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The Magnetic and Aharonov-Bomh Flux Fields of Carbon Monoxide Diatomic Molecule with Energy-Dependent Screened Kratzer Potential

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ABSTRACT

An energy-dependent potential is a type of quantum mechanical potential in which the potential energy explicitly depends on the particle's energy, rather than solely on its spatial coordinates as in conventional potentials. Energy-dependent potentials (EDPs) have gained attention in quantum mechanics due to their ability to model systems where the interaction strength varies with the particle's energy, offering a more flexible description of molecular and nuclear interactions than conventional static potentials. This study analytically solves the two-dimensional Schrödinger equation with an Energy-Dependent Screened Kratzer Potential (EDSKP) using the Nikiforov-Uvarov (NU) method to obtain the energy eigenvalues of a carbon monoxide (CO) diatomic molecule under the influence of Magnetic and Aharonov-Bohm (AB) flux fields. The energy spectra are computed for different quantum numbers, showing that the energy levels decrease with increasing magnetic and AB-flux field strength. This decrease is more pronounced when the energy slope parameter is negative, indicating a field-induced stabilization of the molecule. Conversely, the energy levels increase rapidly when the energy slope parameter is positive, reflecting a stiffening interaction. These behaviors are graphically confirmed and offer insights into the quantum mechanical response of molecules under external perturbations. By adjusting the potential parameters, the well-known screened Kratzer potential model is recovered. In the absence of external fields and with a substitution for the magnetic quantum number, the energy eigenvalue of the three-dimensional Schrödinger equation is retrieved as a special case, which aligns with previous studies. These results provide useful perspectives for molecular physics, quantum control, and materials science.

Keywords:
Energy-Dependent Screened Kratzer Potential,
Greene-Aldrich Approximation Scheme,
Nikiforov-Uvarov Method,
Magnetic,
AB-flux fields.

INTRODUCTION

It is widely recognized that both relativistic and non-relativistic equations involving various potential models have been effectively used to investigate a wide range of quantum systems (Abu-Shady and Ikot, 2019; Abu-Shady, Abdel-Karim and Khokha, 2018; Abu-Shady, 2016; Das, 2016; Edet and Okoi, 2019; Edet *et al*., 2019, 2020; Ikot *et al*., 2020; Inyang *et al*., 2020, 2021; Ntibi *et al*., 2020; Okoi, Edet and Magu, 2020; William, Inyang and Thompson, 2020; Ibrahim, Izam and Jabil, 2023). These studies have contributed significantly to the understanding of quantum information-theoretic entropies (Amadi *et al*., 2020; Yamano, 2024; Inyang *et al*., 2022; Edet *et al*., 2022; Idiodi and Onate, 2016; Martinez-Flores, 2021; Olendski, 2019; Onate *et al*., 2018, 2019, 2020, 2021), thermodynamic properties (Ibrahim, Izam and Jabil, 2024; Edet *et al*., 2020; Ikot *et al*., 2020; Edet and Ikot, 2021), mass spectra of heavy quarkonia (Allosh *et al*., 2021; Omugbe *et al*., 2022; Inyang *et al*., 2021; Rani, Bhardwaj and Chand, 2018) among others. These contributions are essential in various fields of physics, including molecular physics, nuclear physics, solid-state physics, and chemical physics (Dong and Dong, 2002). One of the recently proposed potential models is the Screened Kratzer Potential (SKP), introduced by Ikot *et al*. (2019), which has gained attention due to its ability to effectively describe molecular interactions under external field conditions.

$$V(r) = -2D_e\left(\frac{A}{r} - \frac{B}{2r^2}\right)e^{-\alpha r}, \quad A \equiv r_e, \quad B \equiv r_e^2, \qquad (1)$$

wherein D_e is the dissociation, r_e is the equilibrium bond length, r is the interatomic distance and α is the screening parameter. Moreover, considerable attention has been devoted by many researchers to the investigation of energy-dependent potentials in both relativistic and non-relativistic quantum equations, aimed at solving various quantum systems (García, García, and Peña, 2009; Yekken and Lombard, 2010; Yekken, Lassaut, and Lombard, 2013; Hassanabadi Rajabi and Zarrinkamar, 2011; Hassanabadi *et al*., 2012; Lombard, Mares and Volpe, 2007; Lombard and Mares, 2009; Gupta and Mehrotra, 2012; Budaca, 2016; Boumali and Labidi, 2018). A wide range of mathematical techniques has been employed to obtain solutions, including the Parametric Nikiforov-Uvarov method (Kaushal, Rajendrasinh and Ajay, 2020), the Nikiforov-Uvarov (NU) method (Nikiforov & Uvarov, 1988; Ikot, Hassanabadi, & Abbey, 2015; Eshghi, Mehraban and Ikhdair, 2015; Miranda, Sun and Dong, 2010; Zhang, Sun and Dong, 2010), the Supersymmetric approach (Onate and Ojonubah, 2016; Onate *et al*., 2016; Zhang, Li and Jia, 2008; Zhang, Li and Jia, 2011), the Factorization method (Anita *et al*., 2015), the Asymptotic Iteration Method (AIM) (Bayrak, Boztosun and Ciftci, 2007), the Qiang–Dong proper quantization rule (Qiang and Dong, 2010), and the Exact Quantization Rule (EQR) method (Ma and Xu, 2005), among others. In addition, recent studies have explored the quantum behavior of charged particles subjected to uniform magnetic and Aharonov-Bohm (AB) flux fields perpendicular to the plane of confinement. Interest in the study of non-relativistic and relativistic charged particles in magnetic fields has grown significantly due to its wide-ranging applications in areas such as graphene physics (Eshghi and Mehraban, 2016, 2017; Kryuchkov and Kukhar, 2014), chemical physics (Baura, Sen and Chandra, 2013), and molecular vibrational and rotational spectroscopy (Arda and Sever, 2012). Inspired by (Ikot *et al*., 2019) recent work, we propose another version of potential model known as the Energy-Dependent Screened Kratzer Potential (EDSKP), given by:

$$V(r,E) = -2D_e\left(\frac{a}{r}(1+\beta E) - \frac{a^2}{2r^2}(1+\beta E)\right)e^{-\alpha r}, \quad a \equiv r_e, \quad a^2 \equiv r_e^2, \qquad (2)$$

The energy-dependent screened kratzer potential may be simplified to the Screened Kratzer Potential (SKP) when the energy slope parameter is set to $\beta = 0$.

To the best of our knowledge, the influence of magnetic and AB-flux fields, along with the energy slope parameter of the energy-dependent screened Kratzer potential, on the CO diatomic molecule has not been studied in the existing literature. This study addresses that gap. Also, in this study we are interested by offering answers to the subsequent questions; How do increasing magnetic and AB-flux fields affect the energy eigenvalues of a CO diatomic molecule under an energy-dependent screened Kratzer potential? What role does the energy slope parameter play in modifying the energy spectrum of the CO diatomic molecule in external fields?

Review of the Nikiforov-Uvarov (NU) Method

Originally developed by (Nikiforov and Uvarov, 1988), the NU method is a mathematical technique used to reduce Schrödinger-type differential equations into second-order linear differential equations through an appropriate coordinate transformation, typically expressed as $s = s(r)$, of the form:

$$\psi''(s) + \frac{\tilde{\tau}(s)}{\sigma(s)}\psi'(s) + \frac{\tilde{\sigma}(s)}{\sigma^2(s)}\psi(s) = 0 \qquad (3)$$

wherein $\tilde{\tau}(s)$ is a polynomial of at most first-degree, while $\sigma(s)$ and $\tilde{\sigma}(s)$ are polynomials of at most second-degree and $\psi(s)$ is a function of hypergeometric-kind. In order to find the solution to Eq. (3), we assume:

$$\psi(s) = \phi(s)y(s) \qquad (4)$$

and Eq. (4) substitute into Eq. (3), obtaining the hypergeometric-type equation:

$$\sigma(s)y'' + \tau(s)y' + \lambda y = 0 \qquad (5)$$

where

$$\tau(s) = \tilde{\tau}(s) + 2\pi(s), \qquad \lambda = \lambda_n = -n\tau' - \frac{n(n-1)}{2}\sigma'', \quad n = 0,1,2,\ldots \qquad (6)$$

and $\pi(s)$ is defined as:

$$\pi(s) = \frac{\sigma'(s) - \tilde{\tau}(s)}{2} \pm \sqrt{\left(\frac{\sigma'(s) - \tilde{\tau}(s)}{2}\right)^2 - \tilde{\sigma}(s) + k\sigma(s)} \qquad (7)$$

which must have a negative derivative.

Eq. (5) has polynomial solutions $y_n(s)$ that are given by the Rodrigues relation:

$$y_n(s) = \frac{C_n}{\rho(s)}\frac{d^n}{ds^n}\left[\sigma^n(s)\rho(s)\right] \qquad (8)$$

where C_n is the normalization constant and $\rho(s)$ is called the density or weight function and must satisfy the condition:

$$\frac{d}{ds}\left[\sigma(s)\rho(s)\right] = \tau(s)\rho(s) \qquad (9)$$

The function $\pi(s)$ satisfies:

$$\pi(s) = \frac{\sigma'(s) - \tilde{\tau}(s)}{2} \pm \sqrt{\left(\frac{\sigma'(s) - \tilde{\tau}(s)}{2}\right)^2 - \tilde{\sigma}(s) + k\sigma(s)} \qquad (10)$$

where $\tau(s)$ and the parameter λ are defined as:

$$\tau(s) = \tilde{\tau}(s) + 2\pi(s) \tag{11}$$

and

$$\lambda = k + \pi'(s) \tag{12}$$

The function $\pi(s)$ is a polynomial of first degree at most and thus the expression under the square root in Eq. (11) must be a square of a polynomial of first degree. The determination of k is thus important in the calculation of $\pi(s)$. Equating Eq. (12) and with Eq. (6), we obtain the energy eigenvalues.

Solution of the 2D Schrodinger Equation with Energy-Dependent Screened Kratzer Potential

The 2D SE for a charged particle moving in the presence of external magnetic and AB-flux fields with the EDSKP takes the form (Ibrahim, Izam and Jabil, 2023; Rampho et al., 2020):

$$\left(\vec{p} + \frac{e}{c}\vec{A}\right)^2 \psi(\vec{r}) = 2\mu\left[E_{nm} + 2D_e\left(\frac{a}{r}(1+\beta E) - \frac{a^2}{2r^2}(1+\beta E)\right)e^{-\alpha r}\right]\psi(\vec{r}) \tag{13}$$

wherein e and μ are the charge of the particle and reduced mass of the system respectively and E_{nm} is the energy level and $\vec{A}$ is the vector potential that takes the form:

$$\vec{A} = \left(\frac{\vec{B}e^{-\alpha r}}{1-e^{-\alpha r}} + \frac{\Phi_{AB}}{2\pi r}\right)\hat{\phi} \tag{14}$$

where $\vec{B} = B\hat{z}$ is the external magnetic field and $\Phi_{AB} = \eta$ is the additional magnetic flux. In order to solve the 2D SE, we make ansatz of 2D cylindrical wave function as:

$$\psi(\vec{r}) = (2\pi r)^{-\frac{1}{2}}e^{im\phi}\aleph_{nm}(r)m \in \mathbb{Z} = 0, \pm 1, \pm 2, \ldots \tag{15}$$

in which m is the magnetic quantum number. Substituting Eqs. (15) and (14) into Eq. (13), we find

$$\aleph''_{nm}(r) + \begin{bmatrix} \frac{2\mu E_{nm}}{\hbar^2} + \frac{2\mu}{\hbar^2}\left(\frac{2D_e a(1+\beta E)e^{-ar}}{r} - \frac{D_e a^2(1+\beta E)e^{-ar}}{r^2}\right) \\ + \frac{2m\tau\vec{B}e^{-ar}}{\hbar(1-e^{-ar})r} - \frac{\tau^2\vec{B}^2e^{-2ar}}{\hbar^2(1-e^{-ar})^2} - \frac{\tau^2\vec{B}\eta e^{-ar}}{\hbar^2(1-e^{-ar})\pi r} - \frac{\left[(m+\kappa)^2 - \frac{1}{4}\right]a^2}{(1-e^{-ar})^2} \end{bmatrix}\aleph_{nm}(r) = 0 \tag{16}$$

in which following parameters are established as

$$\tau = -\frac{e}{c}, \phi_0 = \frac{hc}{e} \text{ and } \kappa = \frac{\eta}{\phi_0}.$$

For applying the NU technique of Eq. (3), the differential equation in Eq. (16) must be converted into the following hypergeometric-type equation:

$$\aleph''(z) + \frac{\tilde{\tau}}{\sigma}\aleph'(z) + \frac{\tilde{\sigma}}{\sigma^2}\aleph(z) = 0 \tag{17}$$

The solutions of this equation must satisfy $\aleph(0) = 0$ and $\aleph(\infty) \to 0$ boundary conditions. Now the use of the approximation scheme suggested by Greene-Aldrich (Greene and Aldrich, 1976) given as:

$$\frac{1}{r^2} \approx \frac{a^2}{(1-e^{-ar})^2}, \Rightarrow \frac{1}{r} \approx \frac{a}{(1-e^{-ar})} \tag{18}$$

and via the usage of the coordinate-transformation of the form $z = e^{-ar} \in [0,1]$for $[0,\infty]$then substituting Eq. (18) into Eq. (16), We get:

$$\frac{d^2\aleph_{nm}(r)}{dz^2} + \frac{(1-z)}{z(1-z)}\frac{d\aleph_{nm}(r)}{dz} + \frac{1}{z^2(1-z)^2}\begin{bmatrix} -(\varepsilon_{nm} + \Sigma_1 + \Sigma_4)z^2 + (2\varepsilon_{nm} + \Sigma_1 - \Sigma_2 + \Sigma_3 - \Sigma_5)z \\ -(\varepsilon_{nm} + \Sigma_6) \end{bmatrix}\aleph_{nm}(r) = 0 \tag{19}$$

To simplify calculations and make them more convenient, we use the following abbreviations for mathematical purposes.

$$-\varepsilon_{nm} = \frac{2\mu E_{nm}}{\hbar^2 a^2}, \Sigma_1 = \frac{4\mu r_e D_e(1+\beta E)}{\hbar^2}, \Sigma_2 = \frac{2\mu r_e^2 D_e(1+\beta E)}{\hbar^2},$$

$$\Sigma_3 = \frac{2m\tau\vec{B}}{\hbar a}, \Sigma_4 = \frac{\tau^2\vec{B}^2}{\hbar^2 a^2}, \Sigma_5 = \frac{\tau^2\vec{B}\eta}{\hbar^2 a\pi}, \Sigma_6 = (m+\kappa)^2 - \frac{1}{4} \tag{21}$$

comparing Eq. (19) and Eq. (17), we obtain the following polynomials:

$$\tilde{\tau}(z) = 1 - z$$

$$\sigma(z) = z(1-z)$$

$$\tilde{\sigma}(z) = -(\varepsilon_{nm} + \Sigma_1 + \Sigma_4)z^2 + (2\varepsilon_{nm} + \Sigma_1 - \Sigma_2 + \Sigma_3 - \Sigma_5)z - (\varepsilon_{nm} + \Sigma_6) \tag{22}$$

Substituting these polynomials of Eq. (21) into Eq. (11), $\pi(z)$becomes:

$$\pi(z) = -\frac{z}{2} \pm \sqrt{(a-k)z^2 + (b+k)z + c} \tag{23}$$

where

$$a = \frac{1}{4} + \varepsilon_{nm} + \Sigma_1 + \Sigma_4, \qquad b = -(2\varepsilon_{nm} + \Sigma_1 - \Sigma_2 + \Sigma_3 - \Sigma_5)z, \qquad c = \varepsilon_{nm} + \Sigma_6 \tag{24}$$

To determine the constant k, and according with the NU method, the discriminant of the expression under the square-root of the Eq. (22) must be equal to zero. As such, we have that:

$$k_\pm = -(2\Sigma_6 - \Sigma_1 + \Sigma_2 - \Sigma_3 + \Sigma_5) \pm 2\sqrt{\varepsilon_{nm} + \Sigma_6}\sqrt{\frac{1}{4} + \Sigma_2 - \Sigma_3 + \Sigma_4 + \Sigma_5 + \Sigma_6} \tag{25}$$

Substituting Eq. (24) into Eq. (22), we have:

$$\pi(z) = -\frac{z}{2} \pm \begin{cases} (\sqrt{a_2} - \sqrt{a_3})z - \sqrt{a_2} \\ (\sqrt{a_2} + \sqrt{a_3})z - \sqrt{a_2} \end{cases}$$

$$for k_+ = -(a_1) + 2\sqrt{a_2}\sqrt{a_3}$$

$$for k_- = -(a_1) - 2\sqrt{a_2}\sqrt{a_3} \tag{26}$$

where

$$a_1 = 2\Sigma_6 - \Sigma_1 + \Sigma_2 - 3\Sigma_3 + \Sigma_5, \qquad a_2 = \varepsilon_{nm} + \Sigma_6, \qquad a_3 = \frac{1}{4} + \Sigma_2 - \Sigma_3 + \Sigma_4 + \Sigma_5 + \Sigma_6 \tag{27}$$

However, based on the understanding of the NU method, we select the expression $\pi(z)_-$, that indicates the function $\tau(z)$ has a negative derivative. This is given by

$$\pi(z)_- = \sqrt{a_2} - z\left(\frac{1}{2} + \sqrt{a_2} + \sqrt{a_3}\right) \tag{28}$$

and

$$\tau(z) = 1 + 2\sqrt{a_2} - 2z\left(1 + \sqrt{a_2} + \sqrt{a_3}\right) \tag{29}$$

Moreover, the constant λ is obtained from Eq. (12) as follows:

$$\lambda = -(a_1) - 2\sqrt{a_2}\sqrt{a_3} - \left(\frac{1}{2} + \sqrt{a_2} + \sqrt{a_3}\right) \quad (30)$$

If an integer $n \geq 0$, is a unique solution to the hypergeometric-type equation of degree n_r then it can be obtained by considering the equation:

$$\lambda = \lambda_n = -n\tau' - \frac{n(n-1)}{2}\sigma'', (n = 0,1,2\ldots), \quad (31)$$

and $\lambda_m \neq \lambda_n$ for $m = 0,1,2,\ldots,n-1$, then we have

$$\lambda = -(a_1) - 2\sqrt{a_2}\sqrt{a_3} - \left(\frac{1}{2} + \sqrt{a_2} + \sqrt{a_3}\right) = 2n\left(1 + \sqrt{a_2} + \sqrt{a_3}\right) + n(n-1) \quad (32)$$

$$\varepsilon_{nm} = -\Sigma_6 + \left(\frac{\left(n+\frac{1}{2}+\sqrt{\frac{1}{4}+\Sigma_2-\Sigma_3+\Sigma_4+\Sigma_5+\Sigma_6}\right)}{2} - \frac{(\Sigma_1-\Sigma_4-\Sigma_6)}{2\left(n+\frac{1}{2}+\sqrt{\frac{1}{4}+\Sigma_2-\Sigma_3+\Sigma_4+\Sigma_5+\Sigma_6}\right)}\right)^2 \quad (33)$$

(32)

Substituting Eq. (20) into Eq. (27) gives the energy eigenvalues of the energy-dependent screened Kratzer potential in the form:

$$E_{nm} = \frac{\hbar^2 a^2}{2\mu}\left((m+\kappa)^2 - \frac{1}{4}\right) - \frac{\hbar^2 a^2}{2\mu}\left(\frac{(n+\Xi)}{2} - \frac{\left(\frac{4\mu r_e D_e(1+\beta E)}{\hbar^2\alpha} - \frac{\tau^2\vec{B}^2}{\hbar^2 a^2} - (m+\kappa)^2 - \frac{1}{4}\right)}{2(n+\Xi)}\right)^2 \quad (34)$$

$$\Xi = \frac{1}{2} + \sqrt{\frac{2\mu r_e^2 D_e(1+\beta E)}{\hbar^2} - \frac{2m\tau\vec{B}}{\hbar a} + \frac{\tau^2\vec{B}^2}{\hbar^2 a^2} + \frac{\tau^2\vec{B}\eta}{\hbar^2 a\pi} + (m+\kappa)^2} \quad (35)$$

This finding is novel, and to our knowledge, no previous study has reported on this result. Therefore, given that there is no existing literature to compare this study, we focus on investigating the three-dimensional Schrödinger equation of Eq. (33) by substituting $m = \ell + \frac{1}{2}$, where ℓ is the rotational quantum number and $\beta = 0$ we can determine the energy eigenvalues as:

$$E_{n\ell} = \frac{\hbar^2 a^2 \ell(\ell+1)}{2\mu} - \frac{\hbar^2 a^2}{2\mu}\left(\frac{(n+\sigma)}{2} - \frac{\left(\frac{4\mu r_e D_e}{\hbar^2\alpha} - \ell(\ell+1)\right)}{2(n+\sigma)}\right)^2 \quad (36)$$

Where

$$\sigma = \frac{1}{2} + \sqrt{\frac{2\mu r_e^2 D_e}{\hbar^2} + \ell(\ell+1) + \frac{1}{4}} \quad (37)$$

Eq. (35) is very consistent with the energy eigenvalues obtained in Eq. (29) by (Ikot *et al*., 2019).

RESULTS AND DISCUSSION

In this study, we performed numerical computations for the CO diatomic molecule using the fitting parameters: $D_e = 10.842073641$eV, $r_e = 1.1283\,\dot{A}$, $\alpha = 2.29940\,\dot{A}^{-1}$ and $\mu = 6.860586a.m.u$ from Ibekwe et al. (2020). Tables 1–3 present the calculated energy levels of the CO molecule under external fields for various values of the energy slope parameter in the energy-dependent screened Kratzer potential.

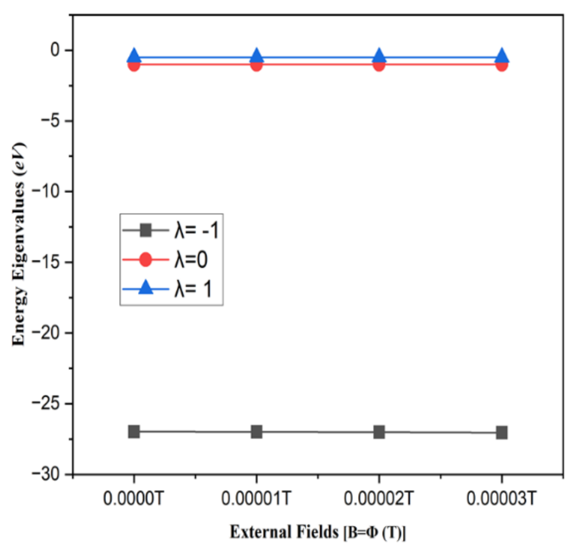

Figure 1: The energy eigenvalues of CO diatomic molecule as a function of External fields

Table 1: Energy Levels $(E_{nm})$of Carbon Monoxide (CO)under the influence of Magnetic and AB-flux Fields when Energy slope Parameter is $\beta = -1$

	$\vec{B} = \vec{\eta} = 0T$		$\vec{B} = \vec{\eta} = 0.00001T$		$\vec{B} = \vec{\eta} = 0.00002T$		$\vec{B} = \vec{\eta} = 0.00003T$	
n	$m = 0$	$m = 1$	$m = 0$	$m = 1$	$m = 0$	$m = 1$	$m = 0$	$m = 1$
0	-27.00588589	-26.97354320	-27.01113985	-26.98435164	-27.02690157	-27.00566820	-27.05317064	-27.03749226
1	-38.13794425	-38.10083597	-38.14400773	-38.11331072	-38.16219751	-38.13791245	-38.19251174	-38.17463856
2	-53.02917092	-52.98784863	-53.03595023	-53.00179668	-53.05628718	-53.02930324	-53.09017895	-53.07036439
3	-72.21519943	-72.17037594	-72.22257353	-72.18554795	-72.24469470	-72.21546798	-72.28155968	-72.26013150

Table 2: Energy Levels $(E_{nm})$of Carbon Monoxide (CO)under the influence of Magnetic and AB-flux Fields when Energy slope Parameter is $\beta = 0$

	$\vec{B} = \vec{\eta} = 0T$		$\vec{B} = \vec{\eta} = 0.00001T$		$\vec{B} = \vec{\eta} = 0.00002T$		$\vec{B} = \vec{\eta} = 0.00003T$	
n	$m = 0$	$m = 1$	$m = 0$	$m = 1$	$m = 0$	$m = 1$	$m = 0$	$m = 1$
0	-0.9931115857	-0.9918542620	-0.9933192185	-0.9922814794	-0.9939422212	-0.9931242623	-0.9949809302	- 0.9943830518
1	-1.064891417	-1.063645049	-1.065105503	-1.064085597	-1.065747864	-1.064954613	-1.066818832	-1.066252531
2	-1.138872806	-1.137637251	-1.139093264	-1.138090968	-1.139754739	-1.138985892	-1.140857559	-1.140322451
3	-1.215029997	-1.213805118	-1.215256748	-1.214271845	-1.215937099	-1.215192360	-1.217071373	-1.216567084

Table 3: Energy Levels $(E_{nm})$of Carbon Monoxide (CO)under the influence of Magnetic and AB-flux Fields when Energy slope Parameter is $\beta = 1$

	$\vec{B} = \vec{\eta} = 0T$		$\vec{B} = \vec{\eta} = 0.00001T$		$\vec{B} = \vec{\eta} = 0.00002T$		$\vec{B} = \vec{\eta} = 0.00003T$	
n	$m = 0$	$m = 1$	$m = 0$	$m = 1$	$m = 0$	$m = 1$	$m = 0$	$m = 1$
0	-0.5020559707	-0.5014228710	-0.5021613957	-0.5016398391	-0.5024777845	-0.5020679670	-0.5030054802	-0.5027077112
1	-0.5272944521	-0.5266851900	-0.5274018690	-0.5269062989	-0.5277242382	-0.5273425617	-0.5282619180	-0.5279944549
2	-0.5523297851	-0.5517442739	-0.5524391044	-0.5519693459	-0.5527671861	-0.5524133884	-0.5533144046	-0.5530768995
3	-0.5771053774	-0.5765435658	-0.5772165042	-0.5767724127	-0.5775500140	-0.5772238584	-0.5781062989	-0.5778984242

In tables 1 – 3, it is observed that for a given quantum states (n and m),the energy of CO diatomic molecule decreases as the magnetic and AB-flux fields increases. However, if one pays close attention to the behavior of the energy spectra as it varies with the energy slope parameterβ. It is immediately evident that the energy increases with a positive value of the energy slope parameter. This trend is also depicted in Figure 1, in which we plot the behavior of the energy eigenvalues of CO diatomic molecule as a function of the magnetic and AB-flux fields. One also can observe that the energy increases with a positive value of the energy slope parameter.

CONCLUSION

This work presents the effect of magnetic and AB-flux fields on the energy levels of a CO diatomic molecule. The Schrödinger equation is solved using the Nikiforov-Uvarov method within an energy-dependent screened Kratzer potential framework. The results reveal that energy eigenvalues decrease with increasing magnetic and AB-flux fields, indicating a stabilization of bound states due to external field interaction. Conversely, the increase in energy with a positive energy slope parameter demonstrates that energy-dependent potentials can induce a stiffer interaction, elevating energy levels. These effects are graphically confirmed in Fig. 1, validating the theoretical predictions. The physical meaning of these findings lies in understanding how external fields modify molecular behavior-stabilizing or energizing the system depending on parameter tuning. This offers valuable insight into field-controlled quantum systems. The relevance of this study extends to high-field physics, quantum control applications, and molecular spectroscopy, particularly in environments with confined or engineered electromagnetic conditions. The ability to adjust molecular energy levels via external parameters makes these systems potential candidates for sensor design, coherent quantum control, and reactive molecular engineering. Additionally, by manipulating potential parameters, the well-known screened Kratzer potential is recovered, and in the absence of fields, the model reduces to the standard three-dimensional Schrödinger equation, aligning well with existing literature. These findings encourage future investigations into more complex molecular systems influenced by quantum field effects.

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