

Reply to "Comment on 'Fine-structure and analytical quantum-defect wave functions'"

V. Alan Kostelecký

Department of Physics, Indiana University, Bloomington, Indiana 47405

Michael Martin Nieto

Theoretical Division, Los Alamos National Laboratory, University of California, Los Alamos, New Mexico 87545

D. Rodney Truax

Department of Chemistry, University of Calgary, Calgary, Alberta, Canada T2N 1N4

(Received 27 March 1989)

The preceding Comment by Goodfriend [Phys. Rev. A **41**, 1730 (1990)] contains three criticisms of our model for analytical quantum-defect wave functions *vis-à-vis* the atomic Fues potential of Simons [J. Phys. Chem. **55**, 756 (1971)]. We rebut the first two criticisms explicitly. This makes the third criticism moot. We stand by our results.

The preceding Comment¹ by Goodfriend discusses our papers²⁻⁵ on the supersymmetry-inspired quantum-defect model (QDM). The Comment especially criticizes our latest paper⁵ in three respects. It claims that (i) reference was not given to literature with mathematical solutions of our type, (ii) our model is equivalent to the 1971 atomic Fues potential (AFP) of Simons,⁶ and hence (iii) our wave functions yield "unreliable" expectation values. The latter claim is only on the grounds of Goodfriend's assertion that the AFP wave functions are unreliable.

We will rebut the first two assertions explicitly; the rebuttal of point (ii) thereby will make the assertion (iii) moot.

(i) *History.* In Ref. 7 of our previous paper,⁴ we observe that the mathematical solutions exist in the classic work of Infeld and Hull.⁷ This work was published some 20 years before Simons's paper.

Note also that in 1967 Parsons and Weisskopf⁸ proposed on physical grounds that the alkali-metal atoms should have the principle-quantum-number labeling of the AFP.

(ii) *Physics.* Our model is not the same as Simons's, even though the casual reader might think so. The truth of this assertion is related to one of the fundamental concepts of modern quantum mechanics: isospectral Hamiltonians.⁹⁻¹⁶ The point is that there are an infinite number of physically inequivalent potentials that have the same energy eigenvalues. To establish the physics one needs not only the eigenvalues but also the scattering data, e.g., wave functions and therefore transition probabilities.

We will show in general and also by specific example that Simons's wave functions and transition probabilities are inequivalent to ours. This proves the inequivalence of the two models.

To begin, we establish the two models in compatible notation. We use spectroscopic notation (n, l) to denote energy levels. The lowest physical value of n in a given series is denoted n_{\min} , e.g., $n_{\min} = 3$ for the sodium s and p levels. A caret is used to denote the value of an AFP

quantity in our QDM notation.

The effective potential in the QDM is

$$V^{\text{QDM}} = [l^*(l^* + 1) - l(l + 1)]/y^2, \quad (1)$$

where

$$l^* = l - \delta(l) + I(l), \quad (2)$$

$$y = \frac{2\mu e^2}{\hbar^2} r.$$

Here, $\delta(l)$ is the quantum defect, and the integer $I(l)$ is constrained to lie in the range

$$\delta(l) - l - \frac{1}{2} < I(l) \leq n_{\min} - l - 1 \quad (3)$$

by the requirement that the kinetic energy, the potential energy, and the wave functions are separately normalizable.⁴ The QDM eigenenergies are¹⁷

$$E_n^{\text{QDM}} = -\frac{1}{4n^{*2}}, \quad (4)$$

where

$$n^* = n - \delta(l) \quad (5)$$

with

$$n = n_{\min}, n_{\min} + 1, \dots \quad (6)$$

The effective potential in the AFP is

$$V^{\text{AFP}} = 2B_l/y^2 \equiv [\hat{l}^*(\hat{l}^* + 1) - l(l + 1)]/y^2, \quad (7)$$

where B_l is Simons's eigenenergy-matching parameter. The AFP eigenenergies are

$$E_n^{\text{AFP}} = -\frac{1}{4\hat{n}^{*2}}, \quad (8)$$

where

$$\hat{n}^* = P + \frac{1}{2} + [(l + \frac{1}{2})^2 + 2B_l]^{1/2} \quad (9)$$

with

$$P = n - n_{\min} = 0, 1, 2, \dots \quad (10)$$

By definition,

$$n^* = \hat{n}^* \quad (11)$$

This relates the quantum defect $\delta(l)$ and the parameter B_l . (See Ref. 18.) It also means that any equivalence of the QDM and the AFP eigenfunctions would depend on l^* being equal to \hat{l}^* . From Eqs. (5), (7), (9), and (11) we obtain

$$\hat{l}^* = n - \delta(l) - P - 1 \quad (12)$$

Therefore, by comparing Eqs. (2), (10), and (12) we find that the equality of l^* and \hat{l}^* holds if and only if

$$I(l) = n_{\min} - l - 1 \quad (13)$$

However, from Eq. (3) we see that in general this condition is *not* satisfied. This proves the inequivalence of the QDM and the AFP.

To emphasize this proof, we consider the particular case of the $3s$ -to- $2p$ transition probability in lithium. (See Table I of Ref. 4.) For the QDM, the radial wave functions are

$$\begin{aligned} \psi^{\text{QDM}}(3s) &= R_{2.6, -0.4} \quad (14) \\ \psi^{\text{QDM}}(2p) &= R_{1.95, 0.95} \end{aligned}$$

where the normalized eigenfunctions R_{n^*, l^*} are given in Eq. (11) of Ref. 4. In contrast, for the AFP one has

$$\begin{aligned} \psi^{\text{AFP}}(3s) &= R_{2.6, 0.6} \quad (15) \\ \psi^{\text{AFP}}(2p) &= R_{1.95, 0.95} \end{aligned}$$

The inequivalence of the two models is already apparent.

Continuing, nevertheless, using Eqs. (13)–(15) of Ref. 4 to calculate the dipole matrix elements and hence the transition probabilities Γ , one finds (in units of 10^8 Hz) the different results

$$\begin{aligned} \Gamma^{\text{QDM}} &= 0.337 \quad (16) \\ \Gamma^{\text{AFP}} &= 0.478 \end{aligned}$$

Note that our QDM value agrees well with the accepted value $\Gamma^{\text{acc}} = 0.349$.

(iii) *Reliability of results.* As mentioned above, Goodfriend's third criticism concerning the reliability of our results is logically in error, given the discussion in (ii), and is therefore moot. In fact, Goodfriend's argument against our model is based on his assertion that applying his Simons-like pseudopotential to the excited states of the hydrogen atom yields incorrect results. This last is irrelevant to our model. For the hydrogen atom, our model necessarily reduces to the standard solutions because the quantum defect and the integer $I(l)$ are zero.

To summarize, the Rydberg levels for our potential are determined by n and by the quantum defect $\delta(l)$; those of Simons's potential depend on an integer P , the angular quantum number l , and a phenomenological parameter B_l . Even though the two descriptions agree on the eigenenergies, they are in general inequivalent because they can yield different eigenfunctions.

The new physics in our papers differentiates itself from standard physics in that our wave functions may have nonstandard nodal structures. Thus, given a Y_{lm} , the associated R_{nL} do not necessarily have $L = l$. This means the calculated results can be different. In fact, our results display good large-distance Coulomb character, as can be seen from the numerical successes of our model.^{3,4} These successes have led to the use of our eigenfunctions as trial wave functions for detailed numerical many-body calculations.¹⁹

An argument in favor of our potential is the good agreement we find⁴ with many-body calculations for transition probabilities in different atomic systems. Furthermore, our potential naturally incorporates the Landé formula.⁵

In conclusion, we stand by our results.

¹P. Goodfriend, Phys. Rev. A **41**, 1730 (1990).

²V. A. Kostecký and M. M. Nieto, Phys. Rev. Lett. **53**, 2285 (1984).

³V. A. Kostecký and M. M. Nieto, Phys. Rev. A **32**, 1293 (1985).

⁴V. A. Kostecký and M. M. Nieto, Phys. Rev. A **32**, 3243 (1985).

⁵V. A. Kostecký, M. M. Nieto, and D. R. Truax, Phys. Rev. A **38**, 4413 (1988).

⁶G. Simons, J. Chem. Phys. **55**, 756 (1971).

⁷L. Infeld and T. E. Hull, Rev. Mod. Phys. **23**, 21 (1951).

⁸R. G. Parsons and V. F. Weisskopf, Z. Phys. **202**, 492 (1967).

⁹There is an impressive body of work on isospectral Hamiltonians. We refer the reader to Bargmann's paper (Ref. 10) on phase-equivalent potentials, Schrödinger's discussion (Ref. 11) of the factorization method, the work of Abraham and Moses (Ref. 12) concerning the inverse method of Gel'fand and Levitan (Ref. 13), and Pursey's analysis (Ref. 14) of various families of isospectral Hamiltonians. Indeed, the

mathematical connections between the inverse method, the factorization method, and supersymmetric quantum mechanics (Ref. 15) helped motivate our papers (Refs. 2–5) under discussion here.

¹⁰V. Bargmann, Rev. Mod. Phys. **21**, 488 (1949).

¹¹E. Schrödinger, Proc. R. Ir. Acad., Sect. A **46**, 9 (1940). This work was championed by Infeld and Hull (Ref. 7). Its mathematics is that of supersymmetric quantum mechanics (Ref. 16).

¹²P. B. Abraham and H. E. Moses, Phys. Rev. A **22**, 1333 (1980).

¹³I. M. Gel'fand and B. M. Levitan, Izv. Akad. Nauk SSSR Ser. Mat. **15**, 309 (1951) [Bull. Acad. Sci. USSR, Math. Ser. **1**, 253 (1955)].

¹⁴D. L. Pursey, Phys. Rev. D **33**, 1048 (1986).

¹⁵M. M. Nieto, Phys. Lett. B **145**, 208 (1984).

¹⁶E. Witten, Nucl. Phys. B **185**, 513 (1981).

¹⁷Note that the reason for the factor of $\frac{1}{4}$ in Eq. (4) is that we have used (Refs. 2–5) units of *two* inverse Bohr radii, instead

of atomic or rydberg units. See, for example, the discussion around Eq. (3.71) of C. Quigg and J. L. Rosner, *Phys. Rep.* **56**, 167 (1979).

¹⁸Given numerical values of $\delta(l)$, Eqs. (5), (6), (9), and (11) should allow the determination of the values of B_l in Simons's tables (Ref. 6). However, there is a slight numerical ambiguity because Rydberg atoms do not really have constant $\delta(l)$ or B_l throughout an entire series. For example, the sodium 3s to 7s eigenvalues are $n^* = 1.626, 2.643, 3.647, 4.649, 5.650, \dots$

We have chosen to expand about the asymptotic value $\delta(l) = 1.35$ represented by the 7s and higher states. This implies the value $B_l = 0.536$. In contrast, Simons chose to expand about the value defined by the 3s state. He took $B_l = 0.510$, which implies the value $1.37 = \delta(l)$. Either expansion is valid.

¹⁹R. E. H. Clark and A. L. Merts, *J. Quant. Spectrosc. Radiat. Transfer* **38**, 287 (1987).