

Bohr's molecular model and the melding of classical and quantum mechanics

With considerable interest I read the article "Bohr's molecular model, a century later" by Anatoly Svidzinsky, Marlan Scully, and Dudley Herschbach (PHYSICS TODAY, January 2014, page 33). It is always interesting to see how our current understanding sheds new light on the revolutionary scientific ideas of the past. I agree with the authors that although quantum mechanics is the real basis for atomic- and molecular-physics computations, the old Bohr model that treats electrons in atoms like tiny planets moving around the sun-nucleus is intuitively clear and very attractive.

As I see it, the aim of the article is to show how to use Bohr's approach to treat not only simple atoms but molecules. An important point in that approach is reconciliation of quantum mechanics with Bohr's ideas. The authors claim that in infinite dimensions, quantum mechanics "morphs into classical mechanics."

I cannot say, however, that the infinite-dimension system is a clarifying model to describe physical or chemical objects. I do not see that the reference to chromodynamics (and to Edward Witten's article in PHYSICS TODAY, July 1980, page 38) is a clarifying one. Far from convincing are statements like "Hence the large- D limit, where $1/D \rightarrow 0$, is closer to the real world ($1/D = 1/3$) than is the oft-used $D = 1$ regime. Indeed, results obtained at large D usually resemble those for $D = 3$." I confess it sounds too lacking in rigor to be convincing.

Letters and commentary are encouraged and should be sent by email to ptletters@aip.org (using your surname as the Subject line), or by standard mail to Letters, PHYSICS TODAY, American Center for Physics, One Physics Ellipse, College Park, MD 20740-3842. Please include your name, work affiliation, mailing address, email address, and daytime phone number on your letter and attachments. You can also contact us online at <http://contact.physicstoday.org>. We reserve the right to edit submissions.

But the large- D limit per se is not what bothers me. Of great concern is the assumption that the radial part of the D -dimensional Schrödinger equation in Hartree units looks like this:

$$\left\{ -\frac{1}{2} \frac{\partial^2}{\partial r^2} + \frac{[l + (D-3)/2][l + (D-1)/2]}{2r^2} - \frac{Z}{r} \right\} \phi = E\phi, \quad (1)$$

where Z is the nuclear charge and l is the angular momentum.

Equation 1 has no sense for $D = 1$. Indeed, in one dimension, a finite angular momentum requires infinite speed of a rotating particle. Therefore, for $D = 1$, the correct equation is

$$\left(-\frac{1}{2} \frac{d^2}{dx^2} - \frac{Z}{r} \right) \phi = E\phi, \quad (2)$$

which does not follow from equation 1 at $D = 1$.

But most important is that equation 1 implies that the Coulomb potential does not depend on D . That could have been considered correct before it became clear that the Coulomb law follows from Maxwell's equations when one considers a field generated by a point-like electric charge. So to obtain the Coulomb law for a two-dimensional space, one has to consider Maxwell equations in a two-dimensional world. For a point-like charge, those equations lead to a $1/(\ln r)$ instead of $1/r$ dependence. If one takes into account the D -dependence of the Coulomb potential, derivations performed in the PHYSICS TODAY article become meaningless. Indeed, when using an unrealistic equation 1, how can one believe that it illuminates Bohr's quite realistic and physical postulates?

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■ **Permit me to add** some information to the article entitled, "Bohr's molecular model, a century later." The authors discuss the idea of "dimensional scaling," approximating the spectra of

atoms and molecules by employing perturbation theory to expand around the infinite-dimension/classical limit. That technique of approximating the Schrödinger equation, originally called the $1/N$ expansion, was developed and applied to numerous problems in the 1980s, including simple atoms, quarkonium, and the hydrogen molecule.¹⁻³ It grew out of attempts in the 1970s to formulate quantum chromodynamics in the limit of a large number of colors. The use of the $1/N$ expansion in atomic physics was discussed by Edward Witten (PHYSICS TODAY, July 1980, page 38), who pointed out that his discussion was based on work that applied the method to hydrogen and helium atoms.¹

The work in reference 1 made use of algebraic methods for the analysis, but the coordinate space method was also developed and was initially used to treat the strong-field Zeeman effect.² A nice description of the status of the field at the time was given by Laurence Yaffe (PHYSICS TODAY, August 1983, page 50). Many additional applications of that method in the physics literature may be found in reference 4.

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■ **Anatoly Svidzinsky**, Marlan Scully, and Dudley Herschbach have illustrated well how the molecular theory might have looked had quantum mechanics not been invented. It's worth noting that Niels Bohr was not alone in his attempts to extend semiclassical mechanics to systems more complex than the hydrogen atom. From 1913 to 1925, many semiclassical models of two-electron systems were proposed.

As we see from the authors' figure 3a, Bohr assumed that electrons in hydrogen molecules move around the molecular axis out of phase. It is a remarkable

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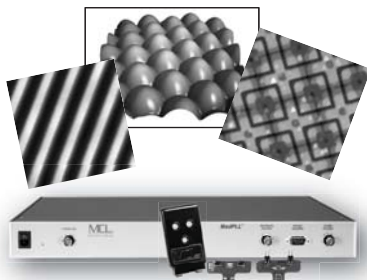
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fact that Werner Heisenberg put forward in 1922 a two-electron atomic model that had electrons moving similarly out of phase and that ascribed a fractional quantum number ($\frac{1}{2}$) to the bending mode of the configuration.¹ Although Heisenberg's model predicted the ground-state helium level, which was in excellent agreement with the spectroscopic data, Bohr opposed the model, since a noninteger quantum number was considered sacrilege. For the same reason, Bohr never published his own results. However, the asynchronous two-electron atomic model turned out to be the fertile one, though the corresponding classical configurations can have very complex structure.²

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■ Svidzinsky, Scully, and Herschbach

reply: We agree with M. Y. Amusia that a statement we made about the infinite dimension limit is "lacking in rigor." It was intended simply to provide heuristic insight into why, for a wide variety of problems, the large- D limit has proven to be a useful starting approximation to obtain results for $D = 3$.

Amusia's other concerns are answered in a 1975 paper on a D -scaling treatment of helium by David Herrick and Frank Stillinger.¹ They gave a rigorous derivation of the D -dimensional hydrogen atom Hamiltonian, shown as equation 1 in Amusia's letter. That solution applies for $D \geq 2$, as implied in the figure included in box 1 of our article. Herrick and Stillinger also showed that for the correct $D \rightarrow 1$ limit, the Z/r term becomes a δ -function. In D -scaling, contrary to Amusia's assumption, the $D = 3$ form of Coulomb's law can be used for dimensional continuation to the large- D limit. The D -dependent similarity transformation affects the Laplacian, not the potential energy. Both theory and application are amply presented in references given in our article (particularly references 8–11). D -scaling, using just elementary algebra, has attained correlation energies for multielectron atoms with accuracy comparable to or better than conventional electronic calculations.²

The papers of Leonard Mlodinow³ and several other authors, especially the earlier paper by Herrick and Stil-

linger,¹ fostered the development of D -scaling for electronic structure. Since the kinship of Bohr's model to dimensional scaling was not recognized until 2005, we did not dwell on that history, other than citing the tutorial article by Edward Witten. The treatment of H_2 that Mlodinow cites in the second part of his reference 3 is a deliberately drastic approximation and gives less than 40% of the bond dissociation energy.

As emphasized by Petar Grujic, the bold, perplexing enterprise by Niels Bohr motivated much further work melding classical and quantum mechanics. We note that D -scaling has a distinctive character. It might aptly be termed "semiquantum" rather than semiclassical. Although in the large- D limit the equations become classical, quantum mechanics is hidden in the D -dependent units adopted for distance and energy. At that limit, electrons take fixed positions in the D -scaled space and the first-order correction in $(1/D)$ has them execute harmonic vibrations about those positions. In the prequantum era, such behavior was postulated by Gilbert Lewis and Irving Langmuir,⁴ motivated by chemical arguments but disdained by physicists and considered incompatible with the Bohr model.

References

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