Chapter 10
Molecular Dynamics Simulation of Strongly Correlated Dusty Plasmas

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Abstract This chapter gives a tutorial introduction to the molecular dynamics (MD) technique as a first-principle description of classical many-particle dynamics. The goal is to provide practical insight into the current status of theoretical dusty plasma research as well as to present the necessary ingredients for a successful MD simulation in one place. As typical examples of the application of MD, we concentrate on two directions of current research interest: (1) the structural properties of spherical dust crystals in traps and (2) the transport properties such as diffusion of liquid unconfined, infinite dust systems.

10.1 Introduction

The field of mesoscopic and macroscopic complex (dusty) plasmas has become an important part of plasma physics in recent years. The research interest was initiated in 1994 by the experimental discovery of a new state of (soft) matter – the plasma (Wigner) crystal [1–4]. In a sheath of a noble gas radio-frequency discharge, highly charged dust grains of micrometer size were investigated for the first time under laboratory conditions. Due to their high charge of several thousand elementary charges, these microspheres are strongly coupled and enable the researchers to observe liquid behavior with short-range order and even macroscopic Coulomb crystals of hcp, fcc, and bcc lattice structure.

The occurrence of dusty plasma effects exceeds by far basic research interests and has practical importance in micro- and nanotechnology [5]. In the industrial plasma processing, the presence of charged dust particulates can completely change characteristic plasma parameters such as electron and ion densities, temperature, and plasma potential. This makes it difficult to run technological processes at optimum...
settings [6]. Additionally, self-assembling of dust particles plays a crucial role in the fabrication of microchips and solar cells, where growing dust particulates can have both devastating as well as advantageous effects. On the one hand, during the manufacture of highly integrated electronic circuits, the so-called chip-killing particles can destroy the damageable plasma-etched nanostructures [7], while on the other hand dust grains included in polymorphous solar cells reduce the degradation of these cells [8]. Besides these technological situations, dusty plasmas are, for example, of great interest in various astrophysical phenomena. For instance, the formation and stability mechanisms of dusty plasma systems are of central interest for the understanding of protoplanetary, protostellar, and accretion disk formation, as well as planetary ring systems [9, 10].

In contrast to the mainly weakly coupled macroscopic plasmas in space and technology, in this chapter, we focus on the numerical simulation and analysis of strongly coupled plasmas such as spherical Coulomb and Yukawa balls in traps (see Fig. 10.1 for an example and Chap. 7 for details). These finite systems are subject of exceptional current interest since their recent experimental generation, for example, in dusty plasmas [11]. As a second example, we will concentrate on dynamical processes (transport quantities) in macroscopic dusty plasmas. In particular, we discuss the question about the occurrence of superdiffusion in the transition region from a purely three-dimensional to a quasi-two-dimensional system [3].

10.2 Basics of Molecular Dynamics Simulation

The molecular dynamics (MD) method was originally introduced by B.J. Alder and T.E. Wainwright in the late 1950s with the aim to calculate many-body correlations of classical hard-sphere systems exactly by means of “electronic computers [sic]” [12–14] (see Fig. 10.2). Many valuable insights concerning the collective behavior of interacting many-body systems emerged from their studies with the