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Complex dynamics of atomic clusters

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Abstract. Potential energy fluctuations in small atomic clusters have long-ranged temporal correlations, which lead to $1/f$ noise in the power spectra. The relaxation dynamics in clusters has a hierarchical organization, resulting from different processes at the surface and core. A cellular dynamical model is proposed to understand the origin of such fluctuations.

Keywords. Atomic clusters; multiple relaxations; $1/f$ noise.

1. Introduction

The molecular dynamics (MD) technique (Alder and Wainwright 1957; Allen and Tildesley 1987) is a powerful method of studying the liquid state through computer simulation (Catlow *et al* 1990). MD studies have addressed a variety of issues in relation to liquids, notable among which are the determination of correlation functions (Rahman 1964) that are normally not accessible to experimental techniques. In addition, simulations of ensembles of atoms or molecules have given valuable insight into microscopic dynamics and its connection with statistical mechanical observables.

One system where such studies have been extremely useful is liquid water (Stillinger and Rahman 1974; Tanaka and Ohmine 1987; Ohmine *et al* 1988; Sasai *et al* 1992). The dynamics of water has long been known to be complex, and indeed, realistic models (Stillinger 1980) for liquid water have introduced ideas of fickering clusters (Frank and Wen 1987) and random networks (Sceats and Rice 1982) in order to accommodate the strong directional properties of the hydrogen bond. Recent work which focused on the anomalously large heat capacity of water (Sasai *et al* 1992) showed that the relaxation processes in water were similar to those in atomic clusters. Both systems appear to have a distribution or hierarchy of relaxation times corresponding to a distribution of different activation processes, rather than a single relaxation pathway.

Atomic clusters, being intermediate in size between bulk matter and isolated molecules, offer new insights into phenomena such as freezing or melting (Berry *et al* 1984). In recent years, considerable attention has been focussed on clusters (Sugano 1991; Schmidt *et al* 1992) and the interest, which has been diverse and extensive, has ranged from the preparation of new types of molecules such as the fullerenes, to the study of electronic structure, stability and dynamics.

The dynamics of clusters is the subject of this paper. In particular, we study the properties of inert gas atoms bound by weak interatomic forces, and examine the

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