John von Neumann Institute for Computing

Condensed Matter

K. Binder, H. Müller-Krumbhaar

published in

NIC Symposium 2001, Proceedings,
Horst Rollnik, Dietrich Wolf (Editor),
John von Neumann Institute for Computing, Jülich,
NIC Series, Vol. **9**, ISBN 3-00-009055-X, pp. 243-245, 2002.

http://www.fz-juelich.de/nic-series/volume9

Condensed Matter

K. Binder[1] **and H. Müller-Krumbhaar**[2]

[1] Institut für Physik, Universität Mainz, 55099 Mainz, Germany

[2] Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich, Germany

Condensed matter physics deals with fundamental properties of solids and liquids. The solution of problems in this field clearly bears high technological potential but it also provides a substantial intellectual challenge. The formation of structures, the appearence of different types of spatial order and disorder, the occurence of transitions between various phases of condensed matter, the temporal evolution and the characterization of thermal and quantum fluctuations associated with various states of condensed matter are confronting us with many important unanswered questions. It is not so much the individual phenomenon occuring in a specific substance but rather the systematics within classes of materials and across these classes which require explanation.

In principle all properties of interest in condensed matter physics depend simply on the interaction of the electrons which can be regarded as the glue between the ionic cores. However, the exponential growth of the quantum-mechanical problem with the number of particles so far prohibits a numerical solution of an interacting quantum-system of more than some hundred particles even in simplified model-systems. One must, therefore, resort to effective interactions between atoms in order to treat large systems. Characteristic aspects of the effective interactions between the particles forming the solid or liquid are the typical range of interaction, local degrees of freedom, local and global symmetries of order parameters.

Typical phenomena of condensed matter physics are directly associated with the enormous number of interacting particles involved, leading to the complicated correlations between the particles even when the direct interactions are of short range. This is a main reason for the continuous need of virtually unlimited computer-ressources for the detailed investigations of model-systems for condensed matter phenomena, and it is a strong driving-force for the development of highly efficient numerical algorithms.

Computer-simulation in condensed matter problems start at the quantum-mechanical level with density-functional models for metals or semiconductors, the so-called models for first-principles calculations. With these models one may now calculate electronic and structural ground-state properties of large classes of materials with surfaces and layer-structures, including compound-materials. A second class of quantum-models starts from an effective Hamiltonian, e.g. of Hubbard-type, which gives the interactions of the many-body system in simplified form. The main objective for these model-studies is the explanation of correlation effects giving rise to collective phenomena like electronic excitations, metal-insulator transitions or superconductivity. A third set of models defines effective interactions between atoms or molecules, serving as basis for classical simulations with molecular dynamics or Monte Carlo methods. The various levels of large-scale computation in condensed matter physics and the enormous progress achieved in recent years are reflected in the following articles.

Starting from a Hubbard model, the Mott-Hubbard metal-insulator transition is studied in the article of Blümer et al. using the quantum-mechanical dynamical mean field approximation (DMFT), with extensions for realistic materials by combining DMFT with the local-density-functional approximation (LDA). This LDA+DMFT Quantum-Monte-Carlo calculation gives remarkably good results for photo-emission and X-ray absorption associated with the strongly correlated electrons in vanadium-oxide.

The mechanism of high-temperature superconductivity (HTSC) is addressed in the contribution by Dorneich et al. This is a numerical study of an effective bosonic model which describes the low-energy physics of a 'projected' SO(5)-theory. The theory unifies the three-dimensional order parameter of the antiferromagnetic phase with the two-dimensional order parameter of the superconducting phase. The large-scale numerical simulations use a technique of stochastic series expansions. The resulting phase diagram looks very similar to the one of real HTSC-cuprates.

Electronic correlations coexisting with dynamical electron-phonon interactions is a central mechanism in physical properties of novel materials like organic polymers, charge-ordered nickelates or collossal magnetoresistance manganites. In the article of Fehske et al. exact diagonalization results for the typical Hamiltonians are presented. As a successful interdisciplinary cooperation the implementation of efficient parallel diagonalization methods for very large matrices also resulted from this project.

A microscopic many-body theory describing the optical and electronic properties of semiconductors and heterostructures is described in the contribution of Meier et al.. The importance of correlations beyond the Hartree-Fock-level for polarization-dependent pump-probe and four-wave mixing experiments have been convincingly demonstrated by these massively parallel computer simulations. Optical properties of semiconductors are of high technological significance in information technology. A very efficient method to calculate optical spectra for complicated geometries such as quantum wires, superlattices in electric and magnetic fields or excitations on rough solid surfaces is presented by Glutsch. The calculations have given convincing agreement with experiments.

The structure of solids and magnetism on an atomic scale is discussed by Hergert et al. on the basis of quantum-mechanical density-functional calculations for electronic properties, accompanied by molecular dynamics simulations for metallic nanostructures. It is demonstrated that a large number of materials properties like surface diffusion barriers, magnetic moments and strain and stress effects can now be reliably calculated for real materials like cobalt deposited on copper and other metals like gold and silver.

Janke et al. study classical spin-glasses as typical representatives of disordered materials, where the possible states of the system are separated by high barriers of the free energy. A multi-overlap algorithm gave substantial new insight concerning the excitations over these barriers, statistically rare events. The method proved to be particularly powerful in the study of the tails of the distribution function.

A related investigation by Binder et al. discusses similarities and differences between glasses and spin-glasses using Monte Carlo and molecular dynamics studies on various model systems. A crucial point is the dramatic slowing down of thermal equilibration, as the glass-temperature is approached from above. Detailed comparisons also with experiments on silica-glass are presented.

Liquid crystals provide a wealth in possible phases and dynamical processes due to the non-spherical symmetry of their molecules. Because of their unusual electric, elastic and

rheological properties they are of high technological interest. As an example, the interface between the nematic and the isotropic phase was studied by Akino et al. via molecular dynamics. An unexpectedly complex spectrum of capillary waves was observed, with significant deviations from capillary wave theory.

Systems of liquid crystals with different molecular shapes like chiral or banana-shape were studied by Memmer in order to unveil the relationship between molecular symmetry and macroscopic phases. A rich polymorphism of phases could be characterized in dependence on temperature, pressure, chirality parameter and molecular structure.

The examples presented here span a whole range of condensed matter physics, from the electronic structure of "hard" materials such as semiconductors and metals to the phase diagrams of "soft matter" - systems, such as liquid crystals. This underlines the significance of large-scale simulations as an increasingly flexible tool which can yield important insights into problems that are relevant both for physics and materials science.