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Condensed Matter

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Condensed matter physics provides an understanding of macroscopic properties of solid or liquid matter in terms of the properties of nuclei and electrons of the constituting atoms. While in principle the problem is well understood - quantum mechanics of interacting many-body systems together with statistical mechanics provides the appropriate framework - in practice the problem is extremely complicated. Thus, a full first principles approach, where one would solve the Dirac or Schrödinger equation for a system of $N \approx 10^{22}$ nuclei (as contained in 1 cm^3 of condensed matter at typical conditions) plus the appropriate number of electrons, and then uses this information within the formalism of statistical thermodynamics, is by no means feasible. This will not become feasible during the next decades, even if the exponential increase of the computational power of the available hardware with time continues.

In this situation, the problem needs to be reduced from the level of nuclei and electrons interacting with Coulomb forces to the level of effective Hamiltonians, where many of the original degrees of freedom have been eliminated, at the cost of admitting effective phenomenological parameters in the model Hamiltonian, which are not explicitly known a priori for real materials. Examples of this idea are the use of pseudopotentials describing the interaction between valence electrons and ionic cores in electronic structure calculations, or the use of the Hubbard Hamiltonian or the t-J model useful for the description of high-T_c-superconductors. While the latter models keep still some important quantum-mechanical effects, the behavior of many systems at elevated temperatures can be understood in terms of models for which classical statistical mechanics suffices (such as Ising- or Potts models on lattices, or off-lattice models for fluids, solids and liquid crystals). However, all these problems have in common that nontrivial correlations develop between important degrees of freedom and analytical approximations of mean-field type (such as Hartree-Fock-theory of a many electron system, molecular field theory for the Heisenberg model of ferromagnetism, or van der Waals theory for a liquid-gas transition, etc.) are typically inadequate.

In this situation, large scale computer simulation is the method of choice. However, one must recall that the methods developed for this task are all comparatively young, and so further improvement of these methods is still of very great importance, and plays a significant role in the research presented here as well. The oldest of the common simulation methods is the importance sampling Monte Carlo method, which at the time of writing (2003) had its 50 year anniversary. Still this method has challenging difficulties to over-

come, in particular when one uses it for the study of phase transitions (these difficulties are due to finite size effects, critical slowing down, and - in the case of quenched disorder - the need to take an average over a huge sample of configurations of the random disorder). Therefore, there is a need to develop very efficient simulation codes, and large resources of computer time on massively parallel supercomputers, such as the NIC has provided, are absolutely crucial. The articles by Dreher et al. (where phase transitions of model colloids are discussed), and by Janke et al. (where bond-diluted Ising and Potts models and their phase transitions are studied) illustrate those issues.

The second "classical" simulation technique, Molecular Dynamics based on the numerical integration of Newton's equation of motion for a description of an interacting many-body system in terms of classical mechanics, now is about 40 years old, but still one of the main tools to deal with complex properties of many-body systems, in particular when dynamic properties are in the focus of the study (e.g. the article by Horbach et al., addressing transport coefficients of mixtures) or when one considers driven systems far from equilibrium (e.g. the article by Germano and Schmid, addressing the nematic-isotropic interface in a sheared liquid-crystalline system, or the article by Dreher et al., where the rupture of metallic nanowires is investigated). An interesting variant of Molecular Dynamics, suitable to study processes too slow to be observable directly on the time scales accessible by standard Molecular Dynamics simulation, is the "Targeted Dynamics" approach: an example is provided by the article by Oberbrodhage and Morgner, where a suitable force acting on a formamide molecule drives it through a slab of liquid benzyl alcohol.

Further articles address problems in condensed matter physics where the quantum nature of the latter cannot be ignored. Although density functional theory for the calculation of the quantum mechanical ground state energy of a many-body system is now also about 40 years old and well-established (its foundation has been honored by a Nobel Prize for W. Kohn a few years ago), there is still room for this method to improve and extend it, and apply it to complex problems of interest for materials science. The article by Schmidt et al. dealing with uracil adsorption on Si (001) surfaces as a prototype for functionalized surfaces is a nice example. However, one has to resort to different techniques when one wishes to explain many-body effects arising in linear and non-linear optical spectroscopy of semiconductor heterostructures, as described in the article by Meier et al. Electron populations in quantum wells and quantum wires and their motion are studied simulating the wave packet dynamics. Here the low dimensionality of the problem makes the approach feasible. For other problems of the dynamics of quantum systems, such as the dynamics of Bose-Einstein condensates with long-range attractive interactions (see the article by Kalinski et al.) one has to resort to a numerical solution of a time-dependent mean field theory (the Gross-Pitaewski equation) to make progress. In this way, the formation kinetics of "supersolids" could be elucidated.

Turning again to lattice models of magnets with quenched disorder, but including the quantum nature of the coupled spins, it is clear that the difficulty of the problem is considerably higher than for the (quasi-classical) Ising and Potts models with quenched disorder, mentioned above. Here an interesting alternative to quantum Monte Carlo methods, the strong disorder renormalization group approach, is presented in the article by Lin et al., and very promising progress in the understanding of these random quantum magnets is reported.

Finally, we mention a particularly challenging correlated electron problem, namely the

understanding of high T_c superconductivity. It is widely believed that suitable models to study this problem are the Hubbard model or the t-J-model, respectively. The article by Lavalle et al. demonstrates applying Quantum Monte Carlo methods for the one-dimensional version of the t-J model that spin and charge separation in the excitation spectrum occurs. Apart from "spinons" and "holons" also "antiholons" are identified, which are not just charge conjugated to the holons but seem to be generic new excitations. Finally, Dorneich et al. present a variant of the Quantum Monte Carlo method, based on Stochastic Series Expansion, and apply it to the so-called "projected SO (5) Hamiltonian", suggesting that the full SO (5) symmetry is in fact restored at the bicritical point of that model.

We hope that this introduction has given the reader some idea of the wide variety of problems that need large scale computations in condensed matter physics. A key point is that most progress does not come simply from "brute force", but also needs clever algorithmic developments together with deliberately designed effective models. Due to all these ingredients, the field is particularly fascinating and lively, the calculations described in the following articles are by no means routine work, and they have a substantial impact both for the foundations of condensed matter physics and for materials science.