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 $1/D \to 0$, 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.

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:

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

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

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

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?

M. Y. Amusia
(amusia@012.net.il)
Hebrew University
Jerusalem
Ioffe Physical-Technical Institute
St. Petersburg, Russia

■ **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.

References

1. L. D. Mlodinow, N. Papanicolaou, *Ann. Phys.* **128**, 314 (1980); **131**, 1 (1981).
2. C. M. Bender, L. D. Mlodinow, N. Papanicolaou, *Phys. Rev. A* **25**, 1305 (1982).
3. T. Imbo, U. Sukhatme, *Phys. Rev. D* **31**, 2655 (1985); M. Kumar, A. Srivastava, J. K. Bhattacharjee, K. Banerjee, *Phys. Lett. A* **117**, 226 (1986).
4. A. Chatterjee, *Phys. Rep.* **186**, 249 (1990).

Leonard Mlodinow
Pasadena, California

■ **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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