Research Square

Preprints are preliminary reports that have not undergone peer review. They should not be considered conclusive, used to inform clinical practice, or referenced by the media as validated information.

Solutions of Schrodinger Equation And Thermodynamic Properties of Potassium Dimer Based On Formular Method

C. P. Onyenegecha (chibueze.onyenegecha@futo.edu.ng)
Federal University of Technology Owerri

E. N. Omoko
Federal University of Technology Owerri

I. J. Njoku
Federal University of Technology Owerri

E. E. Oguzie
Federal University of Technology Owerri

C. J. Okereke
Federal University of Technology Owerri

Research Article

Keywords: thermodynamic, potassium, molecular, probability

Posted Date: August 19th, 2021

DOI: https://doi.org/10.21203/rs.3.rs-763444/v1

License: This work is licensed under a Creative Commons Attribution 4.0 International License.
Read Full License

Solutions of Schrodinger equation and thermodynamic properties of Potassium Dimer based on Formular method

C. P. Onyenegecha* E. N. Omoko, I. J. Njoku, E. E. Oguzie, C.J. Okereke

School of Physical sciences, Federal University of Technology Owerri, Nigeria.

*email: chibueze.onyenegecha@futo.edu.ng.

The study presents the thermodynamic properties of the $X^1\sum_g^+$ state of potassium (K_2) dimer with molecular Deng-Fan potential. The bound state energy solution of the radial Schrodinger equation is obtained via the formula method. The partition function and other thermodynamic properties are evaluated. The numerical values of energy are found to be in agreement with results obtained from other methods in literature. The results further show that the partition function increases as temperature decreases, which implies a decrease in the probability of finding a particle in a state with quantum number, *n*.

The vibrational energy and partition functions of a certain potential model are basic requirements in statistical mechanics and thermodynamics. The partition function [1] can be evaluated by direct approach or by approximate methods, provided that the energy levels are known. In the last few years, the study of thermodynamic properties has drawn a lot of attention from researchers [2-6]. In a recent study, Njoku et al. [7] investigated the thermodynamic properties with Hua potential. Using Poisson summation approach, the authors in Ref.[8], studied the thermodynamic properties of Deng-Fan-Eckart potential for some diatomic molecules. Bakhiti et al. [9] evaluated the thermodynamic properties of O_2 and H_2 molecules with the multiparameter exponential-type potential, and obtained results identical with experimental reports. The thermodynamic properties of a hyperbolic Poschl-Teller potential has been studied [10]. Chabi and Boumali [11] have evaluated the thermal properties of the Morse potential using the Euler MacLauarin method. The thermodynamic properties for modified Rosen- Morse potential has been reported [12]. Jia et al. [13] discussed thermodynamic properties with the improved Manning-Rosen potential for a Lithium dimer. In a related study, the authors in Ref. [14] investigated the thermodynamic properties for a sodium dimer with improved Rosen-Morse potential. However, thermodynamic properties for a potassium dimer with Deng-Fan potential are not yet reported, to the best of our knowledge.

This paper focuses on Deng-Fan potential [15], proposed by Deng and Fan as an extension of Morse model for studying the properties of diatomic molecules. Many interesting works on Deng-Fan potential are found in Refs. [16-24]. Motivated by previous works in literature, we obtain the energy spectra of the Deng-Fan potential using the formula method [25] and then apply our result to the study of thermodynamic properties for $X^1\sum_g^+$ state of the K_2 molecule. The Deng-Fan model studied in this work is [15]

$$V(r) = D_e\left(1-\frac{b}{e^{\alpha r}-1}\right)^2; b = e^{\alpha r_e}-1, \tag{1}$$

where D_e, α, r_e, b and r are the dissociation energy, range of potential, equilibrium internuclear distance, position of minimum r_e and internuclear distance, respectively.

Review of Formula Method

The formula method was proposed by Falaye et al. [25] to solve wave equations. For a second order differential equation

$$\frac{d^2\psi(s)}{ds^2}+\frac{c_1-c_2 s}{s(1-c_3 s)}\frac{d\psi(s)}{ds}+\frac{\xi_1 s^2+\xi_2 s+\xi_3}{s^2(1-c_2 s)^2}\psi(s)=0, \tag{2}$$

the condition for energy equation as proposed by Falaye et al. [25] is

$$\left[\frac{c_4^2-c_5^2-\left[\frac{1-2n}{2}-\frac{1}{2c_3^2}\left(c_2-\sqrt{(c_3-c_2)^2-4\xi_1}\right)\right]^2}{2\left[\frac{1-2n}{2}-\frac{1}{2c_3^2}\left(c_2-\sqrt{(c_3-c_2)^2-4\xi_1}\right)\right]}\right]^2-c_5^2=0, c_3\neq 0, \tag{3}$$

where

$$\left.\begin{aligned} c_4^2 &= \frac{(1-c_1)+\sqrt{(1-c_1)^2-4\xi_3}}{2} \\ c_5^2 &= \frac{1}{2}+\frac{c_1}{2}-\frac{c_2}{2c_3}+\sqrt{\left(\frac{1}{2}+\frac{c_1}{2}-\frac{c_2}{2c_3}\right)^2-\left(\frac{\xi_1}{c_3^2}+\frac{\xi_2}{c_3}+\xi_3\right)} \end{aligned}\right\}. \tag{4}$$

The wave function is given by

$$\psi(s)=N_n s^{c_4^2}(1-c_3 s)^{c_5^2}\,{}_2F_1\left(-n, n+2\left(c_4^2+c_5^2\right)+\frac{c_2}{c_3}-1; 2c_4^2+c_1; c_3 s\right), \tag{5}$$

where N_n is the normalization constant.

For $c_1=c_2=c_3=1$, the simplified energy equation is given by [26]

$$\sqrt{-\xi_3}\left(1+\sqrt{1-4\left(\xi_1+\xi_2+\xi_3\right)}+2n\right)=\xi_3-\xi_1-n(n+1)-n\sqrt{1-4\left(\xi_1+\xi_2+\xi_3\right)}-\left(\frac{1}{2}+\frac{1}{2}\sqrt{1-4\left(\xi_1+\xi_2+\xi_3\right)}\right)^2. \tag{6}$$

Solutions of Schrodinger equation

In spherical coordinates, the Schrodinger equation is given by

$$-\frac{\eta^2}{2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\Psi(r,\theta,\phi)=E_{nl}\Psi(r,\theta,\phi), \tag{7}$$

where E, η, μ and Ψ are respectively the energy, reduced Planck constant, reduced mass and wave function of the system. Choosing $\Psi(r,\theta,\phi) = \frac{R(r)}{r}\psi_{nl}(\theta,\phi)$ as the solution to (7), the radial part of the Schrodinger equation with the centrifugal term is obtained as

$$\frac{d^2R_{nl}(r)}{dr^2} + \left[\frac{2\mu}{\eta^2}\left(E_{nl} - V(r)\right) - \frac{l(l+1)}{r^2}\right]R_{nl}(r) = 0\,, \tag{8}$$

where n and l are the radial and orbital angular momentum quantum number, respectively.

Substituting Eq. (1) in Eq. (8) gives

$$\frac{d^2R_{nl}(r)}{dr^2} + \left[\frac{2\mu}{\eta^2}\left(E_{nl} - D_e\left(1 - \frac{b}{e^{\alpha r} - 1}\right)^2\right) - \frac{l(l+1)}{r^2}\right]R_{nl}(r) = 0\,. \tag{9}$$

Eq. (9) is solvable if we adopt the following approximation [27]

$$\frac{1}{r^2} \approx \alpha^2\left[d_0 + \frac{e^{-\alpha r}}{\left(1 - e^{-\alpha r}\right)^2}\right]; d_0 = \frac{1}{12.0015}, \alpha r \to 1 \tag{10}$$

If we put Eq. (10) in Eq. (9) and use transformation, $s = e^{-\alpha r}$, we have

$$\frac{d^2R_{nl}(s)}{ds^2} + \frac{(1-s)}{s(1-s)}\frac{dR_{nl}(s)}{ds} + \frac{As^2 + Bs + C}{s^2(1-s)^2}R_{nl} = 0 \quad , \tag{11}$$

where,

$$\left.\begin{aligned} A &= \frac{2\mu}{\alpha^2\eta^2}\left(E_{nl} - D_e - 2D_e b - D_e b^2\right) - d_0 l(l+1) \\ B &= \frac{2\mu}{\alpha^2\eta^2}\left(-2E_{nl} + 2D_e + 2D_e b\right) + 2d_0 l(l+1) - l(l+1) \\ C &= \frac{2\mu}{\alpha^2\eta^2}\left(E_{nl} - D_e\right) - d_0 l(l+1) \end{aligned}\right\}. \tag{12}$$

Since $c_1 = c_2 = c_3 = 1$, we use the simplified energy Eq.(6) to obtain non-relativistic energy of Deng-Fan model as

$$E_{nl} = D_e + \frac{\alpha^2\eta^2 d_0 l(l+1)}{2\mu}$$

$$-\frac{\alpha^2\eta^2}{2\mu}\left[\frac{\frac{-4\mu D_e b}{\alpha^2\eta^2}+\frac{1}{2}+n(n+1)+l(l+1)+\left(n+\frac{1}{2}\right)\sqrt{2(l+1)^2+\frac{8\mu D_e b^2}{\alpha^2\eta^2}}}{1+2n+\sqrt{2(l+1)^2+\frac{8\mu D_e b^2}{\alpha^2\eta^2}}}\right]^2. \qquad (13a)$$

The corresponding wave function is given as

$$R(s) = N_n s^{\sqrt{-C}}(1-s)^{\frac{1}{2}+\sqrt{2(l+1)^2+\frac{8\mu D_e b^2}{\alpha^2\eta^2}}}\,{}_2F_1\left(-n, n+2\left(\sqrt{-C}+\frac{1}{2}+\sqrt{2(l+1)^2+\frac{8\mu D_e b^2}{\alpha^2\eta^2}}\right); 2\sqrt{-C}+1; s\right). \qquad (13b)$$

Thermodynamic properties

The first step to investigate the thermodynamic properties of the Deng-Fan model is to set-up the vibrational partition function ($l = 0$) given by

$$Z(\beta,\lambda) = \sum_{n=0}^{\lambda} e^{-\beta E_n}, \beta = \frac{1}{k_B T} \qquad (14)$$

where k_B is the Boltzmann constant, E_n is the vibrational energy of the Deng-Fan potential. Simplifying Eq. (13a) gives

$$E_n = D_e - \frac{\alpha^2\eta^2}{2\mu}\left(\frac{(n+\chi)}{2}+\frac{\Omega}{2(n+\chi)}\right)^2, \qquad (15)$$

where,

$$\left.\begin{aligned}\chi &= \frac{1}{2}+\frac{1}{2}\sqrt{1+\frac{8\mu D_e b^2}{\alpha^2\eta^2}}\\ \Omega &= \frac{-2\mu D_e b(2+b)}{\alpha^2\eta^2}\end{aligned}\right\}. \qquad (16)$$

Substituting Eq. (15) into Eq. (14) gives

$$Z(\beta,\lambda) = \sum_{n=0}^{\lambda}\exp\left(-\beta\left(D_e - \frac{\alpha^2\eta^2}{2\mu}\left(\frac{(n+\chi)}{2}+\frac{\Omega}{2(n+\chi)}\right)^2\right)\right). \qquad (17)$$

In classical limit with $\rho = n+\chi$, the partition function is

$$Z(\beta,\lambda)\int_0^{\lambda} e^{P_1\beta + P_2\rho^2\beta + \frac{P_3\beta}{\rho^2}}\, d\rho\,, \tag{18}$$

where,

$$P_1 = \frac{\alpha^2\eta^2\Omega^2}{2\mu} - D_e, P_2 = \frac{\alpha^2\eta^2\Omega^2}{8\mu}, P_3 = \frac{\alpha^2\eta^2}{8\mu}. \tag{19}$$

Evaluation of Eq. (18) gives

$$Z(\beta,\lambda) = \frac{1}{2} e^{\left(\beta P_2\rho^2 + P_1\beta\right)}\sqrt{\beta P_3}\left(\frac{2\lambda e^{\frac{\beta P_3}{\lambda^2}}}{\sqrt{\beta P_3}} - \frac{2\sqrt{\beta P_3}\sqrt{\pi}\, erfi\left(\frac{\sqrt{\beta P_3}}{\lambda}\right)}{\sqrt{\beta P_3}} - 2\sqrt{\pi}\right). \tag{20}$$

The imaginary error function $erfi(x)$ is defined by

$$erfi(x) = \frac{erf(ix)}{i} = \frac{2}{\sqrt{\pi}}\int_0^x e^{t^2}\, dt. \tag{21}$$

Other thermodynamic properties are obtained as:

4.1 *Vibrational Internal Energy*

$$U(\beta,\lambda) = -\frac{\partial \ln Z(\beta,\lambda)}{\partial\beta} \tag{22}$$

$$= -\frac{\left(erfi\left(\frac{\sqrt{\beta P_3}}{\lambda}\right)+1\right)\sqrt{\beta P_3}\left(\frac{1}{2}+\beta\left(P_2\rho^2+P_1\right)\right)\sqrt{\pi} - e^{\frac{\beta P_3}{\lambda^2}}\lambda\left(P_2\rho^2+P_1\right)\beta}{\beta\left(\sqrt{\beta P_3}\left(erfi\left(\frac{\sqrt{\beta P_3}}{\lambda}\right)+1\right)\sqrt{\pi} - \lambda e^{\frac{\beta P_3}{\lambda^2}}\right)}.$$

4.2 *Vibrational Free Energy*

$$F(\beta,\lambda) = -\frac{1}{\beta}\ln Z(\beta,\lambda)$$

$$= -\frac{\ln\left(e^{\beta}\left(P_2\rho^2+P_1\right)\sqrt{\beta P_3}\left(\frac{\lambda e^{\frac{\beta P_3}{\lambda^2}}}{\sqrt{\beta P_3}} - \sqrt{\pi}\, erfi\left(\frac{\sqrt{\beta P_3}}{\lambda}\right) - \sqrt{\pi}\right)\right)}{\beta}. \tag{23}$$

4.3 *Vibrational Entropy*

$$S(\beta,\lambda)=k\ln Z(\beta,\lambda)-k\beta\frac{\partial\ln Z(\beta,\lambda)}{\partial\beta}$$

$$=\frac{k\ln\left(e^{\beta\left(P_2\rho^2+P_1\right)}\sqrt{\beta P_3}\left(\frac{\lambda e^{\frac{\beta P_3}{\lambda^2}}}{\beta P_3}-\sqrt{\pi}\,erfi\left(\frac{\sqrt{\beta P_3}}{\lambda}\right)-\sqrt{\pi}-\beta\lambda-\left(P_2\rho^2+\rho_1\right)e^{\frac{\beta P_3}{\lambda^2}}\right)\right)}{\left(\beta\left(\sqrt{\beta P_3}\left(erfi\left(\frac{\sqrt{\beta P_3}}{\lambda}\right)+1\right)\sqrt{\pi}-\lambda e^{\frac{\beta P_3}{\lambda^2}}\right)\right)}. \quad (24) \quad .$$

4.4 *Vibrational Specific Heat Capacity*

$$C(\beta,\lambda)=k\beta^2\frac{\partial^2\ln Z(\beta,\lambda)}{\partial\beta^2}$$

$$=\frac{\left(\left(\sqrt{\beta P_3}\left(\frac{1}{2}+\beta\left(P_2\rho^2+P_1\right)\right)\left(erfi\left(\frac{\sqrt{\beta P_3}}{\lambda}\right)+1\right)\sqrt{\pi}-\lambda e^{\frac{\beta P_3}{\lambda^2}}\left(P_2\rho^2+P_1\right)\beta\right)^2 k\right)}{\left(\beta\left(\sqrt{\beta P_3}\left(erfi\left(\frac{\sqrt{\beta P_3}}{\lambda}\right)+1\right)\sqrt{\pi}-\lambda e^{\frac{\beta P_3}{\lambda^2}}\left(P_2\rho^2+P_1\right)\beta\right)^2\right)} \quad . \quad (25)$$

4.5 Probability Function

$$P_r=\frac{e^{-\beta E_n}}{Z(\beta,\lambda)}. \quad (26)$$

Discussions

Using Eq. (13a), we compute numerical values as presented in tables 1 and 2. These values conforms with results obtained using other methods [18, 28, 29, 30]. The results obtained by formula method are very close to those reported using the N-U [28], SUSY [26], and WKB [18] methods and hence more accurate than those obtained by numerical methods [30]. The reason for this is that the authors in Ref. [30] used conventional approximation [31], which has less accuracy than the approximation used in the present work [18].

The experimental values for potassium dimer are chosen from Ref.[32]. These values are used as inputs to evaluate the partition functions and thermodynamic properties. The thermal properties are plotted in figs. 1-10. In figs. 11 and 12, the probability of finding the potassium molecule in a state with quantum number, *n*, is plotted against β and upper bound vibrational energy level, λ,

respectively. Fig 1. Shows the vibrational partition function, Z as a function of β. Z is observed to increase sharply as β increases, which implies that as temperature decreases, the partition function increases for different values of λ. The observation on fig. 2 shows Z increasing monotonically as λ increases for all β. Fig. 2 also confirms the observation in fig. 1. In fig. 3, the internal energy U is observed to decrease as β increases. In fig. 4, U shows a reverse trend against λ to that seen against β. In fig. 5, the vibrational free energy, F, increases as β increases. The variation of F against λ (fig.6), shows a reverse trend as F decreases with an increase in λ. The entropy, S, is observed to be directly proportional to β in fig. 7. In fig. 8, S, increases as λ increases for all β. In fig. 9, the vibrational specific heat capacity, C, is seen to decrease monotonically as β increases, implying that at lower temperatures, C has lower values for the potassium dimer. The opposite trend is observed in fig. 10 as C, increases with increasing λ up to λ=100, but beyond that point, a constant value is maintained for C for all β. As predicted by the trend of Z in fig. 1, the probability, P_r, decreases sharply as β increases (fig. 11) due to an increase in Z. In fig. 12, P_r, also decreases sharply as λ increases up to λ=100, but maintains a constant value approaching zero beyond that point. This implies that the system is less likely to be found in an energy state with $\lambda < 100$.

Conclusions

In the present paper, the thermodynamic properties of potassium dimer is studied with Deng-Fan model. The radial Schrodinger equation is solved approximately using the formula method and a suitable approximation for the centrifugal term. The vibrational partition function and other thermodynamic functions are deduced. The thermodynamic functions are plotted against β and λ. The results of this study can be applied to molecular and chemical physics.

Author Contributions

C.P.O, E. E. O and I.J.N designed and wrote the manuscript. C.J.O and E.N.O did the computations, prepared the tables and plots.

Competing interest

The authors declare no competing interests.

References

1 Strekalov, M. L, An accurate closed-form expression for the partition function of Morse oscillators. *Chem. Phys*. Lett **439**, 209-212 (2007).

2 Hassanabadi, H., Sargolzaeipor, S., Yazarloo, B.H. Thermodynamic properties of the three-dimensional Dirac oscillator with Aharonov–Bohm field and magnetic monopole potential. *Few-Body Syst*. **56**, 115-124 (2015).

3 Okorie, U.S., Ikot, A.N., Onyeaju, M.C., Chukwuocha, E.O. A study of thermodynamic properties of quadratic exponential-type potential in D-dimensions. Rev. Mex. Fis. **64**, 608-614 (2018).

4 Ebomwonyi, O., Onate, C.A., Ekong, S.A., Onyeaju, M.C. Thermodynamic Properties for the Carbon Monoxide Molecule under the Influence of the Coulomb-Hulthen-Pöschl-Teller Potential. J. Sci. Technol. Res. **1**, 122-136 (2019).

5 Okorie, U.S., Ikot, A.N., Onyeaju, M.C., Chukwuocha, E.O. Bound state solutions of Schrödinger equation with modified Mobius square potential (MMSP) and its thermodynamic properties. J. Mol. Mod. **24**, 289-302 (2018).

6 Louis, H., Ita, B.I., Nzeata, N.I. Approximate solution of the Schrödinger equation with Manning-Rosen plus Hellmann potential and its thermodynamic properties using the proper quantization rule. Eur. Phys. J. Plus **134**, 315 (2019)

7 Njoku, I.J., Onyenegecha, C.P., Okereke, C .J., Ukewuihe, U.M., Nwaneho, F.U. Approximate solutions of Schrodinger equation and thermodynamic properties with Hua potential. Res. Phys. **24**, 104208 (2021)

8. Edet, C.O., Okorie, U. S., Osobonye, G., Ikot, A.N., Rampho, G.J. Thermal properties of Deng–Fan– Eckart potential model using Poisson summation approach. R. Sever. J. Math. Chem. **58**, 989-1013 (2020).

9. Bakhti, H., Diaf, A., Hachama, M. Computing thermodynamic properties of the O_2 and H_2 molecules with multi-parameter exponential-type potential. Com. Theor. Chem. **1185**, 112879 (2020).

10. Okorie, U.S., Ikot, A.N., Chukwuocha, E.O., Onyeaju, M.C., Amadi, P.O., Sithole, M.J., Rampho, G.J. Energies spectra and thermodynamic properties of hyperbolic Poschl-Teller potential (HPTP) model. Int. J. Thermophys. **41**, 91-106 (2020).

11. Chabi, K., Boumali, A. Thermal properties of three-dimensional Morse potential for some diatomic molecules via Euler-Maclaurin approximation. Rev. Mex. Fis. **66**, 110-120 (2020).

12. Dong, S.H., Irrison, M.C. Energy spectrum for a modified Rosen-Morse potential solved by proper quantization rule and its thermodynamic properties. J. Math. Chem. **50,** 881-892 (2012).

13. Jia, C.S., Zhang, L.H., Wang, C. W. Thermodynamic properties for the lithium dimer. Chem. Phys. Lett. **667**, 211-215 (2017).

14. Song, X.Q., Wang, C. W., Jia, C. S. Thermodynamic properties for the sodium dimer. Chem. Phys. Lett. **673**, 50-55 (2017).

15. Deng, Z.H., Fan, Y.P. A potential function of diatomic molecules. Shandong Univ. J. **7**, 162-165 (1957).

16. Ikhdair, S.M. An approximate κ state solutions of the Dirac equation for the generalized Morse potential under spin and pseudospin symmetry. J. Math. Phys. **52**, 052303 (2011a).

17. Zhang, L.H., Li, X.P., Jia, C.S. Approximate analytical solutions of the Dirac equation with the generalized Morse potential model in the presence of the spin symmetry and pseudo-spin

symmetry. Phys. Scr. **80**, 035003 (2009).
18. Zhang, L.H., Li, X.P., Jia, C.S. Approximate solutions of the Schrödinger equation with the generalized Morse potential model including the centrifugal term. Int. J. Quant. Chem. **111**, 1870-1878 (2011).
19. Dong, S.H. Relativistic Treatment of Spinless Particles Subject to a Rotating Deng—Fan Oscillator. Commun. Theor. Phys, **55**, 969-971 (2011).
20. Oluwadare, O.J., Oyewumi, K.J., Akoshile, C.O., Babalola, O.A. Approximate analytical solutions of the relativistic equations with the Deng–Fan molecular potential including a Pekeris-type approximation to the (pseudo or) centrifugal term. Phys. Scr. **86**, 035002 (2012).
21. Oluwadare, O.J., Oyewumi, K.J., Babalola, O.A. Exact S-Wave Solution of the Klein-Gordon Equation with the Deng-Fan Molecular Potential using the Nikiforov-Uvarov (NU) Method. Afr. Rev. Phys. **7**, 165-170 (2012b).
22. Yazarloo, B.H., Lu, L., Liu, G., Zarrinkamar, S., Hassanabadi, H. The Nonrelativistic Scattering States of the Deng-Fan Potential. Adv. High Energy Phys. **2013**, 317605, (2013).
23. Tazimi, N., Ghasempour, A. Bound State Solutions of Three-Dimensional Klein-Gordon Equation for Two Model Potentials by NU Method. Adv. High Energy Phys. **2020**, 2541837, 1-10 (2020).
24. Awoga, O.A., Ikot, A.N., Emah, J.B. Bound state solutions of deformed generalized Deng-Fan potential plus deformed Eckart potential in D-dimensions. Rev. Mex. Fis. **59**, 229-235 (2013).
25. Falaye, B.J., Ikhdair, S.M., Hamzavi, M. Formula Method for Bound State Problems. Few-Body Syst. **56**, 63-72 (2015).
26. Onate, C.A., Adebimpe, O., Lukman, A.F., Adama, I.J., Davids, E.O., Dopamu, K.O. Approximate solutions of the Dirac equation with Coulomb-Hulthén-like tensor interaction. Res. Phys. **11**, 1094-1099 (2018).
27. Hamzavi, M., Ikhdair, S.M., Thylwe, K.E. Equivalence of the empirical shifted Deng–Fan oscillator potential for diatomic molecules. J. Math. Chem. **51**, 227-238 (2013).
28. Oyewumi, K.J., Oluwadare, O.J., Sen, K.D., Babalola, O.A. Bound state solutions of the Deng–Fan molecular potential with the Pekeris-type approximation using the Nikiforov–Uvarov (N–U) method. J. Math. Chem. **51**, 976-991 (2013).
29. Omugbe, E. Non-relativistic Energy Spectrum of the Deng-Fan Oscillator via the WKB Approximation Method. AJOPACS. **8**, 26-36 (2020).
30. Dong, S.H., Gu, X.Y. Arbitrary *l* state solutions of the Schrödinger equation with the Deng-Fan molecular potential. J. Phys. Conf. Ser. **96**, 012109 (2008)
31. Greene, R.L., Aldrich, C. Variational wave functions for a screened Coulomb potential. Phys. Rev. A. **14**, 2363-2366 (1976).
32. Ikot, A.N., Chukwuocha, E.O., Onyeaju, M.C., Onate, C.A., Ita, B.I., Udoh, M.E. Thermodynamics properties of diatomic molecules with general molecular potential. Pram. J. Phy. **90**, 22-30 (2018).

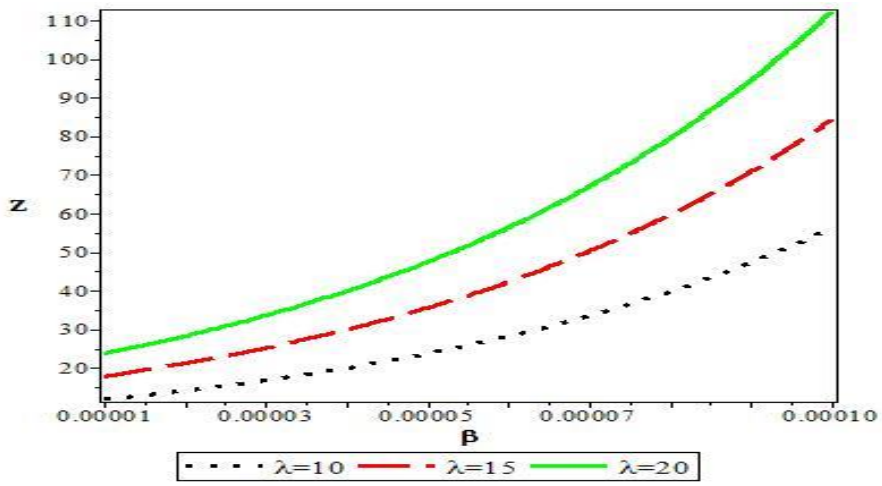

Fig. 1.Vibrational partition function Z as a function of β for the K_2 dimer.

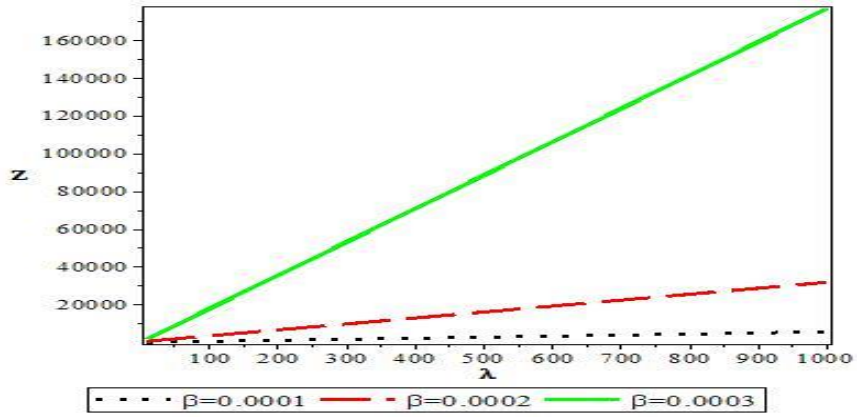

Fig. 2. Vibrational partition function Z as a function of λ for K_2 dimer.

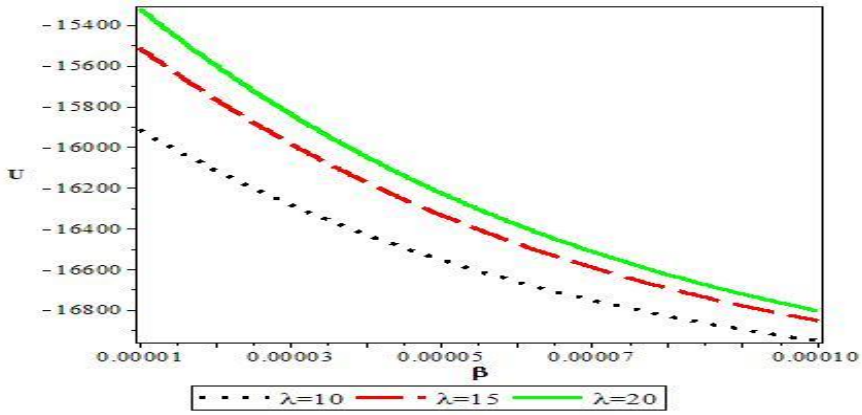

Fig. 3. Vibrational internal energy U as a function of β for K_2 dimer.

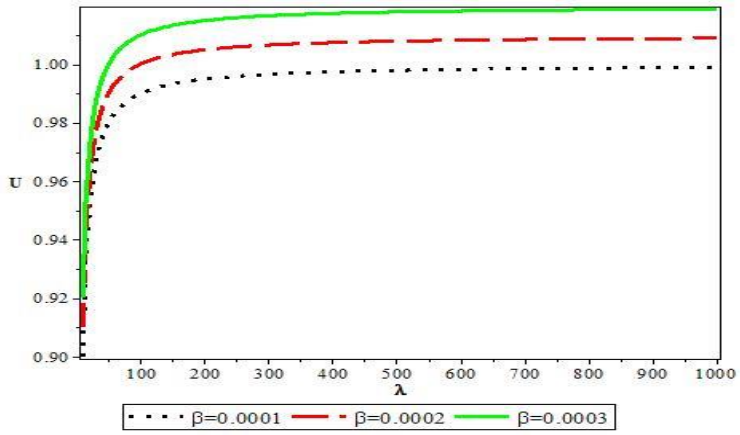

Fig. 4. Vibrational internal energy U as a function of λ for K_2 dimer.

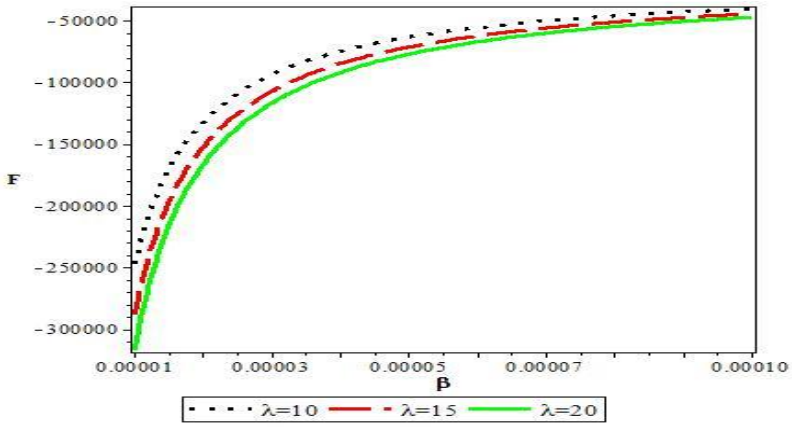

Fig. 5. Vibrational free energy F as a function of β for K_2 dimer

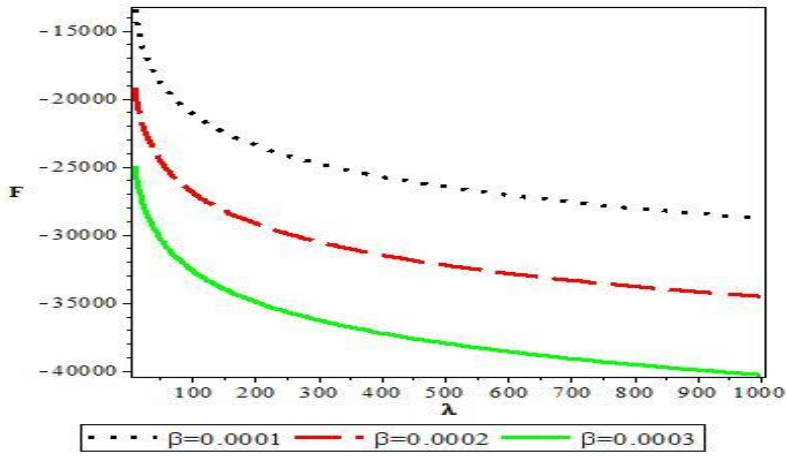

Fig. 6. Vibrational free energy F as a function of λ for K_2 dimer

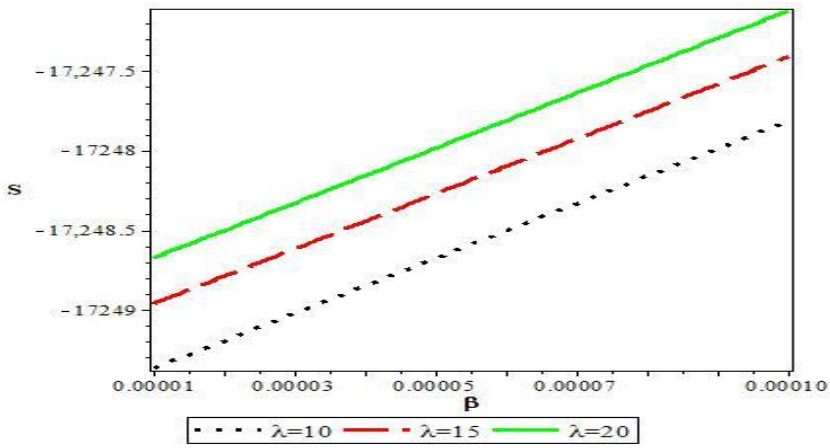

Fig. 7. Vibrational entropy S as a function of β for K_2 dimer

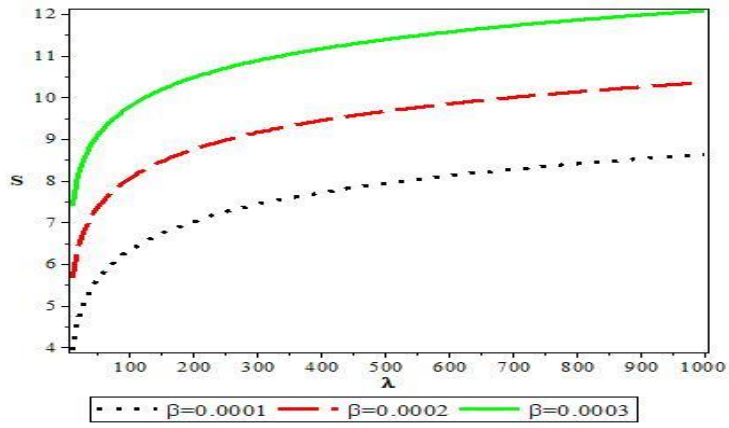

Fig. 8. Vibrational entropy S as a function λ for K_2 dimer

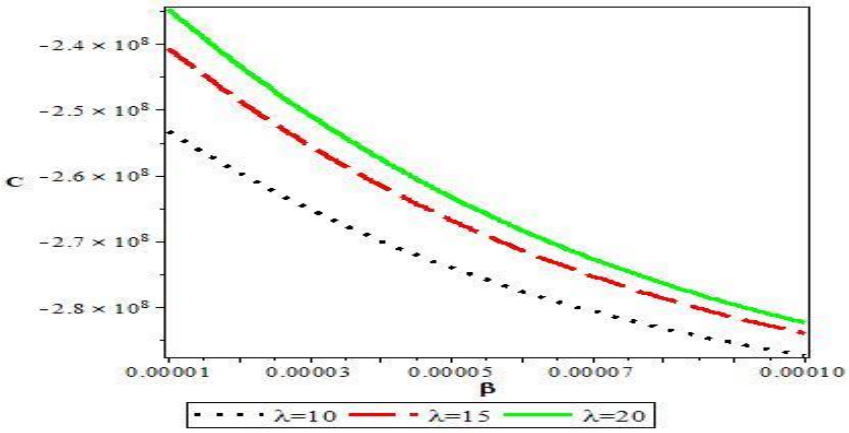

Fig. 9. Vibrational specific heat C as a function of β for K_2 dimer

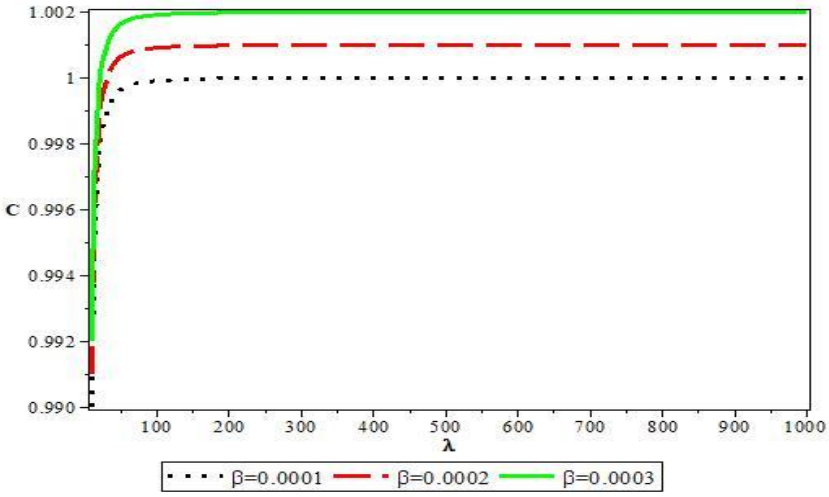

Fig. 10. Vibrational specific heat C as a function of λ for K_2 dimer

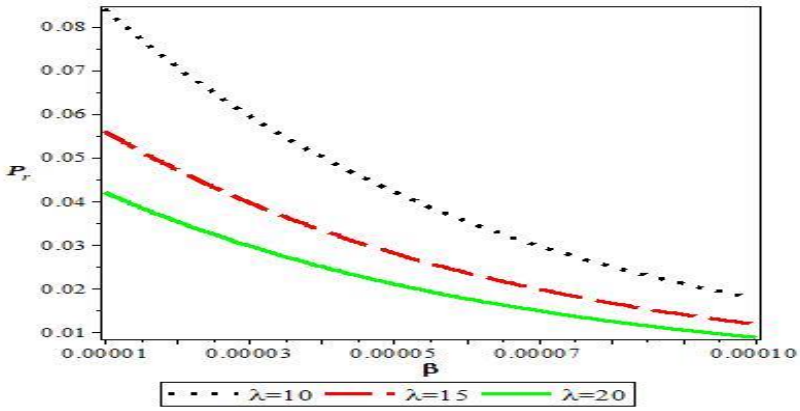

Fig. 11. Probability function as a function of β for K_2 dimer

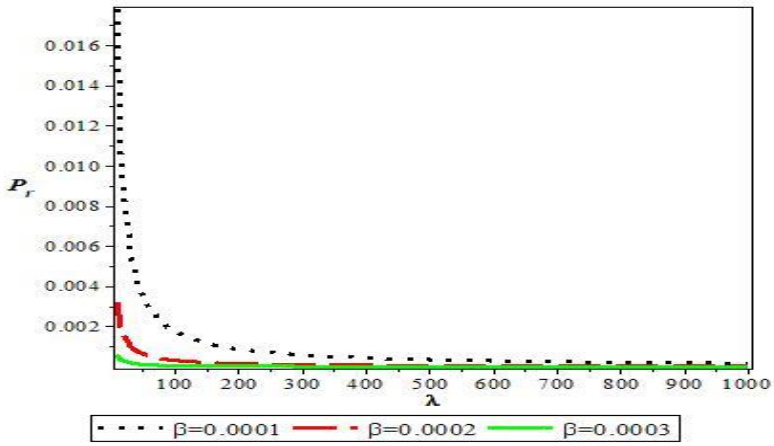

Fig. 12. Probability function as a function of λ for K_2 dimer

Table 1. Numerical results of energy of the Deng-Fan potential with D_e=15 r_e=0.4

State	α	Present	N–U method [22]	SUSY method [26]	Numerical method[36]	Functional method[36]	WKB Method[23]
2p	0.05	7.860804480	7.860804493	7.86080	7.8628	7.8606	7.860830507
	0.10	7.953304375	7.953304454	7.95330	7.95537	7.95247	7.953408639
	0.15	8.045099590	8.045099870	8.04510	8.04724	8.04322	8.045333800
	0.20	8.136203335	8.136203772	8.13620	8.13842	8.13287	8.136619920
	0.25	8.226628510	8.226629167	8.22663	8.22892	8.22142	8.227279483
	0.30	8.316388070	8.316389030	8.31639	8.31874	8.30889	8.317325475
3p	0.05	10.99776303	10.99776305	10.9978	10.9998	10.9976	10.99778906
	0.10	11.16256038	11.16256046	11.1626	11.1647	11.1617	11.16266460
	0.15	11.32424845	11.32424872	11.3242	11.32647	11.3224	11.32448272
	0.20	11.48283720	11.48283762	11.4828	11.48513	11.4795	11.48325379
	0.25	11.63833602	11.63833667	11.6383	11.64068	11.6331	11.63898698
	0.30	11.79075407	11.79075502	11.7908	9.67565	11.7833	11.79169146
3d	0.05	10.21598019	10.21598027	10.21598	10.21651	10.2154	10.21600623
	0.10	10.35353919	10.35353947	10.35354	10.35409	10.351	10.35364341
	0.15	10.48935365	10.48935439	10.48935	10.48992	10.4837	10.48958790
	0.20	10.62346247	10.62346374	10.62346	10.62403	10.6135	10.62387907
	0.25	10.75590446	10.75590641	10.75591	10.75645	10.7403	10.75655542
	0.30	10.88671867	10.88672151	10.88672	10.88719	10.8642	10.88765606
4p	0.05	10.99776303	12.49760242	12.4976	12.4992	12.4974	12.49762844
	0.10	11.16256038	12.69679604	12.69680	12.69851	12.696	12.69690015
	0.15	11.32424845	12.88834813	12.88835	12.8901	12.8865	12.88858217
	0.20	11.48283720	13.07224462	13.07224	13.07400	13.0689	13.07266080
	0.25	11.63833602	13.24847044	13.24847	13.2501	13.2433	13.24912075
4d	0.05	12.09829019	12.09829027	12.09829	12.0989	12.0977	12.09831623
	0.10	12.28500913	12.28500942	12.28501	12.2857	12.2825	12.28511332
	0.15	12.46641864	12.46641937	12.46642	12.46715	12.4608	12.46665293
	0.20	12.64256629	12.64256756	12.64257	12.64324	12.6326	12.64298290
4f	0.05	11.82078608	11.82078623	11.82079	11.8209	11.8195	11.82081212
	0.10	11.99796061	11.99796121	11.99796	11.9981	11.993	11.99806481
	0.15	12.17169516	12.17169661	12.17170	12.1718	12.1604	12.17192945
	0.20	12.34206965	12.34207217	12.34207	12.3421	12.3221	12.34248626
5p	0.10	13.54214241	13.54214250	13.54214	13.5434	13.5413	13.54224659
	0.20	13.92898591	13.92898633	13.92899	13.9301	13.9257	13.92940251
5d	0.10	13.30679661	13.30679690	13.30680	13.3075	13.3043	13.30690079
	0.20	13.69266269	13.69266395	13.69266	13.6931	13.6827	13.69307930
5f	0.10	13.14759711	13.14759771	13.14760	13.1478	13.1426	13.14770129
	0.20	13.53343974	13.53344225	13.53344	13.5333	13.5134	13.53385635
5g	0.10	13.03797518	13.03797622	13.03798	13.0379	13.0296	13.03807936
	0.20	13.42710848	13.42711266	13.42711	13.42667	13.3938	13.42752509
6p	0.10	14.05208851	14.05208861	14.05209	14.0530	14.0513	
6d	0.10	13.90704816	13.90704846	13.90705	13.9075	13.9045	
6f	0.10	13.81118934	13.81118995	13.81119	13.8113	13.8062	
6g	0.10	13.74661180	13.74661283	13.74661	13.7466	13.7383	

Table 2. Numerical results of energy of the Deng-Fan potential with D_e=15 r_e=0.8

State	α	Present	N–U method [22]	SUSY method [26]	Numerical method[36]	Functional method[36]	WKB Method[23]
2p	0.05	4.14088726	4.140887263	4.140887	4.14208	4.14068	4.140913461
	0.1	4.21918001	4.219180128	4.219180	4.2204	4.21835	4.219284120
	0.15	4.29739295	4.297393199	4.297393	4.2987	4.29552	4.297627357
	0.2	4.37554608	4.375546508	4.375547	4.3769	4.37221	4.375962693
	0.25	4.45365901	4.453659654	4.453660	4.4551	4.44845	4.454309954
	0.3	4.53175086	4.531751791	4.531752	4.5332	4.52425	4.532688242
3p	0.05	7.532791565	7.532791561	7.532792	7.5350	7.53258	7.532817713
	0.1	7.724764155	7.724764274	7.724764	7.7271	7.72393	7.724868277
	0.15	7.915178410	7.915178655	7.915179	7.9177	7.9133	7.915412795
	0.2	8.104040205	8.104040627	8.104041	8.1066	8.10071	8.104456816
	0.25	8.291353525	8.291354169	8.291354	8.2841	8.28615	8.292004474
	0.3	8.477120375	8.477121312	8.477121	8.4799	8.46962	8.478057760
3d	0.05	5.739751180	5.739751228	5.739751	5.7404	5.73913	5.739777356
	0.1	5.845769945	5.845770281	5.845770	5.8465	5.84327	5.845874062
	0.15	5.950677420	5.950678133	5.950678	5.9515	5.94505	5.950911804
	0.2	6.054532350	6.054533598	6.054534	6.0553	6.04453	6.054948991
	0.25	6.157393365	6.157395321	6.157395	6.1582	6.14177	6.158044321
	0.3	6.259318950	6.259321745	6.259322	6.2601	6.23682	6.260256322
4p	0.05	9.613013085	9.613013087	9.613013	9.6156	9.6128	9.613039208
	0.1	9.883523580	9.883523698	9.883524	9.8862	9.88269	9.883627711
	0.15	10.14855548	10.14855572	10.14856	10.1514	10.1467	10.14878985
	0.2	10.40805734	10.40805775	10.40806	10.4111	10.4047	10.40847394
	0.25	10.66197324	10.66197388	10.66197	10.665	10.6568	10.66262419
4d	0.05	8.493343435	8.493343486	8.493344	8.4948	8.49272	8.493369573
	0.1	8.707110650	8.707110984	8.707111	8.7087	8.70461	8.707214778
	0.15	8.917806885	8.917807599	8.917808	8.9194	8.91218	8.918041256
	0.2	9.125503845	9.125505093	9.125505	9.1272	9.11551	9.125920478
4f	0.05	7.434705685	7.434705812	7.434706	7.4351	7.43346	7.434731843
	0.1	7.586418155	7.586418806	7.586419	7.5868	7.58142	7.586522280
	0.15	7.735730835	7.735732273	7.735732	7.7361	7.72448	7.735965234
	0.2	7.882755005	7.882757512	7.882758	7.8831	7.86276	7.883171622
5p	0.1	11.30207232	11.30207244	11.30207	11.3047	11.3012	11.30217646
	0.2	11.91322333	11.91322375	11.91322	11.9161	11.9099	11.91363994
5d	0.1	10.52008575	10.52008608	10.52009	10.5219	10.5176	10.52018988
	0.2	11.06937035	11.06937161	11.06937	11.0713	11.0594	11.06978698
5f	0.1	9.796657385	9.796658033	9.796658	9.7975	9.79166	9.796761519
	0.2	10.27303457	10.27303707	10.27304	10.2738	10.253	10.27345118
5g	0.1	9.152222285	9.152223355	9.152223	9.1524	9.14389	9.152326416
	0.2	9.552865320	9.552869479	9.552869	9.5528	9.51954	9.553281943
6p	0.1	12.27979910	12.27979921	12.27980	12.2822	12.279	
6d	0.1	11.73643831	11.73643864	11.73644	11.7383	11.7339	
6f	0.1	11.24481428	11.24481492	11.24481	11.2459	11.2398	
6g	0.1	10.81533122	10.81533228	10.81533	10.8158	10.807	