Approximate Analytical Solutions to Relativistic and Nonrelativistic Pöschl-Teller Potential with its Thermodynamic Properties

Sameer M. Ikhdair

Department of Electrical and Electronic Engineering, Near East University, 922022 Nicosia, Northern Cyprus, Turkey.

and

Department of Physics, Faculty of Science, An-Najah National University, New Campus, Nablus, West Bank, Palestine.

Babatunde J. Falaye

Theoretical Physics Section, Department of Physics, University of Ilorin, P. M. B. 1515, Ilorin, Nigeria.

Adenike G. Adepoju

Physics Section, Holy Marry College, Ifo, Ogun State, Nigeria.

Abstract

We apply the asymptotic iteration method (AIM) to obtain the solutions of Schrödinger equation in the presence of Pöschl-Teller (PT) potential. We also obtain the solutions of Dirac equation for the same potential under the condition of spin and pseudospin (p-spin) symmetries. We show that in the nonrelativistic limits, the solution of Dirac system converges to that of Schrödinger system. Rotational-Vibrational energy eigenvalues of some diatomic molecules are calculated. Some special cases of interest are studied such as $S$-wave case, reflectionless-type potential and symmetric hyperbolic PT potential. Furthermore, we present a high temperature partition function in order to study the behavior of the thermodynamic functions such as the vibrational mean energy $U$, specific heat $C$, free energy $F$ and entropy $S$.

Keywords: Dirac equation; Schrödinger equation; Pöschl-Teller potential; AIM method; thermodynamic property

1 Introduction

The exact solutions of various quantum potential models have attracted much attention from many authors since they contain all necessary information to study quantum models. As well-known, there are several traditional techniques used to solve Schrödinger-like differential equation
with various quantum potentials \[1, 2, 3, 4, 5, 6\]. Few of these methods include the asymptotic iteration method (AIM) \[7, 8\], the Nikiforov-Uvarov (NU) method \[9, 10, 11, 12\]. The algebraic techniques are related to the inspection of the Hamiltonian of quantum system as in the supersymmetric quantum mechanics (SUSYQM) \[13, 14, 15\] and closely to the factorization method \[16, 17\]. Other methods are based on the proper and exact quantization rule \[18, 19, 20, 21\] and the SWKB method \[22\]. Except for the previous methods, quasilinearization method (QLM) is dealing with physical potentials numerically \[23, 24\].

In the present work, we investigate the Schrödinger equation and Dirac equation for the PT potential within the framework of AIM \[7, 8\]. This potential has been investigated by some authors under different wave equations of quantum mechanics which include the Klein-Gordon, the Dirac and the Schrödinger equations for the vibrational \(\ell = 0\) and rotational \(\ell \neq 0\) states \[25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35\]. The priority purpose for studying this potential is due fact that it has been used to accounted for the physics of many systems which includes the excitons, quantum wires and quantum dots \[36, 37, 38, 39, 40, 41, 42\]. For certain ranges of parameters it behaves like the Kratzer potential.

In recent years, an asymptotic iteration method for solving second order homogeneous linear differential equations has been proposed \[7, 8\]. This method is a powerful tool in finding the eigensolutions (energy eigenvalues and wave functions) of all solvable quantum potential models \[7, 8\]. This method has been so far applied to solve both the relativistic the non-relativistic quantum mechanical problems \[13, 14, 15, 16, 17, 18\]. The purpose of this work is to apply AIM to obtain approximate energy levels and wave functions of the PT potential in the framework Schrödinger equation and Dirac equation with the spin and p-spin symmetries by considering an appropriate approximation to the centrifugal (pseudo centrifugal) kinetic energy term and study its thermal properties including vibrational mean energy \(U\), specific heat \(C\), free energy \(F\) and entropy \(S\) as given in Ref. \[49\]. Further, the nonrelativistic limit is obtained and some special cases of this potential are investigated.

This paper is organized as follows: In Section 2, we briefly outline the methodology. In Section 3, we present the bound state solutions of the Schrödinger equation with the PT potential. Furthermore, we consider the solution of the PT potential in the framework of the Dirac equation under the spin and p-spin symmetries. The nonrelativistic limit is also obtained. Section 4 presents eigensolutions for some special cases. The thermodynamic properties of the Schrödinger equation with PT potential are investigated in section 5. Section 6 is devoted for our numerical results and discussions. Finally we give our conclusion in Section 7.
2 Method of Analysis

One of the calculational tools utilized in solving the Schrödinger-like equation including the centrifugal barrier and/or the spin-orbit coupling term is the so called asymptotic iteration method (AIM). For a given potential the idea is to convert the Schrödinger-like equation to the homogeneous linear second-order differential equation whose solution is a special function and having the form [7]:

\[ y''(x) = \lambda_o(x)y'(x) + s_o(x)y(x), \]  

(1)

where \( \lambda_o(x) \) and \( s_o(x) \) have sufficiently many continuous derivatives and defined in some interval which are not necessarily bounded. The differential equation (1) has a general solution [7, 8]

\[ y(x) = \exp \left( -\int^x \alpha(x')dx' \right) \left[ C_2 + C_1 \exp \left( \int^x \left[ \lambda_o(x'') + 2\alpha(x'') \right] dx'' \right) \right]. \]  

(2)

If \( k > 0 \), for sufficiently large \( k \), we obtain the \( \alpha(x) \)

\[ \frac{s_k(x)}{\lambda_k(x)} = \frac{s_{k-1}(x)}{\lambda_{k-1}(x)} = \alpha(x), \quad k = 1, 2, 3, \ldots \]  

(3)

where

\[ \lambda_k(x) = \lambda'_{k-1}(x) + s_{k-1}(x) + \lambda_o(x)\lambda_{k-1}(x), \]

\[ s_k(x) = s'_{k-1}(x) + \lambda_o(x)\lambda_{k-1}(x), \quad k = 1, 2, 3, \ldots \]  

(4)

The energy eigenvalues are obtained from the quantization condition of the method together with equation (4) and can be written as follows:

\[ \delta_k(x) = \lambda_k(x)s_{k-1}(x) - \lambda_{k-1}(x)s_k(x) = 0, \quad k = 1, 2, 3, \ldots \]  

(5)

The energy eigenvalues are then obtained from (5), if the problem is exactly solvable. If not, for a specific \( n \) principal quantum number, we choose a suitable \( x_0 \) point, determined generally as the maximum value of the asymptotic wave function or the minimum value of the potential and the approximate energy eigenvalues are obtained from the roots of this equation for sufficiently large values of \( k \) with iteration.

3 Bound State Solutions

3.1 Schrödinger equation for PT potential

The PT potential we shall study is defined as [34, 50, 51, 52, 56]

\[ V(r) = \frac{A}{\cosh^2(\alpha r)} + \frac{B}{\sinh^2(\alpha r)}, \quad 0 < \alpha r < \frac{\pi}{2} \]  

(6)
where $A$, $B$ and $\alpha$ are constant coefficients. If we insert this potential into the Schrödinger equation, the radial part of the Schrödinger equation takes the following form:

$$\frac{d^2 R_{n\ell}(r)}{dr^2} + \left[ \frac{2\mu}{\hbar^2} E_{n\ell} - \frac{2\mu A}{\cosh^2(\alpha r)} - \frac{2\mu B}{\sinh^2(\alpha r)} - \frac{\ell(\ell + 1)}{r^2} \right] R_{n\ell}(r) = 0,$$

(7)

where $n$ and $\ell$ denote the radial and orbital angular momentum quantum numbers, respectively, and $E_{n\ell}$ denote the bound-state energy eigenvalues. It is clear that the above equation cannot be exactly solved for $\ell \neq 0$ because of the centrifugal barrier. To obtain the exact bound-state solution, we have to include some approximation to deal with the centrifugal term. It is found that the following [30, 35]

$$\frac{1}{r^2} \approx \alpha^2 \left[ 4d_0 + \frac{1}{\sinh^2(\alpha r)} \right],$$

(8)

where $d_0 = 1/12$, is a good approximation to the centrifugal term in short potential range. Now, if we replace $1/r^2$ with equation (8) and further defining the following notations

$$A_1 = \frac{2\mu A}{\hbar^2}, \quad B_1 = \frac{2\mu B}{\hbar^2} + \ell(\ell + 1)\alpha^2, \quad K_1 = \frac{2\mu}{\hbar^2} E_{n\ell} - 4\ell(\ell + 1)\alpha^2 d_0,$$

(9)
equation (7) can be easily transformed into

$$\frac{d^2 R_{n\ell}(r)}{dr^2} + \left[ K_1 - \frac{A_1}{\cosh^2(\alpha r)} - \frac{B_1}{\sinh^2(\alpha r)} \right] R_{n\ell}(r) = 0.$$

(10)

In order to solve with the AIM, equation (10) must be transformed into form of equation (1).

The reasonable wave function we propose is as follows

$$R_{n\ell}(r) = \cosh \gamma(\alpha r) \sinh \beta(\alpha r) F_{n\ell}(r),$$

(11)

where $\gamma = \frac{1}{2} \left( 1 + \sqrt{1 - \frac{4A_1}{\alpha^2}} \right)$ and $\beta = \frac{1}{2} \left( 1 - \sqrt{1 + \frac{4B_1}{\alpha^2}} \right)$. On putting this wave function into equation (10), we then arrive at the following second-order homogeneous linear differential equation of the form

$$F''_{n\ell}(z) + 2\alpha \left[ \frac{\gamma \sinh(\alpha r)}{\cosh(\alpha r)} + \frac{\beta \cosh(\alpha r)}{\sinh(\alpha r)} \right] F'_{n\ell}(z) + K_2 F_{n\ell}(z) = 0,$$

(12)

where we have introduced a new parameter $K_2 = K_1 + \alpha^2(\beta + \gamma)^2$ for the sake of simplicity. Now, before we apply the AIM, let us introduce a new variable of the form $z = \sinh(\alpha r)$ in order to avoid the cumbersome calculations. Therefore, equation (12) can be re-written as

$$F''_{n\ell}(z) + \frac{(2\gamma + 1)z^2 + 2\beta(z^2 + 1)}{z(z^2 + 1)} F'(z) + \frac{K_2}{\alpha^2(1 + z^2)} F(z) = 0.$$

(13)

By making a comparison between equations (11) and (12), we can write $\lambda_0(z)$ and $s_0(z)$ values and be using equation (11), we can calculate $\lambda_k(z)$ and $s_k(z)$ as

$$\lambda_0(z) = \frac{(2\gamma + 1)z^2 + 2\beta(z^2 + 1)}{z(z^2 + 1)},$$

4
\[ s_0(z) = \frac{K_2}{\alpha^2(z^2 + 1)}, \]
\[ \lambda_1(z) = 2z^2 \frac{2\gamma + 1}{(z^2 + 1)^2} + 2\frac{\beta}{z^2} - \frac{2\gamma + 1}{z^2 + 1} - \frac{K_2}{\alpha^2(z^2 + 1)} + \left( \frac{2\gamma + 1 + 2\beta}{z^2 + 1} \right)^2, \]
\[ s_1(z) = \frac{K_2(3 + 2\beta + 2\gamma)z^2 + 2\beta}{\alpha^2z(1 + z^2)}, \]
\[ \ldots \] etc. \hspace{1cm} (14)

By using the quantization condition given by equation (5), we can establish the following relations

\[ \delta_1 = 0 \Rightarrow K_2 = 0, \]
\[ \delta_2 = 0 \Rightarrow K_2 = -4\alpha^2(\gamma + \beta + 1), \]
\[ \delta_3 = 0 \Rightarrow K_2 = -4\alpha^2(\gamma + \beta + 2), \]
\[ \delta_4 = 0 \Rightarrow K_2 = -4\alpha^2(\gamma + \beta + 3), \]
\[ \ldots \] etc. \hspace{1cm} (15)

We generalize the above expression by induction and substituting for \( K_2 \), the eigenvalues becomes

\[ K_1 + \alpha^2(\gamma + \beta + 2n)^2 = 0, \quad n = 0, 1, 2, \ldots \] \hspace{1cm} (16)

By using the notations in equation (9), we obtain a more explicit expression for the energy eigenvalue equation as:

\[ E_{n\ell} = \frac{2\alpha^2\hbar^2}{\mu} \left[ \ell(\ell + 1)d_0 - \left( n + 1 + \frac{1}{2}\sqrt{1 - \frac{8\mu}{\alpha^2\hbar^2} - \frac{1}{4}(2\ell + 1)^2 + \frac{8\mu B}{\alpha^2\hbar^2}} \right)^2 \right]. \] \hspace{1cm} (17)

Now, let us study the eigenfunction of the system. To perform this task, the differential equation we wish to solve should be transformed to the form [8]:

\[ y''(x) = 2 \left( \frac{Ax^{N+1}}{1 - bx^{N+2}} - \frac{m + 1}{x} \right) y'(x) - \frac{Wx^N}{1 - bx^{N+2}}, \] \hspace{1cm} (18)

where \( A, b \) and \( m \) are constants. The general solution of equation (18) can be found as [8]

\[ y_n(x) = (-1)^n C_2(N + 2)^n(\sigma)_n 2F_1(-n, \ell + n; \sigma; bx^{N+2}), \] \hspace{1cm} (19)

where the following parameters have been used

\[ (\sigma)_n = \frac{\Gamma(\sigma + n)}{\Gamma(\sigma)} , \quad \sigma = \frac{2m + N + 3}{N + 2} \quad \text{and} \quad t = \frac{(2m + 1)b + 2A}{(N + 2)b}. \] \hspace{1cm} (20)

By comparing equations (19) with (13), we can easily determine the parameters \( A, b, N, m \) and \( \sigma \). Consequently, the radial eigenfunction for the Schrödinger equation with the PT potential can be found as

\[ R_{n\ell}(r) = 2^n(-1)^n C_2 \cosh^{\gamma}(\alpha r) \sinh^{\beta}(\alpha r) \frac{(\beta + n)!}{\beta!} 2F_1(-n, \beta + \gamma + n; \beta + 1; -\sinh(\alpha r)), \] \hspace{1cm} (21)

where \( C_2 \) is the normalization factor.
3.2 Dirac equation for the PT potential

Using Dirac wave equation and Dirac spinor wave functions, the two-coupled second-order ordinary differential equations for the upper and lower components of the Dirac wave function can be obtained as

\[ \left( \frac{d}{dr} + \frac{\kappa}{r} \right) F_{\nu\kappa}(r) = [M + E_{\nu\kappa} - \Delta(r)] G_{\nu\kappa}(r), \]  
\[ \left( \frac{d}{dr} - \frac{\kappa}{r} \right) G_{\nu\kappa}(r) = [M - E_{\nu\kappa} + \Sigma(r)] F_{\nu\kappa}(r). \]  

where \( \Delta(r) = V(r) - S(r) \) and \( \Sigma(r) = V(r) + S(r) \). On solving equation (22), we obtain the following Schrödinger-like differential equation with coupling to the \( r^{-2} \) singular term and satisfying \( F_{\nu\kappa}(r) \):

\[
\left[ \frac{d^2}{dr^2} - \frac{\kappa(\kappa + 1)}{r^2} + \frac{d\Delta(r)}{dr} \left( \frac{d}{dr} + \frac{\kappa}{r} \right) - (M + E_{\nu\kappa} - \Delta(r)) (M - E_{\nu\kappa} + \Sigma(r)) \right] F_{\nu\kappa}(r) = 0,
\]

(24)

where \( E_{\nu\kappa} \neq -M \) when \( \Delta(r) = 0 \) and \( \kappa(\kappa + 1) = \ell(\ell + 1) \). Since \( E_{\nu\kappa} = +M \) is an element of the positive energy spectrum of the Dirac Hamiltonian, this relation with upper spinor component is not valid for the negative energy spectrum solution. Furthermore, a similar equation satisfying \( G_{\nu\kappa}(r) \) can be obtained as:

\[
\left[ \frac{d^2}{dr^2} - \frac{\kappa(\kappa - 1)}{r^2} + \frac{d\Sigma(r)}{dr} \left( \frac{d}{dr} - \frac{\kappa}{r} \right) - (M + E_{\nu\kappa} - \Delta(r)) (M - E_{\nu\kappa} + \Sigma(r)) \right] G_{\nu\kappa}(r) = 0,
\]

(25)

where \( E_{\nu\kappa} \neq +M \) when \( \Sigma(r) = 0 \) and \( \kappa(\kappa - 1) = \tilde{\ell}(\tilde{\ell} + 1) \). Since \( E_{\nu\kappa} = -M \) is an element of the negative energy spectrum of the Dirac Hamiltonian, this relation with the lower spinor component is not valid for the positive energy spectrum solution. In the next subsections, we shall study the PT potential within the framework the Dirac theory in the presence of spin and p-spin symmetries.

3.2.1 Bound states in pseudospin symmetry limit

Under the condition of the p-spin symmetry, i.e., \( \frac{d\Sigma(r)}{dr} = 0 \), equation (25) turns to

\[
\left[ \frac{d^2}{dr^2} - \frac{\kappa(\kappa - 1)}{r^2} - (M + E_{\nu\kappa} - \Delta(r)) (M - E_{\nu\kappa} + C_{ps}) \right] G_{\nu\kappa}(r) = 0.
\]

(26)

Now taking \( \Delta(r) \) as the PT potential, using approximation expression (8), defining the following parameters

\[
\tilde{A}_3 = (E_{\nu\kappa} - M - C_{ps}) \frac{A}{\alpha^2}, \quad \tilde{B}_3 = (E_{\nu\kappa} - M - C_{ps}) \frac{B}{\alpha^2} + \kappa(\kappa - 1),
\]

\[
\tilde{K}_3 = 4\kappa(\kappa - 1)d_0 + \frac{1}{\alpha^2} (M - E_{\nu\kappa} + C_{ps}) (M + E_{\nu\kappa}),
\]

(27)
and introducing a new transformation of the form \( z = \cosh^2(\alpha r) \), equation (26) can be transformed easily to

\[
G''_{nk}(z) + \left[ \frac{1 - 2z}{2z(1 - z)} \right] G'_{nk}(z) + \frac{1}{4z(1 - z)} \left[ \frac{\tilde{A}_3}{z} - \frac{\tilde{B}_3}{1 - z} + \tilde{K}_3 \right] G_{nk}(z) = 0. \tag{28}
\]

In order to solve this equation with AIM, the wave function satisfies the boundary conditions is being proposed as

\[
G_{nk}(z) = (1 - z)\tilde{\gamma}_2 z^{\tilde{\beta}_2} g_{nk}(z), \tag{29}
\]

where \( \tilde{\gamma}_2 = \frac{1}{4} \left( 1 - \sqrt{1 + 4\tilde{B}_3} \right) \) and \( \tilde{\beta}_2 = \frac{1}{4} \left( 1 - \sqrt{1 - 4\tilde{A}_3} \right) \). Inserting this wave function into equation (28), leads us to write

\[
g''_{nk}(z) + 2 \left( \frac{\tilde{\beta}_2 + \frac{1}{2}}{z(1 - z)} - \frac{\tilde{\beta}_2 + \gamma_2 + \frac{1}{2}}{1 - z} \right) g'_{nk}(z) + \left( \frac{K_3 - 4(\tilde{\beta}_2 + \gamma_1)^2}{4z(1 - z)} \right) g_{nk}(z) = 0. \tag{30}
\]

Following same procedures as in the previous section, we can use equation (30) to calculate the \( \lambda_k(z) \) and \( s_k(z) \) then combine the result with the quantization condition given by equation (5). This yields

\[
s_0\lambda_1 - s_1\lambda_0 = 0 \quad \Rightarrow \quad \tilde{A}_3 = 4(\tilde{\gamma}_2 + \tilde{\beta}_2)^2
\]
\[
s_1\lambda_2 - s_2\lambda_1 = 0 \quad \Rightarrow \quad \tilde{A}_3 = 4(\tilde{\gamma}_2 + \tilde{\beta}_2 + 1)^2
\]
\[
s_2\lambda_3 - s_3\lambda_2 = 0 \quad \Rightarrow \quad \tilde{A}_3 = 4(\tilde{\gamma}_2 + \tilde{\beta}_2 + 2)^2
\]
\[
\ldots \text{etc.} \tag{31}
\]

By generalizing the above expression and using the notations in equation (27), the relativistic energy spectrum becomes

\[
4\alpha^2 \left[ d_{0k}(\kappa - 1) - \left[ n + \frac{1}{2} + \frac{1}{4} \sqrt{1 + \frac{4A}{\alpha^2} (M - E + C_{ps})} - \frac{1}{4} \sqrt{(2\kappa - 1)^2 - \frac{4B}{\alpha^2} (M - E_{nk} + C_{ps})} \right]^2 + (M + E_{nk}) (M - E_{nk} + C_{ps}) = 0, \tag{32}
\]

which is identical to Ref. [35] if \( B \to \alpha^2 B(B - \alpha)/(2M) \) and \( A \to -\alpha^2 A(A + \alpha)/(2M) \). Let us now turn to the calculations of the corresponding wave functions for this system. Thus using the procedure described by equation (18)-(20), the wave functions can be easily found as

\[
G_{nk}(r) = \tilde{N}_{nk} \frac{\Gamma \left( \frac{2\tilde{\beta}_2 + n + \frac{1}{2}}{\Gamma(2\tilde{\beta}_2 + \frac{1}{2})} \right) \cosh^{2\beta_2}(\alpha r) \sinh^{2\gamma_2}(\alpha r) 2F_1 \left( -n, 2(\tilde{\beta}_2 + \gamma_2) + n; 2\tilde{\beta}_2 + \frac{1}{2}; \sinh^2(\alpha r) \right)}{\cos^{2\beta_2}(\alpha r) \sinh^{2\gamma_2}(\alpha r) 2F_1 \left( -n, 2(\tilde{\beta}_2 + \gamma_2) + n; 2\tilde{\beta}_2 + \frac{1}{2}; \sinh^2(\alpha r) \right)}, \tag{33}
\]

where \( \tilde{N}_{nk} \) is the normalization constant.
3.2.2 Bound states in spin symmetry limit

Under the condition of the spin symmetry, i.e., \( \frac{d\Delta(r)}{dr} = 0 \), equation (24) reduces to

\[
\left[ \frac{d^2}{dr^2} - \frac{\kappa(\kappa + 1)}{r^2} - (M - E_{n\kappa} + \Sigma(r))(M + E_{n\kappa} - C_s) \right] F_{n\kappa}(r) = 0. \tag{34}
\]

Now taking the sum potential as the PT potential along with the approximation expression given by equation (8) and then introducing a new parameter of the form \( z(r) = \sinh(\alpha r) \), the equation (26) can be easily decomposed into a Schrödinger-like equation in the spherical coordinates for the upper-spinor component \( F_{n\kappa}(r) \),

\[
F''_{n\kappa}(z) + \frac{1 - 2z}{2z(1 - z)} F'_{n\kappa}(z) + \frac{1}{4z(1 - z)} \left[ \frac{A_3}{z} - \frac{B_3}{1 - z} + K_3 \right] F_{n\kappa}(z) = 0, \tag{35}
\]

where

\[
A_3 = (E_{n\kappa} + M - C_s) \frac{A}{\alpha^2}, \quad B_3 = (E_{n\kappa} + M - C_s) \frac{B}{\alpha^2} + \kappa(\kappa + 1),
\]

\[
K_3 = 4\kappa(\kappa + 1) + \frac{1}{\alpha^2} (M + E_{n\kappa} - C_s)(M - E_{n\kappa}). \tag{36}
\]

In order to avoid repetition of algebra, a first inspection for the relationship between the present set of parameters \((A_3, B_3, K_3)\) and the previous set \((\tilde{A}_3, \tilde{B}_3, \tilde{K}_3)\) enable us to know that the positive solution for the above equation (35), can be easily obtain by using the parameter parameter map \([57, 58]\)

\[
G_{n\kappa} \leftrightarrow F_{n\kappa}, \quad V(r) \rightarrow -V(r), \quad E_{n\kappa} \rightarrow -E_{n\kappa}, \quad \kappa \rightarrow \kappa + 1 \quad \text{and} \quad C_{ps} \rightarrow -C_s. \tag{37}
\]

Using the above transformations and following the previous results, we obtain the relativistic energy spectrum as

\[
4\alpha^2 \left[ d_0\kappa(\kappa + 1) - \left[ n + \frac{1}{2} + \frac{1}{4} \sqrt{1 - 4A M + E - C_s \alpha^2} - \sqrt{(2\kappa + 1)^2 + \frac{4B}{\alpha^2} (M + E_{n\kappa} - C_s)} \right]^2 \right] + (M - E_{n\kappa})(M + E_{n\kappa} - C_s) = 0, \tag{38}
\]

which is identical to Ref. [35] if \( B \rightarrow \alpha^2 B(B - \alpha)/(2M) \) and \( A \rightarrow -\alpha^2 A(A + \alpha)/(2M) \), and the corresponding wave functions as

\[
F_{n\kappa}(r) = N_{n\kappa} \frac{\Gamma \left( \frac{2\beta_2 + n + 1}{2} \right)}{\Gamma \left( \frac{2\beta_2 + 1}{2} \right)} \cosh^{2\beta_2}(\alpha r) \sinh^{2\gamma_2}(\alpha r) _2F_1 \left( -n, 2(\beta_2 + \gamma_2) + n; 2\beta_2 + \frac{1}{2}; \sinh^2(\alpha r) \right), \tag{39}
\]

where \( N_{n\kappa} \) is the normalization constant.

4 Some special cases of the PT potential

In this section, we shall study four special cases of the energy eigenvalues \([32]\) and \([33]\) for the p-spin and spin symmetry, respectively.
4.1 S-wave case

By considering the case $\ell = 0 \ (\kappa = 1)$ and $\ell = 0 \ (\kappa = -1)$, the relativistic energy spectra for the exact p-spin ($C_{ps} = 0$) and exact spin symmetry ($C_s = 0$) become

$$M^2 - E^2_{n,+1} = 4\alpha^2 \left[ n + \frac{1}{2} + \frac{1}{4} \sqrt{1 + \frac{4A}{\alpha^2}(M - E_{n,+1})} - \frac{1}{4} \sqrt{1 + \frac{4B}{\alpha^2}(M - E_{n,+1})} \right]^2,$$  \hspace{1cm} (40)

and

$$M^2 - E^2_{n,-1} = 4\alpha^2 \left[ n + \frac{1}{2} + \frac{1}{4} \sqrt{1 - \frac{4A}{\alpha^2}(M + E_{n,-1})} - \frac{1}{4} \sqrt{1 + \frac{4B}{\alpha^2}(M + E_{n,-1})} \right]^2,$$  \hspace{1cm} (41)

respectively. Equation (41) is the same as the energy equation obtained by equation (22) of Ref. [50] and (35) of Ref. [51] by taking $A \rightarrow -2\alpha(A + \alpha)$, $B \rightarrow 2\alpha(B - \alpha)$.

4.2 Reflectionless-type potential

Choosing $B = 0, A = -\eta(\eta+1)/2$ in potential (1) then it becomes the reflectionless-type potential [59, 60]

$$V(r) = -\frac{\eta(\eta + 1)}{2\cosh^2(\alpha r)},$$  \hspace{1cm} (42)

where $\eta$ is an integer. The eigenvalue equation for exact p-spin and spin symmetry become

$$M^2 - E^2_{n,+1} = 4\alpha^2 \left[ n + \frac{1}{2} + \frac{1}{4} \sqrt{1 - \frac{4\eta(\eta + 1)}{\alpha^2}(M - E_{n,+1})} \right]^2,$$  \hspace{1cm} (43)

and

$$M^2 - E^2_{n,-1} = 4\alpha^2 \left[ n + \frac{1}{2} + \frac{1}{4} \sqrt{1 + \frac{4\eta(\eta + 1)}{\alpha^2}(M + E_{n,-1})} \right]^2,$$  \hspace{1cm} (44)

respectively.

4.3 Symmetric hyperbolic modified PT potential

On putting $\alpha = 1, B = 0, A = \frac{1}{4} - \eta^2$ in the potential equation (1), we have [59, 60]

$$V(r) = \frac{1}{\cosh^2(r)},$$  \hspace{1cm} (45)

with the relativistic energy equation

$$M^2 - E^2_{n,+1} = 4 \left[ n + \frac{1}{4} + \frac{1}{4} \sqrt{1 + (1 - 4\eta^2)(M - E_{n,+1})} \right]^2,$$  \hspace{1cm} (46)

and

$$M^2 - E^2_{n,-1} = 4 \left[ n + \frac{1}{4} + \frac{1}{4} \sqrt{1 - (1 - 4\eta^2)(M + E_{n,-1})} \right]^2,$$  \hspace{1cm} (47)

for p-spin and spin symmetries, respectively.
4.4 The non-relativistic limit

As it can be seen, the nonrelativistic Schrödinger equation is bosonic in nature, i.e., spin does not involve in it. On the other hand, relativistic Dirac equation is for a spin−1/2 particles. It implicitly suggests that there may be a certain relationship between the solutions of the two fundamental equations [61]. de Souza Dutra et al [61] also noted that there is possibility of obtaining approximate nonrelativistic (NR) solutions from relativistic (R) ones. Very recently, H. Sun [61] proposed a little bit crude but meaningful approach for deriving the bound state solutions of NR Schrödinger equation (SE) from the bound state of R equations. The essence of the approach was that, in NR limit, the SE may be derived from the R one when the energies of the two potential $S(r)$ and $V(r)$ are small compared to the rest mass $mc^2$, then the NR energy approximated as $E^{NR} \rightarrow E - mc^2$ and NR wave function is the $\psi^{NR}(r) \rightarrow \psi(r)$. That is, its NR energies, $E^{NR}$ can be determined by taking the NR limit values of the R eigenenergies $E$. Therefore, taking $C_s = 0$, and using the following transformations $M + E_{n\kappa} \rightarrow 2\mu$ and $M - E_{n\kappa} \rightarrow -E_{n\ell}$ together with $\kappa \rightarrow \ell$ [61], the relativistic energy equation (38) reduces to

$$E_{n\ell} = \frac{2\alpha^2}{\mu} \left[ \ell(\ell + 1)d_0 - \left( n + \frac{1}{2} + \frac{1}{4} \sqrt{1 - \frac{8\mu A}{\alpha^2}} - \frac{1}{4} \sqrt{(2\ell + 1)^2 + \frac{8\mu B}{\alpha^2}} \right)^2 \right], \quad (48)$$

where $\hbar = 1$. Let us remark that the non-relativistic solution is identical with the one we obtained for Schrödinger case in equation (17). Similarly, we find the non-relativistic of equations (44) and (47) as

$$E_n = -\frac{2\alpha^2}{\mu} \left[ n + \frac{1}{4} + \frac{1}{4} \sqrt{1 + 4\mu \frac{\eta(\eta + 1)}{\alpha^2}} \right]^2, \quad (49)$$

and

$$E_n = -\frac{2}{\mu} \left[ n + \frac{1}{4} + \frac{1}{4} \sqrt{1 - 2\mu (1 - 4\eta^2)} \right]^2, \quad (50)$$

for reflectionless-type and symmetric hyperbolic modified PT potential, respectively. It should be noted that equations (49) and (50) can be obtained as special cases of equation (17).

5 Thermodynamic properties of the Schrödinger-PT problem

In this section, we study the thermodynamic properties of the PT potential model. The eigenvalues $E_{n\ell}$ of this system that we obtained by equation (17) can be re-written as

$$E_{n\ell} = \frac{2\alpha^2 \hbar^2}{\mu} \left[ \ell(\ell + 1)d_0 - [n - \zeta]^2 \right], \quad n = 0, 1, 2, ....... < n_{max} = [\zeta], \quad (51)$$

where we have introduced $\zeta = \frac{1}{4} \sqrt{1 + \frac{8\mu B}{\alpha^2 \hbar^2}} - \frac{1}{4} \sqrt{1 - \frac{8\mu A}{\alpha^2 \hbar^2}} - \frac{1}{2} + \sqrt{\ell(\ell + 1)d_0}$ for mathematical simplicity and $[\zeta]$ means the largest integer inferior to $\zeta$. Secondly, we obtain the vibrational
partition function calculated by

\[ Z(\beta, \zeta) = \sum_{n=0}^{\zeta} e^{-\beta E_n}, \quad \beta = \frac{1}{kT}, \]  

(52)

where \( k \) is the Boltzman constant. Now, the substitution of equation (51) into equation (52) yields:

\[ Z(\beta, \zeta) = e^{-2\alpha^2h^2(\ell+1)\beta d_0} \sum_{n=0}^{\zeta} e^{\frac{(n-\zeta)^2}{\gamma}}, \quad \gamma = \frac{\tau}{\sqrt{\beta}}, \quad \tau = \frac{1}{\alpha h} \sqrt{\frac{\mu}{2}}, \]  

(53)

Since \( e^{-2\alpha^2h^2(\ell+1)\beta d_0} \approx 1 \), the partition function \( Z \) can therefore be written as

\[ Z(\beta, \zeta) = \sum_{n=0}^{\zeta} e^{\frac{(n-\zeta)^2}{\gamma}}. \]  

(54)

In the classical limit, at high temperature \( T \) for large \( \zeta \) and small \( \beta \), the sum can be replaced by the following integral

\[ Z(\beta, \zeta) = \gamma \int_{0}^{\zeta} e^{y^2} dy = \frac{\sqrt{\pi} \tau \text{Erfi}\left(\frac{\zeta \sqrt{\beta}}{2}\right)}{2\sqrt{\beta}}, \quad y = \frac{(n - \zeta)}{\gamma}, \]  

(55)

Having determined the vibrational partition function, we can easily obtain the thermodynamic properties for the system as follows:

1. The vibrational mean energy \( U \)

\[ U(\beta, \zeta) = \frac{\partial}{\partial \beta} \ln Z(\beta, \zeta) = \frac{1}{2\beta} \left[ 1 - \frac{\chi}{\text{DawsonF}(\chi)} \right] \]

\[ = \frac{2\chi}{\sqrt{\pi} \text{Erfi}(\chi)} \left[ \frac{e^{\chi^2}}{2\beta} - \frac{\sqrt{\pi} \text{Erfi}(\chi)}{4\beta^2} \right], \quad \chi = \chi(\beta, \zeta) = \frac{\zeta}{\tau} \sqrt{\beta}, \]  

(56)

which implies that \( U(\beta, \zeta) = -\zeta^2/(3\tau^2) \) when \( \beta << 1 \).

2. The vibrational specific heat \( C \)

\[ C(\beta, \zeta) = \frac{\partial}{\partial T} U(\beta, \zeta) = -k\beta^2 \frac{\partial}{\partial \beta} U(\beta, \zeta) \]

\[ = \frac{1}{2} k \left[ 1 - \frac{\chi \left[ 2\chi e^{\chi^2} + \sqrt{\pi} (1 - 2\chi^2) \text{Erfi}(\chi) \right]}{4e^{\chi^4} \text{DawsonF}(\chi)^2} \right] \]  

(57)

which yields \( C(\beta, \zeta) = 0 \) when \( \beta << 1 \).

3. The vibrational mean free energy \( F \). It can be calculated as

\[ F(\beta, \zeta) = -kT \ln Z(\beta, \zeta) = -\frac{1}{\beta} \ln \left( \frac{\sqrt{\pi} \tau \text{Erfi}(\chi)}{2\sqrt{\beta}} \right) \]  

(58)
4. The vibrational entropy $S$

$$S(\beta, \zeta) = k_1 n Z(\beta, \zeta) + k T \frac{\partial}{\partial T} \ln Z_{\text{vib}}(\beta, \zeta)$$

$$= k_1 n Z(\beta, \zeta) - k_2 \frac{\partial}{\partial \beta} \ln Z(\beta, \zeta)$$

$$= \frac{1}{2} k \left[ 1 - \frac{\chi}{\text{DawsonF}(\zeta)} + 2 \log \left( \frac{\tau \text{Erfi}(\chi)}{\sqrt{\beta}} \right) + \log \left( \frac{\pi}{4} \right) \right].$$  (59)

Here, in this section, we have obtained the thermodynamics properties in terms of two mathematical functions namely: the Dawson function and the imaginary error function. In mathematics, the Dawson function or Dawson integral (named for John M. Dawson) can be denoted as

$$F(x) = e^{-x^2} \int_0^x e^{y^2} dy = \frac{\sqrt{\pi}}{2} e^{-x^2} \text{erfi}(x).$$  (60)

Thus the Dawson’s integral is implemented in Mathematica as `DawsonF[x]`. On the other hand, the imaginary error function is an entire function defined by

$$\text{erfi}(x) = i \text{erf}(ix),$$  (61)

where $\text{erf}$ denotes the error function (also called the Gauss error function) is a special function (non-elementary) of sigmoid shape which occurs in probability, statistics and partial differential equations. In mathematics, the error function can be denoted as

$$\text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt.$$  (62)

The imaginary error function is implemented in Mathematica as `Erfi[x]`.

6 Numerical Results

The experimental data of $\mu$ (in amu) and $\alpha$ (in $\text{Å}^{-1}$) are taken from the recent literature [63] as inputs in expression (17) to calculate the energy states $E_{n\ell}$ (in eV) of 12 molecules; namely, $I_2$, $CO$, $TiH$, $TiC$, $N_2$, $NO$, $CrH$, $NiC$, $O_2$, $LiH$, $VH$, and $ScN$ for different values of the vibrational $n$ and rotational $\ell$ quantum numbers. The experimental data are presented in Table 1. The calculated energy values are listed Table 2 shows that the PT potential is suitable to describe the diatomic molecules. We selected quantum no $n = 0, n = 5, n = 7$ so as to cover wide energy spectrum in order to see the behavior of energy for large states.

In Figure 1 we plot the variation of the vibrational energy levels with the potential parameter $\alpha$ for $ns$ states, where $n = 1, 2, 3, 4$. The energy is purely attractive (negative). It is found that energy is increasing in the positive direction with increasing $n$ when $\alpha < 0.1$. However, when $\alpha > 0.1$, the energy is sharply changing toward the negative direction with the increasing of
energy state \( n \), i.e., it becomes strongly attractive. For given \( \zeta \) and unit of \( \tau \), the dependence of the vibrational partition function \( Z \) on \( \beta \) and \( \zeta \) are shown for 4 diatomic molecules; namely, \( N_2 \), \( TiH \), \( NiC \) and \( I_2 \), in Figures 2 and 3, respectively. It is found that the \( Z \) increases monotonically as \( \beta \) and \( \zeta \) increase for the first three molecules and linearly increases for the \( I_2 \) molecule. This means that \( I_2 \) is not sensitive to the various values \( \zeta \) and \( \beta \) in Figures 2 and 3, respectively. It is shown in Figures 4 and 5 that the vibrational mean energy \( U \) decrease monotonically with the increasing parameters \( \beta \) and \( \zeta \), respectively. The vibrational specific heat \( C \) \(( k = 1 \)\) first increases with the increasing \( \beta \) and \( \zeta \) to the maximum value and then decreases with it as shown in Figures 6 and 7. In the \( I_2 \) molecule, \( C \) increases monotonically for wide range of \( \beta \). The vibrational free energy \( F \) increases and then decreases with the increasing parameter \( \beta \) in long (short) range for small (large) values of \( \zeta \) as shown in Figure 8. On the other hand, \( F \) decreases with the increasing \( \zeta \) for various values of \( \beta \) and overlapping at a specific value of \( \zeta \) as shown in Figure 9. It is shown in Figure 10 that the entropy \( S(k = 1) \) decreases with the parameter \( \beta \) for various values of \( \zeta \) and overlapping at some specific value \( \beta \) in the range. On the other hand, \( S \) first increases with the \( \zeta \) to the maximum value and then decreases with it as shown in Figure 11. The curves for different \( \beta \) are splitting away from each others at higher values of \( \zeta \).

7 Conclusion

In this work, we have solved the Schrodinger equation for the PT potential in the framework of AIM by considering an approximation to deal with the centrifugal term and obtained the energy eigenvalues and the wave functions. The method is also used to obtain approximate energy states and wave functions of the spin-1/2 particle in the field of PT potential and Coulomb-like coupling interaction under spin and p-spin symmetries. Some special cases of interest of the present solution are obtained as the \( s \) wave case, reflectionless-type potential, symmetric hyperbolic PT potential and the nonrelativistic solution. Further, the nonrelativistic ro-vibrational energy levels of 12 diatomic molecules are obtained using a set parameter values in Table 1 for each molecule. Our results are displayed in Table 2. We plotted the variation of vibrational energy levels with the potential parameter \( \alpha \) in Figure 1. On the other hand, we have derived the vibrational partition function \( Z \) and then calculated the thermodynamic parameters like the vibrational mean energy \( U \), specific heat \( C \), free energy \( F \) and the entropy \( S \). The variations of these thermodynamic parameters with \( \beta \) and \( \zeta \) are shown in Figures 2-11 for 4 diatomic molecules in presence of PT potential field. The behaviour of the thermodynamic properties changes from one diatomic molecule to another.

Acknowledgements
S. M. Ikhdair thanks the partial support provided by the Scientific and Technical Research Council of Turkey (TUBITAK).

References

[1] D. ter Haar, Problems in Quantum Mechanics, 3rd edition (Pion Ltd, London, 1975).

[2] H. Hassanabad, E. Maghsoodi, S. Zarrinkamar and H. Rahimov, Adv. High Energy Phys. 2012 (2012) 707041.

[3] S. M. Ikhdair and M. Hamzavi, Z. Naturforsch. 68a (2013) 279.
   M. Hamzavi, S. M. Ikhdair and K. -E. Thylwe, Z. Naturforsch. 67a (2012) 567.

[4] O. J. Oluwadare, K. J. Oyewumi, C. O. Akoshile and O. A. Babalola, Phys. Scr. 86 (2012) 035002.

[5] K. J. Oyewumi and C. O. Akoshile, Eur. Phys. J. A 45 (2010) 311.

[6] S. M. Ikhdair, M. Hamzavi and A. A. Rajabi, Int. J. Mod. Phys. E. 22 (2013) 1350015.

[7] H. Ciftci, R. L. Hall and N. Saad, J. Phys. A: Math Gen. 36 (2003) 11807.

[8] H. Ciftci, R. L. Hall and N. Saad, Phys. Lett. A: 340 (2005) 388.

[9] A. F. Nikiforov and V. B. Uvarov, Special Functions of Mathematical physics (Basle, Birkhauser, 1988).

[10] O. Aydogdu, E. Maghsoodi and H. Hassanabadi, Chin. Phys. B 22 (2013) 010302.

[11] S. M. Ikhdair, Int. J. Mod. Phys. C 20 (2009) 1563.

[12] H. Hassanabad, E. Maghsoodi, S. Zarrinkamar and H. Rahimov, Chin. Phys. B 21 (2012) 120302.

[13] F. Cooper, A. Khare and U. Sukhatme, Phys. Rep. 251 (1995) 267.

[14] H. Hassanabadi, L. L. Lu, S. Zarrinkamar, G. Liu and H. Rahimov Acta Pol. A 122 (2012) 650.

[15] E. Maghsoodi, H. Hassanabadi and O. Aydogdu, Phys. Scr. 86 (2012) 015005

[16] L. Infeld and T. E. Hull, Rev. Mod. Phys. 23 (1951) 21.

[17] S. H. Dong, Factorizaion Method in Quantum Mechanics, (Springer, Amsterdam, 2007).
[18] Z. Q. Ma and B. W. Xu, Europhys. Lett. 69 (2005) 685.

[19] Z. Q. Ma and B. W. Xu, Acta Phys. Sin. 55 (2006) 1571 (in Chinese).

[20] W. C. Qiang and S. H. Dong, Europhys. Lett. 89 (2010) 10003.

[21] S. M. Ikhdair and R. Sever, J. Math. Chem. 45 (2009) 1137.

[22] A. Comtet, A. Bandrauk and D. Compbell, Phys. Lett. B 150 (1985) 159.

[23] R E. Bellman and R. E. Kalaba, Quasilinearization and Nonlinear Boundary Value Problems (elsevier, New York, 1965).

[24] E. Z. Leverts and V. B. Mandelzweig, Ann. Phys. (N. Y.) 324 (2009) 388 and references therein.

[25] S. Odake and R. Sasaki, J. Phys. A: Math. Theor. 44 (2011) 195203.

[26] Y. Xu, S. He and C. -S. Jia, Phys. Scr. 81 (2010) 045001.

[27] G. Wei and S.-H. Dong, Eur. Phys. J. A 43 (2010) 185.

[28] T. Chen, Y. Diao and C. -S. Jia, Phys. Scr. 79 (2009) 065014.

[29] G. Wei and S. -H. Dong, Phys. Lett. A 373 (2009) 2428.

[30] C. -S. Jia, T. Chen and L. Cui, Phys. Lett. A 373 (2009) 1621.

[31] Z. -Y. Chen, M. Li and C. -S. Jia, Mod. Phys. Lett. A 23 (2009) 1863.

[32] S. -H. Dong, W. Qiang and J. Garcia-Ravelo, Int. J. Mod. Phys. A 23 (2008) 1537.

[33] O. Yesiltas, Phys. Scr. 75 (2007) 41.

[34] H. Hassanaabadi, H. B.Yazarloo and L. L. Lu, Chin. Phys. Lett. 29 (2012) 020303.

[35] H. Hassanaabadi, E. Maghsoodi, S. Zarrinkamar and H. Rhimov, J. Math. Phys. 53 (2012) 022104.

[36] S. M. Ikhdair, Eur. Phys. J. A 39 (2009) 307.

[37] Y. Hasan and M. Tomak, Phys. Rev. B 72 (2005) 115340.

[38] A. Rodriuez and J. Cervero, Phys. Rev. B 74 (2006) 104201.
[39] H. Yildirim and M. Tomak, J. Appl. Phys. 99 (2006) 093103.

[40] W. Xie, Commun. Theor. Phys. 46 (2006) 1101.

[41] J. Radovanovic et al., Phys. Lett. A 269 (2000) 179.

[42] M. Mora Ramos, M. Barseghyan and C. A. Duque, Physica E 43 (2010) 338.

[43] B. J. Falaye, Cent. Eur. J. Phys. 10 (2012) 960.

[44] B. J. Falaye, Few Body Sys 53 (2012) 557.

[45] B. J. Falaye, Few Body Sys 53 (2012) 563.

[46] B. J. Falaye, J. Math. Phys. 53 (2012) 082107.

[47] O. Bayrak and I. Boztosun, Phys. Scr. 76 (2007) 92.

[48] O. Bayrak, I. Boztosun and H. Ciftci, Int. J. Quantum Chem. 107 (2007) 540.

[49] S. H. Dong, M. Lozada-Casson, J. Yu, F. Jimenez-Angles and A. L. Rivera, Int. J. Quant. Chem. 107 (2007) 366.

[50] C. S. Jia, P. Guo, Y. F. Diao, L. Z. Yi, and X. J. Xie, Eur. Phys. J. A 34 (2007) 41.

[51] X. C. Zhang, Q.W. Liu, C.S. Jia, L.Z. Wang, Phys. Lett. A 340 (2005) 59.

[52] C. S Jia, Y. Li, Y. Sunb, J. Y. Liu and L. T. Sun, Phys. Lett. A 311 (2003) 115.

[53] S. M. Ikhdair, J. Math. Phys. 52 (2011) 052303.

[54] S. M. Ikhdair, Cent. Eur. J. Phys. 10 (2012) 361.

[55] S. M. Ikhdair and R. Sever, J. Phys. A: Math. Theor. 44 (2011) 355301.

[56] M. Hamzavi and S. M. Ikhdair, Mol. Phys. 110 (2012) 3031.

[57] C. Berkdemir and Y. -F. Cheng, Phys. Scr. 79 (2009) 035003.

[58] S. M. Ikhdair and R. Sever, J. Math. Phys. 52 (2011) 122108.

[59] K. J. Oyewumi, T. T. Ibrahim, S. O. Ajibola and D A Ajadi JVR 5 (2010)19.

[60] X. Q. Zhao, C. S. Jia, and Q. B. Yang, Phys. Lett. A 337 (2005) 189.
[61] H. Sun, Phys. Lett. A 374 (2009) 116.
    H. Sun, Bull. Korean Chem. Soc. 31 (2010) 3573.
    A. de Souza Dutra and G. Chen, Phys. Lett. A 349 (2006) 297.
    A. S. de Castro, Phys. Lett. A 338 (2005) 81.
    R. L. Hall, Phys. Lett. A 372 (2007) 12.
    R. L. Hall and W. Lucha, Phys. Lett. A 374 (2010) 1980.
    S. M. Ikhdair and R. Sever, J. Math. Chem. 42 (2007) 461.
    S. M. Ikhdair and R. Sever, Ann. Phys. (Leibzig) 16 (2007) 218.
    S. M. Ikhdair and R. Sever, Int. J. Mod. Phys. C 19 (2008) 221.
    S. M. Ikhdair, Chin. J. Phys. 46 (2008) 291.
    S. M. Ikhdair and R. Sever, Cent. Eur. J. Phys. 6 (2008) 141.

[62] M. Abramowitz and I. A. Askey (Eds.) Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables, 9th printing. New York: Dover, pp. 295 and 297, 1972.

[63] K. J. Oyewumi, and K. D. Sen, J. Math. Chem. 50 (2012) 1059.

Table 1: Model parameters for a few diatomic molecules.

| Molecules | $\mu$ (in amu) | $\alpha$ (in Å$^{-1}$) |
|-----------|----------------|----------------------|
| $I_2$     | 6.345225620    | 1.36440              |
| $CO$      | 6.860586600    | 2.29940              |
| $TiH$     | 0.987371000    | 1.32468              |
| $TiC$     | 9.000679600    | 1.52550              |
| $N_2$     | 7.003356600    | 2.69860              |
| $NO$      | 7.484418000    | 2.75340              |
| $CrH$     | 0.988976600    | 1.52179              |
| $NiC$     | 9.974265600    | 2.25297              |
| $O_2$     | 7.997457040    | 2.81510              |
| $LiH$     | 0.880122100    | 1.12600              |
| $VH$      | 0.988005900    | 1.44370              |
| $SiN$     | 10.68277100    | 1.50680              |
Table 2: Energy spectra $E_{n\ell}$ (in eV) of 12 diatomic molecules for any arbitrary choices of $n$ and $\ell$ quantum numbers with $\hbar c = 1973.29eV\cdot\AA$, $A = -2$ and $B = 3$.  

| n | $\ell$ | $I_2$ | CO | TiH | TiC | $N_2$ | NO |
|---|---|---|---|---|---|---|---|
| 0 | 0 | -2.0161700249 | -2.0575615376 | -2.08801628475 | -2.03207234893 | -2.06701616738 | -2.06628076793 |
| 5 | -1.86617831309 | -1.52226413799 | -1.30060734002 | -1.72400386632 | -1.4511793674 | -1.45722010494 |
| 10 | -1.72206229469 | -1.08736269276 | -0.6970620992 | -1.4412459707 | -0.94397059248 | -0.95429245499 |
| 5 | -2.33037239432 | -3.36982420049 | -4.21935759111 | -2.72413935420 | -3.62461728776 | -3.60342077313 |
| 10 | -2.1699136299 | -2.67343449186 | -3.06093305312 | -2.36545044489 | -2.79149784389 | -2.7812426402 |
| 7 | -2.0151700249 | -2.0575615376 | -2.08801628475 | -2.03207234893 | -2.06701616738 | -2.06628076793 |
| 5 | -2.46285504258 | -3.98490713462 | -5.27966285506 | -3.02931337126 | -4.3693328865 | -4.33554810662 |
| 10 | -2.2978377436 | -3.22410506241 | -3.97283205546 | -2.65037685127 | -3.44930217618 | -3.42961923507 |
| 7 | -2.1365147714 | -2.5481894467 | -2.8510969660 | -2.29673034463 | -2.6379095888 | -2.6297431655 |

Figure 1: The variation of the energy eigenvalues as a function of potential parameter $\alpha$. 

18
Figure 2: Vibrational partition function $Z$ of $N_2$, $TiH$, $NiC$ and $I_2$ diatomic molecules as a function of $\beta$ for different $\zeta$. 
Figure 3: Vibrational partition function $Z$ of $N_2$, $TiH$, $NiC$ and $I_2$ diatomic molecules as a function of $\zeta$ for different $\beta$.

Figure 4: Vibrational mean energy $U$ of $N_2$, $TiH$, $NiC$ and $I_2$ diatomic molecules as a function of $\beta$ for different $\zeta$. 
Figure 5: Vibrational mean energy $U$ of $N_2$, $TiH$, $NiC$ and $I_2$ diatomic molecules as a function of $\zeta$ for different $\beta$.

Figure 6: Vibrational specific heat $C$ of $N_2$, $TiH$, $NiC$ and $I_2$ diatomic molecules as a function of $\beta$ for different $\zeta$. 
Figure 7: Vibrational specific heat $C$ of $N_2$, TiH, NiC and $I_2$ diatomic molecules as a function of $\zeta$ for different $\beta$.

Figure 8: Vibrational free energy $F$ of $N_2$, TiH, NiC and $I_2$ diatomic molecules as a function of $\beta$ for different $\zeta$. 
Figure 9: Vibrational free energy $F$ of $N_2$, $TiH$, $NiC$ and $I_2$ diatomic molecules as a function of $\zeta$ for different $\beta$.

Figure 10: Vibrational mean energy $S$ of $N_2$, $TiH$, $NiC$ and $I_2$ diatomic molecules as a function of $\beta$ for different $\lambda$. 

23
Figure 11: Vibrational free energy $S$ of $N_2$, $TiH$, $NiC$ and $I_2$ diatomic molecules as a function of $\zeta$ for different $\beta$. 