SOLUÇÃO ANALÍTICA DA EQUAÇÃO DE SCHRÖDINGER EM COORDENADA BISFÉRICA PARA POTENCIAL MOBIUS SQUARE PLUS MODIFIED YUKAWA USANDO O MÉTODO DE ANÁLISE FUNCIONAL NIKIFOROV UVAROV (NUFA) COM SUAS PROPRIEDADES DE TERMODINÂMICA PARA MOLECULAS DIATÔMICAS

ANALYTICAL SOLUTION OF SCHRÖDINGER EQUATION IN BISPHERICAL COORDINATE FOR MOBIUS SQUARE PLUS MODIFIED YUKAWA POTENTIAL USING NIKIFOROV UVAROV FUNCTIONAL ANALYSIS (NUFA) METHOD WITH ITS THERMODYNAMICS PROPERTIES FOR DIATOMIC MOLECULES

SOLUSI ANALITIS PERSAMAAN SCHRÖDINGER DALAM KOORDINAT BISPERICAL UNTUK POTENSIAL MOBIUS SQUARE PLUS YUKAWA TERMODIFIKASI MENGGUNAKAN METODE NIKIFOROV UVAROV FUNCTIONAL ANALYSIS (NUFA) DENGAN SIFAT TERMODINAMIKANYA UNTUK MOLEKUL DIATOMIK

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RESUMO

Introdução: A solução analítica da equação de Schrödinger em coordenadas bisféricas tem atraído grande interesse para pesquisadores da física teórica no ramo da física quântica. A energia e a função de onda são soluções da equação de Schrödinger que são muito importantes porque contém todas as informações necessárias sobre o comportamento dos sistemas quânticos. **Objetivo.** Este estudo teve como objetivo obter energia, funções de onda radial e propriedades termodinâmicas para moléculas diatômicas da parte radial da equação de Schrödinger em coordenadas bisféricas para o quadrado de Mobius modificado mais potencial de Yukawa usando o método Nikiforov Uvarov Functional Analysis (NUFA). **Métodos:** O método de separação variável foi aplicado para reduzir a equação de Schrödinger em coordenadas bisféricas à parte radial e parte angular da equação de Schrödinger. A equação de Schrödinger da parte radial em coordenadas bisféricas foi resolvida usando o método Nikiforov Uvarov Functional Analysis (NUFA) para obter a equação de energia e a função de onda radial. Além disso, a função de partição vibracional Z foi obtida a partir da equação de energia. A energia vibracional média U , o calor vibracional específico C , a energia vibracional livre F e a entropia vibracional S foram obtidas a partir da função de partição vibracional Z . **Resultados e Discussão:** Os resultados mostraram que o aumento dos parâmetros de n e α causou a diminuição da energia, mas o aumento dos parâmetros de L e m_0 causou o aumento da energia. O número quântico radial n e a faixa de potencial α tiveram o maior efeito nas funções de onda. Os parâmetros n_{max} , T e α tiveram efeito na função de partição vibracional Z , energia média vibracional U , calor específico vibracional C , energia livre vibracional F e entropia vibracional S . **Conclusões:** A partir dos resultados deste estudo, pode-se concluir que a energia, função de onda radial e propriedades termodinâmicas para moléculas diatômicas foram obtidas usando o método Nikiforov Uvarov Functional Analysis (NUFA).

Palavras-chave: Equação de Schrödinger, coordenada bisférica, quadrado Mobius mais potencial Yukawa modificado, método Nikiforov Uvarov Functional Analysis (NUFA), propriedades termodinâmicas.

ABSTRACT

Background: The analytical solution of the Schrödinger equation in bispherical coordinates has attracted a great deal of interest for theoretical physics researchers in the branch of quantum physics. The energy and wave function are solutions of the Schrödinger equation which are very important because it contains all necessary information regarding the behavior of quantum systems. **Aim:** This study aimed to obtain energy, radial wave functions and thermodynamic properties for diatomic molecules from the radial part of the Schrödinger equation

in bispherical coordinates for the modified Mobius square plus Yukawa potential using the Nikiforov Uvarov Functional Analysis (NUFA) method. **Methods:** The variable separation method was applied to reduce the Schrodinger equation in bispherical coordinates to the radial part and angular part Schrodinger equation. The Schrodinger equation of the radial part in bispherical coordinates was solved using the Nikiforov Uvarov Functional Analysis (NUFA) method to obtain the energy equation and radial wave function. Furthermore, the vibrational partition function Z was obtained from the energy equation. The vibrational mean energy U , vibrational specific heat C , vibrational free energy F , and vibrational entropy S were obtained from the vibrational partition function Z . **Results and Discussion:** The results showed that the increase of parameters of n and α caused the decrease of energy, but the increase of parameters of L and m_0 caused the increase of energy. The radial quantum number n and the potential range α had the most effect to the wave functions. The parameters n_{max} , T , and α had effect to the vibrational partition function Z , vibrational mean energy U , vibrational specific heat C , vibrational free energy F , and vibrational entropy S . **Conclusions:** From the results of this study, it can be concluded that the energy, radial wave function, and thermodynamic properties for diatomic molecules have been obtained using the Nikiforov Uvarov Functional Analysis (NUFA) method.

Keywords: *Schrödinger equation, bispherical coordinate, Mobius square plus modified Yukawa potential, Nikiforov Uvarov Functional Analysis (NUFA) method, Thermodynamics properties.*

ABSTRAK

Latar Belakang: Solusi analitis dari persamaan Schrödinger dalam koordinat bispherical telah menarik banyak minat bagi peneliti fisika teori dalam cabang fisika kuantum. Energi dan fungsi gelombang merupakan solusi dari persamaan Schrödinger yang sangat penting karena mengandung semua informasi yang diperlukan mengenai perilaku sistem kuantum. **Tujuan:** Penelitian ini bertujuan untuk mendapatkan energi, fungsi gelombang radial dan sifat termodinamika untuk molekul diatomik dari persamaan Schrödinger bagian radial dalam koordinat bispherical untuk potensial Mobius square plus Yukawa termodifikasi menggunakan metode Nikiforov Uvarov Functional Analysis (NUFA). **Metode:** Metode pemisahan variabel diterapkan untuk mereduksi persamaan Schrodinger dalam koordinat bispherical menjadi persamaan Schrodinger bagian radial dan bagian sudut. Persamaan Schrodinger bagian radial dalam koordinat bispherical diselesaikan menggunakan metode Nikiforov Uvarov Functional Analysis (NUFA) untuk mendapatkan persamaan energi dan fungsi gelombang radial. Selanjutnya fungsi partisi getaran diperoleh dari persamaan energi. Energi rata-rata getaran, kapasitas panas getaran, energi bebas getaran, dan entropi getaran diperoleh dari fungsi partisi getaran. **Hasil dan Diskusi:** Hasil penelitian menunjukkan bahwa peningkatan parameter n dan α menyebabkan penurunan energi, sedangkan peningkatan parameter L dan m_0 menyebabkan peningkatan energi. Bilangan kuantum radial n dan potensial range α memiliki pengaruh paling besar terhadap fungsi gelombang. Parameter n_{max} , T , dan α berpengaruh terhadap fungsi partisi getaran Z , energi rata-rata getaran U , kapasitas panas getaran C , energi bebas getaran F , dan entropi getaran S . **Kesimpulan:** Dari hasil penelitian ini, dapat disimpulkan bahwa energi, fungsi gelombang dan sifat termodinamika untuk molekul diatomik telah diperoleh menggunakan metode Nikiforov Uvarov Functional Analysis (NUFA).

Kata kunci: *Persamaan Schrödinger, koordinat bispherical, Potensial Mobius square plus Yukawa termodifikasi, Metode Nikiforov Uvarov Functional Analysis (NUFA), Sifat termodinamika.*

1. INTRODUCTION:

There had been increasing interest in theoretical physics to obtain the exact solution of the Schrödinger equation in spacetimes with non-spherical topology. The primary purposes of this interest are to obtain the energy eigenvalue and the wave function in quantum systems. Various methods have been used to solve the Schrödinger equation, such as the factorization method (Dong, 2007), supersymmetry of quantum mechanics (SUSYQM) (Ahmadov *et al.*, 2018), Nikiforov–Uvarov method (NU) (Ikot *et al.*, 2013), Asymptotic Iteration Method (AIM) (Bayrak and Boztosun, 2007), and Hypergeometry (Hidayat *et al.*, 2019).

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Schrödinger equation, such as the factorization method (Dong, 2007; Sadeghi, 2007; Mir-Kasimov, 2013), supersymmetry of quantum mechanics (SUSYQM) method (Ahmadov *et al.*, 2018; Abu-Shady and Ikot, 2019; Hassanabadi *et al.*, 2012), Nikiforov–Uvarov method (NU) (Ikot *et al.*, 2013; Berkdemir, 2012; Deta *et al.*, 2013), Asymptotic Iteration Method (AIM) (Bayrak and Boztosun, 2007; Rostami and Motavali, 2008; Falaye, 2012), and Hypergeometry method (Hidayat *et al.*, 2019; Nurhidayati *et al.*, 2018; Dianawati *et al.*, 2019).

The factorization method is a type of basic technique that reduces the dynamic equations of a particular system to simple equations that are easier to solve. The basic idea is to consider a pair of first-order differential equations that can be

obtained from certain second-order differential equations with boundary conditions. This method is only applicable to the discrete energy spectrum because the continuous energy levels are not counted. This method can also write down the desired eigenvalues and normalized eigenvalues of a given Hamiltonian without using traditional quantum mechanical treatment methods such as the power series method or by solving second-order differential equations to get the correct solution of the studied quantum system (Dong, 2007).

The Supersymmetry of quantum mechanics (SUSYQM) method is a method for determining the eigenvalues and eigenstates of known analytical potentials that can be solved using the formalism of algebraic operators without having to solve the Schrödinger differential equation with the standard series method. However, operator methods have been applied only to one-dimensional problems and spherical symmetry. Supersymmetry (Dutt *et al.*, 1988; Sohnius, 1985), by definition, is the symmetry between fermions and bosons. The supersymmetric field theoretical model consists of a set of quantum and lagrangian fields that show symmetry. Lagrangian is determined through the principle of action, equations of motion, and dynamic behavior of particles (Cari *et al.*, 2016).

Nikiforov–Uvarov method (NU) is a method that reduces second-order linear differential equations to general equations in their hypergeometric form. This method has been used successfully to solve many differential equations of quantum mechanics, including the Schrödinger equation, the Dirac Relativistic equation, the Klein - Gordon equation, the Duffin - Kemmer - Petiau equation (DKP), and the spinless-Salpeter equation. The Nikiforov–Uvarov method (NU) is a simpler and more accurate direct method for determining the energy equation and the appropriate wave function (Onyenegecha *et al.*, 2020).

The Asymptotic Iteration method (AIM) is a technique for solving analytically and approaching second-order linear differential equations, especially the problem of eigenvalues that often appears in theoretical physics and mathematics. This method can be solved using the asymptotic aspect of the iterative method (Ismail and Saad, 2020).

The Hypergeometric method is that any second-order ordinary differential equation with at most three ordinary singular points can be brought into the hypergeometric differential equation

through the appropriate change of the variable. The solution of hypergeometric differential equations includes many of the most interesting mathematical physics special functions. Solutions for hypergeometric differential equations are constructed from hypergeometric series (Mubeen *et al.*, 2014).

The method of separation of variables in various coordinate systems was a classic approach to find the exact solutions of the Schrödinger equation that had been widely studied. One such set of coordinates was the bispherical coordinate system.

The variable separation method is one of the most widely used techniques for solving partial differential equations. It is based on the assumption that the solutions of equations are separable; that is, the final solution can be represented as the product of several functions, each of which depends only on one independent variable. If this assumption is wrong, then a clear violation of mathematical principles will be evident from the analysis (Arfken *et al.*, 2005). The method of separating variables in various coordinate systems is a classic approach to finding the correct solution of the Schrödinger equation in the form of a partial differential equation. The Schrödinger solution in the coordinate system with the variable separation method produces a partial differential equation that can be separated, namely the radial part equation and the angular part equation. One such set of coordinates is the bispherical system, but it would be said that some of the uses of this coordinate system have been hidden. Although the usual way of separating variables is suitable for some circumstances, there are other ways that are more suitable for certain classes of problems, particularly some of the problems attracting branches of macroscopic field theory, including electrostatics and magnetostatics (Stoy, 1989).

The bispherical coordinates are one of the non-spherical coordinates that have the spheres are designated by $\mu = \text{const}$, half-planes by $\phi = \text{const}$. The surfaces $\theta = \text{const}$ are spindles if $\eta < \frac{\pi}{2}$, a sphere at $\eta = \frac{\pi}{2}$, and apple-shaped surfaces if $\eta > \frac{\pi}{2}$ (Moon and Spencer, 1971). Bispherical coordinates use to solve other types of equations, such as Gegenbauer differential equations, to solve irrotational fluid motion (Deo and Tiwari, 2008). Other applications to solve the Poisson-Boltzmann theory numerically determine the force between spherical colloid particles (Carnie *et al.*, 1994) and investigate heat transfer by conduction from the spheroidal and bispherical oblate surfaces into an infinite stationary medium (Jafari

et al., 2019).

On the other hand, the result of the energy equation from the solution of the radial part of the Schrödinger equation in bispherical coordinates can solve many problems, calculations of thermodynamic quantities (Irikura, 2014; Skouteri *et al.*, 2016), investigating isotope effects (Lasaga *et al.*, 2008), and calculating the equilibrium constant of gas-phase reaction (Buchowiecki, 2012). The route to these calculations is through partition functions. Acquiring a closed-form expression of the partition function is very useful and informative. The vibrational partition function can be calculated by direct summation over all possible vibrational energy levels. Many attempts have been made in the literature to obtain the analytical expression of the partition function for the potential energy function for diatomic and polyatomic molecules in various mathematical methods, such as the cumulant expansion approach (Strekalov, 2004), Poisson summation formula (Jia *et al.*, 2017; Song *et al.*, 2017), and Wigner-Kirkwood approach (Stratt and Miller, 1977; Korsch, 1979).

Therefore, this study aimed to find the energy spectrum equations and radial wave function equations, and also thermodynamic properties corresponding such as vibrational partition function, vibrational mean energy, vibrational specific heat, vibrational free energy, and vibrational entropy for diatomic molecules affected by the Mobius square plus modified Yukawa potential.

2. MATERIALS AND METHODS:

2.1 Review Before Bispherical Coordinates

Spherical coordinates are the most common and simple coordinates used to solve the Schrödinger equation to obtain the energy and wave function equations. Spherical coordinates also have symmetrical properties, so they are easier to solve using Schrödinger (Suparmi, 2011; Suparmi *et al.*, 2020). Spherical coordinates, also called the polar coordinates of a sphere, are a system of curved coordinates to describe the position on a sphere. The definition θ is the azimuthal angle in the xy plane of the x -axis with $0 \leq \theta < 2\pi$ (denoted λ if it is called longitude), ϕ is the polar angle (also known as the zenithic angle and colatitude, with $\phi = 90^\circ - \delta$ where δ is the latitude) of the positive z -axis with $0 \leq \phi \leq \pi$, and r being the distance (radius) from a point to the origin (Walton, 1967; Arfken, 1985). However, non-spherical coordinates such as bispherical

coordinates can also be solved using the Schrödinger equation. The solution to the Schrödinger equation in bispherical coordinates is described in Section 2.3.

2.2. Bispherical Coordinate

Cartesian coordinates (μ, η, ϕ) relate to bispherical (μ, η, ϕ) which have four parameters namely $-\infty \leq \mu \leq +\infty$, $0 \leq \eta \leq \pi$, $0 \leq \phi < 2\pi$, and $0 < a < +\infty$. Cartesian coordinates are related to bispherical coordinates by (Stoy, 1989)

$$x = \frac{a \sin \eta \cos \phi}{\cosh \mu - \cos \eta} \quad (\text{Eq. 1})$$

$$y = \frac{a \sin \eta \sin \phi}{\cosh \mu - \cos \eta} \quad (\text{Eq. 2})$$

$$z = \frac{a \sinh \mu}{\cosh \mu - \cos \eta} \quad (\text{Eq. 3})$$

$$\mu = \tanh^{-1} \left(\frac{2az}{(x^2 + y^2 + z^2 + a^2)} \right) \quad (\text{Eq. 4})$$

$$\eta = \tan^{-1} \left(\frac{2a(x^2 + y^2)^{\frac{1}{2}}}{(x^2 + y^2 + z^2 - a^2)} \right) \quad (\text{Eq. 5})$$

$$\phi = \tan^{-1} \left(\frac{y}{x} \right) \quad (\text{Eq. 6})$$

The two poles $\mu \rightarrow \pm\infty$ are located on the z axis at $z = \pm a$. The surface $\mu = \mu_o$ is a sphere of radius $a \operatorname{cosech} |\mu_o|$ whose center is located on the z axis at $z = a \coth \mu_o$. The surface $\mu = 0$ is a sphere of infinite radius with center at $x = y = 0, z = \pm\infty$, which includes the central plane $z = 0$.

The surface $\eta = \eta_o$ is a fourth-order surface composed of arcs of circles rotated about the z axis. For $\eta > \frac{1}{2}\pi$ there are sharp points at the poles, for $\eta = \frac{1}{2}\pi$ there is a sphere, and for $\eta < \frac{1}{2}\pi$ there are dimples at the poles. When $\eta = 0$ then $|z| > a$ for the z axis, and when $\eta = \pi$ then $|z| < a$ for the z axis. All surfaces of constant η go through the two poles. Surfaces of constant ϕ are half-planes whose only boundaries are the z axis (Stoy, 1989).

2.3. The solution of the Schrödinger equation in bispherical coordinate

The general time-independent Schrödinger equation with mass (m) and vector potential $V(\mu)$ is given by (Taskin and Koçak, 2010)

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(\mu) \right] \psi = E\psi \quad (\text{Eq. 7})$$

The square of the distance element in curvilinear coordinate space can be written as a quadratic form in the differentials dq_i (Arfken *et al.*, 2005)

$$\begin{aligned} ds^2 &= dr \cdot dr = dr^2 = \sum_{ij} \frac{\partial r}{\partial q_i} \cdot \frac{\partial r}{\partial q_j} dq_i dq_j \\ &= g_{11} dq_1^2 + g_{12} dq_1 dq_2 + g_{13} dq_1 dq_3 \\ &+ g_{21} dq_2 dq_1 + g_{22} dq_2^2 + g_{23} dq_2 dq_3 \\ &+ g_{31} dq_3 dq_1 + g_{32} dq_3 dq_2 + g_{33} dq_3^2 = \sum_{ij} g_{ij} dq_i dq_j \end{aligned} \quad (\text{Eq. 8})$$

Eq. (8) was called metric or Riemannian. Eq. (8) can be written in a more explicitly form as follows

$$\begin{aligned} g_{ij}(q_1, q_2, q_3) &= \frac{\partial x}{\partial q_i} \frac{\partial x}{\partial q_j} + \frac{\partial y}{\partial q_i} \frac{\partial y}{\partial q_j} \\ &+ \frac{\partial z}{\partial q_i} \frac{\partial z}{\partial q_j} = \frac{\partial r}{\partial q_i} \cdot \frac{\partial r}{\partial q_j} \end{aligned} \quad (\text{Eq. 9})$$

By setting the orthogonal coordinate system, $g_{ij} = 0$ for $i \neq j$ and $g_{ii} = h_i^2$ in Eq. (9). Therefore, this will be gotten as follows

$$\begin{aligned} ds^2 &= (h_1 dq_1)^2 + (h_2 dq_2)^2 + (h_3 dq_3)^2 \\ &= \sum_i (h_i dq_i)^2 \end{aligned} \quad (\text{Eq. 10})$$

The scale factor was obtained from Eq. (10) as follows

$$ds_i = h_i dq_i, \quad \frac{\partial r}{\partial q_i} = h_i \hat{q}_i \quad (\text{Eq. 11})$$

The area and volume elements can be developed from Eq. (11) as follows

$$\begin{aligned} d\sigma_{ij} &= ds_i ds_j = h_i h_j dq_i dq_j \\ ; d\tau &= ds_1 ds_2 ds_3 = h_1 h_2 h_3 dq_1 dq_2 dq_3 \end{aligned} \quad (\text{Eq. 12})$$

By applying Eq. (11), the gradient in curvilinear coordinates can be obtained as follows

$$\begin{aligned} \nabla \psi(q_1, q_2, q_3) &= \hat{q}_1 \frac{\partial \psi}{\partial s_1} + \hat{q}_2 \frac{\partial \psi}{\partial s_2} + \hat{q}_3 \frac{\partial \psi}{\partial s_3} \\ &= \hat{q}_1 \frac{1}{h_1} \frac{\partial \psi}{\partial q_1} + \hat{q}_2 \frac{1}{h_2} \frac{\partial \psi}{\partial q_2} + \hat{q}_3 \frac{1}{h_3} \frac{\partial \psi}{\partial q_3} = \sum_i \hat{q}_i \frac{1}{h_i} \frac{\partial \psi}{\partial q_i} \end{aligned} \quad (\text{Eq. 13})$$

By applying Eq. (12), the divergence in curvilinear coordinates can be obtained as follows

$$\begin{aligned} \nabla \cdot V(q_1, q_2, q_3) &= \lim_{d\tau \rightarrow 0} \frac{\int V \cdot d\sigma}{\int d\tau} \\ &= \frac{1}{h_1 h_2 h_3} \left[\frac{\partial}{\partial q_1} (V_1 h_2 h_3) + \frac{\partial}{\partial q_2} (V_2 h_3 h_1) \right. \\ &\quad \left. + \frac{\partial}{\partial q_3} (V_3 h_1 h_2) \right] \end{aligned} \quad (\text{Eq. 14})$$

The laplacian equation was obtained by combining Eq. (13-14) and using $V = \nabla \psi(q_1, q_2, q_3)$ as follows

$$\begin{aligned} \nabla^2 \psi &= \nabla \cdot \nabla \psi = \left[\frac{1}{h_1 h_2 h_3} \frac{\partial}{\partial q_1} \left(\frac{h_2 h_3}{h_1} \frac{\partial \psi}{\partial q_1} \right) \right. \\ &\quad \left. + \frac{\partial}{\partial q_2} \left(\frac{h_3 h_1}{h_2} \frac{\partial \psi}{\partial q_2} \right) + \frac{\partial}{\partial q_3} \left(\frac{h_1 h_2}{h_3} \frac{\partial \psi}{\partial q_3} \right) \right] \end{aligned} \quad (\text{Eq. 15})$$

Eq. (1-3) and Eq. (9) were used to obtain the scale factor of the bispherical coordinates with $g_{ii} = h_i^2$ as follows (Gongora and Koo, 1996; Gilbert and Giacomini, 2019)

$$\begin{aligned} h_\mu &= h_\eta = \frac{a}{\cosh \mu - \cos \eta}; \\ h_\phi &= \frac{a \sin \eta}{\cosh \mu - \cos \eta} \end{aligned} \quad (\text{Eq. 16})$$

Eq. (16) was inserted into Eq. (15), the operator Laplacian in bispherical coordinate can be obtained as follows

$$\begin{aligned} \nabla^2 \psi &= \frac{1}{h_\mu^3} \left[\frac{\partial}{\partial \mu} \left(h_\mu \frac{\partial \psi}{\partial \mu} \right) \right. \\ &\quad \left. + \frac{1}{\sin \eta} \frac{\partial}{\partial \eta} \left(h_\mu \sin \eta \frac{\partial \psi}{\partial \eta} \right) + \frac{h_\mu}{\sin^2 \eta} \frac{\partial^2 \psi}{\partial \phi^2} \right] \end{aligned} \quad (\text{Eq. 17})$$

Eq. (17) will be simplified by introducing a new wave function as $\psi = \sqrt{\cosh \mu - \cos \eta} F$ that it was reduced to

$$\begin{aligned} \nabla^2 \psi &= \frac{(\cosh \mu - \cos \eta)^{5/2}}{a^2} \\ &\quad \left[\frac{\partial^2 F}{\partial \mu^2} + \frac{1}{\sin \eta} \frac{\partial}{\partial \eta} \left(\sin \eta \frac{\partial F}{\partial \eta} \right) + \frac{1}{\sin^2 \eta} \frac{\partial^2 F}{\partial \phi^2} - \frac{F}{4} \right] \end{aligned} \quad (\text{Eq. 18})$$

Eq. (18) and $\psi = \sqrt{\cosh \mu - \cos \eta} F$ were inserted into Eq. (7). Therefore, Eq. (7) can be written as

$$\frac{(\cosh \mu - \cos \eta)^2}{a^2} \left[-\frac{F}{4} + \frac{\partial^2 F}{\partial \mu^2} + \frac{1}{\sin \eta} \frac{\partial}{\partial \eta} \left(\sin \eta \frac{\partial F}{\partial \eta} \right) + \frac{1}{\sin^2 \eta} \frac{\partial^2 F}{\partial \phi^2} \right] - \frac{2m}{\hbar^2} V(\mu) F = -\frac{2m}{\hbar^2} E F \quad (\text{Eq. 19})$$

Eq. (19) is a Schrödinger equation in bispherical coordinate that can be solved analytically and exactly by introducing variable mass

$$m = \frac{m_0 (\cosh \mu - \cos \eta)^2}{a^2} \quad (\text{Eq. 20})$$

Where m_0 is reduced mass parameter, Eq. (20) was inserted into Eq. (19). Therefore, Eq. (19) can be written as

$$\frac{\partial^2 F}{\partial \mu^2} + \frac{1}{\sin \eta} \frac{\partial}{\partial \eta} \left(\sin \eta \frac{\partial F}{\partial \eta} \right) + \frac{1}{\sin^2 \eta} \frac{\partial^2 F}{\partial \phi^2} - \frac{2m_0}{\hbar^2} V(\mu) F - \left(\frac{1}{4} - \frac{2m_0}{\hbar^2} E \right) F = 0 \quad (\text{Eq. 21})$$

Eq. (21) can be solved using the variable separation method and setting the new wave function $F = M(\mu)H(\eta)P(\phi)$ to obtain three parts with different direction as μ, η, ϕ in Schrödinger equation in bispherical coordinates is given as

$$\frac{\partial^2 M}{\partial \mu^2} - \frac{2m_0}{\hbar^2} V(\mu) M - \left(\frac{1}{4} - \frac{2m_0}{\hbar^2} E \right) M = -\frac{1}{H \sin \eta} \frac{\partial}{\partial \eta} \left(\sin \eta \frac{\partial H}{\partial \eta} \right) - \frac{1}{P \sin^2 \eta} \frac{\partial^2 P}{\partial \phi^2} \quad (\text{Eq. 22})$$

$$= \lambda_1 = L(L+1) - \frac{\sin \eta}{H} \frac{\partial}{\partial \eta} \left(\sin \eta \frac{\partial H}{\partial \eta} \right) + \frac{2m_0}{\hbar^2} V(\eta) \sin^2 \eta \quad (\text{Eq. 23})$$

$$-\lambda_1 \sin^2 \eta = \lambda_2 \quad \frac{\partial^2 P}{\partial \phi^2} - \frac{2m_0}{\hbar^2} V(\phi) P = \lambda_2 P \quad (\text{Eq. 24})$$

The radial part of the Schrödinger equation in bispherical coordinate in Eq. (22) was simplified to

$$\frac{\partial^2 M}{\partial \mu^2} - \frac{2m_0}{\hbar^2} V(\mu) M - E' M = 0 \quad (\text{Eq. 25})$$

With

$$E' = \frac{1 + 4L(L+1)}{4} - \frac{2m_0}{\hbar^2} E \quad (\text{Eq. 26})$$

2.4 Nikiforov Uvarov Functional Analysis (NUFA) Method

The Schrödinger equation is transformed into a second-order differential equation of the form with an appropriate coordinate transformation of the form (Tezcan and Sever, 2008)

$$\frac{d^2 \psi(s)}{ds^2} + \frac{\bar{\tau}(s)}{\sigma(s)} \frac{d\psi(s)}{ds} + \frac{\bar{\sigma}(s)}{\sigma^2(s)} \psi(s) = 0 \quad (\text{Eq. 27})$$

where $\sigma(s)$ and $\bar{\sigma}(s)$ are polynomials at most second degree and $\bar{\tau}(s)$ is a first-degree polynomial. In this method, one defines

$$\pi(s) = \frac{(\sigma' - \bar{\tau})}{2} \pm \sqrt{\left(\frac{\sigma' - \bar{\tau}}{2} \right)^2 - \bar{\sigma} + k\sigma} \quad (\text{Eq. 28})$$

and

$$\lambda = k + \pi'(s) \quad (\text{Eq. 29})$$

Where λ and k are constants. Since the square root in the polynomial π in Eq. (28) must be a square then this defines the constant k . By Replacing k into Eq. (28), Eq. (28) can be defined as

$$\tau(s) = \bar{\tau}(s) + 2\pi(s) \quad (\text{Eq. 30})$$

Since $\rho(s) > 0$ and $\sigma(s) > 0$, hence the derivative of τ should be negative (Tezcan and Sever, 2008), this leads to the choice of the solution. If λ in Eq. (29) is

$$\lambda = \lambda_n = -n\tau' - \frac{[n(n-1)\sigma'']}{2}; n = 0, 1, 2, \dots \quad (\text{Eq. 31})$$

The hypergeometric type equation has a particular solution with degree n . The solution of Eq. (27) can be obtained with the product of two independent parts

$$\psi(s) = \phi(s)y(s) \quad (\text{Eq. 32})$$

where $y(s)$ can be written as

$$y_n(s) = \frac{B_n}{\rho(s)} \frac{d^n}{ds^n} [\sigma^n(s) \rho(s)] \quad (\text{Eq. 33})$$

and $\rho(s)$ should satisfy the condition

$$\frac{d}{ds} [\sigma(s) \rho(s)] = \tau(s) \rho(s) \quad (\text{Eq. 34})$$

The other factor is defined as

$$\frac{\phi'(s)}{\phi(s)} = \frac{\pi(s)}{\sigma(s)} \quad (\text{Eq. 35})$$

The following equation is a general form of the Schrödinger equation written for any invariant shape potential reduces to the second-order differential equation is given as (Tezcan and Sever, 2008)

$$\frac{\partial^2 \psi}{\partial s^2} + \frac{\alpha_1 - \alpha_2 s}{s(1 - \alpha_3 s)} \frac{\partial \psi}{\partial s} + \frac{-\xi_1 s^2 + \xi_2 s - \xi_3}{s^2(1 - \alpha_3 s)^2} \psi = 0 \quad (\text{Eq. 36})$$

When Eq. (36) was compared with Eq. (27), Eq. (36) was obtained as follows

$$\begin{aligned} \bar{\tau} &= \alpha_1 - \alpha_2 s; \sigma = s(1 - \alpha_3 s) \\ \bar{\sigma} &= -\xi_1 s^2 + \xi_2 s - \xi_3 \end{aligned} \quad (\text{Eq. 37})$$

In this work, it had applied the Nikiforov Uvarov Functional Analysis (NUFA) method to obtain the energy equation and the wave function in the Schrödinger equation in bispherical coordinates for the Mobius square plus modified Yukawa potential. Then, it also had applied the energy equation results for the Mobius square plus modified Yukawa potential used to calculate the vibrational partition function Z , and investigated thermodynamic properties such as the vibrational mean energy U , vibrational specific heat C , vibrational free energy F , and vibrational entropy S for the diatomic molecules CO, NO, O₂, and I₂.

The radial part of Schrödinger equation in bispherical coordinates for the Mobius square plus modified Yukawa potential was solved using the Nikiforov Uvarov Functional Analysis (NUFA) method to obtain the energy and wave function equations. Then, the vibrational partition function Z was solved using the energy equation. The vibrational mean energy U , vibrational specific

heat C , vibrational free energy F , and vibrational entropy S were obtained from the vibrational partition function Z .

3. RESULTS AND DISCUSSION:

The Mobius square plus modified Yukawa potentials is defined as follows (Boonserm and Visser, 2011; Yukawa, 1935; Antia *et al.*, 2015)

$$V = \frac{(a + be^{-ar})^2}{(c + de^{-ar})^2} + \frac{g + e^{-ar}}{r} \quad (\text{Eq. 38})$$

Where a, b, c, d, g are the potential parameter and α is the potential range. By setting $r \rightarrow \mu$ for the special case in bispherical coordinate in Eq. (38), the form of Mobius square plus modified Yukawa potentials in bispherical coordinate can be obtained as follows

$$V(\mu) = \frac{(a + be^{-\alpha\mu})^2}{(c + de^{-\alpha\mu})^2} + \frac{g + e^{-\alpha\mu}}{\mu} \quad (\text{Eq. 39})$$

By setting in Eq. (39)

$$\frac{1}{\mu} = \frac{\alpha c}{c \left(1 + \frac{d}{c} e^{-\alpha\mu} \right)} \quad (\text{Eq. 40})$$

Where

$$1 + \frac{d}{c} = 0 \rightarrow -\frac{d}{c} = 1; z = -\frac{d}{c} e^{-\alpha\mu} \rightarrow z = e^{-\alpha\mu} \quad (\text{Eq. 41})$$

By applying Eq. (40) in Eq. (39), Eq. (39) becomes

$$\begin{aligned} V(\mu) &= \frac{(a + be^{-\alpha\mu})^2}{c^2 \left(1 + \frac{d}{c} e^{-\alpha\mu} \right)^2} + \frac{(g + e^{-\alpha\mu}) \alpha c}{c \left(1 + \frac{d}{c} e^{-\alpha\mu} \right)} \\ &= \frac{a^2 + 2abe^{-\alpha\mu} + b^2(e^{-\alpha\mu})^2}{c^2 \left(1 + \frac{d}{c} e^{-\alpha\mu} \right)^2} + \frac{\alpha g + \alpha e^{-\alpha\mu}}{\left(1 + \frac{d}{c} e^{-\alpha\mu} \right)} \end{aligned} \quad (\text{Eq. 42})$$

Eq. (42) was inserted into Eq. (25). Therefore, Eq. (25) can be written as

$$\frac{\partial^2 M}{\partial \mu^2} - \frac{2m_0}{\hbar^2} \left[\frac{a^2 + 2abe^{-\alpha\mu} + b^2(e^{-\alpha\mu})^2}{c^2 \left(1 + \frac{d}{c}e^{-\alpha\mu}\right)^2} + \frac{\alpha g + \alpha e^{-\alpha\mu}}{\left(1 + \frac{d}{c}e^{-\alpha\mu}\right)} \right] M \quad (\text{Eq. 43})$$

$$-E'M = 0$$

by setting new variables as

$$\frac{\partial}{\partial \mu} = \frac{\partial}{\partial z} \frac{\partial z}{\partial \mu} = -\alpha z \frac{\partial}{\partial z};$$

$$\frac{\partial^2}{\partial \mu^2} = -\alpha z \frac{\partial}{\partial z} \left(-\alpha z \frac{\partial}{\partial z} \right) = \alpha^2 z^2 \frac{\partial^2}{\partial z^2} + \alpha^2 z \frac{\partial}{\partial z} \quad (\text{Eq. 44})$$

Eq. (41) and Eq. (44) were inserted into Eq. (43). Therefore, Eq. (43) can be written as

$$\alpha^2 z^2 \frac{\partial^2 M}{\partial z^2} + \alpha^2 z \frac{\partial M}{\partial z} - \frac{2m_0}{\hbar^2} \left\{ \frac{a^2 + 2abz + b^2 z^2}{c^2 (1-z)^2} + \frac{\alpha(g+z)}{(1-z)} \right\} M - E'M = 0 \quad (\text{Eq. 45})$$

Eq. (45) was divided by $\alpha^2 z^2$. Therefore, Eq. (45) can be written as

$$\frac{\partial^2 M}{\partial z^2} + \frac{(1-z)}{z(1-z)} \frac{\partial M}{\partial z} - \frac{1}{z^2 (1-z)^2} \left\{ \frac{2m_0}{\hbar^2 \alpha^2 c^2} \left[a^2 + \alpha c^2 g + (2ab + \alpha c^2) z \right] - \alpha c^2 g z + (b^2 - \alpha c^2) z^2 \right\} M - \frac{E'(1-z)^2}{\alpha^2 z^2 (1-z)^2} M = 0 \quad (\text{Eq. 46})$$

Eq. (46) can be written as

$$\frac{\partial^2 M}{\partial z^2} + \frac{(1-z)}{z(1-z)} \frac{\partial M}{\partial z} + \frac{1}{z^2 (1-z)^2} \left[- \left(\frac{E'}{\alpha^2} + \frac{2m_0 b^2}{\hbar^2 \alpha^2 c^2} - \frac{2m_0}{\hbar^2 \alpha} \right) z^2 + \left(\frac{2m_0 g}{\hbar^2 \alpha} - \frac{2m_0}{\hbar^2 \alpha} \right) z - \left(\frac{4m_0 ab}{\hbar^2 \alpha^2 c^2} + \frac{2E'}{\alpha^2} \right) - \left(\frac{2m_0 a^2}{\hbar^2 \alpha^2 c^2} + \frac{2m_0 g}{\hbar^2 \alpha} + \frac{E'}{\alpha^2} \right) \right] M = 0 \quad (\text{Eq. 47})$$

By comparing Eq. (36)-(37) and (47). Therefore, Eq. (47) can be written as

$$\frac{\partial^2 M}{\partial z^2} + \frac{1-z}{z(1-z)} \frac{\partial M}{\partial z} + \frac{-\xi_1 z^2 + \xi_2 z - \xi_3}{z^2 (1-z)^2} M = 0 \quad (\text{Eq. 48})$$

With

$$\xi_1 = \frac{E'}{\alpha^2} + \frac{2m_0 b^2}{\hbar^2 \alpha^2 c^2} - \frac{2m_0}{\hbar^2 \alpha} \quad (\text{Eq. 49a})$$

$$\xi_2 = \frac{2m_0 g}{\hbar^2 \alpha} - \frac{2m_0}{\hbar^2 \alpha} - \frac{4m_0 ab}{\hbar^2 \alpha^2 c^2} + \frac{2E'}{\alpha^2} \quad (\text{Eq. 49b})$$

$$\xi_3 = \frac{2m_0 a^2}{\hbar^2 \alpha^2 c^2} + \frac{2m_0 g}{\hbar^2 \alpha} + \frac{E'}{\alpha^2} \quad (\text{Eq. 49c})$$

$$\alpha_1 = \alpha_2 = \alpha_3 = 1 \quad (\text{Eq. 49d})$$

Eq. (48) was multiplied by $z(1-z)$. Therefore, Eq. (48) can be written as

$$z(1-z) \frac{\partial^2 M}{\partial z^2} + (1-z) \frac{\partial M}{\partial z} + \frac{-\xi_1 z^2 + \xi_2 z - \xi_3}{z(1-z)} M = 0 \quad (\text{Eq. 50})$$

By setting a new wave function

$$M(z) = z^\chi (1-z)^\gamma f \quad (\text{Eq. 51})$$

Substituting Eq. (51) in Eq. (50) gives the following equation

$$z(1-z) f'' + \left\{ (1+2\chi - (2\chi+2\gamma+1)z) f' \right\} - \left\{ ((\chi+\gamma)^2 - (\chi+\gamma)) + (\gamma - \xi_1 + \chi) \right\} f + \frac{\{\chi(\chi-1) + \chi - \xi_3\}}{z} f + \frac{\{\gamma(\gamma-1) + \xi_2 - \xi_3 - \xi_1\}}{(1-z)} f = 0 \quad (\text{Eq. 52})$$

To get gauss hypergeometric equation, Eq. (52) was set as follows

$$\xi_2 - \xi_3 - \xi_1 + \gamma(\gamma-1) = 0$$

$$\rightarrow \gamma = \frac{1}{2} \pm \frac{\sqrt{1-4(\xi_2 - \xi_3 - \xi_1)}}{2} \quad (\text{Eq. 53a})$$

$$\chi(\chi-1) + \chi - \xi_3 = 0 \rightarrow \chi = \pm \sqrt{\xi_3} \quad (\text{Eq. 53b})$$

Eq. (53a)-(53b) was inserted into Eq. (52). The hypergeometry differential equation can be obtained as follows

$$z(1-z)f'' + \left\{ (1+2\chi - (2\chi+2\gamma+1)z) f' \right\} - \left\{ (\chi+\gamma)^2 - (\chi+\gamma) + (\gamma-\xi_1+\chi) \right\} f = 0 \quad (\text{Eq. 54})$$

The energy equation is obtained from the last term in Eq. (54) that $a' = -n$ or $b' = -n$. Eq. (54) was obtained as

$$(\chi+\gamma)^2 - (\chi+\gamma) + (\gamma-\xi_1+\chi) = 0 \quad (\text{Eq. 55})$$

$$\rightarrow ((\chi+\gamma) + \sqrt{\xi_1})(\chi+\gamma - \sqrt{\xi_1}) = 0$$

With

$$a' = (\chi+\gamma) + \sqrt{\xi_1}; b' = (\chi+\gamma) - \sqrt{\xi_1} \quad (\text{Eq. 56})$$

$$; c' = 1 + 2\chi$$

Eq. (56) was chosen $a' = -n$. Therefore, Eq. (56) can be written as

$$-n = \chi + \gamma + \sqrt{\xi_1} \quad (\text{Eq. 57})$$

Eq. (53a)-(53b) were inserted into Eq. (57). Therefore, Eq. (57) can be written as

$$-n = \sqrt{\xi_3} + \frac{1}{2} + \frac{1}{2}\sqrt{1-4(\xi_2-\xi_3-\xi_1)} + \sqrt{\xi_1} \quad (\text{Eq. 58})$$

By substituting Eq. (49a)-(49c) in Eq. (58). Therefore, Eq. (58) can be written as

$$-n = \sqrt{\frac{2m_0a^2}{\hbar^2\alpha^2c^2} + \frac{2m_0g}{\hbar^2\alpha} + \frac{E'}{\alpha^2}} + \frac{1}{2} + \frac{1}{2}\sqrt{1 + \frac{16m_0ab}{\hbar^2\alpha^2c^2} + \frac{8m_0a^2}{\hbar^2\alpha^2c^2} + \frac{8m_0b^2}{\hbar^2\alpha^2c^2}} + \sqrt{\frac{E'}{\alpha^2} + \frac{2m_0b^2}{\hbar^2\alpha^2c^2} - \frac{2m_0}{\hbar^2\alpha}} \quad (\text{Eq. 59})$$

By setting in Eq. (59)

$$p = \frac{2m_0a^2}{\hbar^2\alpha^2c^2} + \frac{2m_0g}{\hbar^2\alpha} \quad (\text{Eq. 60a})$$

$$o = 1 + \frac{16m_0ab}{\hbar^2\alpha^2c^2} + \frac{8m_0a^2}{\hbar^2\alpha^2c^2} + \frac{8m_0b^2}{\hbar^2\alpha^2c^2} \quad (\text{Eq. 60b})$$

$$j = \frac{2m_0b^2}{\hbar^2\alpha^2c^2} - \frac{2m_0}{\hbar^2\alpha} \quad (\text{Eq. 60c})$$

By substituting Eq. (60a)-(60c) in Eq. (59). Therefore, Eq. (59) can be written as

$$-n = \sqrt{p + \frac{E'}{\alpha^2}} + \frac{1}{2} + \frac{1}{2}\sqrt{o} + \sqrt{\frac{E'}{\alpha^2} + j} \quad (\text{Eq. 61})$$

$$\rightarrow \left(-n - \frac{1}{2} - \frac{1}{2}\sqrt{o} \right) - \sqrt{p + \frac{E'}{\alpha^2}} = \sqrt{\frac{E'}{\alpha^2} + j}$$

By using simple mathematical manipulation, Eq. (61) becomes

$$4p + \frac{4}{\alpha^2}E' = \left(\frac{(j-p)}{\left(n + \frac{1}{2} + \frac{1}{2}\sqrt{o} \right)} - \left(n + \frac{1}{2} + \frac{1}{2}\sqrt{o} \right) \right)^2 \quad (\text{Eq. 62})$$

By substituting Eq. (26) in Eq. (62). Therefore, Eq. (62) can be written as

$$E = -\frac{\hbar^2\alpha^2}{2m_0} \left(\frac{(j-p)}{2\left(n + \frac{1}{2} + \frac{1}{2}\sqrt{o} \right)} - \frac{\left(n + \frac{1}{2} + \frac{1}{2}\sqrt{o} \right)}{2} \right)^2 + \frac{\hbar^2\alpha^2}{2m_0} \left(p + \frac{1}{\alpha^2} \left(\frac{1}{4} + L(L+1) \right) \right) \quad (\text{Eq. 63})$$

Eq. (63) is the energy spectrum equation of the Mobius square plus modified Yukawa potential in bispherical coordinate. Table 1 showed the reduced mass of CO, NO, O₂, and I₂ diatomic molecules. The parameters in Table 1 are taken from reference (Bayrak *et al.*, 2006). The numerical calculation of the energy spectra of some diatomic molecules, such as CO, NO, O₂, and I₂, that are influenced by Mobius square plus modified Yukawa potential, for various values of radial and angular quantum numbers, n, L , potential range α , and mass of the molecules m_0 are shown in Figures 1-2.

The general solution of the wave function is

$$M(z) = z^x(1-z)^y {}_2F_1(a', b', c', z) \quad (\text{Eq. 64})$$

Where

$${}_2F_1(a', b', c', z) = 1 + \frac{a'b'}{c'}z + \frac{a'(a'+1)b'(b'+1)}{c'(c'+1)} \frac{z^2}{2!} + \dots \quad (\text{Eq. 65})$$

By substituting Eq. (41), Eq. (56), and Eq. (65) in Eq. (64), the first three lowest un-normalized wave functions of the quantum system for Mobius

square plus modified Yukawa potentials can be obtained as follows

$$M_0 = (e^{-\alpha\mu})^\chi (1 - e^{-\alpha\mu})^\gamma \quad (\text{Eq. 66a})$$

$$M_1 = (e^{-\alpha\mu})^\chi (1 - e^{-\alpha\mu})^\gamma \quad (\text{Eq. 66b})$$

$$\left(1 - \frac{(\chi + \gamma) - \sqrt{\xi_1}}{1 + 2\chi} e^{-\alpha\mu} \right) \quad (\text{Eq. 66b})$$

$$M_2 = (e^{-\alpha\mu})^\chi (1 - e^{-\alpha\mu})^\gamma \quad (\text{Eq. 66c})$$

$$\left(1 - \frac{2((\chi + \gamma) - \sqrt{\xi_1})}{1 + 2\chi} e^{-\alpha\mu} + \frac{((\chi + \gamma) - \sqrt{\xi_1})((\chi + \gamma) - \sqrt{\xi_1} + 1)}{(1 + 2\chi)(2 + 2\chi)} (e^{-\alpha\mu})^2 \right) \quad (\text{Eq. 66c})$$

The graphs of the wave function for various values of radial n , potential range α , and mass of the molecules m_0 are shown in Figures 3-4 and unnormalized wave function equations expressed in Eq. 66a-66c.

The vibrational partition function can be calculated by the aid of direct summation over all possible vibrational energy levels,

$$Z = \sum_{n=0}^{n_{\max}} e^{-\beta E} \quad (\text{Eq. 67})$$

Where $\beta = \frac{1}{kT}$, k denotes the Boltzmann constant, $n_{\max}$ is the upper bound vibration quantum number and T is the temperature. By substituting Eq. (63) in Eq. (67), the following expression can be obtained as follows

$$Z = \sum_{n=0}^{n_{\max}} e^{-\beta \left[\frac{\hbar^2 \alpha^2}{2m_0} \left(\frac{(j-p)}{2 \left(n + \frac{1}{2} + \frac{1}{2} \sqrt{o} \right)} \right)^2 + \frac{\hbar^2 \alpha^2}{2m_0} \left(p + \frac{1}{\alpha^2} \left(\frac{1}{4} + L(L+1) \right) \right) \right]} \quad (\text{Eq. 68})$$

For a finite summation with the maximum value $n_{\max}$, the Poisson summation formula can be written as (Stekalov, 2007)

$$\sum_{n=0}^{n_{\max}} f(n) = \frac{1}{2} [f(0) - f(n_{\max} + 1)] \quad (\text{Eq. 69})$$

$$+ \sum_{m=-\infty}^{\infty} \int_0^{n_{\max}+1} f(x) e^{-i2\pi mx} dx$$

Under the lowest-order approximation, neglecting the quantum corrections, which include the terms with $m \neq 0$, the summation formula in Eq. (69) can be written becomes

$$\sum_{n=0}^{n_{\max}} f(n) = \frac{1}{2} [f(0) - f(n_{\max} + 1)] + \int_0^{n_{\max}+1} f(x) dx \quad (\text{Eq. 70})$$

In terms of expression of Eq. (70), Eq. (68) can be rewritten as follows

$$Z = \frac{1}{2} \left[e^{-\beta(\omega - \delta k_1^2)} - e^{-\beta(\omega - \delta k_2^2)} \right] + \int_0^{n_{\max}+1} e^{-\beta \left(\omega - \delta \left(\frac{t+x}{2} - \frac{s}{2(t+x)} \right)^2 \right)} dx \quad (\text{Eq. 71})$$

Where $\delta = \frac{\hbar^2 \alpha^2}{2m_0}$, $s = j - p$, $t = \frac{1}{2} + \frac{1}{2} \sqrt{o}$, $\omega = \frac{\hbar^2 \alpha^2}{2m_0} \left(p + \frac{1}{\alpha^2} \left(\frac{1}{4} + L(L+1) \right) \right)$, $k_1 = \frac{t}{2} - \frac{s}{2t}$, and $k_2 = \frac{t+1+n_{\max}}{2} - \frac{s}{2(t+1+n_{\max})}$. Introducing a new variable $\rho = \frac{t+x}{2} - \frac{s}{2(t+x)}$ and substituting it into Eq. (71), the integral part in the right-hand side of Eq. (71) can be rewritten as follows

$$\int_0^{n_{\max}+1} e^{-\beta \left(\omega - \delta \left(\frac{t+x}{2} - \frac{s}{2(t+x)} \right)^2 \right)} dx = e^{-\beta \omega} \int_{k_1}^{k_2} e^{\beta \delta \rho^2} \left(1 + \frac{\rho}{\sqrt{\rho^2 + s}} \right) d\rho \quad (\text{Eq. 72})$$

$$= \frac{e^{-\beta \omega}}{2} \sqrt{\frac{\pi}{\delta \beta}} \left[\begin{aligned} & -\operatorname{erfi}(\sqrt{\beta \delta} k_1) + \operatorname{erfi}(\sqrt{\beta \delta} k_2) \\ & + e^{-\beta \delta s} \operatorname{erfi}(\sqrt{\beta \delta} (k_2^2 + s)) \\ & - e^{-\beta \delta s} \operatorname{erfi}(\sqrt{\beta \delta} (k_1^2 + s)) \end{aligned} \right]$$

The imaginary error function, denoted erfi , is defined as (Pearson, 1983)

$$\operatorname{erfi}(z) = -i \operatorname{erf}(iz) = \frac{2}{\sqrt{\pi}} \int_0^z e^{t^2} dt \quad (\text{Eq. 73})$$

Where erf denotes the usual error function. The imaginary error function is implemented in mathematical software Matlab as $erfi(z)$.

By substituting Eq. (72) into Eq. (71), the following vibrational partition function Z of the Mobius square plus modified Yukawa potential can be obtained as follows

$$Z = \frac{1}{2} e^{-\beta\omega} \left[e^{\beta\delta k_1^2} - e^{\beta\delta k_2^2} + \sqrt{\frac{\pi}{\delta\beta}} \left(-erfi(\sqrt{\beta\delta}k_1) + erfi(\sqrt{\beta\delta}k_2) + e^{-\beta\delta s} erfi(\sqrt{\beta\delta(k_2^2 + s)}) - e^{-\beta\delta s} erfi(\sqrt{\beta\delta(k_1^2 + s)}) \right) \right] \quad (\text{Eq. 74})$$

By using Eq. (74), the vibrational partition function Z is visualized using Matlab as shown in Figures 5-6 for various n_{max} , α , T , and mass of molecule m_0 .

Having obtained the relevant classical vibrational partition function Z in Eq. (74), The well-known thermodynamic formulas are used to calculate the thermodynamic functions for the diatomic molecules system are as follows :

(1) Vibrational mean energy U

$$U = -\frac{\partial \ln Z}{\partial \beta} = -\left[e^{\beta\delta k_1^2} - e^{\beta\delta k_2^2} + \sqrt{\frac{\pi}{\delta\beta}} \left(-erfi(\sqrt{\beta\delta}k_1) + erfi(\sqrt{\beta\delta}k_2) + e^{-\beta\delta s} erfi(\sqrt{\beta\delta(k_2^2 + s)}) - e^{-\beta\delta s} erfi(\sqrt{\beta\delta(k_1^2 + s)}) \right) \right]^{-1} \times \left[-(\omega - \delta k_1^2) e^{\beta\delta k_1^2} + (\omega - \delta k_2^2) e^{\beta\delta k_2^2} - \sqrt{\frac{\pi}{\delta}} \left(\frac{\omega}{\sqrt{\beta}} + \frac{1}{2\beta^{\frac{3}{2}}} \right) \left(-erfi(\sqrt{\beta\delta}k_1) + erfi(\sqrt{\beta\delta}k_2) + e^{-\beta\delta s} erfi(\sqrt{\beta\delta(k_2^2 + s)}) - e^{-\beta\delta s} erfi(\sqrt{\beta\delta(k_1^2 + s)}) \right) \right. \\ \left. - \frac{k_1(\omega - \delta k_1^2)}{\beta} e^{\beta\delta k_1^2} + \frac{k_2(\omega - \delta k_2^2)}{\beta} e^{\beta\delta k_2^2} - \frac{s\sqrt{\pi\delta} e^{-\beta\delta s}}{\sqrt{\beta}} erfi(\sqrt{\beta\delta(k_2^2 + s)}) + \frac{s\sqrt{\pi\delta} e^{-\beta\delta s}}{\sqrt{\beta}} erfi(\sqrt{\beta\delta(k_1^2 + s)}) - \frac{s\sqrt{\pi\delta} e^{-\beta\delta s}}{2\beta^{\frac{3}{2}}} erfi(\sqrt{\beta\delta(k_2^2 + s)}) + \frac{s\sqrt{\pi\delta} e^{-\beta\delta s}}{2\beta^{\frac{3}{2}}} erfi(\sqrt{\beta\delta(k_1^2 + s)}) - \frac{\sqrt{k_1^2 + s}(\omega - \delta k_1^2)}{\beta} e^{\beta\delta k_1^2} + \frac{\sqrt{k_2^2 + s}(\omega - \delta k_2^2)}{\beta} e^{\beta\delta k_2^2} \right] \quad (\text{Eq. 75})$$

By using Eq. (75), the vibrational mean energy U is visualized using Matlab as shown in Figures 7-8 for various n_{max} , α , T , and mass of molecule m_0 .

(2) Vibrational specific heat C

$$C = \frac{\partial U}{\partial T} = -k\beta^2 \frac{\partial U}{\partial \beta} = k\beta^2 \left[e^{\beta\delta k_1^2} - e^{\beta\delta k_2^2} + \sqrt{\frac{\pi}{\delta\beta}} \left(-erfi(\sqrt{\beta\delta}k_1) + erfi(\sqrt{\beta\delta}k_2) + e^{-\beta\delta s} erfi(\sqrt{\beta\delta(k_2^2 + s)}) - e^{-\beta\delta s} erfi(\sqrt{\beta\delta(k_1^2 + s)}) \right) \right]^{-1} \times \left[(\omega - \delta k_1^2) e^{\beta\delta k_1^2} - (\omega - \delta k_2^2) e^{\beta\delta k_2^2} + \sqrt{\frac{\pi}{\delta}} \left(\frac{\omega^2}{\sqrt{\beta}} + \frac{\omega}{2\beta^{\frac{3}{2}}} + \frac{3}{4\beta^{\frac{5}{2}}} \right) \left(-erfi(\sqrt{\beta\delta}k_1) + erfi(\sqrt{\beta\delta}k_2) + e^{-\beta\delta s} erfi(\sqrt{\beta\delta(k_2^2 + s)}) - e^{-\beta\delta s} erfi(\sqrt{\beta\delta(k_1^2 + s)}) \right) \right. \\ \left. + e^{-\beta\delta s} erfi(\sqrt{\beta\delta(k_2^2 + s)}) - \sqrt{\frac{\pi}{\delta}} \left(\frac{\omega}{\sqrt{\beta}} + \frac{1}{2\beta^{\frac{3}{2}}} \right) \left(-erfi(\sqrt{\beta\delta}k_1) + erfi(\sqrt{\beta\delta}k_2) + e^{-\beta\delta s} erfi(\sqrt{\beta\delta(k_2^2 + s)}) - e^{-\beta\delta s} erfi(\sqrt{\beta\delta(k_1^2 + s)}) \right) \right. \\ \left. \times \left(-\sqrt{\frac{\delta}{\pi\beta}} k_1 e^{\beta\delta k_1^2} + \sqrt{\frac{\delta}{\pi\beta}} k_2 e^{\beta\delta k_2^2} + \delta s e^{-\beta\delta s} erfi(\sqrt{\beta\delta(k_2^2 + s)}) - \sqrt{\frac{k_1^2 + s}{\pi\beta}} e^{\beta\delta k_1^2} + \sqrt{\frac{k_2^2 + s}{\pi\beta}} e^{\beta\delta k_2^2} \right) \right. \\ \left. + \frac{k_1(\omega - \delta k_1^2)}{\beta} e^{\beta\delta k_1^2} + \frac{k_2(\omega - \delta k_2^2)}{\beta} e^{\beta\delta k_2^2} - \frac{k_2}{\beta^2} e^{\beta\delta k_2^2} - \frac{s\sqrt{\pi\delta}(\delta s + \omega) e^{-\beta\delta s}}{\sqrt{\beta}} erfi(\sqrt{\beta\delta(k_2^2 + s)}) - \frac{s\sqrt{\pi\delta} e^{-\beta\delta s}}{2\beta^{\frac{3}{2}}} erfi(\sqrt{\beta\delta(k_2^2 + s)}) + \frac{s\sqrt{\pi\delta} e^{-\beta\delta s}}{\beta} e^{\beta\delta k_1^2} \right. \\ \left. + \frac{\sqrt{k_1^2 + s}(\omega - \delta k_1^2)}{\beta} e^{\beta\delta k_1^2} + \frac{\sqrt{k_2^2 + s}}{\beta^2} e^{\beta\delta k_1^2} + \frac{s\sqrt{\pi\delta}(\delta s + \omega) e^{-\beta\delta s}}{\sqrt{\beta}} erfi(\sqrt{\beta\delta(k_2^2 + s)}) + \frac{s\sqrt{\pi\delta} e^{-\beta\delta s}}{2\beta^{\frac{3}{2}}} erfi(\sqrt{\beta\delta(k_2^2 + s)}) - \frac{s\sqrt{\pi\delta} e^{-\beta\delta s}}{\beta} e^{\beta\delta k_2^2} \right. \\ \left. - \frac{\sqrt{k_2^2 + s}(\omega - \delta k_2^2)}{\beta} e^{\beta\delta k_1^2} - \frac{\sqrt{k_2^2 + s}}{\beta^2} e^{\beta\delta k_2^2} \right] \\ - k\beta^2 \left[e^{\beta\delta k_1^2} - e^{\beta\delta k_2^2} + \sqrt{\frac{\pi}{\delta\beta}} \left(-erfi(\sqrt{\beta\delta}k_1) + erfi(\sqrt{\beta\delta}k_2) + e^{-\beta\delta s} erfi(\sqrt{\beta\delta(k_2^2 + s)}) - e^{-\beta\delta s} erfi(\sqrt{\beta\delta(k_1^2 + s)}) \right) \right]^{-2} \times \left[-(\omega - \delta k_1^2) e^{\beta\delta k_1^2} + (\omega - \delta k_2^2) e^{\beta\delta k_2^2} - \sqrt{\frac{\pi}{\delta}} \left(\frac{\omega}{\sqrt{\beta}} + \frac{1}{2\beta^{\frac{3}{2}}} \right) \left(-erfi(\sqrt{\beta\delta}k_1) + erfi(\sqrt{\beta\delta}k_2) + e^{-\beta\delta s} erfi(\sqrt{\beta\delta(k_2^2 + s)}) - e^{-\beta\delta s} erfi(\sqrt{\beta\delta(k_1^2 + s)}) \right) \right. \\ \left. - e^{-\beta\delta s} erfi(\sqrt{\beta\delta(k_2^2 + s)}) - \frac{k_1}{\beta} e^{\beta\delta k_1^2} + \frac{k_2}{\beta} e^{\beta\delta k_2^2} + \frac{s\sqrt{\pi\delta} e^{-\beta\delta s}}{\sqrt{\beta}} erfi(\sqrt{\beta\delta(k_2^2 + s)}) - e^{\beta\delta k_1^2} \left(\frac{\sqrt{k_1^2 + s}}{\beta} \right) - \frac{s\sqrt{\pi\delta} e^{-\beta\delta s}}{\sqrt{\beta}} erfi(\sqrt{\beta\delta(k_2^2 + s)}) + e^{\beta\delta k_2^2} \left(\frac{\sqrt{k_2^2 + s}}{\beta} \right) \right] \quad (\text{Eq. 76})$$

By using Eq. (76), the vibrational specific heat C is visualized using Matlab as shown in Figures 9-10 for various n_{max} , α , T , and mass of molecule m_0 .

(3) Vibrational free energy F

$$\begin{aligned} F &= -kT \ln Z = -\frac{1}{\beta} \ln Z \\ &= -\frac{1}{\beta} \ln \left[\frac{1}{2} e^{-\beta\omega} \left(e^{\beta\delta k_1^2} - e^{\beta\delta k_2^2} \right) \right. \\ &\quad + \sqrt{\frac{\pi}{\delta\beta}} \left(-\operatorname{erfi}(\sqrt{\beta\delta}k_1) + \operatorname{erfi}(\sqrt{\beta\delta}k_2) \right) \\ &\quad + e^{-\beta\delta s} \operatorname{erfi}(\sqrt{\beta\delta(k_2^2 + s)}) \\ &\quad \left. - e^{-\beta\delta s} \operatorname{erfi}(\sqrt{\beta\delta(k_1^2 + s)}) \right] \end{aligned} \quad (\text{Eq. 77})$$

By using Eq. (77), the vibrational free energy F is visualized using Matlab as shown in Figures 11-12 for various n_{max} , α , T , and mass of molecule m_0 .

(4) Vibrational entropy S

$$\begin{aligned} S &= k \ln Z + kT \frac{\partial \ln Z}{\partial T} = k \ln Z - k\beta \frac{\partial \ln Z}{\partial \beta} \\ &= k \ln \left[\frac{1}{2} e^{-\beta\omega} \left(e^{\beta\delta k_1^2} - e^{\beta\delta k_2^2} \right) + \sqrt{\frac{\pi}{\delta\beta}} \left(-\operatorname{erfi}(\sqrt{\beta\delta}k_1) \right. \right. \\ &\quad + \operatorname{erfi}(\sqrt{\beta\delta}k_2) + e^{-\beta\delta s} \operatorname{erfi}(\sqrt{\beta\delta(k_2^2 + s)}) \\ &\quad \left. \left. - e^{-\beta\delta s} \operatorname{erfi}(\sqrt{\beta\delta(k_1^2 + s)}) \right) \right] - k\beta \left[e^{\beta\delta k_1^2} - e^{\beta\delta k_2^2} \right. \\ &\quad + \sqrt{\frac{\pi}{\delta\beta}} \left(-\operatorname{erfi}(\sqrt{\beta\delta}k_1) + \operatorname{erfi}(\sqrt{\beta\delta}k_2) \right) \\ &\quad + e^{-\beta\delta s} \operatorname{erfi}(\sqrt{\beta\delta(k_2^2 + s)}) - e^{-\beta\delta s} \operatorname{erfi}(\sqrt{\beta\delta(k_1^2 + s)}) \left. \right]^{-1} \\ &\quad \times \left[-(\omega - \delta k_1^2) e^{\beta\delta k_1^2} + (\omega - \delta k_2^2) e^{\beta\delta k_2^2} \right. \\ &\quad - \sqrt{\frac{\pi}{\delta}} \left(\frac{\omega}{\sqrt{\beta}} + \frac{1}{2\beta^{\frac{3}{2}}} \right) \times \left(-\operatorname{erfi}(\sqrt{\beta\delta}k_1) + \operatorname{erfi}(\sqrt{\beta\delta}k_2) \right) \\ &\quad + e^{-\beta\delta s} \operatorname{erfi}(\sqrt{\beta\delta(k_2^2 + s)}) - e^{-\beta\delta s} \operatorname{erfi}(\sqrt{\beta\delta(k_1^2 + s)}) \left. \right] \\ &\quad - \frac{k_1}{\beta} e^{\beta\delta k_1^2} + \frac{k_2}{\beta} e^{\beta\delta k_2^2} + \frac{s\sqrt{\pi\delta}e^{-\beta\delta s}}{\sqrt{\beta}} \operatorname{erfi}(\sqrt{\beta\delta(k_1^2 + s)}) \\ &\quad - e^{\beta\delta k_1^2} \left(\frac{\sqrt{k_1^2 + s}}{\beta} \right) - \frac{s\sqrt{\pi\delta}e^{-\beta\delta s}}{\sqrt{\beta}} \operatorname{erfi}(\sqrt{\beta\delta(k_2^2 + s)}) \\ &\quad + e^{\beta\delta k_2^2} \left(\frac{\sqrt{k_2^2 + s}}{\beta} \right) \left. \right] \end{aligned} \quad (\text{Eq. 78})$$

By using Eq. (78), the vibrational entropy S is visualized using Matlab as shown in Figures 13-14 for various n_{max} , α , T , and mass of molecule m_0 .

3.1. Numerical result

Figures 1-2 showed that for four diatomic molecules, CO, NO, O₂, and I₂, for constant angular quantum number L and potential range α , the increase of the value of radial quantum number n causes the decrease of the value of energy spectra, and for the constant values radial quantum number n , and potential range α , the increase of angular quantum number L causes the increase of the value of energy spectra. Figures 1 and 2 showed that the increase of the value of the potential range α causes the decrease of the energy spectra for constant radial and angular quantum number, n . Table 1 and Figures 1-2 showed that the larger of the reduced mass values m_0 corresponds to the higher values of the energy spectra. The spectra energy that is shown in Figures 1-2 were numerically calculated energy spectra by using Eq. (63) for the various values of n , L , α , and molecules mass.

Figures 3-4 showed that the radial quantum number n and the potential range α affect the wave functions. The increase of the radial quantum number, n , causes the increase of the amplitude of the wave functions. The wavelength of the wave function increases by the increase of the value of the potential range α , shown in figures 3-4. Figures 3-4 showed that the CO molecule has a longer wavelength and higher amplitude than others, while I₂ molecule has a shorter wavelength and lower amplitude than others.

Figures 5-6 showed that the upper bound vibration quantum number n_{max} , temperature T , and the potential range α affect the vibrational partition function Z . Figures 5-6 showed that the increase of temperature T causes the decrease of the values of vibrational partition function Z for constant the upper bound vibration quantum number n_{max} and potential range α . Figures 5-6 showed that the increase of the upper bound vibration quantum number n_{max} and potential range α causes the increase of the values of vibrational partition function Z for constant temperature T .

Figures 7-8 showed that the upper bound vibration quantum number n_{max} , temperature T , and the potential range α affect the vibrational mean energy U . Figures 7-8 showed that the increase of temperature T causes the increase of the values of vibrational mean energy U for constant the upper bound vibration quantum

number n_{max} and potential range α . Figures 7-8 showed the increase of the upper bound vibration quantum number n_{max} and potential range α causes the decrease of the values of vibrational mean energy U for constant temperature T .

Figures 9-10 showed that the upper bound vibration quantum number n_{max} , temperature T , and the potential range α affect the vibrational specific heat C . Figures 9-10 showed that the increase of temperature T causes the decrease of the values of vibrational specific heat C for constant the upper bound vibration quantum number n_{max} and potential range α . Figures 9-10 showed the increase of the upper bound vibration quantum number n_{max} and potential range α causes the increase of the values of vibrational specific heat C for constant temperature T .

Figures 11-12 showed that the upper bound vibration quantum number n_{max} , temperature T , and the potential range α affect the vibrational free energy F . Figures 11-12 showed that the increase of temperature T causes the increase of the values of vibrational free energy F for constant the upper bound vibration quantum number n_{max} and potential range α . Figures 11-12 showed the increase of the upper bound vibration quantum number n_{max} and potential range α causes the decrease of vibrational free energy F for constant temperature T .

Figures 13-14 showed that the upper bound vibration quantum number n_{max} , temperature T , and the potential range α affect the vibrational entropy S . Figures 13-14 showed that the increase of temperature T causes the increase of the values of vibrational entropy S for constant the upper bound vibration quantum number n_{max} and potential range α . Figures 13-14 showed the increase of the upper bound vibration quantum number n_{max} and potential range α causes the decrease of the values of vibrational entropy S for constant temperature T .

When compared with the results of previous studies by Antia *et al.* (2015), there are differences in parameter variations, namely the potential parameter range α . The energy results in this study are following the energy results in previous studies conducted by Antia *et al.* (2015) namely for constant angular quantum number L and potential range α , the increase of the value of radial quantum number n causes the decrease of the value of energy spectra, and for the constant values radial quantum number n , and potential range α , the increase of angular quantum number L causes the increase of the value of energy spectra. The increase of the value of the potential

range α causes the decrease of the energy spectra for constant radial and angular quantum number, n . Meanwhile, for the results of the wave function in a previous study by Antia *et al.* (2015) there is a difference, namely the equation of the wave function is different from this study, then the results of the wave function are not explained in detail such as the visualization image of the wave function. Meanwhile, the calculation results of thermodynamic properties such as vibrational partition function Z , vibrational mean energy U , vibrational specific heat C , vibrational free energy F , and vibrational entropy S have not been explained in previous research conducted by Antia *et al.* (2015) so that the calculation of thermodynamic properties for the Mobius square plus modified Yukawa potential such as vibrational partition function Z , vibrational mean energy U , vibrational specific heat C , vibrational free energy F , and vibrational entropy S are the latest ideas described in this paper.

The Schrödinger equation for Mobius square plus modified Yukawa potential in bispherical coordinate was solvable using Nikiforov Uvarov Functional Analysis (NUFA) method. Using new wave function and simple mathematical manipulation, the Schrödinger equation in bispherical coordinate reduced to the usual Schrödinger equation solvable using variable separation method. The energy spectra equation and radial wave function was obtained from the solution of the radial Schrödinger equation for Mobius square plus modified Yukawa potential solved using Nikiforov Uvarov Functional Analysis (NUFA) method. The calculated energy spectra, for radial and angular quantum numbers, n , L , potential range α , and mass of the molecules m_0 showed that the increase of parameters of n and α caused the decrease of the energy eigenvalues, but the increase of parameters of L and m_0 caused the increase of the energy eigenvalues.

From the visualization of the ground state, first and second excited state wave functions, for various values of quantum numbers n , potential range α , and mass of molecule m_0 were shown the radial quantum number n and the potential range α had dominant effect to the wave functions.

It was also shown that the upper bound vibration quantum number n_{max} , temperature T , and the potential range α had effect to the vibrational partition function Z , vibrational mean energy U , vibrational specific heat C , vibrational free energy F and vibrational entropy S .

4. CONCLUSIONS:

1. The energy spectra decrease with increasing parameters n and α . Meanwhile, the energy spectra increase with increasing L and m_0 .
2. The wave function is influenced by the dominant effect of the radial quantum number n and the potential range α .
3. Vibrational partition function Z , vibrational mean energy U , vibrational specific heat C , vibrational free energy F , and vibrational entropy S are influenced by upper bound vibration quantum number n_{max} , temperature T , and potential range α .

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Table 1. The characteristic of spectroscopic and reduces mass for diatomic molecules.

Parameter	CO	NO	O ₂	I ₂
$m_0(\text{amu})$	6.860586000	7.468441000	7.997457504	63.45223502

Figure 1. Spectrum Energy of Mobius square plus modified Yukawa potential (E) for the various n and L quantum numbers, $a = b = c = g = 1$, and $\alpha = 5$ for (a) CO, (b) NO, (c) O₂, and (d) I₂ diatomic molecules.

Figure 2. Spectrum Energy of Mobius square plus modified Yukawa potential (E) for the various n and L quantum numbers, $a = b = c = g = 1$, and $\alpha = 7$ for (a) CO, (b) NO, (c) O_2 , and (d) I_2 diatomic molecules.

Figure 3. The graphs of the un-normalized wave function as a function of radial position, ground state (black line), the first excited (blue line) and second excited (red line) wave functions for $a = b = c = g = 1$, $\alpha = 5$, and $L = 0$, for (a) CO, (b) NO, (c) O_2 , and (d) I_2 diatomic molecules.

Figure 4. The graphs of the un-normalized wave function as a function of radial position, ground state (black line), the first excited (blue line) and second excited (red line) wave functions for $a = b = c = g = 1$, $\alpha = 7$, and $L = 0$, for (a) CO, (b) NO, (c) O₂, and (d) I₂ diatomic molecules.

Figure 5. The graphs of the vibrational partition function Z for the various $n_{\max}$ and T for $a = b = c = g = 1$, $\alpha = 5$, and $L = 0$, for (a) CO, (b) NO, (c) O₂, and (d) I₂ diatomic molecules.

Figure 6. The graphs of the vibrational partition function Z for the various n_{max} and T for $a = b = c = g = 1$, $\alpha = 7$, and $L = 0$, for (a) CO, (b) NO, (c) O_2 , and (d) I_2 diatomic molecules.

Figure 7. The graphs of the vibrational mean energy U for the various n_{max} and T for $a = b = c = g = 1$, $\alpha = 5$, and $L = 0$, for (a) CO, (b) NO, (c) O_2 , and (d) I_2 diatomic molecules.

Figure 8. The graphs of the vibrational mean energy U for the various $n_{\max}$ and T for $a = b = c = g = 1$, $\alpha = 7$, and $L = 0$, for (a) CO, (b) NO, (c) O₂, and (d) I₂ diatomic molecules.

Figure 9. The graphs of the vibrational specific heat C for the various $n_{\max}$ and T for $a = b = c = g = 1$, $\alpha = 5$, and $L = 0$, for (a) CO, (b) NO, (c) O₂, and (d) I₂ diatomic molecules.

Figure 10. The graphs of the vibrational specific heat C for the various $n_{\max}$ and T for $a = b = c = g = 1$, $\alpha = 7$, and $L = 0$, for (a) CO, (b) NO, (c) O₂, and (d) I₂ diatomic molecules.

Figure 11. The graphs of the vibrational free energy F for the various $n_{\max}$ and T for $a = b = c = g = 1$, $\alpha = 5$, and $L = 0$, for (a) CO, (b) NO, (c) O₂, and (d) I₂ diatomic molecules.

Figure 12. The graphs of the vibrational free energy F for the various $n_{\max}$ and T for $a = b = c = g = 1$, $\alpha = 7$, and $L = 0$, for (a) CO, (b) NO, (c) O₂, and (d) I₂ diatomic molecules.

Figure 13. The graphs of the vibrational entropy S for the various $n_{\max}$ and T for $a = b = c = g = 1$, $\alpha = 5$, and $L = 0$, for (a) CO, (b) NO, (c) O₂, and (d) I₂ diatomic molecules.

Figure 14. The graphs of the vibrational entropy S for the various n_{max} and T for $a = b = c = g = 1$, $\alpha = 7$, and $L = 0$, for (a) CO, (b) NO, (c) O₂, and (d) I₂ diatomic molecules.