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13. ABSTRACT *(Maximum 200 words)*

The Workshop on Coupled-Cluster Theory at the Interface of Atomic Physics and Quantum Chemistry brought together two different groups of scientists who had previously had little interaction, but who were linked by the need for high accuracy correlated calculations for electron ic structure in atoms and molecules. One group were experts in coupled-cluster (CC) and many-body perturbation methods (MBPT) approachesa for electron correlation in molecules. and had developed very powerful tools for determining molecular structure and spectra using CC/MBPT methods. The second group was primarily concerned with important applications to weak interactions in atoms. whild employing many-body techniques in their calculations. Many examples were shown that demonstrate numerically the inherent superiority of CC methods for electron correlation compared to most other approaches.

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Final Report

Workshop on Coupled-Cluster Theory at the Interface of Atomic Physics and Quantum Chemistry

August 6–11, 1990

Institute for Theoretical Atomic and Molecular Physics
at the Harvard-Smithsonian Center for Astrophysics
Cambridge, MA

Rodney J. Bartlett
University of Florida
Gainesville, FL

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Institute for Theoretical Atomic and Molecular Physics
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Air Force Office of Scientific Research
University of Florida, Division of Sponsored Research
Floating Point Systems, Portland, OR

This report summarizes the Workshop on Coupled-Cluster Theory at the Interface of Atomic Physics and Quantum Chemistry, held August 6–11, 1990, at the Institute for Theoretical Atomic and Molecular Physics at the Harvard-Smithsonian Center for Astrophysics. The schedule of talks is shown in Appendix A, while the papers to be published in two special issues of Theoretica Chimica Acta are listed in Appendix B.

The workshop brought together two different groups of scientists who had previously had little interaction, but who were linked by the need for high accuracy correlated calculations for electronic structure in atoms and molecules. One group were experts in coupled-cluster (CC) and many-body perturbation (MBPT) approaches for electron correlation in molecules, and had developed very powerful tools for determining molecular structure and spectra using CC/MBPT methods. The second group was primarily concerned with important applications to weak interactions in atoms, while employing many-body techniques in their calculations.

I. Parity Violation in Atoms

The subject of weak interactions in atoms falls into two categories

i. Parity violation in atoms due to neutral weak interactions
ii. Electric Dipole Moment (EDM) of atoms due to parity and time-reversal violation

The standard electroweak unification model of Weinberg and Salem predicts a parity violating neutral weak interaction between the constituents of an atom in addition to the usual electromagnetic interaction.

The neutral weak interaction which is mediated by a particle called Z_0, mixes states of opposite parities; thereby giving rise to an electric dipole transition between states of the same symmetry. Several ingenious experiments have been carried out on atomic cesium, thallium, bismuth and lead to detect such an electric dipole transition. The most accurate experiment to date is on cesium where the electric dipole transition moment has been measured to an accuracy of 2% by Wieman and co-workers. The accuracy of the measurements on bismuth and thallium are soon expected to match that of cesium. The experimental results when combined with accurate relativistic many-body calculations confirm the validity of the standard model. If the combined accuracy of the atomic experiments and calculations improve, it may be possible to draw certain conclusions about a variety of unification models that go beyond the standard model.

It is a well-established fact that an atom can possess a permanent electric dipole moment (EDM) if parity and time-reversal violating interactions between the constituents of an atom exist. Since parity violation has been observed earlier, the significance of observing a permanent EDM is that it would be the first ever direct signature of T violation. Furthermore the combined results of atomic EDM experiments and calculations can shed light on the origin of CP violation; one of the most challenging problems of contemporary physics.

II. Coupled-Cluster Theory

The extreme accuracy required by the parity violation problem requires very high accuracy in the solution of the electron correlation problem. The coupled cluster (CC) method as developed by Coester, Kümmel and Čížek is ideally suited to such levels of accuracy. The progress in the further development of these approaches, as summarized at the workshop in chemistry by Bartlett and in physics by Bishop, has been exceptional. The range of applications and dramatic accuracy achieved in barely a decade attests to the fundamental advantages of CC. However, to treat the parity and time reversal problem with the full power of coupled cluster theory requires that several elements in the theory be formulated, further improved, or implemented. This includes:

- Dirac-Fock based relativistic CC theory
- Open-shell single and multi-reference CC approaches
- CC methods for electronic excited states
- CC methods for the treatment of properties

Each of these requirements further generates several competing approaches discussed at the workshop that can be recommended by various criteria.

In the following some attempt is made to summarize some of the profitable areas of attack identified at the workshop that should lead to important developments in the field.

III. Research Opportunities in Coupled-Cluster Theory

- Multi-reference CC generalizations for potential energy surfaces.

  For excited states, ionization potentials, electron affinities, and Auger spectroscopy, Fock space multi-reference methods (as discussed at the workshop by Mukherjee, Kaldor, Rittby and Bartlett) are nearing a wide and routine level of applicability. Important contributions remain, however, in determining transition moments and in separating the true correlation effects from the somewhat artificial "spectator" terms that emerge in the Fock space theory. For example, the latter prohibits a Fock space MRCC method limited to all single and double excitations (MRCCSD) from giving the correct answer for the two-particle problem, since some Fock space S_3 operators of spectator type appear even for two particles.

  The alternative Hilbert space MRCC (Meissner, Balkova, Bartlett, Paldus, Jeziorski) would not have this problem. However, it replaces the "hierarchical waveoperator" of the Fock space approaches with another operator. In principle, this waveoperator should be simpler to use, as it does not have to simultaneously describe the correct eigenstates of all N-1 and N+1 electron states, in addition to the N electron states. The first results reported using the Hilbert space method were presented at the meeting (Balkova, et al. and Paldus, et al.).

  A very important development presented at the meeting was the generalization of the Hilbert space MRCC to *incomplete* active spaces (Meissner). This makes the theory primed for a burst of computational activity. Although this helps to alleviate the severe problem of

intruder states, it is not resolved. Much activity in this area will be reported in the next few years.

- Besides MRCC methods, excited and ionized states can also be treated by equation-of-motion (EOM) (Bartlett, Mukherjee, Meissner), also called linear response (Monkhorst) coupled-cluster methods. These are potentially of very general applicability. However, they do not provide entirely (size)extensive results for excited states (Meissner, Bartlett). According to Mukherjee's remarks at the workshop, they can be said to be "valence extensive", however, meaning that the extensivity errors should not be nearly as great as in CI type methods. Such methods also offer a route toward time-dependent properties (Liu, Kelly, Sekino). Research in the area of time dependent CC theory is likely to pay important dividends in the future.

- Analytic derivatives and properties.

  In molecular theory, it is essential to analytically evaluate the derivative of the energy with atomic displacement to effectively search potential energy surfaces. The theory for first derivatives of single reference CC methods has been presented since 1984 by Bartlett and co-workers. Implementations for gradients on potential energy surfaces for closed shell molecules have been available since 1987 from Scuseria, Schaefer and co-workers. This procedure also provides a route toward other properties, as first derivatives with respect to other parameters than nuclear displacements, since the method introduces the so-called "relaxed" density that in CC/MBPT takes the place of an ordinary expectation value density as an essential computational and conceptual tool. That is,

$$E^{\alpha} = \langle H^{\alpha} \rangle = \langle o|\Lambda^{\dagger} H^{\alpha} exp(T)|o\rangle$$

  Hence, all "first-order" properties like dipole and quadrupole moments, field gradients, etc. are routinely available. The rôle of $\Lambda^{\dagger}$ is to replace the first-order perturbated wavefunction with a perturbation independent quantity.

  Second-order properties in addition to force constants, like polarizabilities, spin-spin coupling constants, dipole derivatives, and others, are not yet obtainable purely analytically, but would instead require numerical differentiation of analytically computed first derivatives. Clearly, the analytical evaluation of such higher-order properties would be highly desirable. The generalization to higher order analytical derivatives is not easy, although the theory has been presented by Salter and Bartlett, J. Chem. Phys. (1989) and a preliminary implementation for Hessians made (Koch, et al., J. Chem. Phys., 1989). Furthermore, as yet, there are no open-shell coupled-cluster analytical gradient methods yet implemented.

- Alternative unitary cluster ansatz.

  Closely tied to the question of properties in CC theory, is that of alternative ansätze for extensive CC-like wavefunctions. That is, instead of standard CC theory, modifications can be made without jeopardizing the fundamental rationale for CC theory, namely the extensive property, while offering some alternative advantages that normal CC theory does not have. An example is the importance of a stationary principle for an energy functional derived

from an extensive wavefunction ansatz. The unitary CC method falls into this category (Kutzelnigg, Bartlett). Unlike normal CC, where closed form equations are obtained for T amplitudes, the unitary (UCC) approach begins with

$$E = \langle o|exp\left(\tau^{\dagger}\right) H exp(\tau)|o\rangle$$

for τ = T - $T^{\dagger}$, which does not terminate. This necessitates truncation and variation, $\delta E/\delta T^{\dagger}$ to define equations for the amplitudes in T (and τ). However, unlike normal CC theory, such variation results in the UCC wavefunction satisfy the Hellmann-Feynman theorem, i.e.

$$\frac{\partial E}{\partial \alpha} = \langle o|exp\left(\tau^{\dagger}\right) H^{\alpha} exp(\tau)|o\rangle_{TRUNCATED}$$

where the expression for the derivative has to be truncated in the same way as the energy functional itself. This makes it far easier to obtain analytical derivatives. Results were reported (Watts and Bartlett, Chem. Phys. Lett., 1989) and presented at the workshop.

Another advantage to this approach is that Hermitian symmetry is maintained throughout all the equations. This, too, differs substantially from the inherently unsymmetric normal CC method and has the advantage that important higher-order correlation corrections can be introduced much more tractably than they would be in normal CC. In his talk at the workshop, Kutzelnigg uses an error analysis to argue that this is a more accurate procedure.

- Extended CC theory (Arponen and Bishop) is another approach that offers an alternative ansatz in CC theory, with particular relevance to properties. A property like $E^{\alpha} = \partial E/\partial \alpha$, may be written in ECCM as

$$E^{\alpha} = \langle o|exp\left(\tilde{\Sigma}\right) H^{\alpha} (exp\Sigma)|o\rangle_{DL}$$

where the DL indicates a double linked structure. Unlike the unitary approach and closer to the first approach for properties in the normal CC theory, where $exp\left(\tilde{\Sigma}\right)$ is replaced by $\Lambda^{\dagger}$, $\tilde{\Sigma}$ and Σ depend upon different amplitudes, requiring that twice as many be obtained as in the UCC method. However, unlike normal CC, ECCM offers a structure that requires that all amplitude diagrams be connected from above and below. CI coefficients are not generally connected, while normal CC only has the amplitude expressions connected from the bottom. It is argued that this structure is essential in correctly describing more difficult situations including phase transitions (Arponen, Bishop, Kümmel). Also, unlike UCC, the ECCM equations naturally terminate as do the normal CC equations, but with more complicated and higher order contributions.

- The need for a coupled-cluster method that is suitable to relativistic phenomena is apparent. For atoms, relativistic linearized CC methods have been used for partiy violation in Cs, as discussed at this workshop (Blundell, Sapirstein, Hartley and Martensson-Pendrill). Yet the power of CC theory lies in the non-linear terms, so these must be included as well. Also, no attempt to do molecules with a correct relativistic approach has yet been made. The necessity of employing complex orbitals throughout the calculation greatly complicates the

programming, but this is an important area for advancement (Sekino, Das, Mohanty). Mohr emphasized the importance of quantum electrodynamic effects in high-Z ions, particularly electron-electron interactions on the self-energy and two photon exchange corrections.

- The indirect inclusion of additional correlation effects in CC theory also drew attention (Jankowski, Paldus). It was demonstrated that requiring least-squares satisfaction of the single excitation projection of $\exp(T_2)$ along with the double excitation projection, which is an overdetermined set of equations, enables avoiding a singularity that occurs in the linearized (LCCD) equations. Similar techniques could potentially be exploited to include certain effects of triple excitations (an n^7 procedure) indirectly in a computation scheme effectively limited to just single and double excitations (an n^6 procedure.

- The description of open-shell systems with CC theory can be accomplished in single and multi-reference forms. The former benefits from the same ease of application as the single reference closed-shell theory and may be accomplished with an unrestricted Hartree-Fock (HF) reference, a restricted open-shell HF reference (Hubac), or what has been called a quasi-restricted HF (QRHF) reference (Rittby) which constructs a high spin open-shell reference from a set of orbitals taken from another system, usually a closed-shell anion or cation. Since the latter function is not variationally optimum for the atom or molecule, it is only a viable starting point because of the $\exp(T_1)$ operator in a coupled-cluster wavefunction, $exp(T_1 + T_2 + \ldots)|o\rangle$, as $exp(T_1)$ builds in the flexibility to rotate the orbitals as necessary for the problem. In the UHF case, $exp(T)|UHF\rangle$ is not an eigenfunction of spin, while the others satisfy the projected spin eigenfunction property, $\langle ROHF|\hat{S}^2 exp(T)|ROHF\rangle = S(S+1)$ as does the QRHF equivalent. This is often important for highly spin contaminated cases (Bartlett, Rittby, Scuseria).

  Whereas, the wavefunction $exp(T)|ROHF\rangle$ is not a spin eigenfunction of spin, it is possible to rigorously formulate a ROHF based CC method that is. This was discussed by Janssen at the workshop. Another approach that applies to the same problem was discussed by Jeziorski.

- The resolution of intruder state problems in CC theory is critical to viable multi-reference techniques. A particularly incisive analysis was offered by Morgan, who demonstrated its resolution in high-order perturbation theory studies.

- The need for extremely high numerical accuracy in many problems including parity violation recommend the use of new, numerical or explicitly correlated approaches in many-body methods. Drake employed Hylleraas type explicitly correlated functions in his highly accurate results for Rydberg states of He, while Jeziorski and Monkhorst report excellent results for explicitly correlated functions for small molecules. Morrison considered spline type functions to obtain effectively numerical accuracy in many body calculations.

IV. Summary

To try to summarize the meeting briefly, many examples (Scuseria, Bartlett, Paldus) were shown that demonstrate numerically the inherent superiority of CC methods for electron correlation compared to most other approaches. Generally, more accurate energies, frequencies

and properties for molecules are obtained for less computational effort than offered by other *ab initio* techniques. Similarly, far more accurate results for the transition moments for C_s (6s-7s), essential to the parity violation problem are being obtained with even linearized CC methods (Blundell, Sapirstein, Mårtensson-Pendrill).

Attacking even more difficult problems, CC methods were shown to reliably describe spin lattices (Bishop) and various kinds of model systems (Paldus, Čížek) even including the description of phase transitions (Bishop). The conclusion is inescapable. Current CC methods are perhaps the most powerful and accurate available for a wealth of different problems that even transcend electronic structure. Furthermore, the current methods are being continually improved, such as through multi-reference generalization and others discussed above, that offer even greater potential in the future.

V. Acknowledgment

A workshop of this quality cannot be held without the generous assistance of several agencies. We are indebted to the Institute for Theoretical Atomic and Molecular Physics, the National Science Foundation, Award No. 9014077, the Air Force Office of Scientific Research, Grant No. 90–0298, University of Florida, Division of Sponsored Research, and Floating Point Systems, Portland, Oregon. We are particularly appreciative of the assistance, hospitality and facilities offered by the Institute for Theoretical Atomic and Molecular Physics, and particularly its director, Professor Alex Dalgarno, Dr. Kate Kirby and Dr. George Victor. They along with their staff, Ms. Valerie Sorenson and Ms. Verity Parris and my secretary, Mrs. Sue Linsley, were critical in making the meeting a success.

VI. Appendix A — List of Participants and Schedule

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Schedule of Presentations

	Monday, August 6	
7:00-9:00	*RECEPTION*	ITAMP - Perkin Lobby
	Tuesday, August 7	NOTE: all lectures will be held in the Pratt Conference Room #G-03 and G-04
8:45-9:00	Opening Remarks	A. Dalgarno
Session I.	**Coupled-Cluster Theory**	**Chairman: A. Dalgarno**
9:00 -9:45	Origins of Coupled-Cluster Theory	H. Kümmel
9:45-10:30	Origins of Coupled-Cluster Theory for Atoms and Molecules	J. Čížek
	Coffee	
10:45-11:30	Survey of Applications of CC Theory in Chemistry	R. Bartlett
11:30-12:15	Survey of Applications of CC Theory in Physics	R. Bishop
12:15-12:30		Discussion
	Lunch	
Session II.	**Parity Violation, Time Reversal and Related Problems**	**Chairman: G. Victor**
		Contributors:
2:00-2:45	Review of Parity Non-Conserving Phenomena in Atoms and Molecules	A.M. Martensson-Pendrill
2:45-3:30	Calculations of Parity Nonconservation in Atomic Cesium	S. Blundell
	Break	
3:45-4:15	Particle Physics Implications of High-Accuracy Analysis of PNC in Cesium	J. Sapirstein
4:15-4:45	Calculations of PNC and EDM Effects in Cesium and Thallium	A. Hartley
4:45-5:15	Relativistic Many-Body Calculations of Electric Dipole Moments of Alkali Atoms Due to Parity and Time Reversal Violation	B.P. Das

5:15-6:00	A CC Theory Calculation for Parity-nonconserving Transition in Cesium	Contributions from floor Z. Liu (15 min.) *Others* Discussion
	Wednesday, August 8	
Session III.	**Relativistic and QED Effects in Atoms and Molecules**	**Chairman: K. Kirby**
9:00-9:45	Field Theoretic Effects in Highly Charged Ions	J. Sapirstein
9:45-10:30	QED Effects in Atomic Structure	P. Mohr
	Coffee	
10:45-11:30	Energies and QED Effects in the Rydberg States of Helium	G.W.F. Drake
11:30-12:30	Relativistic Many-Body Calculations by Gaussian Spinors	Contributions from floor H. Sekino (15 min.)
	Many-Body Perturbation Theory and Coupled-Cluster Theory Using the Numerical Multiconfiguration Dirac-Fock Basis Set	B.P. Das (15 min.)
	Variational Stability of Dirac-Fock Calculations in Atoms and Molecules	A.K. Mohanty (15 min.)
	Multi-reference CC Method Based on Multiconfiguration Dirac-Fock Wavefunctions	Z. Liu (15 min.) *Others* Discussion
	Lunch	
Session IV.	**Open-Shell Single-Reference CC Methods**	**Chairman: R. Bartlett**
2:00-2:45	Spin-Restricted Open-Shell Coupled-Cluster Theory	B. Jeziorski
2:45-3:30	Restricted Hartree-Fock and Unrestricted Hartree-Fock as Reference States in Many-Body Perturbation Theory: A Critical Comparison of the Two Approaches	I. Hubac
	Break	
3:45-4:15	Spin Restricted Open-Shell CC Methods	C. Jannsen (with H.F. Schaefer)
4:15-6:00		Contributions from floor

	Aspects of Size-Extensivity in the Open-Shell Coupled Cluster Formulation Based on a Single Reference State	D. Mukherjee (15 min.)
	Application of Open-Shell Coupled Cluster Theory to As_2, Ga_2 and GaAs Compounds	G. Scuseria (15 min.)
	Open-Shell Coupled-Cluster Applications with Closed-Shell Reference Functions	U. Kaldor (15 min.)
		Others
		Discussion
	Thursday, August 9	
Session V.	**Multi-Reference CC Methods**	**Chairman: J. Čížek**
9:00-9:45	Multireference Coupled Cluster Approach: An Overview of The Recent Developments	D. Mukherjee
9:45-10:30	Medium- and Large-Scale Applications of Multireference CCM: Feasibility and Performance	U. Kaldor
	Coffee	
10:45-11:30	Towards a State-Universal Multi-Reference Coupled-Cluster Approach: Model Study of a Two-Reference Case	J. Paldus
11:30-12:45		Contributions from floor
	A General Model-Space Coupled-Cluster Method Using a Hilbert Space Approach	L. Meissner (15 min.)
		K. Jankowski (15 min.)
	Complete vs. Incomplete Model Space Multireference Coupled Cluster Method. The Study of Prototype Systems LiH, BeH_2 and H_2O	A. Balkova (15 min.)
	Applications of Multi-Reference Coupled Cluster Theory in Fock Space	M. Rittby (15 min.)
		Others
		Discussion
Session VI.	**Properties in CC Theory**	**Chairman: R. Bishop**
2:00-2:15	Overview	R. Bartlett
2:15-3:00	Equilibrium Structures, Vibrational Frequencies and Energetics of Chemical Reactions as Predicted by Coupled Cluster Methods	G. Scuseria

3:00-3:45	Excitation and Ionization Energies With the Fock Space Coupled-Cluster Method	H. Monkhorst
	Coffee	
4:00-6:00		Contributions from floor
	Demands on Coupled-Cluster Methods for Calculations of Parity Non-Conservating Phenomena	A.M. Martensson-Pendrill (15 min.)
	Properties and Stationarity Conditions in Coupled Cluster Theory	W. Kutzelnigg (15 min.)
	The Quantization of Vibrational-Electronic (V-E) Molecular Hamiltonian	I. Hubac (15 min.)
	Non-Linear Response Property in CC Theory	H. Sekino (15 min.)
	NCM Expectation Value Functional and the Hellmann-Feynman Theorem	J. Arponen (15 min.)
	Application of CC Theory for Atomic Dynamic Polarizabilities	Z. Liu (15 min.)
	Open-Shell Single-Reference Coupled Cluster Calculations With General Reference Determinants	M. Rittby (15 min.)
		Others
		Discussion
7:00 p.m.	*BANQUET* - supported by Floating Point Systems	Agassiz Room - Charles Hotel
	Friday, August 10	
Session VII.	**Extended, Unitary and Other Modified CC Methods**	**Chairman: H. Kümmel**
9:00-9:45	Independent Cluster Methods as Mappings of Quantum Theory into Classical Mechanics: Principles and Future Prospects	J. Arponen
9:45-10:15	Handling of Higher Than Pair Clusters in Single-Reference Approaches	J. Paldus
	Coffee	
10:30-11:00	Unitary Coupled-Cluster Theory	W. Kutzelnigg
11:00-12:30		Contributions from floor
	Practical Applications of the Extended CC Method Using Gauge-Field Techniques	R. Bishop (15 min.)

	A New Cluster Expansion for the Treatment of Strong Relaxation Effects: Core-Hole Ionization Events	D. Mukherjee (15 min.)
	Results of Unitary CC Theory	R. Bartlett (30 min.)
		Others
		Discussion
Session VIII.	**Miscellaneous Topics in Many-Body Theory**	**Chairman: J. Paldus**
2:00-2:45	Peculiarities of the Description of Electron Correlation Effects in Atoms	K. Jankowski
2:45-3:30	Finding and Avoiding Singularities in Perturbation Expansions	J. Morgan
	Break	
3:45-4:30	Error Analysis and Improvement of Coupled-Cluster Theory	W. Kutzelnigg
4:30-6:00		Contributions from floor
	Coments on Regularization and Truncation in ECCM	J. Arponen (15 min.)
	Equation-of-Motion CC Methods for Excited States	R.J. Bartlett (15 min.)
	Gaussian Type Geminals in MBPT/CC Calculations	B. Jeziorski (15 min.)
	Transformation of the Hamiltonian in Excitation Energy Calculations: Comparison Between Fock-Space MRCC and EOMCC Methods	L. Meissner (15 min.)
	A Holomorphic Representation Approach to the CC Parametrizations of Model Field Theories	R. Bishop (15 min.)
		Others
		Discussion
	Saturday, August 11	
Session IX.	**Miscellaneous Topics**	**Chairman: J. Arponen**
9:00-9:30	Some Recent Developments in CC Theory	J. Čížek
9:30-10:00	Spline Calculations of the Photoionization Cross Section of H_3^+	J. Morrison
	Coffee	

10:15-10:45	A CC Approach to Quantum Spin Chains and Lattices	R. Bishop
10:45-11:15	Various Contributions of Quantum Chemistry to Steps in the Muon Catalyzed Fusion Process	H. Monkhorst
11:15-11:45	Comparison of Variational Calculations With Core Polarization Models	G.W.F. Drake
11:45-12:00		Discussion
		Adjourn

VII. Appendix B — Papers to be Published

1. J. Arponen — Independent-Cluster Methods as Mappings of Quantum Theory into Classical Mechanics
2. A. Balkova, S.A. Kucharski, L. Meissner, and R.J. Bartlett — A Hilbert Space Multi-Reference Coupled Cluster Study of the H_4 Model System
3. J. Arponen and R.F. Bishop — A Holomorphic Representation Approach to the Regularization of Model Field Theories in Coupled Cluster Form
4. R.F. Bishop — An Overview of Coupled Cluster Theory and Its Applications in Physics
5. R.F. Bishop, J.B. Parkinson and Y. Xian — A Coupled-Cluster Study of the Ground-State Energy and Properties of an Anisotropic Quantum Spin Lattice Model Exhibiting Antiferromagnetism in Various Phases
6. S.A. Blundell, A.C. Hartley, Z. Liu, A. Martensson-Pendrill and J. Sapirstein — Calculations of the Parity Non-Conserving 6s- > 7s Transition in Caesium
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