Preface

Many-particle physics is at work whenever we delve into the rich phenomenology of the real world, or into laboratory experiments. Nevertheless, our physical description of nature is mostly built upon single-particle theories. For instance, Kepler's laws provide a basic understanding of our solar system, many features of the periodic table can be understood from the solution of a single hydrogen atom, and even complicated microprocessors with an unbearable number of electrons floating through millions of transistors can be developed based on the effective single-particle models of semiconductor physics. These approaches are successful because quite often interactions affect physical systems in a perturbative way. Classical perturbation theory yields corrections to a planet's orbit due to other planets, quantum chemistry relies on various approximation schemes to deal with complicated atoms and small molecules, and solid state theory uses weakly interacting quasiparticles as elementary excitations. This fortunate situation changes, however, when we try to understand more complex or strongly interacting systems, or when we try to explore the nature of matter itself. Condensates of cold bosonic atoms, for example, show subtle many-particle effects, strongly correlated fermions may give rise to high-temperature superconductivity, and the way quarks build up elementary particles (hadronization) is a highly non-trivial few-body problem. Another example are quantum computers, which many scientist envision as a replacement for our present-day microprocessors, and which exploit the entanglement property of quantum many-particle states. Last but not least, we mention the complexity of fusion plasmas, which some day may help feeding our ever-growing hunger for new energy resources. Unfortunately, even the most sophisticated analytical approaches largely fail to describe such systems. Hence, at present, unbiased numerical investigations provide the most reliable tool to address these problems. This is the point where the expert use of large-scale computers comes into play.

The increasing importance of computational many-particle physics calls for a comprehensive introduction into this rapidly developing field suitable for graduate students and young researchers. Therefore, we decided to organize a summer school on "Computational Many-Particle Physics" in September 2006, during the 550th anniversary of the University Greifswald. Generously sponsored by the Wilhelm and Else Heraeus Foundation and hosted by the Max-Planck-Institute for Plasma Physics and the Institute for Physics, we brought together more than 40 students and 20 distinguished scientists working on such diverse fields as fusion plasmas,

statistical physics, solid state theory and high performance computing. The present Lecture Notes summarize and extend the material showcased over a 2-week period of tightly scheduled tutorials, seminars and exercises. The emphasis is on a very pedagogical and systematic introduction to various numerical concepts and techniques, with the hope that the reader may quickly start to program himself. The spectrum of the numerical methods presented is very broad, covering classical as well as quantum few- and many-particle systems. The trade-off between the number of particles, the complexity of the underlying microscopic models and the importance of the interactions determine the choice of the appropriate numerical approach. Therefore, we arranged the book along the algorithms and techniques employed, rather than on the physics applications, which we think is more natural for a book on numerical methods.

We start with methods for classical many-particle systems. Here, molecular dynamics approaches trace the motion of individual particles, kinetic approaches work with the distribution functions of particles and momenta, while hybrid approaches combine both concepts. A prominent example is the particle-in-cell method typically applied to model plasmas, where the time evolution of distribution functions is approximated by the dynamics of pseudo-particles, representing thousands or millions of real particles. Of course, at a certain length scale the quantum nature of the particles becomes important. As an attempt to close the gap between classical and quantum systems, we outline a number of semi-classical (Wigner-function, Boltzmann- and Vlasov-equation based) approaches, which in particular address transport properties. The concept of Monte Carlo sampling is equally important for classical, statistical and quantum physical problems. The corresponding chapters therefore account for a substantial part of the book and introduce the major stochastic approaches in application to very different physical situations. Focussing on solids and their properties, we continue with ab initio approaches to the electronic structure problem, where band structure effects are taken into account with full detail, but Coulomb interactions and the resulting correlations are treated approximately. Dynamical mean field theories and cluster approaches aim at improving the description of correlations and bridge the gap to an exact numerical treatment of basic microscopic models. Exact diagonalization of finite systems gives access to their ground-state, spectral and thermodynamic properties. Since these methods work with the full many-particle Hamiltonian, the study of a decent number of particles or larger system sizes is a challenging task, and there is a strong demand to circumvent these limitations. Along this line the density matrix renormalization group represents a clever technique to restrict the many-particle Hilbert space to the physically most important subset. Finally, all the discussed methods heavily rely on the use of powerful computers, and the book would be incomplete without two detailed chapters on parallel programming and optimization techniques for high performance computing.

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