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Brief Report

On the Screened Kratzer Potential and Its Variants

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Abstract: We argue that several potentials proposed recently for the analysis of the vibrational-rotational spectra of diatomic molecules and their thermodynamic properties exhibit a flaw. One can easily show that the parameters D_e and r_e in those potentials are not the dissociation energy and equilibrium bond length, respectively, as the proposers believe. We show how to overcome the mistake in a simple and quite general way.

Keywords: Kratzer potential; screened Kratzer potential; vibrational-rotational spectrum; dissociation energy; equilibrium bond length

1. Introduction

Several years ago, Kratzer [1] proposed a potential for the analysis of the spectra of diatomic molecules and some time later Fues [2] solved the Schrödinger equation with this potential. For this reason, the potential is commonly called Kratzer potential or Kratzer-Fues potential. A few years later, typical textbooks on spectroscopy [3] scarcely resort to the Kratzer potential and today no spectroscopist would take it seriously. However, several authors have recently shown some interest in the Kratzer potential and even proposed some variants [4–12], like the screened Kratzer potential [4,5,10], the screened cosine Kratzer potential [6], the Hulten-screened Kratzer potential [7], the improved screened Kratzer potential [8], the improved Kratzer potential [9], the shifted screened Kratzer potential [11] and the harmonic plus screened Kratzer potential [12].

The purpose of this note is the discussion of all those molecular potentials. In Section 2 we analyze the potentials just mentioned, in Section 3 we show how to generate them correctly and in Section 4 we summarize the main results and draw conclusions.

2. The Modified Kratzer Potentials

Before discussing the potentials we review a relevant feature of a potential $V(r)$ for a diatomic molecule. According to any textbook on spectroscopy the equilibrium bond length r_e and the dissociation energy D_e are given by [3]

$$\left. \frac{dV(r)}{dr} \right|_{r=r_e} = 0, \quad D_e = \lim_{r \rightarrow \infty} V(r) - V(r_e), \quad (1)$$

to which we should add $V''(r_e) > 0$ because the stationary point at $r = r_e$ should be a minimum.

The Kratzer potential can be written in several equivalent forms; in what follows we choose the expression used in most of the papers mentioned in the introduction:

$$V_K(r) = -2D_e \left(\frac{r_e}{r} - \frac{r_e^2}{2r^2} \right). \quad (2)$$

Note that $V_K(r)$ satisfies equations (1).

The first variant of the Kratzer potential is the Screened Kratzer potential

$$V_{SK}(r) = -2D_e \left(\frac{r_e}{r} - \frac{r_e^2}{2r^2} \right) e^{-\alpha r}, \quad (3)$$

proposed by Ikot et al [4] and used also in other papers [5,10] for some physical applications. In this case, $\alpha \geq 0$ is a screening parameter. One can *easily verify* that $V_{SK}(r)$ does not satisfy equations (1):

$$V'_{SK}(r_e) = \alpha D_e e^{-\alpha r_e}, \quad V_{SK}(r \rightarrow \infty) - V_{SK}(r_e) = D_e e^{-\alpha r_e} \leq D_e. \quad (4)$$

This variant of the Kratzer potential only satisfies equations (1) in the trivial case $\alpha = 0$. Note that $r = r_e$ is not at the minimum of the potential but to the right of it. Consequently, the parameters D_e and r_e in equation (3) are not the dissociation energy and equilibrium bond length, respectively. For this reason, all the physical applications based on such assumption [4,5,10] are of doubtful utility.

Purohit et al [6] proposed the screened cosine Kratzer potential

$$V_{SCK}(r) = -2D_e \left(\frac{r_e}{r} - \frac{r_e^2}{2r^2} \right) e^{-\alpha r} \cosh(\delta \alpha r), \quad (5)$$

where δ is another screening parameter. The authors are not clear about the suitable values of δ and here we assume that $-1 \leq \delta \leq 1$ so that $e^{-\alpha r} \cosh(\delta \alpha r) \rightarrow 0$ when $r \rightarrow \infty$. Purohit et al chose the trivial value $\delta = 0$ and also $\delta = 1$. A straightforward calculation leads to

$$\begin{aligned} V'_{SCK}(r_e) &= \alpha D_e e^{-\alpha r_e} [\cosh(\alpha \delta r_e) - \delta \sinh(\alpha \delta r_e)], \\ V_K(r \rightarrow \infty) - V(r_e) &= D_e e^{-\alpha r_e} \cosh(\alpha \delta r_e). \end{aligned} \quad (6)$$

We appreciate that the parameters D_e and r_e are not de dissociation energy and equilibrium bond length, respectively. Once again we conclude that all the physical results and conclusions derived from this assumption may not be correct [6].

Purohit et al [7] also proposed the Hulthén-screened cosine Kratzer potential

$$V_{HSCK}(r) = -\frac{V_0 e^{-\alpha r}}{1 + e^{-\alpha r}} - 2D_e \left(\frac{r_e}{r} - \frac{r_e^2}{2r^2} \right) e^{-\delta \alpha r} \cosh(\delta \lambda \alpha r), \quad (7)$$

where λ is another screening parameter. Once again, the authors are unclear about the values of the screening constants. Here, we assume that $\alpha \geq 0$, $\delta \geq 0$ and $-1 \leq \lambda \leq 1$. The authors chose $\lambda = 0, 1/2, 1$ in their applications. This potential does not satisfy equations (1) as shown by

$$\begin{aligned} V'_{HSCK}(r_e) &= \alpha \delta D_e e^{-\alpha \delta r_e} [\cosh(\alpha \delta \lambda r_e) - \lambda \sinh(\alpha \delta \lambda r_e)] + \frac{\alpha V_0 e^{\alpha r_e}}{(1 + e^{\alpha r_e})^2}, \\ V_{HSCK}(r \rightarrow \infty) - V_{HSCK}(r_e) &= D_e e^{-\alpha \delta r_e} \cosh(\alpha \delta \lambda r_e) + \frac{V_0}{1 + e^{\alpha r_e}}. \end{aligned} \quad (8)$$

As in the preceding examples, D_e and r_e are not the molecular parameters just mentioned.

Ikot et al [8] also proposed the improved screened Kratzer potential (also known as improved Kratzer potential [9])

$$V_{ISK}(r) = -2D_e \left(\frac{r_e}{r} - \frac{r_e^2}{2r^2} \right) \left[e^{-\frac{\alpha+\delta}{2}r} \cosh\left(\frac{\alpha+\delta}{2}r\right) + \tau \right], \quad (9)$$

where τ is a control parameter with values $-1, 0$ and 1 . This potential can be simplified as

$$V_{ISK}(r) = -2D_e \left(\frac{r_e}{r} - \frac{r_e^2}{2r^2} \right) \left[\frac{e^{-(\alpha+\delta)r}}{2} + \tau + \frac{1}{2} \right]. \quad (10)$$

Despite its improvement, this potential does not satisfy equations (1) because

$$\begin{aligned} V'_{ISK}(r_e) &= \frac{(\alpha + \delta)D_e e^{-\frac{\alpha + \delta}{2}r_e}}{2} \left[\cosh\left(\frac{\alpha + \delta}{2}r_e\right) - \sinh\left(\frac{\alpha + \delta}{2}r_e\right) \right], \\ V_{ISK}(r \rightarrow \infty) - V_{ISK}(r_e) &= D_e \left[e^{-\frac{\alpha + \delta}{2}r_e} \cosh\left(\frac{\alpha + \delta}{2}r_e\right) + \tau \right]. \end{aligned} \quad (11)$$

It is clear that D_e and r_e do not have their intended meaning.

Ibrahim et al [11] invented the shifted screened Kratzer potential

$$V_{SSK}(r) = -2D_e \left(\frac{r_e}{r} - \frac{r_e^2}{2r^2} \right) (2\lambda + \gamma e^{-\alpha r}), \quad (12)$$

where λ and γ are shifting parameters. The expressions

$$V'_{SSK}(r_e) = \alpha \gamma D_e e^{-\alpha r_e}, \quad V_{SSK}(r \rightarrow \infty) - V_{SSK}(r_e) = D_e (\gamma e^{-\alpha r_e} + 2\lambda), \quad (13)$$

undoubtedly show that r_e and D_e are not the equilibrium bond length and dissociation energy, respectively.

Finally, we mention the harmonic plus screened Kratzer potential of Bansal et al [12]

$$V_{HSK}(r) = -2D_e \left(\frac{r_e}{r} - \frac{r_e^2}{2r^2} \right) e^{-\alpha r} + cr^2. \quad (14)$$

Since there are no bound states when $c < 0$ we only consider $c \geq 0$. For $c = 0$ we have the screened Kratzer potential discussed above and for $c > 0$ (the novelty of this proposal) this potential does not predict dissociation because $V_{HSK}(r \rightarrow \infty) = \infty$. Not only there is no dissociation energy but r_e is not the equilibrium bond length because

$$V'_{HSK}(r_e) = \alpha D_e e^{-\alpha r_e} + 2cr_e. \quad (15)$$

In conclusion, we have shown that all the potentials described above suffer from the same flaw: in all of them r_e and D_e are not the equilibrium bond length and the dissociation energy, respectively. In the physical applications the authors substituted the experimental values of the equilibrium bond length and dissociation energy into those model parameters. For this reason the vibrational-rotational energies that they calculated and showed in several tables appear to be of scarce utility. Note that they did not attempt to compare their theoretical results with experimental data. In the next section we show how to modify the potentials discussed above in such a way that the model parameters r_e and D_e have the correct meaning.

3. The Correct Form of the Potentials

Most of the potentials described in the preceding section are particular cases of

$$V_G(r) = \left(\frac{a}{r} + \frac{b}{r^2} \right) f(r), \quad (16)$$

where we assume that $f(r \rightarrow \infty) = 0$. If we substitute this expression into equations (1) we obtain a system of two equations with two unknowns: a and b . Upon solving such system of equations we obtain the desired potential. A straightforward calculation shows that

$$V_G(r) = -\frac{2D_e f(r)}{f(r_e)} \left[\frac{r_e}{r} - \frac{r_e^2}{2r^2} + \frac{r_e f'(r_e)}{2f(r_e)} \left(\frac{r_e^2}{r^2} - \frac{r_e}{r} \right) \right]. \quad (17)$$

We appreciate that this expression yields the Kratzer potential when $f(r) \equiv 1$. When $f(r) = e^{-\alpha r}$ we obtain the correct form of the shifted Kratzer potential

$$V_{SK}(r) = D_e \left[\frac{(\alpha r_e + 1)r_e^2}{r^2} - \frac{(\alpha r_e + 2)r_e}{r} \right] e^{-\alpha(r-r_e)}. \quad (18)$$

One can easily verify that this form of the potential already satisfies equations (1). We can proceed in the same way with the other potentials but we do not deem it necessary.

In closing this section, we mention that the Hulthén-screened cosine Kratzer potential is a particular case of

$$V_{G2}(r) = \left(\frac{a}{r} + \frac{b}{r^2} \right) f(r) + g(r), \quad (19)$$

where, for convenience, we choose $g(r \rightarrow \infty) = 0$. We can easily obtain suitable expressions for a and b as in the preceding case so that the resulting potential will satisfy equations (1).

4. Further Comments and Conclusions

In Section 2 we showed that several potentials proposed recently for the analysis of the rotational-vibrational spectra of diatomic molecules and their thermodynamic properties exhibit a serious flaw. The model parameters r_e and D_e in those potentials are not the equilibrium bond length and dissociation energy, respectively, as the proposers believed. The authors inserted experimental values for those model parameters obtaining potentials that are unsuitable for the intended physical application. For this reason, the results obtained by those authors are of doubtful utility.

In Section 3 we solved the problem in a simple way. We thus arrived at a general expression that gives the correct form of those potentials in which r_e and D_e are the molecular parameters mentioned above. However, it is worth noting that the calculation of vibrational-rotational energies by means of an empirical potential is of no utility whatsoever [3]. Any serious spectroscopist would fit the eigenvalues of the model to the molecular spectrum in order to obtain the desired model parameters. The quality of the model is given by the square deviation of the fit.

References

1. A. Kratzer, Z. Physik **3**, 289 (1920).
2. E. Fues, Ann. Phys. **386**, 281 (1926).
3. G. Herzberg, Molecular Spectra and Molecular Structure. I. Spectra of Diatomic Molecules, Second ed. (Van Nostrand Reinhold, New York, 1950).
4. A. N. Ikot, U. S. Okorie, R. Sever, and G. J. Rampho, Eur. Phys. J. Plus **134**, 386 (2019).
5. A. N. Ikot, C. O. Edet, P. O. Amadi, U. S. Okorie, G. J. Rampho, and H. Y. Abdullah, Eur. Phys. J. D **74**, 159 (2020).
6. K. R. Purohit, R. H. Parmar, and A. K. Rai, Eur. Phys. J. Plus **135**, 286 (2020).
7. K. R. Purohit, R. H. Parmar, and A. K. Rai, J. Mol. Model **27**, 358 (2021).
8. A. N. Ikot, U. S. Okorie, G. J. Rampho, P. O. Amadi, C. O. Edet, I.O. Akpan, H. Y. Abdullah, and R. Horchani, J. Low Temp. Phys. **202**, 269 (2021).
9. G. J. Rampho, A. N. Ikot, C. O. Edet, and U. S. Okorie, Mol. Phys. **119**, e1821922 (2021).
10. C. O. Edet, A. N. Ikot, M. C. Onyeaju, U. S. Okorie, G. J. Rampho, M. L. Lekala, and S. Kaya, Physica E **131**, 114710 (2021).
11. N. Ibrahim, U. S. Okorie, N. Sulaiman, G. J. Rampho, and M. Ramantswana, Front. Phys. **10**, 988279 (2022).
12. M. Bansal, V. Kumar, R. M. Singh, S. B. Bhardwaj, and F. Chand, Mol. Phys. **121**, e2232472 (2023).

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