Bibliography for D-scaling

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Sergeev

All references by Alexey Sergeev.

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Abstract: The usefulness of Moller-Plesset perturbation theory, a standard technique of quantum chemistry, is determined by singularities in the corresponding energy function in the complex plane of the perturbation parameter. A method is developed that locates singularities from fourth-order perturbation series, using quadratic approximants with bilinear conformal mappings. (c) 2006 Elsevier B.V. All rights reserved.

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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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Pade approximants that are obtained from an algebraic equation of arbitrary degree. Numerical results indicate that given enough terms in the asymptotic expansion the rate of convergence of the diagonal staircase approximant sequence increases with the degree. Different branches of the approximants converge to different branches of the function. The success of the high-degree approximants is attributed to their ability to model the function on multiple sheets of the Riemann surface and to reproduce the correct singularity structure in the limit of large perturbation parameter. An efficient recursive algorithm for computing the diagonal approximant sequence is presented.

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choice of basis set. Standard basis sets cannot model dissociation to an electron cluster, but if the basis includes diffuse functions then it can model another critical point corresponding to complete dissociation of all the valence electrons. This point is farther from the origin of the z plane than is the critical point for the electron cluster, but it is still close enough to cause divergence of the perturbation series. For the hydrogen fluoride molecule a critical point is present even without diffuse functions. The basis functions centered on the H atom are far enough from the F atom to model the escape of electrons away from the fluorine end of the molecule. For the Ar atom a critical point for a one-electron ionization, which was not previously predicted, seems to be present at a positive value of the perturbation parameter. Implications of the existence of critical points for quantum-chemical applications are discussed. (C) 2005 American Institute of Physics.

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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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