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Influence of External Magnetic and Aharanov-Bohm (AB) Fields on the Energy Spectra of the Modified Kratzer plus Screened Coulomb Potential

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Abstract

In this article, the modified Kratzer plus screened Coulomb potential is scrutinized taking into consideration the effects of magnetic and AB flux fields within the non-relativistic regime using the Nikiforov-Uvarov-Functional Analysis method (NUFA) method. The energy equation and wave function of the system are obtained in close form. We find that the totality of effects these fields result in removal of degeneracy and raising the bound state energy of the system. More so, it could be concluded that to control the energy spectra of this system, the AB-flux and magnetic field will do so greatly. The results from this study can be applied in condensed matter physics, atomic and molecular physics.

Keywords: NUFA method; Magnetic and AB fields; Modified Kratzer plus screened Coulomb potential

1. Introduction

In the last two decades, research in the direction of non-relativistic quantum mechanics (QM) have drawn the attention of researchers to a great extent. Researchers have focused on the solutions of the Schrödinger equation (SE) with several interaction potential models. This because its solutions provides relevant information about the quantum system [1-10]. More so, solutions of the SE with several have been applied to study many physical systems, example; quantum dots [11], quarks [12], diatomic molecules [13], etc. Amongst the numerous potentials proposed and adopted for such studies over the years is the modified Kratzer plus screened Coulomb potential proposed by Edet et al. [14]. This model is given as;

$$V(r) = D_e \left(\frac{r - r_e}{r}\right)^2 - \frac{Ae^{-\alpha r}}{r}$$
⁽¹⁾

where D_e the energy of dissociation is, r_e is the equilibrium bond length, A is the potential parameter, α is the screening parameter and r is the inter-nuclear distance. A number of authors have adopted this model to carry out some interesting studies. For instance, Edet et al [14] in a maiden consideration applied the model to study the diatomic molecules. Okorie et al [15] applied this model study thermal properties of some diatomic molecules.

Another very interesting area of research within quantum mechanics is the effects of the perturbation of external fields on a quantum system. This line of research of has been a subject of interest since the early days of quantum mechanics. A number of authors have carried out research regarding this concept recently [16-20]. Ikot et al. [21] studied effects of magnetic and AB fields on the energy spectra and thermo-magnetic properties of the screened Kratzer potential (SKP). Edet and Ikot[22] studied the effects of magnetic and AB fields on the energy spectra and thermal properties of some diatomic molecules using the Hulthen-Kratzer potential (HKP) model. Abu-shady et al. [23] investigated the dissociation

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of quarkonia in a thermal QCD medium in the background of AB and strong magnetic fields. Edet and Ikot [4] studied the effects of magnetic and AB fields on the energy spectra and thermomagnetic properties of CO diatomic molecule using screened modified Kratzer. Ikot et al.[25] studied the effects of external magnetic and AB fields on the thermodynamic variable of some diatomic molecules via superstatistics.

In view of this, we are interested in providing answers to the following questions; what happens to the energy spectra of the modified Kratzer plus screened Coulomb potential in the presence of the all-inclusive effect of magnetic and Aharanov- Bohm (AB) fields? What happens when there is a solitary effect? This questions have motivated us to carry out this study.

In the present work, our goal is to solve the SE with the modified Kratzer plus screened Coulomb potential in the presence of magnetic and AB flux fields using the Nikiforov-Uvarov Functional Analysis (NUFA) method. We will discuss the effects of the fields on the energy spectra of the system.

The paper is organized as follows. In section 2, we solve of the 2D Schrödinger equation with the modified Kratzer plus screened Coulomb potential under the combined effects of magnetic and AB flux fields. In section 3, we discuss the effects of the fields on the behavior of the energy spectra of the modified Kratzer plus screened Coulomb potential. Finally, a brief concluding remark is given in section 4.

2. NU-functional analysis (NUFA) method

Ikot et al. [26] proposed the Nikiforov-Uvarov-Functional Analysis method (NUFA) as a simple and elegant method for solving a second order differential equation of the hypergeometric form. The Nikiforov Uvarov (NU) method[27], the parametric NU method [28], and the functional analysis method[29, 30, 31] were used. This method, like the parametric NU method, is simple and straightforward. The NU is well-known for solving a second-order differential equation with the form [28].

$$\psi_n''(s) + \frac{\tilde{\tau}(s)}{\sigma(s)}\psi_n'(s) + \frac{\tilde{\sigma}(s)}{\sigma^2(s)}\psi_n(s) = 0, \qquad (2)$$

where $\sigma(s)$ and $\tilde{\sigma}(s)$ are polynomials, at most of second degree, and $\tilde{\tau}(s)$ is a first-degree polynomial. Tezcan and Sever [28] latter introduced the parametric form of NU method in the form

$$\psi'' + \frac{\alpha_1 - \alpha_2 s}{s(1 - \alpha_3 s)} \psi' + \frac{1}{s^2 (1 - \alpha_3 s)^2} \Big[-\xi_1 s^2 + \xi_2 s - \xi_3 \Big] \psi(s) = 0$$
(3)

where α_i and ξ_i (i = 1,2,3) are all parameters. It can be observed in equation (3) that the differential equation has two singularities at $s \to 0$ and $s \to 1$, thus we take the wave function in the form,

$$\psi(s) = s^{\lambda} \left(1 - s\right)^{\nu} f(s) \tag{4}$$

Substituting equation (4) into equation (3) leads to the following equation,

$$s(1-\alpha s)f''(s) + \left[\alpha_{1} + 2\lambda - (2\lambda\alpha_{3} + 2\nu\alpha_{3} + \alpha_{2})s\right]f'(s) -\alpha_{3}\left(\lambda + \nu + \frac{\alpha_{2}}{\alpha_{3}} - 1 + \sqrt{\left(\frac{\alpha_{2}}{\alpha_{3}} - 1\right)^{2} + \frac{\xi_{1}}{\alpha_{3}}}\right)\left(\lambda + \nu + \frac{\alpha_{2}}{\alpha_{3}^{2}} - 1 + \sqrt{\left(\frac{\alpha_{2}}{\alpha_{3}} - 1\right)^{2} + \frac{\xi_{1}}{\alpha_{3}^{2}}}\right) + \left[\frac{\lambda(\lambda - 1) + \alpha_{1}\lambda - \xi_{3}}{s} + \frac{\alpha_{2}\nu - \alpha_{1}\alpha_{3}\nu + \nu(\nu - 1)\alpha_{3} - \frac{\xi_{1}}{\alpha_{3}} + \xi_{2} - \xi_{3}\alpha_{3}}{(1 - \alpha_{3}s)}\right]f(s) = 0$$
(5)

Equation (5) can be reduced to a Gauss hypergeometric equation if and only if the following functions vanished,

$$\lambda(\lambda - 1) + \alpha_1 \lambda - \xi = 0_3 \tag{6}$$

$$\alpha_{2}v - \alpha_{1}\alpha_{3}v + v(v-1)\alpha_{3} - \frac{\xi_{1}}{\alpha_{3}} + \xi_{2} - \xi_{3}\alpha = 0$$
⁽⁷⁾

Thus, equation (5) becomes

$$s(1-\alpha_{1}s)f''(s) + \left[\alpha_{1}+2\lambda-\left(2\lambda\alpha_{3}+2\nu\alpha_{3}+\alpha_{2}\right)s\right]f'(s) - \alpha_{3}\left(\lambda+\nu+\frac{\alpha_{2}}{\alpha_{3}}-1+\sqrt{\left(\frac{\alpha_{2}}{\alpha_{3}}-1\right)^{2}+\frac{\xi_{1}}{\alpha_{3}}}\right)\left(\lambda+\nu+\frac{\alpha_{2}}{\alpha_{3}^{2}}-1+\sqrt{\left(\frac{\alpha_{2}}{\alpha_{3}}-1\right)^{2}+\frac{\xi_{1}}{\alpha_{3}^{2}}}\right)f(s) = 0$$
(8)

Solving equations (6) and (7) completely give,

$$\lambda = \frac{(1 - \alpha_1) \pm \sqrt{(1 - \alpha_1)^2 + 4\xi_3}}{2}$$
(9)

$$v = \frac{(\alpha_{3} + \alpha_{1}\alpha_{3} - \alpha_{2}) \pm \sqrt{(\alpha_{3} + \alpha_{1}\alpha_{3} - \alpha_{2})^{2} + 4\left(\frac{\xi_{1}}{\alpha_{3}} + \alpha_{3}\xi_{3} - \xi_{2}\right)}}{2}$$
(10)

Equation (8) is the hypergeometric equation type of the form,

$$x(1-x)f''(x) + [c+(a+b+1)x]f'(x) - abf(x) = 0$$
(11)

Using equations (4),(8) and (11), we obtain the energy equation and the corresponding wave equation respectively for the NUFA method as follows:

$$\lambda^{2} + 2\lambda \left(\nu + \frac{\alpha_{2}}{\alpha_{3}} - 1 + \frac{n}{\sqrt{\alpha_{3}}} \right) + \left(\nu + \frac{\alpha_{2}}{\alpha_{3}} - 1 + \frac{n}{\sqrt{\alpha_{3}}} \right)^{2} - \left(\frac{\alpha_{2}}{\alpha_{3}} - 1 \right)^{2} - \frac{\xi_{1}}{\alpha_{3}^{2}} = 0$$

$$(12)$$

$$\psi(s) = Ns^{\frac{(1-\alpha_1)+\sqrt{(1-\alpha_1)^2+4\xi_3}}{2}} (1-\alpha_3 s)^{\frac{(\alpha_3+\alpha_1\alpha_3-\alpha_2)+\sqrt{(\alpha_3+\alpha_1\alpha_3-\alpha_2)^2+4\left(\frac{\xi_1}{\alpha_3^2}+\alpha_3\xi_3-\xi_2\right)}}{2}} {}_2F_1(a,b,c;s)$$
(13)

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where a, b and c are given as follows,

$$a = \sqrt{\alpha_3} \left(\lambda + \nu + \frac{\alpha_2}{\alpha_3} - 1 + \sqrt{\left(\frac{\alpha_2}{\alpha_3} - 1\right)^2 + \frac{\zeta_1}{\alpha_3}} \right)$$
(14)

$$b = \sqrt{\alpha_3} \left(\lambda + \nu + \frac{\alpha_2}{\alpha_3} - 1 - \sqrt{\left(\frac{\alpha_2}{\alpha_3} - 1\right)^2 + \frac{\xi_1}{\alpha_3}} \right)$$
(15)

$$c = \alpha_1 + 2\lambda \tag{16}$$

3. Schrödinger Equation with Modified Kratzer plus Screened Coulomb Potentials (MKSCP) with AB Flux and Magnetic Fields

For a charged particle in an electromagnetic field bearing in mind the effects of the magnetic and AB fields, Edet [33] have established a robust framework that can treat basically all class of exponential-type models. Following the work of Edet [33], we obtain the differential equation of the form;

$$R_{nm}''(r) + \frac{2\mu}{\hbar^{2}} \begin{bmatrix} E_{nm} - D_{e} \left(\frac{r - r_{e}}{r}\right)^{2} + \frac{Ae^{-\alpha r}}{r} - \hbar \omega_{c} \left(m + \xi\right) \frac{e^{-\alpha r}}{\left(1 - e^{-\alpha r}\right)r} - \left(\frac{\mu \omega_{c}^{2}}{2}\right) \frac{e^{-2\alpha r}}{\left(1 - e^{-\alpha r}\right)^{2}} \\ - \frac{\hbar^{2}}{2\mu} \frac{\gamma_{m}}{r^{2}} \end{bmatrix} R_{nm}(r) = 0$$
(17)

for our consideration, where $\gamma_m = (m + \xi)^2 - \frac{1}{4}$, $\xi = \frac{\phi_{AB}}{\phi_0}$ is an integer with the flux quantum $\phi_0 = \frac{hc}{e}$ and $\omega_c = \frac{eB}{\mu c}$ denotes the cyclotron frequency.

Eq. (17) is not exactly solvable due to the presence of centrifugal term. Therefore, we employ the Greene and Aldrich approximation scheme [34, 35] to overcome the centrifugal term. This approximation is given;

$$\frac{1}{r^2} = \frac{\alpha^2}{\left(1 - e^{-\alpha r}\right)^2}$$
(18)

We point out here that this approximation is only valid for small values of the screening parameter α . If we consider the approximation above, the transformation $s = e^{-\alpha r}$, Eq. (17) is rewritten as follows:

$$R_{nm}''(s) + \frac{R_{nm}'(s)}{s} + \frac{\left[-\left(\varepsilon_{nm} + P_2 + P_4\right)s^2 + \left(2\varepsilon_{nm} - P_0 + P_2 - P_3\right)s - \left(\varepsilon_{nm} - P_0 + P_1 + \gamma_m\right)\right]R_{nm}(s)}{\left(s(1-s)\right)^2} = 0$$
(19)

where

$$-\varepsilon_{nm} = \frac{2\mu}{\hbar^2 \alpha^2} \left(E_{nm} - D_e \right), P_0 = \frac{4\mu D_e r_e}{\hbar^2 \alpha}, P_1 = \frac{2\mu D_e r_e^2}{\hbar^2}, P_2 = \frac{2\mu A}{\hbar^2 \alpha}, P_3 = \frac{2\mu \omega_c}{\hbar \alpha} \left(m + \xi \right), P_4 = \left(\frac{\mu \omega_c}{\hbar \alpha} \right)^2$$
(20)

comparing (19) and (3), we obtain the following;

$$\alpha_1 = \alpha_2 = \alpha_3 = 1, \ v = \frac{1}{2} + \sqrt{\frac{1}{4} + P_4 + P_3 + P_1 + \gamma_m} \text{ and } \lambda = \sqrt{\varepsilon_{nm} - P_0 + P_1 + \gamma_m}$$
 (21)

The energy is then obtained from (12) as follows;

$$(\lambda + \sigma) - \left(\sqrt{\varepsilon_{nm} + P_2 + P_4}\right) + n = 0 \tag{22}$$

From which we obtain

$$\varepsilon_{nm} = P_0 - \gamma_m - P_1 + \frac{1}{4} \left[\frac{P_0 - P_1 + P_2 + P_4 - \gamma_m - \left(n + \frac{1}{2} + \sqrt{\frac{1}{4} + P_4 + P_3 + P_1 + \gamma_m}\right)^2}{\left(n + \frac{1}{2} + \sqrt{\frac{1}{4} + P_4 + P_3 + P_1 + \gamma_m}\right)} \right]^2$$
(23)

The energy is explicitly obtained in the form below;

$$E_{nm} = D_e + \frac{\hbar^2 \alpha^2}{2\mu} \left[\gamma_m - \frac{4\mu D_e r_e}{\hbar^2 \alpha} + \frac{2\mu D_e r_e^2}{\hbar^2} \right] - \frac{\hbar^2 \alpha^2}{8\mu} \left[\frac{\frac{4\mu D_e r_e}{\hbar^2 \alpha} - \frac{2\mu D_e r_e^2}{\hbar^2} + \frac{2\mu A}{\hbar^2 \alpha} + \left(\frac{\mu \omega_c}{\hbar \alpha}\right)^2 - \gamma_m - \left(n + \zeta\right)^2}{\left(n + \zeta\right)} \right]^2$$

$$(24)$$
where $\zeta = \frac{1}{2} + \sqrt{\frac{1}{4} + \left(\frac{\mu \omega_c}{\hbar \alpha}\right)^2 + \frac{2\mu \omega_c}{\hbar \alpha} \left(m + \xi\right) + \frac{2\mu D_e r_e^2}{\hbar^2} + \gamma_m}}{\hbar \alpha}$ and *m* is the magnetic quantum number.

The corresponding unnormalized wave function is obtained as

$$R_{nm}(s) = N_{nm}s^{\lambda}(1-s)^{\nu}{}_{2}F_{1}(-n,2(\lambda+\sigma)+n;2\lambda+1;s)$$
(25)

where N_{nm} is the normalization constant and ${}_{2}F_{1}(-n,2(\lambda+\sigma)+n;2\lambda+1;s)$ is the hypergeometric function.

The three-dimensional nonrelativistic energy solutions are obtained by setting $m = \ell + \frac{1}{2}$ where ℓ the rotational quantum number in Eq. (24) to obtain is

$$E_{nm} = D_{e} + \frac{\hbar^{2} \alpha^{2}}{2\mu} \left[\ell \left(\ell + 1 \right) - \frac{4\mu D_{e} r_{e}}{\hbar^{2} \alpha} + \frac{2\mu D_{e} r_{e}^{2}}{\hbar^{2}} \right] - \frac{\hbar^{2} \alpha^{2}}{8\mu} \left[\frac{\frac{4\mu D_{e} r_{e}}{\hbar^{2} \alpha} - \frac{2\mu D_{e} r_{e}^{2}}{\hbar^{2} \alpha} + \frac{2\mu A}{\hbar^{2} \alpha} - \ell \left(\ell + 1 \right) - \left(n + \zeta \right)^{2}}{\left(n + \zeta \right)} \right]^{2}$$
(26)
where $\zeta = \frac{1}{2} + \sqrt{\frac{1}{4} + \frac{2\mu D_{e} r_{e}^{2}}{\hbar^{2}}} + \ell \left(\ell + 1 \right).$

Equation (26) is in excellent agreement with Eq. (23) of Ref. [14] and eq. (19) of ref. [15].

4. Results and discussion

Table 1 shows the numerical energy values for the MKSCP potential under the influence of AB flux and magnetic fields with various values of magnetic quantum numbers. We observe that when both fields are absent, there exist degeneracy in the energy spectra. By introducing only magnetic field to the system, the energy eigenvalues is increased and takes

away the degeneracy as well. Nevertheless, as the strength of the magnetic field is raised so is the energy. This suggests that the energy values of the MKSCP can be altered or regulated to a highest level by the application a strong magnetic field. The application of the AB field only, raises the energy values and degeneracies are eliminated. The energy spectra become more negative and the system becomes strongly attractive as the quantum number n increases for fixed m. The combined effect of both fields is robust and therefore, there is an upward shift in the bound state energy of the system. The combined effect completely eliminates the degeneracy. The complete effects shows that the system is strongly attractive while the localizations of quantum levels change and the eigenvalues increase. Also, the combined effect of the fields is strong and consequently, there is a significant upward shift in the bound state energy of the system. The effect of the magnetic field is seen to be stronger than the combined effect. The same behavior is observed in Table 2 but the energy is dropped in this case due to an increased value of the screening parameter.

Table 1 Energy values for the modified Kratzer plus screened Coulomb potential under the influence of AB flux and external magnetic fields with various values of magnetic quantum numbers. We have used the following fitting parameters; $D_e = 4$, $r_e = 2$, $\hbar = c = e = \mu = A = 1$. And $\alpha = 0.005$

т	п	$\vec{B}=0, \xi=0$	$\vec{B}=5, \xi=0$	$\vec{B}=0, \xi=5$	$\vec{B} = 5, \xi = 5$
0	0	0.186118	3.92029	0.254226	3.92035
	1	1.16769	3.92035	1.2112	3.92039
	2	1.81091	3.92039	1.84039	3.9204
	3	2.25513	3.9204	2.27603	3.92039
-1	0	0.292546	3.92037	0.508885	3.92042
	1	1.23576	3.9204	1.3754	3.92044
	2	1.85707	3.92041	1.95241	3.92043
	3	2.28787	3.92039	2.35587	3.92039
1	0	0.292546	3.92022	0.190682	3.92028
	1	1.23576	3.92031	1.1706	3.92034
	2	1.85707	3.92037	1.81288	3.92038
	3	2.28787	3.9204	2.25653	3.9204

Table 2 Energy values for the modified Kratzer plus screened Coulomb potential under the influence of AB flux and external magnetic fields with various values of magnetic quantum numbers. We have used the following fitting parameters; $D_e = 4$, $r_e = 2$, $\hbar = c = e = \mu = A = 1$ and $\alpha = 0.005$

т	п	$\vec{B}=0, \xi=0$	$\vec{B}=5, \xi=0$	$\vec{B}=0, \xi=5$	$\vec{B} = 5, \xi = 5$
0	0	0.184206	3.84119	0.252376	3.84141
	1	1.15646	3.84142	1.20009	3.84157
	2	1.79352	3.84155	1.82313	3.84162
	3	2.23342	3.84159	2.25445	3.84157
-1	0	0.290731	3.8409	0.188774	3.84113
	1	1.22471	3.84124	1.15938	3.84138
	2	1.83988	3.84147	1.7955	3.84154
	3	2.26636	3.8416	2.23483	3.84159
1	0	0.290731	3.84147	0.507271	3.8417
	1	1.22471	3.8416	1.36472	3.84175
	2	1.83988	3.84164	1.93563	3.8417
	3	2.26636	3.84157	2.33476	3.84155

5. Conclusion

In this research article, the modified Kratzer plus screened Coulomb potential is analyzed with the influence of magnetic and AB flux fields. To this end, the Hamiltonian operator containing the external fields and the potential model is transformed into a second-order differential equation. We solve this differential equation using the NUFA method to get the energy equation and wave function of the system. The effect of the fields on the energy spectra of the system is closely examined. It was found out that the magnetic and AB fields remove degeneracy. The results of this study will find possible applications in condensed matter physics, atomic and molecular physics.

Compliance with ethical standards

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