Bibliography for D-scaling

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Watson

All references by Deborah Watson.

References

[168] M. Dunn, T. C. Germann, D. Z. Goodson, C. A. Traynor, J. D. Morgan, D. K. Watson, and D. R. Herschbach. A LINEAR ALGEBRAIC-METHOD FOR EXACT COMPUTATION OF THE COEFFICIENTS OF THE 1/D EXPANSION OF THE SCHRODINGER-EQUATION. *J. Chem. Phys.*, 101(7):5987–6004, 1994.

Abstract: The 1/D expansion, where D is the dimensionality of space, offers a promising new approach for obtaining highly accurate solutions to the Schrodinger equation for atoms and molecules. The method typically employs an asymptotic expansion calculated to rather large order. Computation of the expansion coefficients has been feasible for very small systems, but extending the existing computational techniques to systems with more than three degrees of freedom has proved difficult. We present a new algorithm that greatly facilitates this computation. It yields exact values for expansion coefficients, with less roundoff error than the best alternative method. Our algorithm is formulated completely in terms of tenser arithmetic, which makes it easier to extend to systems with more than three degrees of freedom and to excited stares, simplifies the development of computer codes, simplifies memory management, and makes it well suited for implementation on parallel computer architectures. We formulate the algorithm for the calculation of energy eigenvalues, wave functions, and expectation values for an arbitrary many-body system and give estimates of storage and computational costs.

[169] M. Dunn and D. K. Watson. WRONG PARITY STATES AND THE MOLECULAR-ORBITAL DESCRIPTION OF DOUBLY-EXCITED 2-ELECTRON ATOMS IN D-DIMENSIONS. *J. Phys. Chem.*, 97(10):2457–2460, 1993.

Abstract: Rost et al. have examined some of the implications of dimensional scaling for the molecular orbital (MO) description of the "right parity" (pi = (-1)L) doubly-excited states of two-electron atoms. They propose a new and simple classification scheme utilizing interdimensional degeneracies, saddle degeneracies, and A-doubling. The present paper extends this description, in D dimensions, to the "wrong parity" (pi = (-1)L+1) states and provides a justification for the extension of the new classification scheme to include the pi = (-1)L+1 states. This is achieved by showing that the MO approximation preserves the exact interdimensional degeneracies between pi = (-1)L and pi = (-1)L+1 states and that there exists approximate interdimensional degeneracies between the pi = (-1)L+1 MO states. It is also pointed out that the phenomenon of LAMBDA-doubling is special to three dimensions, although the lifting of this degeneracy is expected to be small for low dimensions. Despite the fact that the energy level spectrum no longer features LAMBDA-doubling for larger values of D, the internal MO electron center of mass wavefunctions for those states which exhibit LAMBDA-degeneracy at D = 3 are still identical in any dimension. The lifting of this degeneracy does not affect the classification scheme of Rost et al. since it utilizes LAMBDA-doubling at D = 3.

[170] M. Dunn and D. K. Watson. Continuation of the Schrodinger equation for higher angular-momentum states to D dimensions and interdimensional degeneracies. *Few-Body Syst.*, 21(3-4):187–209, 1996.

Abstract: The application of the techniques of dimensional scaling, and in particular the 1/D expansion, to higher angular-momentum states of multielectron atoms requires the generalized Euler angles, which multiply with increasing D to be "factored out" of the wave function. The factorization must be performed in a way that produces from the Schrodinger equation a tractable set of differential equations which admit continuation in the dimension D. In two recent works the authors have achieved the necessary factorization of the wave function by generalizing the Schwartz expansion to N electrons in

D dimensions. The present paper applies the N-electron D-dimensional Schwartz expansion to the two-electron problem in D dimensions. The resulting set of coupled differential equations in the internal variables admit continuation in D, enabling the methods of dimensional scaling to be applied to higher-angular-momentum states. In addition, the coupled differential equations clearly show the complete spectrum of exact interdimensional degeneracies of the two-electron system.

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Abstract: Extending the techniques of dimensional scaling to higher angular momentum states of multielectron atoms requires the derivation, from the Schrodinger equation, of a tractable set of differential equations which admit continuation in the spatial dimension D. This derivation centers on "factoring out," in D dimensions, the rotational degrees of freedom from the internal degrees of freedom in the wave function. A solution to this problem, by generalizing thr Schwartz expansion (Schwartz, Phys. Rev. 123, 1700 (1961)) to N electrons in D dimensions, is presented. The generalization to systems with particles of arbitrary masses is straightforward. (C) 1996 Academic Press, Inc.

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Abstract: In a previous paper the authors have developed a finite expansion for the wave function which allows the methods of dimensional scaling to be applied to higher angular momentum states. The terms in the expansion, though, are not necessarily linearly independent and so the expansion requires a little refining. The sources of linear dependence in the expansion for the wave function are explored and protocols for dealing with them are presented. (C) 1996 Academic Press, Inc.

[173] M. Dunn and D. K. Watson. Large-dimension limit of higher-angular-momentum states of two-electron atoms. *Phys. Rev. A*, 59(2):1109–1124, 1999.

Abstract: To apply the methods of dimensional scaling to higher-angular-momentum states, a formalism needs

to be developed which factors the D-dimensional rotational degrees of freedom from the internal degrees of freedom. The rotational degrees of freedom multiply with increasing dimensionality, while the internal degrees of freedom remain finite in number. A suitable expansion which achieves this has been presented by the authors recently and is an N-electron D-dimensional generalization of the Schwartz expansion. A derivation of the coupled differential equations in the internal variables that result from the application of the Hamiltonian to this wave-function expansion for the atomic two-electron system has been presented by the authors in another recent paper. The coupled differential equations admit continuation in D and clearly show the complete spectrum of exact interdimensional degeneracies of the two-electron system. However, to apply the methods of dimensional scaling to the two-electron system, the system of coupled differential equations have to be solved for large D. This paper concerns itself with this issue. [S1050-2947(97)07608-7].

[174] M. Dunn, D. K. Watson, and J. G. Loeser. Analytic, group-theoretic wave functions for confined, correlated N-body systems with general two-body interactions. *Ann. Phys.*, 321(8):1939–1980, 2006.

Abstract: In this paper, we develop an analytic N-body wave function for identical particles under quantum confinement with a general two-body interaction. A systematic approach to correlation is developed by combining three theoretical methods: dimensional perturbation theory, the FG method of Wilson et. al., and the group theory of the symmetric group. Analytic results are achieved for a completely general interaction potential. Unlike conventional perturbation methods which are applicable only for weakly interacting systems, this analytic approach is applicable to both weakly and strongly interacting systems. This method directly accounts for each two-body interaction, rather than an average interaction so even lowest-order results include beyond-mean-field effects. One major advantage is that N appears as a parameter in the analytical expressions for the energy so results for different N are easy to obtain.

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J. Chem. Phys., 104(24):9870–9875, 1996.

Abstract: When linear Pade summation is applied to eigenvalue perturbation expansions near regions of parameter space where those eigenvalues undergo an avoided crossing, the Padi approximants may yield levels which cross diabatically, rather than displaying the proper avoided behavior. The purpose of this study is to elucidate the reasons for the peculiar behavior of Pade approximants in such situations. In particular: we demonstrate that the diabatic crossing is a natural consequence of using the (single-valued) Pade rational approximant to successfully resum series expansions of the multivalued energy function over much of the parameter space. This is illustrated with a perturbative treatment of the Barbanis Hamiltonian. (C) 1996 American Institute of Physics.

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Abstract: The convergence of large-order expansions in delta = 1/D, where D is the dimensionality of coordinate space, for energies E(delta) of Coulomb systems is strongly affected by singularities at delta = 1 and Pade'-Borel approximants with modifications that that completely remove the singularities at delta = 1 and remove the dominant singularity at delta = 0 are demonstrated. A renormalization of the interelectron repulsion is found to move the dominant singularity of the Borel function F(delta) = Sigma(j)E(j)'/ j!, where E-j' are the the expansion coefficients of the energy with singularity structure removed at d51, farther from the origin and thereby accelerate summation convergence. The ground-state energies of He and H-2(+) are used as test cases. The new methods give significant improvement over previous summation methods. Shifted Borel summation using F-m(delta) = Sigma(j)E(j)'/Gamma(j + 1 - m) is considered. The standard deviation of results calculated with different values of the shift parameter m is proposed as a measure of summation accuracy. (C) 1998 American Institute of Physics. [S0022-2488(98)04210-8].

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Abstract: Large-order dimensional perturbation theory, which yields high accuracy for ground-state energies, is applied here to excited states of the two-electron atom. Expansion coefficients are computed recursively using the moment method, which we formulate in terms of normal coordinates. We consider the first two excited S states of helium, corresponding, at the large-dimension limit, to one quantum in either the antisymmetric-stretch normal mode or the symmetric-stretch normal mode. Comparison with the hydrogenic limit has identified these states as Is 2s 3S and 1s2s 1S, respectively. We sum the 1/D expansions at D = 3, using summation procedures that take into account the dimensional singularity structure of the eigenvalues, and find convergence at D = 3 to the eigenvalues predicted by the hydrogenic assignments, despite apparent qualitative differences between the eigenfunctions at large D and those at D = 3. In the D –¿ infinity limit, the electrons are equidistant from the nucleus. Our results for 1s2s energies appear to imply that the shell structure is properly accounted for by terms in the expansion beyond the lowest order. This robustness of the 1/D expansion suggests that the method will be applicable to many-electron systems.

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Abstract: For a two-electron atom, many D = 3 states have the same energies as D = 5 states of lower angular momentum. Thus the energies of 3P(e), 1P(e), 3D0, and 1D0 states for D = 3 are respectively identical to those for 1S(e), 3S(e), 1P0, and 3P0 states at D = 5. We exploit these interdimensional degeneracies to obtain accurate energies for doubly excited 2pnp P(e) states of helium at D = 3, with n = 2-6, by calculating energy eigenvalues for the singly excited 1s(n -1)s S(e) states at D = 5. We also illustrate how some qualitative aspects of double-excitation spectra can be elucidated in terms of interdimensional degeneracies.

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TRASHELL EXCITED-STATES. *Z. Phys. D-Atoms Mol. Clusters*, 10(2-3):195–210, 1988.

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Abstract: Confined quantum systems involving N identical interacting particles are to be found in many areas of physics, including condensed-matter, atomic, and chemical physics. A beyond-mean-field perturbation method that is applicable, in principle, to weakly, intermediate, and strongly interacting systems has been set forth by the authors in a previous series of papers. Dimensional perturbation theory was used, and in conjunction with group theory, an analytic beyond-mean-field correlated wave function at lowest order for a system under spherical confinement with a general two-body interaction was derived. In the present paper, we use this analytic wave function to derive the corresponding lowest-order, analytic density profile and apply it to the example of a Bose-Einstein condensate.

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Abstract: We present semianalytical many-body results for energies and excitation frequencies for an inhomogeneous Bose-Einstein condensate over a wide range of atom numbers N for both small s-wave scattering lengths, typical of most laboratory experiments, and large scattering lengths, achieved by tuning through a Feshbach resonance. Our dimensional perturbation treatment includes two-body correlations at all orders and yields analytical results through first order by taking advantage of the high degree of symmetry of the condensate at the zeroth-order limit. Because N remains a parameter in our analytical results, the challenge of calculating energies and excitation frequencies does not rise with the number of condensate atoms. In this proof-of-concept paper the atoms are confined in a spherical trap and are treated as hard spheres. Our many-body calculations compare well to Gross-Pitaevskii results in the weakly interacting regime and depart from the mean-field approximation as the density approaches the strongly interacting

regime. The excitation frequencies provide a particularly sensitive test of beyond-mean-field corrections. For example, for N=2000 atoms and an experimentally realized large scattering length of a=0.433a(ho) (a(ho)=root(h) over bar /momega(ho)) we predict a 75% shift from the mean-field breathing mode frequency.

[402] B. A. McKinney, M. Dunn, D. K. Watson, and J. G. Loeser. N identical particles under quantum confinement: a many-body dimensional perturbation theory approach. *Ann. Phys.*, 310(1):56–94, 2004.

Abstract: Systems that involve N identical interacting particles under quantum confinement appear throughout many areas of physics, including chemical, condensed matter, and atomic physics. In this paper, we present the methods of dimensional perturbation theory, a powerful set of tools that uses symmetry to yield simple results for studying such many-body systems. We present a detailed discussion of the dimensional continuation of the N-particle Schrodinger equation, the spatial dimension D –¿ infinity equilibrium (D-0) structure, and the normal-mode (D-1) structure. We use the FG matrix method to derive general, analytical expressions for the many-body normal-mode vibrational frequencies, and we give specific analytical results for three confined N-body quantum systems: the N-electron atom, N-electron quantum dot, and N-atom inhomogeneous Bose-Einstein condensate with a repulsive hard-core potential. (C) 2003 Elsevier Inc. All rights reserved.

[403] B. A. McKinney and D. K. Watson. Semiclassical perturbation theory for two electrons in a D-dimensional quantum dot. *Phys. Rev. B*, 61(7):4958–4962, 2000.

Abstract: Dimensional perturbation theory is applied to the two-electron D-dimensional quantum dot, obtaining accurate values for the ground- and excited-state energies. The expansion parameter is 1/kappa, where kappa=D + 2/l/, D is the effective spatial dimensionality of the quantum dot environment, and I is the relative-motion angular momentum quantum number. In this method, no approximations are made in the treatment of correlation. Analytic approximations for ground- and excited-state energies are obtained from the zeroth- and first-order terms of the perturbation expansion; thus, constituting a semiclassical approach to the quantum dot

from a perturbation formalism. Using this analytic form of the energy, parametrized by D, the effects of the effective quantum dot dimensionality on the energy spectra may be investigated. Systematic corrections are made to the semiclassical approximation by adding higher-order perturbation terms. The method described may be extended to obtain analytic approximations to the ground-state energy of the many-electron D-dimensional quantum dot Hamiltonian by truncating the 1/D expansion to low order.

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Abstract: We introduce dimensional perturbation techniques to Bose-Einstein condensation of inhomogeneous alkalimetal gases. The perturbation parameter is delta=1/kappa, where kappa depends on the effective dimensionality of the condensate and on the angular momentum quantum number. We derive a simple approximation that is more accurate and flexible than the N –¿ infinity Thomas-Fermi ground-state approximation of the Gross-Pitaevskii equation. The approximation presented here is well suited for calculating properties of states in three dimensions and in low-effective dimensionality, such as vortex states in a highly anisotropic trap.

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Abstract: The appearance of avoided crossings among energy levels as a system parameter is varied is signaled by the presence of square-root branch points in the complex parameter-plane. Even hidden crossings, which are so gradual as to be difficult to resolve experimentally, can be uncovered by the knowledge of the locations of these branch points. As shown in this paper, there are two different analytic structures that feature square-root branch points and give rise to avoided crossings in energy. Either may be present in an actual quantum-mechanical problem. This poses special problems in perturbation theory since the analytic structure of the energy is not readily apparent from the perturbation series, and yet the analytic structure must be known beforehand if the perturbation series is to be summed to high accuracy. Determining which analytic structure is present from the

perturbation series is illustrated here with the example of a dimensional perturbation treatment of the diamagnetic hydrogen problem. The branch point trajectories for this system in the complex plane of the perturbation parameter delta (related to the magnetic quantum number and the dimensionality) as the magnetic field strength is varied are also examined. It is shown how the trajectories of the two branch-point pairs as the magnetic field strength varies are a natural consequence of the particular analytic structure the energy manifests in the complex delta-plane. There is no need to invoke any additional analytic structures as a function of the field strength parameter. (C) 2000 American Institute of Physics. [S0022-2488(99)00612-X].

[639] J. R. Walkup, M. Dunn, and D. K. Watson. Energy calculations of low-vertical bar m vertical bar diamagnetic hydrogen states with dimensional perturbation theory. *Phys. Rev. A*, 63(2):4, 2001.

Abstract: In a previous article [J. R. Walkup, M. Dunn, and D. K. Watson, Phys. Rev. A 58, 4668 (1998)] dimensional perturbation theory (DPT) was applied to circular Rydberg states of diamagnetic hydrogen to investigate avoided crossings in its energy spectrum as both the field strength and magnetic quantum number m were swept. Because the DPT perturbation parameter delta = 1/(D + 2m + 1), where D is the dimensionality of the system, is inversely related to m, one might assume that for a given field strength DPT would be effective only when m is large. However, the field-strength expression used in DPT is scaled as a function of m, so it is not obvious a priori whether the effectiveness of DPT diminishes when m is significantly reduced for a given physical field strength. It is shown that for many states of diamagnetic hydrogen DPT can still produce strongly convergent and accurate energy values when m is small, even when m = 0 (delta = 1/2). For those regions where even Pade summation failed to converge adequately, a technique is presented based on economized rational approximants.

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Abstract: The energy levels of diamagnetic hydrogen as a function of two independent parameters, magnetic field

strength B, and angular momentum m, are examined. Avoided crossings appear between these energy levels as either parameter is varied while the other is held fixed. These avoided crossings are directly related to degeneracies (Fermi resonances) occurring at zeroth order in perturbation theory. The mathematical basis of these degeneracies are the square-root branch points that connect the energy levels. It is found that the locations of avoided crossings in either constant-B or constant-in spectra can be predicted by visually scanning the locations of these branch points in the complex-delta plane, where delta= 1/(2 + 2 m) is the perturbation parameter used in this research. [S1050-2947(98)07111-X].

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Abstract: We present a perturbation solution of a model Bose-Einstein Hamiltonian derived by Bohn, Esry, and Greene. In our solution we use 1/N as the perturbation parameter, where N is the number of particles in the condensate. Ground-state energies are reported for parameters approximating the Joint Institute for Laboratory Astrophysics Rb-87 experiments. We predict the critical number of atoms with negative scattering lengths that can be trapped using the effective trap frequency of the first-order equation. The N–¿infinity perturbation limit, which retains a single term beyond the conventional Thomas-Fermi limit, gives ground-state energies that agree to three digits with converged results, thus providing a much improved limit for large N. [S1050-2947(99)00305-4].

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Abstract: Large-order dimensional perturbation theory (DPT) has been used to study the ground and a number of excited states of two-electron atoms for the case L=0. Here we present an application of recent work generalizing DPT to any higher angular-momentum state. In this work we begin the investigation of P-o states, presenting

results for the energies of some of the lowest-lying states and discuss the analytic structure of these energies as functions of 1/D. We also obtain energies of corresponding D-o states with almost no additional effort by making use of interdimensional degeneracies with the P-o states. [S1050-2947(98)06512-3].