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ORIGINAL PAPER

Exact and Poisson summation thermodynamic properties for diatomic molecules with shifted Tietz potential

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Abstract: We obtained in detail the energy spectra of the shifted Tietz potential using factorization method within the framework of non-relativistic quantum mechanics. With this energy, the thermodynamic properties of the electronic state of $3^3\Sigma_g^+$ of Cs_2 diatomic molecules are obtained using exact and Poisson summation formalism for the shifted Tietz potential, with adjustable parameter (optimization) appearing in the shifted Tietz potential function ranging from $C_h = \pm\frac{1}{5}, \pm\frac{1}{8}$ and $\pm\frac{1}{4}$ respectively. Free energy F, internal energy U, entropy S and specific heat C are also calculated. In each case, the exact and Poisson summation states are plotted for the electronic state $3^3\Sigma_g^+$ of Cs_2 diatomic molecules with various optimization parameters.

Keywords: Partition function; Schrodinger equation; Shifted Tietz potential

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1. Introduction

The distribution function needed in statistical mechanics to determine the thermodynamic properties of any physical system is the partition function [1, 2]. Different techniques have been developed by many researchers in finding partition function of some systems. These methods include exact method [3], semi-classical expansion method [4], Pade method [5], Poisson summation method [6] and Wigner–Kirkwood formulation [7]. Analytical expression for the partition function of Morse oscillators had been obtained by Strekalov [8]. Strekalov [9–11] had also derived a simple analytical formula for the partition function and other related works. The thermodynamic properties of modified Rosen–Morse had been solved using proper quantization rule formulation [12]. Onyewumi et al. [13] reported on the thermodynamic properties of the shifted Deng–Fan potential. Also, Lutfuoglu studied the thermodynamics properties of a confined nucleon for different physical systems [14]. Ikdair and Falaye reported on the thermodynamic properties with Poschl–Teller potential [15]. It is well known that knowing the maximum numbers of vibrational and rotational states are the necessary conditions needed to evaluate the partition function for the vibrational and rotational states of diatomic molecules [16]. The partition functions have applications in partially ionized and dissociated gas of stellar atmosphere [17]. Furthermore, Song et al. [18] studied the thermodynamic properties of sodium dimer with Rosen–Morse potential and Jia et al. [19] investigated the thermodynamic properties of lithium dimer with improved Manning–Rosen potential model. In a similar development, Jia et al. [20], on the other hand, obtain the partition function for improved Tietz oscillators.

In this present paper, we are motivated by the current trend in the study of the thermodynamic properties of some diatomic molecules and attempt to obtain the rotational–

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*Corresponding author, E-mail: ndemikotphysics@gmail.com vibrational energy spectrum for shifted Tietz potential model via factorization method [21] and subsequently obtain an expression for the partition function in terms of exact and Poisson summation methods. Other thermodynamic properties for the diatomic molecules will then be calculated using the expression for the partition function.

2. Shifted Tietz–Wei potential and bound state solutions

The shifted Tietz–Wei potential model is given as [22]:

$$V(r) = D_e\left[\frac{Ae^{-b_h(r-r_e)} - Be^{-2b_h(r-r_e)}}{\left(1 - C_h e^{-b_h(r-r_e)}\right)^2}\right], \tag{1}$$

where D_e is the potential well depth, $A = 2(C_h - 1)$, $B = \left(C_h^2 - 1\right)$, C_h is the optimization parameter, r_e is the molecular bond length, r is the internuclear distance, $b_h = \gamma(1 - C_h)$, and γ is the Morse constant. This shifted Tietz–Wei potential is the modification of the conventional Tietz–Wei potential.

The radial part of the Schrodinger equation with a central force potential $V(r)$ reads [23],

$$\frac{\mathrm{d}^2\psi_{vJ}}{\mathrm{d}r^2} + \frac{2\mu}{\hbar^2}\left(E_{vJ} - V(r) - \frac{J(J+1)\hbar^2}{2\mu r^2}\right)\psi_{vJ}(r) = 0 \tag{2}$$

where μ is the reduced mass of a diatomic molecule, E_{vJ} is the rotational–vibrational energy of the diatomic molecules, $\hbar$ denotes the reduced Planck constant, and v and J represent the vibrational and rotational quantum numbers, respectively.

Substituting Eq. (1) into Eq. (2) yields,

$$\begin{aligned}&\frac{\mathrm{d}^2\psi_{vJ}}{\mathrm{d}r^2} + \frac{2\mu}{\hbar^2}\left(E_{vJ} - D_e\left(\frac{Ae^{-b_h(r-r_e)} - Be^{-2b_h(r-r_e)}}{\left(1 - C_h e^{-b_h(r-r_e)}\right)^2}\right)\right.\\ &\quad\left.-\frac{J(J+1)\hbar^2}{2\mu r^2}\right)\psi_{vJ}(r) = 0\end{aligned} \tag{3}$$

In order to solve Eq. (3) analytically for $\ell \neq 0$, we apply Pekeris approximation to get rid of the centrifugal barrier as [24]:

$$\frac{\ell(\ell+1)}{r^2} \approx \frac{\ell(\ell+1)}{r_e^2}\left(D_0 + D_1\frac{e^{-\alpha x}}{1 - C_h e^{-\alpha x}} + D_2\frac{e^{-2\alpha x}}{\left(1 - C_h e^{-\alpha x}\right)^2}\right), \tag{4}$$

where $\alpha = b_h r_e$, $x = \frac{r-r_e}{r_e}$, and the parameters D_0, D_1 and D_2 in the approximation are given as

$$D_0 = 1 + \frac{(1 - C_h)}{b_h r_e}\left[\frac{3}{b_h r_e}(1 - C_h) - (3 + C_h)\right], \tag{5}$$

$$D_1 = \frac{2}{b_h r_e}(1 - C_h)^2\left[(2 + C_h) - \frac{3}{b_h r_e}(1 - C_h)\right], \tag{6}$$

$$D_2 = \frac{(1 - C_h)^3}{b_h r_e}\left[\frac{3}{b_h r_e}(1 - C_h) - (1 + C_h)\right]. \tag{7}$$

Inserting Eq. (4) into Eq. (3) and introducing a new variable $y = \left(1 - C_h e^{-\alpha r}\right)^{-1}$, we get

$$\begin{aligned}&y(1-y)\frac{\mathrm{d}^2\psi_{vJ}}{\mathrm{d}y^2} + (1 - 2y)\frac{\mathrm{d}\psi_{vJ}}{\mathrm{d}y}\\ &+\left(P - \frac{\varepsilon_n}{y(1-y)} + \frac{Q}{y}\right)\psi_{vJ}(y)\\ &= 0\end{aligned} \tag{8}$$

where

$$\varepsilon_n = -\left(\frac{2\mu E_{vJ}}{\hbar^2 b_h^2} - \frac{J(J+1)D_0}{r_e^2 b_h^2}\right), \tag{9a}$$

$$P = \frac{2\mu D_e}{\hbar^2 b_h^2 C_h^2}\left(A - \frac{B}{C_h}\right) + \frac{J(J+1)}{b_h^2 r_e^2 C_h}\left(D_1 + \frac{D_2}{C_h}\right), \tag{9b}$$

$$Q_1 = \frac{2\mu D_e B}{\hbar^2 b_h^2 C_h^2} - \frac{J(J+1)D_2}{b_h^2 r_e^2 C_h} \tag{9c}$$

By taking the wave function of the form, $\psi_{vJ}(y) = y^{\lambda}(1-y)^{\delta}f_{vJ}(y)$ reduced Eq. (8) into the following form,

$$\begin{aligned}&y(1-y)f''(y) + [1 + 2\lambda - (2 + 2\delta + 2\lambda)y]f'(y)\\ &-\left(\lambda + \delta + \frac{1}{2} - \sqrt{\frac{1}{4} - P}\right)\left(\lambda + \delta + \frac{1}{2} + \sqrt{\frac{1}{4} - P}\right)f(y)\\ &+\left[\frac{\lambda^2 + Q_1 - \varepsilon_n}{y(1-y)} + \frac{\delta^2 - \lambda^2 - Q_1}{(1-y)}\right]f(y) = 0\end{aligned} \tag{10}$$

Equation (10) can be reduced to a Gauss hypergeometric equation if and only if the following functions vanished,

$$\delta^2 - \lambda^2 - Q_1 = 0 \tag{11}$$

$$\lambda^2 + Q_1 - \varepsilon_n = 0 \tag{12}$$

Therefore, Eq. (10) becomes,

$$\begin{aligned}&y(1-y)f'' + (1 + 2\lambda - (2\lambda + 2\delta + 2)y)f'\\ &-\left(\lambda + \delta + \frac{1}{2} - \sqrt{\frac{1}{4} - P}\right)\left(\lambda + \delta + \frac{1}{2} + \sqrt{\frac{1}{4} - P}\right)f(y)\\ &= 0\end{aligned} \tag{13}$$

The solution of Eq. (13) can now be expressed as,

$$f(y) = {}_2F_1\left(\lambda+\delta+\frac{1}{2}-\sqrt{\frac{1}{4}-P}, \lambda+\delta+\frac{1}{2}+\sqrt{\frac{1}{4}-P}, 1+2\lambda; y\right) \tag{14}$$

where the hypergeometric function in Eq. (14) turns to a polynomial of degree n as

$$\lambda+\delta+\frac{1}{2}-\sqrt{\frac{1}{4}-P} = -n \tag{15}$$

$$\lambda+\delta+\frac{1}{2}+\sqrt{\frac{1}{4}-P} = -n \tag{16}$$

with $n = 0, 1, 2\ldots$

The implications of these quantization conditions are that the wave function in Eq. (14) may be made to vanish asymptotically under certain conditions. Now using the quantization condition, $\lambda+\delta+\frac{1}{2}-\sqrt{\frac{1}{4}-P} = -n$, and imposing Eqs. (11) and (12), we get

$$\lambda+\delta = -\left(n+\frac{1}{2}-\sqrt{\frac{1}{4}-P}\right) \tag{17}$$

$$\lambda-\delta = \frac{Q_1}{\left(n+\frac{1}{2}-\sqrt{\frac{1}{4}-P}\right)} \tag{18}$$

Solving Eqs. (17) and (18) for λ and δ, we obtain

$$\lambda = \frac{1}{2}\left(\frac{Q_1}{\left(n+\frac{1}{2}-\sqrt{\frac{1}{4}-P}\right)}-\left(n+\frac{1}{2}-\sqrt{\frac{1}{4}-P}\right)\right), \tag{19}$$

$$\delta = -\frac{1}{2}\left(\frac{Q_1}{\left(n+\frac{1}{2}-\sqrt{\frac{1}{4}-P}\right)}+\left(n+\frac{1}{2}-\sqrt{\frac{1}{4}-P}\right)\right) \tag{20}$$

Thus, by virtue of Eqs. (9) and (12) and with the help of Eq. (20), we obtain the energy spectrum equation for the shifted Tietz potential as,

$$E_{vJ} = Q_2-\frac{\hbar^2\alpha^2}{8\mu}\left(\frac{Q_1}{(n+\sigma)}+(n+\sigma)\right)^2 \tag{21}$$

where

$$\sigma = \left(\frac{1}{2}-\sqrt{\frac{1}{4}-\left(\frac{2\mu D_e}{\hbar^2 b_h^2 C_h^2}\left(A-\frac{B}{C_h}\right)+\frac{J(J+1)}{b_h^2 r_e^2 C_h}\left(D_1+\frac{D_2}{C_h}\right)\right)}\right)$$
$$Q_2 = \frac{J(J+1)\hbar^2 D_0}{2\mu r_e^2} \tag{22}$$

3. Partition function and thermodynamic properties

3.1. Exact partition function

The exact vibrational partition function for the shifted Tietz model is given as [25, 26],

$$Z_{\text{vib}}(\beta) = \sum_{n=0}^{\eta} e^{-\beta E_{nl}}, \ \beta = \frac{1}{kT} \tag{23}$$

where $\eta = -\sigma+\sqrt{Q_1}\pm\sqrt{Q_1-Q_2}$, k is the Boltzmann constant, and T is the absolute temperature. Substituting Eq. (21) into Eq. (23), we obtain the partition function for the potential model as,

$$Z_{\text{vib}}(\beta) = \sum_{n=0}^{\eta} e^{A\beta+\frac{\beta B}{(n+\sigma)^2}+\beta C(n+\sigma)^2} \tag{24}$$

where

$$A = \frac{2\hbar^2\alpha^2}{m}\left(\frac{Q_2}{2}-Q_1\right), \ B = \frac{\hbar^2\alpha^2 Q_2^2}{2m}, \ C = \frac{\hbar^2\alpha^2}{2m} \tag{25}$$

In the classical limit, we can replace the sum by an integral as,

$$Z_{\text{vib}}(\beta) = \int_0^{\eta} e^{A\beta+\frac{\beta B}{\rho^2}+\beta C\rho^2}\,\mathrm{d}\rho, \ \rho = n+\sigma$$
$$= \frac{1}{2}e^{\beta C\rho^2+\beta A}\sqrt{\beta B}\left[\frac{2\eta e^{\frac{B}{\eta^2}}}{\sqrt{\beta B}}-\frac{2\sqrt{\beta B}\sqrt{\pi}\,\mathrm{erf}i\left(\frac{\sqrt{\beta B}}{\eta}\right)}{\sqrt{\beta B}}-2\sqrt{\pi}\right] \tag{26}$$

where $\mathrm{erf}i(x)$ is the imaginary error function defined as [27, 28],

$$\mathrm{erf}i(x) = -i\,\mathrm{erf}(ix) = \frac{2}{\sqrt{\pi}}\int_0^x e^{t^2}\,\mathrm{d}t \tag{27}$$

It is worth noting that $\mathrm{erf}(x)$ denotes the error function which is a special function of sigmoid shape [27]. In Maple software, the imaginary error function is given as $\mathrm{erf}i(x)$ and can be used in many numerical calculations.

3.2. Poisson summation partition function

The total contribution of the bound state to the rotational–vibrational partition function of a diatomic molecule at temperature T can be written as,

$$Z(\beta) = \sum_{v=0}^{v_{\max}} e^{-\beta E_{n,J}} \tag{28}$$

where $\beta = (k_B T)^{-1}$ with k_B being the Boltzmann constant and $E_{v,J}$ is the rotational–vibrational energy of the vth bound state. Substituting Eq. (21) into Eq. (27) gives,

$$Z(\beta) = \sum_{v=0}^{v_{\max}} e^{-\beta\left[Q_2 - \frac{\hbar^2\alpha^2}{2\mu}\left(\frac{Q_1}{2(v+\sigma)} + \frac{v+\sigma}{2}\right)^2\right]} \tag{29}$$

where

$$v_{\max} = \sqrt{Q_1} - \frac{1}{2}\left(1 - \sqrt{1-4P}\right) \tag{30}$$

In order to evaluate the partition function of Eq. (29), we write the Poisson summation formula as [2, 8–11, 18–20],

$$\sum_{v=0}^{v_{\max}} f(n) = \frac{1}{2}[f(0) - f(v_{\max}+1)] + \sum_{m=-\infty}^{\infty} \int_0^{v_{\max}+1} f(x) e^{-i2\pi m x} \mathrm{d}x \tag{31}$$

However, for the lowest order approximation the Poisson summation formula becomes [8–11, 18–20],

$$\sum_{v=0}^{v_{\max}} f(n) = \frac{1}{2}[f(0) - f(v_{\max}+1)] + \int_0^{v_{\max}+1} f(x) \mathrm{d}x \tag{32}$$

Applying Eq. (32) for the partition function of Eq. (29), we get

$$Z(\beta) = \frac{1}{2}\left[e^{-\beta\left(Q_2 - p_1 p_2^2\right)} - e^{-\beta\left(Q_2 - p_1 p_3^2\right)} + \int_0^{v_{\max}} \left(e^{-a\beta - \frac{b\beta}{\rho^2} - c\beta\rho^2}\right) \mathrm{d}\rho\right] \tag{33}$$

where

$$p_1 = \frac{\hbar^2\alpha^2}{2\mu},\ p_2 = \left(\frac{Q_1}{2v_{\max}} + \frac{v_{\max}}{2}\right),\ p_3 = \left(\frac{Q_1}{2(v_{\max}+1+\sigma)} + \frac{(v_{\max}+1+\sigma)}{2}\right),$$
$$\rho = x + \sigma,\ a = \frac{\hbar^2\alpha^2 Q_1^2}{4\mu} - Q_2,\ b = \frac{\hbar^2\alpha^2 Q_1^2}{8\mu},\ c = \frac{\hbar^2\alpha^2}{4\mu} \tag{34}$$

Evaluating the integral in Eq. (33), we obtain the Poisson summation rotational–vibrational partition function for the diatomic molecules with shifted Tietz model as,

$$Z(\beta) = \frac{1}{2}\left[e^{-\beta\left(Q_2 - p_1 p_2^2\right)} - e^{-\beta\left(Q_2 - p_1 p_3^2\right)} + e^{-c\beta\rho^2 - a\beta}\sqrt{b\beta}\left(\frac{2v_{\max} e^{-\frac{b\beta}{v_{\max}^2}}}{\sqrt{b\beta}} + \frac{2\sqrt{b\pi\beta}\,\mathrm{erf}\left(\frac{\sqrt{b\beta}}{v_{\max}}\right)}{\sqrt{b\beta}} - 2\sqrt{\pi}\right)\right] \tag{35}$$

4. Results and discussion

In this paper, we consider the electronic state of the $Cs_2\left(3^3\Sigma_g^+\right)$ molecules using the exact partition function of Eq. (26) and that of the Poisson summation partition function of Eq. (35). The experimental values of the $3^3\Sigma_g^+$ states of Cs_2 dimer are taken from Ref. [28]: $D_e = 2722.28\ \mathrm{cm}^{-1}$, $r_e = 5.3474208$ Å and $\omega_e = 28.8918\ \mathrm{cm}^{-1}$. Taking these experimental data as inputs, we compute the exact and Poisson summation partition functions for the Cs_2 dimer as given in Figs. 1, 2, 3, 4, 5 and 6 for different values of the optimization parameter C_h at maximum bound state values of $\eta = v_{\max} = 25$ in each case. For each case in Figs. 1, 2, 3, 4, 5 and 6, it is found that the Poisson and exact partition functions Z increase monotonically as β is increased except in Fig. 3 where the exact and Poisson summation partition functions decrease monotonically with increasing β.

Also using these same experimental data as our input, we plotted the vibrational mean internal energy U,

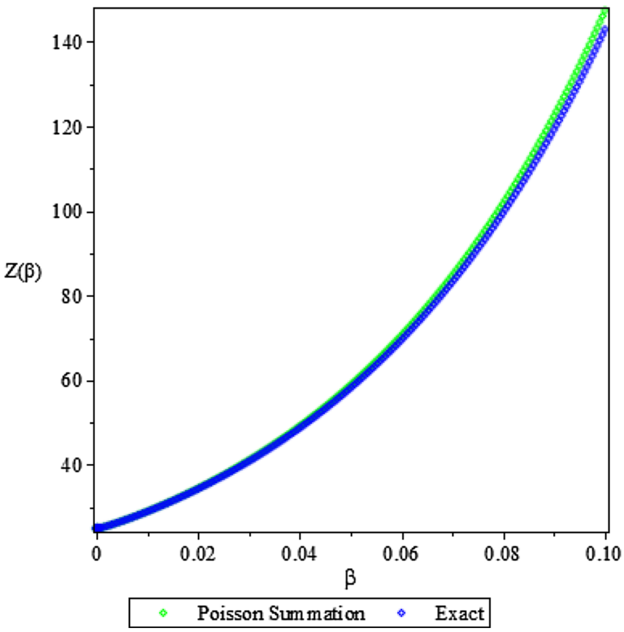

Fig. 1 Plot of the Poisson summation and exact partition functions as a function of β at $\eta = v_{\max} = 25$ given in Eqs. (26) and (33) for the electronic state of $Cs_2\left(3^3\Sigma_g^+\right)$ molecules with shifted Tietz potential where the optimization parameter value of $C_h = \frac{1}{5}$ is used

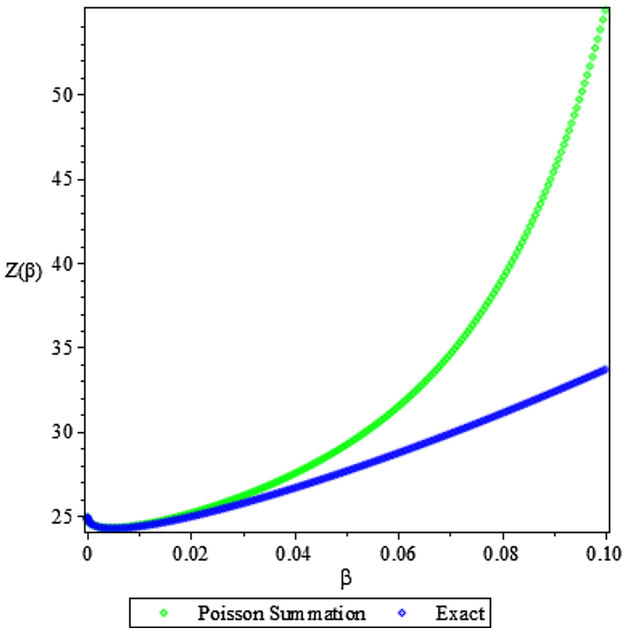

Fig. 2 Plot of the Poisson summation and exact partition functions as a function of β at $\eta = v_{\max} = 25$ given in Eqs. (26) and (33) for the electronic state of $Cs_2\left(3^3\Sigma_g^+\right)$ molecules with shifted Tietz potential where the optimization parameter value of $C_h = \frac{1}{8}$ is used

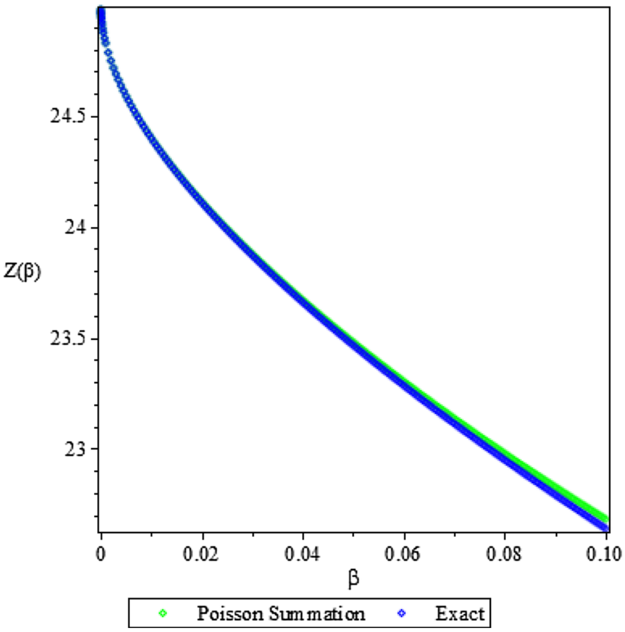

Fig. 3 Plot of the Poisson summation and exact partition functions as a function of β at $\eta = v_{\max} = 25$ given in Eqs. (26) and (33) for the electronic state of the $Cs_2\left(3^3\Sigma_g^+\right)$ molecules with shifted Tietz potential where the optimization parameter value of $C_h = \frac{1}{4}$ is used

vibrational mean free energy F, vibrational specific heat capacity C and vibrational entropy for the $3^3\Sigma_g^+$ states of Cs_2 for upper bound vibration quantum number $v_{\max} = 25$ as a function of β with different optimization parameters C_h in Figs. 7, 8, 9, 10, 11, 12, 13, 14 and 15. In Figs. 7, 8

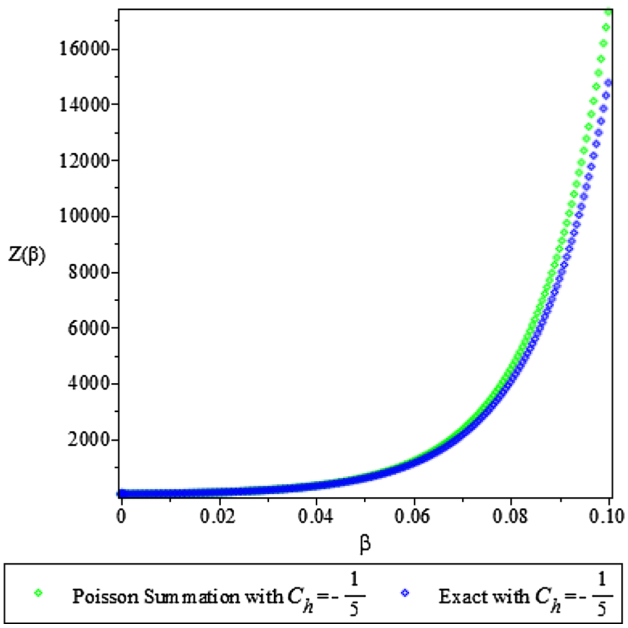

Fig. 4 Plot of the Poisson summation and exact partition functions as a function of β at $\eta = v_{\max} = 25$ given in Eqs. (26) and (33) for the electronic state of the $Cs_2\left(3^3\Sigma_g^+\right)$ molecules with shifted Tietz potential where the optimization parameter value of $C_h = -\frac{1}{5}$ is used

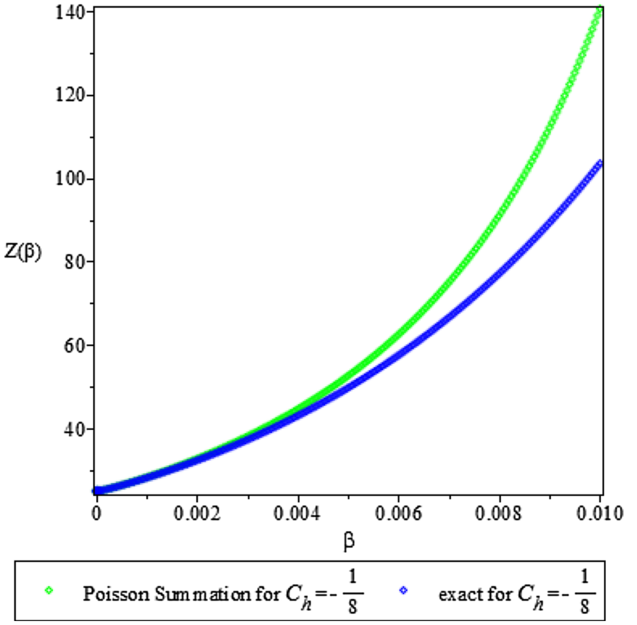

Fig. 5 Plot of the Poisson summation and exact partition functions as a function of β at $\eta = v_{\max} = 25$ given in Eqs. (26) and (33) for the electronic state of the $Cs_2\left(3^3\Sigma_g^+\right)$ molecules with shifted Tietz potential where the optimization parameter value of $C_h = -\frac{1}{8}$ is used

and 9, the vibrational mean energy U monotonically decreases with increasing β parameter at a maximum quantum number of $\eta = v_{\max} = 25$. Interestingly, in Fig. 8, the exact mean free energy decreases with an increase in β, whereas the Poisson mean free energy initially decreases

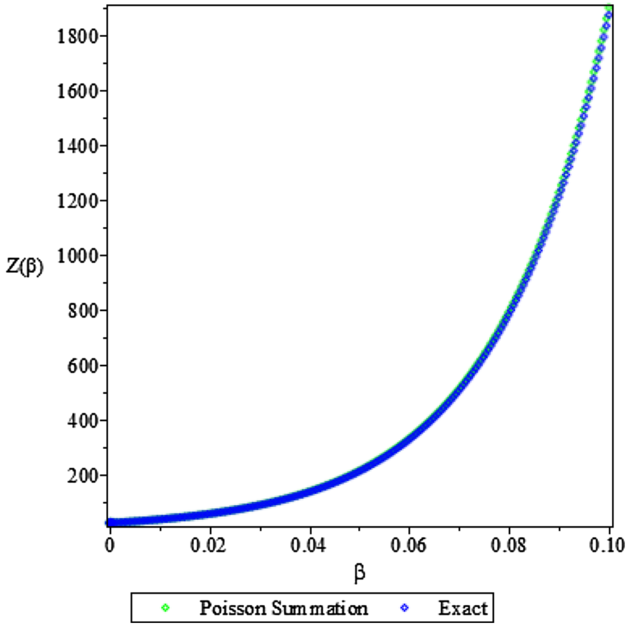

Fig. 6 Plot of the Poisson summation and exact partition functions as a function of β at $\eta = v_{\max} = 25$ given in Eqs. (26) and (33) for the electronic state of the $\mathrm{Cs}_2\left(3^3\Sigma_g^+\right)$ molecules with shifted Tietz potential where the optimization parameter value of $C_h = -\frac{1}{4}$ is used

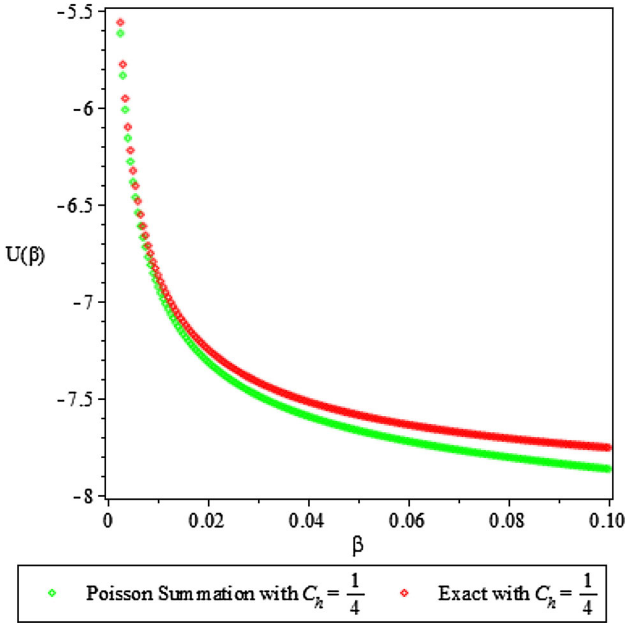

Fig. 7 Vibrational mean energy function as a function of β at $\eta = v_{\max} = 25$ with the optimization parameter value of $C_h = \frac{1}{4}$

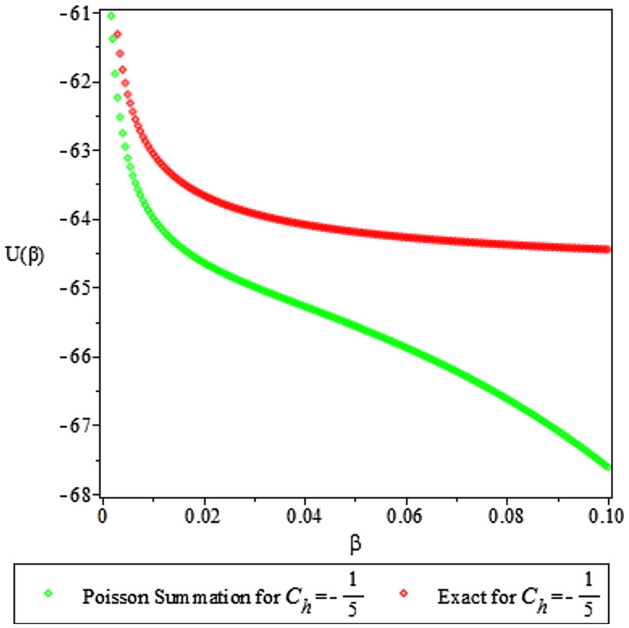

Fig. 8 Vibrational mean energy function as a function of β at $\eta = v_{\max} = 25$ with the optimization parameter value of $C_h = -\frac{1}{5}$

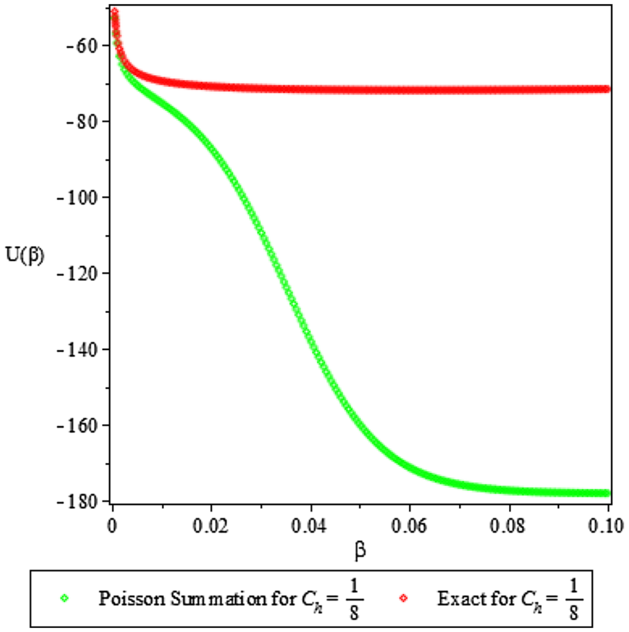

Fig. 9 Vibrational mean energy as a function of β at $\eta = v_{\max} = 25$ with the optimization parameter value of $C_h = \frac{1}{8}$

with an increase in β and thereafter increases with increasing β parameter at $C_h = -\frac{1}{5}$. Also, at the optimization parameter values of $C_h = \pm\frac{1}{8}$ the Poisson mean energy deceases more rapidly with increasing β parameter than the exact mean energy as shown in Fig. 9. As shown in Figs. 10 and 11, the free energy F decreases monotonically with increasing β parameter for each case of exact and Poisson summation. In Fig. 10, the free energy coincides for exact and Poisson summation for different values of the optimization parameter. But when the optimization parameters are fixed at $C_h = \frac{1}{8}$, then there is a clear distinction between the exact and Poisson summation free energies as shown in Fig. 11. The plots of the specific heat are shown in Figs. 12 and 13. The specific heat C in

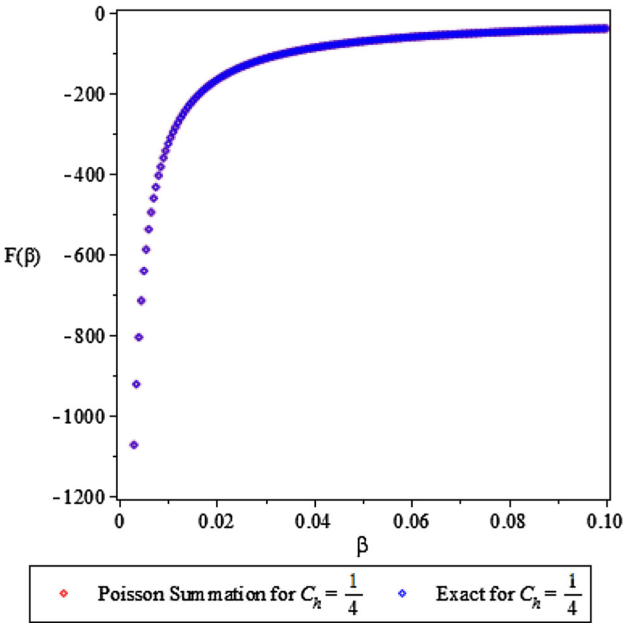

Fig. 10 Vibrational free energy as a function of β at $\eta = v_{\max} = 25$ with the optimization parameter value of $C_h = \frac{1}{4}$

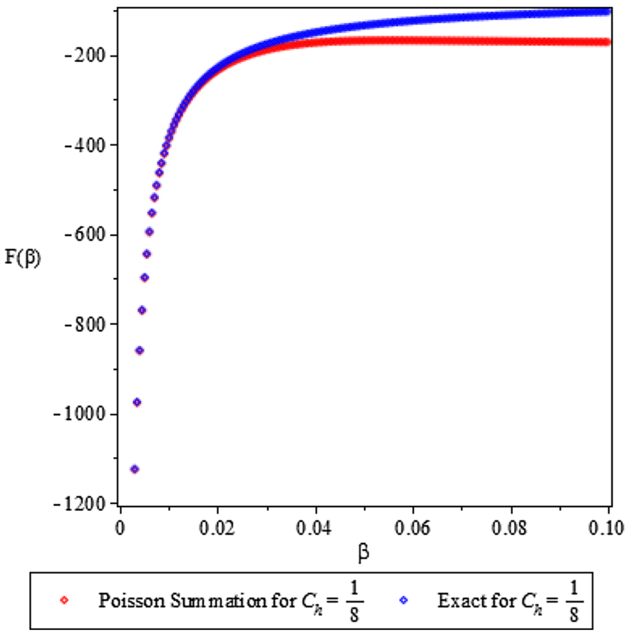

Fig. 11 Vibrational free energy as a function of β at $\eta = v_{\max} = 25$ with the optimization parameter value of $C_h = \frac{1}{8}$

each case decreases with an increase in β except in Fig. 12. In Fig. 12, the exact specific heat decreases with increasing β parameter, whereas the Poisson specific heat first decreases with an increase in β and thereafter increases with increasing β parameter. The plots of the exact and Poisson entropies are shown in Figs. 14 and 15. As shown in Figs. 14 and 15, the entropy S monotonically decreases with increasing β parameter.

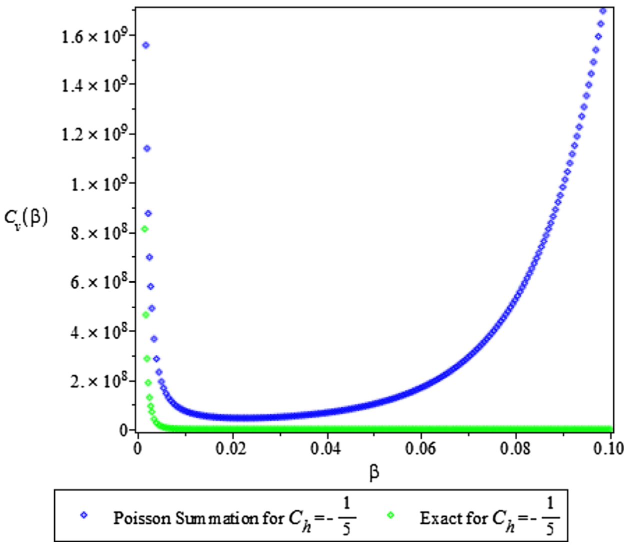

Fig. 12 Vibrational specific heat as a function of β at $\eta = v_{\max} = 25$ with the optimization parameter value of $C_h = -\frac{1}{5}$

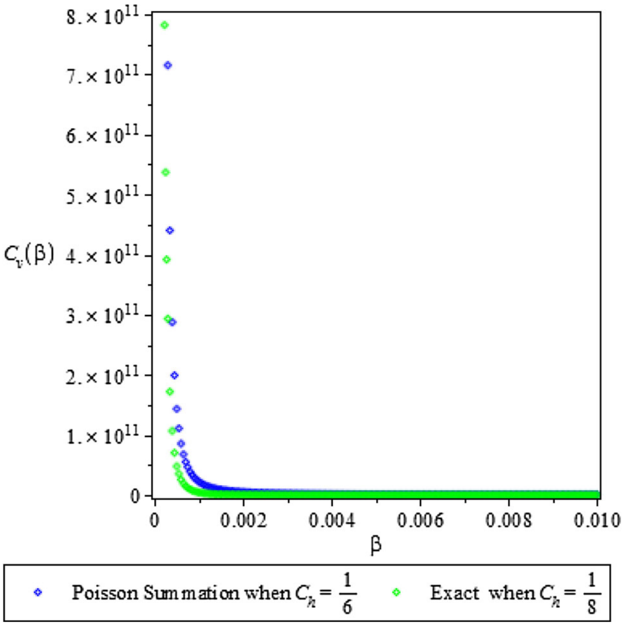

Fig. 13 Vibrational specific heat as a function of β at $\eta = v_{\max} = 25$ with the optimization parameter value of $C_h = \frac{1}{8}$

(1) The vibrational mean energy U

$$U(\beta) = -\frac{\partial \ell n Z(\beta)}{\partial \beta} \tag{36}$$

(2) Vibrational mean free energy F

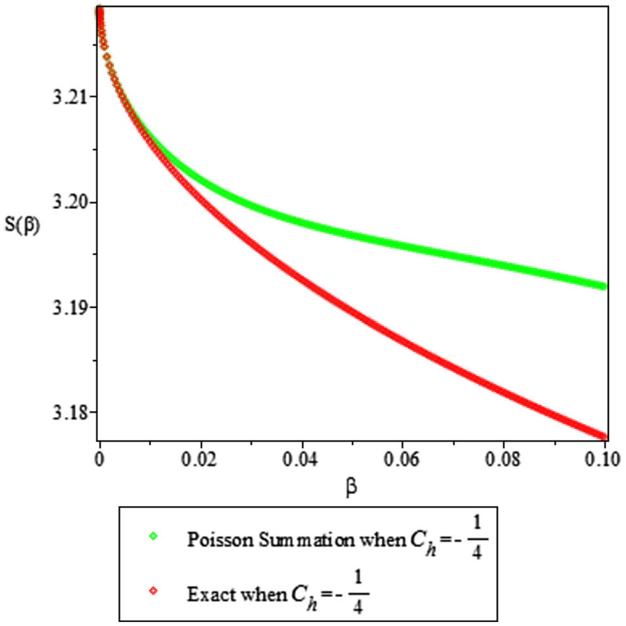

Fig. 14 Vibrational entropy as a function of β at $\eta = v_{\max} = 25$ with the optimization parameter value of $C_h = -\frac{1}{4}$

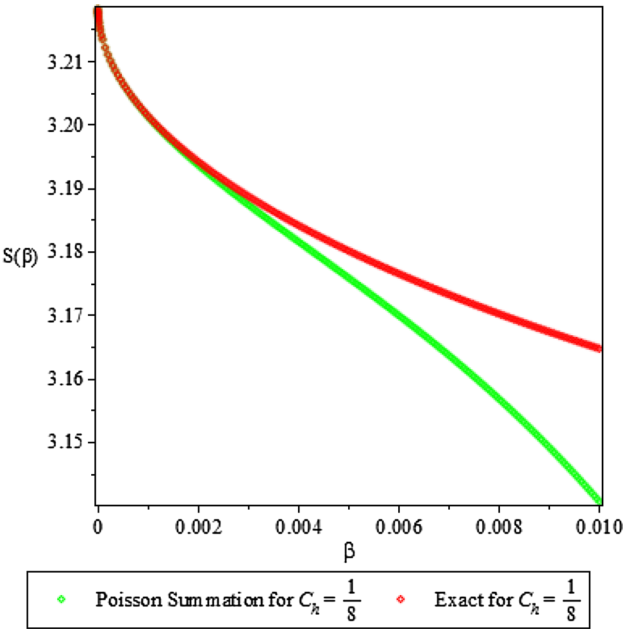

Fig. 15 Vibrational entropy as a function of β at $\eta = v_{\max} = 25$ with the optimization parameter value of $C_h = \frac{1}{8}$

$$F = -\frac{1}{\beta}\ell nZ(\beta) \tag{37}$$

(3) Vibrational specific heat capacity C

$$C = \frac{\partial U}{\partial T} = -k\beta^2 \frac{\partial U(\beta)}{\partial \beta} \tag{38}$$

(4) Vibrational entropy S

$$S = k\ell nZ(\beta) - k\beta \frac{\partial}{\partial \beta}\ell nZ(\beta) \tag{39}$$

5. Conclusions

In this paper, we solved the non-relativistic Schrödinger equation with shifted Tietz potential within the framework of factorization method and obtain the energy spectra in a closed form. In detail, we evaluated the exact and Poisson summation vibrational partition functions Z which we used to study the thermodynamics properties of vibrational mean energy U, vibrational entropy S, vibrational mean free energy F and vibrational specific heat capacity C, for the electronic state of $\left(3^3\Sigma_g^+\right)$ of Cs_2 dimer. The plots of the exact and Poisson summation partition functions and other behaviours of the thermodynamic functions as a function of temperature β with a fixed upper bound vibration quantum number $v_{\max} = \eta = 25$ for the electronic state $3^3\Sigma_g^+$ of Cs_2 dimer are shown in Figs. 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14 and 15. This study can find many other applications in statistical and molecular physics [29–38].

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