

# Bibliography for $D$ -scaling

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## Bohr

All references containing a word “Bohr”.

## References

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- [262] R. D. Harcourt. CHEMICAL BONDING VIA BOHR CIRCULAR ORBITS AND A  $2N \times N$  FACTORIZATION OF  $2N(2)$ . *Theochem-J. Mol. Struct.*, 338:195–213, 1995.

**Abstract:** One type of Bohr orbit approach to descriptions of the electronic structures of atoms and molecules is based on a  $2n \times n$  factorization of the atomic shell-structure formula  $2n(2)$ . It involves  $n$  circular orbits with principal quantum number  $n$ , each of which may accommodate a maximum of  $2n$  electrons. Aspects of a previously published account of this type of orbit theory are reviewed for compounds of main-group elements, and for several transition metal complexes. New types of orbit diagrams are provided for some of the systems considered previously. The theory provides a straightforward representation for the tetrahedral carbon atom. Attention is given to orbit diagrams for a variety of hypercoordinate systems, and to the general reluctance of atoms of first-row elements to form stable hypercoordinate compounds. Orbit diagrams for two elementary triatomic reactions are also provided, and examples are provided of new types of

Bohr orbit calculations of the energies for H-2(+) and H-2.

- [263] R. D. Harcourt and T. M. Klapotke. Tutorial review: Bohr circular orbit diagrams for some fluorine-containing molecules. *J. Fluor. Chem.*, 127(6):712–719, 2006.

**Abstract:** Examples are provided of Bohr circular orbit diagrams to represent the electronic structures of some fluorine-containing molecules. The orbit 2 diagrams are constructed from a  $2n \times n$  factorisation of the atomic shell-structure formula  $2n$ , with  $n = 1, 2, 3$ . Particular attention is given to orbit diagrams and the associated valence bond structures for the hypercoordinate molecules and ions PF<sub>5</sub> and NF<sub>5</sub>, F<sub>3</sub>(-) and XeF<sub>2</sub>, IF<sub>5</sub> and XeF<sub>5</sub><sup>+</sup>, XeF<sub>5</sub><sup>-</sup>, IF<sub>8</sub><sup>-</sup>, XeFg(8)(2-), ReF<sub>8</sub><sup>-</sup> and TaF<sub>8</sub><sup>3-</sup>, ZrF<sub>8</sub><sup>4-</sup>, ZrF<sub>7</sub><sup>3-</sup>, ReF<sub>6</sub><sup>2-</sup>, and high-spin CoF<sub>6</sub><sup>3-</sup>. Aspects of the electronic structures of D-3h-symmetry PF<sub>5</sub> and NF<sub>5</sub> are contrasted via the use of orbital valence bond considerations, and the results of STO-3G valence bond calculations are reported for these species. (c) 2006 Elsevier B.V. All rights reserved.

- [34] J. Avery, T. B. Hansen, M. C. Wang, and F. Antonsen. Sturmian basis sets in momentum space. *Int. J. Quantum Chem.*, 57(3):401–411, 1996.

**Abstract:** The properties of Sturmian basis sets in  $d$ -dimensional direct space and  $d$ -dimensional momentum space are reviewed, as well as the relationship between hydrogenlike Sturmians and hyperspherical harmonics. The kernel of the reciprocal-space Schrodinger equation is expanded in terms of Sturmian basis sets. This expansion allows Shibuya and Wulfman's treatment of many-center Coulomb potentials to be extended to many-center potentials of a general form, and the method is also extended to the calculation of crystal orbitals and band structures. (C) 1996 John Wiley & Sons, Inc.

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**Abstract:** The modification of the Bohr-Sommerfeld quantization rules, which is due to the barrier penetrability, is found. The equation obtained is valid for an arbitrary analytical potential  $U(x)$ , obeying the quasiclassical conditions. It determines both the position  $E(r)$  and the

width-GAMMA of the quasistationary state. A generalization of the Gamow formula for multidimensional systems with separable coordinates is derived. A comparison with exactly solvable models as well as with numerical solutions of the Schrodinger equation for the Stark problem is performed.

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**Abstract:** Bohr’s atomic theory is widely viewed as remarkable, both for its accuracy in predicting the observed optical transitions of one- electron atoms and for its failure to fully correspond with current electronic structure theory. What is not generally appreciated is that Bohr’s original semiclassical conception differed significantly from the Bohr - Sommerfeld theory and offers an alternative semiclassical approximation scheme with remarkable attributes. More specifically, Bohr’s original method did not impose action quantization constraints but rather obtained these as predictions by simply matching photon and classical orbital frequencies. In other words, the hydrogen atom was treated entirely classically and orbital quantized emerged directly from the Planck - Einstein photon quantization condition,  $E = h\nu$ . Here, we revisit this early history of quantum theory and demonstrate the application of Bohr’s original strategy to the three quintessential quantum systems: an electron in a box, an electron in a ring, and a dipolar harmonic oscillator. The usual energy-level spectra, and optical selection rules, emerge by solving an algebraic (quadratic) equation, rather than a Bohr - Sommerfeld integral (or Schroedinger) equation. However, the new predictions include a frozen (zero-kinetic-energy) state which in some (but not all) cases lies below the usual zero-point energy. In addition to raising provocative questions concerning the origin of quantum-chemical phenomena, the results may prove to be of pedagogical value in introducing students to quantum mechanics.

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**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.

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**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.

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**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.

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**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.

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**Abstract:** Since the first attempts to calculate the helium ground state in the early days of Bohr-Sommerfeld quantization, two-electron atoms have posed a series of unexpected challenges to theoretical physics. Despite the seemingly simple problem of three charged particles with known interactions, it took more than half a century after quantum mechanics was established to describe the spectra of two-electron atoms satisfactorily. The evolution of the understanding of correlated two-electron dynamics and its importance for doubly excited resonance states is presented here, with an emphasis on the concepts introduced. The authors begin by reviewing the historical development and summarizing the progress in measuring the spectra of two-electron atoms and in calculating them by solving the corresponding Schrodinger equation numerically. They devote the second part of the review to approximate quantum methods, in particular adiabatic and group-theoretical approaches. These methods explain and predict the striking regularities of two-electron resonance spectra, including propensity rules for decay and dipole transitions of resonant states. This progress was made possible through the identification of approximate dynamical symmetries leading to corresponding collective quantum numbers for correlated electron-pair dynamics. The quantum numbers are very different from the independent particle classification, suitable for low-lying states in atomic systems. The third section of the review describes modern semiclassical concepts and their application to two-electron atoms. Simple interpretations of the approximate quantum numbers and propensity rules can be given in terms of a few key periodic orbits of the classical three-body problem. This includes the puzzling existence of Rydberg series for electron-pair motion. Qualitative and quantitative semiclassical estimates for doubly excited states are obtained for both regular and chaotic classical two-electron dynamics using modern semiclassical techniques. These techniques set the stage for a theoretical investigation of the regime of extreme excitation towards the three-body breakup threshold. Together with periodic orbit spectroscopy, they supply new tools for the analysis of complex experimental spectra.

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**Abstract:** An extensive number of numerical computations of energy  $1/N$  series using a recursive Taylor series method are presented in this paper. The series are computed to a high order of approximation and their behavior on increasing the order of approximation is examined. (C) 2000 American Institute of Physics. [S0022-2488(00)05004-0].

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**Abstract:** We consider the large-D limit of Einstein gravity. It is observed that a consistent leading large-D graph limit exists, and that it is built Lip by a subclass of planar diagrams. The graphs in the effective field theory extension of Einstein gravity are investigated in the same context, and it is seen that all effective field theory extension of the basic Einstein-Hilbert theory will not upset the latter leading large-D graph limit, i.e., the same subclass of planar diagrams will dominate at large-D in the effective field theory. The effective field theory description of large-D quantum gravity limit Will be renormalizable, and the resulting theory will thus be completely well defined up to the Planck scale at similar to  $10^{19}$  GeV. The  $1/D$  expansion in gravity is compared to the Successful  $1/N$  expansion in gauge theory (the planar diagram limit), and dissimilarities and parallels of the two expansions are discussed. We consider the expansion of the effective field theory terms and we make some remarks oil explicit calculations of n-point functions. (C) 2004 Elsevier B.V. All rights reserved.