

COMMENTS

Comments are short papers which criticize or correct papers of other authors previously published in the Physical Review. Each Comment should state clearly to which paper it refers and must be accompanied by a brief abstract. The same publication schedule as for regular articles is followed, and page proofs are sent to authors.

Comment on "Four-parameter exactly solvable potential for diatomic molecules"

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This Comment precludes any chance of discovering a new potential that would allow one to solve the one-dimensional Schrödinger equation in terms of hypergeometric functions. In particular, it argues that the potential function suggested by Hua [Phys. Rev. A **42**, 2524 (1990)] is the well-known Tietz potential, which in turn is a combination of the Rosen-Morse, Morse, and Manning-Rosen potentials presented in a common form.

In a recent publication [1], Hua suggested a "new" analytical function to fit to the adiabatic potentials of diatomic molecules. It is, however, simply the well-known "Tietz potential" [2], which turns into, respectively, the Rosen-Morse [3], Morse [4], and Manning-Rosen [5] potentials for negative, zero, and positive values of the parameter c in Hua's notation. The quality of fits to RKR potentials using the Tietz potential has been emphasized, for example, by Pack [6]. It is, however, commonly overlooked that Tietz simply rediscovered a slightly different form of the known potentials. In fact, by setting $c = \pm e^{bx^0}$ one can represent the potential (7) in Hua's paper as

$$U(r) = \frac{e^{b(r-r^e)} + e^{-b(r-r^e)} - 2}{e^{bx^0} [e^{b(r-x^0-r^e)/2} \pm e^{-b(r-x^0-r^e)/2}]^2}. \quad (1)$$

The standard expressions for both Rosen-Morse [3] and Manning-Rosen [5] potentials are then obtained from (1) by the substitutions

$$e^{\pm b(r-r^e)} = \frac{1}{4} e^{\pm bx^0} \left[\operatorname{ch} \left[\frac{b(r-x^0-r^e)}{2} \right] \pm \operatorname{sh} \left[\frac{b(r-x^0-r^e)}{2} \right] \right]^2. \quad (2)$$

Tietz thus found a single analytical representation for these two potentials with the Morse potential [4] serving as a bridge between the branches. However, to transform the Schrödinger equation to the hypergeometric form (with the boundary conditions imposed at the points 0 and 1), one should use a different change of variables for each branch. On the other hand, at the juncture of the two branches, wave functions are expressed in terms of confluent hypergeometric functions. Therefore the Schrödinger equation with the Tietz potential still has

well-distinguished analytical solutions for different branches.

As proved by the author of this Comment, who performed a general analysis of this problem 20 years ago [7], all practically significant analytical potentials allowing solution of the one-dimensional Schrödinger equation in terms of hypergeometric functions have been already reported in the literature (see Ref. [8] for a more recent exposition of this analysis). The performed analysis precludes any chance of discovering a new potential of such a kind.

It was Lotmar [9] who first demonstrated that the Rosen-Morse potential is expected to provide the best fits in most cases. This was true for the three molecules HgH, CdH, and O₂ selected by Lotman [9], in following Rydberg's famous works [10]. The analysis was significantly simplified by introducing the parameter \sqrt{D}/δ , where D is the dissociation energy and δ is a combination of some spectroscopic constants directly extracted from observed infrared spectra. As proven by Lotmar, $\sqrt{D}/\delta = V'''(r_e)/U_M'''(r_e)$ for an arbitrary potential $V(r)$. [Here we use Hua's notation $U_M(r)$ for the Morse potential.] As follows from Hua's relation (10), $\sqrt{D}/\delta = 1 + c$ for the Tietz potential so that $\sqrt{D}/\delta > 1$ for the Manning-Rosen potential and $\sqrt{D}/\delta < 1$ for the Rosen-Morse potential. Lotmar [9] also showed that $\sqrt{D}/\delta > 1$ for the Pöschl-Teller potential [11]. The experimental data for all three molecules analyzed by Lotmar [9] led to values of this parameter smaller than 1, which unambiguously selected the Rosen-Morse potential over the others. Direct comparison of the Rosen-Morse and Morse potentials with the curve derived by Rydberg [10] from the spectrum of each of the three molecules clearly demonstrated a better agreement of the Rosen-Morse potential with the experimental curve. By analogy, an analysis of Hua's Table II shows that the parame-

ter c is negative for the most molecules, in agreement with Lotmar's conclusions. Only for three molecules HF, H₂, and CO does the Manning-Rosen potential provide better fits to the RKR curves. Taking into account that

the parameter \sqrt{D}/δ turns out to be larger than 1 for these molecules, the Pöschl-Teller potential advocated by Zhirnov and Shadrin [12] should be considered in this case as a possible alternative to the Tietz potential.

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