

USING ASYMPTOTIC ITERATION METHOD (AIM) FOR SOLVING DIFFERENTIAL EQUATIONS: CASE STUDY OF VIBRATIONAL STATES OF DIATOMIC MOLECULE

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ABSTRACT

This paper discusses the new computational technique referred to as the asymptotic iteration method (AIM), and presents numerical computations of exact energy eigenvalues of the Schrödinger equation assuming the Morse potential for some diatomic molecules. The method is used to compute the numerical energies of bound vibrational levels of the ${}^7\text{Li}_2$, H_2 , and N_2 diatomic molecules in the $A^1\Sigma_u^+$, $1^1\Sigma_u^+$ and $A^3\Sigma_u^+$ electronic states.

Keywords: Asymptotic iteration method, differential equations, vibrational states, diatomic molecule

INTRODUCTION

Asymptotic Iteration Method (AIM) was developed by Hakan Ciftci, and his co-workers (Ciftci *et al*, 2003; Ciftci *et al*, 2005) for solving second-order homogeneous linear differential equations that could be put in the form: $y'' = \lambda_0 y' + s_0 y$. The coefficients λ_0 and s_0 are generally functions of the independent variable, subject to conditions: $\lambda_0 \neq 0$; and $s_0 \in C_\infty$. Basically, the method involves finding asymptotic ratio $s_n/\lambda_n = s_{n-1}/\lambda_{n-1} \cong \alpha$, for some large n . The coefficients s_n and λ_n are generated by successive differentiation of y'' , and putting the n^{th} derivative in the form $\lambda_n y' + s_n y$. This asymptotic relation is then used to write down a solution for y . It was recognized very early that the AIM method would be useful for solving very important differential equations of mathematical physics such as Hermite, Laguerre, Legendre and Bessel, hence the focus on solution of Schrodinger equation, with important potentials. The method was first used to find exact solutions for Schrodinger wave equation with harmonic oscillator potential (Ciftci *et al*, 2003). It was subsequently extended to finding exact solutions of Schrodinger equation with complex cubic, quartic and Posch-Teller potentials (Ciftci *et al*, 2005). Other early studies reported on use of AIM for exact eigenvalues of angular spheroidal wave function (Barakat *et al*, 2005), and many other quantum problems. These initial successes led to the use of AIM for investigating the potentials popularly applied to describe physics of atoms and molecules. Some workers employed the AIM to calculate bound states and energies of diatomic molecules, with the anharmonic potential first introduced by P.M. Morse (Morse, 1929) for studying molecular species. The Morse potential has continued to attract workers' interest, and more recently, vibrational energy levels for the nuclear motion of several diatomic molecules have been treated analytically, and sometimes numerically, on the basis of this historically important potential. But as observed by Chabab *et al*. (2012), the accuracy of the obtained results 'seem

model or algorithm dependent'. For instance, these authors noted that Ley-koo *et al*. (1995) and Taseli (1998) used confined system in a spherical box of unit radius, to examine analytically and numerically, the eigenenergies of ${}^7\text{Li}_2$, but the results of Ley-koo *et al*. (1995) were inaccurate because they used too large a spherical box, while Taseli (1998) presented impressive results for ${}^7\text{Li}_2$ eigenenergies accurate to 28 digits. Other recent works used the AIM method for the same molecular species, with eigenvalue accuracies ranging from 14 digits (Barakat *et al*, 2006) to 28 significant figures (Chabab *et al*, 2012).

It may therefore be noted that the AIM has been successfully applied to solve the Schrodinger equation using different potentials to obtain highly accurate numerical results of the energy eigenvalues. Its successes in computing highly accurate numerical results has led to wide acceptance of the AIM as an accurate and easily handled analytic method. As indicated earlier, the vibrational spectrum of ${}^7\text{Li}_2$ diatomic molecule has been computed using the AIM by several workers (Ley-koo *et al*, 1995; Taseli, 1998; Barakat & Abodayeh, 2006; Chabab *et al*, 2012). This research work was undertaken to compare the numerical results of the energy eigenvalues with those obtained by these previous studies, and further extend the computations to other simple diatomic molecules, including H_2 and N_2 , using the asymptotic iteration method (AIM).

MATERIAL AND METHOD

Comprehensive Brief on the Asymptotic Iteration Method (AIM)

Second-order homogeneous linear differential equations of the form $ay'' + by' + cy = 0$ arise naturally in the field of science and engineering. There are many techniques available in different books that can be used to solve these types of differential equations. The main task of the present work is to introduce a new technique, known as the Asymptotic Iteration Method (AIM) as an alternative approach to solve second-order homogeneous linear differential equations.

To solve the second-order homogeneous linear differential equations using the AIM approach, one will rearrange the above equation to this form

$$y'' = -\frac{b}{a}y' - \frac{c}{a}y \quad (1)$$

so as to make comparison with the general expression of the AIM approach below.

$$y'' = \lambda_0 y' + s_0 y \quad (2)$$

Considering the two equations, one can easily identify; $\lambda_0 = -\frac{b}{a}$, and $s_0 = -\frac{c}{a}$.

As an illustration, below is an example by Ciftci *et al.* (2003) on how to solve the second-order homogeneous linear differential equation using the AIM approach.

Suppose we consider the homogenous linear second-order differential equation

$$y'' - 4y' + 3y = 0 \quad (3)$$

The systematic procedure of the AIM begins now by rewriting equation (3) in the form given by equation (4) below and continuously iterate by differentiating from 3rd derivative to (n+2)th derivative;

$$y'' = 4y' - 3y \quad (4)$$

Now let us introduce the constant parameters λ_0 and s_0 from the general AIM expression in (2). The primes of y in equations (2) and (3) denote the first and second derivatives with respect to x . Comparing equation (2) and equation (4), we have $\lambda_0 = 4$ and $s_0 = -3$ and, differentiating (4) with respect to x , gives

$$y''' = \lambda_1 y' + s_1 y \quad (5)$$

where $\lambda_1 = \lambda_0' + s_0 + \lambda_0^2$ and $s_1 = s_0' + s_0 \lambda_0$. Now, $\lambda_0' = 0$ and $s_0' = 0$ because the differential of $\lambda_0 = 4$ and $s_0 = -3$ gives zero.

Substituting the above values in the expression of λ_1 and s_1 gives $\lambda_1 = 0 + (-3) + (4)^2 = 13$, and $s_1 = 0 + (-3)(4) = 12$. Now, rewriting equation (5) by substituting the new values of λ_1 and s_1 from above gives

$$y''' = 13y' - 12y \quad (6)$$

Again, the second derivative of equation (4), gives;

$$y'''' = \lambda_2 y' + s_2 y \quad (7)$$

where $\lambda_2 = \lambda_1' + s_1 + \lambda_0 \lambda_1$, and $s_2 = s_1' + s_0 \lambda_1$. $\lambda_1' = 0$ and $s_1' = 0$ because the differentials of $\lambda_1 = 13$ and $s_1 = -12$ gives zero. Again, substituting the above values in the expression of λ_2 and s_2 gives $\lambda_2 = 0 + (-12) + (4)(13) = 40$ and $s_2 = 0 + (-3)(-12) = -36$. Now, rewriting equation (7) by substituting the new values of λ_2 and s_2 from above gives

$$y'''' = 40y' - 36y \quad (8)$$

Thus, the $(n + 1)^{th}$ and $(n + 2)^{th}$ derivatives, $n = 1, 2, \dots$ is the iteration number, can be written as;

$$y^{n+1} = \lambda_{n-1}(x) y' + s_{n-1}(x) y \quad (9)$$

$$\text{and} \\ y^{n+2} = \lambda_n(x) y' + s_n(x) y \quad (10)$$

where $\lambda_n = \lambda'_{n-1} + s_{n-1} + \lambda_0 \lambda_{n-1}$, and $s_n = s'_{n-1} + s_0 \lambda_{n-1}$. In general, $\lambda_n = \frac{1}{2}(3^{n+2} - 1)$ and $s_n = -\frac{3}{2}(3^{n+1} - 1)$. Note that one can get back the values of $\lambda_0 = 4$ and $s_0 = -3$, $\lambda_1 = 13$ and $s_1 = -12, \dots$ by just substituting the values of $n = 0, 1, \dots$ in the expression of λ_n and s_n above.

$$\alpha(x) = \lim_{n \rightarrow \infty} \frac{s_n}{\lambda_n} = -1 \quad (11)$$

Substituting λ_n , and the expression for $\alpha(x)$ above, in equation (12) below to get the general solution to equation (2) above as seen in equation (13) below, using the elementary method.

$$y(x) = \exp\left(-\int^x \alpha(x_1) dx_1\right) \times [C_2 + C_1 \int^x \exp(\int^{x_1} (\lambda_0(x_2) + 2 \alpha(x_2)) dx_2)] \quad (12)$$

$$y(x) = C_1 e^{3x} + C_2 e^x \quad (13)$$

Formalism of the Asymptotic Iteration Method for Solving Schrödinger Equation with the Morse Potential

As an empirical potential, the Morse potential has been one of the most helpful and convenient models, which provides a qualitative description of the interaction between two atoms in a very substance molecule. Analysis has shown that the rotational energy of a molecule is way smaller than its vibrational energy, and so, in a very pure Morse potential model the rotational energy of a molecule has been omitted (Barakat & Abodayeh, 2006). Hence, we start with the Schrödinger equation given by;

$$\left[-\frac{\hbar^2}{2\mu} \frac{d^2}{dx^2} + V(x)\right] \Psi_n(x) = E_n \Psi_n(x) \quad (14)$$

where E_n are the energy eigenvalues, and $V(x)$ is the Morse potential function given as;

$$V(x) = D_e (e^{-2\beta(x-x_e)} - 2e^{-\beta(x-x_e)}) \quad (15)$$

where D_e is the dissociation energy, x_e is the equilibrium inter-nuclear distance of a diatomic molecule, μ is the reduced mass, and β is an adjustable parameter. Morse potential has a minimum value at $x = x_e$, and it is zero at $x = \infty$. At $x = 0$, $V(0)$ has a finite value of $D_e (e^{2\beta(x_e)} - 2e^{\beta(x_e)})$ that is positive when $\beta x_e > \ln 2$. Equation (14) is the famous one-dimensional Schrödinger equation, if x is defined on the domain $(-\infty < x < +\infty)$, and the eigenfunctions are normalized, that is $\int_{-\infty}^{+\infty} |\Psi(x)|^2 dx = 1$. However, for real diatomic molecules x should range from 0 to ∞ .

Starting with Morse's substitution, i.e. $q = e^{-\frac{\beta(x-x_e)}{2}}$, and rewriting equation (14) in the form;

$$-\frac{d^2 \Psi_n(q)}{dq^2} - \frac{1}{q} \frac{d \Psi_n(q)}{dq} + \frac{8\mu D_e}{\beta^2 \hbar^2} [q^2 - 2] \Psi_n(q) = \frac{8\mu E_n}{\beta^2 \hbar^2 q^2} \Psi_n(q) \quad (16)$$

Furthermore, removing the first derivative by proposing the ansatz

$$\Psi_n(q) = \phi_n(q) \exp\left(-\frac{p(r)}{2}\right); p^{(r)} = \frac{1}{q} \quad (17)$$

This in turn implies,

$$-\frac{d^2\phi_n(q)}{dq^2} + \frac{\epsilon_n(\epsilon_n+1)}{q^2}\phi_n(q) + \gamma^2 u^2 \phi_n(q) = 2\gamma^2 \phi_n(q) \quad (18)$$

where,

$$\epsilon_n(\epsilon_n + 1) = -\frac{1}{4} - \frac{8\mu E_n}{\beta^2 \hbar^2}, \text{ and } \gamma^2 = \frac{8\mu D_e}{\beta^2 \hbar^2} \quad (19)$$

Further still, by introducing the frequency

$$\omega_0 = \beta \sqrt{2 \frac{D_e}{\mu}} \quad (20)$$

of classical small vibrations about the equilibrium position $x = x_e$, and expressing the energy parameters in unit $\hbar\omega_0$; that is;

$$D_e = \Delta \hbar\omega_0; E_n = \epsilon_n \hbar\omega_0 \text{ and } \epsilon_n = -\frac{(\epsilon_n + \frac{1}{2})^2}{16\Delta^2} \quad (21)$$

Now, we can write the eigenvalue problem in a more convenient re-scaled form as;

$$-\frac{d^2\Phi_n(q)}{dq^2} + \frac{\epsilon_n(\epsilon_n+1)}{q^2}\Phi_n(q) + 16\Delta^2 q^2 \Phi_n(q) = 32\Delta^2 \Phi_n(q) \quad (22)$$

In order to guarantee the asymptotic behavior of this eigenvalue problem when $q \rightarrow \infty$, and $q \rightarrow 0$, it is found that $\Phi_n(q)$ should look like

$$\Phi_n(q) = q^{(\epsilon_n+1)} e^{-2\Delta q^2} P_n(q) \quad (23)$$

This implies that the function $f_n(q)$ will satisfy a second-order homogenous linear differential equation of the form;

$$\frac{d^2 P_n(q)}{dq^2} = \left(8\Delta q - \frac{2\epsilon_n+2}{q}\right) \frac{dP_n(q)}{dq} + (12\Delta + 8\Delta\epsilon_n - 32\Delta^2) P_n(q) \quad (24)$$

The systematic procedure of the asymptotic iteration method begins now by rewriting equation (24) in the following form,

$$P_n''(q) = \lambda_0(q) P_n'(q) + s_0(q) P_n(q) \quad (25)$$

where,

$$\lambda_0(q) = \left(8\Delta q - \frac{2\epsilon_n+2}{q}\right), \quad s_0(q) = (12\Delta + 8\Delta\epsilon_n - 32\Delta^2) \quad (26)$$

The primes of $P_n(q)$ in equation (25) denote the second derivatives with respect to q . Now, in order to find the general solution to this equation, we rely on the symmetric structure of the right hand side of equation (25). Thus differentiating equation (25) With respect to q , gives;

$$P_n'''(q) = \lambda_1(q) P_n'(q) + s_1(q) P_n(q) \quad (27)$$

where $\lambda_1(q) = \lambda_0'(q) + s_0(q) + \lambda_0^2(q)$ and $s_1(q) = s_0'(q) + s_0(q)\lambda_0(q)$. Likewise, the calculation of the second derivative of equation (25) yield;

$$P_n''''(q) = \lambda_2(q) P_n'(q) + s_2(q) P_n(q) \quad (28)$$

where $\lambda_2(q) = \lambda_1'(q) + s_1(q) + \lambda_0(q)\lambda_1(q)$ and $s_2(q) = s_1'(q) + s_0(q)\lambda_1(q)$. For $(l+1)^{th}$, and $(l+2)^{th}$ derivatives, $l = 1, 2 \dots$ is the iteration number, one can obtain,

$$P_n^{(l+1)}(q) = \lambda_{l-1}(q) P_n'(q) + s_{l-1}(q) P_n(q) \quad (29)$$

$$P_n^{(l+2)}(q) = \lambda_l(q) P_n'(q) + s_l(q) P_n(q) \quad (30)$$

where

$$\lambda_l(q) = \lambda_{l-1}'(q) + s_{l-1}(q) + \lambda_0(q)\lambda_{l-1}(q) \quad (31a)$$

$$s_l(q) = s_{l-1}'(q) + s_0(q)\lambda_{l-1}(q) \quad (31b)$$

which are called the recurrence relation of equation (25). By taking the natural log of equation (29), we have $\ln P_n^{(l+1)}(q) = \ln[\lambda_{l-1}(q) P_n'(q) + s_{l-1}(q) P_n(q)]$. Now, differentiating this expression with respect to u ;

$$\frac{d}{du} \ln P_n^{(l+1)}(q) = \frac{\lambda_l \left(P_n'(q) + \frac{s_l(q)}{\lambda_l(q)} P_n(q) \right)}{\lambda_{l-1} \left(P_n'(q) + \frac{s_{l-1}(q)}{\lambda_{l-1}(q)} P_n(q) \right)} \quad (32)$$

The ratio of the $(l+2)^{th}$, and $(l+1)^{th}$ can be expressed as;

$$\frac{P_n^{(l+2)}(q)}{P_n^{(l+1)}(q)} = \frac{\lambda_l \left(P_n'(q) + \frac{s_l(q)}{\lambda_l(q)} P_n(q) \right)}{\lambda_{l-1} \left(P_n'(q) + \frac{s_{l-1}(q)}{\lambda_{l-1}(q)} P_n(q) \right)} \quad (33)$$

One can write equation (32) and (33) as;

$$\frac{d}{du} \ln P_n^{(l+1)}(q) = \frac{P_n^{(l+2)}(q)}{P_n^{(l+1)}(q)} = \frac{\lambda_l \left(P_n'(q) + \frac{s_l(q)}{\lambda_l(q)} P_n(q) \right)}{\lambda_{l-1} \left(P_n'(q) + \frac{s_{l-1}(q)}{\lambda_{l-1}(q)} P_n(q) \right)} \quad (34)$$

Equation (34) above is the ratio of $(l+2)^{th}$ and $(l+1)^{th}$ derivatives. For sufficiently large l , and introducing the "asymptotic" aspect of the method; that is,

$$\frac{s_l(q)}{\lambda_l(q)} = \frac{s_{l-1}(q)}{\lambda_{l-1}(q)} \equiv \alpha(q) \quad (35)$$

Thus equation (34) can be reduced to;

$$\frac{d}{dq} \left(P_n^{(l+1)}(q) \right) = \frac{\lambda_l(q)}{\lambda_{l-1}(q)} \quad (36)$$

Clearly, by integrating equation (36), we obtain;

$$P_n^{(l+1)}(q) = C_1 \exp \left(\int \frac{\lambda_l(q)}{\lambda_{l-1}(q)} dq \right) \quad (37)$$

where C_1 is the integration constant. Substituting $\lambda_l(q)$ from equation (31a) and then using the definition of $\alpha(u)$ from equation (35), equation (37) can be rewritten as;

$$P_n^{(l+1)}(q) = C_1 \lambda_{l-1}(q) \exp(\int(\alpha(q) + \lambda_0(q))dq) \quad (38)$$

Substituting equation (38) into equation (29) gives a first-order differential equation of the form

$$P_n'(q) + \alpha(q)P_n(q) = C_1 \exp(\int(\alpha(q) + \lambda_0(q))dq) \quad (39)$$

which, in turn, yield the general solution to equation (25)

$$P_n(q) = \exp(-\int^u \alpha(q')dq') [C_2 + C_1 \int^u \exp(\int\{\lambda_0(q'') + 2\alpha(q'')\}dq'')dq'] \quad (40)$$

where C_2 is the new integration constant. It should be noted that one can construct the eigenfunctions $P_n(q)$ from the knowledge of α .

RESULTS AND DISCUSSION

Numerical Results for the Vibrational Levels of the Morse Potential

The energy eigenvalues of the Morse potential (E_n) were calculated by means of equation (35). To generate the energy eigenvalues E_n , equation (35) is first solved for ϵ_n where the iterations should be terminated by applying a condition $\delta_l(q) = 0$ as a rough calculation to equation (35).

On the other hand, for each iteration, the expression $\delta_l(q) = 0 = s_l(q)\lambda_{l-1}(q) - s_{l-1}(q)\lambda_l(q)$, where the expression above depends on ϵ_n and q . The calculated ϵ_n by means of this condition should, however, be independent of the choice of q . Nevertheless, the choice of q is observed to be critical only to speed of the convergence to ϵ_n , as well as for the stability of the process.

In this work, it is observed that the best starting value for q is the value at which the effective potential of equation (23) takes its minimum value, that is when $q = 1$ (Barakat & Abodayeh, 2006). Therefore, at the end of the iterations, $q = 1$, the results of the AIM for ϵ_n with different values of n are;

$$\epsilon_0 = \frac{-3+8\Delta}{2}, \quad (41a)$$

$$\epsilon_1 = \frac{-7+8\Delta}{2}, \quad (41b)$$

$$\epsilon_2 = \frac{-11+8\Delta}{2}, \quad (41c)$$

$$\epsilon_4 = \frac{-19+8\Delta}{2}, \quad (41d)$$

$$\epsilon_5 = \frac{-23+8\Delta}{2}, \quad (41e)$$

It means that;

$$\epsilon_n = \frac{-4n-3+8\Delta}{2}, \text{ For } n = 0, 1, 2, \dots \quad (42)$$

The parameters ϵ_n were calculated by means of 18 iterations only. Therefore, the exact energy eigenvalues of the Morse potential E_n are;

$$E_n = -\frac{(-2(2n+1)+8\Delta)^2}{64\Delta} \quad (43)$$

The computation results of the energy eigenvalues of equation (43) for three diatomic molecules are represented below:

Table 1: Energy eigenvalues of Morse potential for ${}^7\text{Li}_2$ diatomic molecule in the $A^1 \Sigma_u^+$ electronic state with the parameters $D_e = 1.10842\text{eV}$, $x_0 = 3.10821$, and $\beta = 0.616$.

n	Eigen values for ${}^7\text{Li}_2$
0	-0.6648065682683458
1	-0.11589911441511339
2	-0.018084206708648357
3	-0.3713618451489508
4	-1.1757320297360208
5	-2.4311947604698583
6	-4.137750037350464
7	-6.295397860377837
8	-8.904138229551977
9	-11.963971144872884
10	-15.474896606340561
11	-19.436914613955
12	-23.85002516771621
13	-28.71422826762419
14	-34.029523913678936
15	-39.79591210588045
16	-46.013392844228726
17	-52.68196612872377
18	-59.80163195936557
19	-67.37239033615415
20	-75.39424125908951

Figure 1 below is the graph of ${}^7\text{Li}_2$ diatomic molecule with parameters $D_e = 1.10842\text{eV}$, $x_0 = 3.10821$, and $\beta = 0.616$.

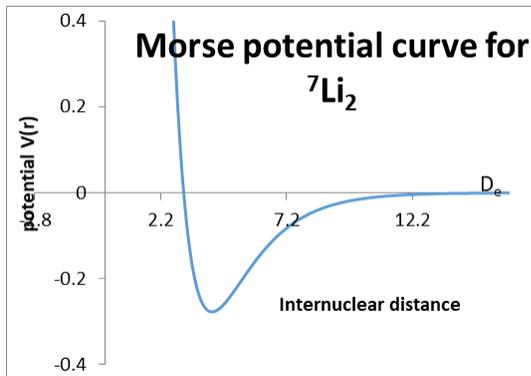


Figure 1: Morse potential curve for ${}^7\text{Li}_2$ diatomic molecule.

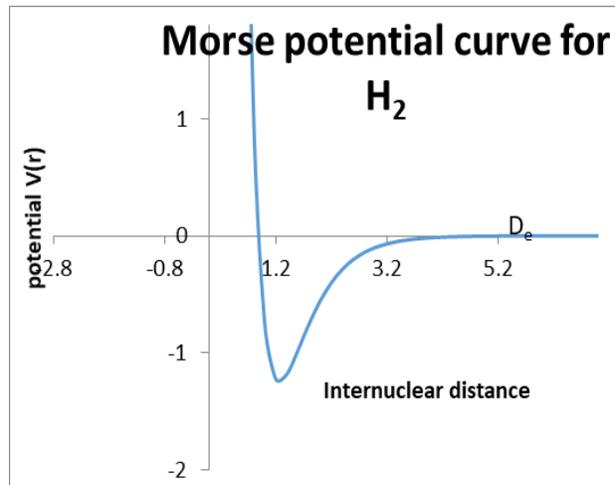


Figure 2: Morse potential curve for H_2 diatomic molecule

Table 2: Energy eigenvalues of Morse potential for H_2 diatomic molecule in the $1^1\Sigma$ electronic state with the parameters $D_e = 4.97177\text{eV}$, $x_0 = 0.89$, and $\beta = 1.85$

n	Eigen values for H_2
0	-4.4843409757289665
1	-3.584908781560692
2	-2.786044393224144
3	-2.0877478107193213
4	-1.4900190340462252
5	-0.9928580632048547
6	-0.5962648981952103
7	-0.3002395390172917
8	-0.10478198567109909
9	-0.009892238156632368
10	-0.015570296473891564
11	-0.12181616062287667
12	-0.3286298306035877
13	-0.6360113064160247
14	-1.0439605880601874
15	-1.5524776755360763
16	-2.1615625688436912
17	-2.8712152679830316
18	-3.681435772954098
19	-4.592224083756891
20	-5.603580200391409

Figure 2 is the graph of H_2 diatomic molecule, with parameters $D_e = 4.97177\text{eV}$, $x_0 = 0.89$, and $\beta = 1.85$.

Table 3: Energy eigenvalues of Morse potential for N_2 diatomic molecule in the $A^3\Sigma_u^+$ electronic state with parameters $D_e = 4.66181\text{eV}$, $x_0 = 1.28$, and $\beta = 2.42$

n	Eigen values for N_2
0	-4.175216809801343
1	-3.282471288212089
2	-2.4969802450335816
3	-1.8187436802658195
4	-1.2477615939088038
5	-0.7840339859625338
6	-0.42756085642701014
7	-0.1783422053022324
8	-0.03637803258820072
9	-0.0016683382849150862
10	-0.0742131223923755
11	-0.2540123849105819
12	-0.5410661258395344
13	-0.935374345179233
14	-1.4369370429296775
15	-2.045754219090868
16	-2.7618258736628047
17	-3.585152006645487
18	-4.515732618038916
19	-5.553567707843091
20	-6.698657276058012

Figure 3 is the graph of N_2 diatomic molecule, with parameters $D_e = 4.66181\text{eV}$, $x_0 = 1.28$, and $\beta = 2.42$.

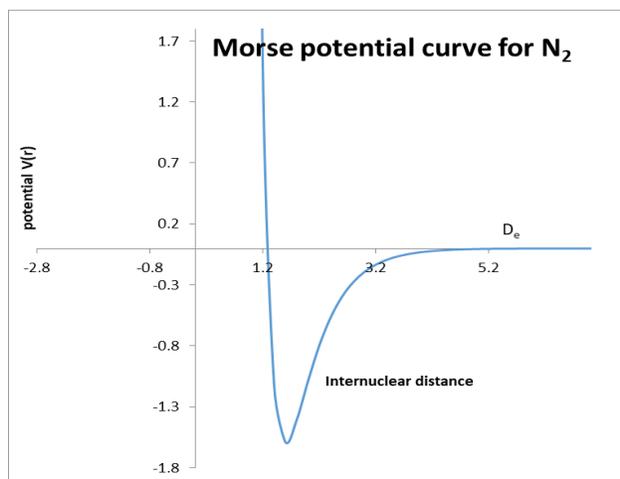


Figure 3: Morse potential curve for N₂ diatomic molecule

In table 1, the results of the computation of vibrational energies of the ⁷Li₂ diatomic molecule in the $A^1 \Sigma_u^+$ electronic state are represented, table 2 is the result of vibrational energies of the H₂ diatomic molecule in the $1^1 \Sigma$ electronic state, and table 3 is the result of vibrational energies of the N₂ diatomic molecule in the $A^3 \Sigma_u^+$ electronic state.

The parameters of the respective Morse potential are explicitly indicated for each diatomic molecule, with the dissociation energy parameter in units of eV. The results of this research work given in the tables above are in excellent agreement with the energy eigenvalues results of Taseli (1998) and Chabab *et al.* (2012).

Morse potential has shown a great ability in the description of diatomic interactions and proven to be successful and accurate in computation. In this work, the energy eigenvalues levels and the corresponding vibrational states of diatomic molecule ⁷Li₂, H₂, and N₂ via the Morse potential are analyzed. For this, the one-dimensional Schrödinger equation is solved by making use of the asymptotic iteration method (AIM).

Note that the unit of the dissociation energy parameters for the respective diatomic molecules in the present work is in eV. On the other hand, the results obtained from AIM calculations are extremely precise and present the energy eigenvalues levels up to 15 decimals.

Morse potential energy curve describes the potential energy of a system, V(x), as the two atoms are brought closer to, or moved away from, one another (see figure 1, figure 2 and figure 3). The point at which the curve flattens out at large inter-nuclear distances is termed the dissociation energy limit, and represents a state where the molecule is no longer bound, being instead, two separate atoms. The dissociation energy, D_e, is the vertical distance between the dissociation limit and the base of the curve, found at the equilibrium bond length.

Finally, the Asymptotic Iteration Method (AIM) is highly accurate, but the technique requires a lot of computational time.

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