

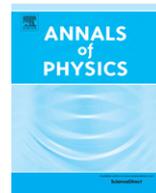


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Nonrelativistic molecular models under external magnetic and AB flux fields

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ABSTRACT

By using the wave function ansatz method, we study the energy eigenvalues and wave function for any arbitrary m -state in two-dimensional Schrödinger wave equation with various power interaction potentials in constant magnetic and Aharonov–Bohm (AB) flux fields perpendicular to the plane where the interacting particles are confined. We calculate the energy levels of some diatomic molecules in the presence and absence of external magnetic and AB flux fields using different potential models. We found that the effect of the Aharonov–Bohm field is much as it creates a wider shift for $m \neq 0$ and its influence on $m = 0$ states is found to be greater than that of the magnetic field. To show the accuracy of the present model, a comparison is made with those ones obtained in the absence of external fields. An extension to 3-dimensional quantum system have also been presented.

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1. Introduction

It is commonly known that the anharmonic and harmonic oscillator potentials play an important role in the history of molecular and quantum chemistry and have also been used to describe the

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molecular structure and molecules [1,2]. Also, the Kratzer-type potential describing the molecular vibrations is important in studying the dynamical variables of diatomic molecules [3]. This potential have a wide applications in various fields of physics and chemistry such as molecular physics, solid-state physics, chemical physics, quantum chemistry, the molecular dynamics study of linear diatomic molecules and the theoretical works on the spectral properties of a diatomic molecule system [4]. Therefore, we found that it is necessary to study the exact bound state solutions of the two-dimensional (2D) solution of the Schrödinger equation for these potentials under the influence of external magnetic and Aharonov–Bohm fields.

The 2D hydrogen model was treated as an atomic spectroscopy and used as a simplified model of the ionization process of the highly excited 3D hydrogen atom by circular-polarized microwaves [5]. The field-free relativistic Coulomb interaction has been studied by many authors by using various techniques [6–8]. The nonrelativistic H-like atom under the influence of magnetic field has been the subject of study over the past years [9–11]. In the presence of a low magnetic field, the quasi-classical solution of the Dirac equation has been obtained by factorization method [12]. In the framework of the variational method, the ground-state Dirac energies and relativistic spinless lowest few states have been calculated for arbitrary strength values of magnetic field [13,14]. The Klein–Gordon wave equation was solved exactly for particular values of magnetic field in which the wave function can be expressed in closed analytical form [15]. The polynomial solutions of the Schrödinger equation was obtained for the ground-state and a few first excited states of 2D hydrogenic atoms for particular values of the magnetic field strength perpendicular to the plane of transversal motion of the electron using a relativistic wave function [16]. Recently, within the framework of power-series solutions, the Klein–Gordon and Dirac equations have been solved for the 2D hydrogen-like systems when an arbitrary external magnetic field is applied [17]. For particular values of magnetic field B , it is found that the exact polynomial solutions can be found using the well-known methods in literature [15,18–22].

Recently, the spectral properties in a 2D charged particle (electron or hole) confined by a PHO potential in the presence of external strong uniform magnetic field \vec{B} along the z direction and Aharonov–Bohm (AB) flux field created by a solenoid have been studied. The Schrödinger equation is solved exactly for its bound states (energy spectrum and wave functions) [23,24]. So, it is natural that the relativistic effects for a charged particle under the action of this potential could become important, especially for a strong coupling. Within this annals, we have also studied the exact analytical bound state energy eigenvalues and normalized wave functions of the spinless relativistic equation with equal scalar and vector pseudo-harmonic interaction under the effect of external uniform magnetic field and AB flux field in the framework of the NU method [25]. Robnik and Romanovsky [26] studied the Schrödinger equation of the hydrogen atom in a strong magnetic field in 2D. Setare and Hatami [27] considered the exact solutions of the Dirac equation for an electron in a magnetic field with shape invariant method. Villalba [28] analyzed the relativistic Dirac electron in the presence of a combination of a Coulomb field, a $1/r$ scalar potential as well as the Dirac magnetic monopole and an Aharonov–Bohm potential using the algebraic method of separation of variables. Schmid-Burrgh and Gail [29] solved the stationary Dirac equation for an electron embedded in a uniform magnetic field and in an electrostatic potential periodic along the field lines. The eigenvalues and width of the lowest band gap are calculated. Kościk and Okopińska have studied quasi exact solutions for two interacting electrons via Coulombic force and confined in an anisotropic harmonic oscillator in 2D anisotropic dot [30]. An ansatz for wave function has been applied to obtain the D -dimensional solutions of radial Schrödinger equation with some anharmonic potentials [31].

Recently, the 2D solution of the Schrödinger equation for the Kratzer potential with and without the presence of a constant magnetic field has been studied for the first time within the framework of the asymptotic iteration method (AIM) [32]. Effect of constant magnetic field on the energy eigenvalues of a particle moving under the Kratzer potential was precisely presented by Aygun et al. [32]. Furthermore, we have studied the spectral properties of the quantum dots by solving the Schrödinger equation for the anharmonic oscillator potential and superposition of pseudoharmonic-linear-Coulomb potential in presence/absence of external uniform magnetic and AB flux fields in the framework of the Nikiforov–Uvarov (NU) method and analytical exact iteration method (AEIM) [33]. Also, we have studied the effect of these external fields on the energy states and wave functions of a

spinless particle with the Cornell (linear-plus-Coulomb) and Killingbeck (Cornell-plus-harmonic oscillator) potentials, respectively [34]. Very recently, we solved the Dirac equation for the anharmonic oscillator potential under the influence of the external magnetic and AB flux fields and obtained the relativistic energy states [35]. The two-dimensional solution of the spinless Klein–Gordon (KG) equation for scalar–vector harmonic oscillator potentials with and without the presence of constant perpendicular magnetic and Aharonov–Bohm (AB) flux fields has been studied within the asymptotic function analysis and NU method [36] and via Laplace transform method [37].

The aim of this work is to extend the works in [33–35] and solve the Schrödinger equation for a general form of potential models in the presence of external magnetic and AB flux fields. This work can be considered as a unified treatment in studying some molecular potentials which find their direct application in molecular physics and chemistry like the diatomic molecules. By using the quasi-exact solutions, we carry out detailed exact 2D and 3D energetic spectrum and wave functions of the Schrödinger equation with a general form of potential models including the well-known molecular interactions in the presence of two external magnetic and Aharonov–Bohm (AB) flux fields. For example, our investigation includes several molecular potentials used to study diatomic molecules such as the pseudo-harmonic interaction, harmonic oscillator, the generalized Kratzer potential, modified Kratzer potential and Mie-type potential.

The outline of our paper is as follows. In Section 2, we give the quasi exact solutions of the 2D Schrödinger equation with a general scalar radial potential form $V(r)$ and vector potential \vec{A} under the influence of external magnetic and AB flux fields. In Section 3, the calculations within the quasi exact solution are obtained for various molecular potentials to obtain the closed analytical energy spectrum and wave functions under external fields and the comparison with exact results is given when fields become zero. Finally, the paper ends with concluding remarks in Section 4.

2. Exact solution to a general potential form under external fields

Consider a 2D charged particles with charge e and effective mass μ interacting via a radially symmetrical interaction potential $V(r, \phi)$ under the influence of external uniform magnetic field, $\vec{B} = B\hat{z}$ and an AB flux field, applied simultaneously. Since we are taking the Hamiltonian in 2D, its adequate to study the system in polar coordinates (r, ϕ) within the plane. Hence, the Schrödinger equation with a vector potential \vec{A} and repulsive interaction potential $V(r, \phi)$ can be written as

$$\left[\frac{1}{2\mu} \left(\vec{p} + \frac{e}{c} \vec{A} \right)^2 + V(r) \right] \psi(r, \phi) = E\psi(r, \phi), \quad (1)$$

with the 2D cylindrical wave function

$$\psi(r, \phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi} u(r), \quad m = 0, \pm 1, \pm 2, \dots, \quad (2)$$

and m is the magnetic quantum number (the eigenvalue of angular momentum). For the solution of Eq. (1), we take the potential $V(r, \phi)$ as radial scalar power form [22,23]

$$V(r) = ar^2 + br + d - \frac{g}{r} + \frac{k}{r^2}, \quad (3)$$

and the vector potential \vec{A} may be represented as a sum of two terms, $\vec{A} = \vec{A}_1 + \vec{A}_2$ such that $\vec{\nabla} \times \vec{A}_1 = \vec{B}$ and $\vec{\nabla} \times \vec{A}_2 = 0$, where $\vec{B} = B\hat{z}$ is the applied magnetic field, and \vec{A}_2 describes the additional magnetic flux Φ_{AB} created by a solenoid. Hence, the vector potentials in the symmetric gauge have the following azimuthal components [24]

$$\vec{A}_1 = \frac{1}{2} \vec{B} \times \vec{r} = \frac{Br}{2} \hat{\phi}, \quad \vec{A}_2 = \frac{\Phi_{AB}}{2\pi r} \hat{\phi}, \quad \vec{A} = \left(\frac{Br}{2} + \frac{\Phi_{AB}}{2\pi r} \right) \hat{\phi}. \quad (4)$$

Substituting the wave function (2) into the Schrödinger equation (1), we obtain a second-order differential equation satisfying the radial part of the wave function; namely $u(r)$,

$$\frac{d^2 u(r)}{dr^2} + \frac{1}{r} \frac{du(r)}{dr} + \left(-\varepsilon^2 - \frac{\beta^2}{r^2} - \gamma^2 r^2 + \frac{g'}{r} - b'r \right) u(r) = 0, \quad (5)$$

with

$$-\varepsilon^2 = E' - d' - \frac{\mu\omega_c}{\hbar} m', \quad (6a)$$

$$\beta^2 = k' + m'^2, \quad (6b)$$

$$\gamma^2 = a' + \left(\frac{\mu\omega_c}{2\hbar} \right)^2, \quad (6c)$$

$$g' = \frac{2\mu}{\hbar^2} g, \quad b' = \frac{2\mu}{\hbar^2} b, \quad E' = \frac{2\mu}{\hbar^2} E, \quad d' = \frac{2\mu}{\hbar^2} d, \quad (6d)$$

$$k' = \frac{2\mu}{\hbar^2} k, \quad a' = \frac{2\mu}{\hbar^2} a$$

and

$$\xi = \frac{\Phi_{AB}}{\Phi_0}, \quad \Phi_0 = \frac{hc}{e}, \quad \omega_c = \frac{eB}{\mu c}, \quad m' = m + \xi. \quad (7)$$

Note that ξ is taken as integer with the flux quantum Φ_0 and ω_c is the cyclotron frequency. The magnetic quantum number (the eigenvalue of angular momentum) m relates to the new quantum number $|\beta|$ (Eq. (6b)). For this system, only two independent integer quantum numbers are required. In addition, the radial wave function $u(r)$ must satisfy the asymptotic behaviors, that is, $u(0) \rightarrow 0$ and $u(\infty) \rightarrow 0$. To make the coefficient of the first derivative vanish in Eq. (5), we may define radial wave function $R(r)$ by means of the equation

$$u(r) = r^{-1/2} R(r), \quad (8)$$

which will lead to the radial wave function $R(r)$ satisfying

$$\frac{d^2 R(r)}{dr^2} + \left(-\varepsilon^2 - \gamma^2 r^2 + \frac{g'}{r} - b'r - \frac{(\beta^2 - 1/4)}{r^2} \right) R(r) = 0. \quad (9)$$

To solve the above radial differential equation for $\beta \neq 0$, we first investigate the asymptotic behavior of $R(r)$. First inspection of Eq. (9) shows that when r approaches 0, the asymptotic solution $R_0(r)$ of Eq. (9) satisfies the differential equation

$$\frac{d^2 R_0(r)}{dr^2} - \frac{(\beta^2 - 1/4)}{r^2} R_0(r) = 0, \quad (10)$$

which assumes the solution $R_0(r) = c_1 r^{\beta+1/2} + c_2 r^{-(\beta+1/2)}$, where c_1 and c_2 are two constants. The term $r^{-(\beta+1/2)}$ is not a satisfactory solution because it becomes infinite as $r \rightarrow 0$ but the term $r^{\beta+1/2}$ is well behaved. Meanwhile, as r approaches ∞ , the asymptotic solution $R_\infty(r)$ of Eq. (9) gives the differential equation

$$\frac{d^2 R_\infty(r)}{dr^2} - (b'r + \gamma^2 r^2) R_\infty(r) = 0, \quad (11)$$

which yields the solution $R_\infty(r) = c_3 \exp[g(p, q, r)]$, where $g(b', \gamma^2, r) = -b'r - \gamma^2 r^2$ is an acceptable physical solution since the solution becomes finite as $r \rightarrow \infty$. Consequently, this asymptotic behavior of $R(r)$ suggests we take an ansatz for the radial wave function [31]

$$R(r) = r^{\beta+1/2} \exp[g(p, q, r)] F(r), \quad (12)$$

with

$$g(p, q, r) = qr + \frac{1}{2}pr^2, \quad q < 0, p < 0 \tag{13a}$$

$$F(r) = \sum_{n=0} a_n r^n. \tag{13b}$$

Substituting Eq. (12) into Eq. (9) and equating the coefficients of $r^{n+\beta+1/2}$ to zero, we can obtain the following recurrence relation,

$$A_n a_n + B_{n+1} a_{n+1} + C_{n+2} a_{n+2} = 0, \tag{14}$$

where

$$A_n = -\varepsilon^2 + q^2 + 2p(n + \beta + 1), \tag{15a}$$

$$B_n = g' + q(2n + 2\beta + 1), \tag{15b}$$

$$C_n = n(n + 2\beta), \tag{15c}$$

and

$$p^2 = \gamma^2, \tag{16a}$$

$$2pq = b'. \tag{16b}$$

It is shown from Eq. (16) that the values of the parameters for $g(p, q, r)$ can be evaluated as

$$p = \pm\gamma, \quad q = \frac{b'}{2p}. \tag{17}$$

To retain a well-behaved solution at the origin and at ∞ , we choose $p = -\gamma$ which enables us to write $q = -b'/(2\gamma)$. On the other hand, for a given s , if $a_s \neq 0$ but $a_{s+1} = a_{s+2} = a_{s+3} = \dots = 0$, where s is the degree of polynomial ($s = 0, 1, 2, \dots$), we then impose the condition $A_s = 0$ from Eq. (14), i.e., from which we can obtain the eigenvalue equation

$$\varepsilon^2 = q^2 + 2p(s + \beta + 1), \tag{18}$$

which can establish the relationship between energies, parameters of the potential and the two fields strength B and ξ . Substituting the values of the parameters defined in (6) into (18) and by using p and q obtained from (17) we may rewrite the energy eigenvalues of the power potential as

$$E_{nm'} = d + \frac{1}{2}\hbar m' \omega_c + \frac{\hbar^2}{2\mu} \sqrt{\frac{8\mu a}{\hbar^2} + \left(\frac{\mu \omega_c}{\hbar}\right)^2} \left(s + 1 + \sqrt{\frac{2\mu k}{\hbar^2} + m'^2} \right) - \frac{2\mu b^2 / \hbar^2}{\left[\frac{8\mu a}{\hbar^2} + \left(\frac{\mu \omega_c}{\hbar}\right)^2 \right]}.$$

Following [31,32], the parameters A_n, B_n and C_n must satisfy the determinant relation for a nontrivial solution:

$$\det \begin{vmatrix} B_0 & C_1 & \dots & \dots & \dots & 0 \\ A_0 & B_1 & C_2 & \dots & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & A_{s-1} & B_s \end{vmatrix} = 0. \tag{19}$$

Note that Eq. (19) leads to the restriction for the flux quantum Φ_0 and the cyclotron frequency ω_c if all other parameters of the model are fixed. However, Eq. (18) allows for calculating the energies for these particular Φ_0 and ω_c .

As an example, the exact solution for $s = 0, 1$ is demonstrated below.

(1) For the simplest polynomial solution ($s = 0$), we can obtain from Eq. (18)

$$\varepsilon_0^2 = -2\gamma(\beta + 1) + \frac{\mu^2 b^2}{\hbar^4 \gamma^2}. \tag{20}$$

On the other hand, it is shown from Eq. (19) that $B_0 = 0$, which leads to the following restriction on the parameters of the potential and β :

$$q = -\frac{g'}{(2\beta + 1)}, \quad (21)$$

and the energy formula can be obtained by substituting Eqs. (6b), (6d) and (17) into Eq. (21)

$$b = \frac{\gamma}{\left(\frac{1}{2} + \sqrt{\frac{2\mu}{\hbar^2}k + m^2}\right)} g. \quad (22)$$

The explicit form of the ground state energy is

$$E_0^{(m')} = d + \frac{1}{2}\hbar m' \omega_c + \frac{\hbar^2}{\mu} \sqrt{\left(\frac{\mu \omega_c}{2\hbar}\right)^2 + \frac{2\mu}{\hbar^2} a} \left(1 + \sqrt{m'^2 + \frac{2\mu}{\hbar^2} k}\right) - \frac{\mu}{2\hbar^2} \frac{b^2}{\left(\frac{2\mu}{\hbar^2} a + \left(\frac{\mu \omega_c}{2\hbar}\right)^2\right)}. \quad (23)$$

The eigenfunction for $s = 0$ can be written as

$$\psi^0(r, \phi) = \frac{1}{\sqrt{2\pi}} a_0 r^{\sqrt{m'^2 + \frac{2\mu}{\hbar^2} k}} \exp\left[-\frac{1}{2} \left(\frac{2\mu b}{\hbar^2 \left(\frac{2\mu}{\hbar^2} a + \left(\frac{\mu \omega_c}{2\hbar}\right)^2\right)^{1/2}} r + \gamma r^2\right)\right] e^{im\phi}, \quad (24)$$

where a_0 is an expansion constant.

(2) When $s = 1$, the eigenvalue from Eq. (18) becomes

$$\varepsilon_1^2 = -2\gamma(\beta + 2) + \frac{\mu^2 b^2}{\hbar^4 \gamma^2},$$

and with the aid of Eq. (6) it reads

$$E_1^{(m')} = d + \frac{1}{2}\hbar m' \omega_c + \frac{\hbar^2}{\mu} \sqrt{\left(\frac{\mu \omega_c}{2\hbar}\right)^2 + \frac{2\mu}{\hbar^2} a} \left(2 + \sqrt{m'^2 + \frac{2\mu}{\hbar^2} k}\right) - \frac{\mu}{2\hbar^2} \frac{b^2}{\left(\frac{2\mu}{\hbar^2} a + \left(\frac{\mu \omega_c}{2\hbar}\right)^2\right)}. \quad (25)$$

Moreover, it is shown from Eq. (19) that $B_0 B_1 - A_0 C_1 = 0$ which provides the restriction on the parameters:

$$\left[g' - \frac{b'}{2\gamma}(2\beta + 1)\right] \left[g' - \frac{b'}{2\gamma}(2\beta + 3)\right] = 2\gamma(2\beta + 1),$$

or alternatively

$$g = \frac{b}{\gamma}(\beta + 1) \pm \frac{\hbar^2}{4\mu} \sqrt{\frac{\mu^2 b^2}{\hbar^4 \gamma^2} + 2\gamma(2\beta + 1)}. \quad (26)$$

The corresponding wave function can be written as

$$\psi^1(r, \phi) = \frac{1}{\sqrt{2\pi}} (a_0 + a_1 r) r^{\sqrt{m^2 + \frac{2\mu}{\hbar^2} k}} \times \exp \left[-\frac{1}{2} \left(\frac{2\mu b}{\hbar^2 \left(\frac{2\mu}{\hbar^2} a + \left(\frac{\mu\omega_c}{2\hbar} \right)^2 \right)^{1/2}} r + \gamma r^2 \right) \right] e^{im\phi}, \tag{27}$$

where a_0 and a_1 are expansion constants.

Following this way, we can obtain a class of exact solutions through taking $s = 0, 1, 2, \dots$ etc. We obtain the energy levels from Eq. (18) with the aid of Eq. (6) as

$$E_{nm'} = d + \frac{1}{2} \hbar m' \omega_c + \frac{\hbar^2}{\mu} \sqrt{\left(\frac{\mu\omega_c}{2\hbar} \right)^2 + \frac{2\mu}{\hbar^2} a} \left(n + 1 + \sqrt{m^2 + \frac{2\mu}{\hbar^2} k} \right) - \frac{\mu}{2\hbar^2} \frac{b^2}{\left(\frac{2\mu}{\hbar^2} a + \left(\frac{\mu\omega_c}{2\hbar} \right)^2 \right)}, \tag{28}$$

and the wave function can be obtained from Eqs. (2), (8), (12) and (13) as

$$\psi(r, \phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi} \exp \left[-\frac{1}{2} \left(\frac{2\mu b}{\hbar^2 \left(\frac{2\mu}{\hbar^2} a + \left(\frac{\mu\omega_c}{2\hbar} \right)^2 \right)^{1/2}} r + \gamma r^2 \right) \right] \times \sum_{n=0} a_n r^{n + \sqrt{m^2 + \frac{2\mu}{\hbar^2} k}}, \tag{29}$$

where a_n ($n = 0, 1, 2, \dots, s$) are expansion constants. We have one set of quantum numbers (n, m, β) for particle. Therefore, expression (24) for the energy levels of the electron may be readily used for studying the thermodynamics properties of quantum structures when the magnetic field turns on or off.

There is a corresponding relationship between 2D and 3D obtained by making a replacement $m = l + 1/2$. Therefore, the bound state energy levels and wave function in 3D have the new forms:

$$E_{nl} = d + \frac{\hbar^2}{\mu} \sqrt{\frac{2\mu}{\hbar^2} a} \left(n + 1 + \sqrt{\left(l + \frac{1}{2} \right)^2 + \frac{2\mu}{\hbar^2} k} \right) - \frac{\mu}{2\hbar^2} \frac{g^2}{\left(n + \frac{1}{2} + \sqrt{\left(l + \frac{1}{2} \right)^2 + \frac{2\mu}{\hbar^2} k} \right)^2}, \tag{30}$$

$$\psi(r, \theta, \phi) = \exp \left[-\frac{1}{2} \left(\frac{2\mu g}{\left(n + \frac{1}{2} + \sqrt{\left(l + \frac{1}{2} \right)^2 + \frac{2\mu}{\hbar^2} k} \right) \hbar^2} r + \gamma r^2 \right) \right] \times \sum_{n=0} a_n r^{n + \sqrt{\left(l + \frac{1}{2} \right)^2 + \frac{2\mu}{\hbar^2} k}} Y_{lm}(\theta, \phi), \tag{31}$$

respectively, where $Y_{lm}(\theta, \phi)$ is the spherical harmonic function with angular momentum quantum numbers being l and m .

3. Applications

The structure of molecules is more complex than atoms, however, we may assume that the ratio of the molecular mass to electron mass to be large, which implies that the energy associated with the motion of the nuclei is much smaller than that associated with the motion of the electrons around the nuclei. Hence, this simplification is the basis of all molecular approximations. It is a good approximation to assume the nuclei to have stable equilibrium arrangement between collapsed structure and dispersed structure while studying the electronic motion. This nuclear structure can be divided into translations and rotations of the quasi-rigid equilibrium arrangement and internal vibrations of the nuclei about equilibrium, the translational motion does not give rise to non-classical features. Thus, the molecular energy levels and wave functions are classified into electronic, vibrational and rotational types [38].

The nuclei in diatomic molecules in general have masses m_1 and m_2 and their relative position vector \vec{r} and cylindrical coordinates r, ϕ, z or spherical coordinates r, θ, ϕ .

We apply our results obtained in the previous section to a class of molecular potentials which includes the pseudo-harmonic interaction, the harmonic oscillator, the generalized Kratzer potential, the modified Kratzer potential and the Mie-type potential. Such potentials are reasonably behaved for both small and large internuclear separations. This set of potential models provides a reasonable description of the rotating diatomic molecules and also will be useful in discussing long amplitude vibrations in large molecules. We will find the energy levels and wave functions of a rotating diatomic molecules in 2D space when applying the magnetic field and also 3D space without magnetic field.

3.1. The pseudoharmonic oscillator

The pseudoharmonic oscillator is an important model not only in classical physics, but also in quantum physics. In non-relativistic quantum mechanics, many authors have adequately studied the problem of the pseudoharmonic oscillator [35,38–40]. It has been studied in 3D [35] using the polynomial solution method, in 2D [40] using the Nikiforov–Uvarov method and in D -dimensions [20] using an ansatz for the wave function. It has the following form [39–42]

$$V(r) = D_e \left(\frac{r}{r_e} - \frac{r_e}{r} \right)^2, \quad (32)$$

which can be simply rewritten in the form of isotropic harmonic oscillator plus square inverse potential

$$V(r) = ar^2 + \frac{k}{r^2} + d, \quad a, k > 0, \quad (33)$$

where $a = D_e r_e^{-2}$, $k = D_e r_e^2$ and $d = -2D_e$. Therefore, the energy formula and wave function from (28) and (29) become

$$E_{nm'} = -2D_e + \hbar\Omega \left(n + \frac{|\beta| + 1}{2} \right) + \frac{1}{2} \hbar m' \omega_c, \quad \Omega = \sqrt{\omega_c^2 + 4\omega_D^2}, \quad (34)$$

$$\psi(r, \phi) = \frac{1}{\sqrt{2\pi}} e^{im'\phi} \exp \left[-\frac{1}{2} \sqrt{\left(\frac{\mu\omega_c}{2\hbar} \right)^2 + \frac{2\mu D_e}{\hbar^2 r_e^2}} r^2 \right] \sum_{n=0} a_n r^{2n + \sqrt{m'^2 + \frac{2\mu D_e r_e^2}{\hbar^2}}}, \quad (35)$$

where $|\beta| = \sqrt{m'^2 + \frac{2\mu D_e r_e^2}{\hbar^2}}$ and $\omega_D = \sqrt{2D_e/\mu r_e^2}$. This is identical to Refs. [23,25,42] for the nonrelativistic pseudo-harmonic in an external uniform magnetic and AB flux fields. Further, in the absence

Table 1

The rovibrational energy levels of the harmonic oscillator for NO, CO, N₂ and CH diatomic molecules with various vibrational n and rotational l quantum states for $D = 3$.

n	l	$E_{nl}^{(\text{NO})}$ (eV)	Ref. [39]	$E_{nl}^{(\text{CO})}$ (eV)	Ref. [39]	$E_{nl}^{(\text{N}_2)}$ (eV)	Ref. [39]	$E_{nl}^{(\text{CH})}$ (eV)	Ref. [39]
0	0	0.08251026	0.0824883	0.10195779	0.1019306	0.10918501	0.1091559	0.16867933	0.1686344
1	0	0.24742511	0.2473592	0.30575368	0.3056722	0.32743034	0.3273430	0.50514181	0.5050072
1	1	0.24784775	0.2477817	0.30623238	0.3061508	0.32792905	0.3278417	0.50872564	0.5085903
2	0	0.41233997	0.4122301	0.50954957	0.5094137	0.54567566	0.5455302	0.84160429	0.8413800
2	1	0.41276261	0.4126526	0.51002827	0.5098923	0.54617437	0.5460288	0.84518812	0.8449631
2	2	0.41360783	0.4134977	0.51098564	0.5108495	0.54717177	0.5470260	0.85235089	0.8521246
3	0	0.57725482		0.71334546		0.76392098		1.17806677	
3	1	0.57767747		0.71382416		0.76441969		1.18165060	
3	2	0.57852269		0.71478153		0.76541710		1.18881337	
3	3	0.57979045		0.71621750		0.76691313		1.19954539	
4	0	0.74216968	0.7419718	0.91714135	0.9168969	0.98216631	0.9819045	1.51452925	1.5141255
4	1	0.74259232	0.7423944	0.91762005	0.9173755	0.98266502	0.9824031	1.51811307	1.5177087
4	2	0.74343754	0.7432395	0.91857742	0.9183327	0.98366242	0.9834003	1.52527585	1.5248701
4	3	0.74470531	0.7445070	0.92001339	0.9197684	0.98515845	0.9848961	1.53600786	1.5356002
4	4	0.74639552	0.7461969	0.92192787	0.9216825	0.98715302	0.9868903	1.55029463	1.5498843
5	0	0.90708453	0.9068427	1.12093724	1.1206384	1.20041163	1.2000916	1.85099173	1.8504983
5	1	0.90750718	0.9072653	1.12141594	1.1211170	1.20091034	1.2005902	1.85457555	1.8540615
5	2	0.90835240	0.9081104	1.12237331	1.1220742	1.20190774	1.2015875	1.86173833	1.8612429
5	3	0.90962017	0.9093779	1.12380928	1.1235099	1.20340377	1.2030832	1.87247034	1.8719729
5	4	0.91131038	0.9110678	1.12572376	1.1254240	1.20539834	1.2050774	1.88675711	1.8862571
5	5	0.91342289	0.9131799	1.12811660	1.1278165	1.20789131	1.2075699	1.90457946	1.9040761

of the external fields, i.e., $B = \Phi_{AB} = 0$, we further obtain,

$$E_{nm} = -2D_e + \frac{\hbar}{r_e} \sqrt{\frac{2D_e}{\mu}} \left(2n + 1 + \sqrt{m^2 + \frac{2\mu D_e r_e^2}{\hbar^2}} \right), \quad (36)$$

$$\psi(r, \phi) = B_{nm} \frac{1}{\sqrt{2\pi}} e^{im\phi} \exp \left[-\frac{1}{2} \sqrt{\frac{2\mu D_e}{\hbar^2 r_e^2}} r^2 \right] \sum_{n=0} a_n r^{2n + \sqrt{m^2 + \frac{2\mu D_e r_e^2}{\hbar^2}}}, \quad (37)$$

and reduces to 3D space if one replaces m by $l + 1/2$ as

$$E_{nl} = -2D_e + \frac{\hbar}{r_e} \sqrt{\frac{2D_e}{\mu}} \left(2n + 1 + \sqrt{\left(l + \frac{1}{2} \right)^2 + \frac{2\mu D_e r_e^2}{\hbar^2}} \right), \quad (38)$$

which is identical to Eq. (15) of Ref. [39].

In our numerical work, we estimate the non-relativistic binding energy levels of the pseudo-harmonic potential for NO, CO, N₂ and CH diatomic molecules with various vibrational n and rotational l quantum numbers, using Eq. (38) in 3D space, with the potential parameter values given in Ref. [38]. We display our results in Table 1 and compare them with Ref. [39]. Further, the energy levels of these diatomic molecules for any arbitrary quantum numbers n and m obtained through Eq. (34) under the external magnetic field B and AB flux field ξ of different strength values. The results are displayed in Table 2 for N₂ and CH molecules. It is noticed from Table 2 that the magnetic field strength $B \neq 0$ has a very small effect on the energy levels when the magnetic quantum number $m = 0$. However, it has a greater effect on the energy levels when $m \neq 0$; leading to a significant splitting to the two degenerate states $m = 1$ and $m = -1$. Therefore, we conclude that only the strong magnetic fields have impact on the $m = 0$. However, the magnetic field of any strength has greater effect on the magnetic quantum number $m \neq 0$. When we set $B = 0$ and $\xi \neq 0$, the Aharonov–Bohm field of any strength has greater influence on the energy levels for any m value. It removes the degeneracy on the $m = 1$ and $m = -1$ and splitting them up and down, respectively. The application of a magnetic field of constant strength and at the same time increasing the strength of AB field leads to an interchange

Table 2

The rovibrational energy levels of the pseudoharmonic oscillator for N₂ and CH diatomic molecules with various *n* and *m* quantum states for *D* = 2 in the presence and absence of external magnetic field, *B* and AB flux field, ξ .

<i>E_{nm}</i> (eV)		N ₂			
<i>n</i>	<i>m</i>	<i>E_{nm}</i> ($\xi = 0, B = 0$)	<i>E_{nm}</i> ($\xi = 0, B = 1$)	<i>E_{nm}</i> ($\xi = 0, B = 2$)	<i>E_{nm}</i> ($\xi = 0, B = 3$)
0	0	0.10912268	0.10912268	0.10912271	0.10912275
1	0	0.32736800	0.32736800	0.32736804	0.32736807
	1	0.32761735	0.32762019	0.32762307	0.32762595
2	-1	0.32761735	0.32761451	0.32761169	0.32760889
	0	0.54561333	0.54561333	0.54561336	0.54561340
	1	0.54586267	0.54586551	0.54586840	0.54587127
3	-1	0.54586267	0.54585983	0.54585702	0.54585421
	0	0.76385865	0.76385865	0.76385869	0.76385872
	1	0.76410800	0.76411084	0.76411372	0.76411659
-1	0.76410800	0.76410516	0.76410234	0.76409953	
<i>E_{nm}</i> (eV)		CH			
<i>n</i>	<i>m</i>	<i>E_{nm}</i> ($\xi = 0, B = 0$)	<i>E_{nm}</i> ($\xi = 1, B = 0$)	<i>E_{nm}</i> ($\xi = 2, B = 0$)	<i>E_{nm}</i> ($\xi = 3, B = 0$)
0	0	0.10912268	0.10937203	0.11012011	0.11136681
1	0	0.32736800	0.32761735	0.32836543	0.32961213
	1	0.32761735	0.32836543	0.32961213	0.33135744
	-1	0.32761735	0.32736800	0.32761735	0.32836543
2	0	0.54561333	0.54586267	0.54661075	0.54785746
	1	0.54586267	0.54661075	0.54785746	0.54960277
	-1	0.54586267	0.54561333	0.54586267	0.54661075
3	0	0.76385865	0.76410800	0.76485608	0.76610278
	1	0.76410800	0.76485608	0.76610278	0.76784809
	-1	0.76410800	0.76385865	0.76410800	0.76485608
<i>E_{nm}</i> (eV)		CH			
<i>n</i>	<i>m</i>	<i>E_{nm}</i> ($\xi = 0, B = 0$)	<i>E_{nm}</i> ($\xi = 0, B = 1$)	<i>E_{nm}</i> ($\xi = 0, B = 2$)	<i>E_{nm}</i> ($\xi = 0, B = 3$)
0	0	0.16823124	0.16823130	0.16823150	0.16823182
1	0	0.50469372	0.50469378	0.50469399	0.50469433
	1	0.50648593	0.50650742	0.50652905	0.50655081
2	-1	0.50648593	0.50646458	0.50644336	0.50642228
	0	0.84115620	0.84115627	0.84115648	0.84115683
	1	0.84294841	0.84296991	0.84299154	0.84301332
3	-1	0.84294841	0.84292706	0.84290585	0.84288478
	0	1.17761867	1.17761875	1.17761897	1.17761934
	1	1.17941089	1.17943239	1.17945403	1.17947582
-1	1.17941089	1.17938954	1.17936834	1.17934729	
<i>E_{nm}</i> (eV)		CH			
<i>n</i>	<i>m</i>	<i>E_{nm}</i> ($\xi = 0, B = 0$)	<i>E_{nm}</i> ($\xi = 1, B = 0$)	<i>E_{nm}</i> ($\xi = 2, B = 0$)	<i>E_{nm}</i> ($\xi = 3, B = 0$)
0	0	0.16823124	0.17002346	0.17539767	0.18434658
1	0	0.50469372	0.50648593	0.51186015	0.52080906
	1	0.50648593	0.51186015	0.52080906	0.53332056
2	-1	0.50648593	0.50469372	0.50648593	0.51186015
	0	0.84115620	0.84294841	0.84832263	0.85727154
	1	0.84294841	0.84832263	0.85727154	0.86978304
3	-1	0.84294841	0.84115620	0.84294841	0.84832263
	0	1.17761867	1.17941089	1.18478511	1.19373402
	1	1.17941089	1.18478511	1.19373402	1.20624552
-1	1.17941089	1.17761867	1.17941089	1.18478511	

in the energy levels for *m* = 0 to become the energy level of *m* = -1 and the energy of the state *m* = 1 becomes the energy of the state *m* = 0.

3.2. The harmonic oscillator

For an isotropic harmonic oscillator with angular frequency ω , the potential function is given by [43]

$$V(r) = \frac{1}{2} \kappa r^2, \quad \kappa = \mu \omega^2. \tag{39}$$

Hence, the energy spectrum formula and wave function become

$$E_{nm'} = \hbar\sqrt{\omega_c^2 + 4\omega^2} \left(n + \frac{1 + m'}{2} \right) + \frac{1}{2}\hbar m' \omega_c, \tag{40}$$

$$\psi(r, \phi) = \frac{1}{\sqrt{2\pi}} e^{im'\phi} \exp \left[-\frac{1}{2} \sqrt{\left(\frac{\mu\omega_c}{2\hbar} \right)^2 + \frac{2\mu D_e}{\hbar^2 r_e^2}} r^2 \right] \sum_{n=0} a_n r^{2n+m'}. \tag{41}$$

This is identical to Refs. [23,25] for the nonrelativistic harmonic oscillator in an external uniform magnetic and AB flux fields. Furthermore, when the fields $B = \Phi_{AB} = 0$, we can obtain,

$$E_{nm} = \hbar\omega (2n + 1 + m), \tag{42}$$

$$\psi(r, \phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi} \exp \left[-\frac{\mu\omega}{2\hbar} r^2 \right] \sum_{n=0} a_n r^{2n+m}. \tag{43}$$

In 3D, the energy formula becomes $E_{nl} = \hbar\omega (2n + l + \frac{3}{2})$.

3.3. Generalized Kratzer potential

The generalized Kratzer potential is given by

$$V(r) = D_e \left(\frac{r - r_e}{r} \right)^2 + \eta, \tag{44}$$

where r_e is the equilibrium separation and D_e is the dissociation energy between diatomic molecules. In the case if $\eta = 0$, this potential reduces to the modified Kratzer potential proposed by Simons et al. [44] and by Molski and Konarski [45]. The modified Kratzer potential is usually used in applications on the molecular spectroscopies. Plíva [46] has demonstrated that the deficiencies of rovibrational energy spectrum based on modified Kratzer potential can be substituted by including correction terms dependent on the vibrational and rotational quantum numbers n and l , respectively. In the case if $\eta = -D_e$, this potential turns to become the Kratzer potential consisting from the attractive Coulomb potential plus repulsive inverse square potential [47]. Now we want to obtain a 2D energy formula and wave function in the presence of the generalized Kratzer potential and magnetic field and AB flux field. So we set the parameters values $a = b = 0, d = D_e + \eta, g = 2r_e D_e$ and $k = r_e^2 D_e$ and use Eqs. (28) and (29) to obtain

$$E_{nm'} = \frac{\hbar\omega_c}{2} \left[m' + \left(n + 1 + \sqrt{\frac{2\mu r_e^2 D_e}{\hbar^2} + m'^2} \right) \right] - \frac{2\mu r_e^2 D_e^2}{\hbar^2} \left(n + \frac{1}{2} + \sqrt{\frac{2\mu r_e^2 D_e}{\hbar^2} + m'^2} \right)^{-2} + D_e + \eta, \tag{45}$$

and

$$\psi(r, \phi) = \exp \left[-\frac{2\mu r_e D_e}{\hbar^2} \left(n + \frac{1}{2} + \sqrt{\frac{2\mu r_e^2 D_e}{\hbar^2} + m'^2} \right)^{-1} r - \frac{\mu\omega_c}{4\hbar} r^2 \right] \times \sum_{n=0} a_n r^{n + \sqrt{\frac{2\mu r_e^2 D_e}{\hbar^2} + m'^2}} \frac{1}{\sqrt{2\pi}} e^{im'\phi}, \tag{46}$$

Table 3

The rovibrational energy levels of the Kratzer–Fues potential for N₂ and CH diatomic molecules with various vibrational n and rotational l quantum states for $D = 3$.

$-E_{nm}$ (eV)			
n	m	N ₂	CH
0	0	11.88375702	3.86419448
1	0	11.77611669	3.70626716
1	1	11.77562811	3.70300883
2	0	11.66993223	3.55782724
2	1	11.66945025	3.55476264
2	2	11.66848639	3.54864946
3	0	11.56517751	3.41812972
3	1	11.56470201	3.41524380
3	2	11.56375110	3.40948682
3	3	11.56232502	3.40088832
4	0	11.46182698	3.28650134
4	1	11.46135783	3.28378047
4	2	11.46041964	3.27835254
4	3	11.45901264	3.27024501
4	4	11.45713719	3.25949862
5	0	11.35985565	3.16233240
5	1	11.35939275	3.15976423
5	2	11.35846705	3.15464074
5	3	11.35707878	3.14698750
5	4	11.35522830	3.13684243
5	5	11.35291603	3.12425536

respectively. Further, when we set $B = 0$ and $\Phi_{AB} = 0$, we obtain

$$E_{nm} = -\frac{2\mu r_e^2 D_e^2}{\hbar^2} \left(n + \frac{1}{2} + \sqrt{\frac{2\mu r_e^2 D_e}{\hbar^2} + m^2} \right)^{-2} + D_e + \eta, \quad (47)$$

and

$$\psi(r, \phi) = \exp \left[-\frac{2\mu r_e D_e}{\left(n + \frac{1}{2} + \sqrt{\frac{2\mu r_e^2 D_e}{\hbar^2} + m^2} \right) \hbar^2} r \right] \sum_{n=0}^{\infty} a_n r^{n + \sqrt{\frac{2\mu r_e^2 D_e}{\hbar^2} + m^2}} \frac{1}{\sqrt{2\pi}} e^{im\phi}. \quad (48)$$

The 3D non-relativistic energy solutions are obtained by setting $m = l + 1/2$ where l is the rotational quantum number, in Eq. (47) to obtain

$$E_{nl} = -\frac{8\mu r_e^2 D_e^2}{\hbar^2} \left(1 + 2n + \sqrt{\frac{8\mu r_e^2 D_e}{\hbar^2} + (2l + 1)^2} \right)^{-2} + D_e + \eta, \quad n = 0, 1, 2, \dots \quad (49)$$

where $l = 0, 1, 2, \dots$ is the rotational quantum number. Note that Eq. (49) is identical to Eq. (36) of Ref. [48] when $N = 3$ and reverts to the rovibrational energy for the Kratzer potential (for $\eta = -D_e$) studied in [49–51] and to energy for the modified Kratzer potential (for $\eta = 0$) studied in [52–54].

In our numerical work, we estimate the non-relativistic binding energy levels of the Kratzer potential for N₂ and CH diatomic molecules with various vibrational n and rotational l quantum numbers in 3D space, with the potential parameter values given in Ref. [38] to see the accuracy of our solution. Our results are displayed in Table 3 and compared with the ones in Ref. [38]. Furthermore the energy levels of these diatomic molecules in the presence of external magnetic field B , and AB flux field, ξ of different strength values with various values of quantum numbers n and m obtained through Eq. (45) are presented in Table 4. It is noticed from Table 4 that the magnetic field strength $B \neq 0$ has very small effect on the energy levels when the magnetic quantum number $m = 0$. However, it has greater influence on the energy levels when $m \neq 0$; it makes splitting to the two degenerate states

Table 4

The rovibrational energy levels of the Kratzer potential for N_2 and CH diatomic molecule with various n and m quantum states for $D = 2$ in the presence and absence of external magnetic field, B and AB flux field, ξ .

$-E_{nm}$ (eV)		N_2			
n	m	$E_{nm}(\xi = 0, B = 0)$	$E_{nm}(\xi = 0, B = 1)$	$E_{nm}(\xi = 0, B = 2)$	$E_{nm}(\xi = 0, B = 3)$
0	0	11.88381894	11.88371512	11.88361129	11.88350747
1	0	11.77617777	11.77607347	11.77596918	11.77586488
	1	11.77593347	11.77582870	11.77572393	11.77561916
	-1	11.77593347	11.77582965	11.77572582	11.77562200
2	0	11.66999248	11.66988771	11.66978294	11.66967818
	1	11.66975149	11.66964625	11.66954101	11.66943577
	-1	11.66975149	11.66964719	11.66954290	11.66943860
3	0	11.56523696	11.56513172	11.56502648	11.56492124
	1	11.56499920	11.56489349	11.56478777	11.56468206
	-1	11.56499920	11.56489443	11.56478966	11.56468489
n	m	$E_{nm}(\xi = 0, B = 0)$	$E_{nm}(\xi = 1, B = 0)$	$E_{nm}(\xi = 2, B = 0)$	$E_{nm}(\xi = 3, B = 0)$
0	0	11.88381894	11.88357129	11.88282838	11.88159041
1	0	11.77617777	11.77593347	11.77520064	11.77397945
	1	11.77593347	11.77520064	11.77397945	11.77227022
	-1	11.77593347	11.77617777	11.77593347	11.77520064
2	0	11.66999248	11.66975149	11.66902854	11.66782383
	1	11.66975149	11.66902854	11.66782383	11.66613766
	-1	11.66975149	11.66999248	11.66975149	11.66902854
3	0	11.56523696	11.56499920	11.56428596	11.56309744
	1	11.56499920	11.56428596	11.56309744	11.56143392
	-1	11.56499920	11.56523696	11.56499920	11.56428596
$-E_{nm}$ (eV)		CH			
n	m	$E_{nm}(\xi = 0, B = 0)$	$E_{nm}(\xi = 0, B = 1)$	$E_{nm}(\xi = 0, B = 2)$	$E_{nm}(\xi = 0, B = 3)$
0	0	3.86462852	3.86445802	3.86428753	3.86411704
1	0	3.70667486	3.70650081	3.70632676	3.70615271
	1	3.70504461	3.70486696	3.70468932	3.70451167
	-1	3.70504461	3.70487408	3.70470355	3.70453302
2	0	3.55821069	3.55803309	3.55785548	3.55767787
	1	3.55667739	3.55649619	3.55631498	3.55613378
	-1	3.55667739	3.55650330	3.55632921	3.55615512
3	0	3.41849082	3.41830965	3.41812848	3.41794732
	1	3.41704692	3.41686216	3.41667740	3.41649264
	-1	3.41704692	3.41686928	3.41669163	3.41651398
n	m	$E_{nm}(\xi = 0, B = 0)$	$E_{nm}(\xi = 1, B = 0)$	$E_{nm}(\xi = 2, B = 0)$	$E_{nm}(\xi = 3, B = 0)$
0	0	3.86462852	3.86289297	3.85769569	3.84906466
1	0	3.70667486	3.70504461	3.70016252	3.69205445
	1	3.70504461	3.70016252	3.69205445	3.68076315
	-1	3.70504461	3.70667486	3.70504461	3.70016252
2	0	3.55821069	3.55667739	3.55208550	3.54445900
	1	3.55667739	3.55208550	3.54445900	3.53383747
	-1	3.55667739	3.55821069	3.55667739	3.55208550
3	0	3.41849082	3.41704692	3.41272269	3.40554035
	1	3.41704692	3.41272269	3.40554035	3.39553666
	-1	3.41704692	3.41849082	3.41704692	3.41272269

$m = 1$ and $m = -1$. Therefore, we conclude that only strong magnetic fields have impact on the $m = 0$. But the magnetic of any strength has greater effect on the magnetic quantum number. When $B = 0$ and $\xi \neq 0$, the AB field of any strength has greater influence on the energy levels for any m value. It removes the degeneracy on the $m = 1$ and $m = -1$ and splitting them up and down, respectively. The application of a magnetic field of constant strength and at the same time increasing the strength of AB field leads to an interchange in the energy levels for $m = 0$ to become the energy level of $m = -1$ and the energy of the state $m = 1$ becomes the energy of the state $m = 0.0$.

Table 5

The rovibrational energy levels of the Mie-type potential for N₂ and CH diatomic molecule with various *n* and *m* quantum states for *D* = 2 in the presence and absence of external magnetic field, *B* and AB flux field, ξ .

-E _{nm} (eV)		N ₂			
<i>n</i>	<i>m</i>	E _{nm} ($\xi = 0, B = 0$)	E _{nm} ($\xi = 0, B = 1$)	E _{nm} ($\xi = 0, B = 2$)	E _{nm} ($\xi = 0, B = 3$)
0	0	11.88381894	11.88371512	11.88361129	11.88350747
1	0	11.77617777	11.77607347	11.77596918	11.77586488
	1	11.77593347	11.77582870	11.77572393	11.77561916
2	-1	11.77593347	11.77582965	11.77572582	11.77562200
	0	11.66999248	11.66988771	11.66978294	11.66967818
	1	11.66975149	11.66964625	11.66954101	11.66943577
3	-1	11.66975149	11.66964719	11.66954290	11.66943860
	0	11.56523696	11.56513172	11.56502648	11.56492124
	1	11.56499920	11.56489349	11.56478777	11.56468206
-1	11.56499920	11.56489443	11.56478966	11.56468489	
<i>n</i>	<i>m</i>	E _{nm} ($\xi = 0, B = 0$)	E _{nm} ($\xi = 1, B = 0$)	E _{nm} ($\xi = 2, B = 0$)	E _{nm} ($\xi = 3, B = 0$)
0	0	11.88381894	11.88357129	11.88282838	11.88159041
1	0	11.77617777	11.77593347	11.77520064	11.77397945
	1	11.77593347	11.77520064	11.77397945	11.77227022
	-1	11.77593347	11.77617777	11.77593347	11.77520064
2	0	11.66999248	11.66975149	11.66902854	11.66782383
	1	11.66975149	11.66902854	11.66782383	11.66613766
	-1	11.66975149	11.66999248	11.66975149	11.66902854
3	0	11.56523696	11.56499920	11.56428596	11.56309744
	1	11.56499920	11.56428596	11.56309744	11.56143392
	-1	11.56499920	11.56523696	11.56499920	11.56428596
-E _{nm} (eV)		CH			
<i>n</i>	<i>m</i>	E _{nm} ($\xi = 0, B = 0$)	E _{nm} ($\xi = 0, B = 1$)	E _{nm} ($\xi = 0, B = 2$)	E _{nm} ($\xi = 0, B = 3$)
0	0	3.86462852	3.86445802	3.86428753	3.86428753
1	0	3.70667486	3.70650081	3.70632676	3.70632676
	1	3.70504461	3.70486696	3.70468932	3.70468932
2	-1	3.70504461	3.70487408	3.70470355	3.70470355
	0	3.55821069	3.55803309	3.55785548	3.55785548
	1	3.55667739	3.55649619	3.55631498	3.55631498
3	-1	3.55667739	3.55650330	3.55632921	3.55632921
	0	3.41849082	3.41830965	3.41812848	3.41812848
	1	3.41704692	3.41686216	3.41667740	3.41667740
-1	3.41704692	3.41686928	3.41669163	3.41669163	
<i>n</i>	<i>m</i>	E _{nm} ($\xi = 0, B = 0$)	E _{nm} ($\xi = 1, B = 0$)	E _{nm} ($\xi = 2, B = 0$)	E _{nm} ($\xi = 3, B = 0$)
0	0	3.86462852	3.86289297	3.85769569	3.84906466
1	0	3.70667486	3.70504461	3.70016252	3.69205445
	1	3.70504461	3.70016252	3.69205445	3.68076315
	-1	3.70504461	3.70667486	3.70504461	3.70016252
2	0	3.55821069	3.55667739	3.55208550	3.54445900
	1	3.55667739	3.55208550	3.54445900	3.53383747
	-1	3.55667739	3.55821069	3.55667739	3.55208550
3	0	3.41849082	3.41704692	3.41272269	3.40554035
	1	3.41704692	3.41272269	3.40554035	3.39553666
	-1	3.41704692	3.41849082	3.41704692	3.41272269

3.4. The Mie-type potentials

This potential has been studied in the *D* dimensions using the polynomial solution and the ansatz wave function method [55,2]. The Mie-type potential has the form [55]

$$V(r) = D_e \left[\frac{k}{j-k} \left(\frac{r_e}{r}\right)^j - \frac{j}{j-k} \left(\frac{r_e}{r}\right)^k \right], \quad j > k, \tag{50}$$

where the parameter D_e determines the interaction energy between two atoms in a solid at $r = r_e$. Taking $j = 2k$ and further setting $k = 1$, the potential reduces to the Coulombic-type form [56–60]

$$V(r) = 2D_e \left(\frac{1}{2} \left(\frac{r_e}{r} \right)^2 - \frac{r_e}{r} \right). \quad (51)$$

Now when taking $a = b = d = 0$, $g = 2r_e D_e$ and $k = r_e^2 D_e$ and using Eqs. (28) and (29) to obtain

$$E_{nm'} = \frac{\hbar\omega_c}{2} \left[m' + \left(n + 1 + \sqrt{m'^2 + \frac{2\mu r_e^2 D_e}{\hbar^2}} \right) \right] - \frac{2\mu r_e^2 D_e^2}{\hbar^2} \left(n + \frac{1}{2} + \sqrt{m'^2 + \frac{2\mu r_e^2 D_e}{\hbar^2}} \right)^{-2}, \quad (52)$$

and

$$\psi(r, \phi) = \exp \left[-\frac{2\mu r_e D_e}{\hbar^2} \left(n + \frac{1}{2} + \sqrt{m'^2 + \frac{2\mu r_e^2 D_e}{\hbar^2}} \right)^{-1} r - \frac{\mu\omega_c}{4\hbar} r^2 \right] \times \sum_{n=0} a_n r^{n + \sqrt{m'^2 + \frac{2\mu r_e^2 D_e}{\hbar^2}}} \frac{1}{\sqrt{2\pi}} e^{im'\phi}, \quad (53)$$

respectively. After setting $B = 0$ and $\Phi_{AB} = 0$, we obtain

$$E_{nm} = -\frac{2\mu r_e^2 D_e^2}{\hbar^2} \left(n + \frac{1}{2} + \sqrt{m^2 + \frac{2\mu r_e^2 D_e}{\hbar^2}} \right)^{-2}, \quad (54)$$

and

$$\psi(\vec{r}, \phi) = \exp \left[-\frac{2\mu r_e D_e}{\hbar^2} \left(n + \frac{1}{2} + \sqrt{m^2 + \frac{2\mu r_e^2 D_e}{\hbar^2}} \right)^{-1} r \right] \times \sum_{n=0} a_n r^{n + \sqrt{m^2 + \frac{2\mu r_e^2 D_e}{\hbar^2}}} \frac{1}{\sqrt{2\pi}} e^{im\phi}. \quad (55)$$

The 3D non-relativistic energy solutions for Mie-type potential are obtained by setting $m = l + 1/2$ where l is the rotational quantum number to obtain

$$E_{nl} = -\frac{2\mu r_e^2 D_e^2}{\hbar^2} \left(n + \frac{1}{2} + \sqrt{\frac{2\mu r_e^2 D_e}{\hbar^2} + \left(l + \frac{1}{2} \right)^2} \right)^{-2}, \quad n = 0, 1, 2, \dots, \quad l = 0, 1, 2, \dots \quad (56)$$

which is identical to Eq. (30) of Ref. [44] when $D = 3$. In Table 5, for the N_2 and CH molecules, when the AB flux field is set to zero and the magnetic field strength increases this result to slightly decreasing of the energy values. However its also noticed that the energy level is shifted (split) slightly up for $m = -1$ whereas shifted down for $m = 1$. On the other hand when B is set to zero and the AB flux field changed, this flux field has a similar influence on the energy states as the magnetic field change in step 1.

4. Concluding remarks

In this paper, we have carried out analysis for the 2D Schrödinger equation with a specific potential function in the presence of external uniform magnetic \vec{B} and AB flux Φ_{AB} fields by using an appropriate wave function ansatz. The restrictions on the potential parameters and β have been given. The problem is then solved in 2D space and the bound state energy solutions are found under the influence of external magnetic and AB flux fields. The 3D bound state energy levels and wave functions are obtained in closed form to show the accuracy of the present model. As an application, we applied the energy formula on the pseudo-harmonic, harmonic, generalized Kratzer, Mie-type and Coulombic potentials models for various strength of external uniform magnetic and AB flux fields. The external fields produce splitting in the energy levels which is essentially dependent on the strength of the applied fields.

As a further application, we generated the non-relativistic energy levels of few diatomic molecules: NO, CO, N₂ and CH for various vibrational n and rotational l quantum numbers. The spectroscopic constant for these molecules are given in Ref. [39] where the 3D pseudo-harmonic potential have been considered. We have developed keen interest in these molecules to enable one in making comparison with the previous work in the absence of external magnetic field. The criterion for selecting these diatomic molecules is nothing but for their intermediate importance in the chemical physics, chemical industry, biological sciences and related areas. NO is an important messenger molecule involved in many pathological and physiological processes within the mammalian body [61]. CO is the simplest oxocarbon and isoelectronic with the cyanide ion and molecular nitrogen. This molecule has received a great deal of attention in clinical section as a biological regulator. N₂ molecules is very essential in industry for production of ammonia, nitric acid and explosives. The emission spectrum of CH can be used to understand double spectral of diatomic molecules.

The energy levels of these diatomic molecules have been calculated in 2D space under the influence of magnetic field and Aharonov–Bohm field. It is noticed that the magnetic field has a small influence on the energy levels when $m = 0$. However, when $m \neq 0$, it removes the degeneracy and makes a narrow shift for the energy states. On the other hand, the effect of the Aharonov–Bohm field is greater as it creates a wider shift for $m \neq 0$ and its influence on $m = 0$ states is found to be greater than that of the magnetic field. The $m \neq 0$ states are much more sensitive to the two fields.

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