

Bibliography for D -scaling

May 8, 2009

(With abstracts)

References

- [001] 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.
- [002] J. P. Ader. MOMENT-METHOD AND THE SCHRÖDINGER-EQUATION IN THE LARGE N LIMIT. *Phys. Lett. A*, 97(5):178–182, 1983.
- [003] A. Aguado, J. J. Camacho, and M. Paniagua. A NUMERICAL PROCEDURE TO OBTAIN ACCURATE POTENTIAL-ENERGY CURVES FOR DIATOMIC MOLECULES. *Theochem-J. Mol. Struct.*, 86:135–144, 1992.

Abstract: The potential energy curves for the X1-SIGMA+ state of C-12-O-16 and Li-6-H-1 were obtained by fitting the Rydberg-Klein-Rees potential in the Chebyshev sense (minimum-maximum approximation) to a simple functional form very similar to a perturbed-Morse-oscillator potential but with a minor number of parameters. Using Hermite orthogonal functions (eigenfunctions of the harmonic oscillator) as the basis set we solved variationally the radial Schrödinger equation to obtain the vibrational energies $E(v)$ and the rotational constants $B(v)$. Using the potential thus determined and the proposed basis set, the matrix elements of the Hamiltonian may be calculated analytically, presenting only round-off errors. The

agreement between the calculated and experimentally determined $E(v)$ and $B(v)$ values is good, the self-consistency of our potentials being very similar to that obtained by other authors.

- [004] L. Akant, G. S. Krishnaswami, and S. G. Rajeev. Entropy of operator-valued random variables: A variational principle for large N matrix models. *Int. J. Mod. Phys. A*, 17(18):2413–2444, 2002.

Abstract: We show that, in 't Hooft's large N limit, matrix models can be formulated as a classical theory whose equations of motion are the factorized Schwinger-Dyson equations. We discover an action principle for this classical theory. This action contains a universal term describing the entropy of the noncommutative probability distributions. We show that this entropy is a nontrivial one-cocycle of the noncommutative analog of the diffeomorphism group and derive an explicit formula for it. The action principle allows us to solve matrix models using novel variational approximation methods; in the simple cases where comparisons with other methods are possible, we get reasonable agreement.

- [005] S. M. Aljaber. QUANTIZATION OF ANGULAR-MOMENTUM IN THE N-DIMENSIONAL SPACE. *Nouvo Cimento Soc. Ital. Fis. B-Gen. Phys. Relativ. Astron. Math. Phys. Methods*, 110(8):993–995, 1995.

Abstract: We consider the most general case of the quantization of angular momentum in the N-dimensional space. We show that a hydrogen atom, when viewed in an N-dimensional, multiply connected space, the angular momentum must be $((N - 1)/2)$ -integral.

- [006] S. M. AlJaber. On the radial-part equation of the wave function in N dimensions. *Nouvo Cimento Soc. Ital. Fis. B-Gen. Phys. Relativ. Astron. Math. Phys. Methods*, 112(5):761–765, 1997.

Abstract: We consider the equation for the radial part of the wave function of the Schrodinger equation in the N-dimensional space. A new effective potential is derived when the equation for the radial part of the wave function is written in the form of a one-dimensional Schrodinger equation.

As a constructive example, we find and discuss the solution, the orthonormality, and the energy eigenvalues of the radial part of the wave function for an infinite spherical potential well in N dimensions.

- [007] S. M. Al-Jaber. Hydrogen atom in N dimensions. *Int. J. Theor. Phys.*, 37(4):1289–1298, 1998.

Abstract: Some aspects of the N-dimensional hydrogen atom are discussed. The complete solution for the energy eigenfunctions is presented and the radial distribution function is examined. Degeneracy of energy levels, expectation Values ($[1/r]$ and $[1/r(2)]$), and the virial theorem are considered. It is shown that the effect of the effective potential manifests itself in some of the aspects being investigated.

- [008] S. M. Al-Jaber. The fine structure of the N-dimensional hydrogen atom. *Nouvo Cimento Soc. Ital. Fis. B-Gen. Phys. Relativ. Astron. Math. Phys. Methods*, 113(5):651–657, 1998.

Abstract: The fine structure of energy levels of a hydrogen atom in N dimensions is given. This is done by calculating the first-order energy correction due to the relativistic correction to kinetic energy, spin-orbit coupling, and Darwin term. Thus we emphasize the role of the topological structure of the configuration space of a physical system on the quantum nature of an observable of the system.

- [009] S. M. Al-Jaber. Fermi gas in D-dimensional space. *Int. J. Theor. Phys.*, 38(3):919–923, 1999.

Abstract: We consider a Fermi gas in D-dimensional space and show how the physical properties of the system behave as a function of the dimension D, in particular, the density of states, the Fermi energy, and the radius of the Fermi hypersphere.

- [100] A. Chatterjee. 1/N EXPANSION FOR THE YUKAWA POTENTIAL REVISITED .2. *J. Phys. A-Math. Gen.*, 19(17):3707–3710, 1986.

- [101] A. Chatterjee. BOUND-STATE ENERGIES OF THE GENERALIZED EXPONENTIAL COSINE-SCREENED COULOMB POTENTIAL. *Phys. Rev. A*, 34(3):2470–2472, 1986.

- [102] A. Chatterjee. LARGE-N LIMIT OF THE KLEIN-GORDON EQUATION FROM THE UNCERTAINTY PRINCIPLE. *Phys. Lett. A*, 120(4):171–173, 1987.
- [103] A. Chatterjee. HYPERVIRIAL 1/N EXPANSION FOR THE BOUND-STATE ENERGY-SPECTRUM OF THE GENERALIZED EXPONENTIAL-COSINE-SCREENED COULOMB POTENTIAL. *Phys. Rev. A*, 35(6):2722–2724, 1987.
- [104] A. Chatterjee. LARGE-N EXPANSIONS IN QUANTUM-MECHANICS, ATOMIC PHYSICS AND SOME O(N) INVARIANT-SYSTEMS. *Phys. Rep.-Rev. Sec. Phys. Lett.*, 186(6):249–370, 1990.
- [105] R. Chattopadhyay, T. K. Das, and P. K. Mukherjee. Hyperspherical harmonics expansion of the ground state of the Ps(-) ion. *Phys. Scr.*, 54(6):601–603, 1996.

Abstract: We have treated the ground state of the positronium negative ion (Ps(-)) by a hyperspherical harmonics expansion method in which the centre of mass motion is properly accounted for. The resulting system of coupled differential equations has been solved by the renormalized Numerov method. We find that the convergence in the Binding Energy (BE) with respect to inclusion of higher hyperspherical partial waves is quite slow for this diffuse system. Using our exact numerical results up to a maximum of 28 for the hyper angular momentum quantum number (K-M) in an extrapolation formula based on the hyperspherical convergence theorems, we get the binding energy of the ground state of Ps(-) as 0.261 6689 au.

- [106] C. Y. Chen, D. S. Sun, C. L. Liu, and F. L. Lu. Scattering states of n-dimensional hydrogen atom. *Acta Phys. Sin.*, 52(4):781–785, 2003.

Abstract: Characteristics of the scattering states of an n-dimensional hydrogen atom have been studied. The normalized wave functions of scattering states on "k/2pi scale" and the calculation formula of phase shift are presented. The analytical properties of phase shift are discussed, and analytical formulas for calculating bound-continuous transition matrix elements are also given. The relevant results of scattering states for the usual hydrogen

atom ($n = 3$) reported in the literature are contained in more general conclusions of this paper as special cases.

- [107] G. Chen. The recursion relations for the N-dimensional harmonic oscillator. *Phys. Lett. A*, 328(2-3):123–126, 2004.

Abstract: Two recursion relations in terms of raising and lowering operators are derived for only the 'principal' and 'angular-momentum' quantum numbers through Laplace transforms. (C) 2004 Elsevier B.V. All rights reserved.

- [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.

- [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.

- [110] T. L. Chen and C. I. Tan. 1/N TOPOLOGICAL EXPANSION FOR LATTICE QCD. *Phys. Lett. B*, 108(2):127–130, 1982.

- [111] T. L. Chen and C. I. Tan. PHASE-STRUCTURE FOR ONE-PLAQUETTE LATTICE QUANTUM CHROMODYNAMICS WITH FERMIONS IN A $1/N$ TOPOLOGICAL EXPANSION. *Phys. Rev. D*, 26(8):2018–2027, 1982.
- [112] S. C. Chhajlany and V. N. Malnev. BOUND-STATES OF ANHARMONIC POTENTIALS. *Phys. Rev. A*, 42(5):3111–3114, 1990.
- [113] H. Christiansen, L. N. Epele, H. Fanchiotti, and C. A. G. Canal. IMPROVED SHIFTED $1/N$ EXPANSION. *Phys. Rev. A*, 40(4):1760–1764, 1989.
- [114] P. Christol, P. Lefebvre, and H. Mathieu. FRACTIONAL-DIMENSIONAL CALCULATION OF EXCITON BINDING-ENERGIES IN SEMICONDUCTOR QUANTUM-WELLS AND QUANTUM-WELL WIRES. *J. Appl. Phys.*, 74(9):5626–5637, 1993.

Abstract: We propose a fractional-dimensional approach of excitonic characteristics in semiconductor quantum wells and quantum-well wires with cylindrical or rectangular cross sections. This type of approach has proved to provide accurate and convenient methods for extracting excitonic binding energies, either from optical spectroscopy experiments, or from simple envelope function calculations. In this paper, we first try and extend the simple description previously developed for single quantum wells and superlattices. Next, we show how the accuracy of the model is dramatically improved by invoking microscopic considerations, in order to describe the anisotropy of the relative motion of confined electron-hole pairs. This original approach allows a rather simple and quick determination of eigenenergies of confined excitons, whatever the quantum numbers of the conduction and valence subbands, and whatever the shape of the confining medium. The results of our calculations compare favorably to those of available variational theories and to experimental findings.

- [115] J. Cizek, R. J. Damburg, S. Graffi, V. Grecchi, E. M. Harrell, J. G. Harris, S. Nakai, J. Paldus, R. K. Propin, and H. J. Silverstone. $1/R$ EXPANSION FOR H_2^+ - CALCULATION OF EXPONENTIALLY SMALL TERMS AND ASYMPTOTICS. *Phys. Rev. A*, 33(1):12–54, 1986.

[116] J. Cizek and E. R. Vrscaj. LARGE ORDER PERTURBATION-THEORY IN THE CONTEXT OF ATOMIC AND MOLECULAR PHYSICS - INTERDISCIPLINARY ASPECTS. *Int. J. Quantum Chem.*, 21(1):27–68, 1982.

[117] H. T. Coelho, J. J. Degroote, and J. E. Hornos. GENERAL THEORETICAL APPROACH TO COULOMBIC 3-BODY SYSTEMS BY THE HYPERSPHERICAL FORMALISM. *Phys. Rev. A*, 46(9):5443–5452, 1992.

Abstract: Coulombic three-body systems are investigated using the hyperspherical adiabatic approach. By using a suitable variable $z = \tan(\alpha/2)$ in the angular differential equation for the determination of the potential curves, we are able to obtain stable series-expansion solutions, valid for small and large values of the hyperspherical radius. The analysis of the mathematical singularities of the differential equations in the variable z offers an insight into the physics of the problem and into the determination of stable converging solutions as well. In order to illustrate our investigation, we apply this study to several carefully chosen systems: He, ddmu, d2+, and excitons bound to a Coulomb center in different semiconductors.

[118] J. M. Cohen and D. Z. Goodson. Unified approach to molecular structure and molecular vibrations. *Int. J. Quantum Chem.*, 59(6):445–456, 1996.

Abstract: First-order dimensional perturbation theory is used to construct a Hamiltonian for the H-2(+) molecule without the Born-Oppenheimer approximation. The physical model that emerges has the three particles undergoing harmonic oscillations about a bent symmetric configuration. Despite its simplicity, the theory yields correct results for the ground-state energy, for the equilibrium internuclear distance, and for vibrational frequencies. Although the standard dimensional continuation of the Schrodinger equation leads to dissociation at large D, this model remains stable due to a quadratic polynomial in 1/D that is included in the potential energy. This Hamiltonian is a suitable starting point for a large-order perturbation expansion in 1/D. (C) 1996 John Wiley & Sons, Inc.

- [119] H. Collins and H. Georgi. A little large N group theory. *Phys. Lett. B*, 394(1-2):152–160, 1997.

Abstract: We discuss the group theory relevant to the ground-state baryons in large N-c QCD. For very large representation, the group generators become classical variables. We find the form of the classical generators for the completely symmetric N index representation of SU(m) as N \rightarrow infinity and derive an integral formula for the matrix elements of an arbitrary polynomial in the group generators between low-spin baryon states in the large N limit.

- [120] J. Cook and B. Derrida. DIRECTED POLYMERS IN A RANDOM MEDIUM - 1/D EXPANSION. *Europhys. Lett.*, 10(3):195–199, 1989.

- [121] J. Cook and B. Derrida. DIRECTED POLYMERS IN A RANDOM MEDIUM - 1/D EXPANSION AND THE N-TREE APPROXIMATION. *J. Phys. A-Math. Gen.*, 23(9):1523–1554, 1990.

- [122] F. Cooper, A. Khare, and U. Sukhatme. SUPERSYMMETRY AND QUANTUM-MECHANICS. *Phys. Rep.-Rev. Sec. Phys. Lett.*, 251(5-6):268–385, 1995.

Abstract: In the past ten years, the ideas of supersymmetry have been profitably applied to many nonrelativistic quantum mechanical problems. In particular, there is now a much deeper understanding of why certain potentials are analytically solvable and an array of powerful new approximation methods for handling potentials which are not exactly solvable. In this report, we review the theoretical formulation of supersymmetric quantum mechanics and discuss many applications. Exactly solvable potentials can be understood in terms of a few basic ideas which include supersymmetric partner potentials, shape invariance and operator transformations. Familiar solvable potentials all have the property of shape invariance. We describe new exactly solvable shape invariant potentials which include the recently discovered self-similar potentials as a special case. The connection between inverse scattering, isospectral potentials and supersymmetric quantum mechanics is discussed and multisoliton solutions of the KdV

equation are constructed. Approximation methods are also discussed within the framework of supersymmetric quantum mechanics and in particular it is shown that a supersymmetry inspired WKB approximation is exact for a class of shape invariant potentials. Supersymmetry ideas give particularly nice results for the tunneling rate in a double well potential and for improving large N expansions. We also discuss the problem of a charged Dirac particle in an external magnetic field and other potentials in terms of supersymmetric quantum mechanics. Finally, we discuss structures more general than supersymmetric quantum mechanics such as para-supersymmetric quantum mechanics in which there is a symmetry between a boson and a para-fermion of order p.

- [123] R. Correale and E. Guadagnini. LARGE-N CHERN-SIMONS FIELD-THEORY. *Phys. Lett. B*, 337(1-2):80–85, 1994.

Abstract: We consider the $SU(N)$ Chern-Simons field theory and study the behaviour of the observables, which are defined by the expectation values of Wilson line operators, in the large-N limit. We determine the structure of the knot invariants which are obtained in this limit and some of their properties are derived; it is proved, for example, that for the product of gauge-invariant operators the factorization property is satisfied. A new relation connecting each knot with its double is derived.

- [124] H. Cox, S. J. Smith, and B. T. Sutcliffe. SOME CALCULATIONS ON THE GROUND AND LOWEST-TRIPLET STATE OF HELIUM IN THE FIXED-NUCLEUS APPROXIMATION. *Phys. Rev. A*, 49(6):4520–4532, 1994.

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 in 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 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.

- [125] R. J. Damburg, R. K. Propin, S. Graffi, V. Grecchi, E. M. Harrell, J. Cizek, J. Paldus, and H. J. Silverstone. 1/R EXPANSION FOR H-2+ - ANALYTICITY, SUMMABILITY, ASYMPTOTICS, AND CALCULATION OF EXPONENTIALLY SMALL TERMS. *Phys. Rev. Lett.*, 52(13):1112–1115, 1984.
- [126] S. R. Das. SOME ASPECTS OF LARGE-N THEORIES. *Rev. Mod. Phys.*, 59(1):235–261, 1987.
- [127] S. R. Das and A. Jevicki. Large-N collective fields and holography. *Phys. Rev. D*, 68(4):13, 2003.

Abstract: We propose that the Euclidean bilocal collective field theory of critical large-N vector models provides a complete definition of the proposed dual theory of higher spin fields in anti-de Sitter spaces. We show how this bilocal field can be decomposed into an infinite number of even spin fields in one more dimension. The collective field has a nontrivial classical solution which leads to an $O(N)$ thermodynamic entropy characteristic of the

lower dimensional theory, as required by general considerations of holography. A subtle cancellation of the entropy coming from the bulk fields in one higher dimension with $O(1)$ contributions from the classical solution ensures that the subleading terms in thermodynamic quantities are of the expected form. While the spin components of the collective field transform properly under dilatational, translational, and rotational isometries of AdS, special conformal transformations mix fields of different spins indicating a need for a nonlocal map between the two sets of fields. We discuss the nature of the propagating degrees of freedom through a Hamiltonian form of collective field theory and argue that nonsinglet states which are present in an Euclidean version are related to nontrivial backgrounds.

- [128] S. Datta and J. K. Bhattacharjee. Spiked harmonic oscillator: N-1 expansion. *Int. J. Mod. Phys. B*, 17(14):2761–2772, 2003.

Abstract: The ground state of the spiked harmonic oscillator with the potential $V(r) = r(2) + \lambda/r(\alpha)$ has been obtained variationally for $\alpha \leq 3$ and recently by a numerical procedure for $\alpha \geq 3$. Due to the Klauder phenomenon at $\alpha = 3$, analytic techniques do not smoothly interpolate between $\alpha \leq 3$ and $\alpha \geq 3$. Here we use the N-1 expansion, where N is the dimensionality of space, to set up an analytic scheme that can be continued across $\alpha = 3$.

- [129] S. Datta, S. Bhattacharyya, and J. K. Bhattacharjee. Hydrogen atom in a magnetic field: large-N expansion. *Phys. Lett. A*, 265(4):241–243, 2000.

Abstract: For a hydrogen atom in a magnetic field, it is known that near the ionisation threshold the energy levels are equispaced with a spacing of $3/2 (\hbar) \overline{\omega(c)}$ where $\omega(c)$ is the cyclotron frequency. We use the large-N expansion to derive this result. (C) 2000 Published by Elsevier Science B.V. All rights reserved.

- [130] J. J. De Groot 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 helium-like 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.

- [131] J. J. De Groote, M. Masili, and J. E. Hornos. Analytical functions for the calculation of hyperspherical potential curves of atomic systems. *Phys. Rev. A*, 62(3):9, 2000.

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.

- [132] F. A. de Saavedra, E. Buendia, F. J. Galvez, and A. Sarsa. Precise variational calculation of some S-states of Coulomb three-body systems with two identical particles. *Eur. Phys. J. D*, 2(2):181–190, 1998.

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.

- [133] F. A. de Saavedra, E. Buendia, F. J. Galvez, and A. Sarsa. Variational calculation of some S-states of Coulomb three-body systems. *Eur. Phys. J. D*, 13(2):201–206, 2001.

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.

- [134] M. deDiosLeyva, A. BrunoAlfonso, A. MatosAbiague, and L. E. Oliveira. Fractional-dimensional space and applications in quantum-confined semiconducting heterostructures. *J. Appl. Phys.*, 82(6):3155–3157, 1997.

Abstract: We present a systematic study of excitonic and impurity states in semiconducting quantum wells within a fractional-dimensional space approach, in which the Schrodinger equation is solved in a noninteger-dimensional space where the interactions are assumed to occur in an isotropic effective environment. In this scheme, the fundamental quantity is the parameter D which defines the fractional dimension associated to the effective medium, and to the degree of anisotropy of the interactions. A direct procedure for determining the fractional dimensionality of the isotropic effective space is proposed in which one may obtain a reliable solution for the energies of the actual physical system under consideration. Explicit calculations of the fractional-dimensional D parameter are made in the case of excitons and impurities in infinite-barrier quantum wells, with exciton and impurity binding energies found in excellent agreement with previous variational results. Calculations are also performed for exciton binding energies in finite-barrier quantum wells with good agreement with recent experimental results. (C) 1997 American Institute of Physics.

- [135] J. Deenen and C. Quesne. DYNAMICAL GROUP OF MICROSCOPIC COLLECTIVE STATES .2. BOSON REPRESENTATIONS IN D-DIMENSIONS. *J. Math. Phys.*, 23(11):2004–2015, 1982.
- [136] J. S. Dehesa, F. J. Galvez, and I. Porras. BOUNDS TO DENSITY-DEPENDENT QUANTITIES OF D-DIMENSIONAL MANY-PARTICLE SYSTEMS IN POSITION AND MOMENTUM SPACES - APPLICATIONS TO ATOMIC SYSTEMS. *Phys. Rev. A*, 40(1):35–40, 1989.
- [137] J. S. Dehesa, R. Gonzalez-Ferez, P. Sanchez-Moreno, and R. J. Yanez. Kinetic energy bounds for particles confined in spherically-symmetric traps with non-standard dimensions. *New J. Phys.*, 9:18, 2007.

Abstract: The kinetic energy of non-relativistic single-particle systems with arbitrary D-dimensional central potentials is found to be bounded from below by means of the orbital hyperangular quantum number, the dimensionality and some radial and logarithmic expectation values of the form $[r(k)]$ and $[r(k)(\ln r)(m)]$. Beyond the intrinsic physico-mathematical interest of this problem, we want to contribute to the current development of the theory of independent particles confined in spherically symmetric traps with non-standard dimensions. The latter has been motivated by the recent experimental achievements of the evaporative cooling of dilute (i.e. almost non-interacting) fermions in magnetic traps.

- [138] J. S. Dehesa, S. Lopez-Rosa, B. Olmos, and R. J. Yanez. Fisher information of D-dimensional hydrogenic systems in position and momentum spaces. *J. Math. Phys.*, 47(5):13, 2006.

Abstract: The spreading of the quantum-mechanical probability distribution density of D-dimensional hydrogenic orbitals is quantitatively determined by means of the local information-theoretic quantity of Fisher in both position and momentum spaces. The Fisher information is found in closed form in terms of the quantum numbers of the orbital. (c) 2006 American Institute of Physics.

- [139] M. F. Delaripelle. GREEN-FUNCTION AND SCATTERING-AMPLITUDES IN MANY-DIMENSIONAL SPACE. *Few-Body Syst.*, 14(1):1–24, 1993.

Abstract: Methods for solving scattering are studied in many-dimensional space. Green function and scattering amplitudes are given in terms of the required asymptotic behaviour of the wave function. The Born approximation and the optical theorem are derived in many-dimensional space. Phase-shift analyses are performed for hypercentral potentials and for non-hypercentral potentials by use of the hyperspherical adiabatic approximation.

- [140] H. J. Devega. LARGE ORDERS IN THE 1-N PERTURBATION-THEORY BY INVERSE SCATTERING IN ONE DIMENSION. *Commun. Math. Phys.*, 70(1):29–42, 1979.

- [141] I. K. Dmitrieva and G. I. Plindov. ELECTRON CORRELATION IN DOUBLY EXCITED S-STATES - LARGE-Z LIMIT. *J. Phys. B-At. Mol. Opt. Phys.*, 21(18):3055–3075, 1988.

- [142] I. K. Dmitrieva and G. I. Plindov. DOUBLY-EXCITED INNER-SHELL STATES OF POSITIVE-IONS - EXACT ENERGY VALUES AND WAVE-FUNCTIONS IN THE LARGE-N LIMIT. *Opt. Spektrosk.*, 77(6):875–879, 1994.

- [143] I. V. Dobrovolska and R. S. Tutik. Logarithmic perturbation theory for radial Klein-Gordon equation with screened Coulomb potentials via h-expansions. *Int. J. Mod. Phys. A*, 19(22):3669–3683, 2004.

Abstract: The explicit semiclassical treatment of logarithmic perturbation theory for the bound-state problem within the framework of the radial Klein-Gordon equation with attractive screened Coulomb potentials, contained time-component of a Lorentz four-vector and a Lorentz-scalar term, is developed. Based upon h-expansions and new quantization conditions a novel procedure for deriving perturbation expansions is offered. Avoiding disadvantages of the standard approach, new handy recursion formulae with the same simple form both for ground and excited states have been obtained. As an example, the perturbation expansions for the energy eigenvalues for the Hulthen

potential containing the vector part as well as the scalar component are considered.

- [144] H. D. Doebner and E. Papp. RELATIVISTIC ENERGY FORMULAS FOR THE COULOMB PLUS AHARONOV-BOHM POTENTIAL AND FURTHER $1/N$ GENERALIZATIONS. *Phys. Lett. A*, 144(8-9):423–426, 1990.
- [145] A. D. Dolgov and V. S. Popov. ANHARMONIC-OSCILLATOR AND ITS DEPENDENCE ON SPACE DIMENSIONS. *Phys. Lett. B*, 86(2):185–188, 1979.
- [146] A. D. Dolgov, V. L. Yeletsy, and V. S. Popov. A NEW APPROACH TO PERTURBATION-THEORY FOR A DISCRETE SPECTRUM (ANHARMONIC-OSCILLATOR). *Zhurnal Eksperimentalnoi Teor. Fiz.*, 79(5):1704–1718, 1980.
- [147] J. D. Doll and W. H. Miller. CLASSICAL-LIMIT QUANTIZATION OF NONSEPARABLE SYSTEMS - MULTIDIMENSIONAL WKB PERTURBATION-THEORY. *J. Chem. Phys.*, 57(10):4428–&, 1972.
- [148] S. H. Dong. The Dirac equation with a Coulomb potential in D dimensions. *J. Phys. A-Math. Gen.*, 36(18):4977–4986, 2003.

Abstract: The Dirac equation is generalized to $D + 1$ spacetime case. The radial equations of this quantum system are obtained and solved exactly by the Tricomi equation approach. The energy levels $E(n, l, D)$ are analytically presented. The dependences of the energy $E(n, l, D)$ on the dimension D are also analysed. It is shown that the energy $E(n, l, D)$ (l not equal 0) is almost independent of the quantum number l , while $E(n, 0, D)$ first decreases and then increases as the dimension D increases. Unexpectedly, there is an absence of bound states for this quantum system with the special case $D = 1$, which is explained in some detail from the fact that the eigenvalues and eigenfunctions do not exist for $D = 1$.

- [149] S. H. Dong. On the Dirac equation with a Coulomb potential in $D+1$ dimensions. *Phys. Scr.*, 67(5):377–380, 2003.

Abstract: The Dirac equation is investigated in $D + 1$ dimensions. The exact Solutions of the Dirac equation with the Coulomb potential are analytically obtained by studying the Tricomi equations.

The eigenvalues and the corresponding fine structure are also discussed.

- [150] S. H. Dong, X. Y. Gu, Z. Q. Ma, and J. Yu. The Klein-Gordon equation with a Coulomb potential in D dimensions. *Int. J. Mod. Phys. E-Nucl. Phys.*, 12(4):555–565, 2003.

Abstract: The solutions of the Klein-Gordon equation with a Coulomb potential in D dimensions are obtained exactly, and the energy levels $E(n, l, D)$ are analytically presented. The dependence of the energy difference $\Delta E(n, l, D)$ for D and $D - 1$ on the dimension D is demonstrated as three different kinds of rules. The dependence of the energy $E(n, l, D)$ on the dimension D is also analyzed. It is shown that the energy $E(n, l, D)$ (l not equal 0) is almost independent of the quantum number l , while $E(n, 0, D)$ first decreases and then increases as the dimension D increases. There is no bound state of the S-wave for $D = 2$.

- [151] S. H. Dong and G. H. Sun. The Schrodinger equation with a Coulomb plus inverse-square potential in D dimensions. *Phys. Scr.*, 70(2-3):94–97, 2004.

Abstract: A D-dimensional Schrodinger equation with a Coulomb plus inverse-square potential is carried out. The relationship between the energy $E(n, l, D)$ and the dimension D is analyzed in great detail. It is shown that the $E(n, 0, D)$ first decreases for D is an element of $(0, 2]$ and then increases for D greater than or equal to 2. The energy $E(n, l, D)$ is almost independent of the quantum number l for large D , but the quantum number l plays some role in the energy $E(n, l, D)$ when the dimension D is not too large.

- [152] S. H. Dong, G. H. Sun, and M. Lozada-Cassou. Dirac equation with a Coulomb plus scalar potential in D+1 dimensions. *Int. J. Quantum Chem.*, 102(2):147–157, 2005.

Abstract: We generalize the Dirac equation to $D + 1$ -dimensional spacetime. The exact solutions of the D-dimensional radial equations with a Coulomb plus scalar potential taking the form $1/r$ are analytically presented by studying the Tricomi equations. The energies $E(n, l, D)$ are exactly presented. The dependences of the energies $E(n, l,$

D) on the dimension D are analyzed in some detail. The energies $E(n, 0, D)$ first decrease and then increase when increasing dimension D , but the energies $E(n, 1, D)$ (l not equal 0) increase when increasing dimension D . The energies $E(n, 0, D)$ are symmetric with respect to $D = 1$ for D is an element of $(0, 2)$. It is shown that the energies $E(n, l, D)$ (l not equal 0) are almost independent of the quantum number l for large D and are completely independent of it if the Coulomb potential is equal to the scalar one. The energies $E(n, l, D)$ almost overlap for large D . The dependences of the energies $E(n, l, v)$ and $E(n, l, s)$ on the vector potential parameter v and scalar potential one s are also studied for $D = 3$. All are found to decrease when these parameters are increased. (C) 2004 Wiley Periodicals, Inc.

- [153] D. J. Doren and D. R. Herschbach. ACCURATE SEMICLASSICAL ELECTRONIC-STRUCTURE FROM DIMENSIONAL SINGULARITIES. *Chem. Phys. Lett.*, 118(2):115–119, 1985.
- [154] D. J. Doren and D. R. Herschbach. CONVERGENCE PROPERTIES AND RESUMMATION OF THE $1/D$ EXPANSION. *Phys. Rev. A*, 34(4):2665–2673, 1986.
- [155] D. J. Doren and D. R. Herschbach. INTERDIMENSIONAL DEGENERACIES, NEAR DEGENERACIES, AND THEIR APPLICATIONS. *J. Chem. Phys.*, 85(8):4557–4562, 1986.
- [156] D. J. Doren and D. R. Herschbach. SPATIAL DIMENSION AS AN EXPANSION PARAMETER IN QUANTUM-MECHANICS. *Phys. Rev. A*, 34(4):2654–2664, 1986.
- [157] D. J. Doren and D. R. Herschbach. 2-ELECTRON ATOMS NEAR THE ONE-DIMENSIONAL LIMIT. *J. Chem. Phys.*, 87(1):433–442, 1987.
- [158] D. J. Doren and D. R. Herschbach. ELECTRONIC-STRUCTURE FROM SEMICLASSICAL DIMENSIONAL EXPANSIONS - SYMMETRY-BREAKING AND BOUND-STATES OF THE HYDRIDE ION. *J. Phys. Chem.*, 92(7):1816–1821, 1988.
- [159] M. R. Douglas. LARGE- N GAUGE-THEORY - EXPANSIONS AND TRANSITIONS. *Nucl. Phys. B*, pages 66–91, 1995.

Abstract: We use solvable two-dimensional gauge theories to illustrate the issues in relating large N gauge theory to string theory. We also give an introduction to recent mathematical work which allows constructing master fields for higher dimensional large N theories. We illustrate this with a new derivation of the Hopf equation governing the evolution of the spectral density in matrix quantum mechanics.

- [160] G. W. F. Drake, M. M. Cassar, and R. A. Nistor. Ground-state energies for helium, H^- , and $Ps(-)$. *Phys. Rev. A*, 65(5):4, 2002.

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.

- [161] P. G. Drazin and Y. Tourigny. Numerical study of bifurcations by analytic continuation of a function defined by a power series. *SIAM J. Appl. Math.*, 56(1):1–18, 1996.

Abstract: A novel computational approach to the investigation of bifurcations; relying on the use of power series in the bifurcation parameter for a particular solution branch, is presented. The first part of the paper is devoted to the description of a series summation technique based on the assumption that the given series is the local representation of a function algebraic in the independent variable. The procedure leads to a special type of Hermite-Pade approximant. Although no mathematical analysis is presented, the numerical evidence suggests that the error decays faster than exponentially with the number of terms of the series used. The procedure's chief merit is its ability to reveal solution branches of the underlying problem in addition to the one represented by the original series. In the final part of the paper, an algorithm is described for numerically generating the required power series where standard perturbation methods are inadequate. Thus, it is shown how path-following techniques may be combined with the basic procedure

for series summation to provide a powerful tool well suited to the numerical analysis of bifurcations in nonlinear problems. Numerical results are presented for a variety of applications, including examples from fluid mechanics.

- [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 states, 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.

- [163] B. Duan, X. Y. Gu, and Z. Q. Ma. Numerical calculation of energies of some excited states in a helium atom. *Eur. Phys. J. D*, 19(1):9–12, 2002.

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.

- [164] B. Duan, X. Y. Gu, and Z. Q. Ma. Energy levels of P-wave states for a D-dimensional helium atom. *Phys. Lett. A*, 322(1-2):96–104, 2004.

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 $|E|$ 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.

- [166] Y. S. Duan, Y. X. Liu, and L. J. Zhang. Corrections to the nonrelativistic ground energy of a helium atom. *Chin. Phys. Lett.*, 21(9):1714–1716, 2004.

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%.

- [167] Z. Dulinski. LARGE NC LIMIT FOR PHYSICAL QUANTITIES IN SU(3) SKYRME MODEL. *Acta Phys. Pol. B*, 19(11):891–897, 1988.

- [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 COMPUTA-

TION OF THE COEFFICIENTS OF THE 1/D EXPAN-
SION 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 tensor arithmetic, which makes it easier to extend to systems with more than three degrees of freedom and to excited states, 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 multi-electron 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.

[171]

M. Dunn and D. K. Watson. Continuation of the wave function for higher angular momentum states to D dimen-

sions .1. The generalized Schwartz expansion. *Ann. Phys.*, 251(2):266–318, 1996.

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 the 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.

[172]

M. Dunn and D. K. Watson. Continuation of the wave function for higher angular momentum states to D dimensions .2. Elimination of linear dependencies. *Ann. Phys.*, 251(2):319–336, 1996.

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.
(c) 2006 Elsevier Inc. All rights reserved.

[175]

M. Dunn, D. K. Watson, J. R. Walkup, and T. C. Germann. On the behavior of Pade approximants in the vicinity of avoided crossings. *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 Pade 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.

- [176] J. Durup. ON THE 1986 NOBEL-PRIZE IN CHEMISTRY. *Laser Chem.*, 7(5-6):239–259, 1987.
- [177] R. Dutt, M. Bag, and Y. P. Varshni. SUPERSYMMETRY-INSPIRED SHIFTED LARGE-N EXPANSIONS FOR THE ENERGY-LEVELS OF THE STATIC SCREENED COULOMB POTENTIAL. *J. Phys. B-At. Mol. Opt. Phys.*, 21(6):927–935, 1988.
- [178] R. Dutt, T. Imbo, and U. Sukhatme. THE 1/N EXPANSION AND NONRELATIVISTIC POTENTIAL PROBLEMS WITH SEVERAL EXPANSION PARAMETERS - APPLICATIONS TO THE ROTATING HARMONIC-OSCILLATOR, ZEEMAN EFFECT AND HELIUM-LIKE ATOMS. *Z. Phys. D-Atoms Mol. Clusters*, 6(3):211–217, 1987.
- [179] R. Dutt, A. Khare, and U. P. Sukhatme. SUPERSYMMETRY-INSPIRED WKB APPROXIMATION IN QUANTUM-MECHANICS. *Am. J. Phys.*, 59(8):723–727, 1991.

Abstract: The supersymmetry-inspired WKB approximation (SWKB) in quantum mechanics is discussed in detail. The SWKB method can be easily applied to any potential whose ground-state wave function is known. It yields eigenvalues that are exact for large quantum numbers n (as any WKB approximation should in the classical limit). Furthermore, for the important special case of "shape-invariant" potentials, the SWKB approach gives the exact analytic expressions for the entire bound-state spectra. A study of some nonshape-invariant,

but solvable, potentials suggests that shape invariance is not only sufficient but perhaps even necessary for the SWKB approximation to be exact. A comparison of the WKB and SWKB predictions for the bound-state spectra of a number of potentials reveals that in many cases the SWKB approach does better than the usual WKB approximation.

- [180] R. Dutt, U. Mukherji, and Y. P. Varshni. SHIFTED $1/N$ EXPANSION FOR THE ENERGY-LEVELS OF LASER-DRESSED COULOMB POTENTIAL OF THE HYDROGEN-ATOM. *J. Phys. B-At. Mol. Opt. Phys.*, 18(16):3311–3318, 1985.
- [181] R. Dutt, U. Mukherji, and Y. P. Varshni. ENERGY-LEVELS AND OSCILLATOR-STRENGTHS FOR THE EXPONENTIAL COSINE SCREENED COULOMB POTENTIAL IN THE SHIFTED LARGE-DIMENSION EXPANSION THEORY. *J. Phys. B-At. Mol. Opt. Phys.*, 19(21):3411–3419, 1986.
- [182] R. Dutt, U. Mukherji, and Y. P. Varshni. SHIFTED LARGE-N EXPANSION FOR THE BOUND-STATES OF THE HELLMANN POTENTIAL. *Phys. Rev. A*, 34(2):777–784, 1986.
- [183] R. Dutt and Y. P. Varshni. SHIFTED LARGE-N EXPANSION FOR THE ENERGY-LEVELS OF NEUTRAL ATOMS. *Z. Phys. D-Atoms Mol. Clusters*, 2(3):207–210, 1986.
- [184] R. Dutt and Y. P. Varshni. VIBRATIONAL AND ROVIBRATIONAL EIGENENERGIES FOR LENNARD-JONES POTENTIALS. *J. Phys. B-At. Mol. Opt. Phys.*, 20(11):2437–2446, 1987.
- [185] S. Edvardsson, D. Aberg, and P. Uddholm. A program for accurate solutions of two-electron atoms. *Comput. Phys. Commun.*, 165(3):260–270, 2005.

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.

[186]

E. Elizalde, S. D. Odintsov, and A. Romeo. Zeta-regularization of the $O(N)$ nonlinear sigma model in D dimensions. *J. Math. Phys.*, 37(3):1128–1147, 1996.

Abstract: The $O(N)$ nonlinear sigma model in a D -dimensional space of the form $R(D-M) \times T-M$, $R(D-M) \times S-M$, or $T-M \times S-P$ is studied, where $R(M)$, $T-M$, and $S-M$ correspond to flat space, a torus, and a sphere, respectively. Using zeta-regularization and the $1/N$ expansion, the corresponding partition functions-for deriving the free energy-and the gap equations are obtained. In particular, the free energy at the critical point on $R(2q+1) \times S-2p+2$ vanishes in accordance with the conformal equivalence to the flat space $R(D)$. Numerical solutions of the gap equations at the critical coupling constants are given for several values of D . The properties of the partition function and its asymptotic behavior for large D are discussed. In a similar way, a higher-derivative nonlinear sigma model is investigated, too. The physical relevance of our results is discussed. (C) 1996 American Institute of Physics.

[187]

M. O. Elout, D. Z. Goodson, C. D. Elliston, S. W. Huang, A. V. Sergeev, and D. K. Watson. Improving the convergence and estimating the accuracy of summation approximants of $1/D$ expansions for Coulombic systems. *J. Math. Phys.*, 39(10):5112–5122, 1998.

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 Padé-Borel approximants

with modifications 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 $F(\delta) = \sum_j E(j)/j!$, where E_j are the expansion coefficients of the energy with singularity structure removed at $d=1$, 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 $F_m(\delta) = \sum_j E(j)/\Gamma(j+1-m)$ 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].

- [188] M. Engelhardt and S. Levit. Variational master field for large- N interacting matrix models - Free random variables on trial. *Nucl. Phys. B*, 488(3):735–774, 1997.

Abstract: Matrices are said to behave as free non-commuting random variables if the action which governs their dynamics constrains only their eigenvalues, i.e. depends on traces of powers of individual matrices. The authors use recently developed mathematical techniques in combination with a standard variational principle to formulate a new variational approach for matrix models. Approximate variational solutions of interacting large- N matrix models are found using the free random matrices as the variational space. Several classes of classical and quantum mechanical matrix models with different types of interactions are considered and the variational solutions compared with exact Monte Carlo and analytical results. Impressive agreement is found in a majority of cases. (C) 1997 Elsevier Science B.V.

- [189] S. Erkoç and R. Sever. $1/N$ EXPANSION FOR A MIE-TYPE POTENTIAL. *Phys. Rev. D*, 33(2):588–589, 1986.
- [190] G. S. Ezra and R. S. Berry. CORRELATION OF 2 PARTICLES ON A SPHERE. *Phys. Rev. A*, 25(3):1513–1527, 1982.

[191] X. J. Fan, Z. F. Yuan, and X. T. Wang. APPLICATION OF THE SHIFTED $1/N$ EXPANSION TO A MORE GENERAL SCREENED COULOMB POTENTIAL. *Chin. Phys. Lett.*, 7(2):61–63, 1990.

[192] U. Fano, D. Green, J. L. Bohn, and T. A. Heim. Geometry and symmetries of multi-particle systems. *J. Phys. B-At. Mol. Opt. Phys.*, 32(6):R1–R37, 1999.

Abstract: The quantum dynamical evolution of atomic and molecular aggregates, from their compact to their fragmented states, is parametrized by a single collective radial parameter. Treating all the remaining particle coordinates in d dimensions democratically, as a set of angles orthogonal to this collective radius or by equivalent variables, bypasses all independent-particle approximations. The invariance of the total kinetic energy under arbitrary d -dimensional transformations which preserve the radial parameter gives rise to novel quantum numbers and ladder operators interconnecting its eigenstates at each value of the radial parameter. We develop the systematics and technology of this approach, introducing the relevant mathematics tutorially, by analogy to the familiar theory of angular momentum in three dimensions. The angular basis functions so obtained are treated in a manifestly coordinate-free manner, thus serving as a flexible generalized basis for carrying out detailed studies of wavefunction evolution in multi-particle systems.

[193] J. M. Feagin and J. S. Briggs. MOLECULAR-ORBITAL DESCRIPTION OF THE STATES OF 2-ELECTRON SYSTEMS. *Phys. Rev. A*, 37(12):4599–4613, 1988.

[194] F. M. Fernandez. On large- N expansions. *J. Phys. A-Math. Gen.*, 35(49):10663–10667, 2002.

Abstract: We show that a recently proposed shifted large- l expansion is exactly the well-known shifted large- N expansion. Results for truncated Coulomb potentials cast doubts on previous conclusions drawn from shifted large- l calculations.

[195] F. M. Fernandez, S. A. Maluendes, and E. A. Castro. $1/N$ EXPANSION FOR A MIE-TYPE POTENTIAL - COMMENT. *Phys. Rev. D*, 36(2):650–650, 1987.

- [196] F. Ferrari. The large N limit of $N=2$ super Yang-Mills, fractional instantons and infrared divergences. *Nucl. Phys. B*, 612(1-2):151–170, 2001.

Abstract: We investigate the large N limit of pure $N = 2$ supersymmetric gauge theory with gauge group $SU(N)$ by using the exact low energy effective action. Typical one-complex dimensional sections of the moduli space parametrized by a global complex mass scale ϵ display three qualitatively different regions depending on the ratio between ϵ and the dynamically generated scale Λ . At large ϵ/Λ , instantons are exponentially suppressed as $N \rightarrow \infty$. When ϵ similar to Λ , singularities due to massless dyons occur. They are densely distributed in rings of calculable thicknesses in the ϵ - plane. At small ϵ/Λ , instantons disintegrate into fractional instantons of charge $1/(2N)$. These fractional instantons give non-trivial contributions to all orders of $1/N$, unlike a planar diagrams expansion which generates a series in $1/N-2$, implying the presence of open strings. We have explicitly calculated the fractional instantons series in two representative examples, including the $1/N$ and $1/N-2$ corrections. Our most interesting finding is that the $1/N$ expansion breaks down at singularities on the moduli space due to severe infrared divergencies, a fact that has remarkable consequences, (C) 2001 Published by Elsevier Science B.V.

- [197] R. A. Ferrell and Scalapin.Dj. STATISTICAL-MECHANICS OF ONE-DIMENSIONAL GINZBURG-LANDAU FIELDS .2. TEST OF SCREENING APPROXIMATION ($N-1$ EXPANSION). *Phys. Rev. A*, 9(2):846–867, 1974.

- [198] G. Ferretti. ON THE LARGE- N LIMIT OF 3D AND 4D HERMITIAN MATRIX MODELS. *Nucl. Phys. B*, 450(3):713–729, 1995.

Abstract: The large- N limit of the hermitian matrix model in three and four euclidean space-time dimensions is studied with the help of the approximate Renormalization Group recursion formula. The planar graphs contributing to wave-function, mass and coupling-constant renormalization are

identified and summed in this approximation. In four dimensions the model fails to have an interacting continuum limit, but in three dimensions there is a non-trivial fixed point for the approximate RG relations. The critical exponents of the three-dimensional model at this fixed point are $\nu = 0.67$ and $\eta = 0.20$. The existence (or non-existence) of the fixed point and the critical exponents display a fairly high degree of universality since they do not seem to depend on the specific (non-universal) assumptions made in the approximation.

- [199] A. Ferron and P. Serra. Stability of two-electron diatomic molecules. *J. Phys. B-At. Mol. Opt. Phys.*, 40(5):995–1002, 2007.

Abstract: We present a detailed study of the ground state behaviour of two-electron diatomic molecules. The ground state stability diagram for diatomic molecules in the Born-Oppenheimer approximation is obtained and the behaviour of the ground state near the stability line is studied. Two different cases are analysed: the homonuclear two-centre two-electron molecule with the internuclear distance as a free parameter and the diatomic two-electron molecule (in this case, the internuclear distance is determined by equilibrium conditions). Analytical and numerical results for these systems are presented.

- [200] A. Ferron, P. Serra, and S. Kais. Dimensional scaling for stability of two particles in a dipole field. *Chem. Phys. Lett.*, 461(1-3):127–130, 2008.

Abstract: We present dimensional scaling calculations for the critical parameters needed to bind one and two-electrons to a finite linear dipole field and the stability diagram for the hydrogen-antihydrogen like molecules. We find that calculations at the large-D limit are much simpler than $D = 3$, yet yield similar results for the critical parameters and the stability diagrams. (C) 2008 Elsevier B. V. All rights reserved.

- [201] A. Ferron, P. Serra, and S. Kais. Critical conditions for stable dipole-bound dianions. *J. Chem. Phys.*, 128(4):6, 2008.

Abstract: We present finite size scaling calculations of the critical parameters for binding two electrons to a finite linear dipole field. This approach gives very accurate results for the critical parameters by using a systematic expansion in a finite basis set. A complete ground state stability diagram for the dipole-bound dianion is obtained using accurate variational and finite size scaling calculations. We also study the near threshold behavior of the ground state energy by calculating its critical exponent.

- [202] A. Ferron, P. Serra, and S. Kais. Stability conditions for hydrogen-antihydrogen-like quasimolecules. *Phys. Rev. A*, 77(5):5, 2008.

Abstract: We present a detailed study of the stability conditions of hydrogen-antihydrogen-like quasimolecules using both variational and finite-size scaling calculations. The stability diagram of the nuclear charge Z as a function of the internuclear distance R shows bound and unbound regions separated by a first-order critical line. Calculations of the leptonic annihilation rate show a peculiar behavior for nuclear charges $Z \leq 2$, which was not observed for the hydrogen-antihydrogen quasimolecule; it goes through a maximum before it decays exponentially for large interhadronic distances. This might have a practical impact on the study of stability of matter-antimatter systems.

- [203] M. R. Flannery and E. Oks. Plasma screening within Rydberg atoms in circular states. *Eur. Phys. J. D*, 47(1):27–31, 2008.

Abstract: A Rydberg atom embedded in a plasma can experience penetration by slowly moving electrons within its volume. The original pure Coulomb potential must now be replaced by a screened Coulomb potential which contains either a screening length R_s or a screening factor $A = R_s^{-1}$. For any given discrete energy level, there is a Critical Screening Factor (CSF) $A(c)$ beyond which the energy level disappears (by merging into the continuum). Analytical results are obtained for the classical dependence of the energy on the screening factor, for the CSF, and for the critical radius

of the electron orbit for Circular Rydberg States (CRS) in this screened Rydberg atom. The results are derived for any general form of the screened Coulomb potential and are applied to the particular case of the Debye potential. We also show that CRS can temporarily exist above the ionization threshold and are therefore the classical counterparts of quantal discrete states embedded into continuum. The results are significant not only to Rydberg plasmas, but also to fusion plasmas, where Rydberg states of multi-charged hydrogen-like ions result from charge exchange with hydrogen or deuterium atoms, as well as to dusty/complex plasmas.

- [204] C. Franck. QUANTUM FLUCTUATION AND PHASE-TRANSITION IN A HARMONIC 2-ELECTRON ATOMIC MODEL WITH VARIABLE DIMENSIONALITY. *Phys. Rev. A*, 47(1):119–125, 1993.

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.

- [205] D. D. Frantz and D. R. Herschbach. LEWIS ELECTRONIC-STRUCTURES AS THE LARGE-DIMENSION LIMIT

- FOR H-2+ AND H-2-MOLECULES. *Chem. Phys.*, 126(1):59–71, 1988.
- [206] D. D. Frantz and D. R. Herschbach. CALCULATION OF H-2+ EIGENPARAMETERS IN ARBITRARY DIMENSIONS. *Computers & Chemistry*, 14(3):225–236, 1990.
- [207] D. D. Frantz and D. R. Herschbach. INTERDIMENSIONAL DEGENERACY AND SYMMETRY-BREAKING IN D-DIMENSIONAL H-2+. *J. Chem. Phys.*, 92(11):6668–6686, 1990.
- [208] D. D. Frantz, D. R. Herschbach, and J. D. Morgan. WRONG-WAY RECURSION YIELDS MORE ACCURATE EIGENPARAMETERS FOR THE HYDROGEN-MOLECULE ION. *Phys. Rev. A*, 40(3):1175–1184, 1989.
- [209] D. E. Freund, B. D. Huxtable, and J. D. Morgan. VARIATIONAL CALCULATIONS ON THE HELIUM ISOELECTRONIC SEQUENCE. *Phys. Rev. A*, 29(2):980–982, 1984.
- [210] R. Friedberg. THE 1-D EXPANSION OF THE EDEN MODEL. *Phys. Lett. A*, 112(3-4):129–132, 1985.
- [211] B. Friedrich and D. Herschbach. Polarizability interaction in molecules and double-well tunneling. *Z. Phys. D-Atoms Mol. Clusters*, 36(3-4):221–228, 1996.

Abstract: Directional superpositions of the rotational states of linear molecules can be created by interaction of the polarizability with the strong electric field of an intense laser beam. The polarizability interaction, proportional to $\cos^2(\theta)$ (with θ the angle between the molecular axis and the direction of the electric field), is a double-well potential, with end-for-end symmetry. The energy levels thus exhibit tunnel-effect splittings. We present an exact treatment, derived by transcription to an oblate spheroidal wave equation. We also develop an accurate semiclassical approximation, in which the action integral and period are evaluated using an effective potential that corresponds to one-dimensional motion. The results pertain both to rotational spectroscopy of nonpolar molecules and to alignment and trapping experiments with either nonpolar or polar molecules.

- [212] G. A. Gallup. ANGULAR MOMENTUM IN N-DIMENSIONAL SPACES. *J. Mol. Spectrosc.*, 3(6):673–682, 1959.
- [213] R. S. Gangyopadhyay. CORRECTION. *Phys. Rev. D*, 33(8):2500–2500, 1986.
- [214] R. S. Gangyopadhyay, R. Dutt, and Y. P. Varshni. NON-RELATIVISTIC POTENTIAL SCATTERING THROUGH THE SHIFTED LARGE-DIMENSION EXPANSION. *Phys. Rev. D*, 32(12):3312–3315, 1985.
- [215] D. A. Garanin, K. Kladko, and P. Fulde. Quasiclassical Hamiltonians for large-spin systems. *Eur. Phys. J. B*, 14(2):293–300, 2000.

Abstract: We extend and apply a previously developed method for a semiclassical treatment of a system with large spin S . A multisite Heisenberg Hamiltonian is transformed into an effective classical Hamilton function which can be treated by standard methods for classical systems. Quantum effects enter in form of multispin interactions in the Hamilton function. The latter is written in the form of an expansion in powers of $J/(TS)$, where J is the coupling constant. Main ingredients of our method are spin coherent states and cumulants. Rules and diagrams are derived for computing cumulants of groups of operators entering the Hamiltonian. The theory is illustrated by calculating the quantum corrections to the free energy of a Heisenberg chain which were previously computed by a Wigner-Kirkwood expansion.

- [216] G. Gaspari, J. Rudnick, and A. Beldjenna. THE SHAPES OF OPEN AND CLOSED RANDOM-WALKS - A 1/D EXPANSION. *J. Phys. A-Math. Gen.*, 20(11):3393–3414, 1987.
- [217] T. C. Germann. AN ACCURATE ANALYTICAL WAVE-FUNCTION FOR CIRCULAR RYDBERG STATES OF THE H ATOM IN A MAGNETIC-FIELD. *J. Phys. B-At. Mol. Opt. Phys.*, 28(17):L531–L536, 1995.

Abstract: By performing first-order perturbation theory about the $m \rightarrow \infty$ limit, we obtain a highly accurate analytical expression for circular Rydberg ($m = n - 1$ much greater than 1) wavefunctions of the hydrogen atom in a uniform magnetic

field. In the $m \rightarrow \infty$ limit, the electron executes a circular orbit about the magnetic field axis; the first-order wavefunction simply corresponds to Gaussian fluctuations about this orbit. To demonstrate the utility of the results derived here, we compare our simple expression for the lifetimes of $m = 25$ and 35 circular states with accurate ab initio results.

- [218] T. C. Germann. Use of dimension-dependent potentials for quasibound states. *J. Chem. Phys.*, 104(13):5100–5108, 1996.

Abstract: Dimensional perturbation theory is applied to the calculation of complex energies for quasibound (resonance) eigenstates, using a modified dimension-dependent potential so that the infinite-dimensional limit better reflects the physical (three-dimensional) nature of the resonant eigenstate. Using the previous approach of retaining the $D=3$ form of the potential for all spatial dimension D , highly accurate results are obtained via Pade-Borel summation of the expansion coefficients when they are complex, but a lesser degree of convergence is found when quadratic Pade summation is applied to real expansion coefficients. The present technique of using a dimension-dependent potential allows complex expansion coefficients to be obtained in all cases, and is demonstrated to provide a marked improvement in convergence. We illustrate this approach on the Lennard-Jones potential and the hydrogen atom in an electric field. (C) 1996 American Institute of Physics.

- [219] T. C. Germann, D. R. Herschbach, M. Dunn, and D. K. Watson. CIRCULAR RYDBERG STATES OF THE HYDROGEN-ATOM IN A MAGNETIC-FIELD. *Phys. Rev. Lett.*, 74(5):658–661, 1995.

- [220] T. C. Germann and S. Kais. LARGE-ORDER DIMENSIONAL PERTURBATION-THEORY FOR COMPLEX ENERGY EIGENVALUES. *J. Chem. Phys.*, 99(10):7739–7747, 1993.

Abstract: Dimensional perturbation theory is applied to the calculation of complex energies for quasibound, or resonant, eigenstates of central potentials. Energy coefficients for an asymptotic expansion in powers of $1/\kappa$, where $\kappa = D +$

2l and D is the Cartesian dimensionality of space, are computed using an iterative matrix based procedure. For effective potentials which contain a minimum along the real axis in the $\kappa \rightarrow \infty$ limit, Hermite-Pade summation is employed to obtain complex eigenenergies from real expansion coefficients. For repulsive potentials, we simply allow the radial coordinate to become complex and obtain complex expansion coefficients. Results for ground and excited states are presented for squelched harmonic oscillator ($V_0 r^2 e^{-r}$) and Lennard-Jones (12-6) potentials. Bound and quasibound rovibrational states for the hydrogen molecule are calculated from an analytic potential. We also describe the calculation of resonances for the hydrogen atom Stark effect by using the separated equations in parabolic coordinates. The methods used here should be readily extendable to systems with multiple degrees of freedom.

- [221] T. C. Germann and S. Kais. Dimensional perturbation theory for Regge poles. *J. Chem. Phys.*, 106(2):599–604, 1997.

Abstract: We apply dimensional perturbation theory to the calculation of Regge pole positions, providing a systematic improvement to earlier analytic first-order results. We consider the orbital angular momentum l as a function of spatial dimension D for a given energy E , and expand l in inverse powers of $\kappa = (D-1)/2$. It is demonstrated for both bound and resonance states that the resulting perturbation series often converges quite rapidly, so that accurate quantum results can be obtained via simple analytic expressions given here through third order. For the quartic oscillator potential, the rapid convergence of the present $l(D;E)$ series is in marked contrast with the divergence of the more traditional $E(D;l)$ dimensional perturbation series, thus offering an attractive alternative for bound state problems. (C) 1997 American Institute of Physics.

- [222] C. C. Gerry and J. B. Togeas. A LARGE-N PHASE INTEGRAL APPROXIMATION FOR COULOMB-TYPE SYSTEMS USING $SO(2,1)$ COHERENT STATES. *J. Phys. A-Math. Gen.*, 19(18):3797–3806, 1986.

[223] C. C. Gerry, J. B. Togeas, and S. Silverman. LARGE-N PHASE-INTEGRAL APPROXIMATION FOR SU(1,1) COHERENT STATES. *Phys. Rev. D*, 28(8):1939–1944, 1983.

[224] R. J. Gillespie and E. A. Robinson. Gilbert N. Lewis and the chemical bond: The electron pair and the octet rule from 1916 to the present day. *J. Comput. Chem.*, 28(1):87–97, 2007.

Abstract: We describe the development of Lewis’s ideas concerning the chemical bond and in particular the concept of the electron pair bond and the octet rule. We show that the concept of the electron pair bond has endured to the present day and is now understood to be a consequence of the Pauli principle. In contrast the octet rule is now regarded as much less important than was originally generally believed, although Lewis himself knew several exceptions and regarded it as less important than what he called the rule of two (the electron pair). The octet rule was more strongly promoted by Langmuir who is also responsible for the term covalent bond. However, many more exceptions to the octet rules than were known to Lewis are now known and the terms hypervalent and hypovalent used to describe such molecules are no longer particularly useful. Today it is realized that bonding electron pairs in many molecules are not as well localized as Lewis believed, nevertheless resonance structures, i.e., plausible alternative Lewis structures, are still often used to describe such molecules. Moreover electrons are not always found in pairs, as for example in linear molecules, which can, however, be satisfactorily described by Linnett’s double quartet theory. The electron density distribution in a molecule can now be analyzed using the ELF and other functions of the electron density to show where electron pairs are most probably to be found in a molecule. (C) 2006 Wiley Periodicals, Inc.

[225] Y. Y. Goldschmidt. THE 1/D EXPANSION FOR THE QUANTUM-MECHANICAL N-BODY PROBLEM - APPLICATION FOR DIRECTED POLYMERS IN A RANDOM MEDIUM. *Nucl. Phys. B*, 393(3):507–522, 1993.

Abstract: In this paper we give a closed form expression for the 1/d corrections to the leading d

$\rightarrow \infty$ approximation for the ground-state energy of an n -body quantum mechanical problem in a general potential (where d is the number of spatial dimensions). We then extend the results to the problem of directed polymers in a random medium where the limit $n \rightarrow 0$ has to be taken in the corresponding n -body problem. In this case the effective two-body potential measures the strength of correlations of the quenched disorder. In the $n \rightarrow 0$ limit a replica-symmetry-breaking solution to the saddle-point equations turns out to be the correct solution in the strong-coupling regime, and we obtain the $1/d$ corrections to the corresponding energy which constitute the gaussian fluctuations about this solution as well as provide information about its basin of stability.

- [226] B. Gonul, O. Ozer, and M. Kocak. Unified treatment of screening coulomb and anharmonic oscillator potentials in arbitrary dimensions. *Commun. Theor. Phys.*, 45(5):807–812, 2006.

Abstract: A mapping is obtained relating radial screened Coulomb systems with low screening parameters to radial anharmonic oscillators in N -dimensional space. Using the formalism of supersymmetric quantum mechanics, it is shown that exact solutions of these potentials exist when the parameters satisfy certain constraints.

- [227] A. Gonzalez. IMPROVED ESTIMATES OF FEW-BODY GROUND-STATE ENERGIES. *Few-Body Syst.*, 8(2):73–76, 1990.

- [228] A. Gonzalez. THE QUANTUM FEW-BODY PROBLEM AND THE $1/D$ METHOD. *Few-Body Syst.*, 10(2):43–57, 1991.

Abstract: Qualitative properties of the ground states and the low-lying spectra of three- and four-body systems are studied in the framework of the $1/D$ method, where D is the dimensionality of space. Special emphasis is laid on model-independent properties and relations between magnitudes. It is shown that the low terms of the $1/D$ expansion often give a good qualitative description of the system, although the $1/D$ series is known to

exhibit poor convergence for $D = 3$. The Post estimate of the ground-state energy, the ordering of Wigner multiplets in the spectrum of resonances of the He-4 nucleus, the Hund rule in the two-electron atom, and other properties follow straightforwardly from the $1/D$ analysis.

- [229] A. Gonzalez and D. Leal. BINDING AND EXCITATION-ENERGIES OF LENNARD-JONES CLUSTERS IN THE $1/D$ -METHOD. *J. Phys. B-At. Mol. Opt. Phys.*, 26(6):1253–1261, 1993.

Abstract: We present simple estimates of the binding energies of clusters of rare-gas atoms and excitation energies of low-lying states in trimers, which are obtained by formally writing the Schrodinger equation in d dimensions and expanding its solution in powers of $1/d$. Comparison with Monte Carlo calculations for Lennard-Jones clusters (Ne(n), Ar(n), Kr(n), Xe(n), $n = 3-7$ and 13) shows good agreement, and suggests that our formulae may be used to estimate the energy of rare-gas atoms interacting through realistic potentials.

- [230] A. Gonzalez and R. Martinez. STRONG INTERACTION RADII OF HADRONS IN THE $1/D$ -EXPANSION. *Rev. Mex. Fis.*, 39(6):893–901, 1993.

Abstract: Within the framework of the nonrelativistic quark model and with the help of the leading term of the $1/d$ -expansion we obtain analytical expressions for the quotients of baryon-to-meson strong interaction radii. Phenomenological relativistic corrections a la Povh and Hufner are shown to lower the non relativistic estimate. Predictions for baryon radii are given and a comparison with experimental results (when available) is made. For some values of the quark masses, our estimate differs from the naive parton result in more than 20%.

- [231] D. Z. Goodson. Self-consistent-field perturbation theory for the Schrodinger equation. *Phys. Rev. A*, 55(6):4155–4163, 1997.

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.

[232]

D. Z. Goodson. Convergent summation of Moller-Plesset perturbation theory. *J. Chem. Phys.*, 112(11):4901–4909, 2000.

Abstract: Rational and algebraic Pade approximants are applied to Moller-Plesset (MP) perturbation expansions of energies for a representative sample of atoms and small molecules. These approximants can converge to the full configuration-interaction result even when partial summation diverges. At order MP2 (the first order beyond the Hartree-Fock approximation), the best results are obtained from the rational [0/1] Pade approximant of the total energy. At MP3 rational and quadratic approximants are about equally good, and better than partial summation. At MP4, MP5, and MP6, quadratic approximants appear to be the most dependable method. The success of the quadratic approximants is attributed to their ability to model the singularity structure in the complex plane of the perturbation parameter. Two classes of systems are distinguished according to whether the dominant singularity is in the positive half plane (class A) or the negative half plane (class B). A new kind of quadratic approximant, with a constraint on one of its constituent polynomials, gives better results than conventional approximants for class B systems at MP4, MP5, and MP6. For CH₃ with the C-H distance at twice the equilibrium value the quadratic approximants yield a complex value for the ground-state electronic energy. This is interpreted as a resonance eigenvalue embedded in the ionization continuum. (C) 2000 American Institute of Physics. [S0021-9606(00)30208-2].

- [233] D. Z. Goodson. Improving the accuracy of ab initio methods with summation approximants and singularity analysis. *Int. J. Quantum Chem.*, 92(1):35–46, 2003.

Abstract: The accuracy of Moller-Plesset (MP) perturbation theory and coupled-cluster (CC) theory can be significantly improved, at essentially no increase in computational cost, by using summation approximants that model the way in which these theories converge to the full configuration interaction limit. Approximants for MP4 and CCSD(T) are presented, their size scaling is analyzed, and the functional analysis of the MP energy, on which the MP4 approximant is based, is discussed. The MP approximants are shown to have a form that is appropriate for describing resonance energies. (C) 2003 Wiley Periodicals, Inc.

- [234] D. Z. Goodson and D. R. Herschbach. ELECTRON CORRELATION CALIBRATED AT THE LARGE DIMENSION LIMIT. *J. Chem. Phys.*, 86(9):4997–5008, 1987.

- [235] D. Z. Goodson and D. R. Herschbach. RECURSIVE CALCULATION OF DIMENSIONAL EXPANSIONS FOR 2-ELECTRON ATOMS. *Phys. Rev. Lett.*, 58(16):1628–1631, 1987.

- [236] D. Z. Goodson and D. R. Herschbach. SUMMATION METHODS FOR DIMENSIONAL PERTURBATION-THEORY. *Phys. Rev. A*, 46(9):5428–5436, 1992.

Abstract: We examine strategies for approximating the sum of a perturbation expansion for Coulombic systems in inverse powers of the spatial dimension D using only the few lowest-order terms. Several summation methods are tested on energy expansions of the following systems: the ground state of He, the ground state of Li^+ , the first two excited S states and the lowest $3P(e)$ state of He, and the ground state of H^{-2+} . The origin of the expansions, the limit $D \rightarrow \infty$, corresponds to a pseudoclassical limit, but lower-order terms are strongly affected by poles at $D = 1$, a hyperquantum limit. Two alternative methods are recommended, weighted truncation and hybrid Pade summation, which exploit these poles to reduce the summation error. In effect, these methods modify a

semiclassical $1/D$ expansion by incorporating corrections that are often large. Weighted truncation appears to be slightly more dependable at very low orders, while hybrid Pade summation is preferable when more than the three lowest-order terms are available or when the residue of the second-order pole at $D = 1$ is known. We demonstrate that the present methods are superior to the shifted-expansion method, which does not correctly model the singularity structure.

[237]

D. Z. Goodson, M. Lopezcabrera, D. R. Herschbach, and J. D. Morgan. LARGE-ORDER DIMENSIONAL PERTURBATION-THEORY FOR 2-ELECTRON ATOMS. *J. Chem. Phys.*, 97(11):8481–8496, 1992.

Abstract: An asymptotic expansion for the electronic energy of two-electron atoms is developed in powers of $\delta=1/D$, the reciprocal of the Cartesian dimensionality of space. The expansion coefficients are calculated to high order (approximately 20 to 30) by an efficient recursive procedure. Analysis of the coefficients elucidates the singularity structure in the $D \rightarrow \infty$ limit, which exhibits aspects of both an essential singularity and a square-root branch point. Pade-Borel summation incorporating results of the singularity analysis yields highly accurate energies; the quality improves substantially with increase in either D or the nuclear charge Z . For He, we obtain 9 significant figures for the ground state and 11 for the $2p^2\ 3P(e)$ doubly excited state, which is isomorphic with the ground state at $D=5$ by virtue of interdimensional degeneracy. The maximum accuracy obtainable appears to be limited only by accumulation of roundoff error in the expansion coefficients. The method invites application to systems with many electrons or subject to external fields.

[238]

D. Z. Goodson, J. D. Morgan, and D. R. Herschbach. DIMENSIONAL SINGULARITY ANALYSIS OF RELATIVISTIC-EQUATIONS. *Phys. Rev. A*, 43(9):4617–4624, 1991.

Abstract: For a nonrelativistic hydrogenic atom, the dimension dependence of the energy levels is non-singular except for a second-order pole at D^*

$= 3 - 2n$, where n is the principal quantum number. For the relativistic Klein-Gordon and Dirac equations, the dimension dependence has a much more complicated singularity structure, involving branch points. For all eigenstates there are branch points at $D+ \pm 2Z\alpha$, where Z is the nuclear charge, α is the fine-structure constant, and $D+$ is independent of n but varies linearly with orbital angular momentum. For most states there is in addition a pair of branch points near D^* but slightly off the real axis. The customary perturbation expansion in terms of $Z\alpha$ gives qualitatively incorrect dimension dependence; it predicts only poles located on the real axis at D^* and $D+$, no matter how high the order of the expansion. The dimensional singularities result from the behavior at $r = 0$. The qualitatively incorrect results occur because the perturbing potential, proportional to α^2/r^2 , overwhelms the unperturbed $1/r$ potential at small r . Because of the complexity of the dimensional singularity structure, the popular "shifted expansion" method for summing the $1/D$ expansion does not work well for these equations. We demonstrate a general method for identifying the dimensional singularities that leads to an exact summation of the $1/D$ expansion for all eigenstates of both the Klein-Gordon and the Dirac equations for a particle in a Coulomb potential.

- [239] D. Z. Goodson and A. V. Sergeev. On the use of algebraic approximants to sum divergent series for Fermi resonances in vibrational spectroscopy. *J. Chem. Phys.*, 110(16):8205–8206, 1999.
- [240] D. Z. Goodson and A. V. Sergeev. Singularity structure of moller-plesset perturbation theory. In *Advances in Quantum Chemistry, Vol 47*, volume 47 of *Advances in Quantum Chemistry*, pages 193–208. Elsevier Academic Press Inc, San Diego, 2004.
- [241] D. Z. Goodson and A. V. Sergeev. Singularity analysis of fourth-order Moller-Plesset perturbation theory. *Phys. Lett. A*, 359(5):481–486, 2006.

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.

[242]

D. Z. Goodson and D. K. Watson. DIMENSIONAL PERTURBATION-THEORY FOR EXCITED-STATES OF 2-ELECTRON ATOMS. *Phys. Rev. A*, 48(4):2668–2678, 1993.

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 $1s\ 2s\ 3S$ 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 $D \rightarrow \infty$ 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.

[243]

D. Z. Goodson, D. K. Watson, J. G. Loeser, and D. R. Herschbach. ENERGIES OF DOUBLY EXCITED 2-ELECTRON ATOMS FROM INTERDIMENSIONAL DEGENERACIES. *Phys. Rev. A*, 44(1):97–102, 1991.

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.

[244] M. S. Gordon and J. H. Jensen. Understanding the hydrogen bond using quantum chemistry. *Accounts Chem. Res.*, 29(11):536–543, 1996.

[245] O. Goscinski and L. Hagg. DIMENSIONAL SCALING OF LOCAL PSEUDOPOTENTIALS. *Theochem-J. Mol. Struct.*, 106:17–21, 1993.

Abstract: The integral equations of Gelfand and Levitan were previously used by Abraham and Moses (Phys. Rev. A, 22 (1980) 1333) to construct a modified local potential $V\text{-pert}(r)$, which in this work is added to a coulombic potential in order to remove the lowest s state from the spectrum. The total modified potential $V\text{-new}(r)$, for excited states is used in conjunction with the shifted $1/D$ expansions of dimensional scaling. It is verified that it is feasible to find the lowest energies and the mean radius for $V\text{-new}$, treating it now as a ground state problem. This indicates that a potential for excited states can be generated by the procedure, with the possibility of using it in the study of excited states and valence states. The potentials applied can be considered as local pseudopotentials.

[246] O. Goscinski and V. Mujica. ADIABATIC COORDINATE SEPARATION AND LARGE N-DIMENSIONAL LIMIT IN 2-ELECTRON IONS. *Int. J. Quantum Chem.*, 29(4):897–908, 1986.

[247] S. Graffi, V. Grecchi, E. M. Harrell, and H. J. Silverstone. THE $1/R$ EXPANSION FOR $H-2+$ - ANALYTICITY, SUMMABILITY, AND ASYMPTOTICS. *Ann. Phys.*, 165(2):441–483, 1985.

[248] F. Green and S. Samuel. CALCULATING THE LARGE-N PHASE-TRANSITION IN GAUGE AND MATRIX MODELS. *Nucl. Phys. B*, 194(1):107–156, 1982.

- [249] G. Grignani, D. Marmottini, and P. Sodano. QCD meson spectrum in the large N-C limit. *Nucl. Phys. B-Proc. Suppl.*, 119:281–283, 2003.

Abstract: A calculation of the low energy mass spectrum of QCD in the large N-C limit is presented. The low-lying states in the meson spectrum up to the fourth order in the strong coupling perturbative expansion are explicitly computed. The 't Hooft limit is smooth and the meson masses are in very good agreement with experiment.

- [250] X. Y. Gu, B. Duan, and Z. Q. Ma. Quantum three-body system in D dimensions. *J. Math. Phys.*, 43(6):2895–2906, 2002.

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 $[\mu, \nu, 0, \dots, 0]$ 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.

- [251] X. Y. Gu, Z. Q. Ma, and S. H. Dong. Exact solutions to the Dirac equation for a Coulomb potential in D+1 dimensions. *Int. J. Mod. Phys. E-Nucl. Phys.*, 11(4):335–346, 2002.

Abstract: The Dirac equation is generalized to $D + 1$ space-time. The conserved angular momentum operators and their quantum numbers are discussed. The eigenfunctions of the total angular momenta are calculated for both odd D and even D cases. The radial equations for a spherically symmetric system are derived. The exact solutions for the system with a Coulomb potential are obtained analytically. The energy levels and the corresponding fine structure are also presented.

- [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. (C) 2002 Elsevier Science B.V. All rights reserved.

[253]

X. Y. Gu, Z. Q. Ma, and J. Q. Sun. Interdimensional degeneracies for a quantum N -body system in D dimensions. *Europhys. Lett.*, 64(5):586–591, 2003.

Abstract: The complete spectrum of exact interdimensional degeneracies for a quantum N -body system in D -dimensions is presented by the method of generalized spherical harmonic polynomials. In an N -body system all the states with angular momentum $[\mu + n]$ in $(D - 2n)$ dimensions are degenerate where $[\mu]$ and D are given and n is an arbitrary integer if the representation $[\mu + n]$ exists for the $SO(D - 2n)$ group and $D - 2n$ greater than or equal to N . There is an exceptional interdimensional degeneracy for an N -body system between the state with zero angular momentum in $D = N - 1$ dimensions and the state with zero angular momentum in $D = N + 1$ dimensions.

[254]

X. Y. Gu, Z. Q. Ma, and J. Q. Sun. Interdimensional degeneracies in a quantum isolated four-body system. *Phys. Lett. A*, 314(1-2):156–162, 2003.

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 isolated 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 μ, ν, τ , 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.

- [255] X. Y. Gu, Z. Q. Ma, and J. Q. Sun. Quantum four-body system in D dimensions. *J. Math. Phys.*, 44(9):3763–3774, 2003.
- Abstract:** By the method of generalized spherical harmonic polynomials, the Schrodinger equation for a four-body system in D-dimensional space is reduced to the generalized radial equations where only six internal variables are involved. The problem on separating the rotational degrees of freedom from the internal ones for a quantum N-body system in D dimensions is generally discussed. (C) 2003 American Institute of Physics.
- [256] H. Guerin. MODIFIED SHIFTED-LARGE-N APPROACH TO AN EXPONENTIAL POTENTIAL. *Phys. Rev. A*, 49(1):599–602, 1994.
- Abstract:** The modified shifted-large-N approach proposed by Bag et al. [Phys. Rev. A 46, 6059 (1992)] for the Morse potential is applied to the exponential (6) [exp(6)] potential, i.e., a potential with an exponential repulsion and an attraction in r^{-6} . Although the method does not provide the exact analytic expressions of the vibrational eigenvalues and eigenfunctions as in the Morse case, it is shown to predict quite accurate results for both the energy eigenvalues and eigenfunctions for the vibrational and rovibrational states of the exp(6) potential. In particular, the wave functions are much more accurate than those provided by the usual shifted-1/N method, which fails to yield their correct behavior. Moreover, in the modified approach, the exp(6) eigenfunctions are given in the same analytical form as the Morse ones.
- [257] W. R. Gutierrez. SINGLET-FIELDS FORMULATION AND THE LARGE-N EXPANSION OF THE QUARK SECTOR OF QCD. *Phys. Rev. D*, 30(12):2622–2627, 1984.
- [258] M. I. Haftel and V. B. Mandelzweig. PRECISE NONVARIATIONAL CALCULATIONS ON THE HELIUM ATOM. *Phys. Rev. A*, 38(12):5995–5999, 1988.
- [259] R. L. Hall. POTENTIAL ENVELOPES AND THE LARGE-N APPROXIMATION. *J. Math. Phys.*, 27(4):1027–1030, 1986.

Abstract: We study the properties of an isolated, self-interacting wormlike polymer chain on the basis of a nonperturbative $1/d$ -expansion, where d denotes the dimension of embedding space. In the absence of an external force, we characterize the dimension R of the chain in embedding space via R similar to $L(\nu)$, where L is the internal size. (A) Long-range, repulsive segmental interactions decaying as $1/r(\alpha)$ may control chain conformations that are either rodlike, $\nu = 1(1 \leq \alpha \leq 2)$, "wrinkled," $1/2 \leq \nu \leq 1(2 \leq \alpha \leq 4)$, or random-walk-like, $\nu = 1/2(\alpha \geq 4)$. (B) For short-range, screened, repulsive interactions, the crossover between rodlike and random-walk-like behavior is controlled by the persistence length whose interaction part we compute focusing on a Debye-Huckel interaction of strength V_0 , with inverse screening length $\kappa(0)$. The induced persistence length varies as $V_0(\beta)\kappa(-\gamma)(0)$, with, as expected, $(\beta, \gamma) = (1, 2)$ when the chain is intrinsically stiff, and, surprisingly, with either $(\beta, \gamma) = (1/6, 7/6)$ or $(\beta, \gamma) = (1, 7)$ when the chain is intrinsically very flexible. The chances of experimentally observing the novel regimes may be limited. For a chain subject to an external stretching force f , we determine the force-extension relation $\zeta = \zeta(f) = \zeta(0) + \Delta\zeta(f)$, where ζ denotes the chain extension, $\zeta(0)$ is the spontaneous extension. (A) If the interaction potential is either screened, or if the decay of a long-range interaction potential is fast, i.e., if $\alpha \geq 4$, the chain spontaneously generates an "effective tension" and responds linearly to weak forces with elastic constants "renormalized" by interactions. By contrast, "tension-free" chains, with either $\nu = 1$, where $\Delta\zeta$ similar to $f(1/2)$, or with $\nu = 2/\alpha$, where $\Delta\zeta$ similar to $f(1/3)$, respond to the weakest force nonlinearly. (B) Near full extension the chain always responds nonlinearly. When the potential is screened, or if $\alpha \geq 4$, we find the $1/\sqrt{f}$ corrections typical of wormlike chains. (C) 2001 American Institute of Physics.

[261] R. D. Harcourt. CIRCULAR ORBIT THEORY OF VALENCE. *Speculations in Science and Technology*, 1(4):339–358, 1978.

[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 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_5 and NF_5 , F_3^- and XeF_2 , IF_5 and XeF_5^+ , XeF_5^- , IF_8^- , $XeFg(8)(2^-)$, ReF_8^- and TaF_8^{3-} , ZrF_8^{4-} , ZrF_7^{3-} , ReF_6^{2-} , and high-spin CoF_6^{3-} . Aspects of the electronic structures of D_{3h} -symmetry PF_5 and NF_5 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.

- [264] A. B. Harris and J. M. Schwarz. 1/d expansion for k-core percolation. *Phys. Rev. E*, 72(4):17, 2005.

Abstract: The physics of k-core percolation pertains to those systems whose constituents require a minimum number of k connections to each other in order to participate in any clustering phenomenon. Examples of such a phenomenon range from orientational ordering in solid ortho-para H-2 mixtures to the onset of rigidity in bar-joint networks to dynamical arrest in glass-forming liquids. Unlike ordinary (k=1) and biconnected (k=2) percolation, the mean field k \geq 3-core percolation transition is both continuous and discontinuous, i.e., there is a jump in the order parameter accompanied with a diverging length scale. To determine whether or not this hybrid transition survives in finite dimensions, we present a 1/d expansion for k-core percolation on the d-dimensional hypercubic lattice. We show that to order 1/d(3) the singularity in the order parameter and in the susceptibility occur at the same value of the occupation probability. This result suggests that the unusual hybrid nature of the mean field k-core transition survives in high dimensions.

- [265] M. Hashimoto. ASYMPTOTIC PERTURBATIONAL EIGENVALUES FOR THE MULTIDIMENSIONAL WAVE-EQUATION IN NONSEPARABLE SYSTEMS. *Opt. Commun.*, 47(4):243–247, 1983.

- [266] M. I. Haysak, Y. L. Griga, and V. I. Lendyel. ONE EFFECTIVE METHOD FOR ACCOUNTING CORRELATIONS IN THE HELIUM ATOM. *Ukr. Fiz. Zhurnal*, 35(10):1470–1477, 1990.

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.

- [267] D. R. Herrick. DEGENERACIES IN ENERGY-LEVELS OF QUANTUM SYSTEMS OF VARIABLE DIMENSIONALITY. *J. Math. Phys.*, 16(2):281–283, 1975.
- [268] D. R. Herrick. VARIABLE DIMENSIONALITY IN GROUP-THEORETIC PREDICTION OF CONFIGURATION MIXINGS FOR DOUBLY-EXCITED HELIUM. *J. Math. Phys.*, 16(5):1047–1053, 1975.
- [269] D. R. Herrick. VARIATIONAL THEORY FOR HIGH RYDBERG STARK IONIZATION THRESHOLD SCALING LAWS IN ATOMIC-HYDROGEN. *J. Chem. Phys.*, 65(9):3529–3535, 1976.
- [270] D. R. Herrick. NEW SYMMETRY PROPERTIES OF ATOMS AND MOLECULES. *Advances in Chemical Physics*, 52:1–115, 1983.
- [271] D. R. Herrick and F. H. Stillinger. VARIABLE DIMENSIONALITY IN ATOMS AND ITS EFFECT ON GROUND-STATE OF HELIUM ISOELECTRONIC SEQUENCE. *Phys. Rev. A*, 11(1):42–53, 1975.
- [272] D. Herschbach. Fifty years in physical chemistry: Homage to mentors, methods, and molecules. *Annu. Rev. Phys. Chem.*, 51:1–39, 2000.

Abstract: A nostalgic account is given of my scientific odyssey, recalling early encounters, some fateful, some just fun, with mentors, methods, and molecules. These include stories of my student years at Stanford, pursuing chemical kinetics with Harold Johnston; graduate study at Harvard, doing molecular spectroscopy with Bright Wilson; and fledgling faculty years at Berkeley, launching molecular beam studies of reaction dynamics. A few vignettes from my "ever after" era on the Harvard faculty emphasize thematic motivations or methods inviting further exploration. An Appendix provides a concise listing of colleagues in research and the topics we have pursued.

- [273] D. R. Herschbach. DIMENSIONAL INTERPOLATION FOR 2-ELECTRON ATOMS. *J. Chem. Phys.*, 84(2):838–851, 1986.
- [274] D. R. Herschbach. NEW DIMENSIONS IN REACTION DYNAMICS AND ELECTRONIC-STRUCTURE - CLOSING REMARKS. *Faraday Discuss.*, 84:465–478, 1987.
- [275] D. R. Herschbach. Dimensional scaling and renormalization. *Int. J. Quantum Chem.*, 57(3):295–308, 1996.
- Abstract:** Chief features of dimensional scaling methods are exemplified by briefly reviewing prototypical applications and recent developments. The pseudoclassical large-D limit usually can be evaluated exactly regardless of the magnitude, nature, and number of strong, nonseparable dynamical interactions. Often, this limit can be accurately linked to $D = 3$ by perturbation or interpolation methods. This is because the dimension dependence of many-body effects tends to be smooth and mild when calibrated by appropriate one- or few-body problems. A simple renormalization procedure applied to atoms with up to N similar to 100 electrons yields a major part of the correlation energy. From Hartree-Fock input, a renormalized nuclear charge is determined which renders the dimensionally scaled energy at $D \rightarrow \infty$ a good approximation to that for $D = 3$ with the actual Z . Prospects are discussed for other means to exploit dimensional scaling, including an analogous renormalization procedure for molecules. (C) 1996 John Wiley & Sons, Inc.
- [276] D. R. Herschbach, J. G. Loeser, and D. K. Watson. PSEUDOMOLECULAR ATOMS - GEOMETRY OF 2-ELECTRON INTRASHELL EXCITED-STATES. *Z. Phys. D-Atoms Mol. Clusters*, 10(2-3):195–210, 1988.
- [277] A. Hibbert. DEVELOPMENTS IN ATOMIC-STRUCTURE CALCULATIONS. *Rep. Prog. Phys.*, 38(11):1217–1338, 1975.
- [278] S. Hikami and E. Brezin. LARGE-ORDER BEHAVIOR OF THE $1/N$ EXPANSION IN ZERO AND ONE DIMENSIONS. *J. Phys. A-Math. Gen.*, 12(6):759–770, 1979.

- [279] A. Holas, P. M. Kozłowski, and N. H. March. KINETIC-ENERGY DENSITY AND PAULI POTENTIAL - DIMENSIONALITY DEPENDENCE, GRADIENT EXPANSIONS AND NONLOCALITY. *J. Phys. A-Math. Gen.*, 24(18):4249–4260, 1991.

Abstract: For arbitrary level filling, the fully non-local kinetic energy density and Pauli potential for the one-dimensional harmonic oscillator can be constructed explicitly. In the present work, these exact results are eventually compared with the low-order gradient expansions. This prompts a fuller study of the dimensionality dependence of low-order gradient expansions for systems with general one-body potentials, and its relevance to the theory of the Pauli potential. One consequence of the present work is to display the generalization to D-dimensions as (D-2)/3D of the three-dimensional Kirzhnits coefficient 1/9 of the von Weizsacker term in the kinetic energy density.

- [280] J. E. Hornos, S. W. Macdowell, and C. D. Caldwell. 2-ELECTRON WAVE-FUNCTIONS IN HYPERSPHERICAL COORDINATES. *Phys. Rev. A*, 33(4):2212–2224, 1986.

- [281] H. Hosoya. NUMBER AND SHAPES OF THE ATOMIC ORBITALS OF 4-DIMENSIONAL AND HIGHER-DIMENSIONAL ATOMS. *J. Mol. Struct.*, 352:561–565, 1995.

Abstract: General and recursive formulae for the degeneracy of the angular momentum I of the atomic orbitals of an n-dimensional atom are derived from the algebraic manipulation of homogeneous polynomials. General rectangular coordinate expressions for the wavefunctions of the p- and d-orbitals of an n-dimensional atom are also obtained. The analytical expressions for the sixteen f-orbitals of a four-dimensional atom are given. The relation between the wavefunctions of these hypothetical atoms and those for the three-dimensional atoms and molecules is discussed.

- [282] H. Hosoya. Hierarchical structure of the atomic orbital wave functions of D-dimensional atom. *J. Phys. Chem. A*, 101(4):418–421, 1997.

Abstract: The hierarchical structure of the set of atomic orbital wave functions of D-dimensional atoms is discussed by using the set of their rectangular coordinate expressions.

- [283] H. Hosoya. Back-of-envelope derivation of the analytical formulas of the atomic wave functions of a D-dimensional atom. *Int. J. Quantum Chem.*, 64(1):35–42, 1997.

Abstract: A simple algebraic manipulation is presented for obtaining the analytical rectangular coordinate expressions of the atomic orbital wave functions with angular quantum number l of a D-dimensional atom, where no hyperspherical harmonics or any differential calculus is involved. A general expression of the D-dimensional f-orbitals is given which supplements the previously obtained result of D-dimensional d-orbitals. (C) 1997 John Wiley & Sons, Inc.

- [284] H. Hosoya. Pascal's triangle, non-adjacent numbers, and D-dimensional atomic orbitals. *J. Math. Chem.*, 23(1-2):169–178, 1998.

Abstract: The topics in chemico-physical problems which are related to Pascal's triangle and asymmetrical Pascal's triangle are collected and their mathematical relations are discussed. The selected topics are: ESR hyperfine splitting, spin-spin coupling of NMR, topological indices of linear and cyclic hydrocarbons, and the number of degeneracy of the atomic orbitals of D-dimensional hydrogen atom. The relation between the Pascal's and asymmetrical Pascal's triangles is also discussed.

- [285] H. Hosoya, F. Kido, and S. Tokita. A new view of hybridized atomic orbitals from n-dimensional world. *Croat. Chem. Acta*, 80(2):251–260, 2007.

Abstract: By taking a birds-eye view from the n-dimensional world (or n-space), it was found that the conventionally used sp, sp(2), and sp(3) hybridized atomic orbitals belong to the sp(n) hybridization and their geometrical shapes correspond to n-simplexes, which are, respectively, the smallest geometrical objects in n-space. Similarly, sp, sp(2)d, and sp(2)d(3) hybridizations are found

to belong to the $sp(n)d(n-1)$ hybridization, whose geometrical shapes correspond to n -cross polytopes (obtained from $2n$ vertices equidistantly located on n rectangular coordinate axes). Another series of n -cube hybridization is also discussed, whose 3-space member is 8-coordinated cubic hybridization, $sp(3)d(3)f$. General analytical forms of the wavefunctions of these three series of hybridized atomic orbitals in n -space are obtained. The periodic table and related problems of atoms and molecules in n -space are discussed.

- [286] S. W. Huang, D. Z. Goodson, M. Lopez-Cabrera, and T. C. Germann. Large-order dimensional perturbation theory for diatomic molecules within the Born-Oppenheimer approximation. *Phys. Rev. A*, 58(1):250–257, 1998.

Abstract: A renormalization of the D -dimensional Hamiltonian is developed to ensure that the large- D limit corresponds to a single well at any value of the internuclear distance R . This avoids convergence problems caused by a symmetry-breaking transition that is otherwise expected to occur when R is approximately equal to the equilibrium bond distance R_{eq} . With larger R giving a double well. This symmetry breaking has restricted the applicability of large-order perturbation theory in $1/D$ to cases where R is significantly less than R_{eq} . The renormalization greatly extends the range of R for which the large-order expansion can be summed. A numerical demonstration is presented for H_2^+ . The $1/D$ expansions are summed using Pade-Borel approximants with modifications that explicitly model known singularity structure.

- [287] S. M. Ikhdair. Exact solutions of the D -dimensional Schrodinger equation for a pseudo-Coulomb potential plus ring-shaped potential. *Chin. J. Phys.*, 46(3):291–306, 2008.

Abstract: We present the exact energy bound state solutions of the Schrodinger equation in D -dimensions for an alternative (often used) pseudo-Coulomb potential plus ring-shaped potential of the form $V(r) = -a/r + b/r^2 + \beta \cos(2\theta)/r^2 \sin(2\theta) + c$. The solution was obtained analytically by means of the Nikiforov-Uvarov method. We give a clear recipe of how to

obtain an explicit solution to the D-dimensional radial and angular parts of the wave functions in terms of orthogonal polynomials. The total energy of the system is different from the pseudo-Coulomb potential because of the contribution of the angular part. The general results obtained in this work can be reduced to the well-known three-dimensional forms given in the literature.

- [288] S. M. Ikhdair. An improved approximation scheme for the centrifugal term and the Hulthen potential. *Eur. Phys. J. A*, 39(3):307–314, 2009.

Abstract: We present a new approximation scheme for the centrifugal term to solve the Schrodinger equation with the Hulthen potential for any arbitrary l-state by means of a mathematical Nikiforov-Uvarov (NU) method. We obtain the bound-state energy eigenvalues and the normalized corresponding eigenfunctions expressed in terms of the Jacobi polynomials or hypergeometric functions for a particle exposed to this potential field. Our numerical results of the energy eigenvalues are found to be in high agreement with those results obtained by using the program based on a numerical integration procedure. The s-wave ($l = 0$) analytic solution for the binding energies and eigenfunctions of a particle are also calculated. The physical meaning of the approximate analytical solution is discussed. The present approximation scheme is systematic and accurate.

- [289] S. M. Ikhdair and R. Sever. BOUND-STATE ENERGIES FOR THE EXPONENTIAL COSINE SCREENED COULOMB POTENTIAL. *Z. Phys. D-Atoms Mol. Clusters*, 28(1):1–5, 1993.

Abstract: The energy eigenvalues of bound states of an electron in the general exponential cosine screened Coulomb potential are obtained using the shifted $1/N$ expansion method. The energies for the states from 1s to 8k are calculated from six to eight significant figures. The energy eigenvalues for the 1s, 2s - 2p, 3s - 3d, and 4s - 4f states are also presented as a function of the screening parameter λ . Results are compared with the ones obtained by other workers. The agreement reduces

roughly for large λ . It is also observed that the convergence of the expansion series increases remarkably as l increases.

- [290] S. M. Ikhdaïr and R. Sever. B-c meson spectrum and hyperfine splittings in the shifted large-N-expansion technique. *Int. J. Mod. Phys. A*, 18(23):4215–4231, 2003.

Abstract: In the framework of potential models for heavy quarkonium, we compute the mass spectrum of the bottom-charmed B-c meson system and spin-dependent splittings from the Schrodinger equation using the shifted-large-N expansion technique. The masses of the lightest vector B-c(*) and pseudoscalar B-c states as well as the higher states below the threshold are estimated. Our predicted result for the ground state energy is 6253(-6)(+15) MeV and are generally in exact agreement with earlier calculations. Calculations of the Schrodinger energy eigenvalues are carried out up to the third order of the energy series. The parameters of each potential are adjusted to obtain best agreement with the experimental spin-averaged data (SAD). Our findings are compared with the observed data and with the numerical results obtained by other numerical methods.

- [291] S. M. Ikhdaïr and R. Sever. Calculation of the B-c leptonic decay constant using the shifted N-expansion method. *Int. J. Mod. Phys. A*, 21(32):6699–6714, 2006.

Abstract: We give a review and present a comprehensive calculation for the leptonic constant $f_B(c)$ of the low-lying pseudoscalar and vector states of B-c-meson in the framework of static and QCD-motivated nonrelativistic potential models taking into account the one-loop and two-loop QCD corrections in the short distance coefficient that governs the leptonic constant of B-c quarkonium system. Further, we use the scaling relation to predict the leptonic constant of the nS-states of the bc system. Our results are compared with other models to gauge the reliability of the predictions and point out differences.

- [292] S. M. Ikhdaïr and R. Sever. A perturbative treatment for the bound states of the Hellmann potential. *Theochem-J. Mol. Struct.*, 809(1-3):103–113, 2007.

Abstract: A new approximation formalism is applied to study the bound states of the Hellmann potential, which represents the superposition of the attractive Coulomb potential $-a/r$ and the Yukawa potential $b\exp(-\delta r)/r$ of arbitrary strength b and screening parameter δ . Although the analytic expressions for the energy eigenvalues E_n yield quite accurate results for a wide range of n , f in the limit of very weak screening, the results become gradually worse as the strength b and the screening coefficient δ increase. This is because that the expansion parameter is not sufficiently small enough to guarantee the convergence of the expansion series for the energy levels. (C) 2007 Elsevier B.V. All rights reserved.

- [293] S. M. Ikhdair and R. Sever. Bound energy for the exponential-cosine-screened Coulomb potential. *J. Math. Chem.*, 41(4):329–341, 2007.

Abstract: An alternative approximation scheme has been used in solving the Schrodinger equation for the exponential-cosine-screened Coulomb potential. The bound state energies for various eigenstates and the corresponding wave functions are obtained analytically up to the second perturbation term.

- [294] S. M. Ikhdair and R. Sever. Bound states of a more general exponential screened Coulomb potential. *J. Math. Chem.*, 41(4):343–353, 2007.

Abstract: An alternative approximation scheme has been used in solving the Schrodinger equation to the more general case of exponential screened Coulomb potential, $V(r) = -(a/r)[1 + (1 + br)e(-2br)]$. The bound state energies of the 1s, 2s and 3s-states, together with the ground state wave function are obtained analytically upto the second perturbation term.

- [295] S. M. Ikhdair and R. Sever. Exact solutions of the radial Schrodinger equation for some physical potentials. *Cent. Eur. J. Phys.*, 5(4):516–527, 2007.

Abstract: By using an ansatz for the eigenfunction, we have obtained the exact analytical solutions of the radial Schrodinger equation for the

pseudoharmonic and the Kratzer potentials in two dimensions. The bound-state solutions are easily calculated from this eigenfunction ansatz. The corresponding normalized wavefunctions are also obtained. (C) Versita Warsaw and Springer-Verlag Berlin Heidelberg. All rights reserved.

- [296] S. M. Ikhdaïr and R. Sever. Polynomial solutions of the Mie-type potential in the D-dimensional Schrodinger equation. *Theochem-J. Mol. Struct.*, 855(1-3):13–17, 2008.

Abstract: The polynomial solution of the D-dimensional Schrodinger equation for a special case of Mie potential is obtained with an arbitrary l not equal 0 states. The exact bound state energies and their corresponding wave functions are calculated. The bound state (real) and positive (imaginary) cases are also investigated. In addition, we have simply obtained the results from the solution of the Coulomb potential by an appropriate transformation. (C) 2008 Elsevier B.V. All rights reserved.

- [297] S. M. Ikhdaïr and R. Sever. Approximate l -state solutions of the D-dimensional Schrodinger equation for Manning-Rosen potential. *Ann. Phys.-Berlin*, 17(11):897–910, 2008.

Abstract: The Schrodinger equation in D-dimensions for the Manning-Rosen potential with the centrifugal term is solved approximately to obtain bound states eigensolutions (eigenvalues and eigenfunctions). The Nikiforov-Uvarov (NU) method is used in the calculations. We present numerical calculations of energy eigenvalues to two- and four-dimensional systems for arbitrary quantum numbers n and l , with three different values of the potential parameter α . It is shown that because of the interdimensional degeneracy of eigenvalues, we can also reproduce eigenvalues of a upper/lower dimensional system from the well-known eigenvalues of a lower/upper dimensional system by means of the transformation $(n, l, D) \rightarrow (n, l \pm 1, D \pm 2)$. This solution reduces to the Hulthen potential case.

- [298] S. M. Ikhdaïr and R. Sever. Exact solutions of the D-dimensional Schrodinger equation for a ring-shaped pseudoharmonic potential. *Cent. Eur. J. Phys.*, 6(3):685–696, 2008.

Abstract: A new non-central potential, consisting of a pseudoharmonic potential plus another recently proposed ring-shaped potential, is solved. It has the form $V(r, \theta) = 1/8 Kr - e(2) (r/r(e) - r(e)/r)(2) + \beta \cos(2)\theta/r(2)\sin(2)\theta$. The energy eigenvalues and eigenfunctions of the bound-states for the Schrodinger equation in D-dimensions for this potential are obtained analytically by using the Nikiforov-Uvarov method. The radial and angular parts of the wave functions are obtained in terms of orthogonal Laguerre and Jacobi polynomials. We also find that the energy of the particle and the wave functions reduce to the energy and the wave functions of the bound-states in three dimensions.

[299]

S. M. Ikhdair and R. Sever. Exact solutions of the modified Kratzer potential plus ring-shaped potential in the d-dimensional Schrodinger equation by the Nikiforov-Uvarov method. *Int. J. Mod. Phys. C*, 19(2):221–235, 2008.

Abstract: We present analytically the exact energy bound-states solutions of the Schrodinger equation in D dimensions for a recently proposed modified Kratzer plus ring-shaped potential by means of the Nikiforov-Uvarov method. We obtain an explicit solution of the wave functions in terms of hyper-geometric functions (Laguerre polynomials). The results obtained in this work are more general and true for any dimension which can be reduced to the well-known three-dimensional forms given by other works.

[300]

S. M. Ikhdair and R. Sever. B-c spectroscopy in the shifted l-expansion technique. *Int. J. Mod. Phys. E-Nucl. Phys.*, 17(4):669–691, 2008.

Abstract: In the framework of static and QCD-motivated model potentials for heavy quarkonium, we present a further comprehensive calculation of the mass spectrum of bc system and its ground state spin-dependent splittings in the context of the shifted l-expansion technique. We also predict the leptonic constant $f_B(c)$, of the lightest pseudoscalar B_c , and $f_{B(c)^*}$, of the vector B_c^* states taking into account the one-loop and two-loop QCD corrections. Furthermore, we use the scaling relation

to predict the leptonic constant of the nS -states of the bc system. Our predicted results are generally in high agreement with some earlier numerical methods. The parameters of each potential are adjusted to obtain best agreement with the experimental spin-averaged data (SAD).

- [301] S. M. Ikhdair and R. Sever. EXACT BOUND STATES OF THE D-DIMENSIONAL KLEIN-GORDON EQUATION WITH EQUAL SCALAR AND VECTOR RING-SHAPED PSEUDOHARMONIC POTENTIAL. *Int. J. Mod. Phys. C*, 19(9):1425–1442, 2008.

Abstract: We present the exact solution of the Klein Gordon equation in D-dimensions in the presence of the equal scalar and vector pseudoharmonic potential plus the ring-shaped potential using the Nikiforov-Uvarov method. We obtain the exact bound state energy levels and the corresponding eigen functions for a spin-zero particles. We also find that the solution for this ring-shaped pseudoharmonic potential can be reduced to the three-dimensional (3D) pseudoharmonic solution once the coupling constant of the angular part of the potential becomes zero.

- [302] S. M. Ikhdair and R. Sever. Exact quantization rule to the Kratzer-type potentials: an application to the diatomic molecules. *J. Math. Chem.*, 45(4):1137–1152, 2009.

Abstract: For arbitrary values of n and l quantum numbers, we present a simple exact analytical solution of the D-dimensional (D a parts per thousand yen 2) hyperradial Schrodinger equation with the Kratzer and the modified Kratzer potentials within the framework of the exact quantization rule (EQR) method. The exact bound state energy eigenvalues ($E(nl)$) are easily calculated from this EQR method. The corresponding normalized hyperradial wave functions ($\psi(nl)(r)$) are also calculated. The exact energy eigenvalues for these Kratzer-type potentials are calculated numerically for a few typical LiH, CH, HCl, CO, NO, O-2, N-2 and I-2 diatomic molecules for various values of n and l quantum numbers. Numerical tests using the energy calculations for the inter dimensional degeneracy ($D = 2 - 4$) for I-2, LiH, HCl, O-2, NO

and CO are also given. Our results obtained by EQR are in exact agreement with those obtained by other methods.

- [303] T. Imbo, A. Pagnamenta, and U. Sukhatme. ENERGY EIGENSTATES OF SPHERICALLY SYMMETRIC-POTENTIALS USING THE SHIFTED $1/N$ EXPANSION. *Phys. Rev. D*, 29(8):1669–1681, 1984.
- [304] T. Imbo, A. Pagnamenta, and U. Sukhatme. BOUND-STATES OF THE YUKAWA POTENTIAL VIA THE SHIFTED $1-N$ EXPANSION TECHNIQUE. *Phys. Lett. A*, 105(4-5):183–187, 1984.
- [305] T. Imbo and U. Sukhatme. LOGARITHMIC PERTURBATION EXPANSIONS IN NONRELATIVISTIC QUANTUM-MECHANICS. *Am. J. Phys.*, 52(2):140–146, 1984.
- [306] T. Imbo and U. Sukhatme. IMPROVED WAVE-FUNCTIONS FOR LARGE- N EXPANSIONS. *Phys. Rev. D*, 31(10):2655–2658, 1985.
- [307] T. D. Imbo. ACCURATE BARYON MASSES FROM MESON MASSES USING POTENTIAL MODELS AND THE $1/D$ EXPANSION. *Phys. Rev. D*, 36(11):3438–3442, 1987.
- [308] T. D. Imbo and U. P. Sukhatme. SUPERSYMMETRIC QUANTUM-MECHANICS AND LARGE- N EXPANSIONS. *Phys. Rev. Lett.*, 54(20):2184–2187, 1985.
- [309] T. Ishinabe, J. F. Douglas, A. M. Nemirovsky, and K. F. Freed. EXAMINATION OF THE $1/D$ EXPANSION METHOD FROM EXACT ENUMERATION FOR A SELF-INTERACTING SELF-AVOIDING WALK. *J. Phys. A-Math. Gen.*, 27(4):1099–1109, 1994.

Abstract: The $1/d$ expansion method for polymer chains is examined by comparing these expansions for several thermodynamic and structural quantities with the results of standard series analysis of exact enumeration data. The comparisons cover a wide range of spatial dimensions d , including non-integer ones, and are performed for particular values of interaction energy. Good agreement is generally found for $d \geq 4$, whereas discrepancies become conspicuous as d decreases to $d = 2$. Reasonable values are obtained for the exponents ν

and γ in $d = 2 - 4$ by applying the coherent-anomaly method of Suzuki to our $1/d$ expansions through fifth order in $d-1$.

[310] I. A. Ivanov. RADIUS OF CONVERGENCE OF THE $1/Z$ -EXPANSION FOR THE GROUND-STATE OF A 2-ELECTRON ATOM. *Phys. Rev. A*, 51(2):1080–1084, 1995.

[311] I. A. Ivanov. Asymptotic description of the Rydberg states with $L \rightarrow 0$ in a two-electron atom. *Eur. Phys. J. D*, 27(3):203–208, 2003.

Abstract: The energies of the levels belonging to a Rydberg series $1snp(1,3)P$ in a two electron atom have been determined by means of the quantum defect theory for a two-electron atom with nuclear charge Z considered as a parameter. Comparison with configuration interaction calculations suggests that the analytic quantum defect expression for the energy levels may be in fact asymptotically exact as $Z \rightarrow 1$, providing an analytic description of the disappearance of the Rydberg states with $L \rightarrow 0$ when Z approaches the value of 1.

[312] N. Iwamoto. GROUND-STATE-ENERGY THEOREM AND THE VIRIAL-THEOREM OF A MANY-PARTICLE SYSTEM IN D -DIMENSIONS. *Phys. Rev. A*, 30(5):2597–2601, 1984.

[313] A. Jakovac. Renormalization of the $O(N)$ model in the $1/N$ expansion in the auxiliary field formalism. *Phys. Rev. D*, 78(8):9, 2008.

Abstract: We study the renormalization of the $O(N)$ model using the auxiliary field formalism (Hubbard-Stratonovich transformation) in the $1/N$ expansion at finite temperature. We provide the general strategy of renormalization for arbitrary order and make a calculation up to next-to-leading order. We show that renormalization is possible for any values of the condensates, prove the temperature independence of the counterterms, and determine the cutoff dependence of the first nontrivial counterterm parts.

[314] M. Jameel. LARGE N -EXPANSION FOR HULTHEN POTENTIAL. *J. Phys. A-Math. Gen.*, 19(10):1967–1971, 1986.

- [315] A. Jevicki and H. Levine. LARGE N CLASSICAL EQUATIONS AND THEIR QUANTUM SIGNIFICANCE. *Ann. Phys.*, 136(1):113–135, 1981.
- [316] A. Jevicki and N. Papanicolaou. CLASSICAL DYNAMICS IN THE LARGE N LIMIT. *Nucl. Phys. B*, 171(3):362–376, 1980.
- [317] A. Jevicki and B. Sakita. COLLECTIVE FIELD APPROACH TO THE LARGE-N LIMIT - EUCLIDEAN FIELD-THEORIES. *Nucl. Phys. B*, 185(1):89–100, 1981.
- [318] B. R. Johnson. THE QUANTUM DYNAMICS OF 3 PARTICLES IN HYPERSPHERICAL COORDINATES. *J. Chem. Phys.*, 79(4):1916–1925, 1983.
- [319] S. Kais and G. Beltrame. DIMENSIONAL SCALING FOR REGGE TRAJECTORIES. *J. Phys. Chem.*, 97(10):2453–2456, 1993.

Abstract: Using dimensional scaling, we were able to obtain a systematic expansion for Regge trajectories in $1/\kappa$, where $\kappa = (D-1)/2$ and D is the number of spatial dimensions. Bound states for the power-law potential were obtained from Regge trajectories by requiring the angular momentum quantum number to take on positive integer values. For scattering states, we calculated the positions of Regge poles for the Lennard-Jones(6,4) and (12,6)potentials. The results to first order in $1/\kappa$ were in good agreement with both semiclassical and quantum calculations. The same expansion was used to obtain the positions of Regge poles for complex optical potentials. The results for the Lennard-Jones (I 2,6) potential perturbed by an imaginary term were in excellent agreement with the semiclassical calculations.

- [320] S. Kais and R. Bleil. CHARGE RENORMALIZATION AT THE LARGE-D LIMIT FOR N-ELECTRON ATOMS AND WEAKLY-BOUND SYSTEMS. *J. Chem. Phys.*, 102(19):7472–7478, 1995.
- [321] S. Kais, D. D. Frantz, and D. R. Herschbach. ELECTRONIC TUNNELING IN H-2+ EVALUATED FROM THE LARGE-DIMENSION LIMIT. *Chem. Phys.*, 161(3):393–402, 1992.

Abstract: We derive a simple, analytic expression for the energy splitting ΔE between

the lowest pair of H_2^+ states ($1s\text{-}\sigma(g)$ and $2p\text{-}\sigma(u)$) that results from electron exchange between two protons. The calculation employs the semiclassical instanton method, with two unorthodox features which markedly simplify the treatment: (1) The double-minimum potential and corresponding wavefunctions that govern the electronic tunneling are evaluated in the large-dimension limit. (2) The time variable is rescaled to cure divergent behavior of fluctuations about the instanton path that otherwise appears because of the potential develops sharp cusps as the internuclear distance increases. By virtue of exact interdimensional degeneracies, the large-D limit yields valid results for a 3D molecule. Indeed, a simple dimensional scaling law gives ΔE for all pairs of g, u states that stem from separated atom states with $m = l = n - 1$, for $n = 1 \rightarrow \infty$. For a wide range of internuclear distances, our analytic expression for ΔE , which pertains to the leading order in \hbar , gives for such states good agreement with comparable semiclassical methods as well as with exact numerical calculations. It is remarkable that use of the effective potential for the large-dimension limit, which is exactly calculable from classical electrostatics, yields quantitative results for electronic tunneling, an intrinsically quantal phenomenon.

[322]

S. Kais, T. C. Germann, and D. R. Herschbach. LARGE-DIMENSION LIMIT YIELDS GENERIC REDUCED POTENTIAL CURVES FOR H_2^+ , H_2 , HHe^+ , AND He_2^{2+} . *J. Phys. Chem.*, 98(43):11015–11017, 1994.

Abstract: Analytic expressions for the $D \rightarrow \infty$ limit previously evaluated for one- and two-electron diatomic molecules are compared with the familiar $D = 3$ potentials as functions of the internuclear distance R for H_2^+ , H_2 , HHe^+ , and He_2^{2+} . We find that the $D = 3$ potential can be obtained from the large-D limit simply by $E(3)(R) E(\infty)(R)/G(R)$, to good approximation, where the function $G(R)$ has the same form for the four molecules. Furthermore, $1 - G(R)$ has a corresponding-states property; when reduced by two parameters, it becomes the same function for

all four molecules, nearly proportional to $x(2)e(-2x)$, with x the scaled internuclear distance. This suggests that the pseudoclassical $D \rightarrow \infty$ limit may provide a useful reference for analysis of intermolecular potentials.

- [323] S. Kais and D. R. Herschbach. DIMENSIONAL SCALING FOR QUASI-STATIONARY STATES. *J. Chem. Phys.*, 98(5):3990–3998, 1993.

Abstract: Complex energy eigenvalues which specify the location and width of quasibound or resonant states are computed to good approximation by a simple dimensional scaling method. As applied to bound states, the method involves minimizing an effective potential function in appropriately scaled coordinates to obtain exact energies in the $D \rightarrow \infty$ limit, then computing approximate results for $D = 3$ by a perturbation expansion in $1/D$ about this limit. For resonant states, the same procedure is used, with the radial coordinate now allowed to be complex. Five examples are treated: the repulsive exponential potential ($e(-r)$); a squelched harmonic oscillator ($r^2e(-r)$); the inverted Kratzer potential (r^{-1} repulsion plus r^{-2} attraction); the Lennard-Jones potential (r^{-12} repulsion, r^{-6} attraction); and quasibound states for the rotational spectrum of the hydrogen molecule ($X^1\Sigma(g)^+$, $v = 0$, $J = 0$ to 50). Comparisons with numerical integrations and other methods show that the much simpler dimensional scaling method, carried to second-order (terms in $1/D^2$), yields good results over an extremely wide range of the ratio of level widths to spacings. Other methods have not yet evaluated the very broad H-2 rotational resonances reported here ($J \rightarrow \infty$), which lie far above the centrifugal barrier.

- [324] S. Kais and D. R. Herschbach. THE $1/Z$ EXPANSION AND RENORMALIZATION OF THE LARGE-DIMENSION LIMIT FOR MANY-ELECTRON ATOMS. *J. Chem. Phys.*, 100(6):4367–4376, 1994.

Abstract: Analytic expressions for the large-dimension limit, when renormalized by introducing a suitable effective nuclear charge $zeta$ yield

accurate $D=3$ nonrelativistic energies for ground states of many-electron atoms. Using Hartree-Fock data to estimate ζ , which typically differs from the actual charge Z by similar to 1% or less, we find this dimensional renormalization method (denoted DR-O) gives results substantially better than the HF input. Comparison of the $1/Z$ expansion for the large- D limit with that for $D=3$ atoms provides expressions for the leading error terms in the renormalized total energy and correlation energy. When configuration mixing occurs in the $Z \rightarrow \infty$ limit (as for Be and many other atoms), we find the renormalization procedure is markedly improved by including the zeroth-order mixing (denoted DR-1); this contributes a term linear in Z . Including the Z -independent term (DR-2) also improves the accuracy when zeroth-order mixing is absent (e.g., ground-state atoms with $N=2, 3,$ and $7-11$) but not otherwise. Correlation energies for atoms and cations with $N=2-18$ electrons and $Z=2-28$ are obtained with a mean error of 26% using just the large- D limit or HF input (DR-O); the mean error improves to only 5% when the leading $1/Z$ term is included (either DR-1 or DR-2). Results much better than the HF approximation are likewise obtained for the ionization potentials and electron affinities of neutral atoms.

[325]

S. Kais, D. R. Herschbach, N. C. Handy, C. W. Murray, and G. J. Laming. DENSITY FUNCTIONALS AND DIMENSIONAL RENORMALIZATION FOR AN EXACTLY SOLVABLE MODEL. *J. Chem. Phys.*, 99(1):417–425, 1993.

Abstract: We treat an analytically solvable version of the "Hooke's Law" model for a two-electron atom, in which the electron-electron repulsion is Coulombic but the electron-nucleus attraction is replaced by a harmonic oscillator potential. Exact expressions are obtained for the ground-state wave function and electron density, the Hartree-Fock solution, the correlation energy, the Kohn-Sham orbital, and, by inversion, the exchange and correlation functionals. These functionals pertain to the "intermediate" density regime ($r(s)$ greater-than-or-equal-to 1.4) for an electron gas. As a test of customary approximations employed in density functional theory, we compare our exact density,

exchange, and correlation potentials and energies with results from two approximations. These use Becke's exchange functional and either the Lee-Yang-Parr or the Perdew correlation functional. Both approximations yield rather good results for the density and the exchange and correlation energies, but both deviate markedly from the exact exchange and correlation potentials. We also compare properties of the Hooke's Law model with those of two-electron atoms, including the large dimension limit. A renormalization procedure applied to this very simple limit yields correlation energies as good as those obtained from the approximate functionals, for both the model and actual atoms.

- [326] S. Kais, D. R. Herschbach, and R. D. Levine. DIMENSIONAL SCALING AS A SYMMETRY OPERATION. *J. Chem. Phys.*, 91(12):7791–7796, 1989.
- [327] S. Kais, J. D. Morgan, and D. R. Herschbach. ELECTRONIC TUNNELING AND EXCHANGE ENERGY IN THE D-DIMENSIONAL HYDROGEN-MOLECULE ION. *J. Chem. Phys.*, 95(12):9028–9041, 1991.

Abstract: Dimensional scaling generates an effective potential for the electronic structure of atoms and molecules, but this potential may acquire multiple minima for certain ranges of nuclear charges or geometries that produce symmetry breaking. Tunneling among such minima is akin to resonance among valence bond structures. Here we treat the D-dimensional H_2^+ molecule ion as a prototype test case. In spheroidal coordinates it offers a separable double-minimum potential and tunneling occurs in only one coordinate; in cylindrical coordinates the potential is nonseparable and tunneling occurs in two coordinates. We determine for both cases the ground state energy splitting $\Delta E(D)$ as a function of the internuclear distance R . By virtue of exact interdimensional degeneracies, this yields the exchange energy for all pairs of g, u states of the $D = 3$ molecule that stem from separated atom states with $m = l = n - 1$, for $n = 1 - j$ infinity. We evaluate $\Delta E(D)$ by two semi-classical techniques, the asymptotic and instanton methods, and obtain good agreement with exact numerical calculations over a wide range of R . We

find that for cylindrical coordinates the instanton path for the tunneling trajectory differs substantially from either a straightline or adiabatic path, but is nearly parabolic. Path integral techniques provide relatively simple means to determine the exact instanton path and contributions from fluctuations around it. Generalizing this approach to treat multielectron tunneling in several degrees of freedom will be feasible if the fluctuation calculations can be made tractable.

- [328] S. Kais, J. P. Neirotti, and P. Serra. Phase transitions and the stability of atomic and molecular ions. *Int. J. Mass Spectrom.*, 182:23–29, 1999.

Abstract: Quantum phase transitions at absolute zero temperature can take place as some parameter in the Hamiltonian of the system is varied. For such transitions, crossing the phase boundary means that the quantum ground state changes in some fundamental way. For the Hamiltonian of N -electron atoms, this parameter is taken to be the nuclear charge. As the nuclear charge reaches a critical point, the quantum ground state changes its characters from being bound to being degenerate or absorbed by a continuum. We describe here a method to calculate the critical nuclear charge for which an atom can bind an extra electron to form a stable negative ion. The estimate of the critical nuclear charge will be used to explain and predict the stability of atomic negative ions. The method can be generalized to predict the stability of molecular negative ions. A detailed calculation for the critical parameters for two center molecular ions is also included. (C) 1999 Elsevier Science B.V.

- [329] S. Kais and P. Serra. Quantum critical phenomena and stability of atomic and molecular ions. *Int. Rev. Phys. Chem.*, 19(1):97–121, 2000.

Abstract: In this review we discuss quantum phase transitions and the mapping between symmetry breaking of electronic structure configurations at the large-dimension limit and mean-field theory of phase transitions. We show that the finite size scaling method can be used for the calculations of the critical parameters of the few-body

Schrodinger equation. In this approach, the finite size corresponds to the number of elements in a complete basis set used to expand the exact eigenfunction of a given Hamiltonian. The critical parameters such as the critical nuclear charges will be used to explain and predict the stability of atomic and molecular negative ions. For N -electron atoms with $2 \leq N \leq 86$, results show that, at most, only one electron can be added to a free atom in the gas phase. However, doubly charged atomic negative ions might exist in a strong magnetic field.

- [330] S. Kais, S. M. Sung, and D. R. Herschbach. ATOMIC ENERGIES FROM RENORMALIZATION OF THE LARGE-DIMENSION LIMIT. *J. Chem. Phys.*, 99(7):5184–5196, 1993.

Abstract: By augmenting Hartree-Fock (HF) results for nonrelativistic ground-state energies of N -electron atoms by analytic expressions for the $D \rightarrow \infty$ limit derived by Loeser, we obtain a simple renormalization procedure which substantially enhances accuracy. A renormalized nuclear charge, $Z(\infty)$, is found which renders the dimensionally scaled energy at $D \rightarrow \infty$ a good approximation to that for $D = 3$ with the actual Z . The renormalized charge is readily evaluated by comparing the HF energy (or any other input approximation) with its $D \rightarrow \infty$ limit. For atoms with any N or Z , the computations are elementary, requiring little more than solution of a quartic equation. With only HF input in addition to the $D \rightarrow \infty$ limit, the renormalization procedure yields about 2/3 or more of the correlation energy, for neutral atoms with $N=Z \leq 86$. Further improvements in the method seem feasible, but will require better means to incorporate shell-structure in the large- D limit.

- [331] S. Kais, S. M. Sung, and D. R. Herschbach. LARGE- Z AND LARGE- N DEPENDENCE OF ATOMIC ENERGIES FROM RENORMALIZATION OF THE LARGE-DIMENSION LIMIT. *Int. J. Quantum Chem.*, 49(5):657–674, 1994.

Abstract: By combining Hartree-Fock results for nonrelativistic ground-state energies of N -electron

atoms with analytic expressions for the large-dimension limit, we have obtained a simple renormalization procedure. For neutral atoms, this yields energies typically threefold more accurate than the Hartree-Fock approximation. Here, we examine the dependence on Z and N of the renormalized energies $E(N, Z)$ for atoms and cations over the range $Z, N = 2 - 290$. We find that this gives for large $Z = N$ an expansion of the same form as the Thomas-Fermi statistical model, $E - Z^{7/3}(C_0 + C(1)Z^{-1/3} + C(2)Z^{-2/3} + C(3)Z^{-3/3} + \dots)$, with similar values of the coefficients for the three leading terms. Use of the renormalized large- D limit enables us to derive three further terms. This provides an analogous expansion for the correlation energy of the for $\Delta E - Z^{4/3}(\Delta C_3 + \Delta C(5)Z^{-2/3} + \Delta C(6)Z^{-3/3} + \dots)$; comparison with accurate values of ΔE available for the range Z less than or equal to 36 indicates the mean error is only about 10%. Oscillatory terms in E and ΔE are also evaluated. (C) 1994 John Wiley & Sons, Inc.

- [332] O. A. Karim. EFFECTIVE-HAMILTONIANS IN THE LARGE- N LIMIT. *Phys. Rev. D*, 28(4):1036–1038, 1983.
- [333] B. M. Karnakov, V. D. Mur, and V. S. Popov. $1/N$ -DECOMPOSITION OF WAVE-FUNCTIONS. *Zhurnal Eksperimentalnoi Teor. Fiz.*, 106(4):976–992, 1994.
- [334] B. M. Karnakov, V. D. Mur, and V. S. Popov. Semiclassical approximation and $1/n$ expansion in quantum-mechanical problems. *Phys. Atom. Nuclei*, 64(4):670–690, 2001.

Abstract: The semiclassical approximation and the technique of $1/n$ expansion are used to calculate the eigenenergies and the wave functions for the radial Schrodinger equation. It is shown that the expressions that are asymptotically exact in the limit $n = n(r) + l + 1 \rightarrow \infty$ and which describe the above eigenenergies and the asymptotic coefficients at the origin and at infinity ensure a satisfactory precision even for states characterized by modest values of the quantum numbers l , and l , including the ground state. (C) 2001 MAIK "Nauka/Interperiodica".

- [335] B. M. Karnakov and S. G. Pozdnyakov. Calculation of wave functions in the subbarrier region using $1/n$ expansion. *Phys. Atom. Nuclei*, 58(12):2088–2095, 1995.

Abstract: A method is developed for calculating wave functions in the subbarrier region on the basis $1/n$ expansion. This method is used to calculate the asymptotic coefficient $c(lp)$ at the origin. To illustrate the accuracy of the method the results are compared with results of numerical calculations for power-law potentials, short-range Yukawa potentials, and exponential potentials. Calculations are performed for node-free states and for states with radial quantum number $p = 1$. The calculated correction of order $1/n$ is shown to considerably increase the accuracy of $1/n$ expansion, especially for $p = 1$ states (at n similar to 1, a zero-order approximation for such states is only an estimate).

- [336] H. A. Kassim and N. S. Al-Maliky. Bound eigenstates in two dimensions for the superposition of the Coulomb and Yukawa potentials by using the shifted $1/N$ method. *J. Phys. B-At. Mol. Opt. Phys.*, 39(14):3057–3071, 2006.

Abstract: The eigenvalue problem for an electron that is moving in a superposition of the attractive Coulomb potential $-A/r$ and the Yukawa potential $Be^{-\lambda r}/r$ is solved by using the shifted $1/N$ method. The calculations of the energy levels have been carried out for both cases of three and the two dimensions. The energy levels for $1s$, $2p(-)$, $3s(-)$, $3p(-)$, $3d(-)$ and $4f(-)$ for the two dimensions case are calculated as a function of the potential strengths A and B and the screening parameter. It is shown that for a given principal quantum number n , the energy eigenvalues increase (decrease) with increasing l for the 3D case and with increasing vertical bar m vertical bar for the 2D and that for $2s$ and $2p(-)$ levels (Lamb shift) is also discussed.

- [337] H. Katsura and H. Aoki. Exact supersymmetry in the relativistic hydrogen atom in general dimensions-supercharge and the generalized Johnson-Lippmann operator. *J. Math. Phys.*, 47(3):7, 2006.

Abstract: A Dirac particle in general dimensions moving in a $1/r$ potential is shown to have an exact

supersymmetry, for which the two supercharge operators are obtained in terms of (a D-dimensional generalization of) the Johnson-Lippmann operator, an extension of the Runge-Lenz-Pauli vector that relativistically incorporates spin degrees of freedom. So the extra symmetry (S(2)) in the quantum Kepler problem, which determines the degeneracy of the levels, is so robust as to accommodate the relativistic case in arbitrary dimensions. (c) 2006 American Institute of Physics.

- [338] S. A. V. Katyurin and O. B. Glinkin. VARIATION ITERATION METHOD FOR ONE-DIMENSIONAL 2-ELECTRON SYSTEMS. *Int. J. Quantum Chem.*, 43(2):251–258, 1992.

Abstract: The variation-iteration method of Svartholm has been applied to the momentum-space Schrodinger equation for one-dimensional two-electron systems. The first and second iteration momentum-space wave functions have been evaluated in analytical forms. The momentum representation of the exact Hartree-Fock ground-state wave function is chosen as the initial function. The influence of electron correlation on the distribution of momentum-space probability density has been studied. It is shown for the one-dimensional McWeeny-Coulson problem that the numerical value of the ground-state energy of the one-dimensional two-electron atom is between the minimum energy values $\epsilon-1/2$ and $\epsilon-1$.

- [339] R. S. Kaushal. SOLUTION OF THE WAVE-EQUATION USING THE $1/N$ EXPANSION AND PERTURBATION-METHODS. *Lettere Al Nuovo Cimento*, 41(13):434–438, 1984.

- [340] D. I. Kazakov and V. S. Popov. On the summation of divergent perturbation series in quantum mechanics and field theory. *J. Exp. Theor. Phys.*, 95(4):581–600, 2002.

Abstract: The possibility of recovering the Gell-Mann-Low function in the asymptotic strong-coupling regime by known first-order perturbation-theory (PT) terms $\beta(n)$ and their asymptotics ($\beta(n)$) over n as $n \rightarrow \infty$ is investigated. Conditions are formulated that are necessary for recovering the required function at the

physical level of rigor: (1) a large number of PT coefficients are known whose asymptotics has already been established, and (2) there is no intermediate asymptotics. Higher orders of PT, their asymptotic behavior, and power corrections are calculated in quantum mechanical problems that involve divergent PT series (including series for a funnel potential, the $\phi^{(0)}(4)$ model, and the Stark effect in a strong field). The scalar field theory $\phi^{(4)}(4)$ is considered in the (MS) over bar and MOM regularization schemes. It is shown that one cannot make any definite conclusion about the asymptotics of the Gell-Mann-Low function as $g \rightarrow \infty$ on the basis of information available for the above theory. (C) 2002 MAIK "Nauka/Interperiodica".

- [341] J. B. Keller. ASYMPTOTIC SOLUTION OF EIGENVALUE PROBLEMS. *Ann. Phys.*, 9(1):24–75, 1960.
- [342] J. Killingbeck. QUANTUM-MECHANICAL PERTURBATION-THEORY. *Rep. Prog. Phys.*, 40(9):963–1031, 1977.
- [343] F. W. King. Progress on high precision calculations for the ground state of atomic lithium. *Theochem-J. Mol. Struct.*, 400:7–56, 1997.

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.

- [344] H. Klar. EQUILIBRIUM ATOMIC-STRUCTURE - ROTATING ATOMS. *Z. Phys. D-Atoms Mol. Clusters*, 3(4):353–358, 1986.

[345] N. A. Kobylinsky, S. S. Stepanov, and R. S. Tutik. NEW SEMICLASSICAL APPROXIMATION FOR QUARKONIA REGGE TRAJECTORIES. *Phys. Lett. B*, 235(1-2):182–186, 1990.

[346] R. D. Koch and J. P. Rodrigues. Systematic $1/N$ corrections for bosonic and fermionic vector models without auxiliary fields. *Phys. Rev. D*, 54(12):7794–7814, 1996.

Abstract: In this paper, colorless bilocal fields are employed to study the large N limit of both fermionic and bosonic vector models. The Jacobian associated with the change of variables from the original fields to the bilocals is computed exactly, thereby providing an exact effective action. This effective action is shown to reproduce the familiar perturbative expansion for the two and four point functions. In particular, in the case of fermionic vector models, the effective action accounts correctly for the Fermi statistics. The theory also is studied nonperturbatively. The stationary points of the effective action are shown to provide the usual large N gap equations. The homogeneous equation associated with the quadratic (in the bilocals) action is simply the two particle Bethe-Salpeter equation. Finally, the leading correction in $1/N$ is shown to be in agreement with the exact S matrix of the model.

[347] A. Konechny and O. T. Turgut. Super-Grassmannian and large N limit of quantum field theory with bosons and fermions. *J. Math. Phys.*, 43(6):2988–3010, 2002.

Abstract: We study a large N -c limit of a two-dimensional Yang-Mills theory coupled to bosons and fermions in the fundamental representation. Extending an approach due to Rajeev we show that the limiting theory can be described as a classical Hamiltonian system whose phase space is an infinite-dimensional super-Grassmannian. The linear approximation to the equations of motion and the constraint yields the 't Hooft equations for the mesonic spectrum. Two other approximation schemes to the exact equations are discussed. (C) 2002 American Institute of Physics.

- [348] V. I. Korobov. Coulomb three-body bound-state problem: Variational calculations of nonrelativistic energies. *Phys. Rev. A*, 61(6):3, 2000.

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.

- [349] V. A. Kostelecky, M. M. Nieto, and D. R. Truax. SUPERSYMMETRY AND THE RELATIONSHIP BETWEEN THE COULOMB AND OSCILLATOR PROBLEMS IN ARBITRARY DIMENSIONS. *Phys. Rev. D*, 32(10):2627–2633, 1985.

- [350] A. V. Koudinov and M. A. Smondyrev. 1/N-EXPANSION FOR THE ANHARMONIC-OSCILLATOR. *Czech. J. Phys.*, 32(5):556–564, 1982.

- [351] R. Krivec. Hyperspherical-harmonics methods for few-body problems. *Few-Body Syst.*, 25(4):199–238, 1998.

Abstract: A review of hyperspherical-harmonics (HH) methods from the standpoint of their applications is given. In the first lecture, the symmetrized and unsymmetrized HH bases and symmetrization methods are presented. The physical obstacles to the straightforward application of the HH expansion are discussed, and expansion acceleration methods are described. In the second lecture, the main HH methods are described, including the correlation function hyperspherical harmonic method (CFHHM), the potential harmonic (PH) methods, and the correlated HH methods (PHH, CHH). The third lecture discusses the advantages and limitations of different HH methods in applications, and

compares the results for specific few-body problems obtained by HH methods as well as non-HH methods.

- [352] A. V. Kudinov and M. A. Smondyrev. QUANTUM-MECHANICAL OSCILLATOR WITH ARBITRARY ANHARMONICITY - $1/N$ EXPANSION AND PERTURBATION-THEORY. *Theor. Math. Phys.*, 56(3):871–878, 1983.
- [353] M. Kumar, A. Srivastava, J. K. Bhattacharjee, and K. Banerjee. MOLECULAR-BINDING IN THE LARGE- N EXPANSION. *Phys. Lett. A*, 117(5):226–228, 1986.
- [354] W. Kutzelnigg. R_{12} -DEPENDENT TERMS IN THE WAVE-FUNCTION AS CLOSED SUMS OF PARTIAL-WAVE AMPLITUDES FOR LARGE- L . *Theor. Chim. Acta*, 68(6):445–469, 1985.
- [355] W. Kutzelnigg. PRESENT AND FUTURE-TRENDS IN QUANTUM CHEMICAL CALCULATIONS. *Theochem-J. Mol. Struct.*, 50(1-2):33–54, 1988.
- [356] G. F. Kventsel and J. Katriel. THOMAS-FERMI ATOM IN N -DIMENSIONS. *Phys. Rev. A*, 24(5):2299–2301, 1981.
- [357] C. H. Lai. PERTURBATIVE RESULTS FROM THE $1/N$ EXPANSION FOR SCREENED COULOMB POTENTIALS. *J. Math. Phys.*, 28(8):1801–1808, 1987.
- [358] W. B. Laing, M. Dunn, and D. K. Watson. Analytic, group-theoretic density profiles for confined, correlated N -body systems. *Phys. Rev. A*, 74(6):13, 2006.

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.

- [359] I. Langmuir. The arrangement of electrons in atoms and molecules. *J. Am. Chem. Soc.*, 41:868–934, 1919.
- [360] J. G. Leopold, I. C. Percival, and A. S. Tworkowski. SEMI-CLASSICAL PERTURBATION-THEORY FOR ENERGY-LEVELS OF PLANETARY ATOMS. *J. Phys. B-At. Mol. Opt. Phys.*, 13(6):1025–1036, 1980.
- [361] G. N. Lewis. The atom and the molecule. *J. Am. Chem. Soc.*, 38:762–785, 1916.
- [362] C. D. Lin and T. Morishita. Few-body problems: The hyperspherical way. *Phys. Essays*, 13(2-3):367–376, 2000.

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.

- [363] D. H. Lin. The path integration of a relativistic particle on a D-dimensional sphere. *J. Phys. A-Math. Gen.*, 30(9):3201–3217, 1997.

Abstract: The fixed-energy amplitude of a relativistic particle near and on the sphere in D dimensions is given by the path integral approach. The Duru-Kleinert equivalence between the project amplitude of a relativistic particle near the surface of spheres in D = 3 and 4 dimensions with the Rosen-Morse and general Rosen-Morse systems are discussed.

- [364] Y. X. Liu, X. H. Zhang, and Y. S. Duan. Detecting extra dimension by helium-like ions. *Mod. Phys. Lett. A*, 23(22):1853–1860, 2008.

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.

- [365] Y. X. Liu, Z. H. Zhao, Y. Q. Wang, and Y. H. Chen. Variational calculations and relativistic corrections to the nonrelativistic ground energies of the helium atom and the helium-like ions. *Acta Phys. Sin.*, 54(6):2620–2624, 2005.

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.

- [366] S. S. Lo and D. A. Morales. A closed-form relation for dimension-dependent two-electron matrix elements of the interelectronic distance. *J. Math. Chem.*, 35(1):21–28, 2004.

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.

- [367] J. G. Loeser. ATOMIC ENERGIES FROM THE LARGE-DIMENSION LIMIT. *J. Chem. Phys.*, 86(10):5635–5646, 1987.
- [368] J. G. Loeser and D. R. Herschbach. DIMENSIONAL INTERPOLATION OF CORRELATION-ENERGY FOR 2-ELECTRON ATOMS. *J. Phys. Chem.*, 89(16):3444–3447, 1985.
- [369] J. G. Loeser and D. R. Herschbach. HARTREE-FOCK APPROXIMATION FOR D-DIMENSIONAL 2-ELECTRON ATOMS. *J. Chem. Phys.*, 84(7):3893–3900, 1986.
- [370] J. G. Loeser and D. R. Herschbach. HILLERAAS-PEKERIS TREATMENT OF D-DIMENSIONAL 2-ELECTRON ATOMS. *J. Chem. Phys.*, 84(7):3882–3892, 1986.
- [371] J. G. Loeser and D. R. Herschbach. DIMENSION DEPENDENCE OF CORRELATION ENERGIES IN 2-ELECTRON ATOMS. *J. Chem. Phys.*, 86(6):3512–3521, 1987.
- [372] J. G. Loeser and D. R. Herschbach. DIMENSIONAL EXPANSIONS FOR 2-ELECTRON ATOMS. *J. Chem. Phys.*, 86(4):2114–2122, 1987.
- [373] J. G. Loeser, J. H. Summerfield, A. L. Tan, and Z. Zheng. CORRELATED ELECTRONIC-STRUCTURE MODELS SUGGESTED BY THE LARGE-DIMENSION LIMIT. *J. Chem. Phys.*, 100(7):5036–5053, 1994.

Abstract: We describe three simple models for electronic structure in many-electron atoms and ions. Each model is parametrized by the spatial dimensionality D , which is ordinarily set to 3. All procedures are motivated by the solution for $D \rightarrow \infty$, a classical limit which can be solved exactly either with or without electron correlation. Each model modifies the $D \rightarrow \infty$ limit treatment to reflect important finite- D effects, but retains the classical character of the limit; the modifications, in order of increasing realism, are designated post-scaling, pre-scaling, and pre-structuring. The three models yield pointlike electronic structures somewhat reminiscent of pre-quantal atomic models. However, all electronic positions have components outside the D -dimensional

physical subspace, a feature which significantly enhances the ability of a localized structure to represent the true solution and to model it quantitatively. Specific calculations reported are total and correlation energies for atoms with Z less-than-or-equal-to 92 (computed by post-scaling and pre-scaling), correlation corrections to ionization potentials and electron affinities for Z less-than-or-equal-to 54 (post-scaling), and the asymptotic behavior of correlation energies for $Z \rightarrow \infty$ (post-scaling).

[374]

J. G. Loeser, Z. Zhen, S. Kais, and D. R. Herschbach. DIMENSIONAL INTERPOLATION OF HARD-SPHERE VIRIAL-COEFFICIENTS. *J. Chem. Phys.*, 95(6):4525–4544, 1991.

Abstract: We examine the dependence on spatial dimension D of the Mayer cluster integrals that determine the virial coefficients $B(n)$ for a fluid of rigid hyperspheres. The integrals vary smoothly with D , and can be characterized analytically in both the low- D and high- D limits. Dimensional interpolation (DI) allows one to evaluate individual Mayer cluster integrals at $D = 2$ and $D = 3$ to within about 1%. The resulting low-order virial coefficients have an accuracy intermediate between those of the Percus-Yevick and hypernetted chain approximations. Much higher accuracy can be achieved by combining the DI and HNC approximations, using DI to evaluate those integrals omitted by HNC. The resulting low-order virial coefficients are more accurate than those given by any existing integral equation approximation. At higher order, the accuracy of the individual cluster integrals is insufficient to compute reliable virial coefficients from the Mayer expansion. Reasonably accurate values can still be computed, however, by taking partial sums of the Ree-Hoover reformulation of the Mayer expansion. We report hard disk virial coefficients through B_{15} and hard sphere values through B_{10} ; the maximum errors with respect to known values are about 1.2 and 4.3%, respectively. The new coefficients are in good agreement with those obtained by expanding certain equations of state which fail to diverge until unphysical densities (those beyond closest packing),

and so help to explain the surprising accuracy of some of these equations. We discuss the possibility that the exact virial expansion has a radius of convergence which corresponds to an unphysical density. Several new equations of state with desirable analytic or representational characteristics are also reported.

- [375] M. Lopezcabrera, D. Z. Goodson, D. R. Herschbach, and J. D. Morgan. LARGE-ORDER DIMENSIONAL PERTURBATION-THEORY FOR H₂⁺. *Phys. Rev. Lett.*, 68(13):1992–1995, 1992.

Abstract: An asymptotic expansion for the electronic energy of H-2(+) is developed in inverse powers of D, the spatial dimension, and the singularity structure in the D \rightarrow infinity limit is elucidated by analysis of the coefficients at large order (approximately 30 to 45). For the ground state and several excited states, Pade-Borel summation yields an accuracy of eight or more significant figures.

- [376] M. Lopezcabrera, A. L. Tan, and J. G. Loeser. SCALING AND INTERPOLATION FOR DIMENSIONALLY GENERALIZED ELECTRONIC-STRUCTURE. *J. Phys. Chem.*, 97(10):2467–2478, 1993.

Abstract: Simple electronic structure problems generalized with respect to the spatial dimensionality D have two singular limits, D \rightarrow 1 and D \rightarrow infinity. Suitable scalings render the limiting solutions finite and reveal their complementary characters: D \rightarrow 1 gives point (delta function) interactions between particles, while D \rightarrow infinity yields point probability distributions between those particles. A single scaling that treats both limits simultaneously allows one to construct approximate D = 3 solutions by interpolation between the much simpler limits. In this paper we show how to construct and utilize such a uniform scaling. We construct the scaling, solve the limits, and interpolate to D = 3 for six model problems: Yukawa potential, hydrogen atom in a spherical cavity, H-2⁺, Hartree-Fock H-2, and Hartree-Fock two-electron atoms in weak magnetic and electric fields. The interpolated D = 3 energies and properties are typically accurate to

within a few percent, except for cases where the $D \rightarrow \infty$ limit gives multiple or unstable solutions. Extensions and improvements are also discussed.

- [377] J. D. Louck. GENERALIZED ORBITAL ANGULAR MOMENTUM AND THE N-FOLD DEGENERATE QUANTUM-MECHANICAL OSCILLATOR .2. THE N-FOLD DEGENERATE OSCILLATOR. *J. Mol. Spectrosc.*, 4(4):298–333, 1960.
- [378] J. D. Louck. GENERALIZED ORBITAL ANGULAR MOMENTUM AND THE N-FOLD DEGENERATE QUANTUM-MECHANICAL OSCILLATOR .3. RADIAL INTEGRALS. *J. Mol. Spectrosc.*, 4(4):334–341, 1960.
- [379] J. D. Louck and W. H. Shaffer. GENERALIZED ORBITAL ANGULAR MOMENTUM AND THE N-FOLD DEGENERATE QUANTUM-MECHANICAL OSCILLATOR .1. THE TWOFOLD DEGENERATE OSCILLATOR. *J. Mol. Spectrosc.*, 4(4):285–297, 1960.
- [380] Y. E. Lozovik, V. D. Mur, and N. B. Narozhnyi. $1/Q$ expansion for the energy spectrum of quantum dots. *J. Exp. Theor. Phys.*, 96(5):932–939, 2003.

Abstract: A new method is proposed for calculating the energy spectrum and the wave functions of N - electron quantum dots with an arbitrary confining potential. The method consists in expansion with respect to a dimensionless quantum parameter $1/Q$, which is expressed in terms of the ratio of the characteristic Coulomb energy of electron - electron interaction to the characteristic energy of one- particle transition in a confining potential. Two- electron quantum dots with a parabolic confining potential in an external magnetic field are considered. Strongly correlated states of the system and the spin rearrangement in a strong magnetic field are analyzed. Analytic expressions are obtained for the energy and the wave functions of the system. It is shown that restriction of the analysis only to the first three terms in the quantum-parameter expansion gives an accuracy of one percent when calculating the energy even for values of Q on the order of unity, i. e., for the presently implementable GaAs quantum dots. The expressions for energy obtained are in a good agreement with the experimental data for quantum dots in

a perpendicular magnetic field. (C) 2003 MAIK ”
Nauka/ Interperiodica”.

- [381] J. Lu. Analytic quantum mechanics of diatomic molecules with empirical potentials. *Phys. Scr.*, 72(5):349–352, 2005.

Abstract: The Schrodinger equations of diatomic molecules with empirical potential functions are solved approximately by means of the hypergeometric series method. The potential functions may fit the experimental Rydber-Klein-Rees curve more closely than the Morse function. Rigorous solutions of Schrodinger equations are also obtained with a similar method for zero total angular momentum. The eigenfunctions of diatomic molecules, expressed in terms of Jacobi polynomial, are employed as the orthonormal basis sets, and analytic expressions of matrix elements for the position and momentum operators are given in closed form.

- [382] M. A. Luty. BARYONS WITH MANY COLORS AND FLAVORS. *Phys. Rev. D*, 51(5):2322–2331, 1995.

- [383] Z. Q. Ma, S. H. Dong, X. Y. Gu, J. A. Yu, and M. Lozada-Cassou. The Klein-Gordon equation with a coulomb plus scalar potential in D dimensions. *Int. J. Mod. Phys. E-Nucl. Phys.*, 13(3):597–610, 2004.

Abstract: The solutions of the Klein-Gordon equation with a Coulomb plus scalar potential in D dimensions are exactly obtained. The energy $E(n, l, D)$ is analytically presented and the dependence of the energy $E(n, l, D)$ on the dimension D is analyzed in some detail. The positive energy $E(n, 0, D)$ first decreases and then increases with increasing dimension D. The positive energy $E(n, l, D)$ (l not equal 0) increases with increasing dimension D. The dependences of the negative energies $E(n, 0, D)$ and $E(n, l, D)$ (l not equal 0) on the dimension D are opposite to those of the corresponding positive energies $E(n, 0, D)$ and $E(n, l, D)$ (l not equal 0). It is found that the energy $E(n, 0, D)$ is symmetric with respect to $D = 2$ for D is an element of $(0, 4)$. It is also found that the energy $E(n, l, D)$ (l not equal 0) is almost independent of the angular momentum quantum number l for large D and is completely independent of the angular momentum quantum number l if the Coulomb potential

is equal to the scalar one. The energy $E(n, l, D)$ is almost overlapping for large D .

- [384] G. H. Machtoub. New approach to three-body Coulomb problem with nonzero total angular momentum. *Int. J. Mod. Phys. C*, 12(6):835–850, 2001.

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 $\text{He}+$.

- [385] M. J. Maeso, J. R. Solana, J. Amoros, and E. Villar. EQUATIONS OF STATE FOR D-DIMENSIONAL HARD-SPHERE FLUIDS. *Mater. Chem. Phys.*, 30(1):39–42, 1991.

Abstract: An equation of state, a kind of generalized Pade approximant, first proposed for the hard-sphere fluid in three dimensions is extended to the two-, four-, and five-dimensional cases in addition to the trivial one-dimensional case (hard rods). The corresponding equations of state show good to excellent agreement with existing simulation data.

- [386] J. Makarewicz. 2 PARTICLES ON A SPHERE AS A RIGID-BENDER MODEL OF THE HELIUM ATOM. *Phys. Lett. A*, 121(2):83–86, 1987.

- [387] Y. M. Makeenko. LARGE N . *Lecture Notes in Physics*, 181:67–105, 1983.

- [388] S. A. Maluendes, F. M. Fernandez, and E. A. Castro. MODIFIED $1/N$ EXPANSION. *Phys. Lett. A*, 124(4-5):215–219, 1987.

- [389] S. A. Maluendes, F. M. Fernandez, and E. A. Castro. MODIFIED LARGE-N EXPANSION. *Phys. Rev. A*, 36(3):1452–1453, 1987.
- [390] S. A. Maluendes, F. M. Fernandez, A. M. Meson, and E. A. Castro. LARGE-ORDER SHIFTED $1/N$ EXPANSIONS. *Phys. Rev. D*, 34(6):1835–1839, 1986.
- [391] G. Mandal, S. J. Rey, and S. R. Wadia. Quantum aspects of GMS solutions of non-commutative field theory and large N limit of matrix models. *Eur. Phys. J. C*, 24(3):495–514, 2002.
- Abstract:** We investigate quantum aspects of Gopakumar-Minwalla-Strominger (GMS) solutions of non-commutative field theory (NCFT) in the large non-commutativity limit, $\theta \rightarrow \infty$. Building upon a quantitative map between the operator formulation of 2- (respectively, $(2 + 1)$ -) dimensional NCFTs and large-N matrix models of $c = 0$ (respectively, $c = 1$) non-critical strings, we show that GMS solutions are quantum mechanically sensible only if we make an appropriate joint scaling of θ and N. For 't Hooft's scaling, GMS solutions are replaced by large-N saddle-point solutions. GMS solutions are recovered from saddle-point solutions in the small 't Hooft coupling regime, but are destabilized in the large 't Hooft coupling regime by quantum effects. We make comparisons between these large-N effects and the recently studied infrared effects in NCFTs. We estimate the $U(N)$ symmetry breaking effects of the gradient term and argue that they are suppressed only in the small 't Hooft coupling regime.
- [392] N. H. March. ASYMPTOTIC RELATION BETWEEN EIGENVALUE SUM AND CHEMICAL-POTENTIAL FOR ELECTRONS MOVING IN BARE POINT-CHARGE POTENTIALS IN D-DIMENSIONS. *Phys. Rev. A*, 30(6):2936–2939, 1984.
- [393] N. H. March. SCALING PROPERTIES OF TOTAL ENERGY OF HEAVY POSITIVE-IONS IN D-DIMENSIONS. *J. Math. Phys.*, 26(3):554–555, 1985.
- [394] N. H. March. DIMENSIONALITY DEPENDENCE OF ENERGY OF HEAVY POSITIVE-IONS AND THE $1/Z$ EXPANSION. *Phys. Rev. A*, 34(6):5106–5107, 1986.

[395] N. H. March. Semiclassical theory of atoms and molecules in intense external fields. In *Atoms and Molecules in Intense Fields*, volume 86 of *Structure and Bonding*, pages 63–96. Springer-Verlag Berlin, Berlin 33, 1997.

[396] N. Marshall, G. W. Semenoff, and R. J. Szabo. CRITICAL-BEHAVIOR OF A FERMIONIC RANDOM-MATRIX MODEL AT LARGE-N. *Phys. Lett. B*, 351(1-3):153–161, 1995.

Abstract: We study the large-N limit of adjoint fermion one-matrix models. We find one-cut solutions of the loop equations for the correlators of these models and show that they exhibit third order phase transitions associated with m-th order multi-critical points with string susceptibility exponents $\gamma(\text{str}) = -1/m$. We also find critical points which can be interpreted as points of first order phase transitions, and we discuss the implications of this critical behaviour for the topological expansion of these matrix models.

[397] M. Masili, J. E. Hornos, and J. J. Degroote. HYPER-SPHERICAL ADIABATIC APPROACH FOR THE HELIUM ATOM. *Phys. Rev. A*, 52(4):3362–3365, 1995.

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.

[398] V. P. Maslov and O. Y. Shvedov. Large-N expansion as a semiclassical approximation to the third-quantized theory. *Phys. Rev. D*, 60(10):4, 1999.

Abstract: The semiclassical theory for the large-N field models is developed from an unusual point of view. Analogously to the procedure of the second quantization in quantum mechanics, the functional Schrodinger large-N equation is presented in

a third-quantized form. The third-quantized creation and annihilation operators depend on the field $\phi(x)$. If the coefficient of the ϕ^4 term is of order $1/N$ (this is the usual condition of applicability of the $1/N$ expansion), one can rescale the third-quantized operators in such a way that their commutator will be small, while the Heisenberg equations will not contain large or small parameters. This means that the classical equation of motion is an equation on the functional $\Phi[\phi(\cdot)]$. This equation, being a nonlinear analogue of the functional Schrödinger equation for the one-field theory, is investigated. The exact solutions are constructed and the renormalization problem is analyzed. We also perform a quantization procedure about found classical solutions. The corresponding semiclassical theory is a theory of a variable number of fields. The developed third-quantized semiclassical approach is applied to the problem of finding the large- N spectrum. The results are compared with formulas obtained by known methods. We show that not only the known but also new energy levels can be found. [S0556-7821(99)00613-8].

- [399] P. A. Massaro. DARBOUX FUNCTIONS AND PERTURBATIVE THEORY FOR GROUND-STATE ENERGY OF 2-ELECTRON ATOMS. *J. Phys. B-At. Mol. Opt. Phys.*, 10(3):391–398, 1977.
- [400] T. Matsui, H. Kleinert, and S. Ami. 2-LOOP EFFECTIVE ACTION OF $O(N)$ SPIN MODELS IN $1/D$ EXPANSION. *Phys. Lett. B*, 143(1-3):199–206, 1984.
- [401] B. A. McKinney, M. Dunn, and D. K. Watson. Beyond-mean-field results for atomic Bose-Einstein condensates at interaction strengths near Feshbach resonances: A many-body dimensional perturbation-theory calculation. *Phys. Rev. A*, 69(5):15, 2004.

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 $a=0.433a(\hbar\omega)$ ($a(\hbar\omega)=\sqrt{\hbar}$ over $\bar{m}\omega(\hbar\omega)$) 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 $D \rightarrow \infty$ 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 $\kappa = D + 2/1$, 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.

- [404] B. A. McKinney and D. K. Watson. Bose-Einstein condensation in variable dimensionality. *Phys. Rev. A*, 65(3):7, 2002.

Abstract: We introduce dimensional perturbation techniques to Bose-Einstein condensation of inhomogeneous alkalimetal gases. The perturbation parameter is $\delta = 1/\kappa$, where κ 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 $N \rightarrow \infty$ 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.

- [405] L. R. Mead and N. Papanicolaou. GENERALIZED HOLSTEIN-PRIMAKOFF THEORY FOR ANHARMONIC LATTICES. *J. Phys. A-Math. Gen.*, 16(17):4135–4146, 1983.
- [406] L. R. Mead and N. Papanicolaou. HOLSTEIN-PRIMAKOFF THEORY FOR MANY-BODY SYSTEMS. *Phys. Rev. B*, 28(3):1633–1636, 1983.
- [407] C. Micu and E. Papp. Applying the $1/N$ -energy solution of the Harper equation to the derivation of thermodynamic properties of Bloch electrons. *Int. J. Mod. Phys. B*, 12(32):3503–3520, 1998.

Abstract: The novel $1/N$ -energy solution to the Harper equation presented recently is applied to the derivation of thermodynamic properties of Bloch electrons on a two-dimensional lattice penetrated by a perpendicular uniform magnetic field. One proceeds by using an almost typical density of states such as proposed previously for a two-dimensional electron gas. Comparisons with recent data concerning rare earth compounds as well as with results obtained before with the help of Dingle- and quantum-gas densities are done. One assumes that the Fermi level is fixed.

- [408] C. Micu and E. Papp. The derivation of $1/N$ energy-solutions to the Harper-equation and related magnetizations. *Int. J. Mod. Phys. B*, 12(18):1847–1870, 1998.

Abstract: Proofs are given for the first time that the energy-spectrum of the Harper-equation can be derived in a closed implicit form by using the one-dimensional limit of the $1/N$ -description. Explicitly solvable cases are discussed in some more detail for $\Delta = 1$. Here Δ expresses the Harper-parameter discriminating between metallic ($\Delta \geq 1$) and insulator ($\Delta < 1$) phases. Related magnetizations have been established by applying both Dingle- and quantum-gas approaches, now for a fixed value of the Fermi-level. The first description leads to large paramagnetic-like magnetizations oscillating with nearly field-independent amplitudes increasing with the temperature. In the second case one deals with magnetization-oscillations centered around the zero-value, such that the amplitudes decrease both with the field and the temperature.

- [409] A. A. Migdal. LOOP EQUATIONS AND $1/N$ EXPANSION. *Phys. Rep.-Rev. Sec. Phys. Lett.*, 102(4):201–290, 1983.
- [410] K. A. Milton. Vector Casimir effect for a D-dimensional sphere. *Phys. Rev. D*, 55(8):4940–4946, 1997.

Abstract: The Casimir energy or stress due to modes in a D-dimensional volume subject to TM (mixed) boundary conditions on a bounding spherical surface is calculated. Both interior and exterior modes are included. Together with earlier results found for scalar modes (TE modes), this gives the Casimir effect for fluctuating "electromagnetic" (vector) fields inside and outside a spherical shell. Known results for three dimensions, first found by Boyer, are reproduced. Qualitatively, the results for TM modes are similar to those for scalar modes: Poles occur in the stress at positive even dimensions, and cusps (logarithmic singularities) occur for integer dimensions D less than or equal to 1. Particular attention is given the interesting case of $D = 2$.

- [411] J. L. Miramontes and C. Pajares. ON THE LARGE-N LIMITS OF RELATIVISTIC-EQUATIONS. *Nouvo Cimento Soc. Ital. Fis. B-Gen. Phys. Relativ. Astron. Math. Phys. Methods*, 84(1):10–18, 1984.
- [412] L. D. Mlodinow and N. Papanicolaou. $SO(2,1)$ ALGEBRA AND THE LARGE N EXPANSION IN QUANTUM-MECHANICS. *Ann. Phys.*, 128(2):314–334, 1980.
- [413] L. D. Mlodinow and N. Papanicolaou. PSEUDO-SPIN STRUCTURE AND LARGE N-EXPANSION FOR A CLASS OF GENERALIZED HELIUM HAMILTONIANS. *Ann. Phys.*, 131(1):1–35, 1981.
- [414] L. D. Mlodinow and M. P. Shatz. SOLVING THE SCHRÖDINGER-EQUATION WITH USE OF $1/N$ PERTURBATION-THEORY. *J. Math. Phys.*, 25(4):943–950, 1984.
- [415] H. E. Montgomery, N. A. Aquino, and K. D. Sen. Degeneracy of confined D-dimensional harmonic oscillator. *Int. J. Quantum Chem.*, 107(4):798–806, 2007.

Abstract: Using the mathematical properties of the confluent hypergeometric functions, the conditions for the incidental, simultaneous, and

interdimensional degeneracy of the confined D-dimensional ($D \geq 1$) harmonic oscillator energy levels are derived, assuming that the isotropic confinement is defined by an infinite potential well and a finite radius R-c. Very accurate energy eigenvalues are obtained numerically by finding the roots of the confluent hypergeometric functions that confirm the degeneracy conditions. (c) 2006 Wiley Periodicals, Inc.

[416] D. A. Morales. ENERGY EIGENSTATES OF THE ROTATING MORSE OSCILLATOR USING THE SHIFTED $1/N$ EXPANSION. *Chem. Phys. Lett.*, 161(3):253–258, 1989.

[417] D. A. Morales. Analytical formulas for the eigenvalues and eigenfunctions of a d-dimensional hydrogen atom with a potential defined by Gauss' law. *Int. J. Quantum Chem.*, 57(1):7–15, 1996.

Abstract: The solution of the Schrodinger equation for the d-dimensional hydrogen atom in a d-dependent potential defined by Gauss' law has been studied by the shifted $1/d$ method and the delta expansion. These methods provide analytical formulas for the eigenvalues and eigenfunctions which have been tested against "exact" numerical values obtained recently. The comparison shows that the results obtained with the analytical expressions are in excellent accord with the numerical ones and, on the other hand, provide a theoretical justification for a proposed empirical expression for the energies of the two-dimensional hydrogen atom with a logarithmic potential energy function. (C) 1996 John Wiley & Sons, Inc.

[418] D. A. Morales and Z. Parra-Mejias. On the relationship between anharmonic oscillators and perturbed Coulomb potentials in N dimensions. *Can. J. Phys.*, 77(11):863–871, 1999.

Abstract: The relation between the perturbed Coulomb problem in N dimensions and the sextic anharmonic oscillator in N' dimensions is presented and generalized in this work. We show that by performing a transformation, containing a free parameter, on the equations for the two problems we can relate the two systems in dimensions that have not been previously linked. Exact solutions can be obtained for the N-dimensional systems from

known three-dimensional solutions of the two problems. Using the known ground-state wave functions for these systems, we construct supersymmetric partner potentials that allow us to apply the supersymmetric large- N expansion to obtain accurate approximate energy eigenvalues.

- [419] G. Moreno and A. Zepeda. 1- N EXPANSION FOR A YUKAWA POTENTIAL. *J. Phys. B-At. Mol. Opt. Phys.*, 17(1):21–27, 1984.
- [420] V. K. Mukhomorov. VIBRATIONAL EIGENSTATES OF ADIABATIC AND STRONG-COUPLED CONTINUUM BIPOLARON - METHOD OF DISPLACED 1- N EXPANSION. *Opt. Spektrosk.*, 74(2):242–256, 1993.
- [421] V. D. Mur and V. S. Popov. 1/ N EXPANSION AND WAVE-FUNCTIONS. *Jetp Lett.*, 45(7):410–413, 1987.
- [422] V. D. Mur and V. S. Popov. THE 1/ N EXPANSION AND WAVE-FUNCTIONS. *Soviet Journal of Nuclear Physics-Ussr*, 47(3):444–449, 1988.
- [423] V. D. Mur and V. S. Popov. SCALING FOR THE STARK-EFFECT IN THE RYDBERG ATOMS. *Jetp Lett.*, 48(2):70–74, 1988.
- [424] V. D. Mur and V. S. Popov. THE 1/ N -EXPANSION AND COHERENT STATES. *Zhurnal Eksperimentalnoi Teor. Fiz.*, 97(6):1729–1740, 1990.
- [425] V. D. Mur and V. S. Popov. PERTURBATION-THEORY FOR QUASI-STATIONARY STATES. *Phys. Atom. Nuclei*, 58(8):1329–1341, 1995.

Abstract: Perturbation theory (to the first order) for quasistationary states is developed in the semiclassical approximation. Formulas for the energy shift ΔE , of a resonance, as well as for the variation of its width $\Delta \Gamma$ due to a perturbative potential ΔU , are obtained. These formulas are valid both for subbarrier and above barrier resonances. The results are illustrated using a number of potentials for which semiclassical expressions can be compared with exact solutions of the Schrodinger equation. The proposed scheme is generalized to a multidimensional case with completely separating variables.

- [426] V. D. Mur, V. S. Popov, and A. V. Sergeev. GENERALIZATION OF THE GAMOW FORMULA TO THE MULTIDIMENSIONAL CASE. *Soviet Journal of Nuclear Physics-Ussr*, 54(4):575–581, 1991.
- Abstract:** A generalization of the Gamow formula for the width GAMMA of a quasistationary level (with energy $E = E(r) - i\text{GAMMA}/2$) is given for the case of multidimensional systems with separable variables. The condition for applicability of this approximation is obtained, and some examples are considered.
- [427] V. D. Mur, V. S. Popov, A. V. Sergeev, and A. V. Shcheblykin. STARK RESONANCES AND SCALING IN RYDBERG ATOMS. *Zhurnal Eksperimentalnoi Teor. Fiz.*, 96(1):91–106, 1989.
- [428] V. D. Mur, V. S. Popov, and A. V. Sergeyev. THE 1/N-EXPANSION IN QUANTUM-MECHANICS. *Zhurnal Eksperimentalnoi Teor. Fiz.*, 97(1):32–46, 1990.
- [429] V. D. Mur, S. G. Pozdnyakov, and V. S. Popov. 1/N-EXPANSION AND WAVE-FUNCTION CALCULATION. *Doklady Akademii Nauk Sssr*, 303(5):1102–1107, 1988.
- [430] V. D. Mur, S. G. Pozdnyakov, and V. S. Popov. 1/N EXPANSION AND WAVE-FUNCTIONS. *Soviet Journal of Nuclear Physics-Ussr*, 51(2):249–252, 1990.
- [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.
- [432] O. Mustafa. THE SHIFTED-1 N-EXPANSION METHOD FOR 2-DIMENSIONAL HYDROGENIC DONOR STATES IN AN ARBITRARY MAGNETIC-FIELD. *J. Phys.-Condes. Matter*, 5(9):1327–1332, 1993.

Abstract: The shifted-1/N-expansion method has been used to study the energy levels for a 2D donor impurity in the presence of an arbitrary magnetic field. Exact analytical expressions for the energy levels at zero- and high-field limits are obtained. The calculations are carried out to the third-order correction of the shifted-1/N-expansion energy series. The results appear to be in excellent agreement with those of Martin et al.

- [433] O. Mustafa. Reply to comment 'On large-N expansion'. *J. Phys. A-Math. Gen.*, 35(49):10671–10673, 2002.

Abstract: Fernandez comments [1] on our pseudo-perturbative shifted-l expansion technique [2, 3] is either unfounded or ambiguous.

- [434] O. Mustafa and T. Barakat. Nonrelativistic shifted-l expansion technique for three- and two-dimensional Schrodinger equation. *Commun. Theor. Phys.*, 28(3):257–264, 1997.

Abstract: The shifted-l expansion techniques (SLET) has been developed to get eigenvalues of Schrodinger equation in three (3D) and two dimensions (2D). SLET simply consists of $1/(l)$ over bar as a perturbation parameter, where (l) over bar = $l - \beta$. β is a suitable shift, l is the angular-momentum quantum number for the 3D-case, $l = m$ for the 2D-case, and m is the magnetic quantum number. Unlike the shifted large-N expansion theory (SLNT), SLET seems to be applicable to a wider number of problems of significant interest in physics.

- [435] O. Mustafa and T. Barakat. Relativistic shifted-l expansion technique for Dirac and Klein-Gordon equations. *Commun. Theor. Phys.*, 29(4):587–594, 1998.

Abstract: The shifted-l expansion technique (SLET) is extended to solve for Dirac particle trapped in spherically symmetric scalar and/or 4-vector potentials. A parameter $\lambda = 0, 1$ is introduced in such a way that one can obtain the Klein-Gordon (KG) bound states from Dirac bound states. The I-vector Coulomb, the scalar linear, and the equally mixed scalar and 4-vector power-law potentials are used in KG and Dirac equations. Exact numerical results are obtained for

the Q-vector Coulomb potential in both KG and Dirac equations. Highly accurate and fast converging results are obtained for the scalar linear and the equally mixed scalar and 4-vector power-law potentials.

- [436] O. Mustafa and S. C. Chhajlany. GROUND-STATE ENERGIES OF HYDROGENIC ATOMS IN A UNIFORM MAGNETIC-FIELD OR ARBITRARY STRENGTH. *Phys. Rev. A*, 50(4):2926–2929, 1994.

Abstract: The ground-state energies of hydrogenic atoms in a uniform magnetic field of arbitrary strength have been calculated accurately. A claim relating the energy eigenvalues of the nonseparable Hamiltonian $H = -\Delta^2/2 - Z/r + \lambda^2(x^2 + y^2)/2$ to those of the spherically symmetric Hamiltonian $H' = -\Delta^2/2 - Z/r + \lambda^2 r^2/2$ has been introduced and justified at the weak- and strong-magnetic-field limits. Moreover, the shifted $1/N$ expansion technique has been used to calculate the energy eigenvalues of H' .

- [437] O. Mustafa and S. H. Mazharimousavi. d-dimensional generalization of the point canonical transformation for a quantum particle with position-dependent mass. *J. Phys. A-Math. Gen.*, 39(33):10537–10547, 2006.

Abstract: The d-dimensional generalization of the point canonical transformation for a quantum particle endowed with a position-dependent mass in the Schrodinger equation is described. Illustrative examples including the harmonic oscillator, Coulomb, spiked harmonic, Kratzer, Morse oscillator, Poschl-Teller and Hulthen potentials are used as reference potentials to obtain exact energy eigenvalues and eigenfunctions for target potentials at different position-dependent mass settings.

- [438] O. Mustafa and S. H. Mazharimousavi. Quantum particles trapped in a position-dependent mass barrier; a d-dimensional recipe. *Phys. Lett. A*, 358(4):259–261, 2006.

Abstract: We consider a free particle. $V(r) = 0$, with a position-dependent mass $m(r) = 1/(1 + \sigma^2 r^2)$ in the d-dimensional Schrodinger equation. The effective potential turns out to be a generalized Poschl-Teller potential that admits

exact solution. (c) 2006 Elsevier B.V. All rights reserved.

- [439] O. Mustafa and M. Odeh. Part of the D-dimensional spiked harmonic oscillator spectra. *J. Phys. A-Math. Gen.*, 33(29):5207–5217, 2000.

Abstract: The pseudoperturbative shifted-l expansion technique (PSLET) is generalized for states with an arbitrary number of nodal zeros. Interdimensional degeneracies, emerging from the isomorphism between the angular momentum and the dimensionality of the central force Schrodinger equation, are used to construct part of the D-dimensional spiked harmonic oscillator bound-state spectra. PSLET results are found to compare excellently with those from direct numerical integration and generalized variational methods.

- [440] O. Mustafa and M. Odeh. 2D H-atom in an arbitrary magnetic field via pseudoperturbation expansions through the quantum number l. *Commun. Theor. Phys.*, 33(3):469–476, 2000.

Abstract: The pseudoperturbative shifted-l expansion technique is introduced to determine nodeless states of the 2D Schrodinger equation with arbitrary cylindrically symmetric potentials. Exact energy eigenvalues and eigenfunctions for the 2D Coulomb and harmonic oscillator potentials are reproduced. Moreover, exact energy eigenvalues, compared with those obtained by numerical solution (V.M. Villalba and R. Pine, *J. Phys.: Condens. Matter* 8 (1996) 8067), were obtained for the hybrid of the 2D Coulomb and oscillator potentials.

- [441] O. Mustafa and M. Odeh. Anharmonic oscillators energies via artificial perturbation method. *Eur. Phys. J. B*, 15(1):143–148, 2000.

Abstract: A new pseudoperturbative (artificial in nature) methodical proposal [15] is used to solve for Schrodinger equation with a class of phenomenologically useful and methodically challenging anharmonic oscillator potentials $V(q) = \alpha(o)q(2) + \alpha q(4)$. The effect of the [4, 5] Pade approximant on the leading eigenenergy term is stud-

ied. Comparison with results from numerical (exact) and several eligible (approximation) methods is made.

- [442] O. Mustafa and M. Odeh. Energy levels of neutral atoms via a new perturbation method. *Czech. J. Phys.*, 51(3):199–210, 2001.

Abstract: The energy levels of neutral atoms supported by potential $V(r) = -Z \exp(-\alpha r)/r$ (Yukawa potential) are studied, using both dimensional and dimensionless quantities, via a new analytical methodical proposal (devised to solve for nonexactly solvable Schrodinger equation). Using dimensionless quantities, by scaling the radial Hamiltonian through γZr and $\alpha' = \alpha / Z$, we report that the scaled screening parameter α' is restricted to have values ranging from zero to less than 0.4. On the other hand, working with the scaled Hamiltonian enhances the accuracy and extremely speeds up the convergence of the energy eigenvalues. The energy levels of several new eligible scaled screening parameter α' values are also reported.

- [443] O. Mustafa and R. Sever. APPROACH TO THE SHIFTED $1/N$ EXPANSION FOR THE KLEIN-GORDON EQUATION. *Phys. Rev. A*, 43(11):5787–5789, 1991.

Abstract: A different approach to the shifted $1/N$ expansion technique is developed to deal with the Klein-Gordon particle trapped in a spherically symmetric potential. Properly modifying the definition of the perturbative expansion of the energy eigenvalue, and without making any approximation in the determination of the parameters involved, we obtain sufficiently good results compared with the exact ones for the Coulomb problem. The calculations are carried out to the second-order correction of the energy series.

- [444] O. Mustafa and R. Sever. SHIFTED $1/N$ EXPANSION FOR THE KLEIN-GORDON EQUATION WITH VECTOR AND SCALAR POTENTIALS. *Phys. Rev. A*, 44(7):4142–4144, 1991.

Abstract: The shifted $1/N$ expansion method has been extended to solve the Klein-Gordon equation

with both scalar and vector potentials. The calculations are carried out to the third-order correction in the energy series. The analytical results are applied to a linear scalar potential to obtain the relativistic energy eigenvalues. Our numerical results are compared with those obtained by Gunion and Li [Phys. Rev. D 12, 3583 (1975)].

- [445] O. Mustafa and R. Sever. APPROACH TO THE SHIFTED $1/N$ EXPANSION FOR SPIN-1/2 RELATIVISTIC PARTICLE. *Journal of Quantitative Spectroscopy & Radiative Transfer*, 49(1):65–69, 1993.

Abstract: A different approach to the shifted $1/N$ expansion method is developed to deal with the Dirac particle trapped in a spherically symmetric potential. The main aspects of our approach are to expand the energy term in a perturbative form and to determine the parameters involved without any approximation. While the formalism is developed for spin-1/2 particles in any spherically symmetric potential, it is applied to the Coulomb case for testing. The calculations are carried out to the third-order correction of the energy eigenvalue series.

- [446] M. K. Nandy. Kolmogorov constant in large space dimensions. *Int. J. Mod. Phys. B*, 16(32):4839–4845, 2002.

Abstract: A large d (space dimension) expansion together with the epsilon-expansion is implemented to calculate the Kolmogorov constant from the energy equation of Kraichnan's direct-interaction approximation using the Heisenberg's eddy-viscosity approximation and Kraichnan's distant-interaction algorithm. The Kolmogorov constant C is found to be $C = C(0)d(1/3)$ in the leading order of a $1/d$ expansion. This is consistent with Fournier, Frisch, and Rose. The constant C_0 evaluated in the above scheme, is found to be $C_0 = (16/27)(1/3)$.

- [447] J. P. Neirotti, P. Serra, and S. Kais. Critical parameters for the heliumlike atoms: A phenomenological renormalization study. *J. Chem. Phys.*, 108(7):2765–2770, 1998.

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, $\lambda(c) = 1/Z(c) = 1.0976 \pm 0.0004$, as well as for the excited $2p(2) P-3$ state, $\lambda(c) = 1.0058 \pm 0.0017$. The results for the critical exponents α and ν are also included. (C) 1998 American Institute of Physics.

[448] M. M. Nieto. HYDROGEN-ATOM AND RELATIVISTIC PI-MESIC ATOM IN N-SPACE DIMENSIONS. *Am. J. Phys.*, 47(12):1067–1072, 1979.

[449] M. M. Nieto. Existence of bound states in continuous $0 \leq D < \infty$ dimensions. *Phys. Lett. A*, 293(1-2):10–16, 2002.

Abstract: In modern fundamental theories there is consideration of higher dimensions, often in the context of what can be written as a Schrodinger equation. Thus, the energetics of bound states in different dimensions is of interest. By considering the quantum square well in continuous D dimensions, it is shown that there is always a bound state for $0 \leq D < 2$. This binding is complete for $D \rightarrow 0$ and exponentially small for $D \rightarrow 2^-$. For $D \geq 2$, a finite-sized well is always needed for there to be a bound state. This size grows like D^{-2} as D gets large. By adding the proper angular momentum tail, a volcano, zero-energy, bound state can be obtained. (C) 2002 Elsevier Science B.V. All rights reserved.

[450] M. P. Nightingale and M. Moodley. Interdimensional degeneracies in van der Waals clusters and quantum Monte Carlo computation of rovibrational states. *J. Chem. Phys.*, 123(1):7, 2005.

Abstract: Quantum Monte Carlo estimates of the spectrum of rotationally invariant states of noble gas clusters suggest interdimensional degeneracy in $N-1$ and $N+1$ spatial dimensions. We derive this property by mapping the Schrodinger eigenvalue problem onto an eigenvalue equation in which D

appears as a continuous variable. We discuss implications for quantum Monte Carlo and dimensional scaling methods. (c) 2005 American Institute of Physics.

- [451] H. Nishimura and M. Ogilvie. The large-N limit of PT-symmetric $O(N)$ models. *J. Phys. A-Math. Theor.*, 42(2):9, 2009.

Abstract: We study a PT-symmetric quantum-mechanical model with an $O(N)$ -symmetric potential of the form $m(x)$ over right arrow $(2)/2 - g(x)$ over right arrow $(2))(2)/N$ using its equivalent Hermitian form. Although the corresponding classical model has finite-energy trajectories that escape to infinity, the spectrum of the quantum theory is proven to consist only of bound states for all N . We show that the model has two distinct phases in the large- N limit, with different scaling behaviors as N goes to infinity. The two phases are separated by a first-order phase transition at a critical value of the dimensionless parameter $m(x)/g(x)$, given by $3 \times 2(1/3)$.

- [452] M. G. K. Njock, M. Nsangou, Z. Bona, S. G. N. Engo, and B. Oumarou. $1/N$ expansions for central potentials revisited in the light of hypervirial and Hellmann-Feynman theorems and the principle of minimal sensitivity. *Phys. Rev. A*, 61(4):25, 2000.

Abstract: The hypervirial and Hellmann-Feynman theorems are used in the methods of $1/N$ expansion to construct Rayleigh-Schrodinger perturbation expansion for bound-state energy eigenvalues of spherical symmetric potentials. An iteration procedure of calculating correction terms of arbitrarily high orders is obtained for any kind of $1/N$ expansion. The recurrence formulas for three variants of the $1/N$ expansion are considered in this work. namely? the $1/n$ expansion and the shifted and unshifted $1/N$ expansions which are applied to the Gaussian and Patil potentials. As a result. their credibility could be reliably judged when account is taken of high-order terms of the eigenenergies. It is also found that there is a distinct advantage in using the shifted $1/N$ expansion over the two other versions. However, the shifted $1/N$ expansion diverges for s states and in certain cases is not

applicable as far as complicated potentials are concerned. In an effort to solve these problems we have incorporated the principle of minimal sensitivity in the shifted $1/N$ expansion as a first step toward extending the scope of applicability of that technique, and then we have tested the obtained approach to some unfavorable cases of the Patil and Hellmann potentials. The agreement between our numerical calculations and reference data is quite satisfactory.

[453]

S. Noorizadeh and G. R. Pourshams. New empirical potential energy function for diatomic molecules. *Theochem-J. Mol. Struct.*, 678(1-3):207–210, 2004.

Abstract: A new empirical potential energy function for diatomic molecules, which has the simple form of $V(r) = (ar(b) + m)/(1 - e(nr))$ is introduced, where a , b , m and n are variational parameters of the function. To obtain the parameters of this function, it was fitted to the points, which were obtained previously from the RKR calculations for a wide range of diatomic molecules in both their ground and excited states. The reliability of the proposed function was checked by calculation of some spectroscopic constants such as bond length (R_e), dissociation energy (D_e), force constant (K_e), rotational constant (B_e), vibrational frequency (ω_e), anharmonicity constant ($\omega_e x_e$) and vibration-rotation coupling constant (α_e) for these molecules. For $\omega_e x_e$ and α_e the results were compared with those of the Morse, Rosen-Morse, Rydberg, Poschl-Teller, Linnett, Frost-Muslin, Varshni, Lippincott and Rafi functions. Our results are consistent with or have less error than those of the above-mentioned functions. (C) 2004 Elsevier B.V. All rights reserved.

[454]

S. Nouri. Determination of Wigner distribution function for the d -dimensional Coulomb problem. *J. Math. Phys.*, 40(3):1294–1299, 1999.

Abstract: In this work we present a theoretical study of the d -dimensional Coulomb problem in quantum phase space. A coordinate transformation in hyperspherical space is used that maps the d -dimensional Coulomb problem into

the D-dimensional harmonic oscillator and the Wigner distribution function for the d-dimensional Coulomb problem is then obtained. This exactly soluble model can shed some light on finite-size features of Wigner's distribution, which will be a vital experience for various dynamic problems. (C) 1999 American Institute of Physics. [S0022-2488(99)03502-1].

- [455] S. Nouri. Generalized coherent states for the d-dimensional Coulomb problem. *Phys. Rev. A*, 60(2):1702–1705, 1999.

Abstract: In this paper a set of generalized coherent states for the d-dimensional Coulomb problem in coordinate representation are constructed. A coordinate transformation in hyperspherical space is used that maps the d-dimensional Coulomb problem into the D-dimensional harmonic oscillator and the generalized coherent states for the d-dimensional Coulomb problem are then obtained. This exactly soluble model can provide an adequate means for a quantum coherency description of the Coulomb problem in arbitrary dimensions, specifically in the special case of the hydrogen atom, in many theoretical and applied related fields such as in coherent scattering. [S1050-2947(99)05008-8].

- [456] M. A. Nunez. Summation of perturbation series of eigenvalues and eigenfunctions of anharmonic oscillators. *Phys. Rev. E*, 68(1):13, 2003.

Abstract: A perturbation approach to compute the bound states of the Schrodinger equation $H\Psi = E\Psi$ with $H = H_0 + \lambda V$ and Ψ parallel to $(x = \pm\infty) = 0$ is studied. The approach involves solving the corresponding Dirichlet problem $H(R)\Psi(R) = E(R)\Psi(R)$ on a finite interval $[-R, R]$ by the Rayleigh-Schrodinger perturbation theory (RSPT). The method is based on the fact that $E(R), \Psi(R)$ converge to E, Ψ as $R \rightarrow \infty$. The model problems to study the summability properties of the RSPT series $E = \sum_{k=0}^{\infty} E^{(k)} \lambda^k$ are the anharmonic oscillators $H = p^2 + x^2 + \lambda dx^{2M}$, with $M = 2, 3, 4$ for which the RSPT produces strongly divergent

series $E = \sum_{k=0}^{\infty} E(k) \lambda^k$. The summation of the latter series with large λ for the octic case is considered as an extremely challenging summation problem, in part, since it was rigorously proven that the Pade approximants cannot converge and the two-point Pade approximants, which combine information of the renormalized weak coupling and strong coupling expansions, give relatively good results. The calculations of this work show that the ordinary Pade approximants from the sole unnormalized E-R series for the octic oscillator give accurate results with small or large λ . The coefficients $E-R(k)$ are calculated with the eigenvalue series of an operator $H-R_n$, whose resolvent converges to that of $H-R$ as $n \rightarrow \infty$. The Pade approximants of the RSPT eigenfunction series $\Psi(R) = \sum_{k=0}^{\infty} \psi(R)(k) \lambda^k$ also provide accurate results for the octic oscillator.

[457]

F. J. Ohkawa. ELECTRON CORRELATION IN THE PERIODIC ANDERSON MODEL IN $D = +\infty$ DIMENSIONS. *Phys. Rev. B*, 46(14):9016–9026, 1992.

Abstract: The periodic Anderson model with strong repulsion is studied. The leading-order effects with respect to $1/d$, d being the dimensionality of the system, are Kondo-effect-type local spin fluctuations and mean-field-approximation-type magnetic orders. The competition between the Kondo effect and the Ruderman-Kittel-Kasuya-Yosida exchange interaction determines whether the ground state is magnetic or paramagnetic. A single-site approximation (SSA) is rigorous for paramagnetic states in $d \rightarrow +\infty$ dimensions. The SSA reduces the problem to solving the Anderson model. A "local" Kondo temperature is defined to show an energy scale of the local spin fluctuations. On the other hand, an SSA including magnetic mean fields is rigorous for magnetic states in $d \rightarrow +\infty$ dimensions. All the other effects are of higher order: Critical and intersite spin fluctuations are $O(1/\sqrt{d})$; and paramagnetic orders are at most $O(1/d)$. The $1/d$ expansion is one of the most useful methods for examining lower-temperature phases in real dimensions.

[458] P. C. Ojha and R. S. Berry. ANGULAR-CORRELATION OF 2 ELECTRONS ON A SPHERE. *Phys. Rev. A*, 36(4):1575–1585, 1987.

[459] E. Oks. Circular Rydberg states of hydrogenlike systems in collinear electric and magnetic fields of arbitrary strengths: an exact analytical classical solution. *Eur. Phys. J. D*, 28(2):171–179, 2004.

Abstract: We derived analytical expressions for the energy of classical Circular Rydberg States (CRS) in collinear electric (F) and magnetic (B) fields of arbitrary strengths. Previously published explicit expressions for the energy E were given only for the region of a weak electric field F and only in the limits of $B \rightarrow 0$ and $B \rightarrow \infty$. We offered formulas for the dependence of the classical ionization threshold $F_c(B)$ and of the energy at this threshold $E_c(B)$ valid for the magnetic field B of an arbitrary strength. We also analyzed the stability of the motion by going beyond the CRS. In addition, for two important particular cases previously studied in the literature – classical CRS in a magnetic field only and classical CRS in an electric field only – we presented some new results as well.

[460] K. J. Oyewumi. Analytical solutions of the Kratzer-Fues potential in an arbitrary number of dimensions. *Found. Phys. Lett.*, 18(1):75–84, 2005.

Abstract: Some aspects of the N dimensional Kratzer-Fues potential are discussed, which is an extension of the combined Coulomb-like potential with inverse quadratic potential in N dimensions. The analytical solutions obtained (eigenfunctions and eigenvalues) are dimensionally dependent, so also, the solutions depend on the value of the coefficient of the inverse quadratic term. The expectation values for $\langle r^{-2} \rangle$, $\langle r^{-1} \rangle$ and the virial theorem for this potential are obtained and the values are also dimensions and parameter dependent.

[461] K. J. Oyewumi, F. O. Akinpelu, and A. D. Agboola. Exactly complete solutions of the pseudoharmonic potential in N-dimensions. *Int. J. Theor. Phys.*, 47(4):1039–1057, 2008.

Abstract: We present analytically the exact solutions of the Schrodinger equation in the N-dimensional spaces for the pseudoharmonic oscillator potential by means of the ansatz method. The energy eigenvalues of the bound states are easily calculated from this eigenfunction ansatz. The normalized wavefunctions are also obtained. A realization of the ladder operators for the wavefunctions is studied and we deduced that these operators satisfy the commutation relations of the generators of the dynamical group SU(1,1). Some expectation values for r^{-2} , r^2 , T , V , H , p^2 and the virial theorem for the pseudoharmonic oscillator potential in an arbitrary number of dimensions are obtained by means of the Hellmann-Feynman theorems. Each solution obtained is dimensions and parameters dependent.

[462]

K. J. Oyewumi and E. A. Bangudu. Isotropic harmonic oscillator plus inverse quadratic potential in N-dimensional spaces. *Arab. J. Sci. Eng.*, 28(2A):173–182, 2003.

Abstract: Some aspects of the N-dimensional isotropic harmonic plus inverse quadratic potential are discussed. The hyperradial equation for isotropic harmonic oscillator Plus inverse quadratic potential is solved by transformation into the confluent hypergeometric equation to obtain the normalized hyperradial Solution. Together with the hyperangular solutions (hyperspherical harmonics), these form the complete energy eigenfunctions of the N-dimensional isotropic harmonic oscillator plus inverse quadratic potential and the energy eigenvalues are also obtained. These are dimensionally dependent. The dependence of the radial solution on the dimensions or the potential strength and the degeneracy of the energy levels are discussed.

[463]

S. Panchanan, R. Roychoudhury, and Y. P. Varshni. Modified shifted $1/N$ expansion for relativistic Yukawa and Hulthen potentials. *Can. J. Phys.*, 74(3-4):136–140, 1996.

Abstract: The shifted $1/N$ expansion technique is applied to the radial Dirac equation. it is shown that the fixing condition $E(1) = 0$ produces an enhanced accuracy for Yukawa and Hulthen potentials. The modified shifted $1/N$ expansion results

are compared with the exact numerical results and results obtained by other approximate methods.

- [464] M. M. Panja, M. Bag, R. Dutt, and Y. P. Varshni. LARGE-N EXPANSION METHOD FOR A SPIN-1/2 PARTICLE IN THE PRESENCE OF VECTOR AND SCALAR POTENTIALS. *Phys. Rev. A*, 45(3):1523–1530, 1992.

Abstract: The shifted large-N technique (SLNT) has been applied to study the relativistic motion of a particle in the presence of vector and scalar interactions with special emphasis on the construction of both large- and small-component Dirac radial wave functions. Numerical results for the binding energy for a particle in the presence of the Coulomb plus linear confining potential compare very well with those obtained by the elaborate analytic approximation method using the Padé-approximation technique. We illustrate that one recovers not only the exact analytic results for binding energies for vector and scalar Coulomb potentials, but also exact wave functions from the leading-order SLNT calculation. This motivates future applications of the same method to more realistic atomic systems governed by screened Coulomb potentials where the knowledge of the large and small components of the radial wave function is essential.

- [465] M. M. Panja and R. Dutt. SHIFTED LARGE-N EXPANSION FOR THE ENERGY-LEVELS OF RELATIVISTIC-PARTICLES. *Phys. Rev. A*, 38(8):3937–3943, 1988.
- [466] M. M. Panja, R. Dutt, and Y. P. Varshni. SHIFTED LARGE-N EXPANSION FOR THE POWER-LAW POTENTIALS IN THE KLEIN-GORDON EQUATION WITH APPLICATIONS. *J. Phys. A-Math. Gen.*, 22(15):2991–3001, 1989.
- [467] M. M. Panja, R. Dutt, and Y. P. Varshni. SHIFTED LARGE-N EXPANSION FOR A RELATIVISTIC SPIN-1/2 PARTICLE IN SCREENED COULOMB POTENTIALS. *Phys. Rev. A*, 42(1):106–115, 1990.
- [468] N. Papanicolaou. PSEUDO-SPIN AND CLASSICAL CORRESPONDENCE FOR FERMI FIELDS. *Ann. Phys.*, 136(1):210–225, 1981.

- [469] E. Papp. QUASI-CLASSICAL APPROACH TO THE VIRIAL-THEOREM AND TO THE EVALUATION OF THE GROUND-STATE ENERGY. *Phys. Rep.-Rev. Sec. Phys. Lett.*, 136(2):103-&, 1986.
- [470] E. Papp. QUASI-CLASSICAL GROUND-STATE ENERGIES FOR QUARKONIA POTENTIALS. *Phys. Rev. A*, 34(1):47-55, 1986.
- [471] E. Papp. QUASI-CLASSICAL APPROACH TO THE SHIFTING PARAMETER OF THE 1/N METHOD. *Phys. Rev. A*, 36(8):3550-3555, 1987.
- [472] E. Papp. SYMMETRY PROPERTIES OF QUASI-CLASSICAL ENERGY-LEVELS. *Phys. Rev. A*, 35(12):4946-4955, 1987.
- [473] E. Papp. QUASICLASSICAL SYMMETRY PROPERTIES .2. *Phys. Rep.-Rev. Sec. Phys. Lett.*, 161(4):171-212, 1988.
- [474] E. Papp. QUASICLASSICAL 1/N FORMULAS TO THE RESONANCE ENERGIES FOR THE STARK-EFFECT IN THE HYDROGEN-ATOM. *Phys. Lett. A*, 132(2-3):127-130, 1988.
- [475] E. Papp. RELEVANT APPROXIMATIONS TO THE GROUND-STATE ENERGY FOR THE QUADRATIC ZEEMAN EFFECT. *Phys. Rev. A*, 37(9):3598-3600, 1988.
- [476] E. Papp. GENERAL 2ND-ORDER 1/N FORMULAS FOR THE ENERGY-LEVELS OF SPHERICALLY SYMMETRIC HAMILTONIANS RELYING ON A NOVEL FIXING OF THE SHIFTING PARAMETER. *Phys. Rev. A*, 38(4):2158-2159, 1988.
- [477] E. Papp. QUASI-CLASSICAL 1/N ENERGY FORMULAS FOR THE SUPERPOSITION BETWEEN THE ATTRACTIVE POTENTIAL $-\lambda_0/x^2$ AND THE REPULSIVE (N-GREATER-THAN-2)-POTENTIAL $-\gamma(N)/x^N$. *Europhys. Lett.*, 9(4):309-313, 1989.
- [478] E. Papp. QUASI-CLASSICAL 1/N ENERGY-FORMULAS FOR RELATIVISTIC 2-BODY SYSTEMS. *Ann. Phys.-Berlin*, 48(5):319-326, 1991.

Abstract: Quickly tractable energy-formulas for relativistic two-body systems are established to first 1/N-order in terms of general classical Hamiltonians (m_1 greater-than-or-equal-to m_2). Arbitrary spherically-symmetrical vector and/or scalar

potentials are assumed. Such Hamiltonians, which have to be converted into related non-relativistic ones, play the role of a dominant zeroth-order approximation (an exact description) in the case of two fermions (two bosons). Proofs have also been given that the $1/N$ -method is quite suitable for the systematic description of order-dependent contributions to the energy of Coulomb-Bethe-Salpeter systems, now to α -6-order.

- [479] E. Papp. $1/N$ ENERGY-FORMULAS FOR RELATIVISTIC 2-BODY COULOMB AND YUKAWA SYSTEMS WITH ARBITRARY MASSES. *Phys. Scr.*, 43(1):14–18, 1991.

Abstract: Energy formulae for two-particle Klein-Gordon systems subjected to Coulomb and Yukawa potentials are derived to first $1/N$ -order. The energies obtained in this manner incorporate the influence of the mass-asymmetry via the parameter $\delta = (m_1(2) - M_2(2))^2$. Certain Coulomb-inspired extrapolations to Dirac-particle systems, having the meaning of dominant contributions, are taken into account. Numerical results are presented.

- [480] E. Papp. CLOSED $1/N$ MASS FORMULAS FOR RELATIVISTIC 2-BODY $Q_1\bar{Q}_2$ SYSTEMS. *Phys. Lett. B*, 259(1-2):19–23, 1991.

Abstract: Proofs are given that the mass spectra of $b\bar{s}$ mesons predicted by Crater and Van Alstine can be reproduced, within relative errors smaller than a few percents, by applying simplified $1/N$ equations, now just in terms of a related phenomenological vectorial Coulomb plus linear potential. Such equations are also useful for a quickly tractable energy description of other relativistic two-body systems with arbitrary masses, for which the constituent Coulomb potential plays a significant role.

- [481] E. Papp. QUANTUM q -DEFORMATIONS OF $1/N$ ENERGY FORMULAS FOR ARBITRARY SPHERICALLY SYMMETRICAL POTENTIALS. *Phys. Lett. A*, 189(5):341–344, 1994.

Abstract: A general q -deformation formula for the expansion parameter of the $1/N$ method

is derived. One proceeds by interpolating between the suitable q -deformed energy of the three-dimensional Coulomb problem and the symmetrized q -deformed energy of the harmonic oscillator in N space-dimensions. Useful q -deformed $1/N$ energy formulae for arbitrary spherically symmetrical $O(N)$ -potentials are presented.

[482] E. Papp. Q-ANALOGS OF THE RADIAL SCHRODINGER-EQUATION IN N -SPACE DIMENSIONS. *Phys. Rev. A*, 52(1):101–106, 1995.

[483] E. Papp. Applying the $1/N$ approximation to the derivation of the band energy of the Harper equation. *Mod. Phys. Lett. B*, 14(11):373–376, 2000.

Abstract: The $1/N$ approach to the Harper equation proposed previously is generalized towards performing the pertinent band-energy description. Leading forms and corrections proceeding to first order in the magnetic field are written down. The energy reflection symmetry has also been discussed.

[484] E. Papp and C. Micu. $1/N$ -ENERGY-SOLUTIONS TO RELATIVISTIC 2-BOSON SYSTEMS WITH AN EXPONENTIAL POTENTIAL. *Z. Naturforsch. Sect. A-J. Phys. Sci.*, 46(8):729–732, 1991.

Abstract: Closed $1/N$ -energy-formulae for relativistic two-boson (m_1 not-equal m_2) systems with a vector exponential potential have been written down to first $1/N$ -order. Numerical estimates and structural properties are presented.

[485] E. Papp and C. Micu. The derivation of $1/N$ equivalent potentials for the radial Schrodinger equation in N space dimensions. *Can. J. Phys.*, 74(3-4):102–107, 1996.

Abstract: Proofs are given that $SO_q(N)$ -motivated q deformations of the expansion parameter of the $1/N$ method can be incorporated into symmetry transformations preserving the radial form of the Schrodinger equation. This opens the way to establish the q deformed energy and the corresponding $1/N$ equivalent potential. So far the number of space dimensions is subject of covariant transformations. An alternative derivation of

the $1/N$ equivalent potential is also done by keeping this number invariant. In this latter case, the stability attributes of q -deformed power-law potentials are discussed in terms of the $q \downarrow 1$ choice.

- [486] G. Parisi and F. Slanina. On the $1/D$ expansion for directed polymers. *Eur. Phys. J. B*, 8(4):603–611, 1999.

Abstract: We present a variational approach for directed polymers in D transversal dimensions which is used to compute the correction to the mean field theory predictions with broken replica symmetry. The trial function is taken to be a symmetrized version of the mean-field solution, which is known to be exact for $D = \text{infinity}$. We compute the free energy corresponding to that function and show that the finite- D corrections behave like $D-4/3$. It means that the expansion in powers of $1/D$ should be used with great care here. We hope that the techniques developed in this note will be useful also in the study of spin glasses.

- [487] S. H. Patil. Hydrogen molecular ion and molecule in two dimensions. *J. Chem. Phys.*, 118(5):2197–2205, 2003.

Abstract: We discuss some general properties of the wave functions of $H-2(+)$ in two dimensions, when the electron is close to the nucleus, and when it is far away from the nucleus. Based on these properties, some simple, parameter-free wave functions are developed for some of the states. They lead to quite accurate energies and give an insight into the structure of $H-2(+)$ in two dimensions. These wave functions and appropriate correlation functions, are then used to develop reliable wave functions for $H-2$ in two dimensions. They provide a clear and interesting comparison with the corresponding results in three dimensions. (C) 2003 American Institute of Physics.

- [488] S. H. Patil. The helium atom and isoelectronic ions in two dimensions. *Eur. J. Phys.*, 29(3):517–525, 2008.

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 inter-electronic 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 perturbative 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.

- [489] S. H. Patil and Y. P. Varshni. Two electrons in a simple harmonic potential. *Can. J. Phys.*, 84(3):181–192, 2006.

Abstract: Some structural properties of energy eigenfunctions of two electrons in a simple harmonic potential are analyzed. Simple expressions are obtained for the energy spectrum based on a model potential, and on a model wave function. These expressions give accurate values for the energy eigenvalues and provide a physical insight into their structure.

- [490] S. Peris. Large- N_c QCD and Pade approximant theory. *Phys. Rev. D*, 74(5):5, 2006.

Abstract: In the large- N_c limit of QCD, the expansion of the vacuum polarization at low energies determines the whole function at any arbitrarily large (but finite) energy. This result is an immediate consequence of the theory of Pade approximants to Stieltjes functions.

- [491] S. Peris, M. Perrottet, and E. de Rafael. Matching long and short distances in large- N_c QCD. *J. High Energy Phys.*, (5):38, 1998.

Abstract: It is shown, with the example of the experimentally known Adler function, that there is no matching in the intermediate region between the two asymptotic regimes described by perturbative QCD (for the very short-distances) and by chiral perturbation theory (for the very long-distances). We then propose to consider an approximation of

large- N_c QCD which consists in restricting the hadronic spectrum in the channels with $J(P)$ quantum numbers $0(-)$, $1(-)$, $0(+)$ and $1(+)$ to the lightest state and to treat the rest of the narrow states as a perturbative QCD continuum; the onset of this continuum being fixed by consistency constraints from the operator product expansion. We show how to construct the low-energy effective Lagrangian which describes this approximation. The number of free parameters in the resulting effective Lagrangian can be reduced, in the chiral limit where the light quark masses are set to zero, to just one mass scale and one dimensionless constant to all orders in chiral perturbation theory. A comparison of the corresponding predictions, to $O(p^4)$ in the chiral expansion, with the phenomenologically known couplings is also made.

[492]

T. M. Perrine, R. K. Chaudhuri, and K. F. Freed. Quadratic Pade approximants and the intruder state problem of multireference perturbation methods. *Int. J. Quantum Chem.*, 105(1):18–33, 2005.

Abstract: Simple and quadratic Pade resummation methods are applied to high-order series from multireference many-body perturbation theory (MR-MBPT) calculations using various partitioning schemes (Moller-Plesset, Epstein-Nesbet, and forced degeneracy) to determine their efficacy in resumming slowly convergent or divergent series. The calculations are performed for the ground and low-lying excited states of (i) CH₂, (ii) BeH₂, at three geometries, and (iii) Be, for which full configuration interaction (0) calculations are available for comparison. The 49 perturbation series that are analyzed include those with oscillatory and monotonic divergence and convergence, including divergences that arise from either frontdoor or backdoor intruder states. Both the simple and quadratic Pade approximations are found to speed the convergence of slowly convergent or divergent series. However, the quadratic Pade method generally outperforms the simple Pade resummation. (c) 2005 Wiley Periodicals, Inc.

[493]

D. Pirjol and T. M. Yan. $1/N_c$ expansion for excited baryons. *Phys. Rev. D*, 57(3):1449–1486, 1998.

Abstract: We derive consistency conditions which constrain the possible form of the strong couplings of the excited baryons to the pions. The consistency conditions follow from requiring the pion-excited baryon scattering amplitudes to satisfy the large- N_c Witten counting rules and are analogous to consistency conditions used by Dashen, Jenkins, and Manohar and others for s-wave baryons. The consistency conditions are explicitly solved, giving the most general allowed form of the strong vertices for excited baryons in the large- N_c limit. We show that the solutions to the large- N_c consistency conditions coincide with the predictions of the non-relativistic quark model for these states, extending the results previously obtained for the s-wave baryons. The $1/N_c$ corrections to these predictions are studied in the quark model with arbitrary number of colors N_c .

[494]

P. V. Pobylitsa. Baryon distribution amplitude: Large- N_c factorization, spin-flavor symmetry and soft-pion theorem. *Phys. Rev. D*, 72(1):20, 2005.

Abstract: The $1/N_c$ expansion for the baryon distribution amplitude is constructed in terms of a specially designed generating functional. At large N_c this functional shows exponential behavior. The exponential factor is universal for all low-lying baryons and baryon-meson scattering states. Simple factorization properties are established for the preexponential term. This factorization agrees with the large- N_c contracted $SU(2N(f))$ spin-flavor symmetry. The consistency of the factorization with the soft-pion theorem for the baryon distribution amplitude is explicitly checked. A relation between the generating functionals for the distribution amplitudes of the nucleon and the Delta resonance is derived.

[495]

V. S. Popov. ON THE THEORY OF THE ABOVE-THE-BARRIER STARK RESONANCES. *Phys. Lett. A*, 173(1):63–68, 1993.

Abstract: A semiclassical $1/n$ -expansion for the Stark effect in a strong electric field ϵ is considered, which gives simple analytic formulae determining the atomic widths $\Gamma(n)(\epsilon)$.

It has been shown that there is a range in which the widths of the Stark resonances depend almost linearly on the applied electric field, which agrees with numerical calculations.

[496]

V. S. Popov. Tunneling and above-barrier ionization of atoms in a laser radiation field. *J. Exp. Theor. Phys.*, 91(1):48–66, 2000.

Abstract: Calculations are made of the energy and angular distributions of photoelectrons during tunneling ionization of an atom or an ion under the action of high-power laser radiation (for all values of the Keldysh parameter γ). Cases of linear, circular, and elliptic polarizations of the electromagnetic wave are considered. The probability of above-barrier ionization of hydrogen atoms in a low-frequency (γ much less than 1) laser field is calculated. Formulas are given for the momentum spectrum of the electrons when an atomic level is ionized by a general type of alternating electric field (for the case of linear polarization). An analysis is made of tunneling interference in the energy spectrum of the photoelectrons. Analytic approximations are discussed for the asymptotic coefficient C_{κ} of the atomic wave function at infinity (for s-wave electrons). (C) 2000 MAIK "Nauka/Interperiodica".

[497]

V. S. Popov, B. M. Karnakov, and V. D. Mur. $1/n$ -expansion for asymptotic coefficients of radial wave functions in quantum mechanics. *Phys. Lett. A*, 224(1-2):15–21, 1996.

Abstract: Using the $1/n$ -expansion, we obtain analytic formulae for the bound state radial wave functions, including its asymptotic coefficients at $r \rightarrow 0$ and $r \rightarrow \infty$, for an arbitrary smooth potential $V(r)$. The formulae are asymptotically exact in the limit $n \rightarrow \infty$ ($n = n(r) + l + 1$ is the principal quantum number and the expansion parameter is $1/n$). Comparison with exact solutions and numerical calculations for the power-law and short-range potentials show that the applicability region of these formulae is usually prolonged up to small quantum numbers, n similar to 1. With growing $n(r)$, the accuracy of the formulae decreases, but the WKB method becomes applicable in this case.

- [498] V. S. Popov, B. M. Karnakov, and V. D. Mur. Quasiclassical theory of atomic ionization in electric and magnetic fields. *Phys. Lett. A*, 229(5):306–312, 1997.

Abstract: Using the "imaginary time" method we have calculated (in the quasiclassical approximation) the probability of ionization of the atomic s-state in static electric and magnetic fields. The Coulomb interaction between the emitted electron and the atomic remainder is taken into account. The results obtained are valid for external fields E and H which are smaller than characteristic atomic fields. The case of mutually orthogonal fields (the Lorentz ionization) is carefully studied. (C) 1997 Elsevier Science B.V.

- [499] V. S. Popov, B. M. Karnakov, and V. D. Mur. Ionization of atoms in electric and magnetic fields and the imaginary time method. *J. Exp. Theor. Phys.*, 86(5):860–874, 1998.

Abstract: A semiclassical theory is developed for the ionization of atoms and negative ions in constant, uniform electric and magnetic fields, including the Coulomb interaction between the electron and the atomic core during tunneling. The case of crossed fields (Lorentz ionization) is examined specially, as well as the limit of a strong magnetic field. Analytic equations are derived for arbitrary fields E and H that are weak compared to the characteristic intraatomic fields. The major results of this paper are obtained using the "imaginary time" method (ITM), in which tunneling is described using the classical equations of motion but with purely imaginary "time." The possibility of generalizing the ITM to the relativistic case, as well as to states with nonzero angular momentum, is pointed out. (C) 1998 American Institute of Physics. [S1063-7761(98)00405-3].

- [500] V. S. Popov and V. D. Mur. PERTURBATION-THEORY FOR QUASI-STATIONARY LEVELS. *Jetp Lett.*, 60(1):66–70, 1994.

Abstract: A perturbation-theory formula is derived for the energies of quasistationary states (resonances) in the semiclassical approximation. This formula is valid for resonances either below or

above the barrier. It is illustrated for several potentials, for which a comparison can be made with exact solutions.

- [501] V. S. Popov, V. D. Mur, and A. V. Sergeev. 1/N-EXPANSION AND SCALING FOR THE STARK-EFFECT IN RYDBERG ATOMS. *Phys. Lett. A*, 149(9):425–430, 1990.

- [502] V. S. Popov, V. D. Mur, and A. V. Sergeev. QUANTIZATION RULES FOR QUASI-STATIONARY STATES. *Phys. Lett. A*, 157(4-5):185–191, 1991.

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 Γ 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.

- [503] V. S. Popov, V. D. Mur, and A. V. Sergeev. QUANTIZATION RULES WITH ALLOWANCE FOR BARRIER PENETRATION. *Zhurnal Eksperimentalnoi Teor. Fiz.*, 100(1):20–44, 1991.

Abstract: A correction to the quasiclassical quantization rules is found which is connected with the taking into account of the barrier penetration. The equation derived defines both the position $E(r)$ and width Γ of the quasistationary level. The results are compared with numerical solutions of the Schrodinger equation and with the exactly soluble models. A generalization of the Gamov formula for systems with separated variables is obtained. The possibility of extending the results to the relativistic case is discussed.

- [504] V. S. Popov, V. D. Mur, and A. V. Sergeev. CRITICAL FIELDS AND ABOVE-BARRIER STARK RESONANCES. *Jetp Lett.*, 59(3):158–162, 1994.

Abstract: Exact values of the critical field $E(c)$ are calculated for a hydrogen atom, including the

case of the ground state. The widths $\text{GAMMA}(n)$ of Stark resonances at $E = E(c)$ are also calculated. In the above-barrier region ($E > E(c)$) the widths $\text{GAMMA}(n)(E)$ are essentially linear functions of the electric field strength.

- [505] V. S. Popov, V. D. Mur, and A. V. Sergeev. THEORY OF STARK-EFFECT IN THE STRONG-FIELD - CRITICAL FIELDS, ABOVE-BARRIER RESONANCES, DEPENDENCE ON DIMENSIONAL SCALING. *Zhurnal Eksperimentalnoi Teor. Fiz.*, 106(4):1001–1030, 1994.
- [506] V. S. Popov, V. D. Mur, A. V. Sergeev, and V. M. Weinberg. STRONG-FIELD STARK-EFFECT - PERTURBATION-THEORY AND 1/N-EXPANSION. *Phys. Lett. A*, 149(9):418–424, 1990.
- [507] V. S. Popov, V. D. Mur, A. V. Shcheblykin, and V. M. Weinberg. 1/N-EXPANSION FOR THE STARK-EFFECT IN STRONG FIELD. *Phys. Lett. A*, 124(1-2):77–80, 1987.
- [508] V. S. Popov and A. V. Sergeev. ASYMPTOTIC FORM OF HIGHER ORDERS OF THE 1/N EXPANSION. *Jetp Lett.*, 57(5):281–285, 1993.
- Abstract:** The asymptotic form of higher orders of the 1/n expansion in quantum mechanics is factorial. The Yukawa potential and the hydrogen atom in electric and magnetic fields are discussed.
- [509] V. S. Popov and A. V. Sergeev. LARGE ORDERS OF THE 1/N EXPANSION IN QUANTUM-MECHANICS. *Phys. Lett. A*, 172(4):193–198, 1993.
- Abstract:** The asymptotics of large orders of the 1/n expansion in quantum mechanics has been found. It is shown that the coefficients $\epsilon(k)$ grow as $k!a(k)$ With $k \rightarrow \infty$, and the dependence of the parameter a on the coupling constant is investigated.
- [510] V. S. Popov and A. V. Sergeev. ASYMPTOTICS OF THE HIGHEST ORDERS OF 1-N-DECOMPOSITION FOR MULTIDIMENSIONAL PROBLEMS. *Zhurnal Eksperimentalnoi Teor. Fiz.*, 105(3):568–591, 1994.
- [511] V. S. Popov and A. V. Sergeev. LARGE ORDERS OF 1/N-EXPANSION FOR MULTIDIMENSIONAL PROBLEMS. *Phys. Lett. A*, 193(2):165–172, 1994.

Abstract: The asymptotics of large orders of the $1/n$ -expansion is investigated for multidimensional problems of quantum mechanics and atomic physics, including those with separable variables (the hydrogen molecular ion H_2^+), and those where separation of variables is impossible (a hydrogen atom in electric and magnetic fields). It is shown that the parameters of the asymptotics can be found by means of calculating sub-barrier trajectories with the help of the "imaginary time" method, as well as by solution of the eikonal equation.

- [512] V. S. Popov and A. V. Sergeev. Effect of a magnetic field on the ionization of atoms. *Jetp Lett.*, 63(6):417–422, 1996.

Abstract: The ionization probability of an atomic s state under the action of static electric and magnetic fields is calculated taking into account the Coulomb interaction between the escaping electron and the atomic core. The structure of the perturbation series for the energy of the level is investigated and the asymptotic behavior of the higher orders of the perturbation theory is found. (C) 1996 American Institute of Physics.

- [513] V. S. Popov and A. V. Sergeev. Ionization of atoms in weak fields and the asymptotic behavior of higher-order perturbation theory. *J. Exp. Theor. Phys.*, 86(6):1122–1126, 1998.

Abstract: Using the imaginary time method, we study the structure of the perturbation series for the hydrogen atom in electric E and magnetic H fields. It is shown that there is a "critical" value of the ratio $\gamma = H/E$ at which the perturbation series for the ground state changes from having a fixed sign (for $\gamma < \gamma(c)$) to having a variable sign (for $\gamma > \gamma(c)$). This conclusion is confirmed by direct higher-order perturbation calculations. The change in the asymptotic regime is explained by competition among the contributions of the various complex trajectories that describe the subbarrier motion of the electrons. Here the parameter $\gamma(c)$ depends on the angle θ between the electric and magnetic fields. (C) 1998 American Institute of Physics.

- [514] V. S. Popov, A. V. Sergeev, V. D. Mur, and A. V. Shcheblykin. ON THE ASYMPTOTICS OF HIGH-ORDER TERMS OF THE $1/N$ EXPANSION. *Phys. Atom. Nuclei*, 57(6):1057–1065, 1994.

Abstract: Analytic and numerical methods for determining the asymptotics of high-order terms of the $1/n$ expansion in quantum-mechanical problems are developed. It is shown that this asymptotics is always of the factorial type. The dependence of parameters of the asymptotics on the form of the potential and on the coupling constant is especially analyzed in the vicinity of the point of collision of classical solutions.

- [515] V. S. Popov, A. V. Sergeev, and A. V. Shcheblykin. ON THE STRUCTURE OF LARGE ORDERS IN $1/N$ -EXPANSION. *Zhurnal Eksperimentalnoi Teor. Fiz.*, 102(5):1453–1468, 1992.

Abstract: The asymptotic behaviour of large orders in $1/n$ -expansion is found for the problems of quantum mechanics. The coefficients of $1/n$ -expansion $\epsilon(k)$ are shown to increase as a factorial $k! a(k)$ at $k \rightarrow \infty$. The a -parameter vs coupling constant dependence is studied. The analytic formulas obtained agree with the numerical calculations. The structure of $1/n$ -expansion is considered in detail for the Yukawa, Hulthen and funnel potentials, as well as for the Stark effect in hydrogen and for the molecular ion H .

- [516] V. S. Popov and A. V. Shcheblykin. HIGHER ORDERS OF THE $1/N$ EXPANSION AND ITS DIVERGENCE. *Soviet Journal of Nuclear Physics-Ussr*, 54(6):968–972, 1991.

Abstract: A numerical investigation is made of the structure of the higher orders of the $1/n$ expansion in problems of quantum mechanics (the funnel and Yukawa potentials, and the Stark effect in the hydrogen atom). It is shown that the coefficients- $\epsilon(k)$ of the $1/n$ expansion have a factorial growth in the limit $k \rightarrow \infty$, and their asymptotic form is obtained.

- [517] V. S. Popov, V. M. Vainberg, and V. D. Mur. DIVERGING PERTURBATION-THEORY SERIES AND CLASSICAL MECHANICS. *Jetp Lett.*, 41(10):539–543, 1985.

- [518] V. S. Popov, V. M. Vainberg, and V. D. Mur. HIGHER ORDERS OF PERTURBATION-THEORY, CLASSICAL MECHANICS, AND THE $1/N$ EXPANSION. *Soviet Journal of Nuclear Physics-Ussr*, 44(4):714–720, 1986.
- [519] V. S. Popov, V. M. Veinberg, V. D. Mur, and A. V. Shcheblykin. $1/N$ -EXPANSION IN QUANTUM-MECHANICS. *Doklady Akademii Nauk Sssr*, 293(4):851–855, 1987.
- [520] V. V. Pupyshev. Selected expansions in the three-body problem. *Phys. Part. Nuclei*, 33(4):435–472, 2002.
- 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.
- [521] P. Pyykko and Y. F. Zhao. THE ELEMENTS OF FLATLAND - HARTREE-FOCK ATOMIC GROUND-STATES IN 2 DIMENSIONS FOR $Z = 1-24$. *Int. J. Quantum Chem.*, 40(4):527–544, 1991.
- Abstract:** The Hartree-Fock problem in two dimensions (2D) has been solved for 1 less-than-or-equal-to Z less-than-or-equal-to 24 using a Gaussian basis and assuming r^{-1} Coulomb interactions. The order of occupation of the one-electron states is $1s \uparrow \downarrow 2s \uparrow 2p \uparrow 3s \uparrow 3p \uparrow 4s$ approximately-less-than $3d \uparrow 4p$ like in the 3D case. The $1s$ shell is found to be particularly small and strongly bound, making the 2D hydrogen a "superhalogen" and the 2D He a "superinert gas." In contrast to 3D, $4s(1)3d2$ and $4s(2)3d3$ configurations are preferred for the 2D "Sc" and "Cu," respectively. The six first 2D atoms have stronger and the later ones weaker valence-bonding energies than do their 3D analogs. It is noted that the 2D Dirac energy expression for a hydrogenlike atom for $m(j) = 1 + 1/2$ agrees with the 3D Klein-Gordon one.
- [522] L. Quiroga, A. Camacho, and A. Gonzalez. 2-DIMENSIONAL MAGNETOEXCITONS - A SHIFTED

1/N APPROACH. *J. Phys.-Condes. Matter*, 7(38):7517–7527, 1995.

Abstract: The energy spectrum of two-dimensional magnetoexcitons has been calculated using the shifted 1/N expansion method (N the space dimension). It is found that even in the leading-term approximation this approach provides remarkably accurate and simple analytic expressions for the magnetoexciton energies for any magnetic field strength and electron-hole mass ratio. For the infinite-hole-mass exciton (hydrogenic impurity) our results show an excellent agreement with previously reported numerical data in the whole magnetic field range. Higher terms in the expansion which allow a systematic improvement of low-energy values are also considered.

[523]

L. Radzihovsky and P. Ledoussal. CRUMPLED GLASS PHASE OF RANDOMLY POLYMERIZED MEMBRANES IN THE LARGE D LIMIT. *J. Phys. I*, 2(5):599–613, 1992.

Abstract: Tethered phantom membranes with quenched disorder in the internal preferred metric are studied in the limit of large embedding space dimension $d \rightarrow \infty$. We find that the instability of the flat phase previously demonstrated via epsilon-expansion is towards a spin-glass-like phase which we call the crumpled glass phase. We propose a spin-glass order parameter that characterizes this phase and derive the free energy which describes the crumpled, flat and crumpled glass phases of the disordered membrane. The crumpled glass phase is described by local tangents which vanish on average, but display a nonzero Edwards-Anderson spin-glass order parameter. From the saddle point equations at large d we obtain the equation of state, phase diagram and the exponents characterizing these phases. We estimate the effects of the higher order corrections in the $1/d$ expansion by utilizing previous results for pure membranes. We use Flory arguments to calculate the wandering exponents and discuss the relevance of self-avoidance in the crumpled glass phase.

[524]

S. J. Rankin. SU(INFINITY) AND THE LARGE-N LIMIT. *Ann. Phys.*, 218(1):14–50, 1992.

- [525] A. R. P. Rau. A NEW BOHR-RYDBERG SPECTRUM OF 2-ELECTRON STATES. *J. Phys. B-At. Mol. Opt. Phys.*, 16(23):L699–L705, 1983.
- [526] A. Ray, K. Mahata, and P. P. Ray. MOMENTS OF PROBABILITY-DISTRIBUTION, WAVEFUNCTIONS, AND THEIR DERIVATIVES AT THE ORIGIN OF N-DIMENSIONAL CENTRAL POTENTIALS. *Am. J. Phys.*, 56(5):462–464, 1988.
- [527] P. P. Ray and K. Mahata. BOUND-STATES OF THE POTENTIAL $V(R)=-ZE^2/(R+BETA)$. *J. Phys. A-Math. Gen.*, 22(15):3161–3165, 1989.
- [528] E. Reyes-Gomez, A. Matos-Abiague, M. De Dios-Leyva, and L. E. Oliveira. The fractional-dimensional space approach: Excitons and shallow impurities in semiconductor low-dimensional systems. *Phys. Status Solidi B-Basic Res.*, 220(1):71–77, 2000.

Abstract: The fractional-dimensional space approach is applied in the study of excitons and shallow impurities in semiconductor low-dimensional systems. In this scheme, a real anisotropic semiconductor heterostructure in a three-dimensional environment is treated as isotropic in an effective fractional-dimensional space, and the value of the fractional dimension is associated to the degree of anisotropy of the actual three-dimensional semiconductor system. When a magnetic field is applied along the growth direction of the semiconductor heterostructure, it introduces an additional degree of confinement and anisotropy besides the one imposed by the heterostructure barrier potential. The fractional dimension is then related to the anisotropy introduced both by the heterostructure barrier potential and magnetic field. In this work, we present results for excitons in GaAs-(Ga,Al)As quantum wells and symmetric-coupled double quantum wells, and shallow-impurity states in GaAs-(Ga,Al)As quantum wells and superlattices under growth-direction applied magnetic fields. Results are shown to be in good agreement with available experimental measurements and previous variational calculations.

- [529] E. Reyes-Gomez, A. Matos-Abiague, C. A. Perdomo-Leiva, M. de Dios-Leyva, and L. E. Oliveira. Excitons and

shallow impurities in GaAs-Ga_{1-x}Al_xAs semiconductor heterostructures within a fractional-dimensional space approach: Magnetic-field effects. *Phys. Rev. B*, 61(19):13104–13114, 2000.

Abstract: The fractional-dimensional space approach is extended to study exciton and shallow-donor states in symmetric-coupled GaAs-Ga_{1-x}Al_xAs multiple quantum wells. In this scheme, the real anisotropic "exciton (or shallow donor) plus multiple quantum well" semiconductor system is mapped, for each exciton (or donor) state, into an effective fractional-dimensional isotropic environment, and the fractional dimension is essentially related to the anisotropy of the actual semiconductor system. Moreover, the fractional-dimensional space approach was extended to include magnetic-field effects in the study of shallow-impurity states in GaAs-Ga_{1-x}Al_xAs quantum wells and superlattices. In our study, the magnetic field was applied along the growth direction of the semiconductor heterostructure, and introduces an additional degree of confinement and anisotropy besides the one imposed by the heterostructure barrier potential. The fractional dimension is then related to the anisotropy introduced both by the heterostructure barrier potential and magnetic field. Calculations within the fractional-dimensional space scheme were performed for the binding energies of 1s-like heavy-hole direct exciton and shallow-donor states in symmetric-coupled semiconductor quantum wells, and for shallow-impurity states in semiconductor quantum wells and superlattices under growth-direction applied magnetic fields. Fractional-dimensional theoretical results are shown to be in good agreement with previous variational theoretical calculations and available experimental measurements.

[530]

S. T. Rittenhouse and C. H. Greene. The degenerate Fermi gas with density-dependent interactions in the large-N limit under the K-harmonic approximation. *J. Phys. B-At. Mol. Opt. Phys.*, 41(20):10, 2008.

Abstract: We present a simple implementation of a density-dependent, zero-range interaction in a degenerate Fermi gas using hyperspherical co-

ordinates in the large particle number limit. The method produces a 1D effective potential that accurately describes the ground-state energy as a function of the hyperradius of the two spin component gas throughout the vicinity of the unitarity regime. In the unitarity regime the breathing mode frequency is found to limit to the non-interacting value. A dynamical instability, similar to the Bosenova, is predicted to be possible for a gas containing more than three spin components, for large, negative, two-body scattering lengths. While the situation is less clear for the gas with three components, collapse might also be possible.

[531] J. P. Rodrigues. NUMERICAL-SOLUTION OF LATTICE SCHWINGER-DYSON EQUATIONS IN THE LARGE-N LIMIT. *Nucl. Phys. B*, 260(2):350–380, 1985.

[532] J. P. Rodrigues. Large N spectrum of two matrices in a harmonic potential and BMN energies. *J. High Energy Phys.*, (12):19, 2005.

Abstract: The large N spectrum of the quantum mechanical hamiltonian of two hermitean matrices in a harmonic potential is studied in a framework where one of the matrices is treated exactly and the other is treated as a creation operator impurity in the background of the first matrix. For the free case, the complete set of invariant eigenstates and corresponding energies are obtained. When $g(\text{YM}(2))$ interactions are added, it is shown that a full string tension corrected BMN type hamiltonian is obtained.

[533] A. Romeo. MULTIDIMENSIONAL EXTENSION OF A WENTZEL-KRAMERS-BRILLOUIN IMPROVEMENT FOR SPHERICAL QUANTUM BILLIARD ZETA-FUNCTIONS. *J. Math. Phys.*, 36(8):4005–4011, 1995.

Abstract: Some insight is offered into the dimensional dependence of the Wentzel-Kramers-Brillouin (WKB) and improved-WKB approximations introduced by Steiner in connection with hyperspherical (originally circular) quantum billiards. The accuracy of every new D-dimensional picture is estimated by examining the residues of the spectral zeta-function poles. (C) 1995 American Institute of Physics.

[534] Rosenthal, C. M. SOLUTION OF DELTA FUNCTION MODEL FOR HELIUMLIKE IONS. *J. Chem. Phys.*, 55(5):2474–2481, 1971.

[535] P. Rossi, M. Campostrini, and E. Vicari. The large- N expansion of unitary-matrix models. *Phys. Rep.-Rev. Sec. Phys. Lett.*, 302(4):144–209, 1998.

Abstract: The general features of the $1/N$ expansion in statistical mechanics and quantum field theory are briefly reviewed both from the theoretical and from the phenomenological point of view as an introduction to a more detailed analysis of the large- N properties of spin and gauge models possessing the symmetry group $SU(N) \times SU(N)$. An extensive discussion of the known properties of the single-link integral (equivalent to YM2 and one-dimensional chiral models) includes finite- N results, the external field solution, properties of the determinant, and the double scaling limit. Two major classes of solvable generalizations are introduced: one-dimensional closed chiral chains and models defined on a $d-1$ dimensional simplex. In both cases, large- N solutions are presented with emphasis on their double scaling properties. The available techniques and results concerning unitary-matrix models that correspond to asymptotically free quantum field theories (two-dimensional chiral models and four-dimensional QCD) are discussed, including strong-coupling methods, reduced formulations, and the Monte Carlo approach. (C) 1998 Elsevier Science B.V. All rights reserved.

[536] J. M. Rost. BINDING-ENERGIES OF WEAKLY BOUND SYSTEMS FROM COMPLEX DIMENSIONAL SCALING. *J. Phys. Chem.*, 97(10):2461–2463, 1993.

Abstract: In the limit of infinite spatial dimension D , the particles of a system become perfectly localized at the minimum of an effective potential surface. Perturbation theory in $1/D$ has been used successfully to predict binding energies and electronic structure in the physical three-dimensional space. For weakly bound systems which are neutral if one particle is removed the large dimensional approach has not been applicable because the effective potential surface exhibits a saddle point rather

than a global minimum. We show that the extension to complex dimensional scaling can theoretically handle this situation and gives good practical estimates for the binding energies of three-particle Coulomb systems, calculated here as an application of the new method.

- [537] J. M. Rost. THE MOLECULAR-PROPERTIES OF THE POSITRONIUM NEGATIVE-ION. *Hyperfine Interact.*, 89(1-4):343–354, 1994.

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(-).

- [538] J. M. Rost, S. M. Sung, D. R. Herschbach, and J. S. Briggs. MOLECULAR-ORBITAL DESCRIPTION OF DOUBLY EXCITED ATOMIC STATES GENERALIZED TO ARBITRARY DIMENSION. *Phys. Rev. A*, 46(5):2410–2419, 1992.

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 $D - l$, $D + 2$ is equivalent to $m - l$, $m + 1$, 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.

- [539] B. Roy. SHIFTED $1/N$ EXPANSION FOR ENERGY EIGENVALUES OF THE EXPONENTIAL COSINE SCREENED COULOMB POTENTIAL. *Phys. Rev. A*, 34(6):5108–5111, 1986.
- [540] B. Roy, P. Roy, and R. Roychoudhury. ON SOLUTIONS OF QUANTUM EIGENVALUE PROBLEMS - A SUPERSYMMETRIC APPROACH. *Fortschritte Phys.-Prog. Phys.*, 39(3):211–258, 1991.
- Abstract:** We study solutions of various quantum mechanical eigenvalue problems using the formalism of one dimensional supersymmetric quantum mechanics. The problems studied includes among other problems the non-polynomial oscillator and the doubly anharmonic oscillator potentials. The solutions obtained here are of two types - exact analytical solutions and approximate solutions. The method of obtaining exact solutions have been shown to be general enough to be applied to a large class of potentials. The method of obtaining approximate solutions have been studied in details and their accuracy have been compared with exact numerical results.
- [541] B. Roy and R. Roychoudhury. THE SHIFTED $1/N$ EXPANSION AND THE ENERGY EIGENVALUES OF THE HULTHEN POTENTIAL FOR $L = 0$. *J. Phys. A-Math. Gen.*, 20(10):3051–3055, 1987.
- [542] B. Roy and R. Roychoudhury. SHIFTED $1/N$ EXPANSION FOR THE DIRAC-EQUATION FOR VECTOR AND SCALAR POTENTIALS. *J. Phys. A-Math. Gen.*, 23(15):3555–3561, 1990.
- [543] B. Roy, R. Roychoudhury, and P. Roy. SHIFTED $1/N$ EXPANSION APPROACH TO THE INTERACTION $V(R)=R^2+\Lambda R^2/(1+GR^2)$. *J. Phys. A-Math. Gen.*, 21(7):1579–1588, 1988.
- [544] R. Roychoudhury and S. Panchanan. MODIFIED $1/N$ EXPANSION FOR THE DIRAC-EQUATION FOR SCREENED COULOMB POTENTIAL. *Z. Naturfors. Sect. A-J. Phys. Sci.*, 48(11):1081–1085, 1993.

Abstract: It is shown that if one chooses the shift parameter correctly then the lowest order term in the modified I/N expansion for the Dirac equation as formulated by Stepanov and Tutik gives accurate results for Coulomb like potentials. Explicit eigenvalues have been obtained for the screened Coulomb potential $V(r) = -\epsilon_0/r[1 - \lambda(1 - 1/z)/(1 + \lambda)]$, and these are compared with exact numerical results and the results obtained by the choice of shift suggested by Stepanov and Tutik.

- [545] R. Roychoudhury and Y. P. Varshni. ROTATING OSCILLATOR - SHIFTED 1/N EXPANSION AND SUPERSYMMETRIC CONSIDERATIONS. *Phys. Rev. A*, 37(7):2309–2313, 1988.
- [546] R. Roychoudhury and Y. P. Varshni. RELATIVISTIC 1/N EXPANSION FOR THE DIRAC-EQUATION. *Phys. Rev. A*, 39(11):5523–5527, 1989.
- [547] R. K. Roychoudhury and Y. P. Varshni. SHIFTED 1/N EXPANSION AND EXACT-SOLUTIONS FOR THE POTENTIAL $V(R)=-Z/R+GR+LAMBDA-R^2$. *J. Phys. A-Math. Gen.*, 21(13):3025–3034, 1988.
- [548] P. Sablonniere. B-splines and Hermite-Pade approximants to the exponential function. *J. Comput. Appl. Math.*, 219(2):509–517, 2008.

Abstract: This paper is the continuation of a work initiated in [P. Sablonniere, An algorithm for the computation of Hermite-Pade approximations to the exponential function: divided differences and Hermite-Pade forms. *Numer. Algorithms* 33 (2003) 443-452] about the computation of Hermite-Pade forms (HPF) and associated Hermite-Pade approximants (HPA) to the exponential function. We present an alternative algorithm for their computation, based on the representation of HPF in terms of integral remainders with B-splines as Peano kernels. Using the good properties of discrete B-splines, this algorithm gives rise to a great variety of representations of HPF of higher orders in terms of HPF of lower orders, and in particular of classical Pade forms. We give some examples illustrating this algorithm, in particular, another way of constructing quadratic HPF already

described by different authors. Finally, we briefly study a family of cubic HPF. (C) 2007 Elsevier B.V. All rights reserved.

- [549] L. Saelen, R. Nepstad, J. P. Hansen, and L. B. Madsen. The N-dimensional Coulomb problem: Stark effect in hyper-parabolic and hyperspherical coordinates. *J. Phys. A-Math. Theor.*, 40(5):1097–1104, 2007.

Abstract: We calculate the first-order energy shifts for the N-dimensional hydrogen atom exposed to a static electric field. The results are compared with numerical diagonalization of the Hamiltonian in a finite basis. Using simple scaling relations, we show how corrections to arbitrarily high order may be obtained from known results for the three-dimensional Coulomb problem.

- [550] B. Saha, S. Bhattacharyya, T. K. Mukherjee, and P. K. Mukherjee. Radial and angular correlation in heliumlike ions. *Int. J. Quantum Chem.*, 92(5):413–418, 2003.

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.

- [551] L. L. Salcedo, S. Levit, and J. W. Negele. MEAN FIELD SOLUTION OF QCD2 IN THE LARGE-N LIMIT. *Nucl. Phys. B*, 361(3):585–625, 1991.

Abstract: Two-dimensional QCD in the large- N limit is formulated as a Hartree-Fock problem and solved numerically on a lattice. Calculation of single-particle wave functions and the one-body density matrix displays the structure of baryons. Insight into the Skyrme model is provided by showing that in the limit of small quark mass, the baryon is accurately approximated by a spatially varying chiral rotation of the vacuum wave function, where the chiral angle satisfies the sine-Gordon equation. The meson spectrum is calculated in the random phase approximation. The same mean field theory is also applied to chiral and non-chiral Gross-Neveu models, where it agrees with known analytical results.

[552] A. G. Samuelson. A molecular abacus for electrons. *Curr. Sci.*, 81(2):155–157, 2001.

[553] P. Sanchez-Moreno, R. Gonzalez-Ferez, and J. S. Dehesa. Improvement of the Heisenberg and Fisher-information-based uncertainty relations for D -dimensional central potentials. *New J. Phys.*, 8:8, 2006.

Abstract: The Heisenberg and Fisher-information-based uncertainty relations are improved for stationary states of single-particle systems in a D -dimensional central potential. The improvement increases with the squared orbital hyperangular quantum number. The new uncertainty relations saturate for the isotropic harmonic oscillator wavefunction.

[554] C. Sandorfy. Remembering the old times of theoretical chemistry. *Chem. Listy*, 97(4):182–191, 2003.

Abstract: After recalling the early stages of quantum chemistry, a more detailed and systematic description of the post-war period (approx. 1945-1960) follows. The essential features of both pi-electron and sigma-electron eras are described: the simplest versions as well as procedures including electron repulsion are considered. Then attention is paid to valence and Rydberg excited states. The review is closed by remarks on hydrogen bonds and other weak intermolecular interactions.

[555]

A. Scardicchio, F. H. Stillinger, and S. Torquato. Estimates of the optimal density of sphere packings in high dimensions. *J. Math. Phys.*, 49(4):15, 2008.

Abstract: The problem of finding the asymptotic behavior of the maximal density $\phi(\max)$ of sphere packings in high Euclidean dimensions is one of the most fascinating and challenging problems in discrete geometry. One century ago, Minkowski obtained a rigorous lower bound on $\phi(\max)$ that is controlled asymptotically by $1/2(d)$, where d is the Euclidean space dimension. An indication of the difficulty of the problem can be garnered from the fact that exponential improvement of Minkowski's bound has proved to be elusive, even though existing upper bounds suggest that such improvement should be possible. Using a statistical-mechanical procedure to optimize the density associated with a "test" pair correlation function and a conjecture concerning the existence of disordered sphere packings [S. Torquato and F. H. Stillinger, *Exp. Math.* 15, 307 (2006)], the putative exponential improvement on $\phi(\max)$ was found with an asymptotic behavior controlled by $1/2((0.77865 \text{ center dot})d)$. Using the same methods, we investigate whether this exponential improvement can be further improved by exploring other test pair correlation functions corresponding to disordered packings. We demonstrate that there are simpler test functions that lead to the same asymptotic result. More importantly, we show that there is a wide class of test functions that lead to precisely the same putative exponential improvement and therefore the asymptotic form $1/2((0.77865 \text{ center dot})d)$ is much more general than previously surmised. This class of test functions leads to an optimized average kissing number that is controlled by the same asymptotic behavior as the one found in the aforementioned paper. (c) 2008 American Institute of Physics.

[556]

T. C. Scott, M. Aubert-Frecon, and J. Grotendorst. New approach for the electronic energies of the hydrogen molecular ion. *Chem. Phys.*, 324(2-3):323-338, 2006.

Abstract: Herein, we present analytical solutions for the electronic energy eigenvalues of the hydro-

gen molecular ion H_2^+ , namely the one-electron two-fixed-center problem. These are given for the homonuclear case for the countable infinity of discrete states when the $(2)Sigma^+$ states. In this case, these solutions are the roots of a set of two coupled three-term magnetic quantum number m is zero, i.e., for, recurrence relations. The eigen-solutions are obtained from an application of experimental mathematics using Computer Algebra as its principal tool and are vindicated by numerical and algebraic demonstrations. Finally, the mathematical nature of the eigenenergies is identified. (c) 2005 Elsevier B.V. All rights reserved.

- [557] G. W. Semenoff and K. Zarembo. Adjoint non-Abelian coulomb gas at large N . *Nucl. Phys. B*, 480(1-2):317–337, 1996.

Abstract: The non-Abelian analog of the classical Coulomb gas is discussed. The statistical mechanics of arrays of classical particles which transform under various representations of a non-Abelian gauge group and which interact through non-Abelian electric fields are considered. The problem is formulated on the lattice and, for the case of adjoint charges, it is solved in the large- N limit. The explicit solution exhibits a first-order confinement-deconfinement phase transition with computable properties. In one dimension, the solution has a continuum limit which describes 1+1-dimensional quantum chromodynamics (QCD) with heavy adjoint matter.

- [558] A. V. Sergeev. $1/N$ EXPANSION FOR THE 3-BODY PROBLEM. *Soviet Journal of Nuclear Physics-Ussr*, 50(4):589–592, 1989.

- [559] A. V. Sergeev and D. Z. Goodson. Self-consistent field perturbation theory of molecular vibrations. *Mol. Phys.*, 93(3):477–484, 1998.

Abstract: Perturbation theory is used to perform non-iterative calculations of energy eigenvalues of the coupled ordinary differential equations that result from imposing separability assumptions in terms of normal coordinates on vibrational wavefunctions. Various model Hamiltonians with 2 or 3 coupled normal modes are studied and

the increase of computational cost with the number of degrees of freedom is analysed. Quadratic Pade approximants of the perturbation expansions are rapidly convergent, and directly yield complex numbers for resonance eigenvalues. For a 3-mode system, results are obtained within partial separability assumptions, with a pair of modes left coupled. Large-order perturbation theory with partial separability is suggested as an alternative to low-order exact perturbation theory.

- [560] A. V. Sergeev and D. Z. Goodson. Semiclassical self-consistent field perturbation theory for the hydrogen atom in a magnetic field. *Int. J. Quantum Chem.*, 69(2):183–192, 1998.

Abstract: A recently developed perturbation theory for solving self-consistent field equations is applied to the hydrogen atom in a strong magnetic field. This system has been extensively studied using other methods and is therefore a good test case for the new method. The perturbation theory yields summable large-order expansions. The accuracy of the self-consistent field approximation varies according to field strength and quantum state but is often higher than the accuracy from adiabatic approximations. A new derivation is presented for the asymptotic adiabatic approximation, the most useful of the adiabatic approaches. This derivation uses semiclassical perturbation theory without invoking an adiabatic hypothesis. (C) 1998 John Wiley & Sons, Inc. *Int J Quant Chem* 69: 183-192, 1998.

- [561] A. V. Sergeev and D. Z. Goodson. Summation of asymptotic expansions of multiple-valued functions using algebraic approximants: Application to anharmonic oscillators. *J. Phys. A-Math. Gen.*, 31(18):4301–4317, 1998.

Abstract: The divergent Rayleigh-Schrodinger perturbation expansions for energy eigenvalues of cubic, quartic, sextic and octic oscillators are summed using algebraic approximants. These approximants are generalized 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.

- [562] A. V. Sergeev and D. Z. Goodson. Singularities of Moller-Plesset energy functions. *J. Chem. Phys.*, 124(9):11, 2006.

Abstract: The convergence behavior of Moller-Plesset (MP) perturbation series is governed by the singularity structure of the energy, with the energy treated as a function of the perturbation parameter. Singularity locations, determined from quadratic approximant analysis of high-order series, are presented for a variety of atoms and small molecules. These results can be used as benchmarks for understanding the convergence of low-order methods such as MP4 and for developing and testing summation methods that model the singularity structure. The positions and types of singularities confirm previous qualitative predictions based on functional analysis of the Schrodinger equation. (c) 2006 American Institute of Physics.

- [563] A. V. Sergeev, D. Z. Goodson, S. E. Wheeler, and W. D. Allen. On the nature of the Moller-Plesset critical point. *J. Chem. Phys.*, 123(6):11, 2005.

Abstract: It has been suggested [F. H. Stillinger, *J. Chem. Phys.* 112, 9711 (2000)] that the convergence or divergence of Moller-Plesset perturbation theory is determined by a critical point at a negative value of the perturbation parameter z at which an electron cluster dissociates from the nuclei. This conjecture is examined using configuration-interaction computations as a function of z and using a quadratic approximant analysis of the high-order perturbation series. Results are presented for the He, Ne, and Ar atoms and the hydrogen fluoride molecule. The original theoretical analysis

used the true Hamiltonian without the approximation of a finite basis set. In practice, the singularity structure depends strongly on the 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.

[564]

A. V. Sergeev and S. Kais. Variational principle for critical parameters of quantum systems. *J. Phys. A-Math. Gen.*, 32(39):6891–6896, 1999.

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 hydrogen-like basis sets.

[565]

P. Serra and S. Kais. Critical phenomena for electronic structure at the large-dimension limit. *Phys. Rev. Lett.*, 77(3):466–469, 1996.

Abstract: We show that the symmetry breaking of the electronic structure configurations at the

large-D limit is completely analogous to the standard phase transitions and critical phenomena in statistical mechanics. Electronic structure at the large-D limit exhibits critical points with mean field critical exponents ($\beta = 1/2$, $\alpha = 0$ (dis), $\delta = 3$, and $\gamma = 1$). The complete mapping is presented for the Hartree-Fock two-electron atom in weak electric field and the two Coulomb center problems.

- [566] P. Serra and S. Kais. Multicritical phenomena for the hydrogen molecule at the large-dimension limit. *Chem. Phys. Lett.*, 260(1-2):302–308, 1996.

Abstract: We show that symmetry breaking of the electronic structure configurations for the Hartree-Fock hydrogen molecule at the large-dimension limit can be described as standard phase transitions. The phase diagram in the internuclear distance-nuclear charge plane shows three different stable phases corresponding to different electronic structure configurations. This phase diagram is characterized by a bicritical point where the two continuous phase transition lines join a first order transition line.

- [567] P. Serra and S. Kais. Mean field phase diagrams for one-electron molecules. *J. Phys. A-Math. Gen.*, 30(5):1483–1493, 1997.

Abstract: We describe a simple model for symmetry breaking of electronic structure configurations of one-electron systems. This model involves generalizing the problem to D-dimensional space and finding the solution at $D \rightarrow \infty$, a semiclassical limit which can be solved exactly. The large-D limit model reduces the problem to a variational calculation which is equivalent to mean-field theories of critical phenomena in statistical mechanics. We show that symmetry breaking of electronic structure configurations can be described as standard phase transitions. Rich phase diagrams with multicritical points are reported for both linear and planar one-electron systems.

- [568] P. Serra and S. Kais. Phase transitions for N-electron atoms at the large-dimension limit. *Phys. Rev. A*, 55(1):238–247, 1997.

Abstract: Symmetry breaking of electronic structure configurations for N-electron atoms in weak magnetic and electric fields at the large-dimension limit is described in terms of standard phase transitions. This symmetry breaking, which leads to ionization, is completely analogous to phase transitions and critical phenomena in statistical mechanics. This analogy is shown by allowing the nuclear charge to play a role analogous to temperature in statistical mechanics. For the exact solution of N-electron atoms at the large-dimension limit, the symmetry breaking is shown to be a first-order phase transition. For the special case of two-electron atoms, the first-order transition shows a triple point where three phases with different symmetry coexist. Treatment of the Hartree-Fock solution reveals a different kind of symmetry breaking where second-order phase transitions exist for N=2. We show that Hartree-Fock two-electron atoms in a weak external electric field exhibit a critical point with mean field critical exponents ($\beta = 1/2$, $\alpha = 0(\text{dis})$, $\delta = 3$, and $\gamma = 1$).

[569]

P. Serra, S. Kais, and J. P. Neirotti. Finite-size scaling method for the stability of atomic and molecular ions. *Physica A*, 283(1-2):65–73, 2000.

Abstract: Phase transitions at absolute: zero temperature can take place as some parameter in the Hamiltonian of the system is varied. For the Hamiltonian of N-electron atoms, this parameter is taken to be the nuclear charge. As the nuclear charge reaches a critical point, the quantum ground state changes its characters from being bound to being degenerate or absorbed by a continuum. We describe the large-dimension approximation and the finite-size scaling method to calculate the critical nuclear charge for which an atom can bind an extra electron to form a stable negative ion. Results show that, at most, only one electron can be added to a free atom in the gas phase. The existence of doubly charged atomic negative ions in a strong magnetic field will be discussed. (C) 2000 Elsevier Science B.V. All rights reserved.

- [570] R. Sever and C. Tezcan. 1/N EXPANSION FOR A MORE GENERAL SCREENED COULOMB POTENTIAL. *Phys. Rev. A*, 36(3):1045–1049, 1987.
- [571] R. Sever and C. Tezcan. 1/N EXPANSION FOR THE EXPONENTIAL-COSINE-SCREENED COULOMB POTENTIAL. *Phys. Rev. A*, 35(6):2725–2728, 1987.
- [572] R. Sever and C. Tezcan. HYPERVIRIAL 1/N EXPANSION FOR A MORE GENERAL SCREENED COULOMB POTENTIAL. *Phys. Rev. A*, 37(8):3158–3161, 1988.
- [573] S. Shaik. The Lewis legacy: The chemical bond - A territory and heartland of chemistry. *J. Comput. Chem.*, 28(1):51–61, 2007.

Abstract: Is chemistry a science without a territory? I argue that "chemical bonding" has been a traditional chemical territory ever since the chemical community amalgamated in the seventeenth century, and even before. The modern charter of this territory is Gilbert Newton Lewis, who started the "electronic structure revolution in chemistry." As a tribute to Lewis, I describe here three of his key papers from the years 1913, 1916, and 1923, and analyze them. Lewis has defined the quantum unit, the "electron pair bond," for construction of a chemical universe, and in so doing he charted a vast chemical territory and affected most profoundly the mental map of chemistry for generations ahead. Nevertheless, not all is known about the chemical bond" the chemical territory is still teaming with new and exciting problems of in new materials, nanoparticles, quantum dots, metalloenzymes, bonding at surface-vapor interfaces, and so on and so forth. (C) 2006 Wiley Periodicals, Inc.

- [574] N. L. Sharma and M. H. Lee. WAVE VECTOR DEPENDENT SUSCEPTIBILITY OF A FREE-ELECTRON GAS IN D-DIMENSIONS AND THE SINGULARITY AT 2KF. *J. Math. Phys.*, 27(6):1618–1623, 1986.
- [575] Q. C. Shi and S. Kais. Finite size scaling for critical parameters of simple diatomic molecules. *Mol. Phys.*, 98(19):1485–1493, 2000.

Abstract: We use the finite size scaling method to study the critical points, points of non-analyticity,

of the ground state energy as a function of the coupling parameters in the Hamiltonian. In this approach, the finite size corresponds to the number of elements in a complete basis set used to expand the exact eigenfunction of a given molecular Hamiltonian. To illustrate this approach, we give detailed calculations for systems of one electron and two nuclear centres, $Z(+)\text{e}(+)Z(+)$. Within the Born-Oppenheimer approximation, there is no critical point, but without the approximation the system exhibits a critical point at $Z = Z(c) = 1.228\ 279$ when the nuclear charge, Z , varies. We show also that the dissociation occurs in a first-order phase transition and calculate the various related critical exponents. The possibility of generalizing this approach to larger molecular systems using Gaussian basis sets is discussed.

[576]

Q. C. Shi and S. Kais. Quantum criticality at the large-dimensional limit: Three-body coulomb systems. *Int. J. Quantum Chem.*, 85(4-5):307–314, 2001.

Abstract: We present quantum phase transitions and critical phenomena at the large-dimension (D) limit for three-body ABA Coulomb systems with charges (Q, q, Q) and masses (M, m, M). The Hamiltonian depends linearly on two parameters $\lambda = Q/q$ and $k = [1 + (m/M)]^{-1}$. The system exhibits critical points with mean field critical exponents ($\alpha = 0, \beta = 1/2, \delta = 3, \gamma = 1$). We calculate the critical curve $\lambda(c)$ (κ) through which all systems undergo a continuous-phase transition from the symmetrical configuration, the two like particles have the same distance from the reference particle, to the unsymmetrical phase. The critical curve at $D \rightarrow \infty$ limit is a convex function of κ and very similar to the one obtained at $D = 3$ with variational calculations. We also calculated the line of zero angular correlation in the mass polarization term, which separates the symmetrical phase to an atom-like region and a molecule-like region. (C) 2001 John Wiley & Sons, Inc.

[577]

Q. C. Shi, S. Kais, and D. R. Herschbach. Electron localization-delocalization transitions in dissociation of the

C-4(-) anion: A large-D analysis. *J. Chem. Phys.*, 120(5):2199–2207, 2004.

Abstract: We present a study, employing high level ab initio methods, of electron localization-delocalization transitions along the dissociation path of the C-4(-) anion to C-2 and C-2(-). We find that at the equilibrium geometry, the symmetrical and nonsymmetrical configurations of the linear C-4(-) anion are almost isoenergetic. However, along a collinear dissociation path, the dipole moment drops abruptly to zero when the separation between the two middle carbon nuclei reaches about $R=2.15$ Angstrom. The dipole moment remains zero until about $R=2.78$ Angstrom, and then continuously increases as dissociation proceeds. This behavior is analogous to critical phenomena: The abrupt drop to zero of the dipole moment resembles a first-order phase transition, the later steady rise resembles a continuous phase transition. We show that a simple sub-Hamiltonian model, corresponding to the large-dimension limit for an electron in the field of four collinear carbon atoms, exhibits both kinds of phase transitions along the dissociation path. (C) 2004 American Institute of Physics.

[578]

Q. C. Shi, S. Kais, F. Remacle, and R. D. Levine. On the crossing of electronic energy levels of diatomic molecules at the large-D limit. *J. Chem. Phys.*, 114(22):9697–9705, 2001.

Abstract: Analytical and numerical results are presented for the intersection of electronic energies of the same space symmetry for electrons in the field of two Coulomb centers in D-dimensions. We discuss why such crossings are allowed and may be less "exceptional" than one could think because even for a diatomic molecule there is more than one parameter in the electronic Hamiltonian. For a one electron diatomic molecule at the large-D limit, the electronic energies are shown analytically to diverge quadratically from the point of intersection. The one electron two Coulomb centers problem allows a separation of variables even when the charges on the two centers are not equal. The case of two electrons, where their Coulombic repulsion precludes an exact symmetry, is therefore treated in the large-D limit. It is then found that,

in addition to the quadratic intersection, there is also a curve crossing where the energies diverge linearly. (C) 2001 American Institute of Physics.

- [579] A. Simoes. In between worlds: G.N. Lewis, the shared pair bond and its multifarious contexts. *J. Comput. Chem.*, 28(1):62–72, 2007.

Abstract: In this paper, I will look at the rather convoluted discovery process which gave birth to the concept of the shared electron pair bond as developed by G.N. Lewis, to be subsequently appropriated by the American founders of quantum chemistry, and highlight the complex relations between conceptual development and the different contexts in which ideas are created and presented. I will show how the successive installments of Lewis's model of the chemical bond were supported by and gained credence from an epistemological background in which Lewis explored the relations of chemistry to physics. Furthermore, they were shaped by the changing public contexts in which the successive metamorphoses of the ideas took place and their epistemological background was outlined and explored. The complexities which are always associated with a discovery process can therefore be illuminated if one pays attention to different interactive realms—the conceptual, epistemological, and the presentational one. (C) 2006 Wiley Periodicals, Inc.

- [580] B. Simon. LARGE ORDERS AND SUMMABILITY OF EIGENVALUE PERTURBATION-THEORY - A MATHEMATICAL OVERVIEW. *Int. J. Quantum Chem.*, 21(1):3–25, 1982.

- [581] A. Sinha, R. Roychoudhury, and Y. P. Varshni. Shifted $1/N$ expansion for confined quantum systems. *Can. J. Phys.*, 78(2):141–152, 2000.

Abstract: In this paper we formulate the shifted $1/N$ expansion method for constrained quantum mechanical systems with spherically symmetric potentials. As an example, we apply our technique to the confined Hulthen potential $V(r) = -Z \delta e(-\delta r)/1-e(-\delta r)$ for different values of the confinement parameter b and the screening parameter δ . It is found that the agreement between

our results and the exact numerical values is reasonably good.

[582] M. Sinharoy, R. S. Gangopadhyay, and B. Duttaroy. LOW-ENERGY POTENTIAL SCATTERING AND THE LIMIT OF LARGE DIMENSIONALITY. *J. Phys. A-Math. Gen.*, 17(13):L687–L690, 1984.

[583] H. Stahl. Quadratic Hermite-Pade polynomials associated with the exponential function. *J. Approx. Theory*, 125(2):238–294, 2003.

Abstract: The asymptotic behavior of quadratic Hermite-Pade polynomials $p(n)$, $q(n)$, $r(n)$ is an element of P_n associated with the exponential function is studied for $n \rightarrow \infty$. These polynomials are defined by the relation $p(n)(z) + q(n)(z)e(z) + r(n)(z)e(2z) = O(z^{3n+2})$ as $z \rightarrow 0$, (*) where $O((.))$ denotes Landau's symbol. In the investigation analytic expressions are proved for the asymptotics of the polynomials, for the asymptotics of the remainder term in (*), and also for the arcs on which the zeros of the polynomials and of the remainder term cluster if the independent variable z is rescaled in an appropriate way. The asymptotic expressions are defined with the help of an algebraic function of third degree and its associated Riemann surface. Among other possible applications, the results form the basis for the investigation of the convergence of quadratic Hermite-Pade approximants, which will be done in a follow-up paper. (C) 2003 Elsevier Inc. All rights reserved.

[584] S. S. Stepanov and R. S. Tutik. A NEW $1/N$ -EXPANSION PROCEDURE. *Zhurnal Eksperimentalnoi Teor. Fiz.*, 100(2):415–421, 1991.

Abstract: An effective method is developed for calculating the $1/N$ -expansion coefficients of arbitrary high orders both for the ground and radially excited states of the discrete spectrum of the Schrodinger equation. The method is based on the semiclassical interpretation of the $1/N$ -expansion. The explicit application of the expansion over the Planck's constant clarifies the cause of the complementarity in the $1/N$ -approach and WKB approximation. The transition to the Riccati equation and

h-expansion allows to apply the quantization condition for involving the wavefunction nodes, what results in the simple recursive relations. In the example of the funnel - shaped potential the calculations are given for the first ten coefficients in the $1/n$ -expansion scheme for energy with the various values of the orbital and radial quantum numbers.

[585]

S. S. Stepanov and R. S. Tutik. A NEW TECHNIQUE FOR DERIVING THE LARGE-N SOLUTION OF THE KLEIN-GORDON EQUATION. *J. Phys. A-Math. Gen.*, 24(9):L469-L474, 1991.

Abstract: A new procedure for deriving the energy values of the Klein-Gordon equation with a potential having both scalar and vector components is described. Using the h-expansion and the quantization condition recursion formulae were obtained which can readily be applied to any $1/N$ -expansion scheme. These formulae have simple structures both for background and excited states and provide, in principle, the calculation of $1/N$ -corrections up to an arbitrary order. Contrary to the methods elaborated formerly our technique does not involve converting the initial equation to the shortened, Schrodinger-like form. For the Coulomb potential the solutions of the Klein-Gordon and shortened equations are compared.

[586]

S. S. Stepanov and R. S. Tutik. $1/N$ -EXPANSION FOR THE KLEIN-GORDON EQUATION. *Zhurnal Eksperimentalnoi Teor. Fiz.*, 101(1):18-25, 1992.

Abstract: An effective method for calculating the $1/N$ -expansion coefficients for the discrete spectrum of the Klein - Gordon equation is developed. Based on the use of the h-expansion and quantization conditions, the method leads to the simple recurrence formulae which allow to derive the coefficients of arbitrary high orders both for the ground and radially excited states. As an example, the calculations of the energy eigenvalues for the Coulomb interaction and the funnel-shaped potential are considered within the $1/n$ -expansion scheme.

- [587] S. S. Stepanov and R. S. Tutik. A NEW APPROACH TO THE 1/N-EXPANSION FOR THE DIRAC-EQUATION. *Phys. Lett. A*, 163(1-2):26–31, 1992.

Abstract: The difficulties associated with the application of the 1/N-expansion to the Dirac equation have been resolved by applying the method of hBAR-expansion. This technique does not involve converting the initial equation into a Schrodinger-like or Klein-Gordon-like form. Obtained recurrence formulae have a simple form both for the ground and excited states, and allow one to find the 1/N-corrections of an arbitrary order in any of the 1/N-expansion schemes. The method restores the exact results for the Coulomb potential.

- [588] S. S. Stepanov and R. S. Tutik. EXPANSION WITH RESPECT TO \hbar FOR BOUND-STATES OF THE SCHRODINGER-EQUATION. *Theor. Math. Phys.*, 90(2):139–145, 1992.

Abstract: A WKB-complementing hBAR expansion for bound states of the radial Schrodinger equation is discussed. A recursive method for calculating the quantum corrections of any order to the energy of the classical motion is presented. The use of quantization conditions makes it possible to write down recursion relations in an equally simple form for the ground and radially excited states. The connection between the approach and the 1/N expansion is considered. It is shown that the method can also be used for analysis in the (l, E) plane in the form of a hBAR expansion for Regge trajectories.

- [589] F. H. Stillinger. AXIOMATIC BASIS FOR SPACES WITH NON-INTEGER DIMENSION. *J. Math. Phys.*, 18(6):1224–1234, 1977.

- [590] F. H. Stillinger. PLANCKS-CONSTANT EXPANSIONS FOR BOUND-STATES. *Phys. Rev. A*, 43(7):3317–3324, 1991.

Abstract: Planck's constant \hbar is a fundamental physical parameter that establishes the scale of quantum phenomena. Bound-state energy eigenvalues for several well-known systems (e.g., harmonic oscillators, Morse oscillators, and square-well potentials) are formally analytic functions of

\hbar in the neighborhood of $\hbar = 0$, and any "physical" state can be reached in principle by analytic continuation. This paper explores the possibility of developing power series in \hbar for atomic and molecular energies, with analytic continuation to access physical states. For this purpose it is necessary to modify Coulomb interactions at short range to keep the potential bounded below. As a result the \hbar expansions appear naturally as Rayleigh-Schrodinger perturbation series in anharmonicity about collective harmonic-oscillator states. Physical eigenvalues emerge in the strong-coupling limit, and Pade approximants seem to be analytical tools well suited for entering the regime. Some basic implementation details are presented for application to the modified hydrogen atom, the two-electron isoelectronic atomic sequence, and many-electron atoms.

- [591] U. Sukhatme and T. Imbo. SHIFTED $1/N$ EXPANSIONS FOR ENERGY EIGENVALUES OF THE SCHRÖDINGER-EQUATION. *Phys. Rev. D*, 28(2):418–420, 1983.
- [592] U. P. Sukhatme, B. M. Lauer, and T. D. Imbo. POTENTIAL SCATTERING AND LARGE- N EXPANSIONS. *Phys. Rev. D*, 33(4):1166–1173, 1986.
- [593] J. H. Summerfield, G. S. Beltrame, and J. G. Loeser. A simple model for understanding electron correlation methods. *J. Chem. Educ.*, 76(10):1430–1438, 1999.
- [594] J. H. Summerfield and J. G. Loeser. Dimension-dependent two-electron Hamiltonian matrix elements. *J. Math. Chem.*, 25(2-3):309–315, 1999.

Abstract: Since the birth of quantum mechanics the ground state electronic energy of the two-electron atom has received special attention. This is because the two-electron system is the simplest atom to include electron-electron interactions. These interactions are key to understanding many-electron systems. This paper adds to the knowledge of two-electron atoms by presenting closed form solutions for Hamiltonian matrix elements at arbitrary spatial dimension, D . The basis functions are the D -dependent hydrogenic wavefunctions: $1s(2), 2p(2), 3d(2), 4f(2)$. The

electron-electron repulsion integrals are solved by the Fourier integral transform.

[595]

S. M. Sung and D. R. Herschbach. HIDDEN SYMMETRY AND EXPLICIT SPHEROIDAL EIGENFUNCTIONS OF THE HYDROGEN-ATOM. *J. Chem. Phys.*, 95(10):7437–7448, 1991.

Abstract: The Schrodinger equation for a hydrogenic atom is separable in prolate spheroidal coordinates, as a consequence of the "hidden symmetry" stemming from the fixed spatial orientation of the classical Kepler orbits. One focus is at the nucleus and the other a distance R away along the major axis of the elliptic orbit. The separation constant α is not an elementary function of Z or R or quantum numbers. However, for given principal quantum number n and angular momentum projection m , the allowed values of α and corresponding eigenfunctions in spheroidal coordinates are readily obtained from a secular equation of order $n - m$. We evaluate $\alpha(n,m;ZR)$ and the coefficients $g(l, \alpha)$ that specify the spheroidal eigenfunctions as hybrids of the familiar nlm_i hydrogen-atom states with fixed n and m but different l values. Explicit formulas and plots are given for α and $g(l, \alpha)$ and for the probability distributions derived from the hybrid wave functions, $\text{SIGMA}(l)g(l, \alpha)nlm_i$, for all states up through $n = 4$. In the limit $R \rightarrow \infty$ these hybrids become the solutions in parabolic coordinates, determined simply by geometrical Clebsch-Gordan coefficients that account for conservation of angular momentum and the hidden symmetry. We also briefly discuss some applications of the spheroidal eigenfunctions, particularly to exact analytic solutions of two-center molecular orbitals for special values of R and the nuclear charge ratio $Z(a)/Z(b)$.

[596]

S. M. Sung and J. M. Rost. CHEMICAL-BINDING FROM THE INFINITE DIMENSIONAL LIMIT. *J. Phys. Chem.*, 97(10):2479–2483, 1993.

Abstract: The electronic structure of molecules calculated in the limit of infinite spatial dimensions is related to properties in three-dimensional

space. In the spirit of the electrostatic theorem, we introduce the concept of antibinding and binding regions to visualize chemical binding. In addition, criteria are developed to determine the ionic or covalent character of the bond. The computational effort requires only the minimization of a multidimensional potential surface at the infinite dimensional limit, yet detailed information can be extracted. Numerical examples are given for the one-electron diatomic molecule.

[597]

A. A. Suvernev and D. Z. Goodson. Dimensional perturbation theory for vibration-rotation spectra of linear triatomic molecules. *J. Chem. Phys.*, 107(11):4099–4111, 1997.

Abstract: A very efficient large-order perturbation theory is formulated for the nuclear motion of a linear triatomic molecule. All coupling between vibration and rotation is included. To demonstrate the method, all of the experimentally observed rotational energies, with values of J almost up to 100, for the ground and first excited vibrational states of CO₂ and for the ground vibrational states of N₂O and of OCS are calculated. The perturbation expansions reported here are rapidly convergent. The perturbation parameter is $D^{-1/2}$, where D is the dimensionality of space. Increasing D is qualitatively similar to increasing the angular momentum quantum number J . Therefore, this approach is especially suited for states with high rotational excitation. The computational cost of the method scales only in proportion to $JN(\text{nu})^{5/3}$, where N - nu is the size of the vibrational basis set. (C) 1997 American Institute of Physics.

[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 H₂ 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 inter-electron 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.

- [602] K. Szalewicz, K. Patkowski, and B. Jeziorski. Intermolecular interactions via perturbation theory: From diatoms to biomolecules. In *Intermolecular Forces and Clusters Ii*, volume 116 of *Structure and Bonding*, pages 43–117. Springer-Verlag Berlin, Berlin, 2005.
- [603] R. Szmytkowski. Closed forms of the Green's function and the generalized Green's function for the Helmholtz operator on the N-dimensional unit sphere. *J. Phys. A-Math. Theor.*, 40(5):995–1009, 2007.
- Abstract:** The Green's function for the Helmholtz differential operator $\Delta + \lambda(\lambda + N - 1)$ on the N-dimensional (with $N \geq 1$) hyperspherical surface S_N of unit radius is investigated. Its closed form is shown to be $G^{(N)}(\lambda; n, n') = \pi/(N - 1) S_N \sin(\pi \lambda) C_{-\lambda}^{((N-1)/2)}(-n \cdot n')$, where S_N is the area of S_N , $C_{-\lambda}^{(\alpha)}$ is the Gegenbauer function of the first kind, while n and n' are radius vectors, with respect to the centre of S_N , of the observation and source points, respectively. The Green's function $G^{(N)}(\lambda; n, n')$ fails to exist whenever λ is such that it holds that $\lambda(\lambda + N - 1) = L(L + N - 1)$, with L is an element of \mathbb{N} . For these exceptional cases, the generalized (known also as 'modified' or 'reduced') Green's function $G^{(L)}(\lambda; n, n')$ is considered. It is shown that $G^{(L)}(\lambda; n, n')$ may be expressed compactly in terms of the Gegenbauer polynomial $C_L^{((N-1)/2)}(n \cdot n')$ and the derivative $[6C_{\lambda}^{((N-1)/2)}(-n \cdot n')/6\lambda]_{\lambda=L}$. Explicit expressions for the derivatives $[6C_{\lambda}^{(n)}(x)/6\lambda]_{\lambda=L}$ and $[6C_{\lambda}^{((n+1)/2)}(x)/6\lambda]_{\lambda=L}$, with n is an element of \mathbb{N} , are found and used to transform the functions $G^{(L)}((2n+1); n, n')$ and $G^{(L)}((2n+2); n, n')$ to potentially more useful forms.
- [604] A. Z. Tang and F. T. Chan. SHIFTED $1/N$ EXPANSION FOR THE HULTHEN POTENTIAL. *Phys. Rev. A*, 35(2):911–914, 1987.
- [605] G. Tanner, K. Richter, and J. M. Rost. The theory of two-electron atoms: between ground state and complete fragmentation. *Rev. Mod. Phys.*, 72(2):497–544, 2000.

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 experi-

mental spectra.

- [606] C. Tezcan and R. Sever. A General Approach for the Exact Solution of the Schrodinger Equation. *Int. J. Theor. Phys.*, 48(2):337–350, 2009.

Abstract: The Schrodinger equation is solved exactly for some well known potentials. Solutions are obtained reducing the Schrodinger equation into a second order differential equation by using an appropriate coordinate transformation. The Nikiforov-Uvarov method is used in the calculations to get energy eigenvalues and the corresponding wave functions.

- [607] K. W. Thompson. DETERMINATION OF GROUND-STATE OF 3-BODY SYSTEMS. *Phys. Rev. A*, 17(5):1583–1591, 1978.

- [608] O. I. Tolstikhin and M. Matsuzawa. Exploring the separability of the three-body Coulomb problem in hyperspherical elliptic coordinates. *Phys. Rev. A*, 63(6):23, 2001.

Abstract: An approximate symmetry of the three-body Coulomb problem which reveals itself via approximate separability of the hyperspherical adiabatic (HSA) eigenvalue problem in hyperspherical elliptic (HSE) coordinates (η , ξ) and thus is intimately related to the HSA approximation is discussed. The additional integral of motion responsible for this separability is specific to the Coulomb interaction and generalizes the Laplace-Runge-Lenz vector known from the two-body Coulomb problem and the integral of separation constant of the two-center Coulomb problem. In the zeroth approximation, this symmetry leads to a completely separable representation of the three-body wave function, where each state is labeled by a pair of HSE quantum numbers ($n(\eta)$, $n(\xi)$) that generalize the spheroidal quantum numbers for diatomic molecules, on the one hand, and the Herrick-Lin quantum numbers for two-electron atoms, on the other. This approximation is illustrated by calculations for a number of three-body Coulomb systems for states with zero total angular momentum. Taking into account the nonadiabatic couplings as well as the nonseparable

part of the Coulomb potential by mixing a few separable states permits one to obtain accurate results for systems with arbitrary masses and charges of particles and for a wide spectrum below the three-body breakup threshold.

- [609] E. Toprak and O. T. Turgut. Large N limit of SO(N) scalar gauge theory. *J. Math. Phys.*, 43(3):1340–1352, 2002.

Abstract: In this paper we study the large N-c limit of SO(N-c) gauge theory coupled to a real scalar field following ideas of Rajeev [Int. J. Mod. Phys. A 9, 5583 (1994)]. We will see that the phase space of this resulting classical theory is Sp(1)(H)/U(H+) which is the analog of the Siegel disk in infinite dimensions. The linearized equations of motion give us a version of the well-known 't Hooft equation of two dimensional quantum chromodynamics. (C) 2002 American Institute of Physics.

- [610] S. Torquato and F. H. Stillinger. Exactly solvable disordered sphere-packing model in arbitrary-dimensional Euclidean spaces. *Phys. Rev. E*, 73(3):8, 2006.

Abstract: We introduce a generalization of the well-known random sequential addition (RSA) process for hard spheres in d-dimensional Euclidean space R-d. We show that all of the n-particle correlation functions of this nonequilibrium model, in a certain limit called the "ghost" RSA packing, can be obtained analytically for all allowable densities and in any dimension. This represents the first exactly solvable disordered sphere-packing model in an arbitrary dimension. The fact that the maximal density $\phi(\infty)=1/2(d)$ of the ghost RSA packing implies that there may be disordered sphere packings in sufficiently high d whose density exceeds Minkowski's lower bound for Bravais lattices, the dominant asymptotic term of which is $1/2(d)$. Indeed, we report on a conjectural lower bound on the density whose asymptotic behavior is controlled by $2(-0.778\ 65\dots)d$, thus providing the putative exponential improvement on Minkowski's 100-year-old bound. Our results suggest that the densest packings in sufficiently high dimensions may be disordered rather than periodic, implying

the existence of disordered classical ground states for some continuous potentials.

- [611] C. A. Traynor and D. Z. Goodson. DIMENSIONAL SCALING FOR H-2(+) WITHOUT THE BORN-OPPENHEIMER APPROXIMATION. *J. Phys. Chem.*, 97(10):2464–2466, 1993.

Abstract: The standard dimensional continuation of the Schrodinger equation, in which the kinetic energy is generalized to arbitrary D, while the potential energy is left unchanged, leads to dissociation of H-2+ in the limit of large D if the nuclei are allowed to move freely. In general, the definition chosen for the D-dimensional Schrodinger equation is arbitrary as long as the correct equation results at D = 3. We propose a mild dimension dependence for the potential of the internuclear repulsion. This yields a stable and physically reasonable chemical bond in the limit D \rightarrow infinity and can therefore be used as the starting point for a dimensional perturbation theory without the Born-Oppenheimer approximation.

- [612] D. F. T. Tuan. DOUBLE PERTURBATION THEORY FOR HE-LIKE SYSTEMS. *J. Chem. Phys.*, 50(6):2740–&, 1969.

- [613] R. S. Tutik. EXACT SOLUTION OF THE N-DIMENSIONAL GENERALIZED DIRAC-COULOMB EQUATION. *J. Phys. A-Math. Gen.*, 25(8):L413–L417, 1992.

Abstract: An exact solution to the bound state problem for the N-dimensional generalized Dirac-Coulomb equation, whose potential contains both the Lorentz-vector and Lorentz-scalar terms of the Coulomb form, is obtained.

- [614] V. M. Vainberg, V. A. Gani, and A. E. Kudryavtsev. High-order perturbation theory for the hydrogen atom in a magnetic field. *J. Exp. Theor. Phys.*, 86(2):305–311, 1998.

Abstract: The states of a hydrogen atom with principal quantum numbers n less than or equal to 3 in a constant uniform magnetic field H are studied. Coefficients in the expansion of the energy of these states in powers of H-2 up to the 75th order are obtained. Series for the energies of the states

and the wave functions are summed to values of H on the order of the atomic magnetic field. A generalization of the moment method upon which these calculations are based can be used in other cases in which a hydrogen atom is perturbed by a potential with a polynomial dependence on the coordinates. (C) 1998 American Institute of Physics.

- [615] V. M. Vainberg, V. D. Mur, V. S. Popov, and A. V. Sergeev. STRONG-FIELD STARK-EFFECT. *Jetp Lett.*, 44(1):9–13, 1986.
- [616] V. M. Vainberg, V. D. Mur, V. S. Popov, A. V. Sergeev, and A. V. Shcheblykin. THE $1/N$ EXPANSION IN QUANTUM-MECHANICS. *Theor. Math. Phys.*, 74(3):269–278, 1988.
- [617] V. M. Vainberg, V. D. Mur, V. S. Popov, and A. V. Shcheblykin. $1/N$ -DECOMPOSITION FOR THE STARK-EFFECT IN A STRONG FIELD. *Doklady Akademii Nauk Sssr*, 299(5):1116–1120, 1988.
- [618] V. M. Vainberg, V. S. Popov, and A. V. Sergeyev. $1/N$ -EXPANSION FOR THE HYDROGEN-ATOM IN AN EXTERNAL-FIELD. *Zhurnal Eksperimentalnoi Teor. Fiz.*, 98(3):847–860, 1990.
- [619] S. M. Valone. A DIMENSIONALLY SCALED GENERALIZATION OF CONSTRAINED SEARCH ENERGY DENSITY FUNCTIONALS. *Int. J. Quantum Chem.*, 49(5):591–600, 1994.
- Abstract:** A dimensionally scaled generalization of constrained search density functional theory allows access to some simple model problems. These might be valuable for testing and perhaps improving conventional density functionals. One specific model problem is solved: When extrapolated to infinite numbers of spatial dimensions, the energy density functional for spherically symmetric, two-electron systems can be calculated to arbitrary accuracy. (C) 1994 John Wiley and Sons, Inc.
- [620] P. D. Vandermerwe. SEMICLASSICAL THEORY OF THE HELIUM ATOMIC SPECTRUM. *J. Chem. Phys.*, 81(12):5976–5985, 1984.
- [621] P. D. Vandermerwe. ELECTRON CORRELATIONS IN DOUBLY EXCITED HELIUM. *J. Chem. Phys.*, 82(11):5293–5293, 1985.

- [622] P. D. Vandermerwe. ELECTRON CORRELATIONS IN THE DOUBLE-EXCITED HELIUM ISOELECTRONIC SEQUENCE. *Phys. Rev. A*, 34(4):3452–3453, 1986.
- [623] P. D. Vandermerwe. STRUCTURAL ARRANGEMENT OF QUARKS IN 3-PARTICLE SYSTEMS. *Phys. Rev. D*, 33(11):3383–3390, 1986.
- [624] P. D. Vandermerwe. DILEPTONIC-HELIUM GROUND-STATE ENERGY. *Phys. Rev. A*, 38(3):1187–1192, 1988.
- [625] P. D. Vandermerwe. EXOTIC ATOMS AS A PROTOTYPE OF THE GENERAL 3-PARTICLE COULOMB PROBLEM. *Phys. Rev. A*, 40(4):1785–1794, 1989.
- [626] P. D. Vandermerwe. ISOTOPIC SCALING FEATURES OF MOLECULAR-IONS AND THEIR DESCENDANTS. *Phys. Lett. A*, 168(5-6):405–408, 1992.
- Abstract:** An analytic treatment of the ground-state energy of homonuclear molecular ions, based on the large-dimensional approach, is presented. It encodes scaling features for these systems and their three-particle counterparts.
- [627] P. D. T. Vandermerwe. CRITICAL COUPLING AND SYMMETRY BREAKDOWN IN 3-PARTICLE ELECTROMAGNETIC SYSTEMS. *Phys. Rev. A*, 36(7):3446–3448, 1987.
- [628] P. I. Vandermerwe. THE HYDROGEN-ATOM AS PROTOTYPE OF THE LARGE-N EXPANSION. *Lettere Al Nuovo Cimento*, 37(3):86–88, 1983.
- [629] Y. P. Varshni. EIGENERGIES OF THE $R^2 + \text{LAMBDA} R^2 / (1 + GR^2)$ POTENTIAL OBTAINED BY THE SHIFTED $1/N$ EXPANSION. *Phys. Rev. A*, 36(7):3009–3014, 1987.
- [630] Y. P. Varshni. COMPARISON OF $1/N$ EXPANSION AND SHIFTED $1/N$ EXPANSION FOR EIGENERGIES OF AN ATOMIC POTENTIAL. *Phys. Rev. A*, 38(3):1595–1598, 1988.
- [631] Y. P. Varshni. COMPARISON OF METHODS FOR IMPROVING THE $1/N$ EXPANSION. *Phys. Rev. A*, 40(4):2180–2183, 1989.
- [632] Y. P. Varshni. EIGENERGIES AND OSCILLATOR-STRENGTHS FOR THE HULTHEN POTENTIAL. *Phys. Rev. A*, 41(9):4682–4689, 1990.

- [633] Y. P. Varshni. WKB APPROXIMATION FOR THE ROTATING MORSE OSCILLATOR. *Can. J. Phys.*, 71(3-4):122–127, 1993.

Abstract: The WKB approximation is applied to the rotating Morse oscillator. Results are presented for the ground state of the H-2 molecule and are compared with those obtained by several other methods. The WKB method gives the best results for $v \geq 5$. At smaller values of v , the WKB results are only slightly less accurate than the best ones.

- [634] Y. P. Varshni. BOUND-STATES FOR THE ROTATING RYDBERG OSCILLATOR. *Chem. Phys.*, 188(2-3):197–204, 1994.

Abstract: Three methods for calculating the levels of the rotating Rydberg oscillator are compared: Two versions of the shifted $1/N$ expansion and the WKB method. Results are presented for the ground state of the H-2 molecule. The WKB method gives the best results for a majority of the levels. In other cases the WKB results are only slightly less accurate than the best ones.

- [635] V. M. Veinberg and V. S. Popov. SUMMATION OF PERTURBATION-SERIES AND CLASSICAL MECHANICS. *Doklady Akademii Nauk Sssr*, 289(5):1095–1099, 1986.

- [636] F. Vinette and J. Cizek. PERTURBATION ENERGY EXPANSION USING HYPERVIRIAL THEOREM AND SYMBOLIC COMPUTATION FOR THE N-DIMENSIONAL HYDROGEN-ATOM IN AN EXTERNAL SPHERICALLY SYMMETRIC FIELD. *Comput. Phys. Commun.*, 52(1):35–41, 1988.

- [637] E. R. Vrscay. RAYLEIGH-SCHRODINGER PERTURBATION EXPANSIONS FOR A HYDROGEN-ATOM IN A POLYNOMIAL PERTURBATION. *Int. J. Quantum Chem.*, 32(5):613–620, 1987.

- [638] J. R. Walkup, M. Dunn, and D. K. Watson. Branch-point structure and the energy level characterization of avoided crossings. *J. Math. Phys.*, 41(1):218–239, 2000.

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 δ (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 δ -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.

- [640] J. R. Walkup, M. Dunn, D. K. Watson, and T. C. Germann. Avoided crossings of diamagnetic hydrogen as functions of magnetic field strength and angular momentum. *Phys. Rev. A*, 58(6):4668–4682, 1998.

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- m spectra can be predicted by visually scanning the locations of these branch points in the complex- δ plane, where $\delta = 1/(2 + 2m)$ is the perturbation parameter used in this research. [S1050-2947(98)07111-X].

- [641] L. Y. Wang, X. Y. Gu, Z. Q. Ma, and S. H. Dong. Exact solutions to D -dimensional Schrodinger equation with a pseudoharmonic oscillator. *Found. Phys. Lett.*, 15(6):569–576, 2002.

Abstract: The exact solutions to the Schrodinger equation with a pseudoharmonic oscillator in an arbitrary dimension D is presented.

- [642] Z. W. Wang and X. X. Guan. Variational calculation of the energy for helium-like ground state from $Z=2$ to 5. *J. Chin. Chem. Soc.*, 48(3):515–520, 2001.

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.

- [643] S. Watanabe, M. Ledourneuf, and L. Pelamourgues. HYPERSPHERICAL ANALYSIS OF ELECTRONIC CORRELATIONS IN MULTIPLY-EXCITED STATES. *Journal De Physique*, 43(NC2):223–241, 1982.

- [644] S. Watanabe and C. D. Lin. DEMONSTRATION OF MOLECULE-LIKE MODES OF DOUBLY EXCITED-STATES IN HYPERSPHERICAL COORDINATES. *Phys. Rev. A*, 34(2):823–837, 1986.

- [645] D. K. Watson and D. Z. Goodson. DIMENSIONAL PERTURBATION-THEORY FOR WEAKLY-BOUND SYSTEMS. *Phys. Rev. A*, 51(1):R5–R8, 1995.

- [646] D. K. Watson and B. A. McKinney. Improved large- N limit for Bose-Einstein condensates from perturbation theory. *Phys. Rev. A*, 59(5):4091–4094, 1999.

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 $N \rightarrow \infty$ 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].

- [647] Q. Wei, S. Kais, and D. Herschbach. Dimensional scaling treatment of stability of atomic anions induced by superintense, high-frequency laser fields. *J. Chem. Phys.*, 127(9):6, 2007.

Abstract: We show that dimensional scaling, combined with the high-frequency Floquet theory, provides useful means to evaluate the stability of gas phase atomic anions in a superintense laser field. At the large-dimension limit ($D \rightarrow \infty$), in a suitably scaled space, electrons become localized along the polarization direction of the laser field. We find that calculations at large D are much simpler than $D=3$, yet yield similar results for the field strengths needed to bind an "extra" one or two electrons to H and He atoms. For both linearly and circularly polarized laser fields, the amplitude of quiver motion of the electrons correlates with the detachment energy. Despite large differences in scale, this correlation is qualitatively like that found between internuclear distances and dissociation energies of chemical bonds. (C) 2007 American Institute of Physics.

- [648] Q. Wei, S. Kais, and D. Herschbach. Dimensional scaling treatment of stability of simple diatomic molecules induced by superintense, high-frequency laser fields. *J. Chem. Phys.*, 129(21):8, 2008.

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 ($D \rightarrow \infty$) 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.

- [649] V. M. Weinberg, V. D. Mur, V. S. Popov, and A. V. Sergeev. HYDROGEN-ATOM IN A STRONG ELECTRIC-FIELD. *Zhurnal Eksperimentalnoi Teor. Fiz.*, 93(2):450–462, 1987.
- [650] W. N. Whitton. ANALYTIC CONTINUATION OF A GROUP OF EIGENVALUES. *Mol. Phys.*, 36(4):941–972, 1978.
- [651] E. Witten. BARYONS IN THE 1-N EXPANSION. *Nucl. Phys. B*, 160(1):57–115, 1979.
- [652] E. Witten. INSTANTONS, THE QUARK-MODEL, AND THE 1-N EXPANSION. *Nucl. Phys. B*, 149(2):285–320, 1979.
- [653] E. Witten. QUARKS, ATOMS, AND THE 1-N EXPANSION. *Phys. Today*, 33(7):38–43, 1980.
- [654] E. Witten. LARGE N CHIRAL DYNAMICS. *Ann. Phys.*, 128(2):363–375, 1980.
- [655] K. Wodkiewicz. FERMI PSEUDOPOTENTIAL IN ARBITRARY DIMENSIONS. *Phys. Rev. A*, 43(1):68–76, 1991.

Abstract: The theory of zero-range potentials is investigated in an arbitrary number of dimensions. Except for the trivial one-dimensional case the zero-range potentials are described by nonlocal operators called Fermi pseudopotentials. It is shown that in odd dimensions the Fermi pseudopotentials involve a very simple regularization operator. In even dimensions with the help of dimensional regularization, explicit formulas for the

Fermi pseudopotentials are derived. The Green's functions, the propagators, and the exact solutions of the Lippmann-Schwinger equations are derived in explicit forms. In odd dimensions $d = 1$ and 3 the Fermi pseudopotentials can be applied to describe multiphoton processes of atoms and molecules with very short-range interactions. In even dimension $d = 2$ the Fermi pseudopotential can be applied to describe tunneling from laser-driven quantum wells. Physical applications involving higher d are also possible.

- [656] L. G. Yaffe. LARGE N LIMITS AS CLASSICAL MECHANICS. *Rev. Mod. Phys.*, 54(2):407–435, 1982.
- [657] L. G. Yaffe. LARGE-N QUANTUM-MECHANICS AND CLASSICAL LIMITS. *Phys. Today*, 36(8):50–57, 1983.
- [658] Z. Yalcin, M. Aktas, and M. Simsek. Exact solutions of the Schrodinger equation for S-1,S-3 states of He atom with Fues-Kratzer-type potential. *Int. J. Quantum Chem.*, 76(5):618–625, 2000.

Abstract: In this article exact solutions of a two-electron Schrodinger equation for the Coulomb potential were extended to the Fues-Kratzer-type potential: $((Z) \text{ over cap}(\Omega)/r) + ((A) \text{ over cap}/r(2))$. 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.

- [659] Z. C. Yan and J. Y. Zhang. Energies of the hydrogen molecular ions in high-angular-momentum states. *J. Phys. B-At. Mol. Opt. Phys.*, 37(5):1055–1059, 2004.

Abstract: The one-centre three-body nonadiabatic method (Yan et al 2003 Phys. Rev. A 67 062504) is extended to the hydrogen molecular ions in higher angular momentum states. The nonrelativistic energies are reported for H-2(+), D-2(+),

T-2(+) HD+, HT+ and DT+ in their lowest excited L-states with L ranging from 2 to 12. The accuracy for the calculated energies is at the level of a few parts in 10^{17} to 10^{20} .

- [660] R. J. Yanez, W. Vanassche, and J. S. Dehesa. POSITION AND MOMENTUM INFORMATION ENTROPIES OF THE D-DIMENSIONAL HARMONIC-OSCILLATOR AND HYDROGEN-ATOM. *Phys. Rev. A*, 50(4):3065–3079, 1994.

Abstract: The position- and momentum-space entropies of the isotropic harmonic oscillator and the hydrogen atom in D dimensions are shown to be related to some entropy integrals which involve classical orthogonal polynomials. These integrals are exactly calculated for Chebyshev polynomials and only in an approximate way for Gegenbauer polynomials. The physical entropies are explicitly obtained in the ground state and in a few low-lying excited states. Finally, the dimensionality dependence of the ground-state entropies of the two above-mentioned quantum-mechanical systems is analyzed (numerically) and the values of the entropies in a large class of excited states of the D-dimensional ($D = 1, 2, 3$) harmonic oscillator and hydrogen atom are tabulated and discussed.

- [661] T. Yoneya and H. Itoyama. INTERNAL COLLECTIVE MOTIONS AND THE LARGE-N LIMIT IN FIELD-THEORIES. *Nucl. Phys. B*, 200(3):439–456, 1982.

- [662] E. P. Yukalova and V. I. Yukalov. SELF-SIMILAR APPROXIMATION FOR AN ANHARMONIC-OSCILLATOR OF ARBITRARY DIMENSIONALITY. *Phys. Lett. A*, 175(1):27–35, 1993.

Abstract: The quartic anharmonic oscillator in a space of arbitrary dimensionality is considered by the method of self-similar approximations. This method, invoking only two terms of the perturbation theory, is shown to be capable of providing quite a good accuracy, within an order of 10^{-3} , for all energy levels and all anharmonicity constants. A comparison with other known analytical methods, using the same number of perturbative terms, proves that the self-similar approximations are more accurate.

- [663] K. Zarembo. Lattice gauged principal chiral field at large N. *Theor. Math. Phys.*, 104(1):777–782, 1995.

Abstract: The lattice model of a principal chiral field interacting with gauge fields which have no kinetic term is considered. The complete set of equations for collective field variables is derived in the large N limit. The continuum limit and the phase structure of the model are discussed.

- [664] G. J. Zeng, K. L. Su, and M. Li. MOST GENERAL AND SIMPLEST ALGEBRAIC RELATIONSHIP BETWEEN ENERGY EIGENSTATES OF A HYDROGEN-ATOM AND A HARMONIC-OSCILLATOR OF ARBITRARY DIMENSIONS. *Phys. Rev. A*, 50(5):4373–4375, 1994.

- [665] Y. H. Zhao and C. L. Zhao. High-order perturbed corrections with scaling transformation. *Chin. Phys. B*, 17(8):2783–2789, 2008.

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 $r \rightarrow r/Z$ 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.

- [666] M. Znojil. MODIFIED RAYLEIGH-SCHRODINGER PERTURBATION-THEORY. *Phys. Rev. A*, 35(6):2448–2454, 1987.

- [667] M. Znojil. A quick perturbative method for Schrodinger equations. *J. Phys. A-Math. Gen.*, 30(24):8771–8783, 1997.

Abstract: Within the framework of perturbation theory we propose, firstly, an iterative method which may serve as a source of optimal unperturbed solutions in both one and more dimensions. It combines the Runge-Kutta and Newton algorithm and its efficiency is illustrated on a few quartic oscillators. Secondly, admitting also an arbitrary perturbation of potentials we generalize the existing Runge-Kutta one-dimensional Rayleigh-Schrodinger constructions of energies and wavefunctions to more dimensions.

- [668] M. Znojil and U. Gunther. Dynamics of charged fluids and $1/l$ perturbation expansions. *J. Phys. A-Math. Theor.*, 40(26):7375–7388, 2007.

Abstract: Some features of the calculation of fluid dynamo systems (spherically symmetric $\alpha(2)$ -dynamos) in magnetohydrodynamics are studied, the problem connected with the presence of mixed (Robin) boundary conditions is addressed and a new treatment for it is proposed. The perturbation formalism of large- l expansions is shown to be applicable and its main technical steps are outlined.

- [669] M. Znojil, D. Yanovich, and V. P. Gerdt. New exact solutions for polynomial oscillators in large dimensions. *J. Phys. A-Math. Gen.*, 36(23):6531–6549, 2003.

Abstract: A new type of exact solvability is reported. The Schrodinger equation is considered in a very large spatial dimension D much greater than 1 and its central polynomial potential is allowed to depend on 'many' ($= 2q$) coupling constants. In a search for its bound states possessing an exact and elementary wavefunction (proportional to a harmonic-oscillator-like polynomial of a freely varying, i.e., not just small, degree N), the 'solvability conditions' are known to form a complicated nonlinear set which requires a purely numerical treatment at a generic choice of D , q and N . Assuming that D is large we discovered and demonstrate that this problem may be completely factorized and acquires an amazingly simple exact solution at all N and up to $q = 5$ at least.