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SUSYQM APPROACH TO ENERGY SPECTRA AND WAVE FUNCTIONS OF THE TIETZ POTENTIAL

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Abstract

In this paper, ideas of the supersymmetric quantum mechanics (SUSYQ) has been used to obtain closed form analytical expression for bound state energy eigenvalues of the Tietz potential. The corresponding normalized eigenfunction was obtained by ansatz method. The Greene-Aldrich approximation model was used to deal with the centrifugal term of the effective potential energy function. Bound state energy eigenvalues were calculated for arbitrary rotational and vibrational quantum numbers, the results obtained are in excellent agreement with existing data for bound state eigen energies of the Tietz potential in the literature. The results obtained in the work may be useful in many areas of physics which include nuclear physics, atomic physics, chemical physics and solid-state physics.

Keywords: Energy eigenvalues, eigenfunctions, shape invariance, super potential, SUSYQM, Tietz potential

1 Introduction

The nonrelativistic and relativistic wave equations of a system are of enormous importance in quantum mechanics because of the valuable information that can be deduced from them [1-3]. Information such as thermodynamic properties [4, 5], information theoretic measures [6, 7], fisher information [8] and optical properties [9] of the system require a knowledge of the wave function, the list is too vast that we can only mention but a few.

Generally, the interaction between a quantum mechanical system and its environment is described by a potential energy system (simply referred to as potential). By solving the Schrödinger wave equation for a given potential energy model, wave functions representing the system are readily obtained [3, 10]. One major challenge in this area of research is that *exact solution* of the Schrödinger equation for a prescribed potential is governed by the presence of the centrifugal or pseudo-spin orbit term in the effective potential of the equation [11-13]. The centrifugal term is given as $L\hbar^2/2\mu r^2$, where $L = J(J + 1)$ is the angular momentum of the system, J is the rotational quantum number, μ is the reduced mass of the system and $r \in [0, \infty)$ is the internuclear separation.

Only few potential energy functions have exact solution with the Schrödinger equation for all values of J, the Coulomb potential, harmonic oscillator and Mie-type potential are typical examples [1, 14]. On the other hand, the Schrödinger equation also have exact solution for the state $J = 0$ for most potential energy functions, this is the pure vibrational state solution [7, 13]. A host of other potential energy functions have no exact solution for nonzero rotational quantum numbers ($J \neq 0$), the number is so enormous.

In the absence of exact solution of the Schrödinger equation, *approximate* numerical or *analytical solutions* are considered [3, 10]. In the course of obtaining approximate analytical solutions, a suitable approximation scheme is used to model the pseudo-spin orbit term [15]. Many solution methods have been proposed in the literature for obtaining analytical solution of the Schrödinger equation for various potential models, some of the solution techniques include: exact and proper quantization rules [16], Nikiforov-Uvarov method [17, 18], path integral method [19] and supersymmetric quantum mechanics (SUSYQM) approach [20-22].

Solutions of Schrödinger equation with different potential energy functions have been obtained in the literature, in the present work, the Tietz potential is considered. Its uses and applications in many areas of physics which include solid-state physics, chemical physics, atomic and molecular physics have been reported elsewhere in the literature [10, 17, 18].

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For example, using the parametric Nikiforov-Uvarov concept, Nikoofard et al. have solved the Schrödinger equation with the Tietz potential, expression of the energy eigenvalues and eigenfunctions was used to study the oscillator strength of the potential [17]. In another development, studies of singlet-triplet transitions of a two-electron quantum dot was achieved for the Tietz potential [10]. Recently, Eyube and collaborators have applied the proper quantization rule to derive J – state solutions and thermodynamic properties of this potential [10]. The Tietz potential is expressed mathematically as [10, 17]

$$\mathrm{V}(r) = \mathrm{V}_0 \left\{ \frac{\sinh \alpha (r - r_e)}{\sinh \alpha r} \right\}^2, \tag{1}$$

where V_0 is the potential strength, α and r_e are the potential screening parameter and equilibrium bond length respectively. The present contribution aims at obtaining energy spectra and wave functions of a rotating Tietz potential withing the frameworks of SUSYQM approach. This paper is structured as follows. In section2, the SUSYQM method is applied in the derivation of energy eigenvalues. Normalized radial wave functions are obtained by ansatz solutions in section 3. In section 4, results of numerical computations were concisely discussed. A brief conclusion of the work is given in section 5

2 SUSYQM approach to energy spectrum of the Tietz potential

In a three-dimensional coordinate system, the radial Schrödinger equation assumes form [3, 10]

$$\mathrm{H}(r)\,\mathrm{u}_{vJ}(r) = \mathrm{E}_{vJ}\,\mathrm{u}_{vJ}(r), \tag{2}$$

where v is the vibrational quantum number, $\mathrm{u}_{vJ}(r)$ is the radial wave function and the Hamiltonian of the system is

$$\mathrm{H}(r) = -\frac{\hbar^2}{2\mu}\frac{\mathrm{d}}{\mathrm{d}r^2} + \mathrm{V}_{\mathrm{eff}}(r), \tag{3}$$

in which the effective potential is

$$\mathrm{V}_{\mathrm{eff}}(r) = \mathrm{V}(r) + \frac{L\hbar^2}{2\mu r^2}. \tag{4}$$

Substituting Eq. (1) into (4), we have

$$\mathrm{V}_{\mathrm{eff}}(r) = \mathrm{V}_0 \left\{ \frac{\sinh \alpha (r - r_e)}{\sinh \alpha r} \right\}^2 + \frac{L\hbar^2}{2\mu r^2}. \tag{5}$$

It is noted that Eq. (2) has exact solution in the presence of Eq. (5) only for the pure vibrational state. However, by employing the Greene-Aldrich approximation scheme to model the pseudo-spin orbit term, approximate analytical solutions of the Schrödinger equation with the effective potential (5) is feasible. For small values of the screening parameter, the centrifugal term can be approximated by

$$\frac{L\hbar^2}{2\mu r^2} \approx \frac{L\hbar^2}{2\mu}\frac{4\alpha^2 \mathrm{e}^{2\alpha r}}{\left(\mathrm{e}^{2\alpha r} - 1\right)^2}. \tag{6}$$

Inserting Eq. (6) in (5) simplifying, we obtained

$$\mathrm{V}_{\mathrm{eff}}(r) = \mathrm{V}_0\, \mathrm{e}^{-2\alpha r_e} \left\{ 1 - \frac{\mathrm{e}^{4\alpha r_e} - 1}{\mathrm{e}^{2\alpha r} - 1} + \frac{\left(\mathrm{e}^{2\alpha r_e} - 1\right)^2 \mathrm{e}^{2\alpha r}}{\left(\mathrm{e}^{2\alpha r} - 1\right)^2} \right\} + \frac{2L\alpha^2\hbar^2}{\mu} \frac{\mathrm{e}^{2\alpha r}}{\left(\mathrm{e}^{2\alpha r} - 1\right)^2}. \tag{7}$$

Note that in arriving at the relation (7), the following identity have been employed

$$\frac{1}{\left(\mathrm{e}^{2\alpha r} - 1\right)^2} \equiv -\frac{1}{\mathrm{e}^{2\alpha r} - 1} + \frac{\mathrm{e}^{2\alpha r}}{\left(\mathrm{e}^{2\alpha r} - 1\right)^2}. \tag{8}$$

Upon substituting Eq. (7) into (3) and replacing the resulting expression into Eq. (2) yields

$$\frac{\mathrm{u}''_{vJ}(r)}{\mathrm{u}_{vJ}(r)} = -\gamma_{vJ} - \frac{\gamma_0}{\mathrm{e}^{2\alpha r} - 1} + \frac{\gamma_1 \mathrm{e}^{2\alpha r}}{\left(\mathrm{e}^{2\alpha r} - 1\right)^2}. \tag{9}$$

where prime denotes derivatives with respect to argument in brackets. For mathematical simplicity, the following notations have been used.

$$\gamma_{vJ} = \frac{2\mu}{\hbar^2}\left(\mathrm{E}_{vJ} - \mathrm{V}_0\, \mathrm{e}^{-2\alpha r_e}\right), \tag{10}$$

$$\gamma_0 = \frac{4\mu \mathrm{V}_0}{\hbar^2}\sinh\left(2\alpha r_e\right), \tag{11}$$

$$\gamma_1 = \frac{8\mu V_0}{\hbar^2}\sinh^2(\alpha r_e) + 4L\alpha^2 . \tag{12}$$

If we assume supersymmetry (SUSY) as one in which $E_{0J} = 0$, Eq. (9) is satisfied by the ground state ($v = 0$) wave function

$$u_{0J}(r) = N_{0J}\exp\left(-\int\phi(r)\,dr\right), \tag{13}$$

where N_{0J} is the normalization constant for the ground state wave function and ϕ is known as the superpotential in the context of SUSYQM [15, 20-22]. Substituting Eq. (13) in (9), we obtain the nonlinear Riccati differential equation given by

$$\phi^2 - \phi' = -\gamma_{0J} - \frac{\gamma_0}{e^{2\alpha r}-1} + \frac{\gamma_1 e^{2\alpha r}}{\left(e^{2\alpha r}-1\right)^2} . \tag{14}$$

In order to solve Eq. (14), we choose a trial wave function of the form

$$\phi = -c_0\left(e^{2\alpha r}-1\right)^{-1} + c_1 , \tag{15}$$

where c_0 and c_1 are constant coefficients. Therefore, replacing Eq. (15) into (14) and comparing coefficients, it is easy to see that

$$c_0 = \alpha\omega , \tag{16}$$

$$c_1 = \frac{\gamma_0}{2c_0} - \frac{c_0}{2} , \tag{17}$$

$$\gamma_{0J} = -\left(\frac{\gamma_0}{2c_0} - \frac{c_0}{2}\right)^2 , \tag{18}$$

where

$$\omega = 1 + \sqrt{1 + \frac{\gamma_1}{\alpha^2}} \equiv 1 + \sqrt{1 + \frac{8\mu V_0}{\alpha^2\hbar^2}\sinh^2(\alpha r_e) + 4L} , \tag{19}$$

with c_0 and c_1 defined by Eqs. (16) and (17) respectively. Next a pair of partner potentials [15, 20-22] is constructed for the Hamiltonian. Thus, we define these partner potentials as

$$V_-(r) \equiv \phi^2 - \phi' = \left(\frac{\gamma_0}{2c_0} - \frac{c_0}{2}\right)^2 - \frac{c_0^2 + 2c_0c_1}{e^{2\alpha r}-1} + \frac{\left(c_0^2 - 2\alpha c_0\right)e^{2\alpha r}}{\left(e^{2\alpha r}-1\right)^2} , \tag{20}$$

$$V_+(r) \equiv \phi^2 + \phi' = \left(\frac{\gamma_0}{2c_0} - \frac{c_0}{2}\right)^2 - \frac{c_0^2 + 2c_0c_1}{e^{2\alpha r}-1} + \frac{\left(c_0^2 + 2\alpha c_0\right)e^{2\alpha r}}{\left(e^{2\alpha r}-1\right)^2} . \tag{21}$$

If shape invariant condition of SUSYQM holds [15 20-22], then the partner potentials in (20) and (21) are connected by

$$V_+(r, a_0) = V_-(r, a_1) + R(a_1) , \tag{22}$$

where a_1 is a new set of parameters uniquely determined from the old set $c_0 \equiv A$ through the relations $c_1 = c_0 + \alpha$, $c_2 = c_0 + 2\alpha$, …, $c_v = c_0 + v\alpha$. R (c_1) is the remainder term and is independent of r [15, 20-22]. Eq. (22) leads to the relation

$$R(c_j) = \left(\frac{\gamma_0}{2c_{j-1}} - \frac{c_j}{2}\right)^2 - \left(\frac{\gamma_0}{2c_j} - \frac{c_j}{2}\right)^2 , \tag{23}$$

where $j \in \mathbb{Z}^+$. To determine the energy eigenvalues, we define

$$\gamma_{vJ}^{(-)} = \sum_{j=1}^{v} R(c_j) . \tag{24}$$

Substituting (23) in (24) and expanding out the summation, we find

$$\gamma_{vJ}^{(-)} = \left(\frac{\gamma_0}{2c_0} - \frac{c_0}{2}\right)^2 - \left(\frac{\gamma_0}{2c_v} - \frac{c_v}{2}\right)^2 \equiv \left(\frac{\gamma_0}{2c_0} - \frac{c_0}{2}\right)^2 - \left\{\frac{\gamma_0}{2(c_0 + \alpha v)} - \frac{c_0 + \alpha v}{2}\right\}^2 . \tag{25}$$

The energy eigenvalue is obtained from the expression

$$\gamma_{vJ} = \gamma_{0J} + \gamma_{vJ}^{(-)} . \tag{26}$$

Inserting Eqs. (10), (18) and (25) into (26) and simplifying, we have

$$E_{\nu J} = V_0 e^{-2\alpha r_e} - \frac{\alpha^2 \hbar^2}{2\mu}\left(\frac{\eta}{\rho} - \frac{\rho}{2}\right)^2, \tag{27}$$

where

$$\eta = \frac{\gamma_0}{2\alpha^2}, \tag{28}$$

$$\rho = \nu + \omega. \tag{29}$$

3 Radial wave functions of the rotating Tietz potential

Since SUSYQM is only suitable for obtaining energy eigenvalues, the corresponding wave functions of the rotating Tietz potential can be obtained via ansatz solution method. Letting

$$x = e^{-2\alpha r}, \tag{30}$$

where $x \in (0, 1)$, equation (9) is transformed to

$$x(1-x)u''_{\nu J}(x) + (1-x)u'_{\nu J}(x) + \left(\frac{\gamma_0 - \gamma_{\nu J}}{4\alpha^2} + \frac{\gamma_{\nu J}}{4\alpha^2}\frac{1}{x} - \frac{\gamma_1}{4\alpha^2}\frac{1}{1-x}\right)u_{\nu J}(x) = 0. \tag{31}$$

Since Eq. (31) has singularities at $x = 0$ and $x = 1$, we suppose an ansatz solution of the form

$$u_{\nu J}(x) = N_{\nu J}\, x^{\frac{1}{2}\sigma}(1-x)^{\frac{1}{2}\omega}\, \Omega_{\nu J}(x), \tag{32}$$

where σ is a parameter, N_{vJ} is the normalization constant, $\Omega_{\nu J}(x)$ is an unknown function of x and the parameter ω is given by Eq. (19). Replacing Eq. (32) into (31), we obtained the following Gauss hypergeometric differential equation

$$x(1-x)\Omega''_{\nu J}(x) + \{\sigma + 1 - (\sigma + \omega + 1)x\}\Omega'_{\nu J}(x) - \left\{(\sigma + \omega)^2 + \frac{\gamma_0 - \gamma_{\nu J}}{4\alpha^2}\right\}\Omega_{\nu J}(x) = 0, \tag{33}$$

subject to the constraint

$$\sigma\alpha = \left(-\gamma_{\nu J}\right)^{\frac{1}{2}}. \tag{34}$$

Considering bound state solutions, Eq. (33) we obtained the hypergeometric function

$$\Omega_{\nu J}(x) = {}_2F_1(-\nu, \nu + \sigma + \omega; \sigma + 1; x). \tag{35}$$

Normalization condition of wave functions requires that

$$\int_0^\infty P_{\nu J}(r)\, dr = 1, \tag{36}$$

where

$$P_{\nu J}(r) = \left|u_{\nu J}(r)\right|^2, \tag{37}$$

Is the probability density function. Upon substituting Eqs. (37), (32) and then (35) into (36), the result leads to

$$N_{\nu J} = \left(\frac{2\alpha}{M_{\nu J}}\right)^{\frac{1}{2}}, \tag{38}$$

where

$$M_{\nu J} = \int_0^1 x^{\sigma-1}(1-x)^{\omega}\left|{}_2F_1(-\nu, \nu + \sigma + \omega; \sigma + 1; x)\right|^2 dx. \tag{39}$$

Following Qiang and Dong [23], the definite integral in (38) yields

$$M_{\nu J} = \frac{\nu!(2\nu + \sigma)\Gamma(\sigma)\Gamma(\sigma + 1)\Gamma(\nu + \omega)}{(2\nu + \sigma + \omega)\Gamma(\nu + \sigma + 1)\Gamma(\nu + \sigma + \omega)}, \tag{40}$$

where $\Gamma(y)$ is the gamma function of the argument y.

4 Results and Discussion

To enable us confirm the accuracy of our results, we have computed bound state energy eigenvalues as a function of potential strength for arbitrary rotational and vibrational quantum numbers. The results calculated using Eq. (27) are shown in Table 1. Also shown in the table are columns of available literature results for bound state energy eigenvalues of Tietz potential obtained by proper quantization rule (PQR) [10] and by numerical (NUM) method [10, 17]. Evidently, results obtained by the SUSYQM approach are in total agreement with existing data in the literature, thus, affirming the validity of

expression (27) as accurate equation for energy eigenvalues of the Tietz potential. Figure 1 shows graphical representation of eigen energy as a function of vibrational quantum number, the plot reveals that for small values of potential screening parameters and rotational quantum number, bound state energy obtained by the SUSYQM method are in near perfect fit with thos obtained by numerical methods in the literature. In figure 2, we have plotted energy eigenvalues versus rotational quantum number, from the plot, it is evident that for the low ro-vibrational states, energies obtained numerically tends to agree with those obtained by SUSYQM analytical methos, however, the disparity is well pronounced for the high ro-vibrational states. It follows that analytical expression for bound state eigen energies of the Tietz oscillator are valid for small values of screening parameters and low quantum states.

Table 1: Bound state energy eigenvalues (atomic unit) as a function of V_0 for $\alpha = 0.01$, $r_e = 2$, $\hbar = 1$ and $\mu = 5$ along with corresponding literature data

state		$V_0 = 0.1$	$V_0 = 0.2$			$V_0 = 0.4$		
N	J	SUSYQM	SUSTQM	PQR [10]	NUM [17]	SUSTQM	PQR [10]	NUM [17]
0	0	0.039027	0.059294	0.059294	0.059294	0.088263	0.088263	0.088263
1	0	0.068404	0.116235	0.116235	0.116235	0.190727	0.190727	0.190727
1	1	0.074908	0.127523	0.127523	0.127529	0.207801	0.207801	0.207808
2	0	0.080639	0.144408	0.144408	0.144408	0.249787	0.249787	0.249787
2	1	0.083822	0.150593	0.150593	0.150599	0.260242	0.260242	0.260249
2	2	0.087444	0.159111	0.159111	0.159131	0.276865	0.276865	0.276885
3	0	0.086832	0.160332	0.160332	0.160332	0.286861	0.286861	0.286861
3	1	0.088603	0.164068	0.164068	0.164074	0.293713	0.293713	0.293720
3	2	0.090720	0.169384	0.169384	0.169405	0.304811	0.304811	0.304831
3	3	0.092457	0.174507	0.174507	0.174573	0.317141	0.317141	0.317118
4	0	0.090354	0.170164	…	…	0.311615	…	…
4	1	0.091423	0.172579	…	…	0.316338	…	…
4	2	0.092740	0.176097	…	…	0.324098	…	…
4	3	0.093853	0.179587	…	…	0.332890	…	…
4	4	0.094686	0.182580	…	…	0.341364	…	…
5	0	0.092509	0.176622	0.176622	…	0.328926	0.328926	…
5	1	0.093187	0.178261	0.178261	…	0.332311	0.332311	…
5	2	0.094037	0.180691	0.180691	…	0.337936	0.337936	…
5	3	0.094766	0.183152	0.183152	…	0.344406	0.344406	…
5	4	0.095310	0.185304	…	…	0.350750	…	…
5	5	0.095686	0.187070	0.187070	…	0.356488	0.356488	…

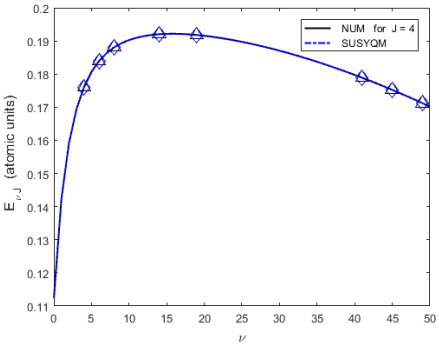

Figure 1: Variation of energy eigenvalues as a function of vibrational quantum number for $\alpha = 0.01$, $r_e = 2$, $\hbar = 1$ and $\mu = 5$

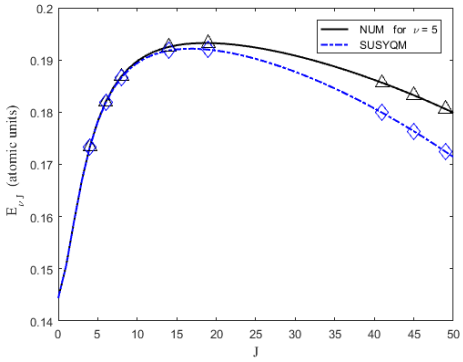

Figure 2: Variation of energy eigenvalues as a function of rotational quantum number for $\alpha = 0.01$, $r_e = 2$, $\hbar = 1$ and $\mu = 5$

5 Conclusion

In the present work, the Schrödinger equation has been solved in the presence of molecular Tietz oscillator to obtain analytical solutions of bound state eigen energies and normalized wave functions in compact form. In order to model the spin-orbit term of the Schrödinger equation, the Greene-Aldrich approximation recipe was considered. By constructing a pair of superpotential to the Hamiltonian of the system, the SUSYQM approach was employed in arriving at the formula for

bound state eigen energies. With the help of our energy equation, bound state energies were computed for the Tietz potential, the results obtained compares favorably with available data in the literature obtained by other methods. This work may be applied in many areas of physics which include: molecular and atomic physics, solid-state physics, statistical physics and chemical physics

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