



Combined effect of AB-flux field and inverse square plus Yukawa potential on diatomic molecules placed at point-like global monopole

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Abstract This paper aims to investigate the combined effect of AB-flux field and inverse square plus Yukawa potential (ISPYP) on the bound state energy levels of diatomic molecules placed at point-like global monopole. Asymptotic iteration method has been employed for numerical calculations. Same quantum system with Kratzer–Feus potential, a particular case of ISPYP, is also discussed here. Pekeris approximation scheme is used to deal with the terms $\frac{1}{r^2}$ and $\frac{1}{r}$.

1 Introduction

During the last two decades, a number of relativistic and non-relativistic investigations have been done on the effect of point-like global monopole (PGM) topological defects on energy spectrum of quantum systems, like diatomic molecules, embedded with some potential fields [1–6]. Some well-known topological defects like domain wall [7], cosmic string [8–11] and global monopole [5, 12–14] have been extensively studied. Shaikh et al. (2023) have discussed on various curvature-restricted geometric properties of PGM spacetime in detail in their recent research work [15]. Some Grand Unified Theories suggest that in the very early stages of the cosmos, topological defects formed during phase transitions via a spontaneous symmetry-breaking mechanism [16, 17]. A global monopole is a heavy object and characterized by spherical symmetry and divergent mass. Some investigations have been done on global monopole in the context of general relativity and quantum mechanical systems [18–27]. Barriola and Vilenkin introduced the concept of the global monopole spacetime in 1989 [28].

In this article, we consider inverse square plus Yukawa potential (ISPYP), combination of inverse quadratic potential and Yukawa potential, which can be expressed by:

$$V_{\text{ISPYP}}(r) = \frac{A}{r^2} + \frac{B}{r} e^{-\mu r}. \quad (1)$$

Here $A = D_0 r_e^2$, $B = -2D_0 r_e$, μ is the screening parameter, D_e is the dissociation energy, r_e is the equilibrium inter-nuclear distance. Though inverse square potential $\frac{A}{r^2}$ has singular features, it has received an immense importance in the field of quantum mechanics [29–39]. This potential is studied in various areas of physics such as Efimov effect [30], dipole-bound anions in polar molecules [31–33], atoms interacting with a charged wire [34, 35], the analysis of the near-horizon structure of black holes [36–38] and the interaction of a dipole in a cosmic string background [39]. The Yukawa potential describes strong interaction between nucleons and it goes down exponentially for larger r . An extensive amount of research has been done on Yukawa potential. Ugalde et al. [40] have calculated the full configuration-interaction energies of the hydrogen anion and the hydrogen molecule when their electrons and nuclei interact through the Yukawa potential. Recently, Ramantswana et al. [41] investigated the thermodynamic properties of some diatomic molecules like CrH, NiC and CuLi under a potential field which is the linear combination of Hulthen and Yukawa potentials. The study was made in the presence as well as in the absence of magnetic and Aharonov-Bohm (AB-flux) fields. They solved the Schrödinger equation in 3D and 2D under the framework of Nikiforov–Uvarov (NU) method and the exact quantization rule (EQR), respectively.

The above potential (1) reduces into Kratzer–Feus potential (KFP) [42–44] when the screening parameter μ takes the value 0:

$$V_{\text{KFP}}(r) = \frac{A}{r^2} + \frac{B}{r}, \quad (2)$$

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i.e., Kratzer–Feus potential is the linear combination of inverse square potential and Coulomb potential. This potential model describes internuclear vibration of a diatomic molecule. Aygun et al. [45] have derived the exact and iterative solutions of the radial Schrödinger equation for a class of potentials $V(r) = \frac{A}{r^2} - \frac{B}{r} + Cr^\kappa$ for various values of κ from -2 to 2 and for any (n, l) -th quantum states. They have also discussed about the particular situation when $C = 0$ but for arbitrary values of A and B . Yalcin et al. [46], Ikhdaïr et al. [47], Shi-hai Dong and Gus-hua Sun [48] investigated on different eigenvalue-related problems and solved Schrödinger equation with the KF potential using some standard methods. It is evident that molecular vibration and rotational spectroscopy have extensive research applications in fields such as biology and environmental science [49]. Various methods like smooth transformation [50, 51], the algebraic approach [52, 53] and series expansion method [54] have been used to study the diatomic molecular potential (2).

The present paper investigated a quantum system installed in a flux field with inverse square plus Yukawa (ISPY) potential and a point-like global monopole spacetime in the curvature. The topological characteristic of the spacetime originated from a point-like global monopole and the combined effect of the flux field with ISPY potential affects the energy spectrum of the quantum system. This system is thoroughly explored in the present investigation, and the same quantum system with Kratzer–Feus potential is presented.

This present paper has been designed in the following manner: Sect. 2 provides a brief overview of the asymptotic iteration method (AIM). In Sect. 3, we discuss the theory of the present problem in detail. Section 4 is devoted to presenting the results and discussing them and in the last section we have made concluding remarks.

2 A brief description of asymptotic iteration method (AIM)

There are some methods like Nikiforov–Uvarov and its functional analysis method, asymptotic iteration method (AIM), supersymmetric quantum mechanics (SUSTQM), quantization rule, Laplace transform and many more available in the literature to solve exact and approximate eigenvalue solutions of the wave equations with potential of various kinds. In the present article, we are interested on asymptotic iteration method (AIM). This method was developed by Ciftci, Hall and Saad [55, 56] and is a very effective technique to solve the non-relativistic radial Schrödinger equation associated with some eigenvalue problems in quantum mechanics. Denoting $\frac{d^2 y}{dx^2}$ by $y''(x)$ and considering the homogeneous linear second-order differential equation of the form:

$$u''(x) = \lambda_0(x)u'(x) + s_0(x)u(x), \quad (3)$$

where $\lambda_0(x) (\neq 0)$ and $s_0(x)$ be the coefficients of $u'(x)$ and $u(x)$, respectively, and they belong to the class of C^∞ functions [56, 57]. The function $s_0(x)$ has sufficiently many continuous derivatives with respect to x . Taking differentiation of Eq. (3) with respect to x , we get,

$$u'''(x) = \lambda_1(x)u'(x) + s_1(x)u(x), \quad (4)$$

where

$$\lambda_1(x) = \lambda_0'(x) + s_0(x) + \lambda_0^2(x); \quad s_1(x) = s_0'(x) + \lambda_0(x)s_0(x). \quad (5)$$

Again differentiating Eq. (4) with respect to x , we get,

$$u''''(x) = \lambda_2(x)u'(x) + s_2(x)u(x), \quad (6)$$

where $\lambda_2(x) = \lambda_1'(x) + s_1(x) + \lambda_1^2(x)$ and $s_2(x) = s_1'(x) + \lambda_1(x)s_1(x)$.

Continuing the same process, we shall get,

$$\begin{aligned} u^{p+1}(x) &= \lambda_{p-1}(x)u'(x) + s_{p-1}(x)u(x), \\ u^{p+2}(x) &= \lambda_p(x)u'(x) + s_p(x)u(x), \end{aligned} \quad (7)$$

where

$$\begin{aligned} \lambda_p(x) &= \lambda_{p-1}'(x) + s_{p-1}(x) + \lambda_{p-1}^2(x) \\ s_p(x) &= s_{p-1}'(x) + s_{p-1}(x)\lambda_{p-1}(x), \quad p = 1, 2, 3, \dots \end{aligned} \quad (8)$$

Now from the ratio of the $(p+2)$ -th and $(p+1)$ -th derivatives, we have,

$$\frac{d}{dx} \ln(u^{p+1}(x)) = \frac{u^{p+2}(x)}{u^{p+1}(x)} = \frac{\lambda_p(x)[u'(x) + \frac{s_p(x)}{\lambda_p(x)}u(x)]}{\lambda_{p-1}(x)[u'(x) + \frac{s_{p-1}(x)}{\lambda_{p-1}(x)}u(x)]} \quad (9)$$

Now introducing the asymptotic condition, i.e., for large values of $p > 0$, we get the relation,

$$\frac{s_p}{\lambda_p} = \frac{s_{p-1}}{\lambda_{p-1}} = \beta(x), \quad p = 1, 2, 3, \dots \quad (10)$$

Here $\beta(x)$ is either a function of x or a constant. From Eqs. (9) and (10), we have,

$$\frac{d}{dx} \ln(u^{p+1}(x)) = \frac{\lambda_p(x)}{\lambda_{p-1}(x)} \tag{11}$$

Equation (11) gives,

$$\begin{aligned} u'(x) + \frac{s_{p-1}}{\lambda_{p-1}}u(x) &= D_1 \exp\left(\int^x (\beta + \lambda_0)dt\right), \text{ from (13)} \\ \Rightarrow u'(x) + \beta(x)u(x) &= D_1 \exp\left(\int^x (\beta + \lambda_0)dt\right), \text{ using (10)} \end{aligned}$$

where D_1 is the integration constant.

After doing some calculations, the general solution of Eq. (3) becomes,

$$u(x) = D_2 \exp\left(-\int^x \beta(t)dt\right) + D_1 \exp\left(-\int^x \beta(t)dt\right) \int^x \exp\left(\int^t [\lambda_0(\kappa) + 2\beta(\kappa)]d\kappa\right)dt, \tag{12}$$

provided the quantization condition,

$$\delta_p(x) = \det \begin{bmatrix} \lambda_p(x) & s_p(x) \\ \lambda_{p-1}(x) & s_{p-1}(x) \end{bmatrix} = 0 \tag{13}$$

holds. The energy eigenvalues are obtained from the above quantization rule (13), if the problem is exactly solvable.

Next, we shall give an idea of eigenfunction from Eq. (3). Putting the homogeneous linear second-order differential Eq. (3) in the following form [55, 58]:

$$u''(x) = 2 \left[\frac{\tau_1 x^{j+1}}{1 - \tau_2 x^{j+2}} - \frac{\chi + 1}{x} \right] u'(x) - \frac{\Omega x^j}{1 - \tau_2 x^{j+2}} u(x). \tag{14}$$

Here j is an integer, χ is real and Ω, τ_1, τ_2 are the coefficients of x^j, x^{j+1} and x^{j+2} , respectively. Then, the exact solution of the above equation can be represented as:

$$u(x) = (-1)^n C_{nl} (j + 2)^n (\sigma)_n {}_2F_1(-n, \rho + n; \sigma; \tau_2 x^{j+2}), \tag{15}$$

where ${}_2F_1$ is the hypergeometric function, C_{nl} is the normalization constant and $(\sigma)_n = \frac{\Gamma(\sigma+n)}{\Gamma(\sigma)}, \rho = \frac{(2\Delta+1)\tau_2+2\tau_1}{(j+2)\tau_2}$ and $\sigma = \frac{2\Delta+j+3}{j+2}$.

3 Theory

The line element of point-like global monopole (PGM) spacetime in spherical coordinates is described as

$$ds_{3D}^2 = \frac{dr^2}{\alpha^2} + r^2 d\theta^2 + r^2 \sin^2\theta d\phi^2, \tag{16}$$

which can be expressed as $ds_{3D}^2 = g_{pq} dx^p dx^q, p, q = 1, 2, 3$ [59–63]. Now, the metric tensors g_{pq} and g^{pq} for the point-like global monopole space-time are

$$g_{pq} = \begin{bmatrix} \frac{1}{\alpha^2} & 0 & 0 \\ 0 & r^2 & 0 \\ 0 & 0 & r^2 \sin^2\theta \end{bmatrix} \text{ and } g^{pq} = \begin{bmatrix} \alpha^2 & 0 & 0 \\ 0 & \frac{1}{r^2} & 0 \\ 0 & 0 & \frac{1}{r^2 \sin^2\theta} \end{bmatrix}. \tag{17}$$

The metric of a three-dimensional sphere is denoted by ds_{3D} and $t \in (-\infty, +\infty), r \in [0, +\infty), \theta \in [0, \frac{\pi}{2}], \phi \in [0, 2\pi)$. Also, $g_{pq} = 0$, for $p \neq q$ means line element of PGM is static, spherically symmetric in coordinates (t, r, θ, ϕ) . The component t is called the time-like component and the other three components r, θ, ϕ are called the spatial components. Here, the topological defect parameter α is connected with the energy scale of symmetry breaking dimensionless parameter η_0 by the relation $\alpha^2 = (1 - 8\pi\eta_0^2)$ [64] and its value is less than 1. It should be noted that, when α tends to 1, the manifold becomes a Minkowski flat space line element, named for the German mathematician Hermann Minkowski (1864-1909), which is a four-dimensional spacetime with a nondegenerate, symmetric bilinear form. Since the Minkowski space provides the natural mathematical background of the special theory of relativity [65], it plays an integral part in contemporary physics. The fact that there are no gravitational fields surrounding the nearby non-relativistic matter in the PGM geometry. This PGM feature aids in measuring some global effects of this geometry broadly. Mazur and Papavassiliou, for instance, estimated the scattering amplitude and the total scattering cross section of mass-less bosonic particles propagating through a global monopole’s gravitational field [66]. On the other hand, H. Ren accurately measured the scattering amplitude of fermions in a global monopole background metric [67]. PGM is not globally flat and has a naked curvature singularity on the axis given by the Ricci scalar, $R = R^\kappa_\kappa = \frac{2(1-\alpha^2)}{r^2}$. In this manifold the surface area of a sphere of radius r is

not $4\pi r^2$. The value of the actual area is $4\pi\alpha^2 r^2$ which is less than $4\pi r^2$. Hence, there is a solid angle deficit $\nabla\Omega = 32\pi^2\eta_0^2$. The surface $\theta = \frac{\pi}{2}$ presents the geometry of a cone, a 3-dimensional geometric shape with a flat and curved surface pointed toward the top, with the deficit angle $\nabla\phi = 8\pi^2\eta_0^2$ and there is no Newtonian-like gravitational potential $g_{tt} = -1$. These are some notable features of a point-like global monopole [68–71].

3.1 Non-relativistic Schrödinger equation of a quantum system confined by AB-flux field with ISPYP or KFP

The time dependent, non-relativistic Schrödinger equation of the present quantum system is given by [1, 59–62]

$$\left[-\frac{D_p(\sqrt{g}g^{pq}D_q)}{2M\sqrt{g}} + V_{eff}(r) \right] \Psi(t, r, \theta, \phi) = i \frac{\partial}{\partial t} \Psi(t, r, \theta, \phi); \quad D_i \equiv \partial_i - ieA_p; \quad p, q = 1, 2, 3 \tag{18}$$

Here e is the electric charge, M denotes the reduced mass of the particle, $g = |g_{pq}| = \frac{r^4 \sin^2\theta}{\alpha^2}$ is the determinant of the metric tensor g_{pq} which contains the topological defect parameter α . If Φ_{mf} and $\Phi_0 (= \frac{2\pi\hbar^2}{e})$ represent the amount of magnetic flux and quantum of magnetic flux, respectively, then the Aharonov-Bohm magnetic flux is expressed as $\Phi = \Phi_{mf}\Phi_0$. Magnetic flux quantum is a property of a superconducting electrical current which tells that the magnetic flux passing through any area bounded by such a current is quantized. It may occur in a superconducting ring such as a hollow cylinder. Inverse of the quantum of magnetic flux is known as Josephson constant and it is denoted by K_J . A_p is the component of the electromagnetic three-vector potential $\mathbf{A} = (A_r, A_\theta, A_\phi) = (0, 0, \frac{\Phi}{2\pi r \sin\theta})$. \mathbf{A} has no radial or θ components. Applying separation of variable method and choosing the wave function $\Psi_{nlm}(r) = e^{-iE_{nl}t} r^{-1} R_{nl}(r) Y_{lm}(\theta, \phi)$, where E_{nl} is the energy eigenvalues for the (n, l) -th state of a quantum particle, $Y_{lm}(\theta, \phi)$ is the spherical harmonic functions, Eq. (18) takes the form:

$$\frac{d^2 R_{nl}(r)}{dr^2} + \frac{2M}{\hbar^2\alpha^2} \left[E_{nl} - V_{ISPYP}(r) - \frac{\hbar^2 l'(l'+1)}{2Mr^2} \right] R_{nl}(r) = 0, \tag{19}$$

which is the radial part of the non-relativistic Schrödinger equation. Here n is the principal quantum number, l is angular momentum quantum number, m is the magnetic quantum number, $l' (= l - \Phi)$ is known as effective orbital quantum number and its value depends on the flux field. Ahmed (2023) has explained the process of shifting in the quantum number $l \rightarrow l'$ in his paper [72]. \hbar denotes the reduced Planck’s constant, $l = 0$ for a non-rotational state or s-wave state and $l \neq 0$ for a rotational state.

Substituting the value of $V_{ISPYP}(r)$ from (1) in Eq. (19), we have,

$$\frac{d^2 R_{nl}(r)}{dr^2} + \frac{2M}{\hbar^2\alpha^2} \left[E_{nl} - \frac{A}{r^2} - \frac{B}{r} e^{-\mu r} - \frac{\hbar^2 l'(l'+1)}{2Mr^2} \right] R_{nl}(r) = 0, \tag{20}$$

The effective potential of the present quantum system is given by:

$$\begin{aligned} V_{eff}(r) &= \frac{1}{\alpha^2} \left[\frac{A}{r^2} + \frac{B}{r} e^{-\mu r} + \frac{\hbar^2 l'(l'+1)}{2Mr^2} \right], \quad A = D_0 r_e^2, \quad B = -2D_0 r_e \\ &= \frac{1}{\alpha^2} \left[\frac{A}{r^2} + \frac{B}{r} e^{-\mu r} + \frac{\hbar^2 (l - \Phi)(l - \Phi + 1)}{2Mr^2} \right]. \end{aligned} \tag{21}$$

Due to the presence of the centrifugal barrier term $\frac{\hbar^2 l'(l'+1)}{2Mr^2}$, it is quite difficult to solve Eq. (20) in exact way for nonzero values of l . So we have considered the Pekeris approximation scheme, the most widely known approximation and with good degree of accuracy, for arbitrary l state [73]. The approximations for $\frac{1}{r^2}$ and $\frac{1}{r}$ are:

$$\frac{1}{r^2} \approx \frac{4\mu^2 e^{-2\mu r}}{(1 - e^{-2\mu r})^2}; \quad \frac{1}{r} \approx \frac{2\mu e^{-\mu r}}{(1 - e^{-2\mu r})}. \tag{22}$$

Using Pekeris approximation, Eq. (20) transforms into:

$$\frac{d^2 R_{nl}(r)}{dr^2} + \left[\frac{2M}{\hbar^2\alpha^2} E_{nl} - 4\mu^2 \left(\frac{2MA}{\hbar^2\alpha^2} + \frac{l'(l'+1)}{\alpha^2} \right) \frac{e^{-2\mu r}}{(1 - e^{-2\mu r})^2} - \frac{4MB\mu}{\hbar^2\alpha^2} \frac{e^{-2\mu r}}{(1 - e^{-2\mu r})} \right] R_{nl}(r) = 0, \tag{23}$$

Now, considering the transformation $\frac{1}{\Xi} = e^{-2\mu r} - 1$, Eq. (20) reduces to

$$\frac{d^2 R_{nl}(\Xi)}{d\Xi^2} + \frac{(2\Xi + 1)}{\Xi(\Xi + 1)} \frac{dR_{nl}(\Xi)}{d\Xi} + \left[\frac{\Lambda + \zeta\Xi + \xi\Xi^2}{\Xi^2(\Xi + 1)^2} \right] R_{nl}(\Xi) = 0 \tag{24}$$

where

$$\zeta - \Lambda - \xi = -\frac{2ME_{nl}}{4\mu^2\hbar^2\alpha^2}; \tag{25}$$

$$\zeta - \xi = \frac{MB}{\hbar^2\alpha^2\mu}; \tag{26}$$

Table 1 Spectroscopic constants of the diatomic molecules studied in the present work [42–44, 74, 75]

Molecules	$D_e(eV)$	$r_e(\text{Å})$	$a(\text{Å}^{-1})$	$M(\text{amu})$
H ₂	4.7446	0.7416	1.9426	0.50391
LiH	2.5152674654	1.5956	1.1280	0.8801221
CO	11.2256	1.1283	2.2994	6.860586
HCl	4.619031371	1.2746	1.8677	0.9801045
NO	8.0437306664	1.1508	2.75340	7.468441
N ₂	11.9381950238	1.0940	2.69860	7.00335
ScH	2.25	1.776	1.41113	0.986040
O ₂	5.156658828	1.208		7.997457504

$$-\xi = \frac{1}{\alpha^2} \left[\frac{2MA}{\hbar^2} + l'(l' + 1) \right] \tag{27}$$

We shall solve the radial Schrodinger equation under the framework of asymptotic iteration method. For this reason, we convert Eq. (24) in the form (3) by taking the transformation $R_{nl}(\Xi) = \Xi^\omega(\Xi + 1)^\beta u_{nl}(\Xi)$ and we have [55, 74, 75],

$$\frac{d^2 u_{nl}(\Xi)}{d\Xi^2} = \left[-\frac{2\beta + 1}{\Xi + 1} - \frac{2\omega + 1}{\Xi} \right] \frac{du_{nl}(\Xi)}{d\Xi} - \frac{(\beta + \omega)^2 + (\beta + \omega) + \xi}{\Xi(\Xi + 1)} u_{nl}(\Xi). \tag{28}$$

Comparing this equation with (3), we get,

$$\begin{aligned} \lambda_0 &= -\frac{2\beta + 1}{\Xi + 1} - \frac{2\omega + 1}{\Xi}, \\ s_0 &= -\frac{(\beta + \omega)^2 + (\beta + \omega) + \xi}{\Xi(\Xi + 1)}. \end{aligned} \tag{29}$$

Following the AIM, we can evaluate the values of λ_1 and s_1 from the relation (5). Using the recurrence relation (8), we obtain $\omega_n^2 = -\Lambda$, $\beta_n^2 = \zeta - \Lambda - \xi$. After finding out the values of β_n and ω_n from the above expressions, we determine the energy eigenvalues of a quantum system under the influence of AB-flux field with ISPYP or KFP in a point-like defect space-time which is stated below.

If $\delta_1 = (n + \frac{1}{2}) + \frac{1}{2}\sqrt{1 - 4\xi}$ and $\delta_2 = \frac{MB}{\alpha^2 \hbar^2}$, then,

Case I: for nonzero values of μ , i.e., when the particles are embedded with ISPYP:

$$E_{nl} = -2\mu B - \frac{\alpha^2 \hbar^2}{2M} \left[\frac{\mu \delta_1^2 - \delta_2}{\delta_1} \right]^2, \tag{30}$$

provided $\sqrt{1 - 4\xi} > 0$ and ξ is given by Eq. (27).

Case II: When $\mu = 0$, i.e., when the molecules are in Kratzer–Feus potential field:

$$E_{nl} = -\frac{\alpha^2 \hbar^2}{2M} \left[\frac{\delta_2}{\delta_1} \right]^2 \tag{31}$$

provided $\sqrt{1 - 4\xi} > 0$ and ξ is given by Eq. (27), $0 < \alpha < 1$.

Comparing Eqs. (14) and (28) to estimate the eigenfunction of the quantum system, we get,

$$\begin{aligned} j &= -1, \tau_1 = -(\beta + 1/2), \tau_2 = -1, \chi = \omega - 1/2, \sigma = 2\omega + 1, \\ \rho &= 2(\beta + \omega) + 1, \Omega = (\beta + \omega)^2 + (\beta + \omega) + \xi, (\sigma)_n = \frac{(2\omega + n)!}{(2\omega)!}. \end{aligned} \tag{32}$$

$$u_{nl}(\Xi) = (-1)^n C_{nl} \frac{(2\omega + n)!}{(2\omega)!} {}_2F_1(-n, 2\beta + 2\omega + n + 1; 2\omega + 1; -\Xi) \tag{33}$$

Hence, the radial part of the required wave function is given by:

$$\begin{aligned} R_{nl}(\Xi) &= \Xi^\omega(\Xi + 1)^\beta u_{nl}(\Xi) \\ &= (-1)^n C_{nl} \frac{(2\omega + n)!}{(2\omega)!} \Xi^\omega(\Xi + 1)^\beta {}_2F_1(-n, 2\beta + 2\omega + n + 1; 2\omega + 1; -\Xi), \end{aligned} \tag{34}$$

where $\Xi^\omega(\Xi + 1)^\beta = \frac{e^{-\mu\beta r}}{(e^{-\mu r} - 1)^{\beta + \omega}}$ and C_{nl} is the normalization constant.

Table 2 Energy eigen values $-E_{nl}$ (in a.u.) of NO, LiH, O₂ and HCl diatomic molecules with Kratzer–Feus potential ($\mu = 0$ in (1)) and $\alpha = 1$, $\Phi = 0$. Here Ref [A]: Doma et al. [42], Ref [B]: Bayrak et al. [43] and Ref [C]: Ibekwe et al. [44]

n	l	Present	Ref [A]	Ref [B]	Present	Ref [A]	Ref [C]
<i>NO</i>				<i>LiH</i>			
0	0	8.0026074754	8.002659243972	8.002659417	2.4672940275	2.467310100790	2.467293680
1	0	7.9214048204	7.921456323005	7.921456839	2.3758028803	2.375818641757	2.380989203
	1	7.9209918062	7.921043308747	7.921043834	2.3740916250	2.374107386003	2.380416619
2	0	7.8414318719	7.841483108610	7.841483956	2.2893079133	2.289323364637	2.281213703
	2	7.8402116722	7.840262908797	7.840263771	2.2844588261	2.284474275211	2.279603547
3	0	7.7626639249	7.762714895928	7.762716066	2.2074518617	2.207467005759	2.187580925
	1	7.7622632629	7.762314233959	7.762315413	2.2059192063	2.205934349403	2.187076666
	3	7.7602605765	7.760311547121	7.760312744	2.1982882758	2.198303413947	2.184558925
4	0	7.6850768917	7.685127597398	7.685129079	2.1299088333	2.129923673518	2.099596786
	2	7.6838930036	7.683943708988	7.683945203	2.1255570259	2.125571862731	2.098175007
	4	7.6811320240	7.681182728848	7.681184246	2.1154731143	2.115487942686	2.094865172
5	0	7.6086472837	7.608697724344	7.608699509	2.0563810592	2.056395599696	2.016815899
	1	7.6082584864	7.608308926962	7.608310719	2.0550029903	2.055017529518	2.016369515
	3	7.6063151001	7.606365540115	7.606367349	2.0481409852	2.048155517864	2.014140642
	5	7.6028195231	7.602869962094	7.602871795	2.0359071693	2.035921689479	2.010141421
<i>O₂</i>				<i>HCl</i>			
0	0	5.1263584908	5.126358490795	5.126358625	4.5418183307	4.541847883485	4.574322886
1	0	5.0666407664	5.066640766392	5.066641151	4.3936979749	4.393727026093	4.402122552
	1	5.0662919381	5.066291938130	5.066292323	4.3912638500	4.391292900595	4.401308521
2	0	5.0079604876	5.007960487581	5.007961116	4.2527070862	4.252735638062	4.239466022
	2	5.0069322711	5.006932271122	5.006932904	4.2457609739	4.245789522965	4.237158875
3	0	4.9502937621	4.950293762100	4.950294624	4.1183953496	4.118423405560	4.085660853
	1	4.9499568798	4.949956879787	4.949957740	4.1161863514	4.116214406181	4.084933001
	3	4.9482731593	4.948273159303	4.948274034	4.1051773314	4.105205379915	4.081297704
4	0	4.8936173815	4.893617381542	4.893618469	3.9903474504	3.990375014951	3.940076275
	2	4.8926241763	4.892624176321	4.892625268	3.9840338609	3.984061421100	3.938009125
	4	4.8903082750	4.890308274954	4.890309388	3.9693810195	3.969408569017	3.933194375
5	0	4.8379087980	4.837908798004	4.837910103	3.8681798599	3.868206938397	3.802136724
	1	4.8375833223	4.837583322339	4.837584627	3.8661690607	3.866196137622	3.801483303
	3	4.8359566060	4.835956606018	4.835957923	3.8561470638	3.856174132198	3.798219664
	5	4.8330312942	4.833031294198	4.833032637	3.8382407871	3.838267839519	3.792359570

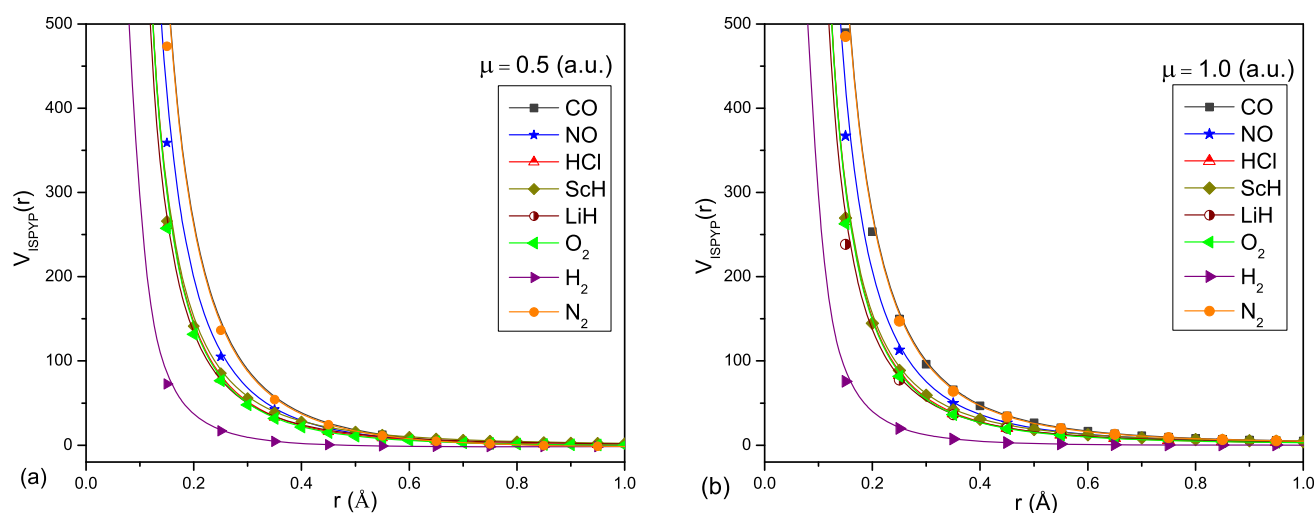
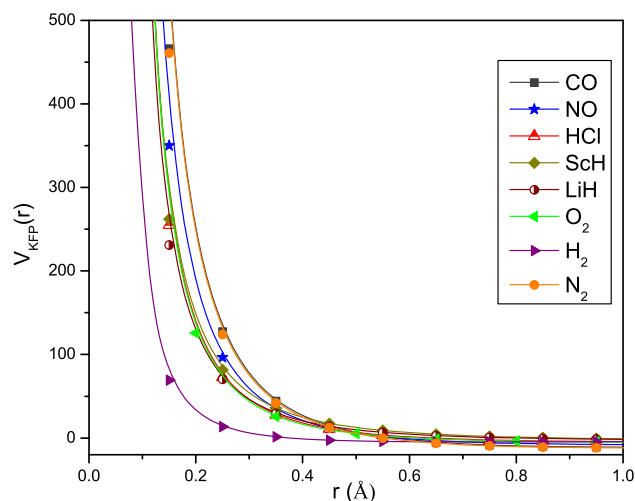


Fig. 1 Inverse square plus Yukawa potential (ISPYP) (1) of the diatomic molecules CO, NO, HCl, ScH, LiH, O₂, H₂, N₂ as a function of r corresponding to (a) $\mu = 0.05$ and (b) $\mu = 1.0$

Table 3 Energy eigen values $-E_{nl}$ (in a.u.) of N_2 , H_2 , CO and ScH diatomic molecules with Kratzer–Feus potential ($\mu = 0$ in (1)) and $\alpha = 1$, $\Phi = 0$. Here Ref [A]: Doma et al. [42]

n	l	N_2		H_2		CO	ScH
		Present	Ref [A]	Present	Ref [A]	Present	Present
0	0	11.8837582290	11.883835079230	4.5591689267	4.559168926667	11.1738890089	2.2114491348
1	0	11.7761178902	11.776194388350	4.2226548035	4.222654803490	11.0716504302	2.1375724919
	1	11.7756293083	11.775705806490	4.2100312296	4.210031229642	11.0711816427	2.1363286701
2	0	11.6699334273	11.670009573639	3.9220682103	3.922068210280	10.9708086490	2.0673368823
	2	11.6684875814	11.668563727603	3.8883646257	3.888364625659	10.9694215738	2.0637918839
3	0	11.5651787034	11.565254498035	3.6524710393	3.652471039349	10.8713383363	2.0005069123
	1	11.5647031900	11.564778984589	3.6423143472	3.642314347183	10.8708822132	1.9993807703
	3	11.5623262119	11.562402006115	3.5923950085	3.592395008530	10.8686021739	1.9937693105
4	0	11.4618281651	11.461903608392	3.4097453298	3.409745329792	10.7732147349	1.9368659083
	2	11.4604208199	11.460496262923	3.3824130533	3.382413053252	10.7718649629	1.9336510161
	4	11.4571383650	11.457213807350	3.3203827164	3.320382716359	10.7687168168	1.9261917425
5	0	11.3598568276	11.359919199001	3.1904350789	3.190435078929	10.6764136433	1.8762141578
	1	11.3593939207	11.359469012927	3.1821421825	3.182142182497	10.6759697325	1.8751913066
	3	11.3570799558	11.357155047390	3.1413502461	3.141350246076	10.6737507352	1.8700941284
	5	11.3529172085	11.352992299136	3.0706347580	3.070634758033	10.6697588786	1.8609903316

Fig. 2 Kratzer–Feus Potential (KFP) (2) of the diatomic molecules CO, NO, HCl, ScH, LiH, O_2 , H_2 , N_2 as a function of r 

4 Results and discussion

Inverse square plus Yukawa potential (ISPYP) (1) and Kratzer–Feus potential (KFP) (2) curves of the diatomic molecules CO, NO, HCl, ScH, LiH, O_2 , H_2 , N_2 as a function of r are plotted in Figs. 1 and 2, respectively. ISPY potential curves are drawn for two different values of $\mu = 0.5$ and $\mu = 1.0$. Figure 3 illustrates profiles of effective potential (21) for the diatomic molecules as a function of r for particular values of α and Φ and different choices of (n, l) and screening parameter μ . Here, we selected two separate sets of values for (n, l) -th state, one is $(3, 2)$ -th state and the other is $(5, 3)$ -th state. Effects of μ , topological defect parameter α and AB-flux field Φ on the effective potential (21) are evident in Fig. 3. In the current investigation, the asymptotic iteration method has been employed to solve the radial component of the Schrödinger equation in relation to the physical problem. The various spectroscopic constants of the diatomic compounds investigated in the present study are shown in Table 1. Units of the

Table 4 Energy eigen values $-E_{nl}$ (in a.u.) of the diatomic molecules N_2 , H_2 , HCl , LiH , NO , CO , ScH and O_2 embedded with inverse square plus Yukawa (ISPY) potential in the Minkowski flat space, i.e., $\alpha = 1$, $\Phi = 0$

$\mu \Rightarrow$		0.10	0.50	1.0	0.10	0.50	1.0
n	l		N_2			H_2	
1	0	9.3088879301	2.3369103119	0.1400582891	3.5482549960	1.4370410560	0.1173905335
	1	9.3084053581	2.3365719761	0.1401706914	3.5357193345	1.4266152918	0.1135581984
2	0	9.2040214278	2.2636748645	0.1656698882	3.2499154259	1.1926300400	0.0415062493
	1	9.2035454764	2.2633438040	0.1657916117	3.2387057696	1.1836095804	0.0393270289
3	1	9.1001211844	2.1916944757	0.1934390451	2.9725860627	0.9734886753	0.0042023797
	2	9.0991824043	2.1910467866	0.1937010156	2.9526359980	0.9580742864	0.0029619779
	3	9.0977745283	2.1900755470	0.1940942643	2.9231390545	0.9353775985	0.0015160883
4	0	8.9985699936	2.1219153024	0.2229474265	2.7423354601	0.7988800280	0.0034748428
	1	8.9981069316	2.1215984408	0.2230874409	2.7332713825	0.7921637455	0.0040954197
	3	8.9957922006	2.1200147104	0.2237880877	2.6887112876	0.7593342074	0.0079238715
	4	8.9939411102	2.1187484194	0.2243492950	2.6539500489	0.7339474690	0.0118324469
5	2	8.8965642737	2.0524109646	0.2550099079	2.5010813510	0.6248065338	0.0393407698
	3	8.8951943654	2.0514816205	0.2554573269	2.4770426129	0.6080408569	0.0453034093
	4	8.8933683521	2.0502430251	0.2560544122	2.4455976337	0.5862838684	0.0538213918
	5	8.8910866885	2.0486956321	0.2568016151	2.4072347545	0.5600161099	0.0653508856
n	l	HCl			LiH		
1	0	3.2951040429	0.4785192178	0.5078177176	1.6409270275	0.0573496305	1.1287114167
	1	3.2927136474	0.4771783261	0.5097565253	1.6392646400	0.0568600717	1.1318869475
2	0	3.1567285959	0.4029143695	0.6283709901	1.5569935502	0.0348919077	1.2983654265
	1	3.1544551228	0.4017076531	0.6304978888	1.5554246569	0.0345177897	1.3017249812
3	1	3.0229111208	0.3339751272	0.7621762253	1.4762645259	0.0179952685	1.4809449906
	2	3.0185906624	0.3318226369	0.7667986352	1.4733070882	0.0174711891	1.4880251564
	3	3.0121279254	0.3286117236	0.7737496712	1.4688870614	0.0167009871	1.4986606569
4	0	2.8997277963	0.2745256403	0.9018949812	1.4028599384	0.0071295309	1.6655131591
	1	2.8976668880	0.2735659948	0.9043767817	1.4014589256	0.0069671866	1.6692216540
	3	2.8873962434	0.2688013334	0.9168183180	1.3944840972	0.0061851528	1.6877921033
	4	2.8792201836	0.2650296650	0.9268103725	1.3889402628	0.0055948989	1.7026817884
5	2	2.7744174242	0.2184122063	1.0620219784	1.3280651870	0.0010119713	1.8740118242
	3	2.7685504165	0.2159004227	1.0699952703	1.3241111945	0.0008392886	1.8856557345
	4	2.7607573974	0.2125806602	1.0806544349	1.3188654090	0.0006346271	1.9012045854
	5	2.7510634825	0.2084777147	1.0940232686	1.3123499425	0.0004195697	1.9206783066
n	l	NO			CO		
1	0	6.1782311922	1.3689651196	0.2250965192	8.6833773809	2.0282021187	0.2295461444
	1	6.1778238182	1.3686931116	0.2252475295	8.6829147288	2.0278867145	0.2296908900
2	0	6.0993614590	1.3165725535	0.2554451000	8.5838674574	1.9606567784	0.2618901268
	1	6.0989603524	1.3163075012	0.2556052178	8.5834112233	1.9603484675	0.2620440756
3	1	6.0213073602	1.2652666977	0.2877275039	8.4852851640	1.8943339018	0.2963779274
	2	6.0205175563	1.2647503795	0.2880658284	8.4843854162	1.8937313504	0.2967041149
	3	6.0193331618	1.2639762130	0.2885736245	8.4830360826	1.8928278112	0.2971936828
4	0	5.9452297011	1.2157981289	0.3214123423	8.3889555379	1.8301127310	0.3324956794
	1	5.9448407572	1.2155466165	0.3215903033	8.3885117959	1.8298182624	0.3326676904
	3	5.9428966494	1.2142896647	0.3224807141	8.3862936523	1.8283464853	0.3335283084
	4	5.9413420963	1.2132848351	0.3231937700	8.3845198171	1.8271697420	0.3342174775
	5	5.8687710932	1.1666340470	0.3575436541	8.2921917058	1.7662020334	0.3712510270

Table 4 continued

<i>n</i>	<i>l</i>	NO				CO	
3	5.8676224463	1.1658997589	0.3581042371	8.2908791624	1.7653393350	0.3717940944	
4	5.8660914768	1.1649212663	0.3588522349	8.2891296242	1.7641895891	0.3725186993	
5	5.8641786639	1.1636990473	0.3597881218	8.2869435363	1.7627532397	0.3734252829	
<i>n</i>	<i>l</i>	ScH				O ₂	
1	0	1.4130741269	0.0091133660	1.6157359883	3.8973781991	0.7520520410	0.2667735933
	1	1.4118737982	0.0089568713	1.6188414749	3.8970346440	0.7518350421	0.2669520823
2	0	1.3453764272	0.0023255055	1.7992913751	3.8395953115	0.7158065433	0.2978324389
	1	1.3442376197	0.0022481129	1.8025309042	3.8392578296	0.7155963568	0.2980200506
3	1	1.2800455777	0.000009536	1.9938615032	3.7824996567	0.6805017603	0.3306241303
	2	1.2778870644	0.000003770	2.0006044787	3.7818366999	0.6800948726	0.3310174588
	3	1.2746588972	0.0000089773	2.0107279777	3.7808426101	0.6794848859	0.3316077941
4	0	1.2201084560	0.0019296004	2.1891206767	3.7270626689	0.6467250221	0.3645356721
	1	1.2190813057	0.0019990269	2.1926169057	3.7267369210	0.6465280481	0.3647411169
	3	1.2139636621	0.0023639136	2.2101146994	3.7251088576	0.6455438530	0.3657690101
	4	1.2098911530	0.0026770055	2.2241327944	3.7238072179	0.6447573059	0.3665921270
5	2	1.1591959321	0.0083216902	2.4058396841	3.6713070521	0.6132716762	0.4007769230
	3	1.1562802902	0.0087481757	2.4167103177	3.6703473437	0.6127005060	0.4014199345
	4	1.1524085829	0.0093322361	2.4312186524	3.6690683499	0.6119395611	0.4022778923
	5	1.1475941949	0.0100869139	2.4493766608	3.6674705989	0.6109893679	0.4033513176

constants are also mentioned in the table. Energy eigen values $-E_{nl}$ (in a.u.) of the eight diatomic molecules with Kratzer–Feus potential ($\mu = 0$ in (1)) are exhibited in Tables 2 and 3 for $\alpha = 1, \Phi = 0$, i.e., in the Minkowski flat space. The comparison of the energy levels is made for NO, HCl, LiH, O₂, H₂, N₂ with the outcomes, accessible from the research work of Doma et al. [42], Bayrak et al. [43] and Ibekwe et al. [44] and we observe that they are in good agreement up to 6–7 decimal places. Small variation in the results occurs due to the choice of the spectroscopic parameters up to different decimal places. In Table 4, negative bound state energy eigenvalues $-E_{nl}$ (in a.u.) of the eight diatomic molecules embedded with inverse square plus Yukawa potential (ISPYP) in the Minkowski flat space have been compiled for $\mu = 0.1, 0.5$ and $\mu = 1.0$. This table demonstrates that, for a particular diatomic molecule except HCl, LiH, ScH and for a specific (*n, l*)-th state, modulus of the energy levels $|-E_{nl}|$ gradually decreases as the values of μ increase.

The effects of a point-like global monopole (PGM) on the energy spectrum $-E_{nl}$ (in a.u.) of the eight diatomic molecules confined by the AB-flux field and embedded with Kratzer–Feus potential ($\mu = 0$) and inverse square plus Yukawa potential are presented in Tables 5, 6, 7 and 8. Three different values of the topological defect parameter $\alpha = 0.20, 0.60, 0.80$ and two distinct amounts of AB-flux field $\Phi = 0.25, 0.75$ have been selected here. We have determined bound state energies of the molecules with ISPYP background for $\mu = 0.50$ and $\mu = 1.0$. Bound state energies of any diatomic molecules embedded with KFP and influenced by a fixed amount of AB-flux field alter from more negative to less negative values when α goes through smaller values to larger values. If the particle is with ISPYP then for a particular (*n, l*)-th state and fixed values of α and Φ , energy level $|-E_{nl}|$ of the diatomic molecules CO, NO, O₂, H₂, N₂ slowly falls down as the screening rises. But the molecules HCl, LiH, ScH experience the opposite scenario. We are able to determine that, the eigenvalue solutions are influenced by the topological defects of the geometry characterize by the parameter α , and the AB-flux field Φ which is an analog of the AB effect [76, 77]. Figures 4, 5, and 6 illustrate some pictorial depictions that can help to effectively understand these phenomena. The energy curves of the particles embedded with ISPYP as a function of the screening parameter $\mu \in [0, 1]$ are shown in Fig. 4. Figures 5 and 6 illustrate the Kratzer–Feus potential and how, when the curves are plotted with respect to α or Φ , the energy eigen levels of the molecules are almost parallel to one another.

Table 5 Topological effects on the energy eigen values $-E_{nl}$ (in a.u.) of N_2 , H_2 diatomic molecules confined by the AB-flux field and embedded with (a) Kratzer–Feus potential, $\mu = 0$; (b) inverse square plus Yukawa potential, $\mu = 0.50$ and (c) inverse square plus Yukawa potential, $\mu = 1.0$

$\alpha \Rightarrow$			0.20	0.60	0.80	0.20	0.60	0.80
n	l			$\Phi = 0.25$			$\Phi = 0.75$	
N_2								
1	1	a	11.9051970085	11.8402418276	11.8079560462	11.9054453397	11.8404881290	11.8082013406
		b	2.4267277166	2.3814228106	2.3589845746	2.4269013340	2.3815941935	2.3591548483
		c	0.1120905532	0.1257364716	0.1328408719	0.1120400290	0.1256830992	0.1327860834
2	2	a	11.8826259195	11.7749813893	11.7216995420	11.8831211623	11.7754699173	11.7221847574
		b	2.4109604896	2.3361233209	2.2993033921	2.4113061683	2.3364616028	2.2996380206
		c	0.1167349119	0.1403198275	0.1528856547	0.1166318986	0.1402073715	0.1527685222
3	2	a	11.8609831992	11.7111069278	11.6372246456	11.8614770896	11.7115914860	11.6377046252
		b	2.3958661018	2.2920013137	2.2412367478	2.3962102917	2.2923352167	2.2415655948
		c	0.1212855216	0.1554551835	0.1740437664	0.1211806102	0.1553371210	0.1739192158
	3	a	11.8596252130	11.7097745999	11.6359049063	11.8603658942	11.7105012865	11.6366247269
		b	2.3949197917	2.2910832874	2.2403326229	2.3954359223	2.2915839914	2.2408257447
		c	0.1215742399	0.1557800621	0.1743864846	0.1214167186	0.1556028181	0.1741995103
4	2	a	11.8393995544	11.6477507993	11.5536596487	11.8398920973	11.6482314307	11.5541344676
		b	2.3808367584	2.2484513599	2.1841755057	2.3811794644	2.2487809269	2.1844986464
		c	0.1259190824	0.1713237539	0.1964937886	0.1258122779	0.1712001277	0.1963618950
	4	a	11.8361990257	11.6446276648	11.5505742808	11.8371836192	11.6455884503	11.5515234485
		b	2.3786101687	2.2463101430	2.1820760444	2.3792950888	2.2469688002	2.1827218565
		c	0.1266143099	0.1721282894	0.1973520474	0.1264002095	0.1718805617	0.1970877925
5	1	a	11.8187343975	11.5857417436	11.4718135866	11.8189800283	11.5859801466	11.4720484816
		b	2.3664694187	2.2060371205	2.1286623096	2.3666400628	2.2061997866	2.1288210926
		c	0.1304451941	0.1876939631	0.2199791905	0.1303908784	0.1876294189	0.2199096378
	3	a	11.8165241805	11.5835965600	11.4696999671	11.8172608275	11.5843115326	11.4704044200
		b	2.3649340810	2.2045735676	2.1272336965	2.3654457683	2.2050613301	2.1277098140
		c	0.1309344948	0.1882753027	0.2206055968	0.1307713028	0.1880814346	0.2203967083
	5	a	11.8123515836	11.5795467213	11.4657097097	11.8135785116	11.5807375552	11.4668830251
		b	2.3620362555	2.2018112512	2.1245373367	2.3628882510	2.2026234024	2.1253300945
		c	0.1318609835	0.1893755528	0.2217909298	0.1315881810	0.1890516562	0.2214420146
H_2								
1	1	a	4.6235010379	4.4120963746	4.3115945800	4.6307598190	4.4188624262	4.3181303209
		b	1.7743395769	1.5950106970	1.5108608532	1.7805490109	1.6007026146	1.5163100688
		c	0.2640459139	0.1809443845	0.1458503928	0.2671073068	0.1834138999	0.1480400326
2	2	a	4.5269227714	4.1934069017	4.0401267120	4.5409705807	4.2059293443	4.0519677295
		b	1.6920431457	1.4129055067	1.2876281968	1.7039758327	1.4232303995	1.2972304586
		c	0.2245949887	0.1085920416	0.0673233714	0.2301823087	0.1123242849	0.0702093658
3	2	a	4.4572194217	4.0109708981	3.8124066067	4.4709437844	4.0226845261	3.8232600636
		b	1.6330319501	1.2640411536	1.1056680726	1.6446247034	1.2735077737	1.1142168333
		c	0.1976602554	0.0604426401	0.0226431904	0.2028581806	0.0631682365	0.0242778624
	3	a	4.4199111987	3.9791145507	3.7828835215	4.4401828187	3.9964264253	3.7989285183
		b	1.6015851852	1.2383626751	1.0824810319	1.6186597310	1.2523050572	1.0950703432
		c	0.1837978648	0.0532977682	0.0184642831	0.1912811879	0.0571316728	0.0206865381
4	2	a	4.3891136520	3.8401864300	3.6034106355	4.4025244221	3.8511594245	3.6133833673
		b	1.5757012907	1.1275749417	0.9437593815	1.5869639644	1.1362514702	0.9513614766
		c	0.1726549269	0.0269311968	0.0019963395	0.1774733112	0.0287183273	0.0024865245

Table 5 continued

$\alpha \Rightarrow$		0.20	0.60	0.80	0.20	0.60	0.80	
n	l		$\Phi = 0.25$			$\Phi = 0.75$		
	4	a	4.3039133934	3.7703973540	3.5399517866	4.3297713010	3.7915920195	3.5592297638
		b	1.5044608330	1.0727044179	0.8956983707	1.5260239345	1.0893103111	0.9102406198
		c	0.1432938717	0.0168163295	0.0001288427	0.1519725550	0.0196559059	0.0004639079
5	1	a	4.3455465190	3.6981347793	3.4272482203	4.3521604286	3.7033263616	3.4318795188
		b	1.5392041089	1.0164825032	0.8117471587	1.5447356189	1.0205008000	0.8151597374
		c	0.1573675984	0.0087163949	0.0024346938	0.1596519097	0.0092148354	0.0021911134
	3	a	4.2869232885	3.6520782155	3.3861461423	4.3062859067	3.6672982313	3.3997320710
		b	1.4903208635	0.9809806757	0.7816071156	1.5064371403	0.9926834073	0.7915403141
		c	0.1377043082	0.0048787763	0.0051807555	0.1440815614	0.0060296552	0.0041557632
	5	a	4.1804425431	3.5682360927	3.3112488399	4.2112013420	3.5924802717	3.3329164194
		b	1.4022301199	0.9170520380	0.7273848989	1.4275811294	0.9354424132	0.7429757082
		c	0.1047835700	0.0006905940	0.0129837960	0.1139112114	0.0015195575	0.0103442945

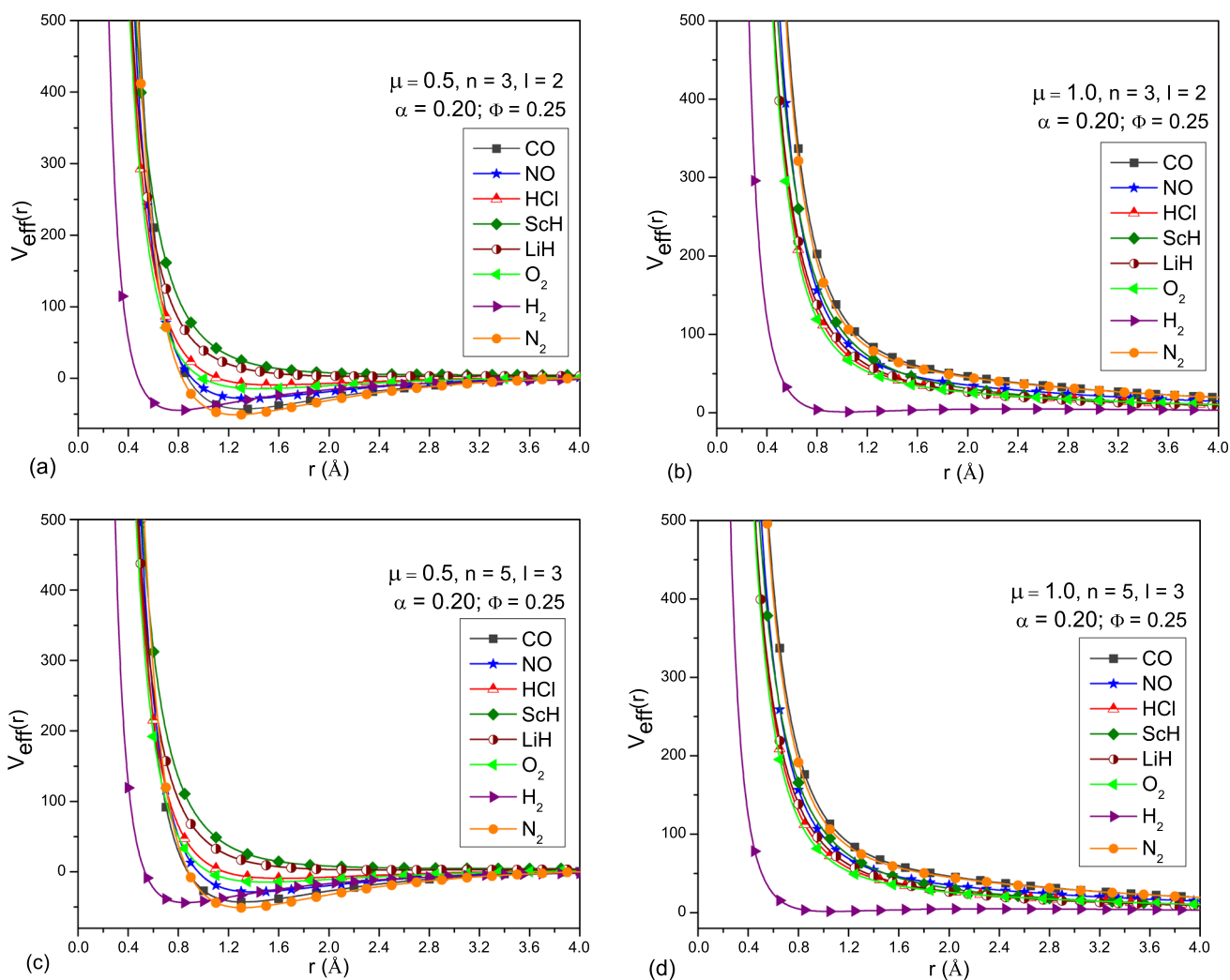


Fig. 3 Effective potential (21) as a function of r of the diatomic molecules CO, NO, HCl, ScH, LiH, O₂, H₂, N₂ corresponding to (a) $n = 3, l = 2, \alpha = 0.20, \Phi = 0.25, \mu = 0.5$; (b) $n = 3, l = 2, \alpha = 0.20, \Phi = 0.25, \mu = 1.0$; (c) $n = 5, l = 3, \alpha = 0.20, \Phi = 0.25, \mu = 0.5$; (d) $n = 5, l = 3, \alpha = 0.20, \Phi = 0.25, \mu = 1.0$

Table 6 Topological effects on the energy eigen values $-E_{nl}$ (in a.u.) of HCl, LiH diatomic molecules confined by the AB-flux field and embedded with (a) Kratzer–Feus potential, $\mu = 0$; (b) inverse square plus Yukawa potential, $\mu = 0.50$ and (c) inverse square plus Yukawa potential, $\mu = 1.0$

$\alpha \Rightarrow$			0.20	0.60	0.80	0.20	0.60	0.80
n	l		$\Phi = 0.25$			$\Phi = 0.75$		
<i>HCl</i>								
1	1	a	4.5709541760	4.4802389248	4.4358536029	4.5722465161	4.4814929678	4.4370890429
		b	0.5792943357	0.5269641181	0.5019319013	0.5800508421	0.5276769357	0.5026234202
		c	0.3791495856	0.4419744691	0.4750015676	0.3782985912	0.4410636104	0.4740613228
2	2	a	4.5359738260	4.3880397754	4.3167364316	4.5385283420	4.3904703038	4.3191079275
		b	0.5589336165	0.4754041402	0.4367200086	0.5604128744	0.4767414455	0.4379892993
		c	0.4236361282	0.5123320053	0.5715055107	0.4009012425	0.5103896417	0.5694681859
3	2	a	4.5058147272	4.3027834972	4.2063415338	4.5083438051	4.3051435262	4.2086226298
		b	0.5415613847	0.4292766125	0.3790090934	0.5430116115	0.4305326395	0.3801736123
		c	0.4236361282	0.5835907295	0.6718465432	0.4218498017	0.5815347504	0.6696613309
	3	a	4.4988744145	4.2963068565	4.2000814005	4.5026573791	4.2998371292	4.2034936796
		b	0.5375878941	0.4258359223	0.3758194735	0.5397525955	0.4277102320	0.3775569405
		c	0.4285631037	0.5892578905	0.6778684637	0.4258730153	0.5861643114	0.6745814942
4	2	a	4.4759554174	4.2199879914	4.1001279223	4.4784593938	4.2222802214	4.1023231553
		b	0.5245315930	0.3859937164	0.3261618807	0.5259531252	0.3871711654	0.3272261648
		c	0.4450948907	0.6588456626	0.7790985271	0.4432690905	0.6566787683	0.7767699642
	4	a	4.4597478309	4.2051496323	4.0859168365	4.4647222177	4.2097040287	4.0902788157
		b	0.5153597817	0.3784010994	0.3193015168	0.5181693351	0.3807260985	0.3214018179
		c	0.4570304049	0.6729902717	0.7942903290	0.4533454584	0.6686270788	0.7896055952
5	1	a	4.4507323703	4.1434583108	4.0015874133	4.4519740584	4.1445736362	4.0026459351
		b	0.5102801462	0.3473907635	0.2796658605	0.5109788115	0.3479432962	0.2801517050
		c	0.4637582450	0.7340228925	0.8887359732	0.4628278418	0.7328870472	0.8875037857
	3	a	4.4395884115	4.1334477021	3.9920863157	4.4432968299	4.1367791180	3.9952482383
		b	0.5040233296	0.3424450997	0.2753186062	0.5061027132	0.3440882385	0.2767626315
		c	0.4721628547	0.7442720634	0.8998502487	0.4693551340	0.7408503708	0.8961405820
	5	a	4.4186909502	4.1146719607	3.9742645978	4.4248167176	4.1201762617	3.9794894345
		b	0.4923568279	0.3332355502	0.2672306907	0.4957676490	0.3359263907	0.2695928115
		c	0.4881892321	0.7637610899	0.9209637403	0.4834552141	0.7580115488	0.9147377134
<i>LiH</i>								
1	1	a	2.4852429619	2.4290533477	2.4016443659	2.4861592069	2.4299386796	2.4025147427
		b	0.0921528175	0.0734438051	0.0649540578	0.0924719306	0.0737251464	0.0652170148
		c	0.9396039199	1.0333367127	1.0816046693	0.9381316374	1.0318060823	1.0800453669
2	2	a	2.4631574708	2.3718258992	2.3280284561	2.4649650783	2.3735338650	2.3296893029
		b	0.0845952130	0.0562146013	0.0443570968	0.0852039905	0.0567008875	0.0447848396
		c	0.9756299752	1.1361022433	1.2200645544	0.9726422627	1.1329234904	1.2167929853
3	2	a	2.4444882116	2.3194839545	2.2605234584	2.4462753035	2.3211356858	2.2621125806
		b	0.0784113800	0.0421844150	0.0285050377	0.0789950718	0.0426007568	0.0288427763
		c	1.0069024207	1.2370073322	1.3591713112	1.0038759125	1.2337175054	1.3557548989
	3	a	2.4395871903	2.3149539124	2.2561650169	2.4422580275	2.3174226264	2.2585402349
		b	0.0768196782	0.0410516027	0.0275877791	0.0776854376	0.0416672989	0.0280860104
		c	1.0152386777	1.2460662093	1.3685776014	1.0106892035	1.2411228521	1.3634448726
4	2	a	2.4260304035	2.2688557225	2.1959125780	2.4277972890	2.2704536613	2.1974340467
		b	0.0724864943	0.0302954073	0.0163070350	0.0730454098	0.0306442466	0.0165588405
		c	1.0385763022	1.3413359971	1.5042119417	1.0355113076	1.3379375380	1.5006547575

Table 6 continued

$\alpha \Rightarrow$		0.20	0.60	0.80	0.20	0.60	0.80	
n	l	$\Phi = 0.25$			$\Phi = 0.75$			
4	a	2.4146083075	2.2585244000	2.1860750352	2.4181112770	2.2616931032	2.1890924081	
	b	0.0689160185	0.0280826758	0.0147215628	0.0700031390	0.0287534533	0.0151999735	
	c	1.0585606872	1.3634790388	1.5273826812	1.0524002606	1.3566560392	1.5202442053	
5	1	a	2.4108397584	2.2225749377	2.1365848484	2.4117151635	2.2233498097	2.1373151761
	b	0.0677543165	0.0209713776	0.0078981979	0.0680234445	0.0211148241	0.0079845262	
	c	1.0652195264	1.4428822332	1.6485597818	1.0636698234	1.4411314027	1.6467141119	
3	a	2.4029897675	2.2156257008	2.1300347624	2.4056007148	2.2179372030	2.1322135631	
	b	0.0653607143	0.0197046574	0.0071436875	0.0661528862	0.0201220501	0.0073907133	
	c	1.0791950900	1.4586630630	1.6651919984	1.0745309361	1.4533981272	1.6596436995	
5	a	2.3883013578	2.2026190823	2.1177736010	2.3926027061	2.2064284279	2.1213648377	
	b	0.0609783046	0.0174301466	0.0058276781	0.0622485457	0.0180831975	0.0062000292	
	c	1.1057306807	1.4885848751	1.6967114450	1.0979075998	1.4797690419	1.6874271393	

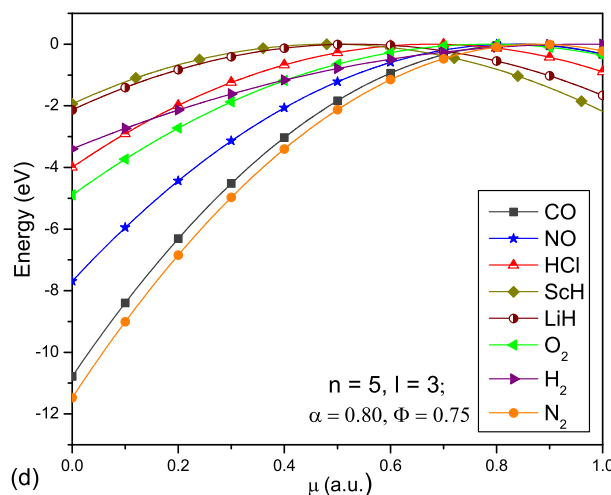
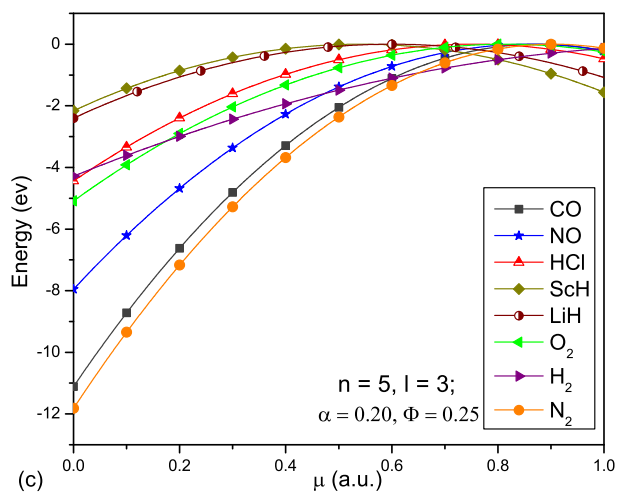
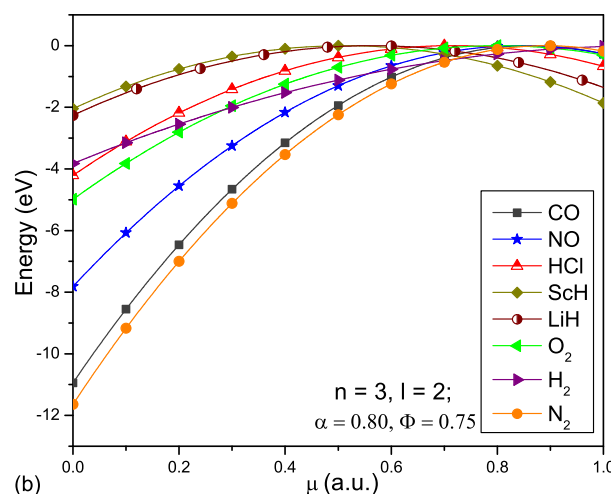
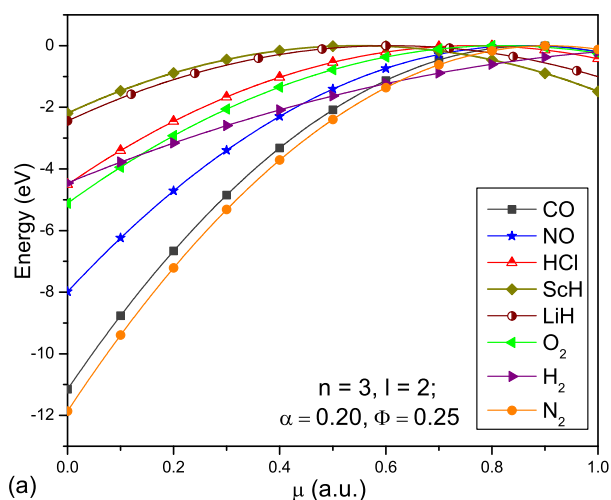


Fig. 4 Energy eigenvalues of the diatomic molecules CO, NO, HCl, ScH, LiH, O₂, H₂, N₂ embedded with ISPYP as a function of μ corresponding to (a) $n = 3, l = 2, \alpha = 0.20, \Phi = 0.25$; (b) $n = 3, l = 2, \alpha = 0.80, \Phi = 0.75$; (c) $n = 5, l = 3, \alpha = 0.20, \Phi = 0.25$; (d) $n = 5, l = 3, \alpha = 0.80, \Phi = 0.75$

Table 7 Topological effects on the energy eigen values $-E_{nl}$ (in a.u.) of NO, CO diatomic molecules confined by the AB-flux field and embedded with (a) Kratzer–Feus potential, $\mu = 0$; (b) inverse square plus Yukawa potential, $\mu = 0.50$ and (c) inverse square plus Yukawa potential, $\mu = 1.0$

$\alpha \Rightarrow$			0.20	0.60	0.80	0.20	0.60	0.80
n	l			$\Phi = 0.25$			$\Phi = 0.75$	
<i>NO</i>								
1	1	a	8.0187721999	7.9697370441	7.9453817379	8.0189825397	7.9699454573	7.9455891962
		b	1.4334959014	1.4008972873	1.3847812673	1.4336361684	1.4010354126	1.3849183302
		c	0.1911175076	0.2078285187	0.2164303574	0.1910475564	0.2077557803	0.2163562338
2	2	a	8.0016487299	7.9204441126	7.8802984333	8.0020680545	7.9208570696	7.8807082542
		b	1.4220893127	1.3683324273	1.3419652299	1.4223683483	1.3686043782	1.3422336861
		c	0.1968615627	0.2254478733	0.2404161213	0.1967197317	0.2252968059	0.2402604835
3	2	a	7.9853115502	7.8723231160	7.8167200007	7.9857295912	7.8727323153	7.8171248718
		b	1.4112293569	1.3367438696	1.3004972356	1.4115069655	1.3370116324	1.3007601683
		c	0.2024332787	0.2434566319	0.2652794421	0.2022895903	0.2433000855	0.2651165595
	3	a	7.9841621634	7.8711980380	7.8156068219	7.9847890606	7.8718116769	7.8162139709
		b	1.4104661589	1.3360077414	1.2997743872	1.4108824077	1.3364092259	1.3001686287
		c	0.2028286473	0.2438873534	0.2657275850	0.2026129507	0.2436523746	0.2654831042
4	2	a	7.9690243535	7.8246393328	7.7539079040	7.9694411161	7.8250448197	7.7543079048
		b	1.4004249813	1.3056429000	1.2598851326	1.4007011682	1.3059065202	1.2601426213
		c	0.2080773665	0.2621041034	0.2912673205	0.2079318260	0.2619421235	0.2910972726
	4	a	7.9663164597	7.8220046949	7.7513089086	7.9671494616	7.8228151630	7.7521084131
		b	1.3986308297	1.3039303945	1.2582124649	1.3991826802	1.3044571298	1.2587269457
		c	0.2090244414	0.2631579952	0.2923736352	0.2087328378	0.2628335321	0.2920330455
5	1	a	7.9535140713	7.7780906936	7.6925415180	7.9537218487	7.7782916347	7.6927391528
		b	1.3901568588	1.2754784296	1.2205578954	1.3902942766	1.2756082221	1.2206839872
		c	0.2135357231	0.2810921394	0.3180575294	0.2134620620	0.2810084862	0.3179689921
	3	a	7.9516445642	7.7762826936	7.6907632643	7.9522676355	7.7768852665	7.6913559237
		b	1.3889205881	1.2743107659	1.2194235280	1.3893325806	1.2746998935	1.2198015588
		c	0.2141991616	0.2818454848	0.3188548209	0.2139779178	0.2815942764	0.3185889660
	5	a	7.9481156732	7.7728698843	7.6874065954	7.9491532567	7.7738733394	7.6883935450
		b	1.3865878091	1.2721074775	1.2172830842	1.3872735951	1.2727551916	1.2179123212
		c	0.2154547187	0.2832707586	0.3203630525	0.2150851122	0.2828512500	0.3199191515
<i>CO</i>								
1	1	a	11.1942510223	11.1325519308	11.1018864355	11.1944893325	11.1327882733	11.1021218020
		b	2.1111298543	2.0692870163	2.0485725223	2.1112918949	2.0694468782	2.0487313027
		c	0.1934553103	0.2111812329	0.2203197429	0.1933885420	0.21111116528	0.2202487648
2	2	a	11.1728024235	11.0705599747	11.0199572542	11.1732776672	11.0710287094	11.0204227784
		b	2.0965590639	2.0274684710	1.9935011287	2.0968816277	2.0277838225	1.9938129180
		c	0.1995179453	0.2298829200	0.2458217122	0.1993824692	0.2297381218	0.2456722968
3	2	a	11.1522447262	11.0098978751	10.9397373878	11.1527186588	11.0103627624	10.9401978380
		b	2.0826183245	1.9867669382	1.9399684886	2.0829394365	1.9870780203	1.9402746413
		c	0.2054280794	0.2490630875	0.2723507510	0.2052907296	0.2489127540	0.2721940112
	3	a	11.1509416193	11.0086196380	10.9384713501	11.1516523671	11.0093168214	10.9391618797
		b	2.0817354742	1.9859116653	1.9391267689	2.0822169911	1.9863781409	1.9395858523
		c	0.2058059988	0.2494767071	0.2727819852	0.2055998232	0.2492510597	0.2725467303
4	2	a	11.1317437153	10.9497330177	10.8603902855	11.1322163417	10.9501940995	10.8608457352
		b	2.0687403645	1.9466174858	1.8874061028	2.0690600297	1.9469243404	1.9395858523
		c	0.2114192724	0.2689598501	0.3001425145	0.2112800537	0.2688040231	0.2999785236

Table 7 continued

$\alpha \Rightarrow$		0.20	0.60	0.80	0.20	0.60	0.80	
n	l		$\Phi = 0.25$			$\Phi = 0.75$		
4	a	11.1286726228	10.9467369353	10.8574307970	11.1296173936	10.9476586316	10.8583412364	
	b	2.0666635199	1.9446238791	1.8854532039	2.0673023684	1.9452371215	1.8860539236	
	c	0.2123251711	0.2699736705	0.3012093846	0.2120462526	0.2696615513	0.3008809453	
5	1	a	11.1121240274	10.8908603143	10.7826917699	11.1123597199	10.8910890021	10.7829170589
		b	2.0554818924	1.9075443895	1.8363178037	2.0556410339	1.9076957527	1.8364653813
		c	0.2172444475	0.2892855750	0.3288848652	0.2171739361	0.2892049643	0.3287993085
	3	a	11.1100032454	10.8888025580	10.7806645940	11.1107100826	10.8894883900	10.7813402342
		b	2.0540500689	1.9061825542	1.8349900301	2.0545272534	1.9066364127	1.8354325363
		c	0.2178794996	0.2900115027	0.3296552983	0.2176677256	0.2897694405	0.3293984027
	5	a	11.1059995344	10.8849178138	10.7768375734	11.1071767965	10.8860600968	10.7779628842
		b	2.0513477232	1.9036123247	1.8324840990	2.0521422309	1.9043679861	1.8332208545
		c	0.2190812494	0.2913848175	0.3311126357	0.2187274941	0.2909806140	0.3306837255

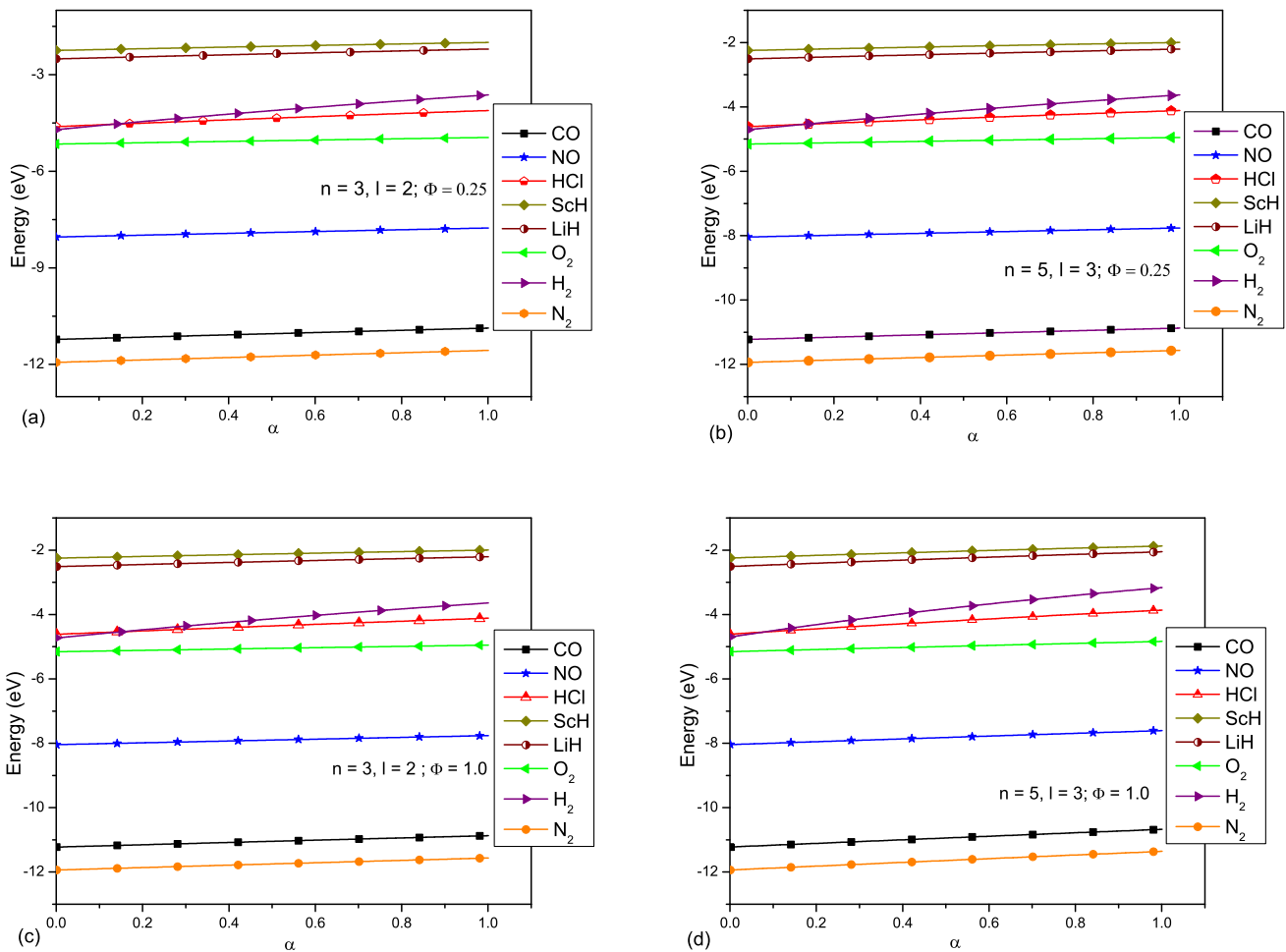


Fig. 5 Energy eigenvalues of the diatomic molecules CO, NO, HCl, ScH, LiH, O₂, H₂, N₂ embedded with Kratzer–Feus potential as a function of topological defect parameter α corresponding to (a) $n = 3, l = 2, \Phi = 0.25$; (b) $n = 5, l = 3, \Phi = 0.25$; (c) $n = 3, l = 2, \Phi = 1.0$; (d) $n = 5, l = 3, \Phi = 1.0$

5 Conclusions

The effects of a point-like global monopole (PGM) on non-relativistic Schrodinger’s particles under the influence of AB-flux field with a potential that is a superposition of the inverse square and the Yukawa potential are investigated in this article. Additionally, the

Table 8 Topological effects on the energy eigen values $-E_{nl}$ (in a.u.) of ScH, O₂ diatomic molecules confined by the AB-flux field and embedded with (a) Kratzer–Feus potential, $\mu = 0$; (b) inverse square plus Yukawa potential, $\mu = 0.50$ and (c) inverse square plus Yukawa potential, $\mu = 1.0$

$\alpha \Rightarrow$			0.20	0.60	0.80	0.20	0.60	0.80
n	l		$\Phi = 0.25$			$\Phi = 0.75$		
<i>ScH</i>								
1	1	a	2.2259742057	2.1807065388	2.1585698385	2.2266355706	2.1813478231	2.1592013756
		b	0.0233480866	0.0153077357	0.0119443312	0.0234767758	0.0154108501	0.0120349514
		c	1.4074697293	1.5111113264	1.5640678092	1.4060003916	1.5095999309	1.5625356785
2	2	a	2.2084590632	2.1346812971	2.0991529911	2.2097659154	2.1359231884	2.1003639907
		b	0.0200560735	0.0087515532	0.0048743125	0.0202939156	0.0089061283	0.0049888432
		c	1.4468471043	1.6229623215	1.7140382767	1.4438779161	1.6198549479	1.7108634006
3	2	a	2.1934109938	2.0922044053	2.0441904559	2.1947045098	2.0934094087	2.0453541999
		b	0.0174091662	0.0042416840	0.0010437179	0.0176300108	0.0043483875	0.0010963481
		c	1.4814036834	1.7323535201	1.8636035040	1.4784065137	1.7291653237	1.8603227928
	3	a	2.1898616977	2.0888978521	2.0409970597	2.1917962478	2.0907001181	2.0427376593
		b	0.0168096967	0.0039553966	0.0009058059	0.0171352541	0.0041102556	0.0009797921
		c	1.4896536939	1.7411280302	1.8726320443	1.4851522729	1.7363406682	1.8677061903
4	2	a	2.1785162045	2.0509828513	1.9913586385	2.1797965652	2.0521524135	1.9924775538
		b	0.0149579333	0.0013687011	0.0000221495	0.0151619613	0.0014289796	0.0000153063
		c	1.5162831197	1.8445262505	2.0180126826	1.5132581496	1.8412586779	2.0146285636
	4	a	2.1702305244	2.0434134473	1.9841166810	2.1727732176	2.0457364678	1.9863392720
		b	0.0136682962	0.0010092824	0.0000971448	0.0140583828	0.0011139120	0.0000684539
		c	1.5359816113	1.8657967877	2.0400385359	1.5299138783	1.8592462445	2.0332559993
5	1	a	2.1659915205	2.0129556261	1.9424332394	2.1666263320	2.0135243511	1.9429723328
		b	0.0130292066	0.0001111156	0.0015895861	0.0131240166	0.0001196934	0.0015584597
		c	1.5461422647	1.9535775842	2.1710586262	1.5446170702	1.9519057202	2.1693168406
	3	a	2.1602949920	2.0078517266	1.9375950815	2.1621904868	2.0095501072	1.9392050697
		b	0.0121926239	0.0000483385	0.0018831356	0.0124681503	0.0000663855	0.0017826087
		c	1.5598855198	1.9686381743	2.1867472979	1.5553011407	1.9636152204	2.1815152256
	5	a	2.1496166135	1.9982822996	1.9285230210	2.1527462867	2.0010872202	1.9311822761
		b	0.0106938127	0.0000000399	0.0025029780	0.0111236579	0.0000047629	0.0023118523
		c	1.5859254103	1.9971532609	2.2164428489	1.5782557715	1.9887573908	2.2077005811
<i>O2</i>								
1	1	a	5.1382376264	5.1021422025	5.0842316946	5.1384157657	5.1023184678	5.0844070322
		b	0.7969698515	0.7742310325	0.7630184558	0.7970825382	0.7743416141	0.7631279943
		c	0.2316542553	0.2489852508	0.2578664678	0.2315705842	0.2488987814	0.2577786089
2	2	a	5.1255469136	5.0658293789	5.0363560369	5.1259018638	5.0661781433	5.0367017616
		b	0.7889537155	0.7515473214	0.7332805589	0.7891776064	0.7517642566	0.7334940693
		c	0.2376618494	0.2671888774	0.2825418533	0.2374925627	0.2670103247	0.2823587208
3	2	a	5.1135220571	5.0305067347	4.9897500037	5.1138757589	5.0308518577	4.9900909405
		b	0.7813795785	0.7296709398	0.7046656210	0.7816020671	0.7298837715	0.7048737274
		c	0.2434398712	0.2856512835	0.3079002012	0.2432687201	0.2854672413	0.3077098167
	3	a	5.1125496297	5.0295578914	4.9888126688	5.1130799988	5.0300753978	4.9893238986
		b	0.7807679874	0.7290858973	0.7040935691	0.7811015367	0.7294049669	0.7044055536
		c	0.2439107889	0.2861576434	0.3084239984	0.2436538789	0.2858814028	0.3081382473
4	2	a	5.1015394676	4.9955522494	4.9437879225	5.1018919269	4.9958937814	4.9441241594
		b	0.7738529356	0.7082097598	0.6767782666	0.7740740276	0.7084185385	0.6769810570
		c	0.2492810678	0.3046700194	0.3342370271	0.2491080581	0.3044805381	0.3340394785

Table 8 continued

$\alpha \Rightarrow$		0.20	0.60	0.80	0.20	0.60	0.80	
n	l	$\Phi = 0.25$			$\Phi = 0.75$			
4	a	5.0992496706	4.9933334334	4.9416035033	5.0999540043	4.9940159352	4.9422754255	
	b	0.7724170250	0.7068538386	0.6754612464	0.7728586245	0.7072708347	0.6758662771	
	c	0.2504068167	0.3059027829	0.3355222041	0.2500602136	0.3055232615	0.3351265600	
5	1	a	5.0902136186	4.9615523384	4.8990383543	5.0903892663	4.9617213685	4.8992041996
		b	0.7667580978	0.6875170699	0.6499524473	0.7668679848	0.6876194922	0.6500512613
		c	0.2548792640	0.3238989927	0.3611824547	0.2547918690	0.3238015918	0.3610801749
	3	a	5.0886333357	4.9600315883	4.8975462545	5.0891599875	4.9605384009	4.8980435194
		b	0.7657696604	0.6865957884	0.6490636278	0.7660990304	0.6869027783	0.6493597996
		c	0.2556663630	0.3247761174	0.3621034762	0.2554038877	0.3244836392	0.3617963685
	5	a	5.0856510369	4.9571616146	4.8947303383	5.0865278201	4.9580053780	4.8955582106
		b	0.7639052903	0.6848581397	0.6473872346	0.7644532712	0.6853688670	0.6478799539
		c	0.2571557791	0.3264354434	0.3638456519	0.2567173529	0.3259470625	0.3633329125

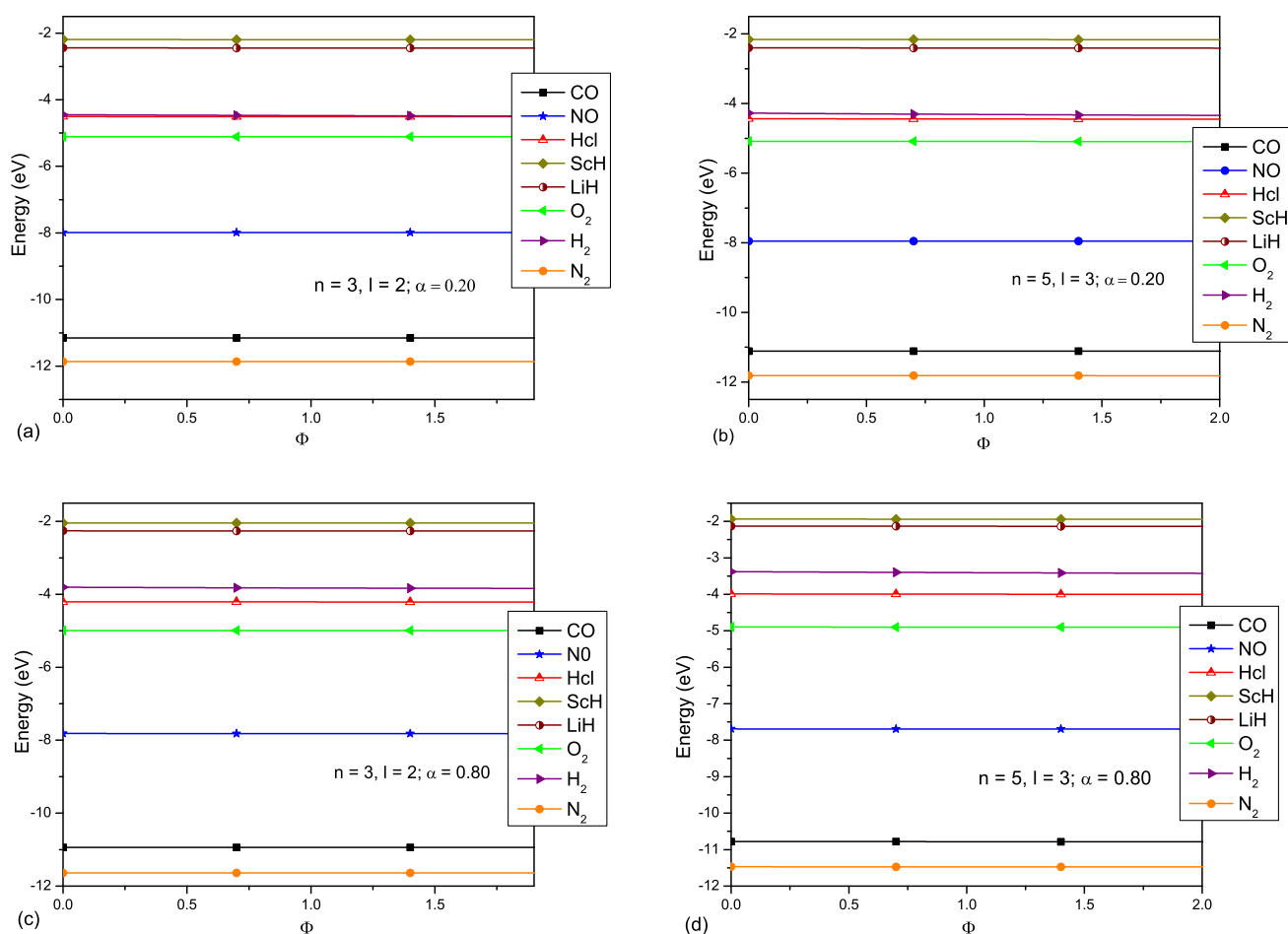


Fig. 6 Energy eigenvalues of the diatomic molecules CO, NO, HCl, ScH, LiH, O₂, H₂, N₂ embedded with Kratzer–Feus potential as a function of AB-flux field corresponding to (a) $n = 3, l = 2, \alpha = 0.20$; (b) $n = 5, l = 3, \alpha = 0.20$; (c) $n = 3, l = 2, \alpha = 0.80$; (d) $n = 5, l = 3, \alpha = 0.80$

same problem was considered under the Kratzer–Feus potential, a particular case of ISPYP. The current investigation is very important and significant in numerous fields of both chemistry and physics. Since the presence of topological defects in PGM geometry and the magnetic flux, shifts the energy spectrum and wave function of the diatomic molecules in comparison with the case in Minkowski flat space background. For mathematical calculations, we employ the asymptotic iteration method. We have exhibited sufficient tables and graphs in this paper, as well as compared our findings with the information obtained from the literature. Our data are consistent

with the data found in the literature review. The current study has the potential to contribute pertinent knowledge to astrophysics, plasma physics, solid-state physics, and molecular physics.

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Author contributions BD contributed to methodology, writing—original draft preparation, formal analysis and investigation, software, and data curation. SKN contributed to conceptualization, methodology, writing, formal analysis and investigation, writing—original draft preparation, writing—review and editing, software, data curation, and supervision. BP contributed to writing—original draft preparation, writing—review and editing, software, and data curation.

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Declarations

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