-Mayer Potential.

I. INTRODUCTION

Many quantum mechanical systems are very complex to describe and difficult to solve exactly, hence the necessity of approximation methods. However, the exact solutions of the Schrödinger equations, which are in effect the bound state solutions of the radial part of the Schrödinger equation, have been playing important roles(in physics and chemistry) in obtaining the wave functions associated with various physical systems and their corresponding energy eigenvalues as well as understanding their non-relativistic dynamic evolutions [1, 2, 3, 4]. Moreover, due to the various types of mathematical challenges being encountered in solving complex systems analytically/exactly [5, 7], different

methods have been developed for solving the Schrödinger equation with various potentials [3]. Among such methods include the asymptotic iteration method (AIM) [8], the supersymmetric approach [9], the algebraic method [10], the variational method [11], the shape invariant method [12], the Nikiforov–Uvarov method (NU) [13] amongst others. The NU method promises to be suitable for obtaining analytical solutions of the Schrödinger equation with the Born-Mayer potential, a potential which plays a vital role in many branches of physics such as atomic, molecular, solid-state physics and chemical physics [15]. Reference [16] presented a theoretical approach to calculate the absorption coefficient of silicon nanostructure. He used quantum mechanical calculation on the interaction of photons with the electrons of the valence

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band; one model is that the oscillator strength of the direct optical transition is enhanced by the quantum confinement effect in silicon nanocrystallites. He discovered that the absorption coefficient showed a peak at high photon energy. Similarly, [17] calculated the optical absorption coefficient of a silicon nanowire using a quantum mechanical model and discovered a very good agreement between theory and experimental data at low photon energies and the discrepancy between experimental data and theory at high photon energies probably due to free carrier absorption as well. In this research work, the radial Schrodinger equation with interacting Born-Mayer potential is used to calculate the energy spectrum of polystyrene silver nanoparticles.

II. REVIEW OF NIKIFOROV-UVAROV (NU) METHOD

The Nikiforov-Uvarov (NU) method is based on solving a second-order linear differential equation by reducing it to a generalized hypergeometric equation. The NU method has been used to solve the Schrödinger, Dirac and Klein-Gordon wave equation for certain kinds of potential [18]. The NU equation is given as

$$\psi''(s) + \frac{\bar{\tau}(s)}{\sigma(s)}\psi'(s) + \frac{\bar{\sigma}(s)}{\sigma^2(s)}\psi(s) = 0$$
 (1)

Where $\sigma(s)$ and $\bar{\sigma}(s)$ are polynomials, at most seconddegree, and $\bar{\tau}(s)$ is a first-degree polynomial. To find a particular solution to (1), we use the following transformation. $\psi(s) = \phi(s)\chi(s)$

This reduces (1) to hypergeometric equation,

$$\sigma(s)\chi''(s) + \tau(s)\chi'(s) + \lambda\chi(s) = 0 \tag{3}$$

Where $\phi(s)$ is defined as a logarithmic derivative

$$\frac{\phi'(s)}{\phi(s)} = \frac{\pi(s)}{\sigma(s)} \tag{4}$$

The other part $\chi(s)$ is the hypergeometric function whose polynomials are given by the Rodrigues relation,

$$\chi_n(s) = \frac{B_n(s)}{\alpha(s)} \frac{d^n}{ds^n} [\sigma^n(s)\alpha(s)]$$
 (5)

Where B_n is a normalization constant and the weight function $\alpha(s)$ must satisfy the condition

$$\frac{d}{ds}(\sigma(s)\alpha(s)) = \tau(s)\alpha(s) \tag{6}$$

The function $\pi(s)$ and the parameter λ required for the NU method are defined as follows:

$$\pi(s) = \frac{\sigma'(s) - \bar{\tau}(s)}{2} \pm \sqrt{\left(\frac{\sigma'(s) - \bar{\tau}(s)}{2}\right)^2 - \bar{\sigma}(s) + k\sigma(s)}$$
(7)
$$\lambda = k + \pi'(s)$$
(8)

On the other hand, to find the value of k, the expression under the square root must be the square of the polynomial. Thus, a new eigenvalue for the second-order differential equation

becomes, $\lambda = \lambda_n = -n\tau'(s) - \frac{n(n-1)}{2}\sigma''(s)$

$$\lambda = \lambda_n = -n\tau(s) - \frac{1}{2}\sigma(s) \tag{9}$$
Where

$$\tau(s) = \tau^{\bar{t}(s)(s)} \tag{10}$$

The derivative of (10) is negative. The energy eigenvalues are obtained by comparing (8) and (9).

III. EXACT SOLUTIONS OF SCHRÖDINGER EQUATION WITH BORN-MAYER POTENTIAL IN SPHERICAL COORDINATE SYSTEM

The Born-Mayer potential for polystyrene and silver nanoparticles [19] may be written as:

$$V(r) = \eta e^{-r/\rho} - \frac{e_0^2}{r} \tag{11}$$

Where η and ρ are empirical constants and r is the distance between the polystyrene and silver nanoparticle.

Without any loss in generality, (11) may be written as:

$$V(r) = \frac{\eta e^{-r/\rho}}{r} - \frac{e_0^2}{r^2}$$
Letting $\frac{e_0^2}{r^2} \to 0$, then (12) reduces to

$$V(r) = \frac{\eta e^{-r/\rho}}{r} \tag{13}$$

The radial part of the Schrodinger equation with the Born-Mayer potential is given as

$$\frac{1}{R(r)}\frac{d}{dr}\left(r^2\frac{d}{dr}R(r)\right) + \frac{2mr^2}{\hbar^2}\left(E + \frac{\eta e^{-r/\rho}}{r}\right) = \lambda(\lambda + 1)$$
(14)

$$\frac{d^2R(r)}{dr^2} + \frac{2}{r}\frac{dR(r)}{dr} + \frac{2m}{\hbar^2}\left(E + \frac{\eta e^{-r/\rho}}{r} - \frac{\hbar^2\lambda(\lambda+1)}{2mr^2}\right)R(r) = 0 (15)$$
This equation cannot be solved analytically for $\lambda \neq 0$ because

of the centrifugal term $\frac{1}{r^2}$.

By employing the Greene-Aldrich approximation scheme of

$$\frac{1}{r^2} \approx \frac{\rho^2}{\left(1 - e^{-\delta}\right)^2} \quad \text{or} \quad \frac{1}{r} \approx \frac{\rho}{\left(1 - e^{-\delta}\right)} \tag{16}$$

$$\delta = \frac{r}{\rho} \tag{17}$$

Let the coordinate transformation be
$$s = e^{-\frac{r}{\rho}}$$
 (18)

and choosing a function in the form of $R(r) \equiv R(s)$, where the transformation $r \rightarrow s$ is valid, then (15) becomes,

$$\left(\frac{1}{\rho^2} s \frac{d}{ds} + \frac{1}{\rho^2} s^2 \frac{d^2}{ds^2} - \frac{2}{r} \frac{1}{\rho} s \frac{d}{ds}\right) R(s) + \frac{2m}{h^2} \left(E + \frac{\eta s}{r} - \frac{h^2 \lambda(\lambda + 1)}{2mr^2}\right) R(s) = 0$$
(19)

$$\frac{d^{2}R(s)}{ds^{2}} + \frac{2\rho}{s}\frac{dR(s)}{ds} + \frac{2m}{\hbar^{2}}\left(E + \frac{\eta\rho^{2}}{s^{2}} - \frac{\hbar^{2}\lambda(\lambda+1)\rho^{2}}{2ms^{4}}\right)R(s) = 0$$
(20)

Putting (16) into (20) reduces to,

$$\frac{d^{2}R(s)}{ds^{2}} + \frac{2\rho}{s} \frac{dR(s)}{ds} + \frac{1}{s^{2}} (-\varepsilon s^{2} + Ps - \gamma)R(s) = 0$$

Where
$$\varepsilon = -\frac{2mE}{\hbar^2 \rho^2}$$
, $P = \frac{2m\eta}{\hbar^2 \rho}$ and $\gamma = \lambda(\lambda + 1)$ (22)

By comparing (21) and (1) we get,

$$\bar{\tau}(s) = 2\rho, \sigma(s) = s \text{ and } \bar{\sigma}(s) = -\varepsilon s^2 + Ps - \gamma$$
 (23)

Substitute (23) into (7) yield

$$\pi(s) = -\frac{1-2\rho}{2} \pm \sqrt{\left(\frac{1-2\rho}{2}\right)^2 - \{-\varepsilon s^2 + Ps - \gamma\} + ks}$$
(24)

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$$\pi(s) = -\frac{1}{2} - \rho \pm \sqrt{\frac{1}{4} - \rho^2 + \varepsilon s^2 - Ps + \gamma + ks}$$
 (25)

If $\rho \to 0$, (25) then reduces to

$$\pi(s) = -\frac{1}{2} \pm \frac{1}{2} \sqrt{4\varepsilon s^2 + 4(k-P)s + 1 + 4\gamma}$$
 (26)

and the values of k is obtained as:

$$k_{+} = P \pm \sqrt{\varepsilon(1 + 4\gamma)} \tag{27}$$

So that (26) becomes:

$$\pi(s) = -\frac{1}{2} \pm \frac{1}{2}$$

$$\frac{1}{2}\sqrt{4\varepsilon s^2 + 4\left(P \pm \sqrt{\varepsilon(1+4\gamma)} - P\right)s + 1 + 4\gamma} \tag{28}$$

The suitable choice of the polynomial $\pi(s)$ to make the derivative of the polynomial $\tau(s)$ to be negative, is chosen as

$$\frac{1}{2}\sqrt{4\varepsilon s^2 + 4(P - \sqrt{\varepsilon(1+4\gamma)} - P)s + 1 + 4\gamma}$$
 (29)

$$\pi(s) = -\frac{1}{2} - \frac{1}{2} \left[2\sqrt{\varepsilon}s - \sqrt{(1+4\gamma)} \right]$$
 (30)

By substituting (15) into (10), obtain
$$\tau(s) = 2\rho + 2\left(-\frac{1}{2} - \frac{1}{2}\left[2\sqrt{\varepsilon}s - \sqrt{(1+4\gamma)}\right]\right)$$
(31)

$$\tau(s) = \left\{ 2\sqrt{(1+4\gamma)} - 4\sqrt{\varepsilon}s \right\} (\rho+1) \tag{32}$$

Differentiate (32) gives

$$\tau'(s) = -4\sqrt{\varepsilon(\rho + 1)} \tag{33}$$

Similarly, by differentiating (30), get

$$\pi'(s) = -2\sqrt{\varepsilon} \tag{34}$$

Substitute (27) and (34) into (8) obtain the expression for λ .

$$\lambda = P - \sqrt{\varepsilon(1+4\gamma)} - 2\sqrt{\varepsilon} \tag{35}$$

Substitute (33) into (9), obtain the expression for

$$\lambda = \lambda_n = -n\left(-4\sqrt{\varepsilon}(\rho+1)\right) - \frac{n(n-1)}{2}\sigma''(s) \tag{36}$$

$$\sigma(s) = s, \sigma'(s) = 1, \text{ and } \sigma''(s) = 0$$
 (37)

Putting (37) into (36) gives

$$\lambda = \lambda_n = -n \left(-4\sqrt{\varepsilon}(\rho + 1) \right) \tag{38}$$

By comparing (35) and (38) yields,

$$\lambda = \lambda_n \tag{39}$$

$$P - \sqrt{\varepsilon(1+4\gamma)} - 2\sqrt{\varepsilon} = -n\left(-4\sqrt{\varepsilon}(\rho+1)\right) \tag{40}$$

And solving (40) gives,

$$\varepsilon = \frac{p^2}{\left\{\sqrt{(1+4\gamma)} + 2 + 4n(\rho+1)\right\}^2}$$
(41)

So that from (22) and (41), we get

$$E = -\frac{\left(\frac{4m^2\eta^2}{\hbar^4\rho^2}\right)\frac{\hbar^2\rho^2}{2m}}{\left\{2+4n(\rho+1)+\sqrt{(1+4\lambda(\lambda+1))}\right\}^2\frac{\hbar^2\rho^2}{2m}}$$
(42)

Which reduces to

$$E = -\frac{m\eta^2}{2h^2(2n(\rho+1)+\lambda)^2} \tag{43}$$

Here $n = 0,1,2,3, \dots$ and λ are integers while η and ρ are empirical constants.

Define the principal quantum number, n_n , as

$$n_p = 2n(\rho + 1) + \lambda \tag{44}$$

The quantum number λ must satisfy $\lambda \leq n_p - 1$ and hence it ranges from 0 to $n_p - 1$. Then (43) becomes

$$E_{n_p} = -\frac{m\eta^2}{4\hbar^2 n_p^2} \tag{45}$$

This expression of (45) represents the bound-state energy levels of the polystyrene nanoparticle for the Born-Mayer Potential, which is similar to the energy equation obtained for nonlinear lattice with nearest neighbour Born-Mayer interaction [21].

To find the corresponding eigenfunctions for the radial equation in (15), it is noted that the polynomial solution of the hypergeometric-type function $\chi_n(s)$ depends on the determination of the weight function $\alpha(s)$. Thus, using (4), we obtain,

$$\frac{d\phi(s)}{ds} \frac{1}{\phi(s)} = \frac{\pi(s)}{\sigma(s)} \tag{46}$$

Substituting (23) and (30) into (46) gives

$$\frac{d\phi(s)}{\phi(s)} = \left(\frac{-1 + \sqrt{(1 + 4\gamma)}}{2s} - \sqrt{\varepsilon}\right) ds \tag{47}$$

$$\phi(s) = s^{\frac{-1+\sqrt{(1+4\gamma)}}{2}} e^{-\sqrt{\varepsilon}s}$$
(48)

$$\sqrt{(1+4\gamma)} = \sqrt{1+4\lambda^2+4\lambda} = 2\lambda+1 \tag{49}$$

So that (48) becomes

$$\phi(s) = s^{\ell} e^{-\sqrt{\varepsilon}s} \tag{50}$$

The weight function can be obtained by expanding (6) and separating the variable to obtain

$$\frac{d\alpha(s)}{\alpha(s)} \frac{1}{ds} = \left(\frac{\tau(s) - d\sigma(s)}{\sigma(s)ds}\right) \tag{51}$$

$$\frac{d\sigma(s)}{ds} = \sigma'(s) = 1, \text{ where } \sigma(s) = s$$
 (52)

and recalling (32), (51) yields

$$\frac{d\alpha(s)}{\alpha(s)} = \left(\frac{2\sqrt{(1+4\gamma)}(\rho+1)}{s} - 1 - 4\sqrt{\varepsilon}(\rho+1)\right)ds \tag{53}$$

which by integrating gives

$$\alpha(s) = s^{2\sqrt{(1+4\gamma)}(\rho+1)}e^{-5\sqrt{\varepsilon}s(\rho+1)}$$
(54)

Substituting (54) into (5) gives the polynomial $\chi(s)$:

$$B_{n}(s)e^{5\sqrt{\varepsilon}s(\rho+1)}s^{-4\ell-2(\rho+1)}\frac{d^{n}}{ds^{n}}\left[s^{-4\ell-2(\rho+1)}e^{-5\sqrt{\varepsilon}s(\rho+1)}\right]$$
(55)

Writing (55) in the format of the Rodrigues relation of the associated Laguerre polynomials given by (56),

$$L_n^k(x) = \frac{1}{n!} e^x x^{-k} \frac{d^n}{dx^n} (e^{-x} x^{n+k})$$
 (56)

$$L_n^{4\ell-2(\rho+1)} \left(5\sqrt{\varepsilon}s(\rho+1) \right) =$$

$$L_n^{4\ell-2(\rho+1)} \left(5\sqrt{\varepsilon}s(\rho+1) \right) = \frac{1}{n!} e^{5\sqrt{\varepsilon}s(\rho+1)} s^{-4\ell-2(\rho+1)} \frac{d^n}{ds^n} \left[s^{-4\ell-2(\rho+1)} e^{-5\sqrt{\varepsilon}s(\rho+1)} \right]$$
(57)

Where $B_n(s) = \frac{1}{n!}$, and,

$$\chi_n(s) = L_n^{4\lambda - 2(\rho + 1)} \left(5\sqrt{\varepsilon}s(\rho + 1) \right) \tag{58}$$

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Substituting (50) and (58) into (2) gives the total eigenfunction of the particle

$$\psi(s) = \Re_{n\ell} s^{\ell} e^{-\sqrt{\varepsilon}s} L_n^{4\ell-2(\rho+1)} \left(5\sqrt{\varepsilon} s(\rho+1) \right)$$
 (59)

Where $\mathfrak{R}_{n\lambda}$ is the normalization constant, which can be evaluated using the normalization condition

$$\int_0^\infty \psi^*(s)\psi(s)ds = 1 \tag{60}$$

IV. RESULT AND DISCUSSION

The radial wave function for polystyrene silver nanoparticles would be obtained considering boundary conditions and physical confinements. The energy state for this system (polystyrene silver nanoparticle) is considered based on the Born-Mayer potential. Fig. 1 shows a sketch of the potential V(r) as a function of the linear coordinate r(m) for polystyrene silver nanoparticles.

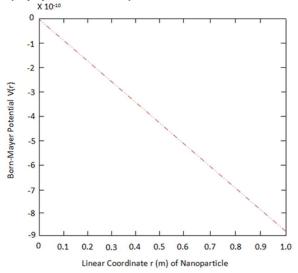


Fig. 1 Sketch of Born-Mayer potential.

Fig. 2 shows that as the principal quantum number (n_p) increases the absolute value of the energy state decreases. This means an electron with the lowest value of " n_p " has more energy and is located on the orbital or wave function closer to the nucleus of the nanoparticle. As the value of " n_p " increases the atomic size of the nanoparticle increases and more orbital or wave functions are formed. At $n_p = 1$ and $E_1 = 138.6$ eV. The periodic nature is that the amplitude of the wave decays all through along the direction of propagation, this is because of the core-shell nature of polystyrene silver nanoparticles, and this creates a perturbation in the wave that results in the decay of the wave as it propagates. at $n_p = 2$ and $E_2 = 68.2$ eV there is partial formation of the wave packet which is due to the high frequency that arises as the wave travels, and it makes the line of propagation of the wave to become compactable and the amplitude decay throughout the direction of propagation.

The wave packet that over crowds at the middle is observed at the energy of $E_3 = 40.09$ eV, $n_p = 3$. This core region (over

crowd) of the wave packet is due to the core region of the polystyrene silver nanoparticle and the shell region (less crowd) of the wave packet indicates the shell region of the polystyrene silver Nanoparticle [20, 21, 22]. Although, at $E_4 = 26.8 \, eV$, $n_p = 4$ the wave packet nature of the probability distribution disappeared but high oscillation is observed due to high frequency and the wave became more compacted while the amplitude decay along the direction of propagation.

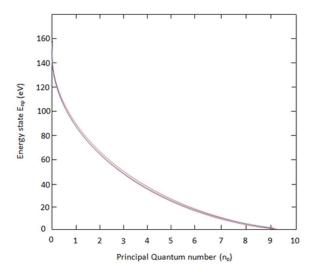


Fig. 2 Energy State $E_{np}(eV)$ versus n_P

At higher states $E_5 = 22.352 \text{ eV}$, $n_p = 5$ some oscillations are lost as the value of n_p increases making the waves to be in phase as they travel. At an energy of $E_6 = 20.022 \ eV$ and n_p = 6 shows a combination of many waves having a distribution of frequencies which reinforced along the direction of propagation. The reinforcement is more pronounced. At the energy of $E_7 = 18.22$ eV and $n_p = 7$, this is due to various components of sinusoidal waves of different phases and amplitudes which interfere constructively only over a small region of space of the core-shell nanoparticle. Hence, the constructive interference became more in the core region of the polystyrene silver nanoparticle. At energies $E_8 = 11.70 \text{ eV}$ and $n_p = 8$, $E_9 = 9.70$ eV and $n_p = 9$. The interference may be due to the repulsion created by the Born-Mayer potential when the wave function of the inner-shell electrons or nuclei begins to overlap. In [20] the study revealed that the energy and the probability distribution near the core centre of polystyrene silver nanoparticles increase as the quantum integer numbers $n_{\rm p}$ are enhanced. Hence, the wave distortions are sensible in the core-shell nanoparticle where the wave number is larger than the shell, because of the semiconductor behavior of the shell; the wave function is a damping wave [23]. The result in this research work is in good agreement with the literature because a sinusoidal wave whose amplitude drops exponentially with the radial distance is observed and this is due to the semiconductor nature of polystyrene silver

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nanoparticle. Also, the formation of the wave packet at the core region of polystyrene silver nanoparticles is due to constructive interference of the sinusoidal waves.

V. CONCLUSION

The Nikiforov Uvarov (NU) method is used to solve the Schrödinger ss with the Born-Mayer potential of the Coreshell polystyrene nanoparticle. The analytical expression for the energy spectrum and the corresponding eigenfunctions were obtained. It is found that the energy eigenvalues are degenerate depending on the allowed quantum numbers $n_{\rm p}$. These results may have many interesting applications in the different quantum mechanical systems such as in the thermodynamic properties of the system.

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