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Condensed Matter

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The physics of condensed matter deals with various physical phenomena (mechanical response, electrical conductivity, magnetism, optical properties, etc.) of solids and liquids, trying to provide a link between macroscopic properties of matter and the basic characteristics of the nuclei and electrons which constitute it. A crucial aspect for many of these phenomena is the fact that this many-body problem cannot be simply reduced to a one-body problem (with an effective field resulting from the other degrees of freedom), since nontrivial correlations, central for a correct description of the system, develop. Since there is no general analytic method which could deal with such correlations, large-scale computer simulation is the most promising tool to tackle such problems.

This crucial role of correlations and the corresponding importance of state-of-the art computer simulation methods to deal with them is very much apparent in the articles which will follow in this section. Note that only a small number of NIC projects dealing with applications in condensed matter physics could be selected for the present section of this volume, due to restricted space. Furthermore, closely related applications can be found in the sections on chemistry, materials science and polymers (soft matter) as well: nontrivial correlations resulting either from the quantum many-body problem or from entropic effects (or both) are present there in a similar way.

Strongly correlated electron systems are a common theme in the papers of Assaad and Hanke, Anders et al. and Keller et al. Assaad and Hanke first describe a methodic advance to deal with the famous "minus sign problem" of Quantum Monte Carlo (QMC) methods, based on a representation of the density matrix in terms of Gaussian operators. This so-called "Gaussian Monte Carlo method" then is applied to gain insight into the phase diagram of the SU(N) Hubbard-Heisenberg model.

A completely different approach in order to deal with strongly correlated electrons is based on a combination of the local density approximation (LDA) of density functional theory with the dynamical mean field theory (DMFT). The resulting equations then also need to be solved by QMC methods. Keller et al. demonstrate that with this approach one can compute properties of real materials, such as photoemission spectra of V_2O_3, and thus explain pertinent experiments.

The third approach we discuss here, applied by Anders et al. in order to understand the conductance in coupled quantum dots, is based on a numerical renormalization group method to solve the effective quantum Hamiltonian near the quantum phase transition that the model exhibits.

An alternative method (namely the density matrix renormalization group) also proves useful for the calculation of spectral properties of strongly correlated electron phonon properties by Schubert et al.

Still another, and very promising, approach on how to deal with strongly correlated quantum systems is based on Stochastic Series Expansion Quantum Monte Carlo (SSE-QMC). Wessel applies this methods to ultracold atom gases in optical lattices to describe the transition from the suprafluid state to the Mott insulator.

Also on a more mesoscopic scale, quantum-mechanical correlations may be very important. Meier et al. give an example for this statement by their treatment of semiconductor nanostructures and their optoelectronic properties. Such nanostructures are discussed in the context of photonic crystals and hence, a hot topic of materials science. The dynamics of electrons and hole excitations, which interact with Coulomb forces, are obtained by numerical solutions of a high-dimensional set of coupled nonlinear differential equations, the so-called semiconductor Bloch equations.

Nontrivial correlations are certainly the key problem when one deals with the statistical mechanics of magnetic systems. While the equilibrium behavior of the two-dimensional Ising model is well understood, Pleimling shows that the dynamical scaling associated with far from equilibrium behavior (domain growth, ageing) exhibits the so-called "local scale invariance" which was recently proposed.

Finally, nontrivial correlations also arise in classical model systems for colloids, as demonstrated by Vink et al. The Asakura-Oosawa (AO) model of colloid-polymer mixtures coarse grains both colloids and polymers as spheres with excluded volume interactions (but polymers may overlap each other with no interaction). The resulting (purely entropically driven) phase separation falls in the universality class of the Ising model. Similarly, hard spherocylinders exhibit phase separation between a nematic and an isotropic phase. Computer simulation techniques were developed allowing to estimate the interfacial tensions for such systems. The relation of this work to simulations of polymeric and other soft matter systems is evident.

At the end of this introduction, we note that successful simulations in condensed matter require several ingredients which are all crucial for obtaining relevant results: clever "model building" needs to be combined with a carefully chosen and optimized algorithm, and only then the computational power of the supercomputer fully pays off. The following papers will illustrate this importance of algorithmic improvements in more detail.