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# Condensed Matter: From the Schrödinger Equation of Many Electrons and Nuclei to Fluid Flow

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In principle, any phenomena in condensed matter could be theoretically understood if one were able to solve the many-body Schrödinger equation of electrons and nuclei (interacting with just the appropriate Coulomb potentials) and use this solution as input to the formalism of (quantum) statistical mechanics. Unlike elementary particle physics, where the nature of some of the basic interactions are still debated, the starting point of the theory of condensed matter is perfectly well defined. However, the problem posed is far beyond reach even of the most powerful computers, also in the foreseeable future, and hence a large variety of approximations is needed, where (i) the Hamiltonian is reduced to some model Hamiltonian (often involving some unknown phenomenological parameters), and the type of model depends very much on the systems one wants to describe, and (ii) implicit approximations are necessary in the simulation methods used to study these models. In fact, depending on the problems that are studied a wide variety of models and simulation methods are encountered, and this fact will become apparent from the articles that will follow in this section. Of course, these articles constitute only a small selection of problems in the science of condensed matter that are studied using the resources of NIC; in addition, we note that many articles that appear in the sections on chemistry, materials science, polymers and soft matter also deal with condensed matter, of course.

Now progress in the simulation studies of condensed matter systems is gained by improvements of algorithms on the one hand, and by better computer hardware (faster processors, larger memory, etc.) on the other hand. In favourable cases, these two aspects combine and allow to deal with problems that were intractable so far.

An example for this statement is the article by Dolfen and Koch on the attempt of a realistic description of the quasi-one-dimensional organic conductor TTF-TCNQ. This system can be modelled as a strongly correlated organic metal, and hence a description in terms of a (slightly extended) Hubbard model results. The appropriate parameters of this model are estimated by all-electron density functional (DFT) methods. The hamiltonian then is diagonalized applying the Lanczos algorithm, to obtain the ground state energy and excitations. However, only finite clusters can be dealt with exactly, to deal with the infinite chain hopping between clusters is treated by a “cluster perturbation theory”, which allows to study fascinating physics like spin-charge separation in the excitation spectrum. It should be emphasized that due to excessive memory requirements this approach was

only feasible using a massively parallel implementation at the Blue Gene/L system JUBL.

Dealing with a strongly correlated electron systems is also the focus of the article by Martin et al. on the numerical simulation of heavy fermion systems. A generic model for such systems is the Kondo lattice model, which is tackled here by a dynamical cluster approximation (a finite sized cluster is embedded in a bath of the remaining electrons), using a quantum Monte Carlo algorithm. Again use of a highly parallelized implementation on high-performance computers is crucial for a success of this study, which allowed first steps towards a study of the magnetic order-disorder transition of this model.

An interesting step on the (long) way towards the solution of the many-body Schrödinger equation is also the *Ab Initio* Molecular Dynamics (AIMD) method, applied in the chapter by Groß to study adsorption of hydrogen molecules on palladium surfaces. Using density functional theory within the generalized gradient approximation, the substrate surface at $T = 0K$ was prepared, and then at least 200 microcanonical Molecular Dynamics (MD) trajectories of the adsorption and desorption of the hydrogen molecules were generated, for each choice of the initial kinetic energy of the molecule. The simulations again need an efficiently parallelized code and unravel the crucial role of the substrate degrees of freedom (clean and hydrogen-precovered surfaces are studied) on the dissociative adsorption process.

When one studies large systems at high temperatures, however, the above types of techniques are still unfeasible, and one must rely on phenomenological potentials that are used in classical MD methods. However, if these potentials are carefully chosen, a reasonably good description of real systems is possible. This fact is demonstrated in the article by Kerrache et al. on the simulation of multicomponent liquids. Two systems are studied: molten silica and AlNi alloys, both in the crystalline state and in the melt. For silica, a new and more accurate potential is defined, from a new fitting scheme to Car Parrinello Molecular Dynamics (CPMD). Like AIMD, the starting point is also DFT, but the dynamics is stochastic rather than microcanonical. For the metallic alloy, a standard embedded-atom potential from the literature is used, but the new methodic aspect in this part of the study is the very accurate estimation of the melting temperature from recording the temperature dependence of the crystal-melt interface velocity. Due to the necessary sample averaging the use of a high performance computer such as JUMP also was indispensable for the success of this project.

While such a chemically realistic description of the dynamics of fluids on the atomistic scale requires MD methods, coarse-grained models of fluids can also be studied by Brownian Dynamics (BD) or Lattice Boltzmann (LB) methods. The latter approach is implemented in the article by Harting and Kunert, where flow in thin channels with rough surfaces is studied, to find out how the slip length depends on the wall roughness. The BD method is applied by Bürzle et al. for the study of transport phenomena of colloids in microchannels: the colloidal particles move as a regular array of several rows, but also transitions from $n$ to $n - 1$ in the number of "lanes" for this motion are observed. Other coarse-grained models concern the phase behaviour of colloidal particles in the periodic potential by laser fields (which is studied by Monte Carlo (MC)) and the structure of lipid bilayers with incorporated proteins (a model for a biological membrane) in solution. Due to the large number of particles ("only" 4800 lipid molecules but 90 000 solvent particles) the need for (geometric) parallelization on a high-performance computer such as JUMP again is clearly apparent.

Advanced MC methods are also the technique of choice in the article by Bittner et al. on free-energy barriers of spin glasses (Ising spins interact with random couplings, assuming either infinite range (SK model) or nearest neighbour forces (EA model)). Due to the extremely slow relaxation and the fact that the free energy barriers are not self-averaging, this problem is by no means simple. Progress is obtained by combining the "multi-overlap algorithm" with "parallel tempering"; thus again the need for a parallel implementation on a high-performance computer such as JUMP immediately becomes apparent. In this way, information can be extracted on how the barrier heights scale with the number of spins in the system.