

Bibliography for D -scaling

May 8, 2009

Svidzinsky

All references by Anatoly Svidzinsky.

References

- [108] G. Chen, S. A. Chin, Y. S. Dou, K. T. Kapale, M. Kim, A. A. Svidzinsky, K. Urtekin, H. Xiong, and M. O. Scully. The two electron molecular bond revisited: From bohr orbits to two-center orbitals. In *Advances in Atomic Molecular, and Optical Physics, Vol 51*, volume 51 of *Advances in Atomic Molecular and Optical Physics*, pages 93–238. Elsevier Academic Press Inc, San Diego, 2005.
- [431] R. K. Murawski and A. Svidzinsky. Quantum-number dimensional-scaling analysis for excited states of multielectron atoms. *Phys. Rev. A*, 74(4):5, 2006.

Abstract: A dimensional-scaling method for the calculation of excited states of multielectron atoms is introduced. By including the principle and orbital quantum numbers in the dimension parameter, we obtain an energy expression for excited states including high angular momentum states. The method is tested on He, Li, and Be. We obtain good agreement with more orthodox quantum mechanical treatments even in the zeroth order.

- [598] A. Svidzinsky, G. Chen, S. Chin, M. Kim, D. X. Ma, R. Murawski, A. Sergeev, M. Scully, and D. Herschbach. Bohr model and dimensional scaling analysis of atoms and molecules. *Int. Rev. Phys. Chem.*, 27(4):665–723, 2008.

Abstract: It is generally believed that the old quantum theory, as presented by Niels Bohr in 1913, fails when applied to few electron systems, such as the H-2 molecule. Here we review recent developments of the Bohr

model that connect it with dimensional scaling procedures adapted from quantum chromodynamics. This approach treats electrons as point particles whose positions are determined by optimizing an algebraic energy function derived from the large-dimension limit of the Schrodinger equation. The calculations required are simple yet yield useful accuracy for molecular potential curves and bring out appealing heuristic aspects. We first examine the ground electronic states of H-2, HeH, He-2, LiH, BeH and Li-2. Even a rudimentary Bohr model, employing interpolation between large and small internuclear distances, gives good agreement with potential curves obtained from conventional quantum mechanics. An amended Bohr version, augmented by constraints derived from Heitler-London or Hund-Mulliken results, dispenses with interpolation and gives substantial improvement for H-2 and H-3. The relation to D-scaling is emphasized. A key factor is the angular dependence of the Jacobian volume element, which competes with interelectron repulsion. Another version, incorporating principal quantum numbers in the D-scaling transformation, extends the Bohr model to excited S states of multielectron atoms. We also discuss kindred Bohr-style applications of D-scaling to the H atom subjected to superstrong magnetic fields or to atomic anions subjected to high frequency, superintense laser fields. In conclusion, we note correspondences to the prequantum bonding models of Lewis and Langmuir and to the later resonance theory of Pauling, and discuss prospects for joining D-scaling with other methods to extend its utility and scope.

- [599] A. A. Svidzinsky, S. A. Chin, and M. O. Scully. Model of molecular bonding based on the Bohr-Sommerfeld picture of atoms. *Phys. Lett. A*, 355(4-5):373–377, 2006.

Abstract: We develop a model of molecular binding based on the Bohr-Sommerfeld description of atoms together with a constraint taken from conventional quantum mechanics. The model can describe the binding energy curves of H-2, H-3 and other molecules with striking accuracy. Our approach treats electrons as point particles with positions determined by extrema of an algebraic energy function. Our constrained model provides a physically appealing, accurate description of multi-electron chemical bonds. (c) 2006 Elsevier B.V. All rights reserved.

- [600] A. A. Svidzinsky, M. O. Scully, and D. R. Herschbach. Simple and surprisingly accurate approach to the chemical bond obtained from

dimensional scaling. *Phys. Rev. Lett.*, 95(8):4, 2005.

Abstract: We present a new dimensional scaling transformation of the Schrodinger equation for the two electron bond. This yields, for the first time, a good description of the bond via D scaling. There also emerges, in the large-D limit, an intuitively appealing semiclassical picture, akin to a molecular model proposed by Bohr in 1913. In this limit, the electrons are confined to specific orbits in the scaled space, yet the uncertainty principle is maintained. A first-order perturbation correction, proportional to $1/D$, substantially improves the agreement with the exact ground state potential energy curve. The present treatment is very simple mathematically, yet provides a strikingly accurate description of the potential curves for the lowest singlet, triplet, and excited states of H-2. We find the modified D-scaling method also gives good results for other molecules. It can be combined advantageously with Hartree-Fock and other conventional methods.

- [601] A. A. Svidzinsky, M. O. Scully, and D. R. Herschbach. Bohr's 1913 molecular model revisited. *Proc. Natl. Acad. Sci. U. S. A.*, 102(34):11985–11988, 2005.

Abstract: It is generally believed that the old quantum theory, as presented by Niels Bohr in 1913, fails when applied to few electron systems, such as the H-2 molecule. Here, we find previously undescribed solutions within the Bohr theory that describe the potential energy curve for the lowest singlet and triplet states of H-2 about as well as the early wave mechanical treatment of Heitler and London. We also develop an interpolation scheme that substantially improves the agreement with the exact ground-state potential curve of H-2 and provides a good description of more complicated molecules such as LiH, Li-2, BeH, and He-2.