

## Research Article

# Solution of the Rovibrational Schrödinger Equation of a Molecule Using the Volterra Integral Equation

Mahmoud Korek<sup>1</sup> and Nayla El-Kork<sup>2</sup>

<sup>1</sup>Department of Physics, Beirut Arab University, P.O. Box 11-5020, Riad El Solh, Beirut 1107 2809, Lebanon

<sup>2</sup>Department of Physics, Khalifa University, P.O. Box 57, Abu Dhabi, UAE

Correspondence should be addressed to Mahmoud Korek; [fkorek@yahoo.com](mailto:fkorek@yahoo.com)

Received 22 May 2018; Revised 28 June 2018; Accepted 30 July 2018; Published 4 October 2018

Academic Editor: Joel Bowman

Copyright © 2018 Mahmoud Korek and Nayla El-Kork. This is an open access article distributed under the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

By using the Rayleigh-Schrödinger perturbation theory the rovibrational wave function is expanded in terms of the series of functions  $\phi_0, \phi_1, \phi_2, \dots, \phi_n$ , where  $\phi_0$  is the pure vibrational wave function and  $\phi_i$  are the rotational harmonics. By replacing the Schrödinger differential equation by the Volterra integral equation the two canonical functions  $\alpha_0$  and  $\beta_0$  are well defined for a given potential function. These functions allow the determination of (i) the values of the functions  $\phi_i$  at any points; (ii) the eigenvalues of the eigenvalue equations of the functions  $\phi_0, \phi_1, \phi_2, \dots, \phi_n$  which are, respectively, the vibrational energy  $E_v$ , the rotational constant  $B_v$ , and the large order centrifugal distortion constants  $D_v, H_v, L_v, \dots$ . Based on these canonical functions and in the Born-Oppenheimer approximation these constants can be obtained with accurate estimates for the low and high excited electronic state and for any values of the vibrational and rotational quantum numbers  $v$  and  $J$  even near dissociation. As application, the calculations have been done for the potential energy curves: Morse, Lenard Jones, Reidberg-Klein-Rees (RKR), ab initio, Simon-Parr-Finlin, Kratzer, and Dunham with a variable step for the empirical potentials. A program is available for these calculations free of charge with the corresponding author.

## 1. Introduction

For the gas-phase of molecules, the rovibrational spectroscopy remains the most accurate and reliable source for understanding the molecular structure and the development of quantum mechanics. The theoretical determination of the rovibrational constants enables the prediction of line positions, which can be used in guiding experimental investigations and greatly facilitating the detection of unknown molecules. The fundamental atomic and molecular data are very important for interpreting observations and modelling the atmospheres of planetary and stellar objects. In the last two decades hundreds of extrasolar planets, cool stars, the atmospheres of exoplanets, and brown dwarfs have been detected where their other proposal uses molecular states.

Since diatomic molecules exhibit very long decoherence times, the molecular electronic states (electronic, vibrational, and/or rotational) are chosen recently to act as the quantum

bits (qubits). A femtosecond laser pulse can be shaped to produce high fidelity binary shaped laser pulses to act as a quantum logic gate on the chosen qubits. By using the vibrational states of a linear molecule of  $N$  atoms as the qubit basis the number of vibrational degrees of freedom is  $3N - 6$ . A huge quantity of spectroscopic data is required to implement experiments using shaped laser pulses for molecular quantum computing. However, these data are still not available in literature.

The quantum mechanical canonical function method is a powerful technique to compute the very large rotation-vibration constants. The vibration rotation energy of an electronic state of a diatomic molecule is commonly represented by  $E_{vJ} = E_v + \lambda B_v + \lambda^2 D_v + \lambda^3 H_v + \lambda^4 L_v + \lambda^5 M_v \dots$ , where  $\lambda = J(J + 1)$ ,  $v$  and  $J$  are, respectively, the vibrational and rotational quantum numbers,  $E_v$  is the pure vibrational energy,  $B_v$  the rotational constant, and  $D_v, H_v, L_v + \dots$  are the centrifugal distortion constants (CDC) related to

a potential energy curve  $U(r)$  and  $v$ . In the conventional approach of the Raleigh-Schrödinger perturbation theory (RSPT) [1] Albritton et al. [2] derived the first analytical expressions of the centrifugal distortion constants (CDC). Because of the complexity and the tedious computation of these expressions, Hutson derived, by using the Numerov difference equation, an algorithm [3] that allows the determination of the constants  $D_v$ ,  $H_v$ ,  $L_v$ , and  $M_v$  only in terms of the vibrational wave function  $\psi_v$ . However, difficulties appeared in this algorithm for some potentials (like the Lennard-Jones potential) in treating high vibrational level (near dissociation for example) [4]. Because of the development in spectroscopic techniques, higher orders are needed [5]. Tellinghuisen [4] introduced an improvement to Huston algorithm, but it was not sufficient to accede these levels and reach large order of the centrifugal distortion constants.

In this work, we present the canonical function method (superposition of difference equation) which is an advantageous technique with respect to other difference equation methods for solving the vibration-rotation eigenvalue problem [6]. Moreover, with this canonical approach with variable step [7], the large order of CDC and the calculation of the vibration-rotation energy levels, even near dissociation [8], for any potential energy curves (either RKR [9], ab initio [10–12], or empirical [13]) and for any electronic state can be done by one single and simple routine. A program is available for these calculations free of charge with the corresponding author, with applications on the six potential energy curves: Morse potential, Lenard Jones potential, RKR potential, ab initio potential, Simon-Parr-Finlin (Kratzer) potential, and Dunham potential. Since the canonical function method is proven to be valid for any type of potential function, the program is structured in different subroutines for the different cited potentials in order to give the possibility to use the same program for other types of potentials that can be added.

## 2. The Theory

**2.1. Vibration-Rotation Canonical Functions.** In the Born-Oppenheimer approximation, the vibration-rotation motion of a diatomic molecule is described by the wave function  $\Psi_{vJ}$  and the energy  $E_{vJ}$  that are, respectively, the eigenfunction and the eigenvalue of the radial Schrödinger equation [18]

$$\frac{d^2\Psi_{vJ}}{dr^2} + \left[ k(E_{vJ} - V(r)) - \frac{J(J+1)}{r^2} \right] \Psi_{vJ}(r) = 0 \quad (1)$$

where  $k = 2\mu/\hbar^2$ ,  $\mu$  is the reduced mass,  $\hbar$  is the Planck constant,  $v$  and  $J$  are the vibrational and rotational quantum numbers, respectively, and  $r$  is the internuclear distance. This equation can be simply represented by

$$\Psi''_{vJ}(x) = f_{vJ}(x) \Psi_{vJ}(x), \quad (2)$$

where  $x = r - r_e(r_e)$  is the value of  $r$  at the equilibrium, and

$$f_{vJ}(x) = -k[E - U(x)] + \frac{\lambda}{(x + r_e)^2} \quad (3)$$

with  $\lambda = J(J+1)$ . Equation (1) is equivalent to the Volterra integral equation [19]

$$\Psi_{vJ}(x) = \Psi_{vJ}(0) + x' \Psi'_\lambda(0) + \int_0^x (x-t) f_{vJ}(t) \Psi_{vJ}(t) dt \quad (4)$$

in the sense that any solution of (4) is solution of (1). By inserting  $\Psi_{vJ}(x)$  by its expression many times in the integral, one can find:

$$\Psi_{vJ}(x) = \Psi_{vJ}(0) \alpha(x) + \Psi'_{vJ}(0) \beta(x) \quad (5)$$

where  $\alpha(x)$  and  $\beta(x)$  are two canonical functions [20, 21] defined by

$$\alpha(x) = \sum_{i=0}^{\infty} A_i(x) \quad (6-1)$$

$$\text{with } A_i = \int_0^x (x-t) f_{vJ}(t) A_{i-1}(t) dt \text{ and } A_0(x) = 1$$

$$\beta(x) = \sum_{i=0}^{\infty} B_i(x) \quad (6-2)$$

$$\text{with } B_i(x) = \int_0^x (x-t) f_{vJ}(t) B_{i-1}(t) dt \text{ and } B_0(x) = x$$

with the well determined initial values

$$\begin{aligned} \alpha(0) &= 1, \\ \alpha'(0) &= 0 \\ \beta(0) &= 0, \\ \beta'(0) &= 1 \end{aligned} \quad (7)$$

The initial value  $\Psi'_{vJ}(0)$  for the unnormalized wave function  $\Psi_{vJ}(x)$  can be deduced from  $\alpha(x)$  and  $\beta(x)$  by using (5), on one hand, and on the other hand the boundary conditions [5]

$$\Psi_{x \rightarrow \infty}^{vJ} \quad (x) \rightarrow 0 \quad (8)$$

We find

$$\frac{\Psi'_{vJ}(0)}{\Psi_{vJ}(0)} = \lim_{x \rightarrow \infty} \frac{-\alpha(x)}{\beta(x)} \quad (9)$$

$$\frac{\Psi'_{vJ}(0)}{\Psi_{vJ}(0)} = \lim_{x \rightarrow -r_e} \frac{-\alpha(x)}{\beta(x)}$$

**2.2. The Rotational Schrödinger Equations.** In the Rayleigh-Schrödinger perturbation theory (RSPT), the eigenvalue and the eigenfunction of (1) are given, respectively, by

$$E_\lambda = \sum_{n=0}^{\infty} e_n \lambda^n \quad (10)$$

$$\Psi_{vJ}(x) = \sum_{n=0}^{\infty} \Phi_n \lambda^n \quad (11)$$

where  $e_0 = E_v$  is the pure vibrational energy,  $e_1 = B_v$  is the rotational constant,  $e_2 = -D_v$ ,  $e_3 = H_v$ , ... are the centrifugal

distortion constants,  $\varphi_0$  is the pure vibrational wave function, and  $\varphi_i$  is the rotational correction.

Therefore, the energy factor  $f_{vj}(x)$  can be written as

$$f_{vj}(x) = \sum_{n=0}^{\infty} \varepsilon_n(x) \lambda^n \quad (12)$$

where

$$\varepsilon_0 = -k(e_0 - U(x)) \quad (13-1)$$

$$\varepsilon_1 = -ke_1 + \frac{1}{(r_0 + x)^2} \quad (13-2)$$

...

$$\varepsilon_n = ke_n \quad \text{for } i \geq 2 \quad (13-n)$$

From this expression of  $f_{vj}(x)$ , the functions  $\alpha(r)$  and  $\beta(r)$  are given by

$$\alpha(r) = \sum_{n=0}^{\infty} a_n(r - r_i)^n \quad (14)$$

$$\beta(r) = \sum_{n=0}^{\infty} b_n(r - r_i)^n \quad (15)$$

By replacing  $\alpha_{vj}(x)$ ,  $\beta_{vj}(x)$  by their expressions (14) and (15) in (5) we find

$$\Psi_{vj}(x) = \Psi_v + \sum_{n=1}^{\infty} \varphi_n(x) \lambda^n \quad (16)$$

A set of Schrödinger equations is obtained by replacing the wave function  $\Psi_{vj}(x)$  by its expression (16) in (2) to obtain a set of Schrödinger equations

$$\varphi''_0(x) - \varepsilon_0(x) \varphi_0(x) = 0 \quad (17-0)$$

$$\varphi''_1(x) - \varepsilon_0(x) \varphi_1(x) = \varepsilon_1(x) \varphi_0(x) \quad (17-1)$$

$$\varphi''_2(x) - \varepsilon_0(x) \varphi_2(x) = \varepsilon_1(x) \varphi_1(x) + \varepsilon_2(x) \varphi_0(x) \quad (17-2)$$

...

$$\varphi''_n(x) - \varepsilon_0(x) \varphi_n(x) = \sum_{m=1}^n \varepsilon_m(x) \varphi_{n-m}(x) \quad (17-n)$$

where the first of these equations is the radial Schrödinger equation of pure vibration. All the other equations are called the rotational Schrödinger equations.

### 2.3. Analytic Expressions of the Rotation Harmonics

**2.3.1. Pure Vibration  $\Psi_v(x)$ .** For one electronic state and for a given potential function, the solution of the vibrational Schrödinger equation (17-0) is given by [21]

$$\Psi_v(x) = \Psi_v(0) \alpha_v(x) + \varphi'_v(0) \beta_v(x) \quad (18)$$

where  $\alpha_v(x)$  and  $\beta_v(x)$  are the pure vibration canonical functions defined by (5) and (7) in which we replace  $f_{vj}(x)$  by  $f_v(x)$  (i.e., we take  $J=0$ ).

**2.3.2. Calculation of the Rotational Harmonics  $\Phi_n(x)$ .** A rotational Schrödinger equation (17-0), (17-1), (17-2), (17-n) is given by

$$\varphi''_n(x) - \varepsilon_0(x) \varphi_n(x) = \sum_{m=1}^n \varepsilon_m(x) \varphi_{n-m}(x) \quad (19)$$

If we multiply this equation by  $x - t$  and integrate it between zero and  $x$ , it will become

$$\begin{aligned} \varphi_n(x) &= \varphi_n(0) + \varphi'_n(0) x \\ &+ \sum_{m=1}^n \int_0^x (x-t) \varepsilon_m(t) \varphi_{n-m}(t) dt \end{aligned} \quad (20)$$

By replacing  $\varepsilon_m(t)$  by its expression (13-1), (13-2), (13-n) in (17-0), (17-1), (17-2), (17-n) we obtain

$$\varphi_n(x) = \varphi_n(0) \alpha_v(x) + \varphi'_n(0) \beta_v(x) + \sigma_n(x) \quad (21)$$

where

$$\sigma_n(x) = \sum_{m=0}^{\infty} k_m^n(x) \quad (22)$$

$$k_0^n(x) = \int_0^x (x-t) \varepsilon_n(t) \varphi_0(t) dt \quad (23-0)$$

$$k_1^n(x) = \int_0^x (x-t) \int_0^t (t-t_1) \varepsilon_n(t) \varphi_0(t) dt dt \quad (23-1)$$

$$k_m^n(x) = \int_0^x (x-t) \varepsilon_n(t) k_{m-1}(t) dt \quad (23-2)$$

for  $x = 0$

$$k_0^n(0) = k_1^n(0) = \dots = k_m^n(0) = \dots = 0 \quad (24)$$

$$k_0^{n'}(0) = k_1^{n'}(0) = \dots = k_m^{n'}(0) = \dots = 0$$

Therefore

$$\sigma_n(0) = \sigma'_n(0) = 0 \quad (25)$$

for the derivation of order  $i$

$$\frac{d^i k_m^n(0)}{dx^i} = 0 \quad \text{for } i \geq 2 \quad (26)$$

and

$$\frac{d^i \sigma_n(0)}{dx^i} \neq 0 \quad (27)$$

For the unnormalized wave function, we chose  $\Psi_v(0) = \varphi_0(0) = 1$ , and by using (16) we obtain

$$\varphi_n(0) = 0 \quad (28)$$

By replacing  $\varphi_n(0)$  by its value in (21) we obtain

$$\varphi_n(x) = \varphi'_n(0) \beta_v(x) + \sigma_n(x) \quad (29)$$

On the other hand, the rotation harmonics must be vanished at the boundaries (8); thus (29) gives

$$\frac{-\sigma_n(x)}{\beta_v(x)} = l_n \quad (30)$$

and the rotation harmonic  $\varphi_n(x)$  is given by [7]

$$\varphi_n(x) = \sigma_n(x) + I_n \beta_v(x) \quad (31)$$

This expression is valid without any restriction for the form of a given potential function.

#### 2.4. Numerical Method

2.4.1. *Calculation of the Vibrational Wave Function  $\Phi_0(r)$ .* For one electronic state and for a given potential function, the vibrational wave function is given by

$$\varphi_0(x) = \varphi_0(0) \alpha_v(x) + \varphi'_0(0) \beta_v(x) \quad (32)$$

The determination of  $\varphi_0(x)$  requires the calculation of  $\alpha_v(x)$ ,  $\beta_v(x)$ , and  $\varphi'_0(x)$ .

(1) *Calculation of  $\alpha_v(x)$  and  $\beta_v(x)$ .* For a given potential, and on one interval,  $I_i = [r_i, r_{i+1}]$  has the polynomial form

$$U(r) = \sum_{n=0}^N \gamma_n(i) (r - r_i)^n \quad (33)$$

The canonical functions  $\alpha(x)$  and  $\beta(x)$  are particular solutions of (17-0), because  $U(x)$  is expanded in polynomial [8];  $\alpha(x)$  and  $\beta(x)$  also can be expanded as

$$\alpha(r) = \sum_{n=0}^{\infty} a_n (r - r_i)^n \quad (34)$$

$$\beta(r) = \sum_{n=0}^{\infty} b_n (r - r_i)^n \quad (35)$$

By representing  $\alpha(r)$  and  $\beta(r)$  by the same function  $y(r)$  for a given potential  $U(r)$  and energy  $E$ , the function  $y(r)$  is given by

$$y(r) = \sum_{n=0}^{\infty} C_n(i) (r - r_i)^n \quad (36)$$

By using (17-0), we obtain the following recursion relation:

$$\begin{aligned} & (n+2)(n+1)C_{n+2}(i) \\ &= -kEC_n(i) + k \sum_{m=0}^n C_m(i) \gamma_{n-m}(i) \end{aligned} \quad (37)$$

with

$$\begin{aligned} C_0(i) &= y(r_i), \\ C_1(i) &= y'(r_i) \end{aligned} \quad (38)$$

The initial values  $y(r_1)$  and  $y'(r_1)$  are given by

$$y(r_i) = \sum_{n=0}^{\infty} C_n(i-1) (r_i - r_{i-1})^n \quad (39)$$

$$y'(r_i) = \sum_{n=0}^{\infty} n C_n(i-1) (r_i - r_{i-1})^{n-1} \quad (40)$$

where  $y(0) = 1, y'(0) = 0$  for  $\alpha$  function and  $y(0) = 0, y'(0) = 1$  for  $\beta$  function

Therefore, the canonical functions  $\alpha(r)$  and  $\beta(r)$  are well determined at any point  $r$ .

(2) *Calculation of  $\Phi'_0$ .* From equation (5), the wave function  $\varphi_0(x)$  is given by

$$\varphi_0(r) = \alpha(r) + \varphi'_0(0) \beta(r) \quad (41)$$

By using the boundary conditions (8) one can find

$$\frac{\varphi'_0(0)}{\varphi_0(0)} = \lim_{r \rightarrow \infty} \frac{-\alpha(r)}{\beta(r)} = \lim_{r \rightarrow \infty} \frac{\alpha'(r)}{\beta'(r)} \quad (42)$$

For the unnormalized wave function  $\varphi_0(0) = 1$ , the vibration function  $\varphi_0(r)$  is determined at any point  $r$ .

2.5. *Diatomic Centrifugal Distortion Constants (CDC).* The rotational equations (17-0), (17-1), (17-2), and (17-n) are all of the form

$$z'' + k(e_0 - v)z = S(r) \quad (43)$$

We multiply this equation by  $\varphi_0$  and integrate between  $r_0$  and  $\infty$ . By making use of (17-0), (17-1), (17-2), and (17-n), we obtain

$$\int_{r_0}^{\infty} (z'' \varphi_0 - z \varphi_0'') dr = \int_{r_0}^{\infty} s(r) \varphi_0(r) dr \quad (44)$$

Then we make use of the boundary conditions for  $\varphi_0$  and  $z$  (at  $r \approx \infty$ ) on one hand, and of (8) on the other hand, and we find

$$z'(r_0) = - \int_{r_0}^{\infty} s(r) \varphi_0(r) dr \quad (45-1)$$

and similarly, for the other boundary condition (at  $r \approx 0$ ),

$$z'(r_0) = - \int_{r_0}^0 s(r) \varphi_0(r) dr \quad (45-2)$$

The continuity condition for  $s(r)$  implies the equality of  $z'(r_0)$  given by (44); therefore

$$- \int_0^{\infty} s(r) \varphi_0(r) dr = - \int_{r_0}^0 s(r) \varphi_0(r) dr, \quad (46)$$

$$\int_0^{\infty} s(r) \varphi_0(r) dr = \langle s | \varphi_0 \rangle = 0$$

This equation gives for the successive value of  $s$

$$\langle \varphi_0 | e_1 - R | \varphi_0 \rangle = 0 \quad (47-0)$$

$$\langle \varphi_0 | e_1 - R | \varphi_1 \rangle + e_2 \langle \varphi_0 | \varphi_2 \rangle = 0 \quad (47-1)$$

...

$$\langle \varphi_0 | e_1 - R | \varphi_{n-1} \rangle + \sum_{m=2}^n e_m \langle \varphi_0 | \varphi_{n-m} \rangle = 0. \quad (47-n)$$

These equations give simple expression of  $e_1, e_2, \dots, e_n$  in terms of  $\varphi_0, \varphi_1, \dots, \varphi_{n-1}$

$$I_0 e_1 = R_0 \quad (48-1)$$

$$I_0 e_2 = R_1 - e_1 I_1 \quad (48-2)$$

$$I_0 e_3 = R_2 - e_1 I_2 - e_2 I_1 \quad (48-3)$$

...

$$I_0 e_n = R_{n-1} - \sum_{m=1}^{n-1} e_m I_{n-m} \quad (48-n)$$

where

$$\begin{aligned} I_n &= \langle \varphi_0 | \varphi_n \rangle, \\ R_n &= \langle \varphi_0 | R | \varphi_n \rangle \end{aligned} \quad (49)$$

Once  $e_0 = E_v$  is given, the determination of  $e_1, e_2, \dots$  is reduced to that of simple definite integrals  $I_0, I_1, I_2, \dots$  and  $R_0, R_1, R_2, \dots$  depending on  $\varphi_0, \varphi_1, \varphi_2, \dots$  [19].

### 3. Results and Discussion

**3.1. Calculated Data.** In order to test the accuracy and the validity of the present method for the calculation of the different rovibrational parameters we used as examples for the empirical potentials Morse potential [14, 15], Lenard Jones potential [4, 8, 22], Dunham Potential [23], and Kratzer potential [24]. For the investigation of the *ab initio* potential [17], we employed the state averaged Complete Active Space Self Consistent Field (CASSCF) followed by Multireference Configuration Interaction (MRCI) method with Davidson correction (+Q), single and double excitations. In these entire calculations, we used the computational chemistry program MOLPRO [25] with the advantage of the graphical user interface GABEDIT [26]. The CASSCF configuration space was used as the reference in the MRCI calculations. The potential energy  $U(r)$  is determined in terms of the internuclear distance  $r$  with a step equal to  $0.02\text{\AA}$ . The Schrödinger equation is solved by using the cubic spline interpolation between every two consecutive points. A Rydberg-Klein-Rees (RKR) potential is obtained experimentally and defined by their turning points [27–29]. The calculation has been done by an interpolation between every two consecutive points also by using the cubic spline interpolation. If the number of the turning points is limited we extrapolate the potential function curve to the right by [30]  $U(x) = a/r^6 + b/r^8 + c/r^{10}$  and to the left by  $U(x) = d/r^{15}$  where the constants  $a, b, c$  can be obtained from literature (if available) and  $d$  is calculated using the used potential energy curve.

The comparison of our calculated values of the vibrational energy levels  $E_v$ , by using the empirical Morse potential for the molecule CO, with those given in [14, 15] shows, respectively, excellent agreements with the relative differences  $0.00\% < \Delta E_v/E_v < 1.25\%$  and  $0.00\% < \Delta E_v/E_v < 0.03\%$  (Table 1). Similar excellent agreement  $\Delta E_v/E_v = 0.00\%$  is

obtained by comparing our calculated values of the different vibrational levels  $E_v$  with those given by Martin et al. [16] of the RKR potential of the molecule  $I_2$  (Table 2). Our method is also tested in case of an *ab initio* potential for the molecule ZnBr [17] (Table 3). Recently [31], we calculated, by using the present method, the rovibrational parameters  $E_v, B_v, D_v$  of the molecule LiSr by using an *ab initio* potential. The comparison of the calculated values of  $E_v$  and  $B_v$  with those available in literature shows the good agreement with the relative differences  $0.1\% < \Delta E_v/E_v < 7.5\%$  for  $E_v$  and acceptable agreement  $10.9\% < \Delta B_v/B_v < 12.9\%$  for  $B_v$ . However, the comparison of our calculated values of  $B_v$ , by the present method, with those given in literature shows a very good agreement with the relative difference  $1.1\% < \Delta B_v/B_v < 2.8\%$  for the molecule NaSr [31].

**3.2. Advantage of the Present Method.** The first explicit analytical expressions for the calculation of the distortion constants were derived by Albritton et al. [2]. The conventional Rayleigh-Schrödinger perturbation approach makes use of the wavefunction expansion given in (11) that leads to the expressions for  $e_1, e_2, e_3, \dots$  as first- and higher-order perturbation energies (10). These expressions of the distortion constants were considered fairly good for low-lying vibrational levels only; for higher levels they failed mainly because of the omission of the contribution from continuum levels.

A modification of the perturbation method enabled Hutson [3] to derive simple expressions for  $e_1, e_2, e_3, \dots$  in terms of the internuclear distance  $r, \phi_0, \phi_1, \phi_2$  and to elaborate an efficient routine to solve the diatomic distortion constants problem by using the Numerov method described by Cooley [32]. By using this method, Tellinghuisen [4] pointed out a “pesky problem of instability” in the computation of  $\phi_1, \phi_2$  in the Hutson approach. Therefore, he described a modification of the Hutson method in order to improve it by eliminating “nuisance instabilities in the nonclassical regions.”

The advantages of the method given in the present work are as follows:

(i) By using the variable step method, for an empirical potential, the number of mesh steps is largely reduced. For *ab initio* and RKR potentials, the step is the distance between two consecutive points. In the present method we step out to the left and to right by starting from an arbitrary origin. The calculation is stopped when the wave function tends to zero (see (42)) which reduces the range of integration.

(ii) The instability problem and its solution presented by Tellinghuisen [4] are both implied by the perturbation formulation as used by Hutson [3] (which indirectly implies an initial value problem for  $\phi_1, \phi_2, \dots$ ). The present work eliminates this instability problem by giving exact analytical initial values for  $\phi_1, \phi_2, \dots$  (see (32) and (41)) at an arbitrary origin.

(iii) The present method is free from any conventional problems related to those of Hutson and Tellinghuisen; it does not imply any trial value or any “matching” problem (or initial values assumptions) on any iteration; it is equally easy for low or high levels.

TABLE 1: The energy eigenvalues  $E_v$ , the rotational constants  $B_v$ , and the centrifugal distortion constants  $D_v$ ,  $H_v$ ,  $L_v$  of the pure vibrational energy levels of the Morse potential of CO molecule.

V	$E_v$ cm <sup>-1</sup>	$\Delta E_v/E_v$	$B_v$ cm <sup>-1</sup>	$D_v \times 10^6$ cm <sup>-1</sup>	$H_v \times 10^{12}$ cm <sup>-1</sup>	$L_v \times 10^{17}$ cm <sup>-1</sup>
0	1081.78 <sup>a</sup>		1.9225	6.11954	5.8008	3.6445
	1081.61 <sup>b</sup>	0.02				
	1081.5857 <sup>c</sup>	0.02				
1	3225.05		1.9050	6.11885	5.6556	3.7160
	3225.05	0.00				
	3224.8568	0.03				
2	5341.84		1.8875	6.11849	5.5100	3.7848
	5342.11	0.00				
	5341.6478	0.00				
3	7432.22		1.8700	6.11844	5.3659	3.8409
	7432.79	0.01				
	7432.0247	0.00				
4	9496.25		1.8525	6.11863	5.2272	3.8678
	9497.09	0.18				
	9496.0550	0.00				
5	11534.03		1.8350	6.11892	5.1007	3.8397
	11535.01	0.01				
	11533.80787	0.00				
6	13545.61		1.8175	6.11910	4.9970	3.7184
	13546.56	0.00				
	13545.3543	0.00				
7	15531.12		1.8001	6.11884	4.9323	3.4491
	15531.72	0.00				
	15530.767	0.00				
8	17490.66		1.7826	6.11761	4.9298	2.9556
	17490.1202	0.00				
9	19424.39		1.7652	6.11467	5.0224	2.2224
	19423.4901	0.00				
10	21332.48		1.7478	6.10895	5.2545	0.8581
	21330.9539	0.01				
11	23195.48		1.7353	6.3063	5.1176	7.4807
	23212.5907	0.07				
12	25046.37		1.7179	6.3265	4.8608	7.7559
	25068.4807	0.09				
13	26870.69		1.7004	6.3476	4.5905	8.0499
	26898.7056	0.10				
14	28668.43		1.6829	6.3695	4.3061	8.3641
	28703.3478	0.00				
15	30439.59		1.6653	6.3922	4.0066	8.7004
	30482.4908	0.14				
16	32184.18		1.6476	6.4159	3.6911	9.0606
	32236.2189	0.16				
17	33902.19		1.6299	6.4405	3.3586	9.4470
	33964.6167	0.18				
18	35593.63		1.6121	6.4661	3.0081	9.8617
	35667.7691	0.21				
19	37258.49		1.5943	6.4927	2.6384	10.307
	37345.7608	0.23				
20	38896.77		1.5764	6.5204	2.2483	10.787
	38998.6766	0.26				

TABLE I: Continued.

V	$E_v$ cm <sup>-1</sup>	$\Delta E_v/E_v$	$B_v$ cm <sup>-1</sup>	$D_v \times 10^6$ cm <sup>-1</sup>	$H_v \times 10^{12}$ cm <sup>-1</sup>	$L_v \times 10^{17}$ cm <sup>-1</sup>
21	40508.47	0.29	1.5584	6.5493	1.8363	11.303
	40626.6001					
22	42093.6	0.32	1.5403	6.5794	1.4011	11.859
	42229.6144					
23	43652.15	0.36	1.5221	6.6108	9.4096	12.460
	43807.8009					
24	45184.13	0.39	1.5039	6.6435	4.5424	13.109
	45361.2396					
25	46689.52	0.43	1.4856	6.6775	6.0978	13.812
	46890.0081					
26	48168.35	0.47	1.4672	6.7131	6.0676	14.573
	48394.1814					
27	49620.59	0.51	1.4488	6.7502	1.1853	15.398
	49873.8318					
28	51046.26	0.55	1.4302	6.7890	1.7992	16.295
	51329.0276					
29	52445.35	0.60	1.4116	6.8295	2.4510	17.270
	52759.8334					
30	53817.87	0.65	1.3929	6.8718	3.1438	18.332
	54166.3090					
31	55163.8	0.70	1.3741	6.9160	3.8807	19.496
	55548.5091					
32	56483.17	0.75	1.3552	6.9623	4.6654	20.757
	56906.4825					
33	57775.95	1.11	1.3362	7.0107	5.5017	22.142
	58240.2716					
34	59042.17	1.12	1.3171	7.0614	6.3942	23.660
	59711.7					
35	60281.79	0.92	1.2979	7.1145	7.3475	25.327
	60835.4299					
36	61494.85	0.98	1.2785	7.1702	8.3670	27.299
	62096.8449					
37	62681.33	1.04	1.2591	7.2286	9.4589	29.181
	63334.1657					
38	63841.23	0.46	1.2396	7.2899	10.630	31.412
	63547.399					
39	64974.55	1.17	1.2200	7.3543	11.887	33.881
	65736.5076					
40	66081.3	1.24	1.2002	7.4220	13.238	36.619
	66901.4905					

<sup>a</sup>The first entry is for the present work.

<sup>b</sup>The second and the <sup>c</sup>third entries are, respectively, for [14, 15].

(iv) The computing “effort” to calculate  $e_1$  is roughly the same as that to obtain  $e_2, e_3, \dots$ . For each constant two new integrals,  $I_n$  and  $R_n$  (see (49)), are required. The effort necessary to calculate  $B_v, D_v, H_v, L_v, M_v \dots$  is roughly equivalent to the average required to solve the vibrational eigenvalue.

(v) Calculation of the energy eigenvalue  $E_v$  near the dissociation energy is another advantage. The spectroscopic

constants used in the present work for Morse potential of the molecule CO [14, 15] are  $\omega_e = 2169.81358$  cm<sup>-1</sup> and  $\omega_e x_e = 13.28831$  cm<sup>-1</sup>. The dissociation energy for this potential is given by  $D_e = \omega_e^2 / 4\omega_e x_e = 88575.80$  cm<sup>-1</sup>. We present in Table SF7 (Supplementary Material file) the vibrational energy levels  $E_v$ , the rotational constants  $B_v$ , and the centrifugal distortion constants  $D_v, H_v, L_v$  of the Morse potential for the molecule CO near dissociation (from

TABLE 2: The energy eigenvalues  $E_v$ , the rotational constants  $B_v$ , and the centrifugal distortion constants  $D_v$ ,  $H_v$ ,  $L_v$  of the pure vibrational energy levels of the RKR potential of the electronic state  $XO_g^+$  of the molecule  $I_2$ .

$v$	$E_v \text{ cm}^{-1}$	$B_v \times 10^2 \text{ cm}^{-1}$	$D_v \times 10^9 \text{ cm}^{-1}$	$-H_v \times 10^{16} \text{ cm}^{-1}$	$-L_v \times 10^{22} \text{ cm}^{-1}$
0	107.10 <sup>a</sup> 107.0981 <sup>b</sup>	3.731	4.547	5.115	2.858
1	320.40 320.3986	3.719	4.572	5.380	3.115
2	532.47 532.4712	3.708	4.597	5.554	3.345
3	743.31 743.3082	3.696	4.624	5.750	3.462
4	952.90 952.9017	3.684	4.651	5.959	3.589
5	1161.24 1161.2438	3.673	4.679	6.282	4.258
6	1368.33 1368.3260	3.661	4.708	6.504	3.546
7	1574.14 1374.1399	3.649	4.739	6.857	5.389
8	1778.68 1778.6764	3.637 3.637	4.770 4.768	7.131 5.57	4.302 3.03
9	1981.93 1981.9263	3.625 3.625	4.803 4.794	7.365 7.18	5.531 3.23
10	2183.88 2183.8800	3.613 3.613	4.837 4.825	7.742 7.50	6.076 3.46
11	2384.53 2384.5275	3.601 3.601	4.872 4.864	7.949 7.85	5.614 3.73
12	2583.86 2583.8536	3.589 3.589	4.909 4.901	8.316 8.32	6.790 4.02
13	2781.86 2781.8628	3.576 3.577	4.947 4.939	8.679 8.64	6.859 4.35
14	2978.53 2978.5290	3.564 3.564	4.987 4.980	9.049 9.08	6.970 4.71
15	3173.84 3173.8461	3.551 3.551	5.029 5.019	9.510 9.54	7.467 5.11
16	3367.80 3367.8023	3.539 3.540	5.072 5.509	10.01 10.04	8.106 5.56
17	3560.38 3560.3875	3.526 3.527	5.117 5.114	10.52 10.57	8.463 6.05
18	3751.58 3751.5835	3.513 3.513	5.163 5.166	11.10 11.13	
19	3941.38 3941.3830	3.121			

<sup>a</sup>The first entry is for the present work.

<sup>b</sup>The second entry is for [16].

$v = 41$  to  $v = 81$ ). Our calculated value for  $E_v = 88575.55 \text{ cm}^{-1}$  for  $v = 81$  is in excellent agreement with that calculated using the formula  $D_e = \omega_e^2/4\omega_e x_e$ .

We are now considering the application of this method as a verification procedure, for additional future and previously characterized molecules. The calculated values of the rovibrational energy levels  $E_{vJ}$  of the potential energy curves Morse,

RKR, and ab initio for different values of  $v$  and  $J$  are given in Tables (SF1, SF2, SF3) in Supplementary Material file. The accuracy of our calculated values of the rotational constants  $B_v$  and the centrifugal distortion constants  $D_v$ ,  $H_v$ ,  $L_v$  for the six considered potentials by using the present software is presented in Tables (SF1, SF4, SF5-SF6) in Supplementary Material file. In these tables, we compare the calculated values

TABLE 3: The eigenvalues  $E_v$ , the rotational constants  $B_v$ , and the centrifugal distortion constants  $D_v$ ,  $H_v$ ,  $L_v$  of the pure vibrational levels of the ab initio potential of the electronic state  $(2)^2\Sigma^+$  of ZnBr molecule.

$v$	$E_v$	$B_v \times 10^2 \text{ cm}^{-1}$	$D_v \times 10^8 \text{ cm}^{-1}$	$H_v \times 10^{14} \text{ cm}^{-1}$	$L_v \times 10^{19} \text{ cm}^{-1}$
0	73.93 <sup>d</sup>	4.45103	1.61218	0.91241	0.14521
1	221.79	4.44744	1.63363	0.90472	0.19051
2	368.99	4.44350	1.66127	0.92463	0.05234
3	515.45	4.43935	1.67943	0.87615	0.27340
4	661.24	4.43481	1.70614	1.00984	0.15840
5	806.32	4.43028	1.71652	0.84228	0.29044
6	950.77	4.42537	1.73609	0.94056	0.11801
7	1094.61	4.42030	1.75034	0.11996	0.47912
8	1237.82	4.41370	1.78434	0.05349	0.84506
9	1380.27	4.40576	1.79032	0.59008	1.70130
10	1522.02	4.39775	1.73959	2.38350	2.47151
11	1663.35	4.39179	1.74384	0.88805	5.98681
12	1804.32	4.38529	1.88228	0.62346	2.15342
13	1944.46	4.37762	1.95563	3.05568	8.56892
14	2083.65	4.37184	1.86765	0.65588	4.32335
15	2222.28	4.36596	1.88941	2.90845	0.21492
16	2360.26	4.35694	1.90747	1.64760	0.79699
17	2497.54	4.34855	1.87664	320136	8.65452
18	2634.29	4.34149	1.96854	0.20066	4.88072
19	2770.33	4.33340	2.00230	1.64988	6.52090
20	2905.64	4.32574	1.95889	0.24895	5.04669
21	3040.34	4.31742	1.98347	0.26314	1.24147
22	3174.38	4.30858	2.00303	2.70697	1.67678
23	3307.78	4.30041	2.03418	0.91178	1.17857
24	3440.52	4.29194	2.06118	1.10390	3.42636
25	3572.59	4.28340	2.05726	0.54873	1.82649
26	3704.00	4.27461	2.07284	0.96785	1.25401
27	3834.77	4.26566	2.09089	1.58438	0.12407
28	3964.89	4.25677	2.10901	0.80808	1.31828
29	4094.36	4.24767	2.11876	1.04840	0.30910
30	4223.18	4.23849	2.12936	0.86572	0.05289
31	4351.37	4.22914	2.13889	1.08629	0.85910
32	4478.92	4.21971	2.15187	1.10438	0.34952
33	4605.84	4.21019	2.16476	0.78563	0.70987
34	4732.14	4.20049	2.17260	0.99447	1.02375
35	4857.80	4.19069	2.18507	1.11534	0.64514
36	4982.85	4.18081	2.19293	0.94266	0.49012
37	5107.27	4.17082	2.20322	1.05993	0.17041
38	5231.08	4.16074	2.21393	0.94721	1.19382
39	5354.28	4.1505	2.22180	0.97556	1.04020
40	5476.87	4.14026	2.23134	1.12858	0.13659
41	5598.85	4.12991	2.24135	0.94846	0.81640
42	5720.22	4.11945	2.24801	1.01250	0.74932
43	5840.99	4.10891	2.25680	1.06147	0.53996
44	5961.17	4.09830	2.26532	0.88668	0.28173
45	6080.74	4.08758	2.27180	1.09059	0.75800
46	6199.73	4.07680	2.28052	1.12210	0.61602
47	6318.12	4.06596	2.28691	0.91408	0.02149
48	6435.92	4.05503	2.29364	1.02652	0.71959
49	6553.13	4.04403	2.30155	1.04383	.25215
50	6669.76	4.03296	2.30781	0.95909	0.10453
51	6785.81	4.02183	2.31237	1.14847	0.87011

TABLE 3: Continued.

v	$E_v$	$B_v \times 10^2 \text{ cm}^{-1}$	$D_v \times 10^8 \text{ cm}^{-1}$	$H_v \times 10^{14} \text{ cm}^{-1}$	$L_v \times 10^{19} \text{ cm}^{-1}$
52	6901.28	4.01063	2.32080	1.05833	0.81187
53	7016.17	3.99938	2.32662	0.95641	0.09161
54	7130.49	3.98806	2.33122	1.13254	0.51320
55	7244.23	3.97669	2.33750	1.03295	0.81658
56	7357.41	3.96527	2.34305	0.93553	0.06755
57	7470.02	3.95378	2.34775	1.09995	0.66094
58	7582.06	3.94225	2.35311	1.13554	0.84554
59	7693.54	3.93068	2.35746	0.95176	0.06318
60	7804.46	3.91905	2.36103	1.09731	0.78457
61	7914.82	3.90737	2.36686	1.11190	0.93709
62	8024.62	3.89566	2.37097	0.90113	0.83185
63	8133.87	3.88389	2.37344	0.99341	0.85369
64	8242.57	3.87209	2.37792	1.14385	0.17720
65	8350.73	3.86026	2.38109	0.98947	0.70085

<sup>a</sup>Data published in [17] calculated by the present software.

of the rovibrational energy levels  $E_{vJ}$  by using (1) and (11). This comparison shows the high accuracy of the present technique.

#### 4. Conclusion

In the present work, the Volterra integral equation is used to solve the rovibrational Schrödinger equation of a diatomic molecule. This method showed that a high order precision is obtained for large order centrifugal distortion constant as  $D_v, H_v, \dots, Q_v, \dots$ . By using the present canonical function approach one can obtain these constants with the high values of vibrational levels even near dissociation by one single and simple routine. This method provides strong evidence for our assumption that the higher order of  $D_v, H_v, L_v, \dots$  and the higher vibrational  $v$  and rotational level  $J$  for any electronic state and any type of potential energy curves (either experimental, empirical, or theoretical) are as accurate as the low-order values.

#### Data Availability

The data used to support the findings of this study are available from the corresponding author upon request.

#### Disclosure

For the calculations, a program is available, free of charge, with the corresponding author.

#### Conflicts of Interest

The authors declare that they have no conflicts of interest.

#### Supplementary Materials

In the supplementary material there are three main files: (1) Read me: Rovib-1 is a program for calculating the

rovibrational energy eigenvalues  $E_{vJ}$ , the rotational constant  $B_v$ , and large order centrifugal distortion constants  $D_v, H_v, L_v, \dots$  of bound levels of different types of potential energy curves: empirical, RKR, and ab initio. (2) Input Data: Table of all the data used in the program. (3) Program, input, output files: In this file the reader can find the following: (i) the Rovib-1 program; (ii) examples of input files for the different kinds of potential energy curves; (iii) examples of output files for the different kinds of potential energy curves. (*Supplementary Materials*)

#### References

- [1] A. Messiah, *Mechanics*, vol. 2, Dunod, Paris, 1972.
- [2] D. L. Albritton, W. J. Harrop, A. L. Schmeltekopf, and R. N. Zare, "Calculation of centrifugal distortion constants for diatomic molecules from RKR potentials," *Journal of Molecular Spectroscopy*, vol. 46, no. 1, pp. 25–36, 1973.
- [3] J. M. Hutson, "Centrifugal distortion constants for diatomic molecules: An improved computational method," *Journal of Physics B: Atomic, Molecular and Optical Physics*, vol. 14, no. 5, pp. 851–857, 1981.
- [4] J. Tellinghuisen, "An improved method for the direct computation of diatomic centrifugal distortion constants," *Journal of Molecular Spectroscopy*, vol. 122, no. 2, pp. 455–461, 1987.
- [5] J. A. Coxon and P. G. Hajigeorgiou, "Isotopic dependence of Born-Oppenheimer breakdown effects in diatomic hydrides: The  $B1\Sigma^+$  and  $X1\Sigma^+$  states of HF and DF," *Journal of Molecular Spectroscopy*, vol. 142, no. 2, pp. 254–278, 1990.
- [6] H. Kobeissi, M. Kobeissi, and A. E. Hajj, "On testing difference equations for the diatomic eigenvalue problem," *Journal of Computational Chemistry*, vol. 9, no. 8, pp. 844–850, 1988.
- [7] M. Dagher and H. Kobeissi, "DIRIGE- a program for calculating eigenvalues and initial values of log derivative eigenfunctions for a diatomic molecule," *Computer Physics Communications*, vol. 46, p. 445, 1987.
- [8] W. Chmaisani, N. El-Kork, and M. Korek, "Theoretical electronic structure of the NaBe molecule," *Chemical Physics*, vol. 491, pp. 33–41, 2017.

- [9] M. Korek and H. Kobeissi, "Diatomic centrifugal distortion constants for large orders at any level: application to the state," *Canadian Journal of Chemistry*, vol. 71, no. 3, pp. 313–317, 1993.
- [10] N. El-Kork, N. Abu el kher, F. Korjeh, J. A. Chtay, and M. Korek, "Electronic structure of the polar molecules XF (X: Be, Mg, Ca) with rovibrational and dipole moment calculations," *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, vol. 177, pp. 170–196, 2017.
- [11] D. Houalla, W. Chmaisani, N. El-Kork, and M. Korek, "Electronic structure calculation of the MgAlk (Alk = K, Rb, Cs) molecules for laser cooling experiments," *Computational and Theoretical Chemistry*, vol. 1108, pp. 103–110, 2017.
- [12] S. Elmoussaoui, N. El-Kork, and M. Korek, "Electronic structure of the ZnCl molecule with rovibrational and ionicity studies of the ZnX (X = F, Cl, Br, I) compounds," *Computational and Theoretical Chemistry*, vol. 1090, pp. 94–104, 2016.
- [13] H. Kobeissi and M. Korek, "One compact analytic expression of the diatomic centrifugal distortion constants to any order," *Journal of Physics B: Atomic, Molecular and Optical Physics*, vol. 26, no. 3, pp. L35–L40, 1993.
- [14] M. Rasoolzadeh and R. Islampour, "Estimation of vibrational energy levels of diatomic molecules (CN, CO and CS) using Numerov algorithm and comparison with the empirical values," *Australian Journal of Basic and Applied Sciences*, vol. 5, no. 12, pp. 2041–2047, 2011.
- [15] S. Chandra, V. U. Maheshwari, and A. K. Sharma, "Einstein A-coefficients for vib-rotational transitions in CO," *Astronomy and Astrophysics Supplement Series*, vol. 117, no. 3, pp. 557–559, 1996.
- [16] F. Martin, R. Bacis, S. Churassy, and J. Vergès, "Laser-induced-fluorescence Fourier transform spectrometry of the XOg+ state of I2: Extensive analysis of the BOu+  $\rightarrow$  XOg+ fluorescence spectrum of 127I2," *Journal of Molecular Spectroscopy*, vol. 116, no. 1, pp. 71–100, 1986.
- [17] S. Elmoussaoui, N. El-Kork, and M. Korek, "Electronic structure with dipole moment and ionicity calculations of the low-lying electronic states of the ZnF molecule," *Canadian Journal of Chemistry*, vol. 95, no. 1, pp. 22–27, 2016.
- [18] G. Herzberg, *Spectra of Diatomic Molecules*, vol. 56, Von Nostrand, Toronto, 1950.
- [19] H. Kobeissi and M. Korek, "Analytic expression of the rotation harmonics in the vibration-rotation wave function of a diatomic molecule," *International Journal of Quantum Chemistry*, vol. 22, no. 1, pp. 23–29, 1982.
- [20] H. Kobeissi and M. Korek, "Diatomic rovibrational matrix elements: analytic expression of the rotational factor for any potential," *Journal of Physics B: Atomic, Molecular and Optical Physics*, vol. 27, no. 16, pp. 3653–3658, 1994.
- [21] M. Korek and H. Kobeissi, "Highly accurate diatomic centrifugal distortion constants for high orders and high levels," *Journal of Computational Chemistry*, vol. 13, no. 9, pp. 1103–1108, 1992.
- [22] J. Lennard-Jones, *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, vol. 198, no. 1, 1949.
- [23] R. H. Tipping and J. F. Ogilvie, "Herman-wallis factors for Raman transitions of  $1\Sigma$ -state diatomic molecules," *Journal of Raman Spectroscopy*, vol. 15, no. 1, pp. 38–40, 1984.
- [24] G. Simons, R. G. Parr, and J. M. Finlan, "New alternative to the Dunham potential for diatomic molecules," *The Journal of Chemical Physics*, vol. 59, no. 6, pp. 3229–3234, 1973.
- [25] H. J. Werner, P. J. Knowles, G. Knizia et al., version .1, a package of ab initio programs, <http://www.molpro.net/info/users>.
- [26] A.-R. Allouche, "Gabedit—a graphical user interface for computational chemistry softwares," *Journal of Computational Chemistry*, vol. 32, no. 1, pp. 174–182, 2011.
- [27] R. Rydberg, "Graphische Darstellung einiger bandenspektroskopischer Ergebnisse," *Zeitschrift für Physik*, vol. 73, no. 5–6, pp. 376–385, 1932.
- [28] O. Klein, "Zur Berechnung von Potentialkurven für zweiatomige Moleküle mit Hilfe von Spektraltermen," *Zeitschrift für Physik*, vol. 76, no. 3–4, pp. 226–235, 1932.
- [29] A. L. G. Rees, "The calculation of potential-energy curves from band-spectroscopic data," *Proceedings of the Physical Society*, vol. 59, no. 6, pp. 998–1008, 1947.
- [30] R. J. Leroy and R. B. Bernstein, "Dissociation energy and long-range potential of diatomic molecules from vibrational spacings of higher levels," *The Journal of Chemical Physics*, vol. 52, no. 8, pp. 3869–3879, 1970.
- [31] N. El-Kork, I. zeid, H. A. Razzouk, S. Atwani, R. Abou arkoub, and M. Korek, "Electronic structure with dipole moment calculations of the high-lying electronic states of BeH, MgH and SrH molecules," *Journal of Physics Communications*, vol. 2, no. 5, p. 055030, 2018.
- [32] J. W. Cooley, "An improved eigenvalue corrector formula for solving the Schrödinger equation for central fields," *Mathematics of Computation*, vol. 15, pp. 363–374, 1961.



Hindawi

Submit your manuscripts at  
[www.hindawi.com](http://www.hindawi.com)

