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# THERMODYNAMIC PROPERTIES OF DIATOMIC MOLECULES: A JOST FUNCTION APPROACH

*A differential equation approach was employed to derive the necessary expression for the regular solution. By utilizing the interplay between the regular solution, the irregular solution, and the Jost function, the Jost function for the Manning–Rosen potential was constructed in its most reduced form. This Jost function was then applied to investigate the bound state energies and thermodynamic properties of both homonuclear and heteronuclear diatomic molecules.*

*K e y w o r d s*: Jost function, diatomic molecule, partition function, internal energy, free energy, specific heat, entropy.

## 1. Introduction

The fundamental importance of molecular structure hinges on accurately representing the potential energy of atoms as a function of their separation distance [1]. Details about the molecule's structure, including bond lengths and vibrational/rotational levels, can be readily derived from its potential energy curve. Initially, authors [2–6] employed meticulous methods to plot energy curves for simple diatomic molecules through careful consideration of energy levels. The problem concerning the accuracy of the above method at low vibrational quantum number was addressed by Crawford and Jorgenson [7] through a power series expansion of potential energy, although the approach still involves considerable computational complexity. On the other hand, except for the simplest molecules like $H_2^+$, $H_2$ *etc.* [8, 9] it is extremely difficult to obtain the potential energy curve through the use of quantum mechanical method [10]. This problem can be resolved by using a suitable empirical or semi-empirical function to represent the potential energy curve with proper criteria [11–13], some of which are necessary and others desirable. The introduction of the empirical functions [14–22] for representing the potential energy curve and studying molecular dynamics has provided new insights into physics. Therefore, many authors [14–22] have used various types of empirical function to study the observables of molecular systems and have reported their results.

Within the non-relativistic domain of quantum mechanics the Schrödinger equation [23, 24] completely describes the motion of particles of a system. The physical background of any quantum mechanical system can be understood by solving the Schrödinger equation analytically with proper physical potentials. The exact analytical solutions of the Schrodinger equation for bound state problem with different physical potentials are often difficult to obtain, and this difficulty has been addressed by sev-

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eral authors through the proper use of approximation techniques. Some of the prominent approximation techniques are the Nikiforov–Uvarov method [25–27], the asymptotic iteration method [28–30], the supersymmetric quantum mechanics technique [31–35], the generalised fractional Nikiforov–Uvarov method [36–38], 1/N expansion method [39–41] *etc.* Many authors [27, 42–47] have extensively investigated the properties of molecular systems by solving their bound state Schrödinger equations using various forms of empirical molecular interactions and innovative techniques. They have successfully derived the bound state energy, which is further utilized to explore various thermodynamic properties of molecular systems. Studies of the thermodynamic properties of diatomic molecules are particularly important for the quality control and product design in industry. For example, the knowledge of specific heat capacities, which determine the concept of heat absorption or release can be employed for the design of any heating and cooling system.

Beyond the conventional methods for obtaining the bound state energy of a diatomic molecule, we adapted the Jost function [48–53] formalism to obtain it. The irregular solution of the radial Schrödinger equation popularly known as the Jost solution [54–56] is crucial for the determination of both the bound state and scattering state observables of quantum mechanical systems under consideration. The behavior near the origin of the Jost solutions (or Jost function) has twofold applications, one of which can be applied to study the scattering phase shifts, whereas the other one is applicable to determine the bound state energy. In the present work we have exploited the Jost function formalism for obtaining the bound state energy of both homonuclear and heteronuclear diatomic molecules, which are then used to investigate their thermodynamic properties. The method adopted here for molecular study is new. After a detailed description of the problems in Section 1, we have analytically deduced the Jost function for the potential under consideration and derived the expression for the bound state energy in its most reduced form in Section 2. The resulting compact expression for the bound-state energy, derived using the Jost function formalism, is then employed to calculate the thermodynamic properties of diatomic molecules, the detailed calculations of which are clearly described in Section 3. Finally, the results along with a brief conclusion containing the main focus of our work, are presented in Section 4.

## 2. Jost Function and Bound State Energy

The theory of the radial Schrödinger equation [23, 24] is a fundamental mathematical framework in quantum scattering theory. Traditionally, researchers employ the partial wave analysis technique to study observables associated with various quantum systems of interest. In addition, the methods of exploration of the regular and irregular solutions of the radial Schrödinger equation for the central potentials in the scattering theory are also of immense importance. The irregular solution of the radial Schrödinger equation, known as the Jost solution, plays a significant role in determining the properties of both scattering states and bound states. The Jost solution is crucial for understanding the asymptotic behavior of wave functions and for constructing the scattering matrix, which encodes information about how particles interact and scatter in a potential field. The behavior of the Jost solution near the origin, referred to as the Jost function, can be used to determine the bound state energy in quantum mechanical bound state problems. By analyzing the Jost function, one can gain insights into the energy levels of bound states and the characteristics of the potential causing these states.

The molecular Manning–Rosen potential [57, 58] reads as

$$V(r) = \frac{\hbar^2}{2mb^2}\left[\frac{\alpha(\alpha-1)e^{-2r/b}}{(1-e^{-r/b})^2} - X\frac{e^{-r/b}}{(1-e^{-r/b})}\right], \quad (1)$$

where $\alpha$, $X$ and $b$ are the adjustable parameters. The dimension of "**b**" is the same as that of length, whereas the other two are dimensionless.

The essential features of the molecular potentials are:

1. It should approach a finite value asymptotically.
2. The potential should be minimal at $r \to r_e$.
3. It must become infinite at $r = 0$.

When the second condition is applied to the potential represented in Eq. (1), one can easily arrive at the result

$$r_e = b \ln\left(1 + \frac{2\alpha(\alpha-1)}{X}\right). \quad (2)$$

The dissociation energy $D_e$, being the amount of energy required to dissociate a diatomic molecule into

its constituent atoms, is related to the $V(r)$ through the standard relation

$$D_e = V(\infty) - V(r_e). \tag{3}$$

By substituting Eqs (1) and (2) into Eq. (3) one obtains

$$D_e = \frac{\hbar^2}{2mb^2}\left[\frac{X^2}{4\alpha(\alpha-1)}\right]. \tag{4}$$

From Eqs (2) and (4), through mathematical manipulations one obtains

$$X = \frac{2m}{\hbar^2} 2D_e b^2 (e^{r_e/b} - 1) \tag{5}$$

and

$$\alpha = \frac{1 - \sqrt{1 + \left(\frac{8m}{\hbar^2}\right) D_e b^2 (e^{r_e/b} - 1)^2}}{2}. \tag{6}$$

The radial Schrödinger wave equation for the regular solution $\phi_\ell(E, r)$ of the potential given in Eq. (1) at all partial waves reads as

$$\left[\frac{d^2}{dr^2} + \frac{2m}{\hbar^2}(E - V(r)) - \frac{\ell(\ell+1)}{r^2}\right]\phi_\ell(E, r) = 0. \tag{7}$$

Using the Green–Aldrich approximation [59]

$$\frac{\ell(\ell+1)}{r^2} = \frac{\ell(\ell+1)}{b^2}\frac{e^{-2r/b}}{(1-e^{-r/b})^2} \tag{8}$$

and Eqs (1), (7) can be written as

$$\left[\frac{d^2}{dr^2} + k^2 - b^{-2}\left(\frac{d(d-1)e^{-2r/b}}{(1-e^{-r/b})^2} - \frac{Xe^{-r/b}}{1-e^{-r/b}}\right)\right] \times$$
$$\times\, \phi_\ell(k, r) = 0, \tag{9}$$

with

$$d = \frac{1 - \sqrt{1 + 4(\alpha(\alpha-1) + \ell(\ell+1))}}{2} \tag{10}$$

and

$$k^2 = \frac{2mE}{\hbar^2}. \tag{11}$$

Using the transformation

$$\phi_\ell(k, r) = b^d (1 - e^{-r/b})^d e^{ikr} g_\ell(k, r). \tag{12}$$

Eq. (9) becomes

$$b^2(1 - e^{-r/b})e^{r/b}\frac{d^2 g_\ell(k,r)}{dr^2} +$$
$$+ \left[2db + 2ikb^2(1 - e^{-r/b})\, e^{r/b}\right]\frac{dg_\ell(k,r)}{dr} +$$
$$+ \Big[2ikbd - d + X\Big] g_\ell(k, r) = 0. \tag{13}$$

Changing the variable to

$$z = 1 - e^{-r/b} \tag{14}$$

converts the Eq. (13) into

$$z(1-z)\frac{d^2 g_\ell(k,z)}{dz^2} + \Big[2d - (2d - 2ikb + 1)z\Big]\frac{dg_\ell(k,z)}{dz} +$$
$$+ \Big[2ikbd - d + X\Big] g_\ell(k, z) = 0. \tag{15}$$

Comparing the above equation with the standard Gauss hypergeometric equation [60, 61]

$$z(1-z)\frac{d^2 y}{dz^2} + \Big[c' - (a' + b' + 1)z\Big]\frac{dy}{dz} - a'b'y = 0, \tag{16}$$

one obtains the solution to Eq. (15):

$$g_\ell(k, z) = {}_2F_1(a',\, b';\, c';\, z), \tag{17}$$

with

$$a' = d - ikb + \sqrt{d^2 - k^2b^2 - d + X}, \tag{18}$$

$$b' = d - ikb - \sqrt{d^2 - k^2b^2 - d + X} \tag{19}$$

and

$$c' = 2d. \tag{20}$$

In view of Eqs (14) and (17), Eq. (12) can be expressed as

$$\phi_\ell(k, r) = b^d (1 - e^{-r/b})^d e^{ikr} \times$$
$$\times\, {}_2F_1(a', b'; c'; 1 - e^{-r/b}). \tag{21}$$

Replacing $d$ with $\omega$ through the relation

$$d = 1 + \omega \tag{22}$$

converts Eq. (21) to

$$\phi_\ell(k, r) = b^{1+\omega}(1 - e^{-r/b})^{1+\omega} \times$$
$$\times\, e^{ikr}\, {}_2F_1(A', B'; C'; 1 - e^{-r/b}), \tag{23}$$

with

$$A' = 1 + \omega - ikb + \sqrt{\omega^2 - k^2b^2 + \omega + X}, \quad (24)$$

$$B' = 1 + \omega - ikb - \sqrt{\omega^2 - k^2b^2 + \omega + X} \quad (25)$$

and

$$C' = 2(1 + \omega). \quad (26)$$

Using the analytical continuation [60] of the Gauss hypergeometric function

$$\begin{aligned} {}_2F_1(a, b; c; z) &= \frac{\Gamma[c]\,\Gamma[c-a-b]}{\Gamma[c-a]\,\Gamma[c-b]} \times \\ &\times {}_2F_1(a,\, b;\, a+b-c+1;\, 1-z) + \\ &+ (1-z)^{c-a-b}\,\frac{\Gamma[c]\,\Gamma[a+b-c]}{\Gamma[a]\,\Gamma[b]} \times \\ &\times {}_2F_1(c-a,\, c-b;\, c-a-b+1;\, 1-z) \end{aligned} \quad (27)$$

and the standard relation

$${}_2F_1(a, b; c; z) = (1-z)^{c-a-b}\,{}_2F_1(c-a, c-b; c; z) \quad (28)$$

Eq. (23) becomes

$$\begin{aligned} \phi_\ell(k, r) = \frac{b^\omega \Gamma[2+2\omega]}{2ik} \Bigg[ & \frac{\Gamma[1+2ikb]}{\Gamma[A'^*]\,\Gamma[B'^*]} \times \\ & \times [1 - e^{-r/b}]^{-\omega} e^{ikr} \\ & \times {}_2F_1(A' - 2\omega - 1, B' - 2\omega - 1;\, 1 - 2ikb;\, e^{-r/b}) - \\ & - \frac{\Gamma[1-2ikb]}{\Gamma[A']\,\Gamma[B']} [1 - e^{-r/b}]^{-\omega} e^{-ikr} \times \\ & \times {}_2F_1(A'^* - 2\omega - 1, B'^* - 2\omega - 1;\, 1 + 2ikb;\, e^{-r/b}) \Bigg]. \end{aligned} \quad (29)$$

The standard relationship between the regular solution and the irregular solution [56] reads as

$$\phi_\ell(k, r) = \frac{1}{2ik}\Big[f_\ell(-k) f_\ell(k, r) - f_\ell(k) f_\ell(-k, r)\Big]. \quad (30)$$

Comparing Eq. (29) with Eq. (30) yields the Jost function:

$$f_\ell(k) = b^\omega \frac{\Gamma[2+2\omega]\,\Gamma[1-2ikb]}{\Gamma[A']\,\Gamma[B']} \quad (31)$$

and Jost Solution:

$$\begin{aligned} f_\ell(k, r) &= [1 - e^{-r/b}]^{-\omega} e^{ikr} \times \\ &\times {}_2F_1(A' - 2\omega - 1,\, B' - 2\omega - 1;\, 1 - 2ikb;\, e^{-r/b}). \end{aligned} \quad (32)$$

The relationship between the Jost solution and the Jost function reads as

$$f_\ell(k) = \lim_{r \to 0} (1 - e^{-r/b})^\omega (1 + 2\omega) f_\ell(k, r). \quad (33)$$

The zeros of the Jost function [54–56] in the upper half of the complex $k$-plane give the bound state energy. In the upper half of the complex $k$-plane one has to replace $k$ by $i\kappa$ and to obtain zeros of the Jost function, one of the arguments of the gamma function in the denominator of Eq. (31) must be a negative integer. Here, we consider $A' = -n$. Through some mathematical manipulation, one arrives at the result

$$\kappa = \frac{A - (n+1)^2 - \omega(2n+1)}{2b(\omega + n + 1)}. \quad (34)$$

The quantity $\kappa$ is related to the bound state energy through the relation

$$\kappa = \sqrt{\frac{2mE_{n\ell}}{\hbar^2}}. \quad (35)$$

Comparing Eq. (34) and Eq. (35), we derive the expression for the energy as

$$E_{n\ell} = -R_1 \left[ \frac{R_2}{(n+d)} - (n+d) \right]^2, \quad (36)$$

with

$$R_1 = \frac{\hbar^2}{8mb^2}, \quad (37)$$

and

$$R_2 = \omega^2 + \omega + X. \quad (38)$$

## 3. Thermodynamic Properties of Diatomic Molecules

The thermodynamic properties of diatomic molecules are of immense importance for the prediction and management of their applications not only in the theoretical realm but also in the experimental domain. The partition function, being the central thermodynamic property of a molecular system, creates a foundation for determining all other thermodynamic properties relevant for industrial application of molecules. In this context we have been interested to deal with the desired expression for the internal energy, free energy, entropy, and specific heat at their most reduced forms for their theoretical study of several diatomic molecules in the next section.

The partition function $Z$ for a diatomic molecule requires the energy eigenvalue expression for the system under consideration, as obtained in the previous section and given in Eq. (36). The expression for the partition function is [62]

$$Z(\beta) = \sum_{n=0}^{n_{\max}} e^{-\beta E_{n,\ell}}, \tag{39}$$

where,

$$\beta = \frac{1}{K_{\rm B}T}, \tag{40}$$

with $K_{\rm B} = 1.38 \times 10^{-23}$ J/K, the Boltzmann constant, and $T$ being the absolute temperature. To evaluate the partition function, we apply the Poisson summation formula [63, 64],

$$\sum_{n=0}^{n_{\max}} f(n) = \frac{1}{2}[f(0) - f(n_{\max}+1)] + \\ + \sum_{m=-\infty}^{+\infty} \int_0^{n_{\max}+1} f(x) e^{-i2\pi m x}\, dx, \tag{41}$$

within the lowest-order approximation, the formula in the above equation becomes

$$\sum_{n=0}^{n_{\max}} f(n) = \frac{1}{2}[f(0) - f(n_{\max}+1)] + \int_0^{n_{\max}+1} f(x)\, dx \tag{42}$$

in view of Eqs (36) and (42), Eq. (39) becomes

$$Z(\beta) = \frac{1}{2}\left[e^{R_1\beta g_1^2} - e^{R_1\beta g_2^2}\right] + \\ + \int_0^{n_{\max}+1} \exp\left[\beta R_1 \left(\frac{R_2}{n+d} - (n+d)\right)^2\right] dn, \tag{43}$$

with

$$n_{\max} = \sqrt{R_2} - d, \tag{44}$$

$$g_1 = \frac{R_2}{d} - d \tag{45}$$

and

$$g_2 = \frac{R_2}{(d + n_{\max} + 1)} - (d + n_{\max} + 1). \tag{46}$$

Introducing two new variables $x$ and $y$ defined by

$$x = n \tag{47}$$

and

$$y = \frac{R_2}{x+d} - (x+d). \tag{48}$$

The integral in Eq. (43) now becomes

$$\int_0^{n_{\max}+1} \exp\left[\beta R_1 \left(\frac{R_2}{n+d} - (n+d)\right)^2\right] dn = \\ = I_1 + I_2, \tag{49}$$

with

$$I_1 = -\frac{1}{2}\int_{g_1}^{g_2} e^{\beta R_1 y^2} dy = \\ = \frac{1}{4}\sqrt{\frac{\pi}{\beta R_1}}\Big(\mathrm{erf}i\Big(\sqrt{\beta R_1} g_1\Big) - \mathrm{erf}i\Big(\sqrt{\beta R_1} g_2\Big)\Big), \tag{50}$$

where

$$\mathrm{erf}i(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{t^2} dt \tag{51}$$

and

$$I_2 = \frac{1}{2}\int_{g_1}^{g_2} e^{\beta R_1 y^2} \left(\frac{y}{\sqrt{y^2 + 4R_2}}\right) dy = \\ = \frac{i e^{-4\beta R_1 R_2}\sqrt{4R_2 + y^2}\,\Gamma\left[\frac{1}{2}, -\beta R_1 (4R_2 + y^2)\right]}{4\sqrt{\beta R_1 (4R_2 + y^2)}}. \tag{52}$$

By using

$$\Gamma\left[\frac{1}{2}, x^2\right] = \frac{\sqrt{\pi}}{2}\mathrm{erf}(x) \tag{53}$$

and

$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}}\left(x - \frac{x^3}{3} + \ldots\right), \tag{54}$$

$I_2$ can be written as

$$I_2 = \frac{1}{4}\, e^{-4\beta R_1 R_2}\left(\sqrt{4R_2 + g_1^2} - \sqrt{4R_2 + g_2^2}\right). \tag{55}$$

Using Eqs (50) and (55), Eq. (43) can be represented as

$$Z(\beta) = \frac{1}{2}\left[e^{R_1\beta g_1^2} - e^{R_1\beta g_2^2}\right] + \\ + \frac{1}{4}\sqrt{\frac{\pi}{\beta R_1}}\Big(\mathrm{erf}i(\sqrt{\beta R_1} g_1) - \mathrm{erf}i(\sqrt{\beta R_1} g_2)\Big) + \\ + \frac{1}{4} e^{-4\beta R_1 R_2}\left(\sqrt{4R_2 + g_1^2} - \sqrt{4R_2 + g_2^2}\right). \tag{56}$$

Again

$$\mathrm{erf}i(t) = -i + \frac{e^{t^2}}{\sqrt{\pi}}\left(t^{-1} + \frac{t^{-3}}{2} + ...\right). \quad (57)$$

Using the above result, one can rewrite

$$\mathrm{erf}i\left(\sqrt{\beta R_1} g_1\right) = -i + \frac{e^{\beta R_1 g_1^2}}{\sqrt{\pi \beta R_1} g_1} \quad (58)$$

and

$$\mathrm{erf}i\left(\sqrt{\beta R_1} g_2\right) = -i + \frac{e^{\beta R_1 g_2^2}}{\sqrt{\pi \beta R_1} g_2}. \quad (59)$$

While deriving the above result, we have neglected the contribution of higher-order terms. By considering only the real parts of the above results, Eq. (56) reads as

$$Z(\beta) = \frac{1}{2}\, e^{R_1 \beta g_1^2}\left(1 + \frac{1}{2R_1 \beta g_1}\right) - \\ - \frac{1}{2}\, e^{R_1 \beta g_2^2}\left(1 + \frac{1}{2R_1 \beta g_2}\right) + \\ + \frac{1}{4}\, e^{-4\beta R_1 R_2}\left(\sqrt{4R_2 + g_1^2} - \sqrt{4R_2 + g_2^2}\right). \quad (60)$$

The internal energy of a system refers to the microscopic energy, which is defined as the sum of all the possible kinds of energy, such as kinetic energy and potential energy of the particles contained within that system. It excludes the kinetic and potential energy associated with the motion of the system in an external electrostatic, gravitational, or electromagnetic field. The internal energy of a system can be expressed in terms of the usual thermodynamic state variables, such as temperature, pressure, and volume

$$U(\beta) = -\frac{\partial}{\partial \beta} \ln(Z). \quad (61)$$

In view of Eq. (60), Eq. (61) results

$$U = -\frac{U_1}{U_2}, \quad (62)$$

with

$$U_1 = \left[R_1 g_1^2\left(1 + \frac{1}{2\beta R_1 g_1}\right) - \frac{1}{2\beta^2 R_1 g_1}\right] e^{\beta R_1 g_1^2} - \\ - \left[R_1 g_2^2\left(1 + \frac{1}{2\beta R_1 g_2}\right) - \frac{1}{2\beta^2 R_1 g_2}\right] e^{\beta R_1 g_2^2} - \\ - 2R_1 R_2 e^{-4\beta R_1 R_2}\left(\sqrt{4R_2 + g_1^2} - \sqrt{4R_2 + g_2^2}\right) \quad (63)$$

and

$$U_2 = \left(1 + \frac{1}{2\beta R_1 g_1}\right) e^{\beta R_1 g_1^2} - \left(1 + \frac{1}{2\beta R_1 g_2}\right) e^{\beta R_1 g_2^2} + \\ + \frac{1}{2} e^{-4\beta R_1 R_2}\left(\sqrt{4R_2 + g_1^2} - \sqrt{4R_2 + g_2^2}\right). \quad (64)$$

Free energy is a thermodynamic parameter that is used to predict how much energy is accessible in a system to do useful work. In order to determine how chemical and physical systems behave at equilibrium in thermodynamics, one uses the concept of free energy which is the energy of the system in the absence of any external energy input. It is commonly defined as the quantity of energy present in the system at constant volume and temperature that can perform useful work

$$F(\beta) = -\frac{1}{\beta} \ln Z(\beta). \quad (65)$$

Substituting Eq. (60) into the above equation yields

$$F(\beta) = -\frac{1}{\beta} \ln\left[\frac{1}{2}\left(1 + \frac{1}{2\beta R_1 g_1}\right) e^{\beta R_1 g_1^2} - \right. \\ - \frac{1}{2}\left(1 + \frac{1}{2\beta R_1 g_2}\right) e^{\beta R_1 g_2^2} + \\ \left. + \frac{1}{4}\, e^{-4\beta R_1 R_2}\left(\sqrt{4R_2 + g_1^2} - \sqrt{4R_2 + g_2^2}\right)\right]. \quad (66)$$

The specific heat of a substance is one of the fundamental concepts that is defined as the amount of thermal energy required to raise the temperature by one unit. The heat capacity of a thermodynamic systems is an extensive property and not a constant because it depends on thermodynamic variables such as pressure, volume, and temperature

$$C(\beta) = K_{\mathrm{B}} \beta^2 \frac{\partial^2}{\partial \beta^2} ln Z(\beta). \quad (67)$$

The above result can be written in a simpler way as

$$C(\beta) = K_{\mathrm{B}} \beta^2 \left[\frac{1}{z}\frac{\partial^2 z}{\partial \beta^2} - U^2(\beta)\right]. \quad (68)$$

The entropy of a system is defined as a measure of disorder or randomness within the system and is used to explain its behavior in terms of temperature and

pressure. It is a measure of thermal energy per unit temperature that is unavailable for performing useful work in the system. In order to provide a quantitative explanation for the direction of spontaneous change, the concept of entropy is introduced

$$S(\beta) = K_{\mathrm{B}} \ln Z(\beta) - K_{\mathrm{B}}\beta \frac{\partial \ln Z(\beta)}{\partial \beta}. \tag{69}$$

## 4. Results and Conclusion

Diatomic molecules have a simpler molecular structure than polyatomic molecules and their simpler structure facilitates precise measurements of bond lengths, bond energies, and spectroscopic properties using techniques such as rotational and vibrational spectroscopy. This simplicity makes them ideal for studying the fundamental principles of chemical bonding, molecular spectroscopy, and quantum mechanics. The simplified electronic structure of diatomic molecules allows for accurate theoretical predictions and computational simulations of molecular properties, which can then be extended to more complex systems such as polyatomic molecules. Diatomic molecules are abundant in astrophysical environments and are often detected in interstellar clouds, planetary atmospheres, and stellar atmospheres. Their simple structure and spectroscopic signatures make them valuable probes for studying the chemical composition and physical conditions of celestial objects. Diatomic molecules exhibit unique reactivity patterns that differ from polyatomic molecules; hence, understanding their reactivity is important for the design of chemical reactions, catalysis, and materials synthesis. The diatomic molecules play crucial roles in various industrial processes such as fertilizer production, fuel production, various scientific processes, environmental processes, as well as medical applications such as anesthesia and breathing gas mixtures. Nitrogen gas is used to create of inert atmospheres for various industrial processes such as metal production, because it prevents oxidation and other chemical reactions that could degrade the product and hence it can also be used for food packaging. Fluorine gas is used in the production of semiconductors and other diatomic molecules also have such applications in different fields due to linear geometry and maximum number of covalent bonds.

The expressions for various thermodynamic quantities mentioned in the previous section are applied to the case study of simple diatomic molecules. In our study we have considered both homonuclear and heteronuclear types of diatomic molecules. We have chosen to explore our model calculation for the study of thermodynamic properties of $H_2$, LiH and HCl molecules. For these computations we have used the parameters presented in Table 1. The computation of both the regular and irregular solutions for all the diatomic molecules under consideration shows similar types of curves when plotted against the radial parameter for various values of $k$. Since the present work is based on the irregular (Jost) solution, for a better understanding as well as visualisation, we have plotted both the real and imaginary parts of the Jost solution for the $H_2$ molecule in Figs 1 and 2. The results for the partition function, the internal energy, free energy, the specific heat and the entropy for all three diatomic molecules are presented in Figs 3–7 as a function of the parameter $\beta$. These results are systematic.


***Fig. 1.*** Real $f_0(k,r)$ vs. $r$ at different values of $k$ for $H_2$ molecule

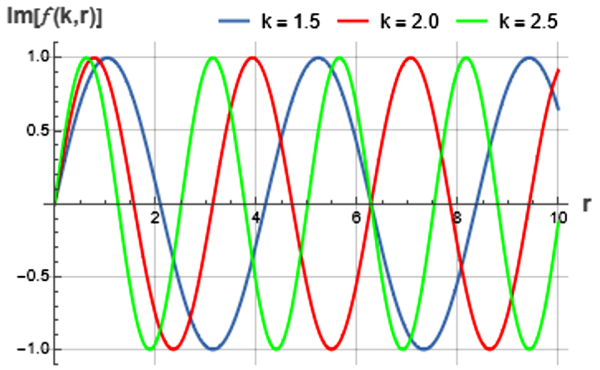


***Fig. 2.*** Imaginary $f_0(k,r)$ vs. $r$ at different values of $k$ for $H_2$ molecule

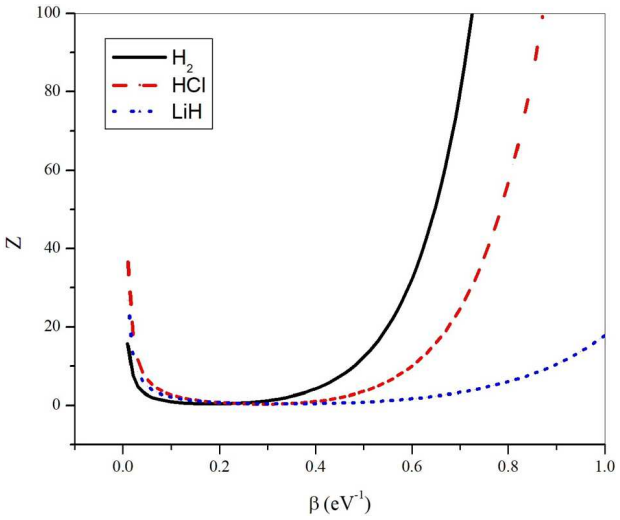


***Fig. 3.*** Partition function ($Z$) vs. $\beta$ (eV$^{-1}$) for $H_2$, HCl and LiH molecules for $b = 0.05$

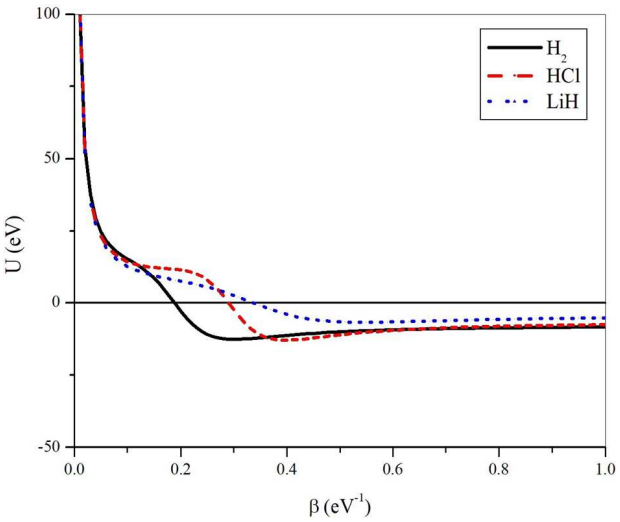


***Fig. 4.*** Internal energy [$U$ (eV)] vs. $\beta$ (eV$^{-1}$) for $H_2$, HCl and LiH molecules for $b = 0.05$

*Table 1.* **Spectroscopic parameters of HCl, LiH and $H_2$ used in the present calculations**

| Molecules | $D_e$, eV | $r_e$, Å | $m$, a.m.u |
|---|---|---|---|
| $H_2$ | 4.7446 | 0.7416 | 0.50391 |
| HCl | 4.619031371 | 1.2746 | 0.9801045 |
| LiH | 2.5152675 | 1.5956 | 0.8801221 |

We have considered the Manning–Rosen potential to study the thermodynamic properties of diatomic molecules such as $H_2$, HCl, and LiH. These molecules

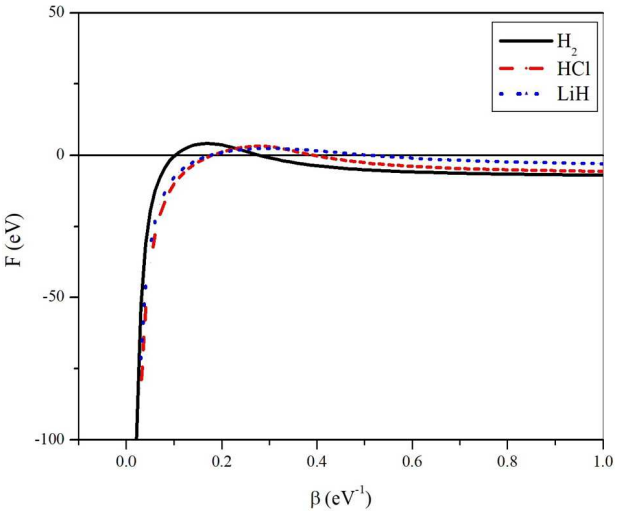


***Fig. 5.*** Free energy [$F$ (eV)] vs. $\beta$ (eV$^{-1}$) for $H_2$, HCl and LiH molecules for $b = 0.05$

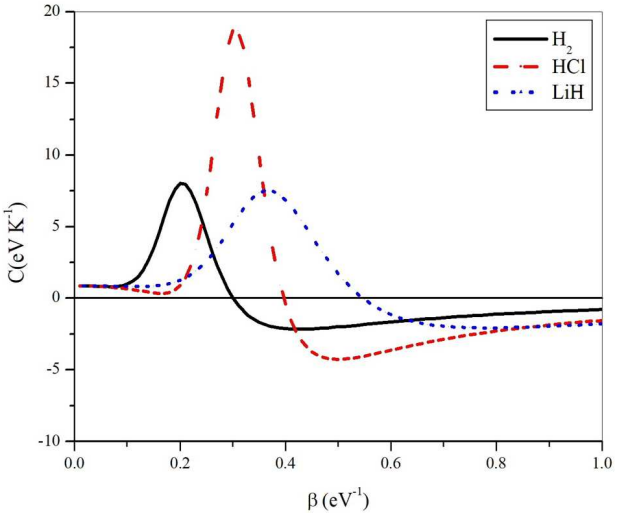


***Fig. 6.*** Specific heat [$C$ (eV K$^{-1}$) $X$ 10$^4$] vs. $\beta$ (eV$^{-1}$) for $H_2$, HCl and LiH molecules for $b = 0.05$

have various important applications in industry and many other scientific fields. Since hydrogen is the lightest element of the modern periodic table, the dihydrogen formed by a covalent bond between two hydrogen atoms is the lightest known molecule which plays significant role in everyday life and a number of industrial processes and acts as a reducing agent for metallic ore reduction. In various chemical industries and the petroleum industries, the application of $H_2$ is vast on a regular basis and the main use of $H_2$ is in the refining of certain fossil fuels, however, one

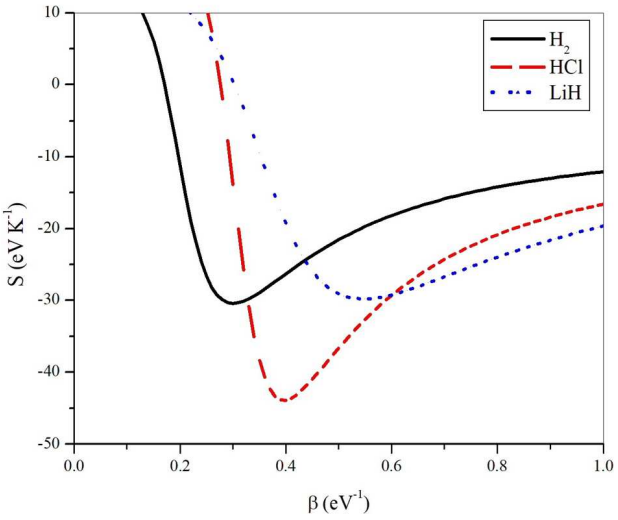


***Fig. 7.*** Entropy [$S$ (eV $K^{-1}$) $X$ $10^5$] vs. $\beta$ (eV$^{-1}$) for $H_2$, HCl and LiH molecules for $b = 0.05$

of the main consumers of this molecule is the petrochemical industry. The food industry uses these diatomic molecules for the production of hydrogenated vegetable oils such as margarine and butter. Other applications of this molecule include fossil fuel processing and ammonia production where ammonia is part of many household cleaning products. The hydrogen fuel cells which are used in spacecraft, remote weather stations and submarines use oxygen and hydrogen to generate electricity and these cells generate only water vapor which is considered as environmentally friendly. The unique properties including strong acidity, solubility and reducing properties of HCl make it usable across various industrial sectors and water treatment. HCl is used in the synthesis of various chemicals such as pigments, fertilizers and it is used as a precursor in the production of a number of organic and inorganic compounds. This molecule is widely used for the pickling and cleaning metals such as iron and steel and for the removal of impurities from metal surfaces. The lithium hydride molecule has applications in various industries, ranging from energy production to metallurgy and chemical synthesis and offers several advantages, including high reactivity and high energy density. LiH has been studied as a potential component in advanced battery technologies. Its high theoretical hydrogen storage capacity and potential use in lithium-ion batteries make it an area of interest for researchers exploring next-generation energy storage solutions. LiH is used as a neutron moderator in some types of nuclear reactors due to its ability to efficiently slow down fast neutrons, and this application is crucial for maintaining the efficiency and safety of nuclear fission processes.

Previously, many authors have studied the thermodynamic properties of various diatomic molecules analytically by solving the bound state Schrödinger equation, but for the first time in the literature we have exploited the Jost function approach to deal with the thermodynamic properties of both homonuclear and heteronuclear diatomic molecules. It is our belief that the present approach to the above problem of interest deserves serious attention from researchers working in this area of physics.

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ТЕРМОДИНАМІЧНІ ВЛАСТИВОСТІ
ДВОАТОМНИХ МОЛЕКУЛ: ПІДХІД ФУНКЦІЇ ЙОСТА

Для диференціального рівняння Шредінґера отримано вираз для регулярного розв'язку. Використовуючи взаємозв'язок між регулярним розв'язком, нерегулярним розв'язком і функцією Йоста, було побудовано функцію Йоста для потенціалу Маннінга–Розена у її найбільш скороченій формі. Цю функцію Йоста було застосовано для дослідження енергій зв'язаних станів і термодинамічних властивостей як гомоядерних, так і гетероядерних двоатомних молекул.

*Ключові слова*: функція Йоста, двоатомна молекула, функція розподілу, внутрішня енергія, вільна енергія, питома теплоємність, ентропія.