Analytic treatment of IR-spectroscopy data for double well potential

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Abstract

A theoretical scheme for the analysis of experimental data on IR spectroscopy for a quantum particle in a double well potential (DWP) is suggested. The analysis is based on the trigonometric DWP for which the exact analytic solution of the Schrödinger equation is available. The corresponding energy levels along with their wave functions are expressed via special functions implemented in *Mathematica* (spheroidal function and its spectrum of eigenvalues). As a result trigonometric DWP makes the calculation of the energy levels an extremely easy procedure. It contains three parameters allowing one to model the most important characteristics of DWP (barrier height and the distance between the minima of the potential) along with the required asymmetry. Our approach provides an accurate calculation of the energy spectrum for hydrogen bonds in chromous acid (CrOOH) and potassium dihydrogen phosphate (KH_2PO_4) along with their polarizability in agreement with available experimental data.

Key words: Schrödinger equation, confluent Heun's function, spheroidal function, hydrogen bond.

1   Introduction

The one-dimensional time-independent Schrödinger equation (SE) for a quantum particle moving in some double-well potential (DWP) is ubiquitous in physics and chemistry (see [1], [2], [3], [4], [5], [6], [7], [8], [9], [10], [11], [12], [13], [14], [15], [16] and refs. therein). On the one hand numerical methods for the solution of SE (see [17], [18] and refs. therein) provide accurate description

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for both one-dimensional and multidimensional problems. On the other hand the exact analytic solutions [3], [4], [5], [6], [7], [8], [9], [10], [11], [12], [13], [14], [16] remain an important tool for understanding the reality. Such solutions are expressed via confluent Heun's function (CHF) [3], [4], [5], [6], [7], [8], [9], [10], [11], [12], [14] (implemented in *Maple*), spheroidal function (SF) [7], [8], [9] or derived via the functional Bethe ansatz [16]. Unfortunately these solutions can be obtained only for some particular DWPs and lack the universality of numerical methods. Trigonometric DWP

$$U(x) = \left(m^2 - \frac{1}{4}\right) \tan^2 x - p^2 \sin^2 x - a \sin x$$

where $-\pi/2 \leq x \leq \pi/2$ is a particular type of DWPs expressed via trigonometric functions for which SE can be exactly solved via SF (implemented in *Mathematica*) or CHF [7], [8], [9]. In the symmetric form $a = 0$ (see examples in Fig.1, Fig.2 and Fig.5) it contains two parameters $\{m, p\}$ allowing one to model the most important characteristics of DWP (barrier height and the distance between the minima of the potential). In the asymmetric form it contains the third (asymmetry $a \neq 0$) parameter. The merit of trigonometric DWP is in the fact that SF [15] is implemented in *Mathematica* along with its spectrum of eigenvalues. As a result the calculation of the energy levels becomes an easy procedure. It is obvious that not all DWPs (in particular those complicated curves of quantum chemical calculations) can be covered by the trigonometric form. On the other hand there are cases in which the IR spectroscopy data can be accurately described by this DWP. Thus it is an additional and complementary tool in the toolkit of the researchers dealing with IR spectroscopy. It enables one to make quick calculations of the energy levels and the wave functions of the system under investigation from the IR spectroscopy data. Also with the rational time consumption it allows one to obtain the characteristics of the system calculated on the basis of the above information, e.g., the behavior of its polarizability on temperature (see below). In the present article we apply SE with trigonometric DWP to the analytic description of the IR-spectroscopy data for symmetric hydrogen bonds (HB) in chromous acid (CrOOH) and potassium dihydrogen phosphate (KH_2PO_4).

SE with DWP is often used for the description of the proton position for HB [19], [20], [21], [22], [23], [24], [25], [26]. The aim of the present article is to show that trigonometric DWP provides the expressions for the energy levels and their corresponding wave functions for HB in CrOOH and KH_2PO_4 along with their polarizability. The tunneling process for a proton is known to yield a dominant contribution **to** the extremely high polarizability of HB [22], [23], [24], [25], [26]. This problem was thoroughly investigated by Zundel and co-authors (see [22], [25], [26] and refs. therein). In [24] the ground-state splitting was calculated by the instanton approach to double Morse potential. For low-barrier HB in CrOOH and KH_2PO_4 the ground state doublet is close

to the barrier top and the instanton method is known to yield very inaccurate results [9] in this case. Our approach provides a more stringent and adequate tool for calculating the ground state splitting. However it should be stressed that the intricate phenomenon of the polarizability of realistic HB is known to be complicated by many other factors arising from their interaction with environment [24], [26]. Besides we are not aware of the experimental data on the polarizability of HB in CrOOH or KH_2PO_4. Thus we can not compare our model calculations with the experiment. Nevertheless the calculation of the polarizability for HB in CrOOH and KH_2PO_4 at room temperature yields the values very close to that calculated from the available experimental data for HB in BrH $\cdots$ N [25]. In our opinion such coincidence can not be fortuitous and is a serious argument in favor of the relationship of trigonometric DWP to the reality.

2 Energy levels, wave functions and polarizability for quantum particle in trigonometric double-well potential

Polarizability $\alpha(T)$ as a function of temperature T is a reaction of the system under consideration to a constant external electric field making DWP intrinsically asymmetric [25]. Thus a self-consistent approach should include an asymmetry term in the Hamiltonian $-\mu(X)F$ where F is the electric field strength and $\mu(X)$ is the dipole moment. The latter is usually assumed to be $\mu(X) = eX$ in the linear approximation. In Appendix 1 we show how to transform the dimensional values into their dimensionless counterparts for trigonometric DWP. We denote the asymmetry parameter

$$a = \frac{16ML^3eF}{\hbar^2\pi^3} \tag{1}$$

Here e is the quantum particle charge, M is the mass of the quantum particle, $\hbar$ is the reduced Planck constant and L is the dimensional boundary of the interval for the spatial variable X (see Appendix 1). Then the dimensionless interaction energy is $-ax$. However the linear approximation can be valid within the interval of a sufficiently small x only. Common knowledge pervading textbooks on physical chemistry ascertains that the realistic behavior of the dipole moment must deflect to more slow growth than the linear one (see, e.g., Fig. 10.54 in [27]). To go beyond the framework of the linear approximation and to model such deflection we replace the linear term by the trigonometric one

$$-ax \longrightarrow -a\sin x \tag{2}$$

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at $-\pi/2 \leq x \leq \pi/2$. The latter approximation is certainly better than the linear one, it is natural for our trigonometric DWP and finally it enables us to proceed with analytic treatment of the problem.

Then SE with trigonometric DWP in dimensionless units (see Appendix 1 for details) takes the form [8], [9]

$$\psi''_{xx}(x) + \left[\epsilon - \left(m^2 - \frac{1}{4} \right) \tan^2 x + p^2 \sin^2 x + a \sin x \right] \psi(x) = 0 \qquad (3)$$

Here $-\pi/2 \leq x \leq \pi/2$, m (an integer number) is the barrier width parameter and p is the barrier height parameter. The solution of (3) is discussed in details in [9]

$$\psi_q(x) = \cos^{1/2} x \; \bar{\Xi}_{mq}(p, a; \sin x) \qquad (4)$$

Here $q = 0, 1, 2, ...$ and $\bar{\Xi}_{mq}(p, a; \sin x)$ is angular generalized (Coulomb) SF [15]. The energy levels are determined by the relationship

$$\epsilon_q = \lambda_{mq}(p, a) + \frac{1}{2} - m^2 - p^2 \qquad (5)$$

Here $\lambda_{mq}(p, a)$ is the spectrum of eigenvalues for the function $\bar{\Xi}_{mq}(p, a; s)$.

With the solution (4) further calculations are straightforward along the general formulas for the dipole moment and the definition of the polarizability [25]. The average dipole moment in the n-th state with taking into account the replacement (2) and with the help of (1.24b) from the part 2 in [15] is

$$\mu_{nn} = - \int_{-\pi/2}^{\pi/2} dx \; \psi_n(x) \; \sin x \; \psi_n(x) = - \int_{-1}^{1} d\eta \; \eta \left[\bar{\Xi}_{mn}(p, a; \eta) \right]^2 = \frac{\partial \lambda_{mn}(p, a)}{\partial a} (6)$$

We denote the dimensionless inverse temperature β and the dimensionless polarizability $\Theta(\beta)$

$$\beta = \frac{\hbar^2 \pi^2}{16 M L^2 k_B T} \qquad\qquad \Theta(\beta) = \frac{\hbar^2 \pi^4}{64 e^2 L^4 M} \alpha(T) \qquad (7)$$

Here k_B is the Boltzmann constant and T is the temperature. The mean dipole moment as a function of the dimensionless inverse temperature is

$$\mu(\beta, a) = \left[\sum_{n=0}^{\infty} \exp(-\beta \epsilon_n) \right]^{-1} \sum_{n=0}^{\infty} \frac{\partial \lambda_{mn}(p, a)}{\partial a} \exp(-\beta \epsilon_n) \qquad (8)$$
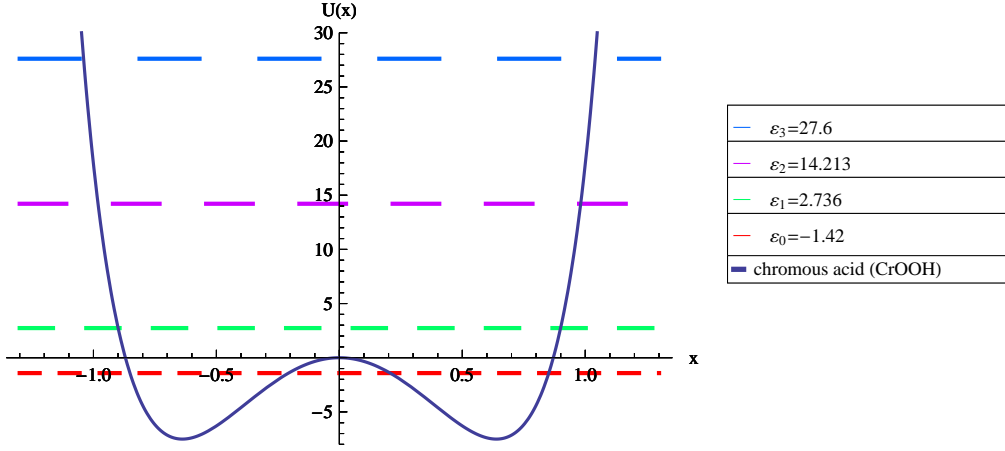
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Fig. 1. The symmetric trigonometric double-well potential at the values of the parameters $m = 5$, $p = 7.716$. The parameters are chosen to describe the potential and the energy levels for the hydrogen bond in chromous acid (CrOOH) (experimental data are taken from [21]). The energy levels $\epsilon_0 = -1.42$, $\epsilon_1 = 2.736$, $\epsilon_2 = 14.213$, $\epsilon_3 = 27.6$ are respectively depicted by the dashes of increasing length. The splitting of the ground state $\epsilon_1 - \epsilon_0 = 4.156$ corresponds to 546 cm^{-1} in dimensional units.

Finally the field zero polarizability is

$$\Theta\left(\beta\right) = \left.\frac{\partial\mu\left(\beta, a\right)}{\partial a}\right|_{a = 0} \tag{9}$$

The stringent procedure for the calculation of $\lambda_{mn}\left(p, a\right)$ is extremely cumbersome [29]. However the requirement to carry out the calculations in the limit $a \to 0$ enables us to simplify them considerably. For an approximate estimate we use the expression from [28], [29] that is valid for $a \to 0$ at low values of m and p. As a result we obtain

$$\lambda_{mn}\left(p, a\right) \approx A_n + B_n\frac{a^2}{2} \tag{10}$$

Here

$$A_n = \lambda_{mn}\left(p, 0\right) \equiv \lambda_{m(n+m)}\left(p\right) \tag{11}$$

where $\lambda_{m(q+m)}\left(p\right) \equiv SpheroidalEigenvalue[q + m, m, ip]$ is the spectrum of eigenvalues for SF written in the designations of [15] and in *Mathematica*
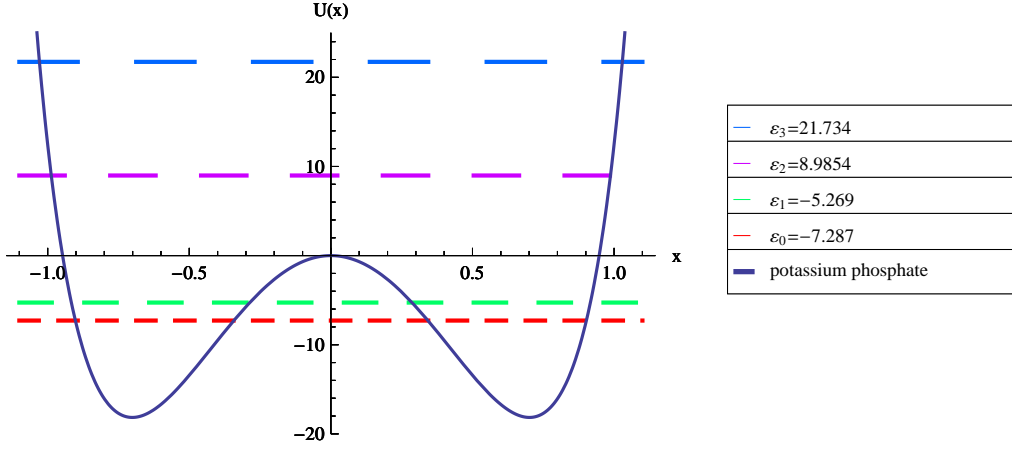
Fig. 2. The symmetric trigonometric double-well potential at the values of the parameters $m = 6$, $p = 10.24$. The parameters are chosen to describe the potential and the energy levels for the hydrogen bond in potassium dihydrogen phosphate (KH_2PO_4) (experimental data are taken from [19], [20]). The energy levels $\epsilon_0 = -7.287$, $\epsilon_1 = -5.269$, $\epsilon_2 = 8.9854$, $\epsilon_3 = 21.734$ are respectively depicted by the dashes of increasing length. The splitting of the ground state $\epsilon_1 - \epsilon_0 = 2.018$ corresponds to 320 cm^{-1} in dimensional units.

notation. For B_n we have from the above mentioned expression [28], [29]

$$B_n \approx \frac{1}{2(n+m)+1} \left[\frac{m^2 - (n+m)^2}{(n+m)\,(2(n+m)-1)} + \frac{(n+m+1)^2 - m^2}{(n+m+1)\,(2(n+m)+3)} \right] (12)$$

With the help of (10) eq. (8) takes the form

$$\mu\left(\beta, a\right) \approx \left\{ \sum_{n=0}^{\infty} \exp\left[-\beta\left(A_n + \frac{a^2 B_n}{2}\right)\right] \right\}^{-1} a \sum_{n=0}^{\infty} B_n \exp\left[-\beta\left(A_n + \frac{a^2 B_n}{2}\right)\right] (13)$$

The latter expression makes the polarizability (9) to be calculable. The results obtained with the help of *Mathematica* [30] are presented in Fig.3 and Fig.4.

3 Results and discussion

In Fig.1 the energy levels for HB in chromous acid (CrOOH) (experimental data are taken from [21]) are presented. In Fig.2 the energy levels for HB
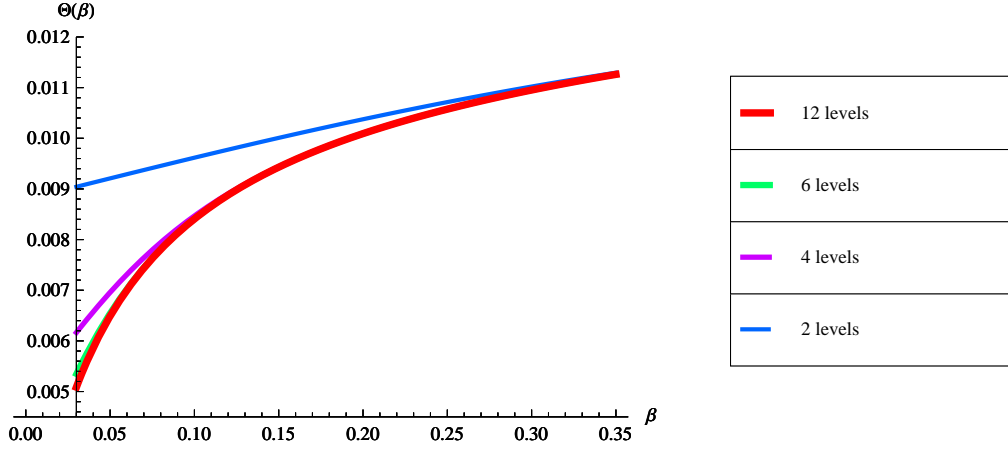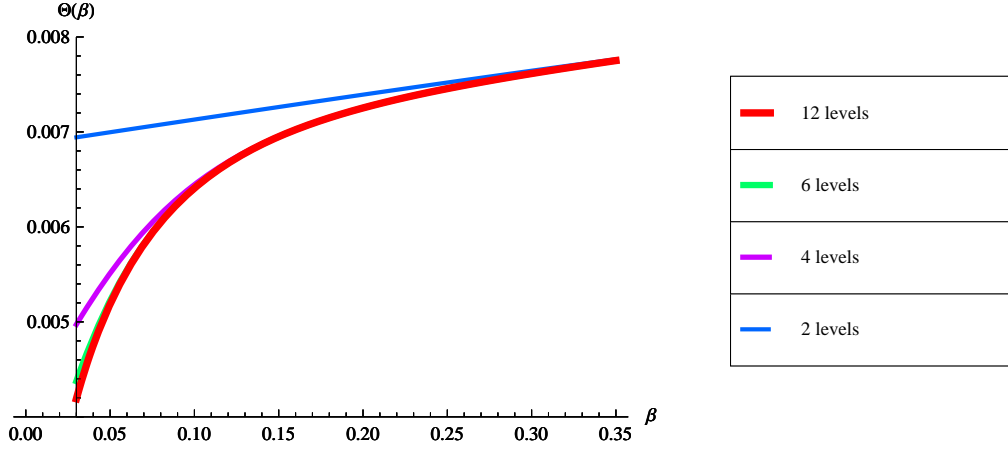
Fig. 3. The dependence of the dimensionless polarizability $\Theta(\beta)$ (9) of the quantum particle in the trigonometric double-well potential on the dimensionless inverse temperature (7) at the values of the barrier height parameter $p = 7.716$ and the barrier width parameter $m = 5$ corresponding to the hydrogen bond in chromous acid (CrOOH). The results for the increasing number of doublets (pairs of energy levels) taken into account in (13) are depicted by the lines of increasing thickness respectively.

in potassium dihydrogen phosphate (KH_2PO_4) (experimental data are taken from [19], [20]) are presented. For HB in CrOOH [21] (KH_2PO_4 [19], [20]) the ground-state splitting is $\Delta E = E_1 - E_0 \approx 546$ cm^{-1} (320 cm^{-1}) while the frequencies for the higher levels are $E_2 - E_1 \approx 1508$ cm^{-1} (2260 cm^{-1}), $E_3 - E_0 \approx 3802$ cm^{-1} (4600 cm^{-1}) and $E_2 - E_0 \approx 2053$ cm^{-1} (2580 cm^{-1}). The ratios

$$\frac{E_2 - E_0}{E_2 - E_1} = \frac{\epsilon_2 - \epsilon_0}{\epsilon_2 - \epsilon_1} = 1.36 \ (1.14); \qquad \frac{E_2 - E_1}{E_1 - E_0} = \frac{\epsilon_2 - \epsilon_1}{\epsilon_1 - \epsilon_0} \approx 2.76 \ (7.06);$$

$$\frac{E_3 - E_0}{E_2 - E_0} = \frac{\epsilon_3 - \epsilon_0}{\epsilon_2 - \epsilon_0} \approx 1.85 \ (1.78)$$

are obtained for our dimensionless energy levels ϵ_q if we take the values for the parameters of DWP $m = 5$ (6) and $p = 7.716$ (10.24).

Fig.3 and Fig.4 show the behavior of the polarizability with the decrease of temperature (increase of β) at the value of the parameters corresponding to HB in CrOOH and KH_2PO_4 respectively. In Fig.3. and Fig.4 the number of doublets (pairs of energy levels) taken into account in (13) means the quantity "N" used for the truncation of the infinite summation in (13). For instance

Fig. 4. The dependence of the dimensionless polarizability $\Theta\left(\beta\right)$ (9) of the quantum particle in the trigonometric double-well potential on the dimensionless inverse temperature (7) at the values of the barrier height parameter $p = 10.24$ and the barrier width parameter $m = 6$ corresponding to the hydrogen bond in potassium dihydrogen phosphate (KH_2PO_4). The results for the increasing number of doublets (pairs of energy levels) taken into account in (13) are depicted by the lines of increasing thickness respectively.

"6 levels" in Fig.3 and Fig.4 means that the series is truncated by $N = 5$ (n=0,...,5) while "12 levels" means that the series is truncated by $N = 11$ (n=0,...,11). The curves in Fig.3 and Fig.4 practically are not altered at increasing the truncation number over $N = 5$ that proves the convergence of the series in (13).

One can conclude that the suggested trigonometric double-well potential for the Schrödinger equation provides accurate analytic calculation of the energy levels, the corresponding wave functions and the polarizability of hydrogen bonds in CrOOH and KH_2PO_4 via special functions implemented in *Mathematica*.

4 Appendix 1

In dimensional units the one-dimensional SE for a quantum particle with the reduced mass M has the form

$$\frac{d^2\psi(X)}{dX^2} + \frac{2M}{\hbar^2}\left[E - V(X)\right]\psi(X) = 0 \tag{14}$$

where $-L \leq X \leq L$ and $V(X)$ is a DWP. The latter is assumed to be infinite at the boundaries of the finite interval for the spatial variable $X = \pm L$. The dimensionless values for the distance x, the potential $U(x)$ and the energy ϵ are introduced as follows

$$x = \frac{\pi X}{2L} \qquad\qquad U(x) = \frac{8ML^2}{\hbar^2\pi^2}V(X) \qquad\qquad \epsilon = \frac{8ML^2E}{\hbar^2\pi^2} \qquad (15)$$

where $-\pi/2 \leq x \leq \pi/2$. As a result we obtain dimensionless SE (3) with trigonometric DWP.

For HB in both chromous acid [21] and potassium dihydrogen phosphate [19], [20] the distance between the oxygen atoms is $2L \approx 2.49$ Å so that for the boundary of trigonometric DWP we have $L \approx 1.245$ Å. The mass of a proton is $M = 1$ amu. From these values we estimate the inverse dimensionless temperature (7) to be $\beta \approx 0.0583$ at $T = 300$ K and $\beta \approx 0.175$ at $T = 100$ K. The calculated value for the dimensionless polarizability in chromous acid at room temperature is $\Theta\,(0.0583) \approx 0.0068$ (see Fig.3). The calculated value for the dimensionless polarizability in potassium dihydrogen phosphate at room temperature is $\Theta\,(0.0583) \approx 0.0054$ (see Fig.4). These values are close to those calculated from the known experimental values: $\Theta\,(0.0583) \approx 0.00676$ obtained from $\alpha\,(300\ K) = 40 \cdot 10^{-24}\ cm^3$ for HB in $BrH \cdots N$ [25].

5   Appendix 2

Another case of making use the trigonometric DWP takes place when the results of non-empirical quantum chemical (ab initio) potential energy surface calculations are available instead of the IR spectroscopy frequencies. To exemplify this case we apply the present approach to the Zundel ion $H_5O_2^+$ (oxonium hydrate) basing on the results of [31]. For obtaining the parameters of the symmetric trigonometric DWP $(a = 0)$ from the data for the Zundel ion presented in [31] we transform the parameters of trigonometric DWP $\{m, p\}$ into the barrier height $B = -U\,(x_{min})$ and width $D = x_{min}^{(1)} - x_{min}^{(2)}$

$$p = \frac{\sqrt{B}}{1 - [\cos\,(D/2)]^2} \qquad\qquad m^2 - \frac{1}{4} = \frac{B\,[\cos\,(D/2)]^4}{\left\{1 - [\cos\,(D/2)]^2\right\}^2}$$

Inversely we obtain

$$D(m,p) = 2\arccos\left(\frac{m^2 - \frac{1}{4}}{p^2}\right)^{1/4} \qquad\qquad B(m,p) = \left(\sqrt{m^2 - \frac{1}{4}} - p\right)^2$$
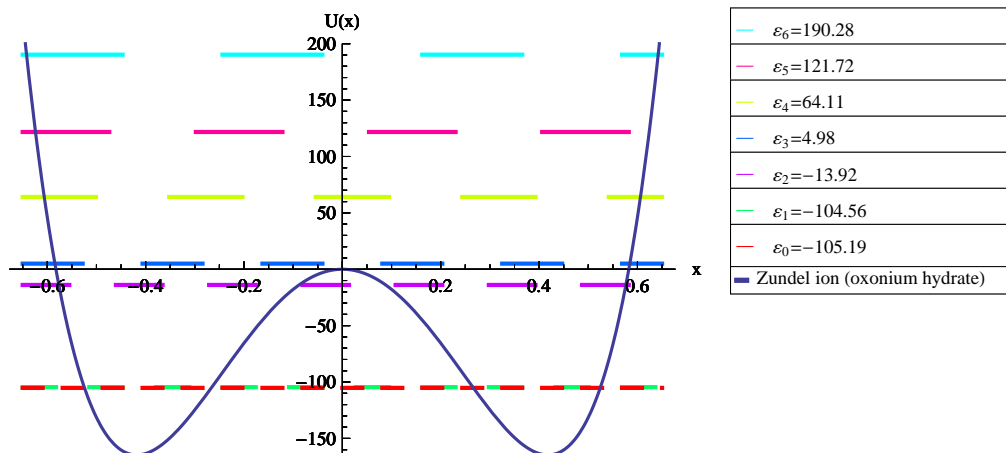
Fig. 5. The symmetric trigonometric double-well potential at the values of the parameters $m = 65$, $p = 77.83$. The parameters are chosen to describe the potential and the energy levels for the hydrogen bond in the Zundel ion (oxonium hydrate) for $R_{OO} = 2.786$ Å (experimental data are taken from [31]). The increasing energy levels are respectively depicted by the dashes of increasing length.

From Fig.1 of [31] we obtain that for $R_{OO} = 2.786$ Å ($2L = 2.786$ Å) the dimensional distance between the minima of DWP is $X_{min}^{(1)} - X_{min}^{(2)} \approx 0.74$ Å. The dimensional barrier height is $V(X_{max}) - V(X_{min}) \approx 3100$ cm^{-1}. We obtain that $B \approx 163.02$ and $D \approx 0.83$. From here we have $p \approx 77.83$ and $m = 65$. The results are presented in Fig.5. As a whole the system of energy levels agrees satisfactorily well with that in Fig2. of [23] for the case $R_{OO} = 2.8$ Å.

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References

[1] M. Razavy, An exactly soluble Schrödinger equation with a bistable potential, American Journal of Physics 48 (1980) 285-288.

[2] V. Jelic, F. Marsiglio, The double-well potential in quantum mechanics: a simple, numerically exact formulation, Eur. J. Phys. 33 (2012) 1651-1666.

[3] Qiong-Tao Xie, New quasi-exactly solvable double-well potentials, J. Phys. A: Math. Theor. 45 (2012) 175302.

[4] C. A. Downing, On a solution of the Schrödinger equation with a hyperbolic double-well potential, J. Math. Phys. 54 (2013) 072101.

[5] Bei-Hua Chen, Yan Wu, Qiong-Tao Xie, Heun functions and quasi-exactly solvable double-well potentials, J. Phys. A: Math. Theor. 46 (2013) 035301.

[6] R.R. Hartmann, Bound states in a hyperbolic asymmetric double-well, J.Math.Phys. 55 (2014) 012105.

[7] A.E. Sitnitsky, Exactly solvable Schrödinger equation with double-well potential for hydrogen bond, Chemical Physics Letters 676C (2017) 169-173.

[8] A.E. Sitnitsky, Analytic description of inversion vibrational mode for ammonia molecule, Vibrational Spectroscopy 93 (2017) 36-41.

[9] A.E. Sitnitsky, Analytic calculation of ground state splitting in symmetric double well potential, Computational and Theoretical Chemistry 1138 (2018) 15-22.

[10] Qian Dong, F.A. Serrano, Guo-Hua Sun, Jian Jing, Shi-Hai Dong, Semiexact solutions of the Razavy potential, Advances in High Energy Physics (2018) 9105825.

[11] Shishan Dong, Qian Dong, Guo-Hua Sun, S. Femmam, Shi-Hai Dong, Exact solutions of the Razavy cosine type potential, Advances in High Energy Physics (2018) 5824271.

[12] Qian Dong, Guo-HuaSun, Jian Jing, Shi-Hai Dong, New findings for two new type sine hyperbolic potentials, Phys.Lett. A383 (2019) 270-275.

[13] Qian Dong, Shi-Shan Dong, E. Hernández-Márquez, R. Silva-Ortigoza, Guo-Hua Sun, Shi-Hai Dong, Semi-exact solutions of Konwent potential, Commun. Theor. Phys. 71 (2019) 231-236.

[14] A. Ishkhanyan, Schrödinger potentials solvable in terms of the confluent Heun functions, Theoretical and Mathematical Physics 188 (2016) 980-993.

[15] I.V. Komarov, L.I. Ponomarev, S.Yu. Slavaynov, Spheroidal and Coloumb spheroidal functions, Moscow, Science, 1976.

[16] D. Agboola, Quasi-exactly solvable double Morse potential and proton tunnelling in hydrogen bonded crystals, presentation (unpublished results).

[17] I.N. Levine, Quantum Chemistry, 7-th ed., Pearson, 2014, section 4.4.

[18] M.R. Hermesa, S. Hirata, Diagrammatic theories of anharmonic molecular vibrations, International Reviews in Physical Chemistry 34 (2015) 7197.

[19] M.C. Lawrence, G.N. Robertson, The temperature and pressure dependence of the proton tunnelling frequency in KPD, J.Phys. C: Solid St.Phys. 13 (1980) L1053-9.

[20] M.C. Lawrence, G.N. Robertson, Estimating the proton potential in KDP from infrared and crystallographic data, Ferroelectrics 34 (1981) 179-186.

[21] M.C. Lawrence, G.N. Robertson, The interpretation of the neutron inelastic scattering and infrared absorption spectra of chromous acid using the double Morse potential model, J.Chem.Phys. 87 (1987) 3375-3380.

[22] E.G. Weidemann and G. Zundel, Field-dependent mechanism of anomalous proton conductivity and the polarizability of hydrogen bonds with tunneling protons, Z. Naturforsch., Teil A, 25 (1970) 627-634.

[23] R. Janoschek, E. G. Weidemann, H. Pfeiffer, G. Zundel, Extremely high polarizability of hydrogen bonds, J. Amer. Chem. Soc. 94 (1972) 2387-2396.

[24] E.S. Kryachko, M. Eckert, G. Zundel, Study of tunnelling in symmetrical double-Morse hydrogen bonds via the instanton-soliton approach: large polarizability and isotopic effect, Journal of Molecular Structure (Theochem), 235 (1991) 157-183.

[25] M. Eckert, G. Zundel, Proton polarizability, dipole moment, and proton transitions of an $AH \cdots B \rightleftharpoons A^- \cdots H^+B$ proton-transfer hydrogen bond as a function of an external electrical field: an ab initio SCF treatment, J.Phys.Chem. 91 (1987) 5170-5177.

[26] G. Zundel, Hydrogen bonds with large proton polarizability and proton transfer processes in electrochemistry and biology, Advances in Chemical Physics 111 (2000) 1-217.

[27] P. Atkins, J.de Paula, R.Friedman, Quanta, Matter, and Change. A molecular approach to physical chemistry, Freeman, 2009.

[28] L.I. Ponomarev, L.N. Somov, The wave functions of continuum for the two-center problem in quantum mechanics, J. Compt. Phys. 20 (1976) 183-195.

[29] J.W. Liu, Analytical solutions to the generalized spheroidal wave equation and the Greens function of one-electron diatomic molecules, J. Math. Phys. 33 (1992) 4026-4036.

[30] Wolfram Research, Inc., Mathematica, Version 11.3, Champaign, IL (2018).

[31] Q.Yu, J.M. Bowman, How the Zundel $H_5O_2^+$ potential can be used to predict the proton stretch and bend frequencies of larger protonated water clusters, J. Phys. Chem. Lett. 7 (2016) 5259-5265.