# Bibliography for $D$-scaling

May 8, 2009

## Helium

All references containing a word "helium".

## References


[1] A. G. Abrashkevich, M. I. Gajsak, V. I. Lendel, V. Y. Pojda, and I. V. Puzynin. MULTICHANNEL COMPUTATION OF THE GROUND-STATE ENERGIES OF HELIUM-LIKE SYSTEMS WITHIN THE HYPERSPHERICAL COORDINATE METHOD. *Phys. Lett. A*, 133(3):140–143, 1988.

[109] G. Chen, Z. H. Ding, A. Perronnet, and Z. G. Zhang. Visualization and dimensional scaling for some three-body problems in atomic and molecular quantum mechanics. *J. Math. Phys.*, 49(6):57, 2008.

> **Abstract:** Three-body problems in atomic and molecular quantum mechanics, comprising one electron-two nuclei and two electron-one nucleus, are studied from their Schrodinger-Born-Oppenheimer models. The following are main topics of interest in this paper: (1) review of foundational mathematical properties of the multiparticle Schrodinger operator, (2) visualization of H-2(+) (hydrogen molecular ion)-like and He (helium)-like molecular and atomic states, and (3) spectrum of He obtained by the large-dimension scaling limit. The authors begin with topic (1) for the tutorial purpose and devote topics (2) and (3) to new contributions of the analytical, numerical, and visualization nature. Relevant heuristics, graphics, proofs, and calculations are presented. (c) 2008 American Institute of Physics.

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**Abstract:** The series solution method developed by Pekeris [Phys. Rev. 112, 1649 (1958); 115, 1216 (1959)] for the Schrodinger equation for two-electron atoms, as generalized by Frost et al. [J. Chem. Phys. 41, 482 (1964)] to handle any three particles with a Coulomb interaction has been used. The wave function is expanded in a triple orthogonal set in three perimetric coordinates. From the Schrodinger equation an explicit recursion relation for the coefficients in the expansion is obtained, and the vanishing of the determinant of these coefficients provides the condition for the energy eigenvalues and for the eigenvectors. The Schrodinger equation is solved and the matrix elements are produced algebraically by using the computer algebra system MAPLE. The substitutions for a particular atom and diagonalization were performed by a program written iu the C language. Since the determinant is sparse, it is possible to go to the order of 1078 as Pekeris did without using excessive memory or computer CPU time. By using a nonlinear variational parameter in the expression used to remove the energy, nonrelativistic energies, within the fixed-nucleus approximation, have been obtained. For the ground-state singlet 1 1S state this is of the accuracy claimed by Frankowski and Pekeris [Phys. Rev. 146, 46 (1966); 150, 366(E) (1966)] using logarithmic terms for Z from 1 to 10, and for the triplet 2(3)S state, energies have been obtained to 12 decimal places of accuracy, which, with the exception of Z = 2, are lower than any previously published, for all Z from 3 to 10.

[130] J. J. De Groote and M. Masili. Low-lying doubly excited states of the helium isoelectronic series. *Few-Body Syst.*, 32(4):249–266, 2003.

**Abstract:** We present within the hyperspherical adiabatic approach a nonadiabatic calculation of the low-lying doubly excited states for heliumlike atomic systems with Z ranging from 2 to 6. Potential curves, channel functions, and nonadiabatic couplings are accurately obtained using a well-established technique. By neglecting the lowest potential curve of each system, the doubly excited states are identified as bound states of the remaining coupled closed channels. We investigate the efficacy of this approximation by comparing the resonance positions with the values obtained when the coupling with the neglected open channel is included in the calculation.

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**Abstract:** We present angular basis functions for the Schrodinger equation of two-electron systems in hyperspherical coordinates. By using the hyperspherical adiabatic approach, the wave functions of two-electron systems are expanded in analytical functions, which generalizes the Jacobi polynomials. We show that these functions, obtained by selecting the diagonal terms of the angular equation, allow efficient diagonalization of the Hamiltonian for all values of the hyperspherical radius. The method is applied to the determination of the S-1(e) energy levels of the Li+ and we show that the precision can be improved in a systematic and controllable way.

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**Abstract:** A generalized Hylleraas basis set with two nonlinear parameters is used to study three-body systems with two equal masses interacting via coulomb forces within the framework of non-relativistic quantum mechanics. Accurate variational bounds for the ground state of some of these systems are obtained improving the rate of convergence of the calculation with respect to an usual Hylleraas basis set. A study of the interparticle densities is also carried out.

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**Abstract:** A generalized Hylleraas-type basis set with three nonlinear parameters is proposed to study three-body systems interacting via coulomb forces within the framework of non-relativistic quantum mechanics. This basis set improves the rate of convergence with respect to previous ones, specially for nonsymmetric systems and excited states of two electron atoms: Accurate binding energies and other properties for S-states of helium-like ions, muonic molecules and the positronium negative ion are reported.

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**Abstract:** A triple basis set in Hylleraas coordinates is used to obtain improved variational bounds for the nonrelativistic energy and other properties of He, H-, and Ps(-). The accuracy, numerical stability, and computational efficiency are compared with recent work based on quasirandom basis sets. The Kato cusp conditions are used to assess the accuracy of the wave functions at short distances.

[162] B. Duan, X. Y. Gu, and Z. Q. Ma. Precise calculation for energy levels of a helium atom in P states. *Phys. Lett. A*, 283(3-4):229–236, 2001.

**Abstract:** The energy levels of a helium atom in P stares, for parahelium and orthohelium with both the odd parity and the even parity, are precisely calculated directly from the Schrodinger equation. The rotational degrees of freedom are separated completely from the internal ones, so that only three internal variables are involved in both the generalized radial functions and equations. By making use of the appropriate internal variables, the singularity in the solutions is removed and the series in calculation converges very fast. (C) 2001 Elsevier Science B.V. All rights reserved.

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**Abstract:** The energies of some excited states with the total angular momentum L = 0, 1 and 2, the total spin of two electrons S = 0 and 1, and the even and odd parities are precisely calculated directly from the Schrodinger equation where the mass of the helium nucleus is finite. Moreover, we find that the solutions to the equation for the excited states have some more nodes, which can be used to distinguish the states with the same spectral term.

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**Abstract:** In this Letter, the lowest energies of a D-dimensional helium atom in P-wave, where the total spin of two electrons is I and 0 and the parity is odd and

even, are directly calculated from the Schrodinger equation with the finite mass of the helium nucleus, respectively. It is found that the lowest energy level of the P-state with spin zero is higher than that of the state with spin one if the parity and the spatial dimension D are the same, and that I E I of the states with the same angular momentum and the parity decreases as D increases. Moreover, the interdimensional degeneracies are confirmed in the calculation, namely the states P-1,3(e) and D-1,3(o) in three dimensions are degenerated with the states S-3,1(e) and P-3,1(o) in five dimensions. (C) 2004 Elsevier B.V All rights reserved.

[165] B. Duan and Z. Q. Ma. Energies of the ground states of S-wave for a D-dimensional helium atom. *Phys. Lett. A*, 312(5-6):363–368, 2003.

**Abstract:** For a helium atom in D dimensions, the lowest energies of S wave with spin 1 and 0 are precisely calculated directly from the Schrodinger equation where the mass of the helium nucleus is finite. Our numerical results are a confirmation of the interdimensional degeneracy between the state S-1, (S-3(e)) in D dimensions and the state (3)Pe (P-1(e)) in D - 2 dimensions, where D greater than or equal to 5. (C) 2003 Elsevier Science B.V. All rights reserved.

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**Abstract:** Considering the nuclear motion, we present the nonrelativistic ground energy of a helium atom by using a simple effective variational wavefunction with a flexible parameter k. Based on the result, the relativistic and radiative corrections to the nonrelativistic Hamiltonian are discussed. The high precision value of the helium ground energy is evaluated to be -2.90338 a.u. with the relative error 0.00034%.

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**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 multi-electron 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:** 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].

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**Abstract:** We present a comprehensible computer program capable of treating non-relativistic ground and excited states for a two-electron atom having infinite nuclear mass. An iterative approach based on the implicitly restarted Arnoldi method (IRAM) is employed. The Hamiltonian matrix is never explicitly computed. Instead the action of the Hamiltonian operator on discrete pair functions is implemented. The finite difference method is applied and subsequent extrapolations gives the continuous grid result. The program is written in C and is highly optimized. All computations are made in double precision. Despite this relatively low degree of floating point precision (48 digits are not uncommon), the accuracy in the results can reach about 10 significant figures. Both serial and parallel versions are provided. The parallel program is particularly suitable for shared memory machines such as the Sun Starcat series. The serial version is simple to compile and should run on any platform.

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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:** Witten's generalization to arbitrary dimension has afforded new insight into the correlated motion of quantum particles [Phys. Today 33, (7), 38 (1980)]. We have used a classically based method to understand the resultant dimensionality dependence of the ground-state energy of the helium atom in the approximation which regards the quantum fluctuations of the system as being harmonic oscillations about a classical, correlated state of minimum effective potential energy. Making an analogy with thermal systems, this provides a "phase diagram" of a single helium atom that features a first-order melting transition, with inverse dimensionality playing the role of temperature. Our approximation gives an understanding of the high-dimensionality behavior of the quantum solution found with a perturbation theory expansion in inverse dimensionality by Goodson and Herschbach [Phys. Rev. Lett. 58, 1628 (1987)]. From comparison with variational quantum ground-state solutions by Loeser and Herschbach [J. Chem. Phys. 84, 3882 (1986)] for atomic

numbers 2, 3, and 6 we find that the harmonic description improves with decreasing nuclear charge.

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**Abstract:** A method is developed for using large-order perturbation theory to solve the systems of coupled differential equations that result from the variational solution of the Schrodinger equation with wave functions of product form. This is a noniterative, computationally efficient way to solve self-consistent-field (SCF) equations. Possible applications include electronic structure calculations using products of functions of collective coordinates that include electron correlation, vibrational SCF calculations for coupled anharmonic oscillators with selective coupling of normal modes, and ab initio calculations of molecular vibration spectra without the Born-Oppenheimer approximation.

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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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**Abstract:** The independent eigenstates of the total orbital angular momentum operators for a three-body system in an arbitrary D-dimensional space are presented by the method of group theory. The Schrodinger equation is reduced to the generalized radial equations satisfied by the generalized radial functions with a given total orbital angular momentum denoted by a Young diagram [mu, nu, 0,..., 0] for the SO(D) group. Only three internal variables are involved in the functions and equations. The number of both the functions and the equations for the given angular momentum is finite and equal to (mu-nu+1). (C) 2002 American Institute of Physics.

[252] X. Y. Gu, Z. Q. Ma, and B. Duan. Interdimensional degeneracies for a quantum three-body system in D dimensions. *Phys. Lett. A*, 307(1):55–59, 2003.

**Abstract:** A new approach is developed to derive the complete spectrum of exact interdimensional degeneracies for a quantum three-body system in D dimensions. The new method gives a generalization of previous methods. 

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> **Abstract:** Complete spectrum of exact interdimensional degeneracies for a quantum isolated four-body system in D dimensions is presented and proved by the method of generalized spherical harmonic polynomials. A quantum isolatd system must be invariant in a global translation and a global rotation. In a quantum isolated four-body system all the states with angular momentum [mu + n, nu + n, tau + n] in (D - 2n) dimensions are degenerate where mu, nu, tau, and D are given and n is an arbitrary integer if the representation [mu + n, nu + n, tau + n] exists for the SO(D - 2n) group and D - 2n greater than or equal to 4. There is an exceptional interdimensional degeneracy for a four-body system between the state with zero angular momentum in D = 3 dimensions and the state with zero angular momentum in D = 5 dimensions. (C) 2003 Elsevier B.V. All rights reserved.

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> **Abstract:** An adiabatic model of a three-particle problem with the use of hyperspherical approach is suggested. The essential point of the proposed model is that the trial solution of the equation for determination of the adiabatic potential satisfies the correct asymptotic parametric dependence on the hyperradius. This enables one both to reproduce a very precise value of the ground state energy and to obtain much better agreement of the theory with the experiment for higher energies of 1sns-configurations for singlet as well as for triplet states.

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**Abstract:** For large values of d = 3N, the radial distribution function of an N-particle system is sharply peaked near the hyperradius r(m) = (d - 2)/2k0, where k0 = (2E)1/2. This fact allows an approximate separation of the hyperradius, leading to many-dimensional hydrogen-like radial solutions. Kindred applications to dimensional scaling are also discussed, where d = DN, with D the spatial dimension. For the large D regime, illustrative analytic formulas are obtained giving the energy and effective nuclear charge for the lowest few S states of the helium atom.

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**Abstract:** A growing repertoire of electronic structure methods employ the spatial dimension D as an interpolation or scaling parameter. It is advantageous to transform the Schrodinger equation to remove all dependence on D from the Jacobian volume element and the Laplacian operator; this introduces a centrifugal term, quadratic in D, that augments the effective potential. Here we explicitly formulate this procedure for S states of an arbitrary many-particle system, in two variants. One version reduces the Laplacian to a quasicartesian form, and is particularly suited to evaluating the exactly solvable D –¿ infinity limit and perturbation expansions about this limit. The other version casts the Jacobian and Laplacian into the familiar forms for D = 3, and is particularly suited to calculations employing conventional Rayleigh-Ritz variational methods.

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**Abstract:** Progress on high precision calculations for the ground state of atomic lithium is reviewed. The following properties are considered: upper and lower bounds to the nonrelativistic ground state energy, the specific

mass shift, the transition isotope shift, relativistic corrections to the ground state energy, the Lamb shift, the ionization potential, the electron affinity, the hyperfine coupling constant, the nuclear magnetic shielding constant, the diamagnetic susceptibility, several polarizability factors, shielding constants, oscillator strength sums, the electron density and spin density, intracule functions, moments [r(i)(n)] and [r(i)(jn)] and form factors. A discussion is also given on some convergence considerations as they apply to high precision calculations on the lithium atom. (C) 1997 Elsevier Science B.V.

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**Abstract:** It is known that variational methods are the most powerful tool for studying the Coulomb three-body bound-state problem. However, they often suffer from loss of stability when the number of basis functions increases. This problem can be cured by applying the multiprecision package designed by D. H. Bailey. We consider variational basis functions of the type exp(-alpha(n)r(1)-beta(n)r(2)-gamma(n)r(12)) with complex exponents. The method yields the best available energies for the ground states of the helium atom and the positive hydrogen molecular ion as well as many other known atomic and molecular systems.

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**Abstract:** Hyperspherical coordinates were first introduced by Pane in the 1960s to understand the basic properties of doubly excited slates of helium atoms, In the past few decades, this approach has been refined and extended to a broad range of few-body atomic and molecular systems. The success story of this general method as first laid out by Fano is reviewed.

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**Abstract:** Considering that gravitational force might deviate from Newton's inverse-square law and become much stronger in small scale, we present a method to detect the possible existence of extra dimensions in the ADD model. By making use of an effective variational wave function,

we obtain the nonrelativistic ground energy of a helium atom and its isoelectronic sequence. Based on these results, we calculate gravity correction of the ADD model. Our calculation may provide a rough estimation about the magnitude of the corresponding frequencies which could be measured in later experiments.

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**Abstract:** Mathematica language is used to make a program that can solve the three-body problem with variational method. Considering the nuclear motion, the nonrelativistic ground energies and the analytic wave functions of the helium atom and the helium-like ions ( H-, He, L+ , Be+ +, B3+, C4+, N5+, O6+) are presented by using a simple effective variational wave function with a flexible parameter k. Based on these results, the influence of a finite nucleus charge radius, the relativistic and radiative corrections on the nonrelativistic Hamiltonian are discussed. The high precision values of the helium atom and the helium-like ions ground energies are evaluated.

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**Abstract:** The evaluation of matrix elements of two electron atoms is fundamental for the study of the electronic properties of those systems. We add to this knowledge by presenting an explicit expression for the matrix elements of the inverse of the interelectronic distance of two-electron atoms in any spatial dimension D. The basis functions used are the D-dependent hydrogenic wavefunctions 1s(2), 2p(2), 3d(2), 4f(2), 5g(2),..., 21y(2),..., extending and including, in this way, the results of the previous basis set 1s(2), 2p(2), 3d(2), 4f(2). The methodology used does not employ Fourier integral transforms as in previous works but hypergeometric transformation formulas.

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**Abstract:** Our approach aims at a general formalism for the quantum description of the three-body Coulomb systems. We seek the exact solutions of 6D Schrodinger equation. For this, we propose a new algorithm for the case of nonzero total angular momentum, taking into account the overall rotation of the system, which is affected indirectly by the Coriolis coupling. We construct a special set of hyperspherical harmonics, which provide much more flexibility in choosing the best basis for the needs of this particular physical problem. The robustness, efficiency, and accuracy of the adopted algorithm are studied in detail. We apply this method to the computation of the nonrelativistic energy levels of the exotic helium (P) over tilde He+.

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**Abstract:** The nonadiabatic ground state for the helium atom is obtained with the hyperspherical adiabatic approach. Potential curves, nonadiabatic couplings, and channel functions are calculated by a numerically exact procedure based on the analytical expansion of the channel functions. The coupled radial equations are solved by standard techniques. The convergence of the procedure is investigated as nonadiabatic couplings are systematically introduced. The inclusion of 11 potential curves and channel functions gives a ground-state energy that differs from the best variational calculation by 0.1 parts per million.

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**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.

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**Abstract:** A mapping between the quantum few-body problem and its classical mechanics pseudo-system analog is used to study the critical parameters for the helium isoelectronic sequence. The critical point is the critical value of the nuclear charge Z(c), for which the energy of a bound state becomes degenerate with a threshold. A finite-size scaling ansatz in the form of a phenomenological renormalization equation is used to obtain very accurate results for the critical point of the ground-state energy, lambda(c) = 1/Z(c) = 1 .0976+/-0.0004, as well as for the excited 2p(2) P-3 state, lambda(c) = 1.0058+/-0.0017. The results for the critical exponents alpha and nu are also included. (C) 1998 American Institute of Physics.

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**Abstract:** The energy levels of the helium atom and isoelectronic ions in two dimensions are considered. The difficulties encountered in the analytical evaluation of the perturbative and variational expressions for the ground state, promote an interesting factorization of the interelectronic interaction, leading to simple expressions for the energy. This expression provides an insight into the general structure and screening effect in the ground state. Some of the considerations are extended to excited states. The dimensionality properties of the energy spectrum of a helium atom, the screening effect and their implications are of significant pedagogical interest in the study of perurbative and variational approaches to analyse the properties of helium atoms, in quantum mechanics and atomic physics, for general graduate students and specialists in atomic physics.

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**Abstract:** The splitting of pair interactions into physical and spurious terms is analyzed and the construction of exact solutions to the Faddeev equations with centrifugal potentials is described. The derivations of the asymptotics for three-body wave functions and their components at triple- and double-collision points are discussed, and essential peculiarities of some variational and spline approximations are clarified.

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**Abstract:** The dynamics of the positronium negative ion is described in a molecular adiabatic approximation. It is shown, how the classification of the spectrum, propensity rules for radiative and non-radiative transitions and conditions for the occurrence of shape resonances can easily be derived within this approach. Propensity rules for two-photon processes are also derived and used to demonstrate the possibility of an absorption experiment from the ground state to excite a S-1(e) shape resonance, which is unique to Ps(-).

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**Abstract:** The molecular-orbital description of two-electron atoms [J. M. Feagin and J. S. Briggs, Phys. Rev. A 37, 4599 (1988)], derived from H-2+ by interchanging the roles of electrons and nuclei, is generalized to D dimensions. For H-2+ itself there exist myriad exact interdimensional degeneracies because D –¿ D + 2 is equivalent to m –¿ m + 1, augmenting by unity the projection of the electronic angular momentum on the internuclear axis. When the molecular orbitals (MO's) are transcribed to treat two-electron motion, additional constraints limit the exact degeneracies to states in D = 3 and 5, but many approximate degeneracies persist. Since the MO description emphasizes rotational properties of the two-electron atom, the link between dimension and orbital angular momentum is a pervasive feature. We use this link to classify groups of quasidegenerate doubly excited atomic energies

and to explain striking similarities among certain pairs of hyperspherical or molecular-orbital two-electron potential curves.

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**Abstract:** in the framework of nonrelativistic variational formalism a new type of basis set is proposed, to estimate separately the effect of radial and angular correlations on the ground-state energy for helium isoelectronic sequence H- to Ar16+. Effect of radial correlation is incorporated by using multiexponential functions arising from product basis sets suitably formed out of Slater-type one-particle orbitals. The angular correlation can be switched on by incorporating an expansion in terms of basis involving interparticle coordinates. With a set of six-term Slater-type one-particle basis and five-term interparticle expansion, the ground-state energy of helium is estimated as -2.9037236 (a.u.) compared with the multiterm variational estimates -2.9037244 (a.u.) due to Pekeris and Thakkar and Smith and Drake. Matrix elements of different operators in the ground state have been calculated and found to be in good agreement with available accurate results. (C) 2003 Wiley Periodicals, Inc.

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**Abstract:** The variational principle for eigenvalue problems with a nonidentity weight operator is used to establish upper or lower bounds on critical parameters of quantum systems. Three problems from atomic physics are considered as examples. Critical screening parameters for the exponentially screened Coulomb potential are found using a trial function with one nonlinear variational parameter. The critical charge for the helium isoelectronic series is found using a Hylleraas-type trial function. Finally, critical charges for the same system subjected to a magnetic field are found using a product of two hydrogenlike basis sets.

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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:** 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 sub-

stantially 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 mo-

tion. 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:** The non-relativistic energies of the ground states in the helium-like systems from Z = 2 to 5 are calculated by using three different basis functions, the Slater-type, the ordered coordinates and the modified angular wave functions in which the angular variational parameters are included. In calculations with the latter two types of basis functions, we only used 168 terms in eight l components. The best value of energy for neutral helium atom in this work is obtained by using the modified angular wave functions. It is determined to be -2.9037161 a.u., which is about 0.00017 a.u. lower than that obtained with the 221-term Slater-type expansions. In cases of the helium-like ions from Z = 3 to 5, the comparison of our calculated results using these three types of basis functions indicates that the results obtained with the modified angular wave functions are better than those with the other two types of basis functions. The convergence pattern in energy with the increasing number of terms in the angular partial wave functions is also analyzed.

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**Abstract:** We present results obtained using dimensional scaling with high-frequency Floquet theory to evaluate the stability of gas phase simple diatomic molecules in superintense laser fields. The large-D limit provides a simple model that captures the main physics of the problem, which imposes electron localization along the polarization direction of the laser field. This localization markedly reduces the ionization probability and can enhance chemical bonding when the laser strength becomes sufficiently strong. We find that energy and structure calculations at the large-dimensional limit (D -¿infinity) for stabilities of H-2(+), H-2, and He-2 in superintense laser fields are much simpler than at D=3, yet yield similar results to those found from demanding ab initio calculations. We also use the large-D model to predict the stability of H-2(-) and the field strength needed to bind the "extra" electron to the H-2 molecule.

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**Abstract:** In this article exact solutions of a two-electron Schrodinger equation for the Coulomb potential were extended to the Fues-Kratzer-type potential: ((Z) over cap(Omega)/r) + ((A) over cap/r(2)). The wave function psi(r, Omega) is expanded into generalized Laguerre polynomials and hyperspherical harmonics. An analytical expression of two-electron systems is given for matrix elements and accurate energy eigenvalues of the excited state of S-1,S-3 helium are calculated by using the hyperspherical harmonics method. The present results are compared with previous theoretical calculations and it is concluded that the convergence of energy eigenvalues is faster. (C) 2000 John Wiley & Sons, Inc.

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**Abstract:** The performance of the so-called superconvergent quantum perturbation theory (Wenhua Hai et al 2000 Phys. Rev. A 61 052105) is investigated for the case of the ground-state energy of the helium-like

ions. The scaling transformation r –¿ r/Z applied to the Hamiltonian of a two-electron atomic ion with a nuclear charge Z (in atomic units). Using the improved Rayleigh-Schrodinger perturbation theory based on the integral equation to helium-like ions in the ground states and treating the electron correlations as perturbations, we have performed a third-order perturbation calculation and obtained the second-order corrected wavefunctions consisting of a few terms and third-order energy corrections. We find that third-order and higher-order energy corrections are improved with decreasing nuclear charge. This result means that the former is quadratically integrable and the latter is physically meaningful. The improved quantum perturbation theory fits the higher-order perturbation case. This work shows that it is a development on the quantum perturbation problem of helium-like systems.

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**Abstract:** The definition of a norm for scattering states is reviewed particularly with respect to the method of complex scaling used to determine resonant states. The meaning of complex expectation values which result from this procedure is illustrated with a simple two-channel model. In a further example autoionizing states of helium are analysed in terms of complex expectation values which are shown to provide a sensitive tool to probe details of complicated dynamics. We also demonstrate how Lewis structures for resonances may be defined through complex expectation values.

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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].

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**Abstract:** In this work we analyze the spectrum of the iso-electronic series of the helium atom by using the hyperspherical adiabatic method. This method allows the study of the energy levels of atomic systems by means of a set of potential curves, similarly to the Born-Oppenheimer approach for molecular systems. The potential curves are defined with respect to a unique radial variable, regardless the number of the system electrons. As a result the analysis and classification of the energy levels proceeds in a simple and intuitive way, which is not observed within the variational and Hartree-Fock methods, The objective of this research is to describe the behavior of the helium-like systems ground state with respect to the nuclear charge value. Besides the hyperspherical method simplification of the results analysis, it is an ab-initio process, whose accuracy is only limited by the truncation of the coupled equation number. Within its simplest approximation, in which all couplings are disregarded, the error obtained for the ground state energy is inferior to 1% and with the introduction of the diagonal coupling the error drops to only 0.3%. Further improvement is obtained with the non-adiabatic couplings, reaching precisions of the order of 10(-3)%.