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EIGENSPECTRA OF GENERALIZED MORSE POTENTIAL INCLUDING THE SPIN-ORBIT COUPLING TERM

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Abstract

We have solved the radial Schrödinger equation with generalized Morse potential including the spin-orbit coupling term by ansatz method. Also we have applied generalized Pekeris approximation scheme to deal with the centrifugal term potential and obtained bound state energy eigenvalues and normalized radial wave functions in closed forms. To test the accuracy of our results, we computed energy eigenvalues for 2p, 3p, 3d, 4p, 4d and 4f quantum states and compared with those in the literature obtained by other approximation schemes and solution methods. In contrast our computed energy eigenvalues are in total agreement with those obtained numerically and by supersymmetric quantum mechanics than those obtained by Nikiforov-Uvarov method. We have also considered the variation of energy eigenvalue with energy determining parameter, α, and the result shows that the energy of the system initially decreases with α up to a critical value after which it begins to increase.

***Keywords*: Eigenspectra, Schrödinger equation, Generalized Morse Potential, Pekeris Approximation**

1. Introduction

Because of the information derivable from energy eigenspectrum and eigenfunctions, emphasis is placed on the solution of Schrödinger equation which is used to describe nonrelativistic spinless particles [1]. It is a well-known fact that exact solutions play an important role in quantum mechanics since they contain all the necessary information regarding the quantum system under investigation, for instance, the exact solution of the Schrödinger equation for a hydrogen atom and for a harmonic oscillator in three dimensions are an important milestone at the beginning stage of quantum mechanics, which provided a strong evidence for supporting the correctness of the quantum theory [2-4]. The Coulomb potential and the harmonic oscillator potential are amongst the few potential models which gives exact solution for all quantum states $n\ell$,of the Schrödinger equation, where n is the principal quantum number and ℓ is the angular momentum quantum number [5]. Not many potential models give exact solution for the case of s-wave (zero angular momentum quantum number) [6-8]. Most potential models have no exact solution with the Schrödinger equation, a common practice for thisclass of potentials is to obtain approximate numerical [5] or analytical solutions [9], the analytical method of solution involves dealing with the spin-orbit coupling term using approximation schemes [10-14]. However, most of the approximation models are only applicable to exponential-type potentials and are restricted to screening parameters of the potential. In this article we have solved the Schrödinger equation with the generalized Morse potential including the spin-orbit coupling term via the generalized Pekeris approximation scheme [9-10, 15-16] which, to the best of our knowledge has not been solved in the existing literatures. There is rather a lengthy list of solution methods of the Schrödinger equation, some of the methods used to solve the Schrödinger equation include: ansatz solution [2-4], Nikiforov-Uvarov method [17-18], exact and proper quantization rules [7, 19], factorization method [20], extended transformation method [21] and asymptotic iteration method [22]. In this paper we have used the ansatz solution method to obtain eigenspectra of generalized Morse potential including the spin-orbit coupling term and compared results with those in literatures.

2 Theoretical Formulation

2.1 The Generalized Morse Potential

The generalized Morse potential [18] is given by:

$$V(r) = D_e\left[1-\frac{b}{1-e^{-\delta(r-r_e)}}\right]^2. \qquad (1)$$

where D_e is the dissociation energy, r_e is the equilibrium internuclear separation, r is the internuclear separation, δ is an adjustable screening parameter and $b = e^{\delta r_e} - 1$. Using the following hyperbolic function relations:

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$$\sinh(x) = \tfrac{1}{2}\left(e^{x} - e^{-x}\right). \tag{2}$$

$$\cosh(x) = \tfrac{1}{2}\left(e^{x} + e^{-x}\right). \tag{3}$$

$$\coth(x) = \frac{\cosh(x)}{\sinh(x)}. \tag{4}$$

together with the identity:

$$\coth^{2}(x) = 1 + \cos ech^{2}(x). \tag{5}$$

Eq. (1) transforms to:

$$V(r) = A - B\coth\tfrac{1}{2}\delta(r - r_e) + C\cos ech^{2}\,\tfrac{1}{2}\delta(r - r_e). \tag{6}$$

where

$$A = \left(1 - 2b + 2b^{2}\right)D_e. \tag{7}$$

$$B = 2b(1 - b)D_e. \tag{8}$$

$$C = b^{2}\,D_e. \tag{9}$$

2.2 The Radial Schrödinger Time Independent Wave Equation with Spin-Orbit Coupling Term

The radial Schrödinger time independent wave equation [9-10] with spin-orbital centrifugal term can be expressed as:

$$\frac{d^{2}R_{n\ell}}{dr^{2}} + \frac{2\mu}{\hbar^{2}}\left\{E_{n\ell} - V(r) - \frac{\ell(\ell+1)\hbar^{2}}{2\mu r_e^{2}}\left(\frac{r_e}{r}\right)^{2}\right\}R_{n\ell} = 0. \tag{10}$$

where μ is the reduced mass of the molecule, $E_{n\ell}$ is the energy eigenvalue and $R_{n\ell}$ is the radial wave function. If we substitute Eq. (6) in Eq. (10), we get:

$$\frac{d^{2}R_{n\ell}}{dr^{2}} + \frac{2\mu}{\hbar^{2}}\left\{E_{n\ell} - \left[A - B\coth\tfrac{1}{2}\delta(r - r_e) + C\cos ech^{2}\,\tfrac{1}{2}\delta(r - r_e)\right] - \frac{\ell(\ell+1)\hbar^{2}}{2\mu r_e^{2}}\left(\frac{r_e}{r}\right)^{2}\right\}R_{n\ell} = 0 \tag{11}$$

Let

$$u = \tfrac{1}{2}\delta(r - r_e). \tag{12}$$

Eq. (11) transforms to:

$$\frac{d^{2}R_{n\ell}}{du^{2}} + \left\{\frac{8\mu}{\delta^{2}\hbar^{2}}(E_{n\ell} - A) + \frac{8\mu B}{\delta^{2}\hbar^{2}}\coth u - \frac{8\mu C}{\delta^{2}\hbar^{2}}\cos ech^{2}\,u - \frac{4\ell(\ell+1)}{\delta^{2}\,r_e^{2}}\left(\frac{r_e}{r}\right)^{2}\right\}R_{n\ell} = 0 \tag{13}$$

Eq. (13) has no exact analytical solution, it can only be solved by approximation technique, and several approximation models have been proposed by researchers to make equations such as this amenable to solution. In this article, we have employed the generalized Pekeris approximation [10, 16] to approximate the factor $(r/r_e)^2$ which occurs in Eq. (13) by terms of a Taylor series expansion given as:

$$\left(\frac{r_e}{r}\right)^{2} \approx c_0 + c_1\left(\Gamma - \alpha_{n\ell}\right) + \tfrac{1}{2}c_2\left(\Gamma - \alpha_{n\ell}\right)^{2}. \tag{14}$$

where Γ and its inverse function, Γ^{-1} are appropriately chosen functions and $\alpha_{n\ell}$ (dimensionless) are elements in the domain of Γ^{-1}.

The constant coefficients: c_0, c_1 and c_2 are defined by Ferreira and Bezerra [16]. In this work we have:

$$c_j = \frac{d^{j}}{dy^{j}}\left[1 + \frac{2\Gamma^{-1}(\Gamma)}{\delta r_e}\right]^{2}\Bigg|_{\Gamma = \alpha_{n\ell}}. \tag{15}$$

$$\Gamma = \coth\tfrac{1}{2}\delta(r - r_e) \equiv \coth u \tag{16}$$

and

$$\Gamma^{-1}(\Gamma) = \coth^{-1}\Gamma. \tag{17}$$

Using Eq. (15) and Eq. (17), we have:

$$c_0 = \frac{\delta^{2} r_e^{2}}{d_{n\ell}^{2}}. \tag{18}$$

$$c_1 = \frac{-4c_0}{\left(1 - \alpha_{n\ell}^{2}\right)d_{n\ell}}. \tag{19}$$

and

$$c_2 = \frac{\left(2\alpha_{n\ell}\,d_{n\ell} - 6\right)c_1}{\left(1 - \alpha_{n\ell}^{2}\right)d_{n\ell}}. \tag{20}$$

where $\alpha_{n\ell} \in (-\infty, -1) \cup (1, \infty)$ and $d_{n\ell} = \delta r_e + 2\coth^{-1}\alpha_{n\ell}$. Substitute Eq. (14) in Eq. (13) and using Eq. (16), we have:

$$\frac{d^2 R_{n\ell}}{du^2} + \left\{ \begin{array}{l} \frac{8\mu}{\delta^2\hbar^2}(E_{n\ell} - A) + \frac{8\mu B}{\delta^2\hbar^2}\coth u - \frac{8\mu C}{\delta^2\hbar^2}\operatorname{cosech}^2 u \\ -\frac{4\ell(\ell+1)}{\delta^2 r_e^2}\left[c_0 - \alpha_{n\ell}c_1 + \tfrac{1}{2}c_2 + \tfrac{1}{2}\alpha_{n\ell}^2 c_2 + (c_1 - \alpha_{n\ell}c_2)\coth u + \tfrac{1}{2}c_2 \operatorname{cosech}^2 u\right] \end{array} \right\} R_{n\ell} = 0 \tag{21}$$

With simplified coefficients, Eq. (21) can be expressed as:

$$\frac{d^2 R_{n\ell}}{du^2} + \left\{ \begin{array}{l} \frac{8\mu}{\delta^2\hbar^2}(E_{n\ell} - A) - \frac{4\ell(\ell+1)}{\delta^2 r_e^2}\left(c_0 - \alpha_{n\ell}c_1 + \tfrac{1}{2}c_2 + \tfrac{1}{2}\alpha_{n\ell}^2 c_2\right) \\ + \left[\frac{8\mu B}{\delta^2\hbar^2} - \frac{4\ell(\ell+1)}{\delta^2 r_e^2}(c_1 - \alpha_{n\ell}c_2)\right]\coth u - \left[\frac{8\mu C}{\delta^2\hbar^2} + \frac{2\ell(\ell+1)}{\delta^2 r_e^2}c_2\right]\operatorname{cosech}^2 u \end{array} \right\} R_{n\ell} = 0 \tag{22}$$

Eq. (22) can be written in compact form as:

$$\frac{d^2 R_{n\ell}}{du^2} + \left(-\eta + \kappa\coth u - \lambda\operatorname{cosech}^2 u\right) R_{n\ell} = 0 \,. \tag{23}$$

where

$$\eta = \frac{8\mu}{\delta^2\hbar^2}(A - E_{n\ell}) + \frac{4\ell(\ell+1)}{\delta^2 r_e^2}\left(c_0 - \alpha_{n\ell}c_1 + \tfrac{1}{2}c_2 + \tfrac{1}{2}\alpha_{n\ell}^2 c_2\right). \tag{24}$$

$$\kappa = \frac{8\mu B}{\delta^2\hbar^2} - \frac{4\ell(\ell+1)}{\delta^2 r_e^2}(c_1 - \alpha_{n\ell}c_2). \tag{25}$$

$$\lambda = \frac{8\mu C}{\delta^2\hbar^2} + \frac{2\ell(\ell+1)}{\delta^2 r_e^2}c_2 \,. \tag{26}$$

In order to solve Eq. (23), let us assume an ansatz solution as used by Rosen and Morse [23]

$$R_{n\ell}(u) = N_{n\ell}\, e^{su} \sinh^{-t} u . \Pi_{n\ell}(u). \tag{27}$$

where $N_{n\ell}$ are normalization constants, s and t are constants to be determined when Eq. (27) is satisfied by Eq. (23) and $\Pi_{n\ell}(u)$ is a function of u. Thus, Eq. (27) gives:

$$R''_{n\ell}(u) = \left\{ \frac{\Pi''_{n\ell}(u)}{\Pi_{n\ell}(u)} + 2(s - t\coth u)\frac{\Pi'_{n\ell}(u)}{\Pi_{n\ell}(u)} + s^2 + t^2 - 2st\coth u + (s^2 + s)\operatorname{cosech}^2 u \right\} R_{n\ell}(u). \tag{28}$$

where prime designate derivatives with respect to u. By putting Eq. (28) in Eq. (23), we obtained:

$$\left\{\Pi''_{n\ell}(u) + 2(s - t\coth u)\Pi'_{n\ell}(u) + \left[s^2 + t^2 - \eta + (\kappa - 2st)\coth u + (t^2 + t - \lambda)\operatorname{cosech}^2 u\right]\Pi_{n\ell}(u)\right\} R_{n\ell}(u) = 0 \tag{29}$$

Eq. (29) can be converted to a more useful form by imposing the following constraints:

$$s^2 + t^2 = \eta \,. \tag{30}$$

and

$$2st = \kappa \,. \tag{31}$$

From Eq. (30) and Eq. (31) get:

$$s = \tfrac{1}{2}\left\{(\eta + \kappa)^{\frac{1}{2}} + (\eta - \kappa)^{\frac{1}{2}}\right\}. \tag{32}$$

$$t = \tfrac{1}{2}\left\{(\eta + \kappa)^{\frac{1}{2}} - (\eta - \kappa)^{\frac{1}{2}}\right\}. \tag{33}$$

Using Eq. (30) and Eq. (31), Eq. (29) reduces to:

$$\Pi''_{n\ell}(u) + 2(s - t\coth u)\Pi'_{n\ell}(u) + (s^2 + s - \lambda)\operatorname{cosech}^2 u \, \Pi_{n\ell}(u) = 0 \,. \tag{34}$$

Introducing the change of variable in Eq. (34) given by:

$$z = \tfrac{1}{2}(1 - \coth u). \tag{35}$$

Eq. (34), gives:

$$z(1 - z)\Pi''_{n\ell}(z) + \{-s + t + 1 - (2t + 2)z\}\Pi'_{n\ell}(z) + (s^2 + s - \lambda)\Pi_{n\ell}(z) = 0 \,. \tag{36}$$

Eq. (36) is the Gaussian hypergeometric differential equation, whose solution is the hypergeometric function given by:

$$\Pi_{n\ell}(z) = {}_2F_1(\sigma, \varsigma; \tau; z). \tag{37}$$

where

$$\sigma = t + \tfrac{1}{2} + \left(\lambda + \tfrac{1}{4}\right)^{\frac{1}{2}} . \tag{38}$$

$$\varsigma = t + \tfrac{1}{2} - \left(\lambda + \tfrac{1}{4}\right)^{\frac{1}{2}} . \tag{39}$$

$$\tau = -s + t + 1. \tag{40}$$

For a polynomial solution [4, 23] either σ or ς or both must be a negative integer, $-n$

Thus, Eq. (38) can be written as:

$$t+\tfrac{1}{2}+\left(\lambda+\tfrac{1}{4}\right)^{\frac{1}{2}}=-n\cdot \tag{41}$$

so that:

$$\Pi_{n\ell}(z)={}_2F_1\left(-n,\, n+2t+1;\, -s+t+1;\, z\right)\cdot \tag{42}$$

2.3 Energy Eigenspectra

Eq. (41) can be recast as:

$$t^2=\left\{n+\tfrac{1}{2}+\left(\lambda+\tfrac{1}{4}\right)^{\frac{1}{2}}\right\}^2. \tag{43}$$

By putting Eq. (33) in Eq. (43) get:

$$\eta=\left\{n+\tfrac{1}{2}+\left(\lambda+\tfrac{1}{4}\right)^{\frac{1}{2}}\right\}^2+\left\{\frac{\tfrac{1}{2}\kappa}{n+\tfrac{1}{2}+\left(\lambda+\tfrac{1}{4}\right)^{\frac{1}{2}}}\right\}^2. \tag{44}$$

From Eq. (24), we get:

$$E_{n\ell}=A-\frac{\delta^2\hbar^2}{8\mu}\eta+\frac{\ell(\ell+1)}{2\mu r_e^2}\left(c_0-\alpha_{n\ell}c_1+\tfrac{1}{2}c_2+\tfrac{1}{2}\alpha_{n\ell}^2\,c_2\right)\cdot \tag{45}$$

Inserting Eq. (25) and Eq. (26) in Eq. (45), the analytical energy eigenvalue is therefore given by:

$$E_{n\ell}=A-\frac{\delta^2\hbar^2}{8\mu}\left\{\left[n+\tfrac{1}{2}+\left(\frac{8\mu C}{\delta^2\hbar^2}+\frac{2\ell(\ell+1)}{\delta^2 r_e^2}c_2+\tfrac{1}{4}\right)^{\frac{1}{2}}\right]^2+\left[\frac{\frac{4\mu B}{\delta^2\hbar^2}-\frac{2\ell(\ell+1)}{\delta^2 r_e^2}\left(c_1-\alpha_{n\ell}c_2\right)}{n+\tfrac{1}{2}+\left(\frac{8\mu C}{\delta^2\hbar^2}+\frac{2\ell(\ell+1)}{\delta^2 r_e^2}c_2+\tfrac{1}{4}\right)^{\frac{1}{2}}}\right]^2\right\} \tag{46}$$

$$+\frac{\ell(\ell+1)}{2\mu r_e^2}\left(c_0-\alpha_{n\ell}c_1+\tfrac{1}{2}c_2+\tfrac{1}{2}\alpha_{n\ell}^2\,c_2\right)$$

2.4 Normalization Constant

The requirement for the normalization of wave functions [24] is given by:

$$\int_0^\infty P_{n\ell}(r)\,dr=1\cdot \tag{47}$$

where

$$P_{n\ell}(r)=\left|R_{n\ell}(r)\right|^2\cdot \tag{48}$$

is the probability density function.

Using Eq. (12), Eq. (35), Eq. (48) and the identity given by Eq. (5), Eq. (47) transforms to:

$$\int_{z_0}^{0} z^{-1}(z-1)^{-1}\left|R_{n\ell}(z)\right|^2 dz=\delta\cdot \tag{49}$$

where

$$z_0=\frac{1}{1-e^{-\delta r_e}}\cdot \tag{50}$$

Eq. (27) when expressed in terms of variable z can be used to eliminate $R_{n\ell}(z)$ in Eq. (49), leading to:

$$N_{n\ell}^2\int_{z_0}^{0} z^{-1}(z-1)^{-1}\left|2^t\, z^{-\frac{1}{2}s+\frac{1}{2}t}\,(z-1)^{\frac{1}{2}s+\frac{1}{2}t}\,\Pi_{n\ell}(z)\right|^2 dz=\delta\cdot \tag{51}$$

It follows that:

$$N_{n\ell}=\left\{\frac{\delta}{\int_{z_0}^{0} z^{-1}(z-1)^{-1}\left|2^t\, z^{-\frac{1}{2}s+\frac{1}{2}t}\,(z-1)^{\frac{1}{2}s+\frac{1}{2}t}\,\Pi_{n\ell}(z)\right|^2 dz}\right\}^{\frac{1}{2}}. \tag{52}$$

3.0 Results and Discussion

Table 1: Comparison of Bound State Energy Eigenvalues (in eV) of the Generalized Morse Potential for 2p, 3p, 3d, 4p, 4d and 4f Quantum States with $\hbar = \mu = e = 2r_e = 1$ and $D_e = 15cm^{-1}$ as a Function of Screening Parameter

State	δ	$\alpha_{n\ell}$	$-E_{n\ell}$ (PM)	$-E_{n\ell}$ [18] (NU)	$-E_{n\ell}$ [18] (NUM)	$-E_{n\ell}$ [18] (SUSY)
2p	0.05	80.048723	7.816795	7.77122	7.8628	7.8608
	0.10	36.436184	7.955375	7.77577	7.95537	7.9533
	0.15	21.849229	8.047245	7.78125	8.04724	8.0451
	0.20	14.701458	8.138425	7.78768	8.13842	8.1362
3p	0.05	80.101563	7.449385	10.9468	10.9998	10.9978
	0.10	40.017966	7.849045	11.0628	11.1647	11.1626
	0.15	26.642249	8.515015	11.1779	11.3265	11.3262
	0.20	19.931503	9.447205	11.2921	11.4851	11.4828
3d	0.05	31.344887	10.216550	10.0723	10.2165	10.316
	0.10	15.290867	10.354150	10.1725	10.3541	10.3535
	0.15	9.693648	10.489950	10.2734	10.4899	10.4894
	0.20	6.676524	10.623949	10.4739	10.624	10.6235
4p	0.05	80.136887	7.332950	12.4651	12.4992	12.4976
	0.10	40.011738	7.954550	12.6344	12.6985	12.6968
	0.15	26.692084	8.990250	12.7986	12.8901	12.8884
	0.20	19.965469	10.440150	12.9579	13.074	13.0722
4d	0.05	36.008121	12.098150	12.0105	12.0981	12.0983
	0.10	17.429241	12.285749	12.1143	12.2857	12.285
	0.15	10.867873	12.467149	12.2176	12.4672	12.4664
	0.20	7.262262	12.643248	12.3204	12.6432	12.6426
4f	0.05	22.996016	11.820850	11.6417	11.8209	11.8208
	0.10	11.053723	11.998149	11.6456	11.9981	11.998
	0.15	6.785111	12.171849	11.6518	12.1718	12.1717
	0.20	4.324315	12.342148	11.6603	12.3421	12.0421

The Table 1 shows energy determining parameter used in our computations and the corresponding bound state (negative) energy eigenvalues obtained using Eq. (46). Also shown in the Table are bound states energy eigenvalues obtained by other methods and approximation schemes in otherrelated literatures, the results show that the present method (PM) is in total agreement with those computed by numerical methods (NUM) [18] as well as those obtained by supersymmetric quantum mechanics (SUSY) [18] than those obtained by Nikiforov-Uvarov (NU) method [18], except for the p states (3p and 4p).

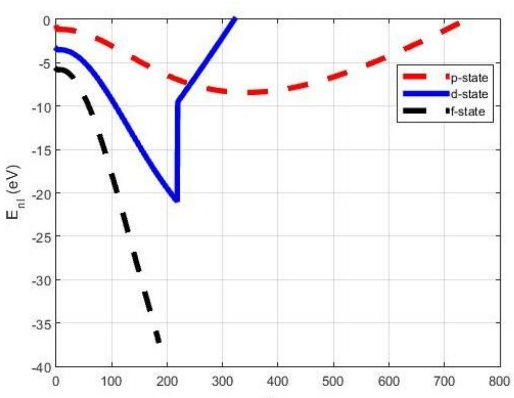

Figure 1 Plot of Energy Eigenvalues versus Energy Determining Parameter

The Figure1 shows plot of energy eigenvalues versus energy determining parameter for p, d and f states for a given screening parameter, these plots clearly suggests a minimum energy eigenvalue in agreement with the remarks by Eyube *et al*. [18]. As a special case, by putting $\ell = 0$ in Eq. (46), the s-wave energy eigenvalue becomes

$$E_{n0} = A - \frac{\delta^2\hbar^2}{8\mu}\left\{\left[n+\tfrac{1}{2}+\left(\frac{8\mu C}{\delta^2\hbar^2}+\tfrac{1}{4}\right)^{\frac{1}{2}}\right]^2 + \left[\frac{\frac{4\mu B}{\delta^2\hbar^2}}{n+\tfrac{1}{2}+\left(\frac{8\mu C}{\delta^2\hbar^2}+\tfrac{1}{4}\right)^{\frac{1}{2}}}\right]^2\right\}. \tag{53}$$

which is clearly independent of α and only varies with n.

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