

## Short Communication

# The Family of Tietz Potentials

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We show that several potential-energy functions based on the exponential function  $e^{-\alpha r}$ ,  $\alpha > 0$ , are either equivalent or identical to the Tietz potential. Some of those potentials exhibit redundant parameters that can be removed without affecting their performance for the description of the vibration-rotation spectra of diatomic molecules.

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## 1. Introduction

Several potentials based on the exponential function  $e^{-\alpha r}$ ,  $\alpha > 0$ , have been proposed in the last decades for the treatment of the vibration-rotation spectra of diatomic molecules. In two papers<sup>[1][2]</sup> we have shown that most of those potentials are equivalent to the Tietz one. To prove this fact we resorted to what we have called normalization method that consists in rewriting a given potential in terms of the equilibrium bond length  $r_e$  and the dissociation energy  $D_e$ . The choice of a particular, well defined, normal form for all potentials facilitated their comparison no matter their intricacy. In addition to prove that all those potentials are equivalent to the Tietz one, we have also shown that most of them exhibit redundant parameters.

A question arises if those potentials are equivalent only when they are written in terms of  $r_e$  and  $D_e$ ; that is to say, if they are required to have a minimum. In this paper we will answer this question by direct comparison of the potentials.

## 2. Normalization method

For the sake of clarity, we first review the normalization method<sup>[1][2]</sup>. Consider a potential  $V(r)$ ,  $r > 0$ , that depends on two or more adjustable parameters. We require that this potential exhibits a minimum

at  $r = r_e$  and a finite value when  $r \rightarrow \infty$  (like most commonly accepted molecular potentials). In order to achieve this goal we force the given analytical function to satisfy the obvious equations

$$V'(r_e) = 0, \lim_{r \rightarrow \infty} V(r) - V(r_e) = D_e > 0, \quad (1)$$

from which we obtain two model parameters in terms of  $r_e$ ,  $D_e$  and the remaining potential parameters.

If  $r_e$  is the minimum of the potential ( $V''(r_e) > 0$ ) we then rewrite it in normal form<sup>[1][2]</sup>

$$V(r) - V(r_e) = D_e[1 - f(r)]^2. \quad (2)$$

Since  $\lim_{r \rightarrow \infty} [1 - f(r)]^2 = 1$  we conclude that the two roots  $f_0(r)$  and  $f_2(r)$  of the quadratic equation (2) behave asymptotically as  $\lim_{r \rightarrow \infty} f_0(r) = 0$  and  $\lim_{r \rightarrow \infty} f_2(r) = 2$ . We always choose  $f_0(r)$  in order to provide a consistent representation of  $V(r)$  in normal form.

As an example, consider the polynomial potential

$$V_P(r) = a + \frac{b}{e^{\alpha r} + d} + \frac{c}{(e^{\alpha r} + d)^2}, \alpha > 0, \quad (3)$$

where  $d \geq -1$  in order to avoid an unphysical singularity in  $0 < r < \infty$ . Clearly,  $a$  is an irrelevant energy shift that does not appear in equations (1); however, it will be useful for comparing  $V_P(r)$  with other potentials. If we solve equations (1) for  $b$  and  $c$  we obtain

$$b = -2D_e(e^{\alpha r_e} + d), c = D_e(e^{\alpha r_e} + d)^2, \quad (4)$$

and the normal form

$$V_P(r) - V_P(r_e) = V_N(r) = D_e \left( 1 - \frac{e^{\alpha r_e} + d}{e^{\alpha r} + d} \right)^2, \quad (5)$$

of the potential (3).

If we define  $k = V''(r_e)$  and  $k_3 = V'''(r_e)$  then the remaining model parameters can be determined from the following equations

$$\begin{aligned} d &= e^{\alpha r_e} \left( \alpha \sqrt{\frac{2D_e}{k}} - 1 \right), \\ \alpha &= \sqrt{\frac{2k}{D_e}} + \frac{k_3}{3k}. \end{aligned} \quad (6)$$

The polynomial potential contains one irrelevant energy shift  $a$  and four adjustable parameters  $b$ ,  $c$ ,  $d$  and  $\alpha$  that can be expressed in terms of  $r_e$ ,  $D_e$ ,  $k$  and  $k_3$  that can be obtained from spectroscopic data<sup>[3]</sup>.

We say that two potentials  $V_1(r)$  and  $V_2(r)$  are equivalent if  $V_1'(r) - V_2'(r) = 0$  for all  $r$ . The reason is that the Hamiltonian operators  $H = T + V_i(r)$ ,  $i = 1, 2$ , where  $T$  is the kinetic-energy operator, have the

same eigenfunctions and their eigenvalues are displaced by the irrelevant energy shift  $\Delta = V_1(r) - V_2(r)$ . Therefore,  $V_1(r)$  and  $V_2(r)$  describe the same physical model. If  $V_1(r)$  is equivalent to  $V_2(r)$  and  $V_2(r)$  is equivalent to  $V_3(r)$  then  $V_1(r)$  is equivalent to  $V_3(r)$  as follow from  $V_1'(r) - V_3'(r) = V_1'(r) - V_2'(r) + V_2'(r) - V_3'(r) = 0$ . A particular case of equivalent potentials is that of identical potentials for which  $\Delta = 0$ .

According to the definition above  $V_P(r)$  is equivalent to  $V_N(r)$  when the potential parameters are given by equation (4). In what follows  $V_P(r, a, b, c, d, \alpha)$  will denote the polynomial potential (3). We keep the irrelevant energy shift  $a$  in order to facilitate comparison with other potentials based on exponential functions because we will look for exact identity. Given a potential  $V_G(r)$  we will rewrite it as  $V_G(r) = V_P(r, a, b, c, d, \alpha)$  indicating the corresponding values of  $a, b, c, d$ , and  $\alpha$ .

### 3. Tietz potential

One of the most relevant potentials for present analysis was proposed by Tietz<sup>[4]</sup> several years ago

$$V_T(r) = D_e + D_e \frac{(a+b)e^{-2\beta r} - be^{-\beta r}}{(1+ce^{-\beta r})^2}, \beta > 0, \quad (7)$$

where  $c \geq -1$  in order to avoid an unphysical singularity in  $0 < r < \infty$ .

We can easily prove that the Tietz potential is identical to the polynomial one:

$$V_T(r) = V_P(r, a', b', c', d', \alpha), a' = D_e, b' = -bD_e, c' = aD_e + bD_e(c+1), \\ d' = c, \alpha = \beta. \quad (8)$$

The simple potential

$$V_S(r) = \frac{A + Be^{-\alpha r}}{(1 - Ce^{-\alpha r})^2} + D, \quad (9)$$

is also identical to the polynomial one as shown by

$$V_S(r) = V_P(r, a, b, c, d, \alpha), a = A + D, b = 2AC + B, c = C(AC + B), \\ d = -C. \quad (10)$$

The potentials  $V_P(r)$  and  $V_S(r)$  are the simplest members of the Tietz family.

### 4. Other potentials based on exponential functions

The Hua potential<sup>[5]</sup>

$$U_H(r) = D_e \left[ \frac{1 - e^{-b(r-r_e)}}{1 - ce^{-b(r-r_e)}} \right]^2, b > 0, \quad (11)$$

is given in terms of four parameters and it also belongs to the Tietz family

$$\begin{aligned} U_H(r) &= V_P(r, a', b', c', d', b), a' = D_e, b' = 2D_e e^{br_e} (c - 1), \\ c' &= D_e e^{2br_e} (c - 1)^2, d' = -ce^{br_e}. \end{aligned} \quad (12)$$

Şimşek and Özçelik<sup>[6]</sup> proposed the four-parameter exponential type potential (FPEP)

$$V_{\text{FPEP}}(r) = \frac{Ae^{\lambda r}}{C + e^{\lambda r}} - \frac{Be^{\lambda r}}{(C + e^{\lambda r})^2}, A, B > 0, \quad (13)$$

that is just another member of the Tietz family

$$V_{\text{FPEP}}(r) = V_P(r, a', b', c', d', \lambda), a' = A, b' = -AC - B, c' = BC, d' = C. \quad (14)$$

Jia et al.<sup>[7]</sup> introduced a deformed five-parameter exponential-type potential (DFPEP)

$$V_{\text{DFPEP}}(r) = P_1 + \frac{P_2}{e^{2\alpha r} + q} + \frac{P_3}{(e^{2\alpha r} + q)^2}, \alpha > 0, \quad (15)$$

that is identical to the polynomial potential

$$V_{\text{DFPEP}}(r) = V_P(r, P_1, P_2, P_3, q, 2\alpha), \quad (16)$$

and consequently is a member of the Tietz family.

Boonserm and Visser<sup>[8]</sup> showed that several potentials are equivalent to the Möbius square potential

$$V(r) = V_0 \left( \frac{A + Be^{-\alpha r}}{C + De^{-\alpha r}} \right)^2. \quad (17)$$

It can be rewritten in terms of the polynomial potential as

$$\begin{aligned} V(r) &= V_P(r, a, b, c, d, \alpha), a = V_0 \frac{A^2}{C^2}, b = V_0 \frac{2A(BC - AD)}{C^3}, \\ c &= V_0 \frac{(AD - BC)^2}{C^4}, d = \frac{D}{C}, \end{aligned} \quad (18)$$

and therefore belongs to the Tietz family.

Falaye et al.<sup>[9]</sup> proposed the shifted Tietz-Wei (sTW) oscillator

$$V_{\text{sTW}}(r) = V_e \frac{2(c_h - 1)e^{-b_h(r-r_e)} - (c_h^2 - 1)e^{-2b_h(r-r_e)}}{[1 - c_h e^{-b_h(r-r_e)}]^2}, b_h > 0, \quad (19)$$

given in terms of four adjustable parameters. It can be rewritten as

$$\begin{aligned} V_{\text{sTW}}(r) &= V_P(r, 0, b', c', d', b_h), b' = 2e^{b_h r_e} (c_h - 1), \\ c' &= e^{2b_h r_e} (c_h - 1)^2, d' = -c_h e^{b_h r_e}, \end{aligned} \quad (20)$$

which proves that it belongs to the Tietz family.

Onate et al.<sup>[10]</sup> proposed the q-deformed six-parameter exponential-type potential model

$$V_{\text{qDSPEP}}(r) = Q_1 - \frac{Q_2}{1 - qe^{-2\alpha r}} + \frac{Q_3 e^{-2\alpha r}}{1 - qe^{-2\alpha r}} - \frac{Q_4 e^{-4\alpha r}}{(1 - qe^{-2\alpha r})^2}, \alpha > 0, \quad (21)$$

that is identical to the polynomial potential as shown by

$$V_{\text{qDSPEP}}(r) = V_P(r, a, b, c, d, 2\alpha), a = Q_1 - Q_2, b = Q_3 - qQ_2, c = -Q_4, \\ d = -q, \quad (22)$$

and also belongs to the Tietz family. Note that if we choose  $Q_2 = 0$  or  $Q_3 = 0$  the performance of the model is not affected. Any one of those parameters is redundant.

Okorie et al.<sup>[11]</sup> proposed the deformed exponential-type potential (DEP)

$$U_{\text{DEP}}(r) = P_1 + \frac{P_2 e^{-2\alpha(r-r_0)}}{1 - qe^{-2\alpha(r-r_0)}} + \frac{P_3 e^{-4\alpha(r-r_0)}}{[1 - qe^{-2\alpha(r-r_0)}]^2}, \quad (23)$$

that is also identical to the polynomial potential

$$U_{\text{DEP}}(r) = V_P(r, a, b, c, d, 2\alpha), a = P_1, b = P_2 e^{2\alpha r_0}, c = P_3 e^{4\alpha r_0}, \\ d = -qe^{2\alpha r_0}, \quad (24)$$

and belongs to the Tietz family. In this case we can choose  $r_0 = 0$  without affecting the performance of the model. This parameter is redundant.

In their research Onyenegecha et al.<sup>[12]</sup> and Yanar et al.<sup>[13]</sup> resorted to the potential

$$V_{\text{MH}}(r) = -V_0 \left( \frac{A + Be^{-2\alpha r}}{1 - e^{-2\alpha r}} \right)^2 + \frac{V_1 e^{-2\alpha r}}{1 - e^{-2\alpha r}}, \quad (25)$$

that is also identical to the polynomial potential

$$V_{\text{MH}}(r) = V_P(r, a, b, c, -1, 2\alpha), a = -V_0 A^2, b = V_1 - 2V_0 A(A + B), \\ c = -V_0(A + B)^2, \quad (26)$$

and belongs to the Tietz family.  $V_{\text{MH}}(r)$  is a three-parameter model because  $d = -1$ . In this case we can choose, for example,  $V_1 = 0$  and  $A = 1$  without affecting the model performance. In other words, two parameters are redundant.

Yanar et al.<sup>[13]</sup> mentioned the apparently more general six-parameter potential-energy function

$$V_{\text{MH+}}(r) = -U_0 \left( \frac{A + Be^{-2\alpha r}}{1 - e^{-2\alpha r}} \right)^2 - \frac{U_1 e^{-2\alpha r}}{1 - e^{-2\alpha r}} + \frac{U_2 e^{-2\alpha r}}{(1 - e^{-2\alpha r})^2}, \quad (27)$$

that had been used earlier by Njoku et al.<sup>[14]</sup> and Onyenegecha et al.<sup>[15]</sup>. This potential can also be reduced to the polynomial potential

$$V_{\text{MH}^+}(r) = V_{\text{P}}(r, a, b, c, -1, 2\alpha), a = -U_0 A^2, b = U_1 + U_2 - 2U_0 A(A + B), \\ c = U_2 - U_0(A + B)^2, \quad (28)$$

and belongs to the Tietz family. It is also a three-parameter model because  $d = -1$ . In this case we can choose  $A = 1$ ,  $U_1 = 0$  and  $U_2 = 0$  without affecting the model performance. There are three redundant parameters.

Yanar et al.<sup>[16]</sup> and Yanar<sup>[17]</sup> made extensive use of the general molecular potential

$$V_{\text{GMP}}(r) = \frac{A - Be^{-\alpha(r-r_e)} + \tilde{q} [C - De^{-\alpha(r-r_e)}]^2}{[1 - qe^{-\alpha(r-r_e)}]^2}, \quad (29)$$

that is also identical to the polynomial potential

$$V_{\text{GMP}}(r) = V(r, a, b, c, d, \alpha), a = A + \tilde{q} C^2, \\ b = e^{\alpha r_e} [2Aq - B + 2C\tilde{q} (Cq - D)], \\ c = e^{2\alpha r_e} [Aq^2 - Bq + \tilde{q} (D^2 - 2CDq + C^2 q^2)], \\ d = -qe^{\alpha r_e}, \quad (30)$$

and belongs to the Tietz family. In this case we can choose  $\tilde{q} = 0$  (or  $C = D = 0$ ) and  $r_e = 0$  without affecting the model performance. Note that when  $\tilde{q} = 0$  and  $r_e = 0$  we obtain the simple potential (9). The parameters  $\tilde{q}$ ,  $C$ ,  $D$  and  $r_e$  are redundant. Note that  $\left. \frac{dV_{\text{GMP}}}{dr} \right|_{r=r_e} \neq 0$  and the equilibrium bond length appears when we use equations (1).

## 5. Conclusions

The results given above show that many potentials built from the exponential function  $e^{-\alpha r}$  are identical (or at least equivalent) to the Tietz potential. When used for the study of the vibration-rotation spectra of diatomic molecules, all of them reduce to an identical expression given in terms of  $r_e$  and  $D_e$  like equation (5) that can be complemented by equations (6). None of those potentials provide any advantage with respect to such physical application.

Some of the potentials discussed in the preceding section exhibit redundant parameters that can be removed without affecting the performance of the model. This is the case of the potentials proposed by Onate et al.<sup>[10]</sup>, Okorie et al.<sup>[11]</sup>, Onyenegecha et al.<sup>[12]</sup>, Yanar et al.<sup>[13]</sup>, Njoku et al.<sup>[14]</sup>, Onyenegecha et al.<sup>[15]</sup>, Yanar et al.<sup>[16]</sup> and Yanar<sup>[17]</sup>.

## References

1. <sup>a, b, c</sup>Fernández FM. "Equivalent Potential-Energy Functions." arXiv:2606.00378 [math-ph].
2. <sup>a, b, c</sup>Fernández FM. "On Some Potentials Based on Exponential Functions." arXiv:2607.25805 [quant-ph].
3. <sup>Δ</sup>Herzberg G (1950). *Molecular Spectra and Molecular Structure. I. Spectra of Diatomic Molecules*. 2nd ed. New York: Van Nostrand Reinhold.
4. <sup>Δ</sup>Tietz T (1963). *J Chem Phys*. **38**:3036.
5. <sup>Δ</sup>Hua W (1990). *Phys Rev A*. **42**:2524.
6. <sup>Δ</sup>Şimşek M, Özçelik S (1994). *Phys Lett A*. **186**:35.
7. <sup>Δ</sup>Jia CS, Zhang Y, Zeng XL, Sun LT (2001). *Commun Theor Phys*. **36**:641.
8. <sup>Δ</sup>Boonserm P, Visser M (2011). *JHEP*. **03**:073.
9. <sup>Δ</sup>Falaye BJ, Ikhdair SM, Hamzavi M (2015). *J Theor Appl Phys*. **9**:151.
10. <sup>a, b</sup>Onate CA, Onyeaju MC, Okorie US, Ikot AN (2020). *Res Phys*. **16**:102959.
11. <sup>a, b</sup>Okorie US, Ikot AN, Chukwuocha EO (2020). *Bull Korean Chem Soc*. **41**:609.
12. <sup>a, b</sup>Onyenegecha CP, Onate CA, Echendu OK, Ibe AA, Hassanabadi H (2020). *Eur Phys J Plus*. **135**:289.
13. <sup>a, b, c</sup>Yanar H, Sahin O, Salti M, Aydogdu O (2024). *Eur Phys J Plus*. **139**:896.
14. <sup>a, b</sup>Njoku IJ, Onyeocha E, Onyenegecha CP, Onuoha M, Egeonu EK, Nwaokafor P. *Int J Quantum Chem*. **123**:e27050.
15. <sup>a, b</sup>Onyenegecha CP, Njoku IJ, Opara AI, Echendu OK, Omoko EN, Eze FC, Okereke CJ, Onyeocha E, Nwaneho FU (2022). *Heliyon*. **8**:e08952.
16. <sup>a, b</sup>Yanar H, Aydoğdu O, Saltı M (2016). *Mol Phys*. **114**:3134.
17. <sup>a, b</sup>Yanar H (2022). *Phys Scr*. **97**:045404.

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