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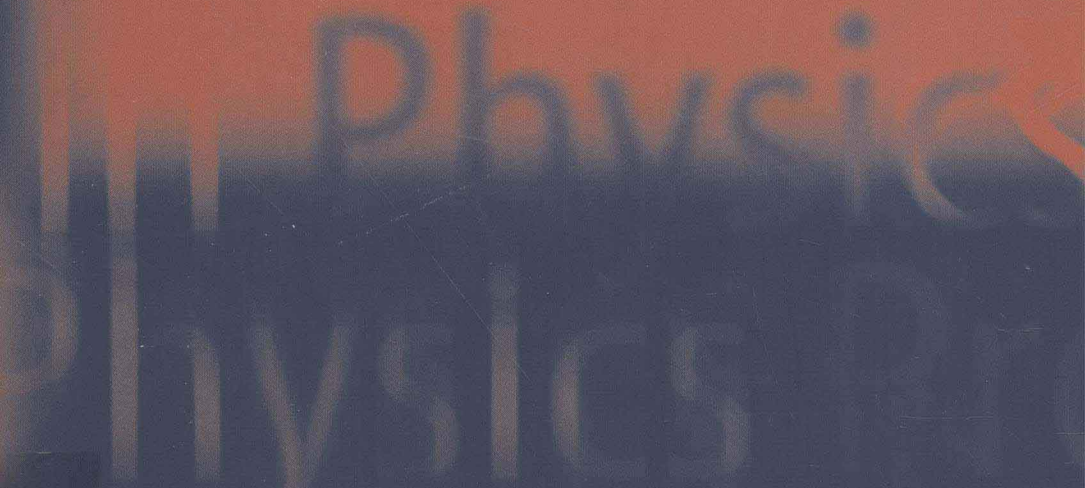
Computer Simulation Studies in Condensed-Matter Physics XIII



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Computer Simulation Studies in Condensed-Matter Physics XIII

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With 100 Figures

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Preface

Almost fifteen years ago, because of the phenomenal growth in the power of computer simulations, The University of Georgia formed the first institutional unit devoted to the use of simulations in research and teaching: The Center for Simulational Physics. As the international simulations community expanded further, we sensed a need for a meeting place for both experienced simulators and neophytes to discuss new techniques and recent results in an environment which promoted extended discussion. As a consequence, the Center for Simulational Physics established an annual workshop on Recent Developments in Computer Simulation Studies in Condensed Matter Physics. This year's workshop was the thirteenth in this series, and the continued interest shown by the scientific community demonstrates quite clearly the useful purpose that these meetings have served. The latest workshop was held at The University of Georgia, February 21–25, 2000, and these proceedings provide a "status report" on a number of important topics. This volume is published with the goal of timely dissemination of the material to a wider audience.

We wish to offer a special thanks to the IBM Corporation for its generous support of this year's workshop. We also acknowledge the Donors of the Petroleum Research Fund, administered by the American Chemical Society, and the National Science Foundation for partial support.

This volume contains both invited papers and contributed presentations on problems in both classical and quantum condensed matter physics. We hope that each reader will benefit from specialized results, as well as profit from exposure to new algorithms, methods of analysis, and conceptual developments.

Athens, GA, USA,
August 2000

D. P. Landau
S. P. Lewis
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Computer Simulation Studies in Condensed-Matter Physics: An Introduction

D.P. Landau, S.P. Lewis, and H.-B. Schüttler

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Computer simulation studies in condensed matter physics play an ever increasing role in many areas of investigation. The "status report" which is contained in this volume is the result of presentations and discussion which took place during the 13th Annual Workshop at the Center for Simulational Physics. The texts of both longer, invited presentations as well as a number of contributed papers are included. The reader will find that the scope of simulational/computational studies is broad and that substantial potential for cross-fertilization of methods between different sub-fields exists.

Part I contains five papers on recent work on interacting quantum systems. In the first paper, Antropov reviews the current status of the application of generalized density functional theory (DFT) to first-principles calculations of dynamical spin correlations, effective local moment spin interaction parameters and quantum spin noncollinear effects. An "adiabatic" approximation scheme is outlined for the DFT treatment of spin dynamics, exploiting the separation of time scales between "slow" low-energy spin and "fast" electronic excitations in magnetic local moment systems. The second paper, by Capriotti and Sorella, presents a Green's function Monte Carlo study of the frustrated spin-1/2 square lattice Heisenberg model with near neighbor antiferromagnetic spin exchange interactions. They focus on the parameter regime where the frustration is strong enough to destroy long-range antiferromagnetic order in the groundstate and compare their results with RVB groundstates. In the next paper, Chandrasekharan and Osborn describe recent approaches for solving or alleviating the sign problem in quantum Monte Carlo simulations, based on so-called meron cluster algorithms. After a pedagogical discussion, they describe special cases, including interacting fermion models, where the sign problem can be eliminated via the meron approach. They also consider cases where a more efficient simulation of quantum lattice models is possible by way of novel representations which initially introduce a minus sign, but which then can be made "minus-sign-free" by the meron approach. The paper by Hellberg describes a new implementation of the Lanczos exact diagonalization approach for calculations of the low-temperature thermodynamics in quantum lattice models. His approach allows the systematic calculation of the many-body energy density of states in a single run of the basic Lanczos iteration process. He applies this approach to the frustrated quantum spin model, proposed to describe the quantum disordered

antiferromagnet CaV_4O_9. Moukouri et al. describe the recent development of the dynamical cluster approximation (DCA) for strongly interacting electron models. This approach reduces the treatment of an infinite lattice to that of a self-consistently embedded finite cluster, without violating fundamental analyticity requirements of the self-energy. The systematic improvement of the DCA approach with increasing embedded cluster size is explicitly illustrated for the single-particle Green's function of the one-dimensional Hubbard model.

Part II contains papers that deal with diverse developments in the methodology of simulation and analysis. The chapter begins with a paper by Adler and Berengolts which presents a novel parallel algorithm for groundstate searches of models in condensed matter physics. A master-slave message-passing arrangement appropriate to diverse systems is employed with good success. De Raedt et al. then describe an approach to the simulation of a quantum computer. They present a program that contains a graphical user interface and solves the time-dependent Schrödinger equation for several Hamiltonians. Examples are shown for a 4-qubit computer. In the following manuscript, Fasnacht and Swendsen discuss methods for dealing with problems in dynamically optimized Monte Carlo methods. They describe a method to detect problems as well as to accelerate decorrelation. Next, Michielsen et al. describe a morphological image analysis method to characterize shape and topology. They show the result of the application of this method to A/B binary polymer blends. In the final paper in this section, Muñoz et al. construct an n-fold way type algorithm which can be applied to systems with continuous degrees of freedom. Test results are shown for the classical Heisenberg model on simple cubic lattices.

Part III of this report focuses on investigations of the effects of defects and disorder on lattices. The section begins with a description by Nieminen et al. of large-scale *ab initio* electronic-structure calculations of the structural, electronic, and local vibrational properties of oxygen impurities in silicon. By studying the energetics of impurity clustering in the silicon lattice, they have identified the structure of the oxygen dimer and have analyzed the atomic geometry of the thermal double donor in silicon. Next, Jain reports on the nonequilibrium dynamics of the disordered, two-dimensional Ising model at zero temperature for both the bond-diluted and $\pm J$ models of disorder. He examines the effect of the existence and type of disorder on the persistence behavior and blocking exhibited by spin systems. The work by Schröder et al. presents an algorithm for computing the exact groundstate of a collection of self-avoiding flux lines in the presence of disorder. Their method is of the combinatorial-optimization class and is based on the minimum cost flow algorithm. In the subsequent paper, Knetter et al. use this algorithm to examine roughening of flux lines in a periodic potential due to the presence of disorder. To close this section, Janke and Johnston present Monte Carlo simulations of spin models with quenched connectivity disorder. They exam-

ine the effect of this type of disorder on critical exponents and analyze the non-self-averaging autocorrelations exhibited by these models.

Part IV is devoted to simulational studies of glasses and fluids. The paper by Hukushima discusses a novel "extended ensemble" approach for model systems with poorly equilibrating Monte Carlo dynamics. The basic idea of this approach is to simulate simultaneously, and equilibrate between, multiple model replicas, each kept at a different temperature. The method is applied to study the ordering in the three-dimensional Ising spin glass. In the following paper, Kob and co-workers report a very interesting application of the parallel tempering ("extended ensemble") method to several glassy systems, including models with both continuous and discrete degrees of freedom. The parallel tempering algorithm speeds up the characteristically slow equilibration of these systems by about 2 orders of magnitude as compared with traditional Monte Carlo and molecular dynamics methods. Then Orkoulas et al. report on a high-resolution study of the hard-core square-well fluid. By means of histogram reweighting techniques, they study higher order free energy derivatives along generalized axes in the temperature-density plane in order to examine the analyticity of the chemical potential along the phase boundary.

Part V contains four different papers describing diverse aspects of nonequilibrium and dynamical systems. In the first paper, Ito discusses the examination of nonequilibrium relaxation processes in simple models to extract information about the location of a phase transition as well as the dynamical critical exponent. Results on the d= 3 Ising model are highlighted. Then, Korniss et al. discuss a massively parallel algorithm for discrete-event simulations. They compare the evolution of the simulated time horizon with that of a growing interface, including both long wavelength and short distance behavior. Monte Carlo simulations of hysteresis in electrochemical systems are then described by Mitchell et al. They sweep the electrochemical potential back and forth across the transition and examine the relationship between hysteresis and slow ordering/disordering kinetics and critical slowing down. In the final paper of this section, Yamakov et al. present a molecular dynamics study of plastic deformation of nanocrystalline Pd at high temperatures. They consider relatively high tensile stress and compare the homogeneous steady-state diffusion creep with the Coble-creep formula.

Part VI of this volume explores the application of computer simulations to polymeric and other complex systems. The opening paper by Laradji presents Langevin-dynamics simulations of a realistic model for a semi-dilute polymer solution near a fluctuating membrane. He investigates the effect of adsorbed polymers on the elastic properties (i.e. surface tension and bending rigidity) of the membrane. Boghosian and Coveney then review the use of lattice-gas cellular automata to simulate the equilibrium and hydrodynamic properties of amphiphilic fluids. They present several examples of dynamical phenomena in such fluids that they have studied using this approach, including domain

growth, interfacial fluctuations, and shear-induced phase transitions. Lastly, Rapaport discusses the role of discrete-particle computer simulations in analyzing the emergent behavior observed generically in many-particle systems. To illustrate the broad scope of these issues, he provides a diverse collection of examples, including Taylor vortices, granular vibrational patterns, micelle formation, and virus capsid assembly.

Part I

Interacting Quantum Systems

Spin Dynamics and Noncollinearity in Molecules and Crystals

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Abstract. In current paper we would like to review current status in the area of electronic structure calculations of the interaction parameters for the magnetic systems with arbitrary magnetic orderings and their dynamical properties. Due to recent advances in the area of temperature and time dependent first-principle calculations we will describe the connection between so called 'ab-initio' approaches and traditional model techniques. We discuss in details what kind of new effects such treatment brings in comparison with traditional classical local moment description.

1 Introduction

In this article we review recent theoretical progress concerning the first-principle evaluation of parameters of magnetic interactions and their time or frequency dependence in both collinear and noncollinear case. For small deviations from equilibrium one can use linear response theory and we will discuss some general first principles methods for doing this. For other situations, such as encountered at high temperatures, the deviation of the spin orientations from their low temperature directions can be severe and the electronic structure can be altered significantly from that of the ground state. Also in such treatment the magnitudes of the local moments will depend on the relative orientation of nearby moments. In these cases one needs a first principles method to evaluate the electronic structure for a large collection of atoms having moments pointing in arbitrary directions. For static equilibrium situations there are methods to evaluate the electronic structure for noncollinear magnetic ordering [1]. For dynamical situations we have previously presented a method to evaluate the time evolution of the magnetic moments [2]. Because of length limitations, we have been rather selective and terse in our presentation. The topics considered are relatively new, and with rapid increases in computing power we expect many of the beginning studies described will be extended to address more complex situations, including the alteration of magnetic interactions caused by extended defects, and also both thermal and nonequilibrium properties.

In Sect. 2 we give a review of some general results from linear response theory as implemented with the multiple scattering formalism. Here we give a general discussion of the formalism and ideas of SD. In Sect. 3 we will derive the expression for the effective exchange parameters in general many-body