Journal of Science Research and Reviews
PRINT ISSN: 1595-9074
E-ISSN: 1595-8329
DOI: https://doi.org/10.70882/josrar.2025.v2i3.83
Homepage: https://josrar.esrgngr.org
Original Research Article

Estimation of Energy Eigenvalues using an Exponential Screened plus Yukawa Potential under the Influence of an External Magnetic Field

***[1]Manga, Peter J., [1]Amusat, Ramoni O., [1]Dibal, Amina A., [1]Adamu, Aliyu and [2]Ubale, Shelk A.**

[1]Department of Physics, University of Maiduguri, Borno – State – Nigeria.
[2]Department of Fine and Applied Art, Aminu Saleh College of Education, Azare Bauchi State - Nigeria
*Corresponding Author's email: 2016peterjohn@unimaid.edu.ng

KEYWORDS
Magnetic Field,
Magnetic Flux,
Partition Function,
Magnetisation,
Magnetic Susceptibility.

CITATION
Manga, P. J., Amusat, R. O., Dibal, A. A., Adamu, A., & Ubale, S. A. (2025). Estimation of Energy Eigenvalues using an Exponential Screened plus Yukawa Potential under the Influence of an External Magnetic Field. *Journal of Science Research and Reviews*, *2*(3), 66-79. https://doi.org/10.70882/josrar.2025.v2i3.83

ABSTRACT
Diatomic molecules play a key role in molecular physics and quantum chemistry because of their simple structure and their usefulness in studying how molecules behave under external factors. Examining the impact of influences like magnetic fields and Aharonov-Bohm (AB) flux on their quantum properties is essential for advancements in areas such as quantum control, molecular spectroscopy, and condensed matter research. In this study, numerical calculations were conducted to validate the computed results, revealing that both the external magnetic field B(T) and flux ϕ_{AB} significantly affect the energy levels of the selected diatomic molecules. At zero temperature, the energy eigenvalues indicate a slight decrease in magnetization (M_{nm}) and magnetic susceptibility (χ_{nm}) under varying magnetic field B(T) and flux ϕ_{AB}, with hydrogen (H_2) exhibiting an overlap at specific field strengths B(T). Magnetization (M_{nm}) generally increases with both magnetic field B(T) and flux ϕ_{AB} as temperature changes, while for Co, it decreases with rising temperature but increases when plotted against temperature as magnetic field B(T) and flux ϕ_{AB} vary. A similar pattern is observed in ScH and ScF. Additionally, partition function results show that temperature, magnetic field B(T) and flux ϕ_{AB} strongly influence the bound state energy eigenvalues, leading to a slight increase in the thermal properties of these diatomic molecules.

INTRODUCTION

The study of diatomic molecules and their energy spectra is a fundamental aspect of quantum mechanics, energy physics and molecular physics. Accurately determining the energy eigenvalues of such molecules is essential for understanding their electronic structure, vibrational motion, and rotational behaviour, which have applications in spectroscopy, chemical bonding analysis, and material science (Abu – shady *et al.*, 2023). Manga *et al.* (2023) utilized the modified Yukawa potential to explore the interaction between pseudovector and pseudoscalar components in determining the neutron-neutron, proton-proton, and proton-neutron coupling constants. Similarly, the application of an appropriate potential function has been employed to refine the screened-kratzer and kratzer potentials, particularly in quantum approximations. In a related study, Ding *et al.* (2011) investigated bound-state and thermal properties using the modified Tietz–Hua potential within the framework of supersymmetric quantum mechanics. Their research focused on the

vibrational energy spectra and thermodynamic characteristics of select diatomic molecules (Ding *et al*. 2011).

Edet *et al*. (2021) examined eigen solutions and various properties of the screened cosine kratzer potential in 2D-dimensional space under both relativistic and nonrelativistic conditions. Their work extended to calculating the rotational and vibrational energy levels of different heteronuclear diatomic molecules. In an earlier study, applied coupling constants to determine the effective radius and scattering length for neutron-neutron and proton-neutron interactions using the Modified Yukawa Potential (Dong, 2023).

Several researchers have explored potential models to analyse the partition function and various information-theoretic measures, such as Tsallis, Renyi, Shannon, and Fisher information entropies. Recently, there has been significant interest in studying potential models in the presence of an Aharonov–Bohm flux and an external magnetic field (Edet *et al.,* 2021) investigated the thermomagnetic properties of the screened-Kratzer potential under these conditions, examining effects such as persistent current, magnetization, and magnetic susceptibility (Ikot *et al.,* 2021).

Ikot *et al*. (2021) further analysed the impact of the Aharonov–Bohm flux and an external magnetic field on the Hellmann plus screened-Kratzer potential, presenting the energy equation in a closed-form solution. Their study extended to the thermomagnetic properties of diatomic molecules, where they derived a normalized wave function expressed in terms of Jacobi polynomials. Additionally, they provided wave function plots and probability density distributions for selected diatomic molecules. The study also covered essential thermomagnetic characteristics, including partition function, vibrational mean energy, vibrational heat capacity, magnetization, persistent current, and magnetic susceptibility (Edet *et al.,* 2021).

In this Study, we focus on four specific diatomic molecules: H_2 (hydrogen), Co (carbon monoxide), ScH (scandium hydride), and ScF (scandium fluoride). The energy eigenvalues of these molecules are influenced by the presence of an exponential screening parameter, the Yukawa potential, and an external magnetic field, making the problem both complex and scientifically significant.

Theoretical Framework of Yukawa potential

In molecular systems, interatomic forces primarily arise due to electrostatic interactions between charged particles such as nuclei and electrons. The Coulomb potential provides a classical description of these interactions, but in many physical environments, such as plasmas, semiconductors, and astrophysical systems, these interactions are often modified due to screening effects caused by surrounding particles. This is where the Yukawa potential becomes useful (Manga *et al.,* 2023).

The Nikiforov-Uvarov-Functional Analysis (NUFA) Method

By employing the concept of NU method, Parametric NU method and Functional analysis method, we deduced a simple and intuitiveness method for solving a second order differential equation of the hypergeometric form called the Nikiforov-Uvarov-Function Analysis (NUFA) method. This method is simple which require little mathematical manipulation just as its counter part of parametric NU method (Edet *et al*. 2021). On the same note, the NU method required finding the square of the polynomials and other conditions this make it complicated, NUFA method said to be easier in obtaining the energy and the wave function once the wave equation is well transformed and the singularities is identified. It is well known that the NU method is deployed for the past decade in solving second-order differential equation of the form (Jia *et al*. 2012).

$$\frac{d^2\Psi(u)}{du^2}+\frac{\bar{\tau}(u)}{\sigma(u)}\frac{d\Psi(u)}{du}+\frac{\bar{\sigma}(u)}{\sigma^2(u)}\Psi(u)=0 \quad (1)$$

Where $\sigma(u)$ and $\bar{\sigma}(u)$ are polynomials of second order and $\bar{\tau}(u)$ is the first order polynomial. Tezcan and sever latter invent the parametric form od NU method in the form (Jia *et al*. 2012).

$$\frac{d^2\Psi(u)}{du^2}+\frac{\eta_1-\eta_2 u}{u(1-\eta_3 u)}\frac{d\Psi(u)}{du}+\frac{1}{u^2(1-\eta_3 u)^2}[-\xi_1 u^2+\xi_2 u-\xi_3]\Psi(u)=0 \quad (2)$$

Where$\eta_{i\ and}\ _{\xi_i}(i=1,2,3)$are all parameters, it can be observed in equation (3) that the differential equation has two singularities at $u\to 0$ and $u\to 1$, thus the wave is express in the form (Jia *et al*. 2012).

$$\Psi(u)=u^{\lambda^0}(1-u)^v f(u) \quad (3)$$

By substituting equation (3) into equation (2) we obtained the following equation.

$$u(1-\eta_3 u)\frac{d^2 f(u)}{du^2}+[\eta_1+2\lambda^0-(2\lambda^0\eta_3+2v\eta_3+\eta_2)u]\frac{d f(u)}{du}-\eta_3\left(\lambda^0+v+\frac{1}{2}\left(\frac{\eta_2}{\eta_3}-1\right)+\sqrt{\frac{1}{4}\left(\frac{\eta_2}{\eta_3}-1\right)^2}+\frac{\xi_1}{\eta_3^2}\right)\left(\lambda^0+v+\frac{1}{2}\left(\frac{\eta_2}{\eta_3}-1\right)-\sqrt{\frac{1}{4}\left(\frac{\eta_2}{\eta_3}-1\right)^2+\frac{\xi_1}{\eta_3^2}}\right)+\left[\frac{\lambda^0(\lambda^0-1)+\eta_1\lambda^0-\xi_3}{u}+\frac{v(v-1)\eta_3+\eta_2 v-\eta_1\eta_3 v-\frac{\xi_1}{\eta_3}+\xi_2-\xi_3\eta_3}{(1-\eta_3 u)}\right]f(u)=0 \quad (4)$$

The expression of equation (4) in the form of gauss hypergeometric equation can be obtain if and only the following function vanished,

$$\lambda^0(\lambda^0-1)+\eta_1\lambda^0-\xi_3=0 \quad (5)$$

$$v(v-1)\eta_3+\eta_2 v-\eta_1\eta_3 v-\frac{\xi_1}{\eta_3}+\xi_2-\xi_3\eta_3=0 \quad (6)$$

Now equation (4) becomes

$$u(1-\eta_3 u)\frac{d^2 f(u)}{du^2}+[\eta_1+2\lambda^0-(2\lambda^0\eta_3+2v\eta_3+\eta_2)u]\frac{d f(u)}{du}-\eta_3\left(\lambda^0+v+\frac{1}{2}\left(\frac{\eta_2}{\eta_3}-1\right)+\sqrt{\frac{1}{4}\left(\frac{\eta_2}{\eta_3}-1\right)^2+\frac{\xi_1}{\eta_3^2}}\right)$$

$$\left(\lambda^0 + v + \frac{1}{2}\left(\frac{\eta_2}{\eta_3} - 1\right) - \sqrt{\frac{1}{4}\left(\frac{\eta_2}{\eta_3} - 1\right)^2 + \frac{\xi_1}{\eta_3^2}}\right) f(u) = 0 \quad (7)$$

By solving equation (5) and (6) we have (Lublinsky *et al.,* 2017).

$$\lambda^0 = \frac{1}{2}\left((1-\eta_1) \pm \sqrt{(1-\eta_1)^2 + 4\xi_3}\right) \quad (8)$$

$$v = \frac{1}{2\eta_3}\left((\eta_3 + \eta_1\eta_3 - \eta_2) \pm \sqrt{(\eta_3 + \eta_1\eta_3 - \eta_2)^2 + 4\left(\frac{\xi_1}{\eta_3} + \eta_3\xi_3 - \xi_2\right)}\right) \quad (9)$$

Equation (7) is the hypergeometric equation of the form (Lublinsky *et al.,* 2017).

$$v(1-v)\frac{d^2 f(v)}{dv^2} + [\gamma_3 + (\gamma_1 + \gamma_2 + 1)v]\frac{d f(v)}{dv} - [\gamma_1\gamma_2]f(v) = 0 \quad (10)$$

Where $\gamma_1, \gamma_2, \gamma_3$ are given as follows,

$$\gamma_1 = \sqrt{\eta_3}\left(\lambda^0 + v + \frac{1}{2}\left(\frac{\eta_2}{\eta_3} - 1\right) + \sqrt{\frac{1}{4}\left(\frac{\eta_2}{\eta_3} - 1\right)^2 + \frac{\xi_1}{\eta_3^2}}\right) \quad (11)$$

$$\gamma_2 = \sqrt{\eta_3}\left(\lambda^0 + v + \frac{1}{2}\left(\frac{\eta_2}{\eta_3} - 1\right) - \sqrt{\frac{1}{4}\left(\frac{\eta_2}{\eta_3} - 1\right)^2 + \frac{\xi_1}{\eta_3^2}}\right) \quad (12)$$

$$\gamma_3 = \eta_1 + 2\lambda^0 \quad (13)$$

Letting either $\gamma_1 \; and \; \gamma_2$ equal to a negative integer $-n$, the hypergeometric functions $f(u)$ turns to a polynomial of degree n. Thus, the hypergeometric function $f(u)$ approaches finite in the following quantum conditions that is $\gamma_1 = -n$, where $n = 0, 1, 3, \ldots, n_{max}$.

From the above quantum conditions, we have (Mulian, 2025),

$$\gamma_1 = \sqrt{\eta_3}\left(\lambda^0 + v + \frac{1}{2}\left(\frac{\eta_2}{\eta_3} - 1\right) + \sqrt{\frac{1}{4}\left(\frac{\eta_2}{\eta_3} - 1\right)^2 + \frac{\xi_1}{\eta_3^2}}\right) = -n \quad (14)$$

$$\lambda^0 + v + \frac{1}{2}\left(\frac{\eta_2}{\eta_3} - 1\right) + \frac{n}{\sqrt{\eta_3}} = -\sqrt{\frac{1}{4}\left(\frac{\eta_2}{\eta_3} - 1\right)^2 + \frac{\xi_1}{\eta_3^2}} \quad (15)$$

Squaring both side of equation (15) and rearranging, we obtain the energy equation for NUFA method as

$$(\lambda^0)^2 + 2\lambda^0\left(v + \frac{1}{2}\left(\frac{\eta_2}{\eta_3} - 1\right) + \frac{n}{\sqrt{\eta_3}}\right) + \left(v + \frac{1}{2}\left(\frac{\eta_2}{\eta_3} - 1\right) + \frac{n}{\sqrt{\eta_3}}\right)^2 - \frac{1}{4}\left(\frac{\eta_2}{\eta_3} - 1\right)^2 - \frac{\xi_1}{\eta_3^2} \quad (16)$$

By substituting equation (8) and (9) into Equation (3), we corresponding NUFA wave equation is given as (Onate *et al*. 2022).

$$\Psi(u) = \mathbb{N}u^{\frac{(1-\eta_1)+\sqrt{(\eta_1-1)^2+4\xi_3}}{2}}(1-\eta_3 u)^{\sqrt{\frac{(\eta_3+\eta_1\eta_2-\eta_2)+4\left(\frac{\xi_1}{\eta_3^2}+\eta_2\xi_3-\xi_2\right)}{2\eta_3}}} 2F_1(\gamma_1, \gamma_2, \gamma_3; u) \quad (17)$$

Application of the NUFA method to modified exponential (Modified Tietz-Wei) plus Yukawa potential

We use the NUFA method to find the energy eigenvalues for selected diatomic molecules based on different principal number quantum number and magnetic quantum number. The Hamiltonian operator of a system of particles characterised by a particle that is charged and confined to move with the improved screened Greene and Aldrich modified exponential plus Yukawa potential under the combined influence of AB and magnetic fields can be express in cylindrical coordinates as follows (Onate *et al.,* 2022).

$$\left(i\hbar\vec{\nabla} - \frac{e}{c}\vec{A}\right)^2 \psi(r,\phi,z) = 2\,\mu\left[E_{nm} + \left(D_0\left(\frac{1+e^{-2\alpha r}}{1-e^{-2\alpha r}}\right) + \frac{D_1 e^{-2\alpha r}}{r} + \frac{\vec{c}}{2}\right)\right]\psi(r,\phi,z) \quad (18)$$

Where E_{nm} donates the energy level, μ is the effective reduce mass of the system, the vector potential is given as $\vec{A}$ which can give as the superposition of two terms $\vec{A} = \overrightarrow{A_1} + \overrightarrow{A_2}$ having the azimuthal component and external magnetic field with $\vec{\nabla} \times \vec{A} = \overrightarrow{B}, \overrightarrow{A_2} = 0$ where $\vec{B}$ is the magnetic field. We choose $\overrightarrow{A_1} = \frac{\vec{B}e^{-2\alpha r}}{1-e^{-2\alpha r}}\hat{\phi}$ and $\overrightarrow{A_2} = \frac{\phi_{A,B}}{2\pi r}\hat{\phi}$ the additional magnetic flux $\phi_{A,B}$ created by a solenoid with $\vec{\nabla}.\overrightarrow{A_2} = 0$. Hence the vector potential can be written as

$$\vec{A} = \left(0, \frac{\vec{B}e^{-2\alpha r}}{1-e^{-2\alpha r}} + \frac{\phi_{A,B}}{2\pi r}, 0\right) \quad (19)$$

This equation can be solved analytically for $m \neq 0$ due to the centrifugal term. We employed the Greene and Aldrich screening Approximation (Jia *et al*. 2012).

$$\frac{1}{r^2} = \frac{4\alpha^2 e^{-2\alpha r}}{(1-e^{-2\alpha r})^2} \Longrightarrow \frac{1}{r} = \frac{2\propto e^{-2\alpha r}}{(1-e^{-2\alpha r})} \quad (20)$$

We substitute equation (19) & (20) into equation (18) and transform it. We have

$$R''(r) + \left[\frac{2\mu E_{nm}}{\hbar^2} + \frac{2\mu}{\hbar^2}\left(D_0\left(\frac{1+u}{1-u}\right) + D_1\left(\frac{2\propto u}{(1-u)}\right) - \frac{m^2 - 1/4\,(4\alpha^2)}{(1-u)^2} - \left(\frac{e}{\hbar c}\right)\frac{4\alpha^2 u^2}{(1-u)^2}\left(B + \frac{\phi_{A,B}}{2\pi}\right) - \frac{e^2}{\hbar^2 c^2}\left(\frac{4\alpha u^2}{(1-u)^2}\right)\left(B + \frac{\phi_{A,B}}{2\pi}\right)^2\right)\right] R_{nm}(r) = 0 \quad (21)$$

We transform equation (21) into hypergeometric equation type of the form

$$\frac{d^2R}{du^2} + \frac{(1-u)}{u(1-u)}\frac{dR}{du} + \frac{1}{u^2(1-u)^2}\{-(\varepsilon_{nm} + B + BD_1 2\alpha + C + D + E + F + G + H)u^2 + (2\varepsilon_{nm} + BD_1 2\alpha)u - \varepsilon_{nm} + BD_0\} = 0 \quad (22)$$

Comparing equation (22) with equation (23) given as.

$$\psi'' + \frac{\eta_1 - \eta_2 u}{u(1-u)}\psi' + \frac{1}{u^2(1-u)^2}\{-\xi_1 u^2 + \xi_2 u - \xi_3\}\psi = 0 \quad (23)$$

$$\xi_1 = \varepsilon_{nm} + B + BD_1 2\alpha + C + D + E + F + G + H \quad (24)$$

$$\xi_2 = 2\varepsilon_{nm} + BD_1 2\alpha \quad (25)$$

$$\xi_3 = \varepsilon_{nm} + BD_0 \quad (26)$$

Where $D_0 = \frac{D_e}{2} > 0, D_e$ is the dissociation energy that describes the depth of the potential well, α is the screening parameter which characterizes the strength of the

potential. D_1 is a real constant which also serve as a control parameter for the potential model, while r is the internuclear distance between the atoms of diatomic molecules (Jia *et al*. 2012).

$$B = \frac{\mu}{2\alpha^2\hbar^2}, \quad C = (m+x)^2, D = \left(\frac{e\,B}{\hbar c}\right), \quad E = \left(\frac{e\,\phi_{AB}}{2\pi\hbar c}\right), F = \frac{e^2B^2}{\hbar^2c^2}, G = \frac{e^2\phi_{AB}B}{2\pi\hbar^2c^2}, H = \frac{e^2{\phi_{AB}}^2}{4\pi^2\hbar^2c^2} \quad (27)$$

$$\lambda^0 = \frac{1}{2}\left((1-\eta_1) \pm \sqrt{(1-\eta_1)^2 + 4}\xi_3\right) \quad (28)$$

$$(\lambda^0)^2 = \varepsilon_{nm} + BD_0 \quad (29)$$

For

$\eta_1 = \eta_2 = \eta_3 = 1$, we have the expression for the coiling velocity as follows

$$v = \frac{1}{2\eta_3}\left((\eta_3 + \eta_1\eta_3 - \eta_2) \pm \sqrt{(\eta_3 + \eta_1\eta_3 - \eta_2)^2 + 4\left(\frac{\xi_3}{\eta_2} + \eta_3\xi_3 - \xi_2\right)}\right) \quad (30)$$

$$v = \frac{1+\sqrt{1+4(B+C+D+E+F+G+H+BD_0)}}{2} \quad (31)$$

The energy eigenvalue equation is deduced from the relation

$$(\lambda^0)^2 + 2\lambda^0\left(v + \frac{1}{2}\left(\frac{\eta_2}{\eta_3} - 1\right) + \frac{n}{\sqrt{\eta_3}}\right) + \left(\left(v + \frac{1}{2}\left(\frac{\eta_2}{\eta_3} - 1\right) + \frac{n}{\sqrt{\eta_3}}\right)^2 + \frac{1}{4}\left(\frac{\eta_2}{\eta_3} - 1\right)^2 - \frac{\xi_1}{\eta_3^2}\right) = 0 \quad (32)$$

$$E_{nm} = D_0 - \frac{2\alpha^2\hbar^2}{\mu}\left(\frac{\gamma - BD_0 - (v+n)^2}{2(v+n)}\right)^2 \quad (33)$$

Thermodynamic Properties

In this section, the thermodynamic properties of the potential model were evaluated. These properties can be derived using the exact partition function as follows (Reiss, 2012).

$$Z(\beta) = \sum_{n=0}^{\lambda} e^{-\beta E_n} \quad (34)$$

Where λ is an upper bound of the vibrational quantum number deduced from $\frac{dE_n}{d_n} = 0$, $\beta = \frac{1}{KT}$ where k and T are Boltzmann constant and temperature respectively. The summation can be replaced with an integral (Ikot *et al*. 2021).

$$Z(\beta) = \int_0^{\lambda} e^{-\beta E_n}\, dn \quad (35)$$

The energy equation can be expressed in terms of a partition function as follows (Ikot *et al*. 2021).

$$Z = e^{-\beta K_1}\int_0^{\lambda} e^{-\frac{\beta}{2}\left(\frac{2K_2K_3^2}{P^2} + K_2P^2\right)}\, dP \quad (36)$$

Magnetisation and Magnetic Susceptibility at Zero Temperature

At absolute zero, magnetization M_{nm} and magnetic susceptibility χ_{nm} reveal key quantum characteristics of a system subjected to an external magnetic field B(T). Magnetization $M_{\mathrm{nm}}(B, \Phi_{\mathrm{AB}})$ describes the material's response to the applied field and is given by (Jia *et al*. 2012)

$$M_{\mathrm{nm}} = -\frac{\partial E}{\partial B} \quad (37)$$

Magnetic susceptibility quantifies how magnetization varies with the magnetic field. At zero temperature, quantum effects become dominant, influencing susceptibility through the system's ground state properties.

$$\chi_{\mathrm{nm}} = \frac{\partial E}{\partial B} \quad (38)$$

Magnetisation and Magnetic Susceptibility at Finite Temperature

At finite temperatures, magnetization (M_{nm}) and magnetic susceptibility (χ_{nm}) are influenced by both thermal fluctuations and quantum effects. It depends on the statistical distribution of energy states with thermal excitations leading to gradual changes in magnetic response compared to the abrupt transitions seen at zero temperature (Umirzakov, 2019).

$$M_{\mathrm{nm}} = \frac{1}{\beta}\frac{\partial Z}{\partial B} \quad (39)$$

Magnetic susceptibility (χ_{nm}) describes how magnetization responds to variations in the applied field.

$$\chi_{\mathrm{nm}} = \frac{\partial M}{\partial B} \quad (40)$$

Numerical computation of energy eigenvalues

The numerical computation for energy eigenvalues is calculated using equation (33) as shown in table (1 - 4) for four diatomic molecules based on the results of spectroscopic analysis by vary magnetic field B(T) and flux ϕ_{AB}. The numerical bound state solutions were carried out for fixed principal quantum number ($n = 0, 1, 2, 3$) with varying magnetic quantum number $m = 0, +1, -1$.

Table 1: The Results of Spectroscopic Analysis (Jia *et al.*, 2012)

Parameters	H_2	Co	ScH	ScF
$\mu(amu)$	0.50391	6.86067	10.68277	13.35894
$D_e(cm^{-1})$	38266	90540	36778.9	47183.43
$\alpha(A^{-1})$	1.9426	2.2940	1.5068	1.46102

Table 2: Numerical Solutions for Energy Eigenvalues of H_2 Diatomic Molecule

H_2 Diatomic Molecule					
m	n	$B=0,\phi_{AB}=0$	$B=3,\phi_{AB}=0$	$B=0,\phi_{AB}=3$	$B=3,\phi_{AB}=3$
0	0	−12.09318	−11.46353	−11.89254	−11.10884
	1	−9.47862	−8.97591	−9.3186	−8.69199
	2	−7.34169	−6.93629	−7.21278	−6.70683
	3	−5.58088	−5.25123	−5.47614	−5.064315
1	0	−12.02567	−11.40175	−11.82689	−11.05017
	1	−9.42480	−8.92649	−9.26621	−8.64497
	2	−7.29835	−6.89637	−7.17054	−6.66879
	3	−5.54567	−5.21873	−5.44180	−5.03330
−1	0	−12.02567	−11.40175	−11.82689	−11.05017
	1	−9.42480	−8.92649	−9.26621	−8.64497
	2	−7.29835	−6.89637	−7.17054	−6.66879
	3	−5.54567	−5.21873	−5.44180	−5.03330

Table 3: Numerical Solution for Energy Eigenvalues of Co Diatomic Molecule

Co Diatomic Molecule					
m	n	$B=0,\phi_{AB}=0$	$B=3,\phi_{AB}=0$	$B=0,\phi_{AB}=3$	$B=3,\phi_{AB}=3$
0	0	0.55234	0.56455	0.55612	0.57190
	1	0.88345	0.89490	0.88700	0.90178
	2	1.19636	1.20709	1.19968	1.21355
	3	1.49211	1.50217	1.49522	1.5082
1	0	0.55360	0.56581	0.55738	0.57315
	1	0.88463	0.89607	0.88818	0.90296
	2	1.19747	1.20820	1.20079	1.21465
	$l3$	1.49314	1.50320	1.49626	1.50926
−1	0	0.55360	0.56581	0.55738	0.57315
	$l1$	0.88463	0.89607	0.88818	0.90296
	2	1.19747	1.20820	1.20079	1.21465
	3	1.49314	1.50320	1.49626	1.50926

Table 4: Numerical Solution for Energy Eigenvalues of ScH Diatomic Molecule

ScH Diatomic Molecule					
m	n	$B=0,\phi_{AB}=0$	$B=3,\phi_{AB}=0$	$B=0,\phi_{AB}=3$	$B=3,\ \phi_{AB}=3$
0	0	−5.97612	−5.96501	−5.97268	−5.95831
	1	−5.66566	−5.65502	−5.66237	−5.64860
	2	−5.36672	−5.35651	−5.36356	−5.35035
	3	−5.07877	−5.06898	−5.07574	−5.06308
1	0	−5.97497	−5.96386	−5.97153	−5.95717
	1	−5.66457	−5.65392	−5.66127	−5.64750
	2	−5.36567	−5.35546	−5.36251	−5.34930
	3	−5.07776	−5.06797	−5.07473	−5.06207
−1	0	−5.97497	−5.96386	−5.97153	−5.95717
	1	−5.66457	−5.65392	−5.66127	−5.64750
	2	−5.36567	−5.35546	−5.36251	−5.34930
	3	−5.07776	−5.06797	−5.07473	−5.06207

Table 5: Numerical Solution for Energy Eigenvalues of ScF Diatomic Molecule

ScF Diatomic Molecule					
m	n	$B=0,\phi_{AB}=0$	$B=3,\phi_{AB}=0$	$B=0,\phi_{AB}=3$	$B=3,\phi_{AB}=3$
0	0	−1.87691	−1.87284	−1.87565	−1.87039
	1	−1.70905	−1.70513	−1.70784	−1.70276
	2	−1.54645	−1.54267	−1.54528	−1.54038
	3	−1.38893	−1.38527	−1.38780	−1.38307
1	0	−1.87649	−1.87242	−1.87523	−1.86997
	1	−1.70865	−1.70473	−1.70744	−1.70236
	2	−1.54606	−1.54228	−1.54489	−1.54000
	3	−1.38855	−1.38490	−1.38742	−1.38270
−1	0	−1.87649	−1.87242	−1.87523	−1.86997
	1	−1.70865	−1.70473	−1.70744	−1.70236
	2	−1.54606	−1.54228	−1.54489	−1.54000
	3	−1.38855	−1.38490	−1.38742	−1.38270

Computational Analysis

The computational analysis was conducted to validate the numerical solutions for the bound state energy eigenvalues of four diatomic molecules under the influence of an external magnetic field B(T) and flux (ϕ_{AB}). This study is framed within the parametric Nikiforov-Uvarov-Functional Analysis (NUFA) approach, utilizing the exponential screened plus Yukawa potential (ESPYP).

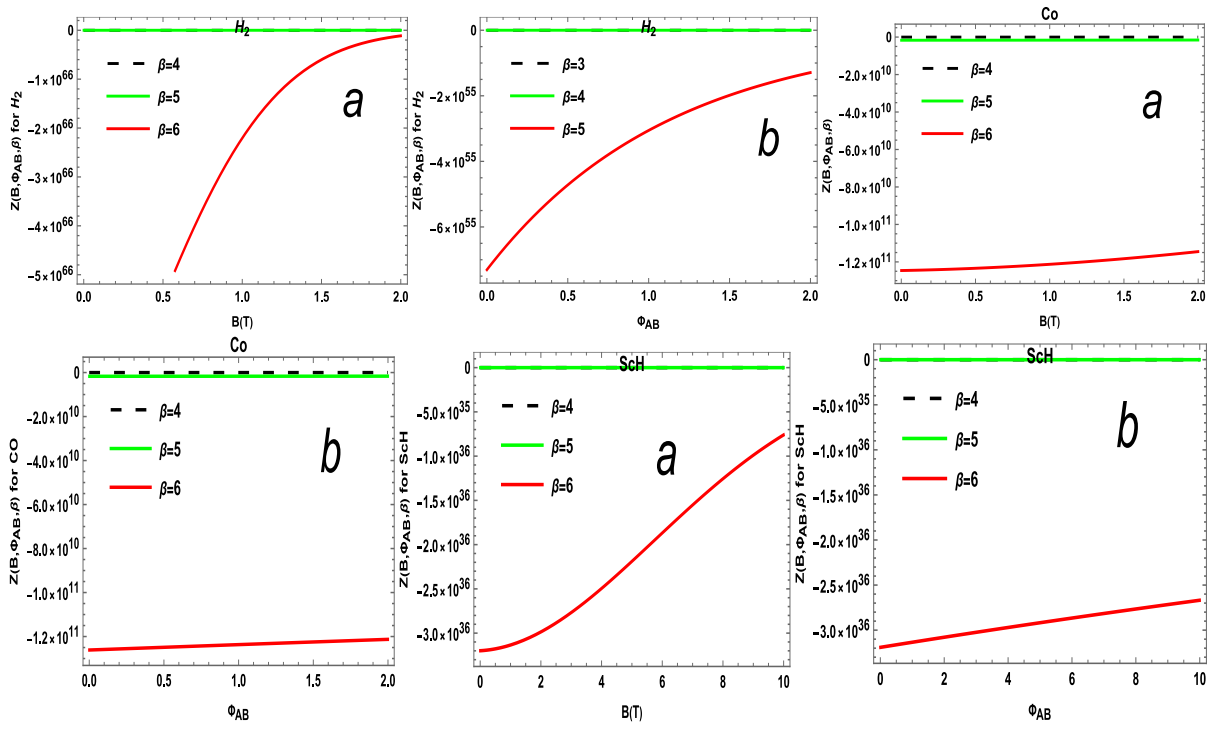
This section is divided into two parts. The first part involves calculating the molecular energy eigenvalues by varying the magnetic field B(T) and flux (ϕ_{AB}) across the four diatomic molecules. The second part focuses on computing the magnetisation and magnetic susceptibility at both zero and finite temperatures under the influence of the external magnetic field B(T) and flux (ϕ_{AB}).

The thermodynamic characteristics of the diatomic molecules are determined by the partition function, expressed as follows.

$$Z=\frac{e^{-\beta(K_1+K_2K_3)}\sqrt{\frac{\pi}{2}}\left(e^{-\sqrt{-\beta K_2}\sqrt{-\beta K_2K_3^2}}A+e^{\sqrt{-\beta K_2}\sqrt{-\beta K_2K_3^2}}B\right)}{2\sqrt{-\beta K_2}} \tag{41}$$

$$A=\left(1+\mathrm{Erf}\left[\frac{P^2\sqrt{-\beta K_2}-\sqrt{-\beta K_2K_3^2}}{\sqrt{2}P}\right]\right) \tag{42}$$

$$B=\left(-1+\mathrm{Erf}\left[\frac{P^2\sqrt{-\beta K_2}+\sqrt{-\beta K_2K_3^2}}{\sqrt{2}P}\right]\right) \tag{43}$$



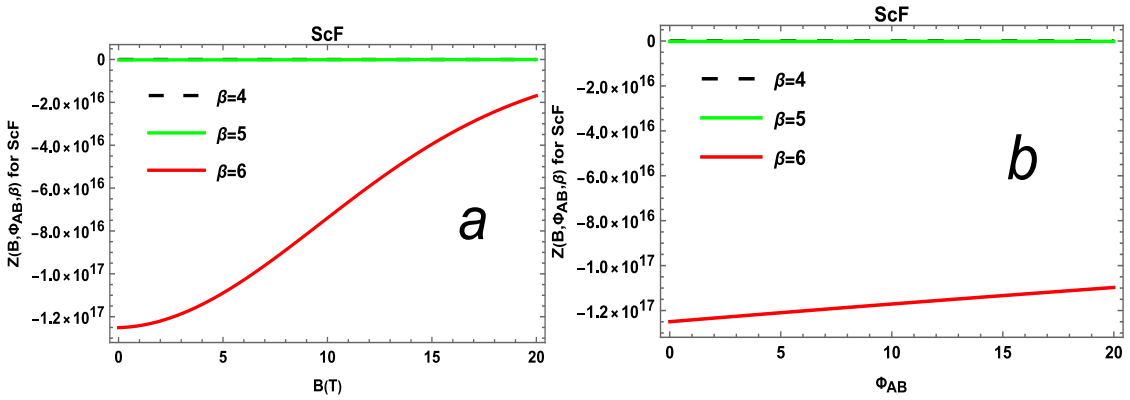
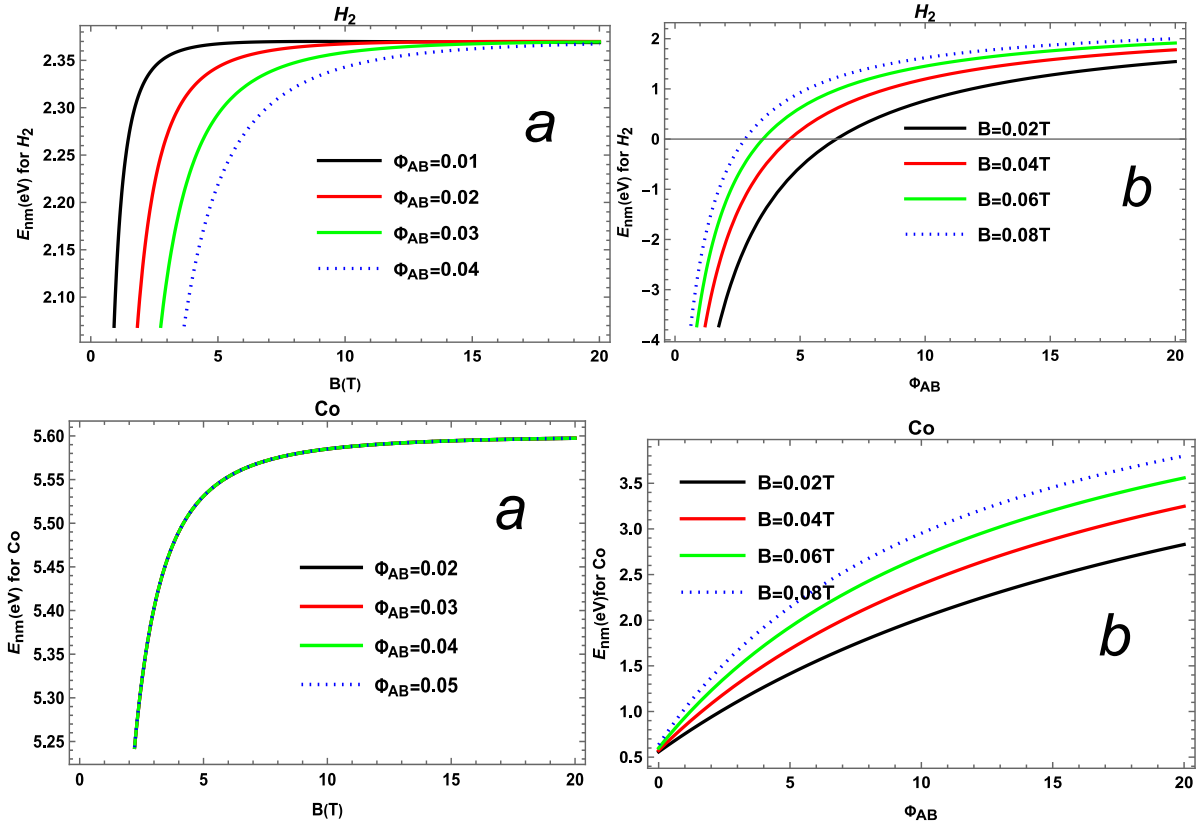


Figure 1: Calculated partition function based on temperature (β) for four diatomic molecules under varying B(T) and flux (ϕ_{AB}).



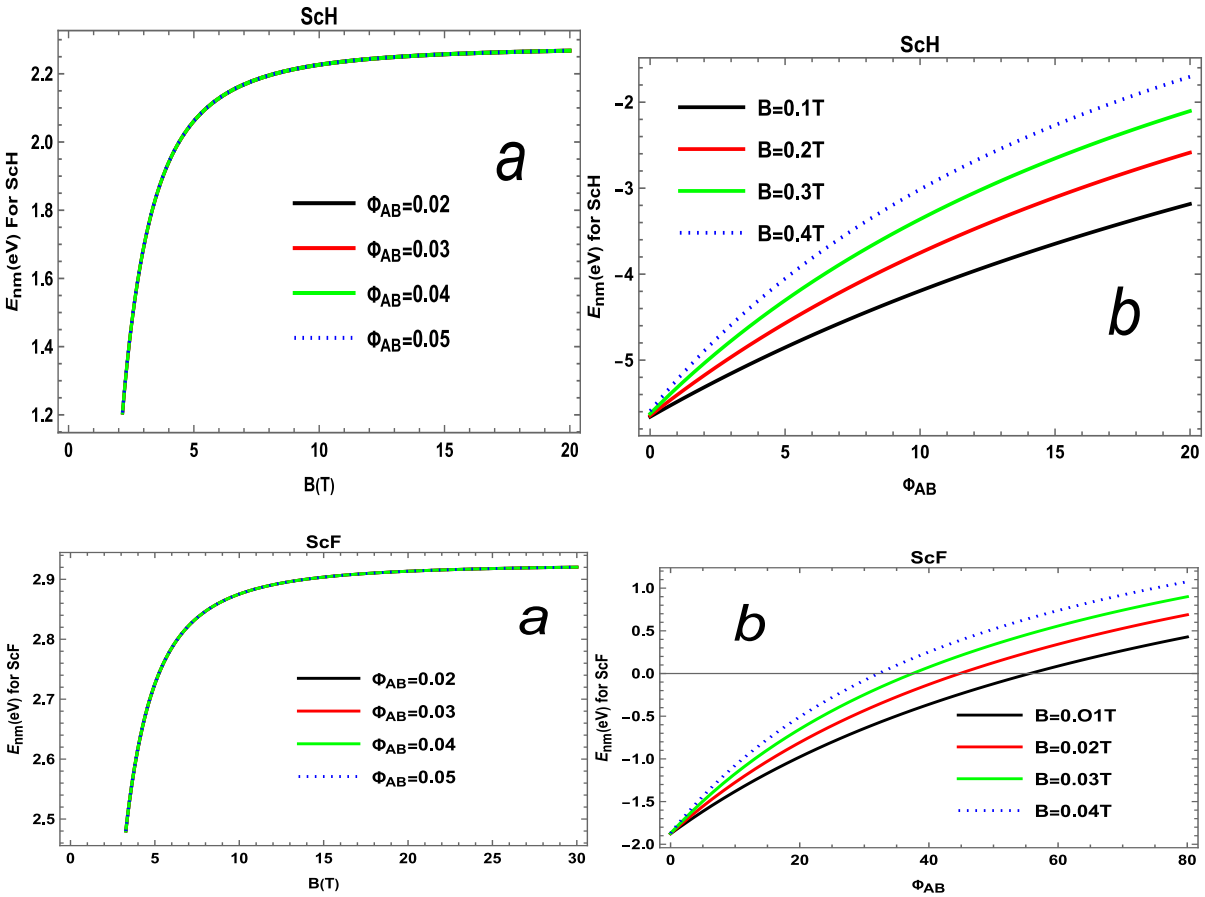
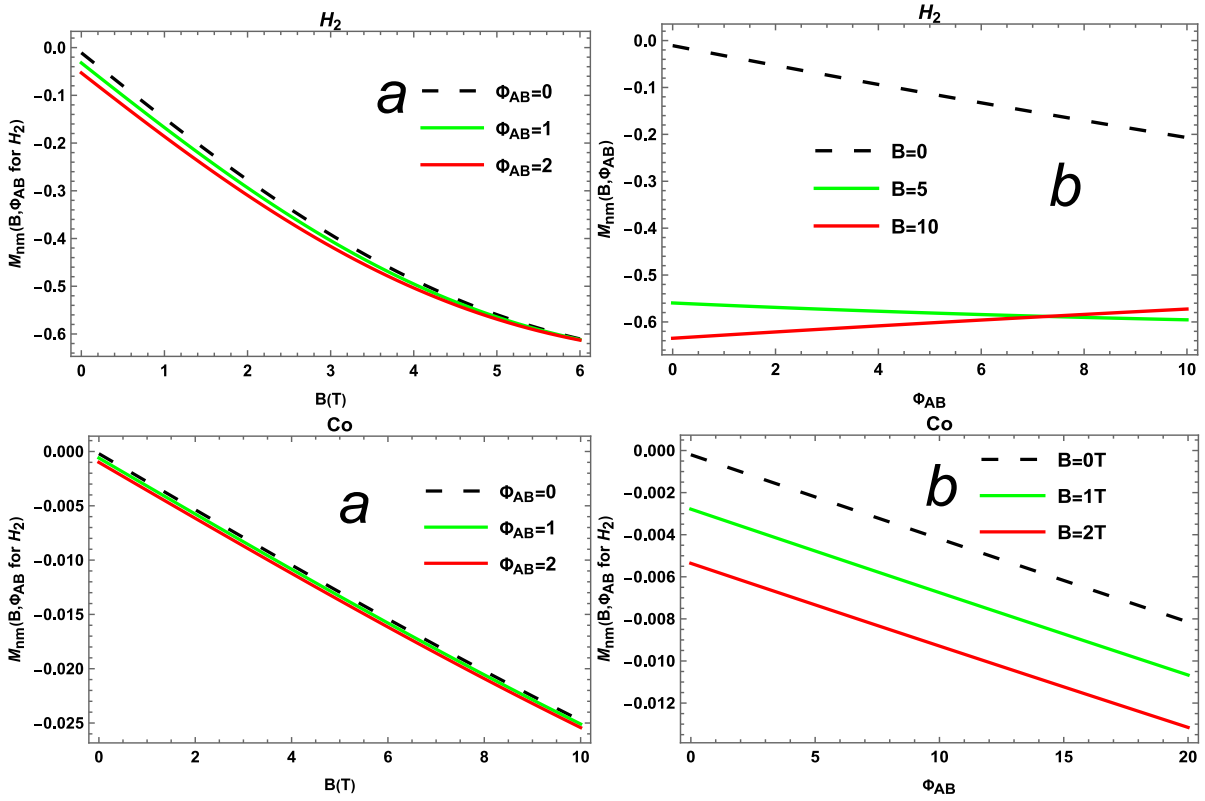


Figure 2: Calculated energy eigenvalues for four diatomic molecules under varying B(T) and flux (ϕ_{AB})



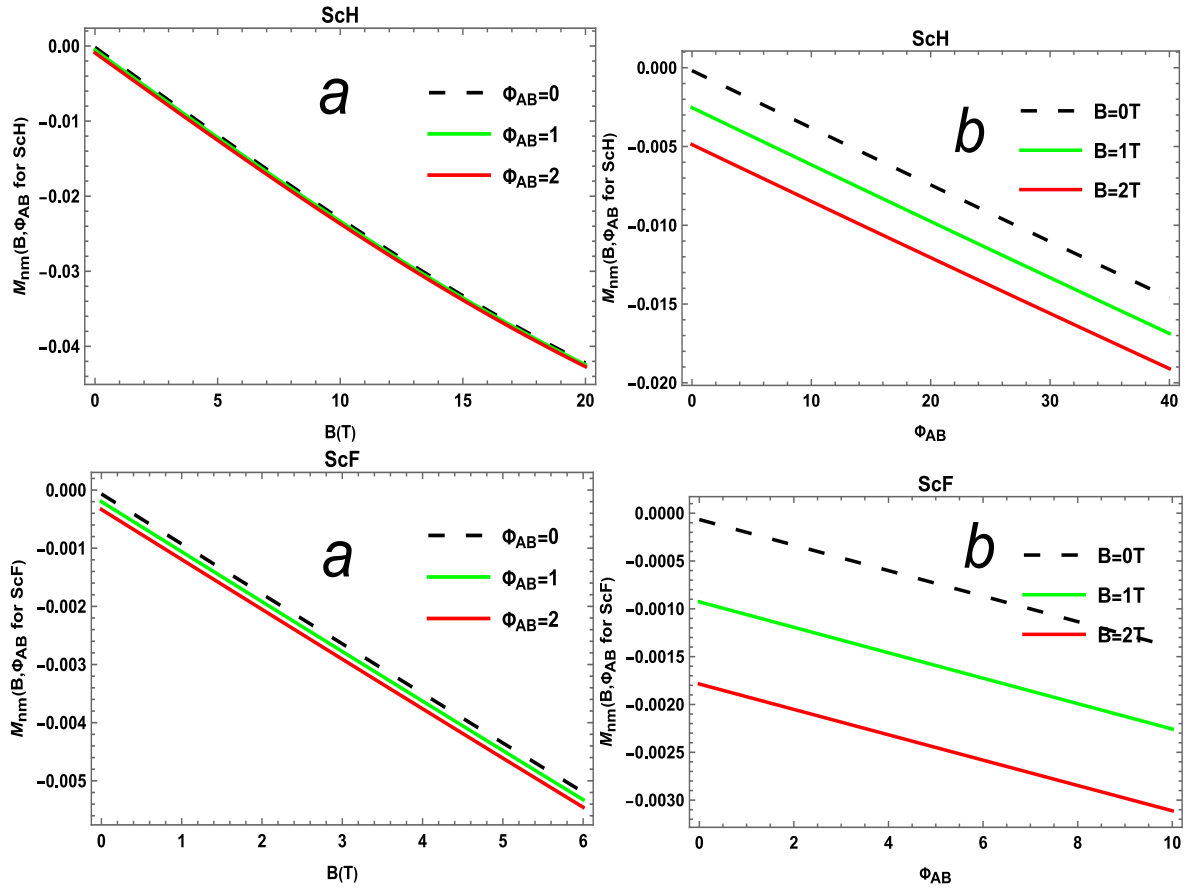
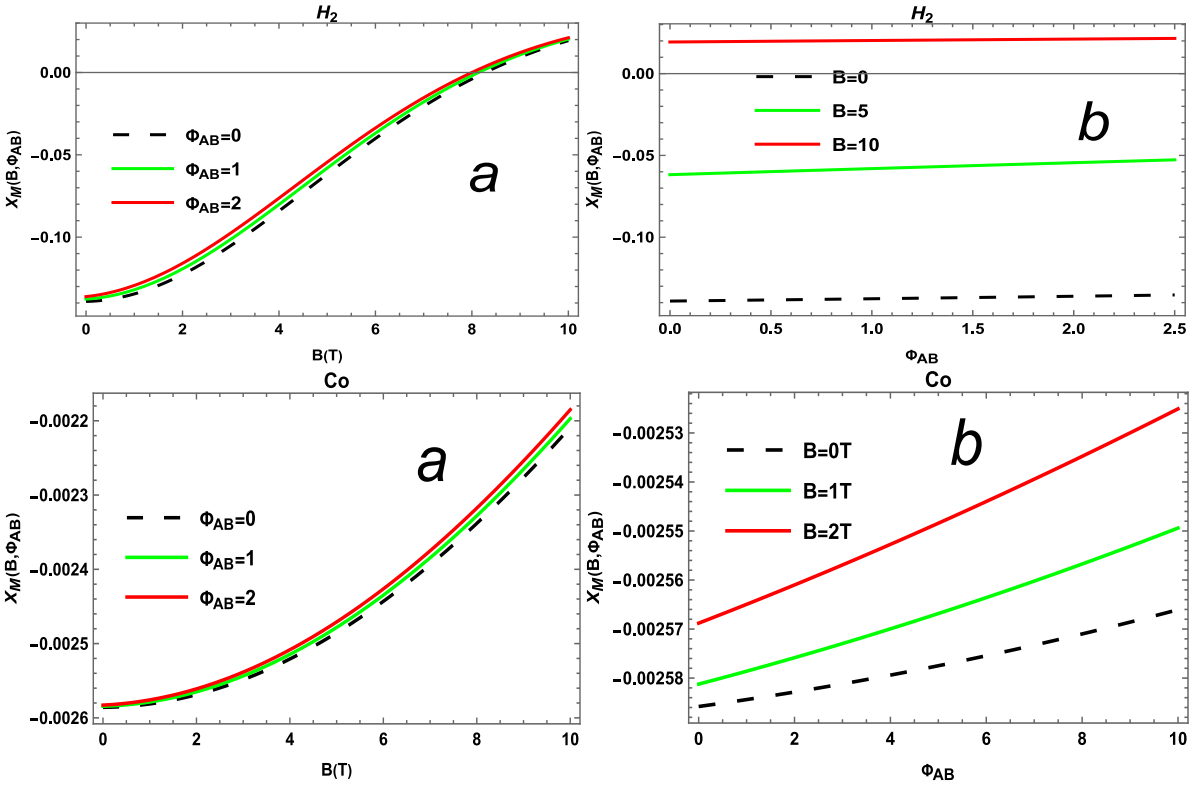


Figure 3: Calculated magnetisation for four diatomic molecules under varying B(T) and flux (ϕ_{AB}) at zero temperature



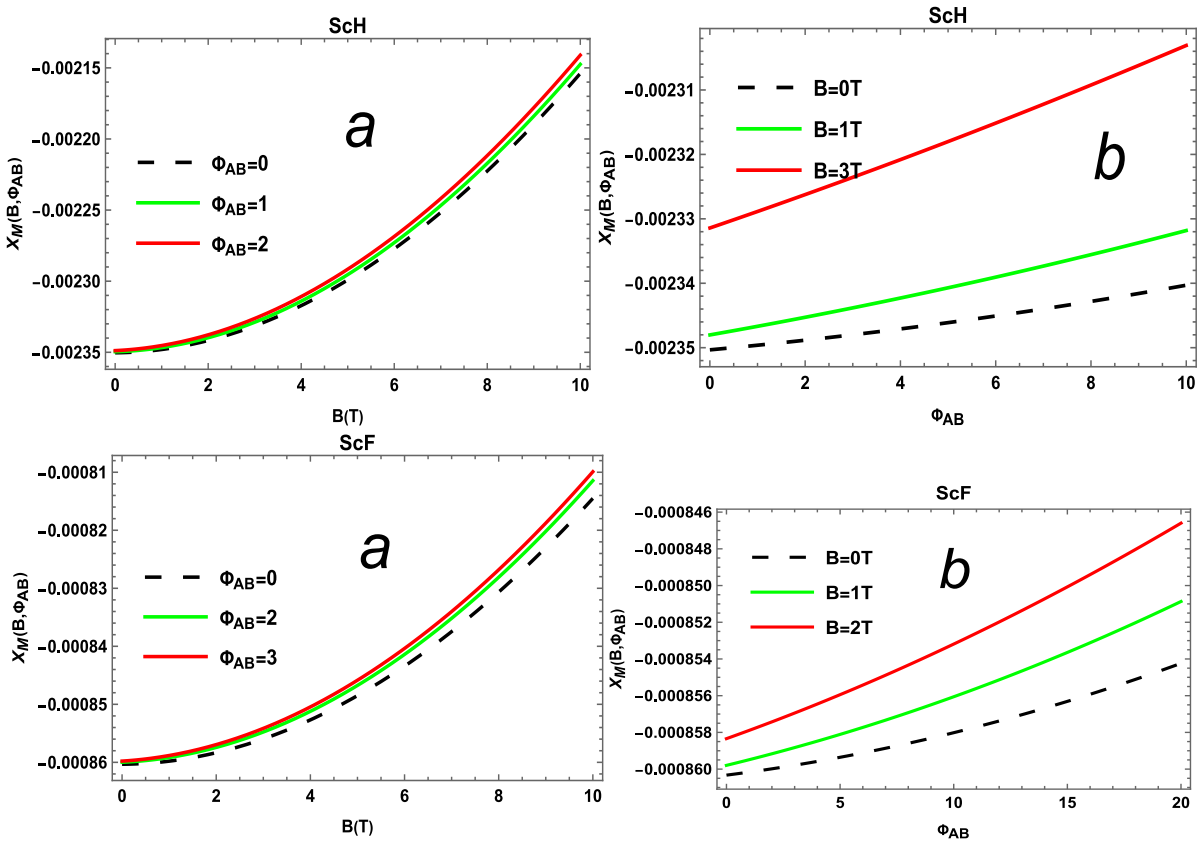
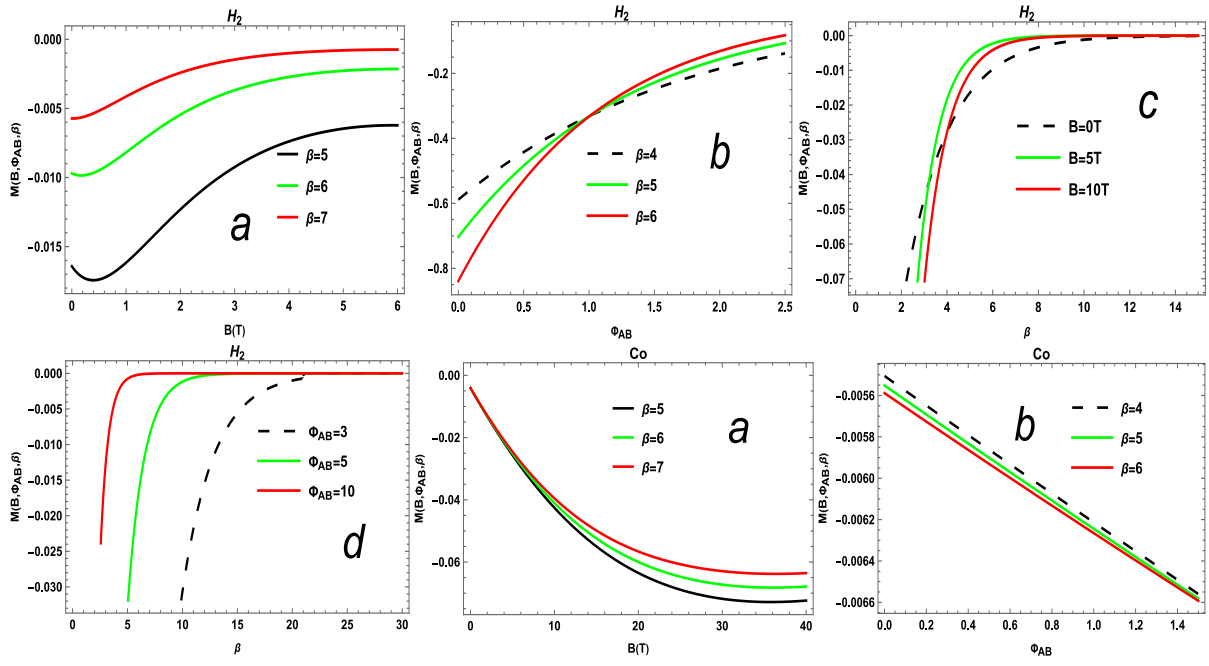


Figure 4: Calculated magnetic susceptibility for four diatomic molecules under varying B(T) and flux (ϕ_{AB}) at zero temperature



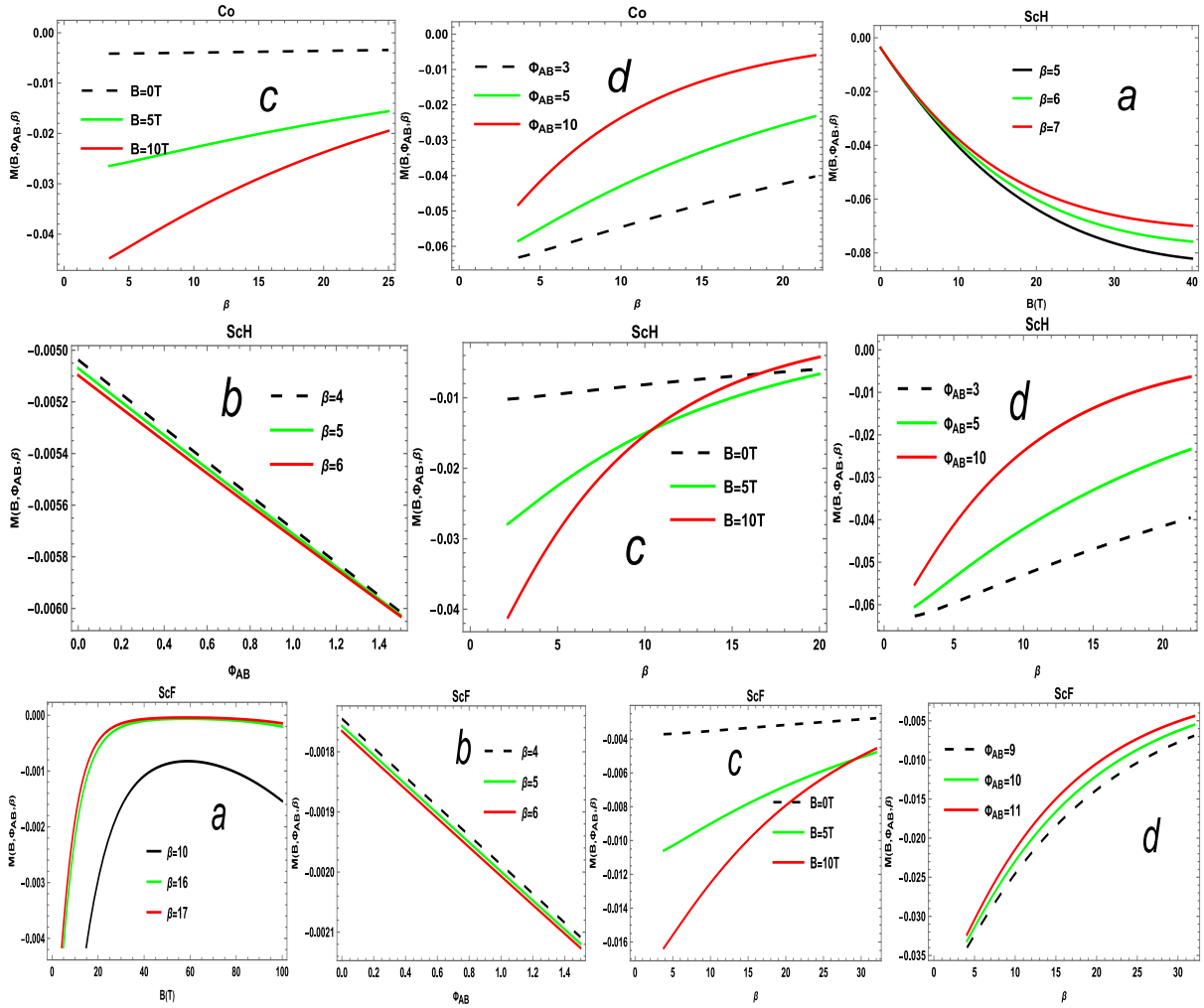
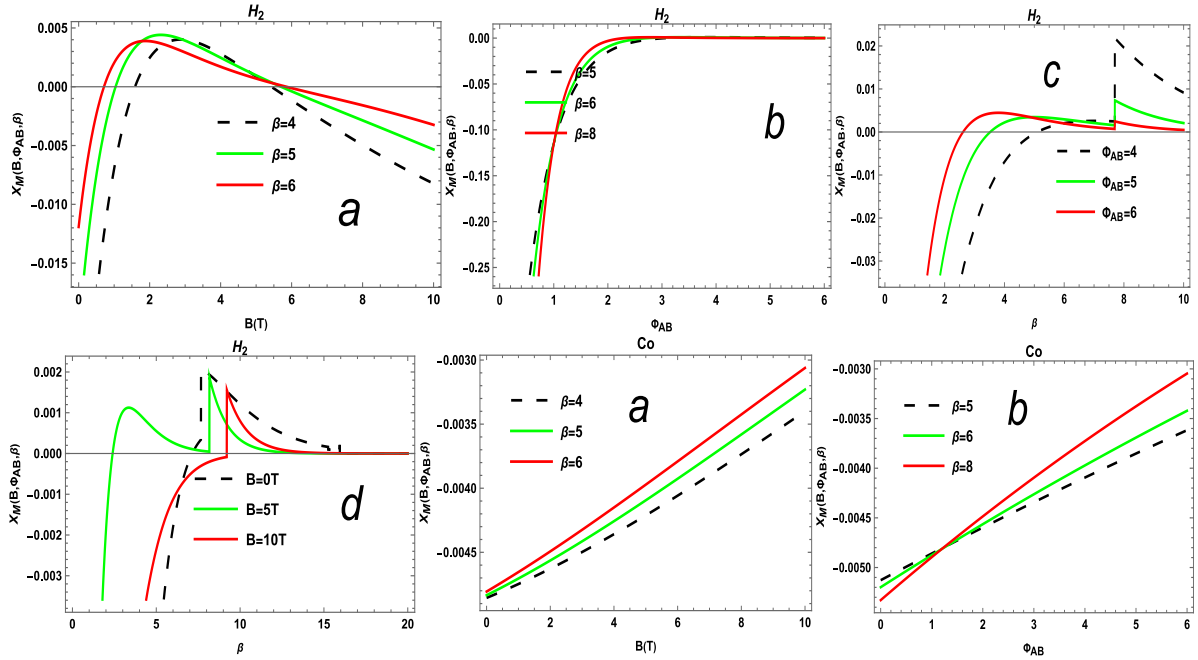


Figure 5: Computed magnetic susceptibility for four different diatomic molecules under varying magnetic field strength B(T) and flux (ϕ_{AB}) at a finite temperature



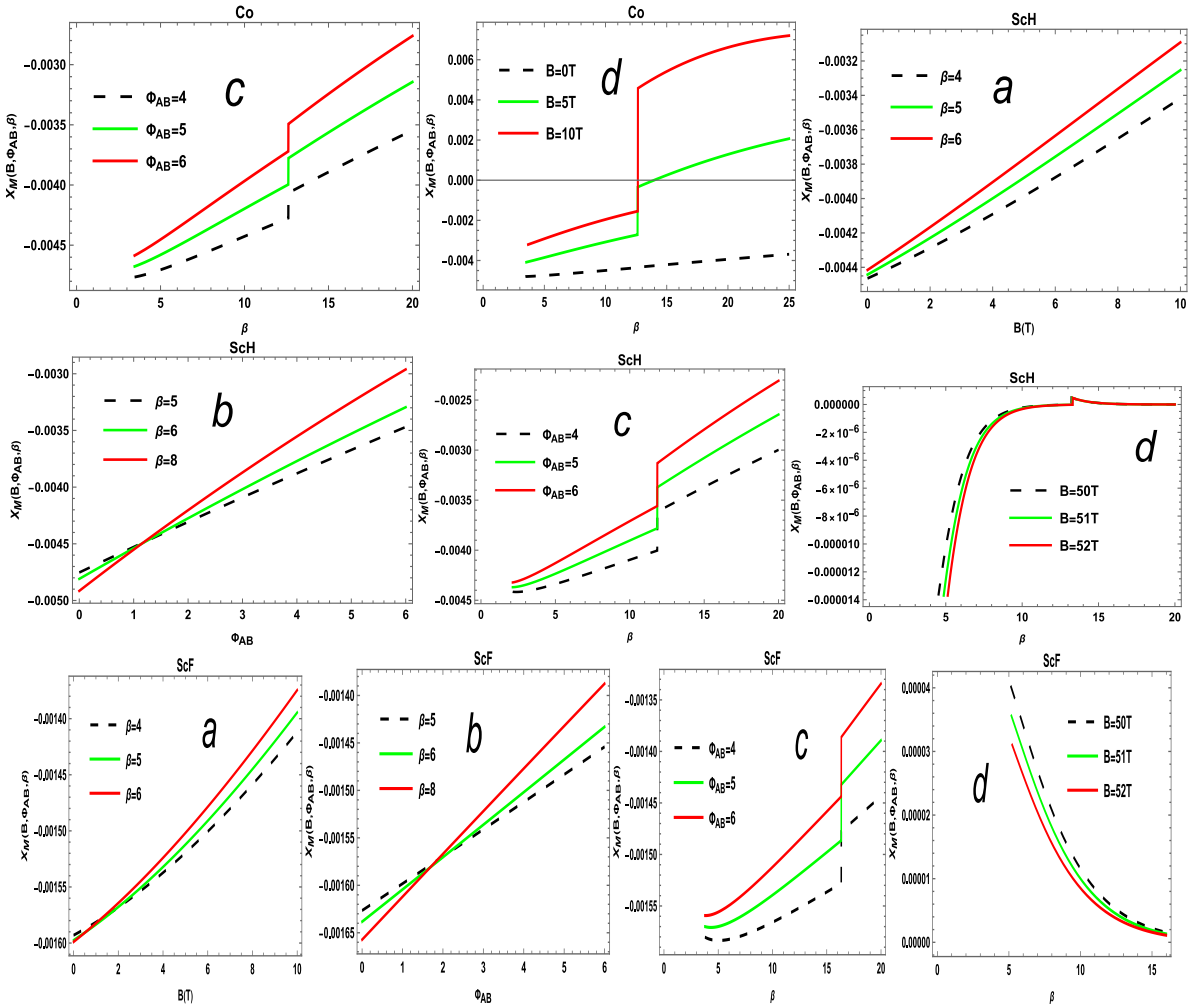


Figure 6: Computed magnetic susceptibility for four different diatomic molecules under varying magnetic field strength B(T) and flux (ϕ_{AB}) at a finite temperature

Discussion of Results

To validate the results of our study, we calculate the energy eigenvalues using equation (33) for various diatomic molecules, such as H_2, Co, ScH *and* ScF and our findings is similar to that of manga *et al.* 2025A; Manga *et al.* 2025B; Manga *et al.* 2023. These computations were performed under an external magnetic field by varying the magnetic field B(T) and magnetic flux (ϕ_{AB}) across different principal and magnetic quantum numbers. More so, we make used of spectroscopic parameters as shown in table 1 obtained from NIST database under the following conversions (Jia *et al.* 2012);

$1\ amu = 931.494028\ MeV/c^2$ (44)

$1\ cm^{-1} = 1.239841875 \times eV\dot{A}$ (45)

The calculated numerical energy eigenvalues are presented in tables (2 – 5), shows that both the external magnetic B(T) and magnetic flux (ϕ_{AB}) significantly influence the energy levels of the (H_2, Co, ScH *and* ScF) diatomic molecules. The upward shifts in energy levels with increasing B(T) and magnetic flux (ϕ_{AB}) indicates their role in modifying the molecular quantum states, which can be critical for understanding magneto-quantum effects in diatomic systems. Figure 1. Show that there is slightly influence of temperature, magnetic field, and magnetic flux on the statistical (thermal) properties of diatomic molecules. Figure 2 demonstrates how external magnetic fields and flux modify the quantum energy states of diatomic molecules with a trend relation. Figure 3 illustrates the impact of magnetic field B(T) and magnetic flux (ϕ_{AB})on the magnetization of diatomic molecules at zero temperature. However, in plot (b) for hydrogen, an overlap occurs at $B = 5\,T$ *and* $B = 10\,T$. Figure 4 shows how external magnetic fields B(T) and magnetic flux (ϕ_{AB}) affect the magnetic susceptibility of diatomic molecules at zero temperature. These variations provide insight into the quantum magnetic properties of molecular systems with a trend relationship, that at zero temperature magnetic suceptibility (χ_{nm}) increases. Figure 5 shows that for H_2 the magnetization (M_{nm}) increases with both the magnetic field B(T) and magnetic flux (ϕ_{AB}). as temperature varies. A similar trend is observed in the relationship between magnetization (M_{nm}) and temperature when B(T) and

magnetic flux (ϕ_{AB}). are varied. In the case of Co, magnetization (M_{nm}) decreases with increasing temperature while varying B(T) and magnetic flux (ϕ_{AB}). However, when plotted against temperature, magnetization (M_{nm}) increases as B(T) and magnetic flux (ϕ_{AB}) change. This behavior is also observed in ScH and ScF.

Figure 5 for H_2 the magnetisation M_{nm} increseases with magnetic field B(T) and magnetic flux (ϕ_{AB}) by varying temperature. Similar trend was observed that the magnetisation (M_{nm}) with temperature increases by varying magnetic field B(T) and magnetic flux (ϕ_{AB}). For Co it was observed that magnetisation (M_{nm}) with magnetic field B(T) and magnetic flux (ϕ_{AB}) decreases by varying temperature. On the same note, the magnetisation (M_{nm}) with temperature increased by varying magnetic field B(T) and magnetic flux (ϕ_{AB}). Similar effect is observed for ScH and ScF. Figure 6 shows that the magnetic susceptibility (χ_{nm}) with temperature increases by varying B(T) and magnetic flux (ϕ_{AB}) and it also shows that magnetic susceptibility (χ_{nm}) with magnetic field B(T) and magnetic flux (ϕ_{AB}) increases by varying temperature, expect plot (d) for ScF, which show that magnetic susceptibility (χ_{nm}) with temperature decreases by varying magnetic field B(T) and magnetic flux (ϕ_{AB}).

CONCLUSION

In summary, this study provides a comprehensive analysis of the energy eigenvalues of H_2, Co, ScH and ScF diatomic molecules influence by external magnetic based the exponential screened Yukawa potential (ESYP). The numerical calculations were used to validate the computation results of four different diatomic molecules. The calculations of the energy eigenvalues were carried-out at zero temperature along side magnetisation (M_{nm}) and magnetic susceptibility (χ_{nm}). We obtained the thermal properties of the diatomic molecules at finite temperature based on partition function. similarly, magnetisation (M_{nm}) and magnetic susceptibility (χ_{nm}). The findings have broad implications across quantum mechanics, spectroscopy, astrophysics, energy physics and material science, contributing to both fundamental and applied research.

REFERENCES

Abu-Shady, M., & Khokha, E. M. (2023). A precise estimation for vibrational energies of diatomic molecules using the improved Rosen–Morse potential. *Scientific Reports*, *13*(1), 11578.

Ding, Y., & Wang, Z. Q. (2011). Bound states of nonlinear Schrödinger equations with magnetic fields. *Annali di Matematica Pura ed Applicata*, *190*(3), 427-451.

Dong, S. H. (2000). Exact solutions of the two-dimensional Schrödinger equation with certain central potentials. *International Journal of Theoretical Physics*, *39*(4), 1119-1128.

Edet, C. O., Amadi, P. O., Onyeaju, M. C., Okorie, U. S., Sever, R., Rampho, G. J., & Ikot, A. N. (2021). Thermal properties and magnetic susceptibility of Hellmann potential in Aharonov–Bohm (AB) flux and magnetic fields at zero and finite temperatures. *Journal of Low Temperature Physics*, *202*(1), 83-105.

Ettah, E. (2021). The Schrödinger Equation with Deng-Fan-Eckart Potential (DFEP): Nikiforov-Uvarov-Functional Analysis (NUFA) Method. *European Journal of Applied Physics*, *3*(5), 58-62.

Ikot, A. N., Okorie, U. S., Amadi, P. O., Edet, C. O., Rampho, G. J., & Sever, R. (2021). The Nikiforov–Uvarov-Functional Analysis (NUFA) Method: A new approach for solving exponential-type potentials. *Few-Body Systems*, *62*(1), 9.

Jia, C. S., Diao, Y. F., Liu, X. J., Wang, P. Q., Liu, J. Y., & Zhang, G. D. (2012). Equivalence of the Wei potential model and Tietz potential model for diatomic molecules. *The Journal of chemical physics*, *137*(1).

Lublinsky, M., & Mulian, Y. (2017). High Energy QCD at NLO: from light-cone wave function to JIMWLK evolution. *Journal of High Energy Physics*, *2017*(5), 1-80.

Manga, P. J., Amusat, R. O., Teru, P. B., Dibal, A. A., Likta, W. E., Omolara, O. V., ... & Ubale, S. A. (2025A). Determination of Thermodynamic Properties via Partition Function Approaches Derived from the Non-Relativistic Schrödinger Equation. *Nigerian Journal of Theoretical and Environmental Physics*, *3*(2), 42-59.

Manga, P. J., Amusat, R. O., Teru, P. B., Likta, E. W., Dibal, A. A., Yahaya, M. N., & Isyaku, S. (2025B). COMPUTING ENERGY FLUCTUATIONS IN DIATOMIC MOLECULES THROUGH THERMODYNAMIC PROPERTIES USING THE PARTITION FUNCTION APPROACH. *Science World Journal*, *20*(2), 760-773.

Manga, P. J., Buteh, S. D., Maina, M., Amusat, R. O., Teru, P. B., Hashimu, M. U., & John, D. S. (2023). Solutions of Schrödinger equation based on Modified Exponential Screened Plus Yukawa Potential (MESPYP) within the frame of parametric Nikiforov-Uvarov method. *Dutse Journal of Pure and Applied Sciences*, *9*(3b), 144-154.

Manga, P. J., Likta, E. W., & Teru, P. B. (2021). Comparative Study on Charged and Neutral Pion-Nucleon Coupling

Constants Using Yukawa Potential Model. *FUDMA JOURNAL OF SCIENCES*, *5*(4), 167-173.

Mulian, Y. (2025). The Magnus expansion for non-Hermitian Hamiltonians. *arXiv preprint arXiv:2505.09559*.

Onate, C., Okon, I. B., Onyeaju, M. C., & Antia, A. D. (2022). Approximate solutions of the Schrodinger Equation for a Momentum-Dependent potential. *Journal of the Nigerian Society of Physical Sciences*, 242-250.

Reiss, H. R. (1980). Effect of an intense electromagnetic field on a weakly bound system. *Physical Review A*, *22*(5), 1786.

Umirzakov, I. (2019). Incorrectness of analytical solution of Schrodinger equation for diatomic molecule with shifted Tietz-Wei potential. *arXiv preprint arXiv:1902.04977*.