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Reply to "Comment on 'Analytical wave functions for atomic quantum-defect theory' "

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The preceding paper, by Martin and Barrientos [Phys. Rev. A **43**, 4061 (1991)], comments on our supersymmetry-inspired model of atomic physics. We relate this to other Comments [Rau, Phys. Rev. Lett. **56**, 95 (1986) and Goodfriend, Phys. Rev. A **41**, 1730 (1990)] and point out that, although the mathematics and physics of the 1974 Simons model [J. Chem. Phys. **60**, 645 (1974)] is similar to ours, it is not identical. This is elucidated by explicitly comparing our symmetry-based approach to the more phenomenological approach of Martin and Barrientos.

I. INTRODUCTORY REMARKS

The preceding paper by Martin and Barrientos (MB) is the third in a series[1–3] of independent Comments on our supersymmetry-inspired model of atomic systems.[4–9] In Sec. II we address the present Comment[3] in detail. However, we first wish to point out that logically, all three Comments cannot be correct because their assertions are contradictory.

It is important to emphasize that in pointing out the contradictory nature of these Comments we are not attempting to reopen the previous discussions. The reader is free to review the previous Comments (Refs. 1 and 2) versus our responses[7,9] to make an independent decision as to which, if any, of the stated arguments are correct. (However, note that our wave functions have since been used as trial wave functions for many-body calculations.[10])

The present Comment (III) declares that our supersymmetry-inspired model and its results have all been obtained before. As opposed to the 1971 Simons model,[11] supposedly our results are contained in the 1974 Simons model[12] and in papers developing in the 1974 model.[13–15] We reply to these remarks in detail in Sec. II, below.

Let us now elucidate the contradictions between the three Comments. First, Comment III agrees that our work is correct. Therefore, there is a conflict between Comment III and Comments I and II, which both claim that our work is incorrect.

Second, observe that Simons himself declared that his 1971 and 1974 models are inequivalent. In his 1974 paper Simons wrote,[12] "The new model is related to, but distinct from, standard quantum-defect treatments and pseudopotential calculations," referring explicitly to his 1971 paper.[11] Therefore, it is evident that Comment II and the present Comment (III), which claim, respectively, that our supersymmetry-inspired model is equivalent to the 1971 Simons model and the 1974 Simons model, cannot both be right.[16]

II. DETAILED REPLY

Our point of departure, that of finding and using a new symmetry (supersymmetry) in atomic physics, is complementary to that of the Simons school. This symmetry approach has been widely adopted in quantum mechanics, in both physics and chemistry, since Pauli showed that the matrix formalism of Heisenberg yields the Balmer formula. He did this by using the O(4) symmetry of the hydrogen atom, which is embedded in O(4,1).

Nowhere does Comment III, or the authors' other papers cited therein, discuss a supersymmetry or indeed any symmetry at all. Thus, even if the details of our results were identical to those of the Simons school, saying there is nothing new is the same as saying there is nothing in Pauli's work that is not in Schrödinger's work.

In addition to this, one of the complaints in Comment III about our work can be used to demonstrate subtle but explicit differences between our two programs.

Comment III complains that we make the "somewhat misleading remark" that for a given Rydberg series one can approximate $\delta(l)$ as a constant. They prefer to use a different $\delta(l,n)$ for every state, especially the low-lying ones. This use means they have a different potential for every level and effectively introduces an additional parameter in the system.[17] Therefore, more symmetry is lost. Further, this means that Comment III advocates *eigenvectors that are not orthogonal.* That is, $R(n^*,l^*,\delta_1)$ is not orthogonal to $R(n^*+\text{ integer}, l^*,\delta_2)$ if $\delta_1 \neq \delta_2$. Our eigenvectors are orthogonal, which is a manifestation of the symmetry we are studying.

The above, by itself, makes the two programs distinct, independent of the fundamentally different philosophy. Even so, if one wants to look in more detail at the symmetry breaking, we have explicitly stated that exact quantum defects may be used instead and we cited examples of this usage.[6] Also, it should be noted that we have considered the application of these ideas to ions both in our original publication[4] and later.[8,18]

Another distinction between the two programs is the physical intuition for the preferred nodal-modifying parameter, $I(l)$ in our case and $c(l)$ in the case of the program advocated by MB in Comment III. Our bias is towards the exact supersymmetry integers, which are intimately tied to the Pauli principle.[4,6] For sodium this would be $I(0)=2$ and $I(1)=1$. MB's program in Comment III prefers the choice $|\delta(l)-c(l)| \leq 0.5$. For sodium this would be $c(0)=1$ and $c(1)=1$. These two prescriptions result in different detailed predictions for physical quantities such as transition probabilities.

For example, consider the transition probability for Na $4s \rightarrow 3p$, with accepted value 0.251×10^8 Hz.[19] It is predicted to be 0.247×10^8 Hz in our preferred supersymmetry prescription. In the preferred prescription of MB advocated in Comment III, this transition probability is predicted to be either 0.0819×10^8 or 0.202×10^8 Hz, respectively, depending on whether one uses the more symmetric $\delta(l)$ or the more phenomenological $\delta(l,n)$.

The similarity of the underlying mathematical formalisms of the two programs does not, by itself, imply equivalence. In Ref. 9 we explained the relevance to this point of an important result of modern quantum mechanics. This result is that even an identical spectrum does not imply the same physics because the scattering data can be different. Indeed, such differences can arise from solutions to the same differential equation, differing only in the parameters involved. (It is important to mention the 1967 paper of Parsons and Weisskopf.[20] This paper, which predates even Simon's 1971 model, proposed on physical grounds the type of anomalous nodal structures in Rydberg atoms that we are considering.[21])

III. CONCLUDING REMARKS

In the final two paragraphs of Comment III, MB are largely objecting to our lack of citation of certain related recent literature, in particular their own work. However, this objection is not entirely reasonable given MB's own lack of citation.

For instance, MB have never referred to the above 1967 paper of Parsons and Weisskopf.[20] Further, our tables[6] on Li and Na were not only published before those of MB (Ref. 15) but are also more extensive. It is easy to overlook relevant and related publications.

In conclusion, we find the work of Simons and his school to be interesting and complementary to our symmetry-based approach. Our supersymmetry model enables an understanding in terms of the Pauli principle of the physical basis of apparently anomalous nodal structure in atomic systems. Supersymmetry permits physical insight into the complexities of many-body systems.

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[21] We also mention the program of R. M. Sternheimer, Phys. Rev. A **15**, 817 (1975); **20**, 18 (1979), and references therein.