Statistical properties of Fermionic Molecular Dynamics

H. Feldmeier, J. Schnack
GSI Darmstadt

Molecular dynamic models are expected to describe multifragmentation of nuclei seen in heavy–ion collisions. These reactions show large fluctuations, for example in the mass distribution, which are beyond an ensemble–averaged mean–field treatment. In this context it is important to understand the statistical properties of molecular dynamic models especially at low temperatures.

There are two aspects of this. One concerns the thermo*static* properties of a molecular dynamic model where the attribute thermostatic refers to the properties of the static canonical statistical operator, which are contained in the partition function $Z(T) = \mathrm{Tr}(\exp\{-\underset{\sim}{H}/T\})$. Once the partition function is calculated within a given model its thermostatic properties can be deduced by standard methods like partial derivatives of $\ln Z(T)$ with respect to temperature T or other parameters contained in the Hamilton operator $\underset{\sim}{H}$.

In the case of Fermionic Molecular Dynamics (FMD) [1] the trace in the partition function can be evaluated exactly because the model is based on antisymmetric many–body states which form an overcomplete set covering the whole Hilbert space. As the calculation of the trace does not depend on the representation all thermostatic properties like Fermi–Dirac distribution, specific heat, mean energy as a function of temperature etc. ought to be correct and fully quantal using FMD trial states.

The issue of our investigations [2] is the other and even more important aspect, namely the dynamical behaviour of a molecular dynamic model. A dissipative system which is initially far from equilibrium is expected to equilibrate towards the canonical ensemble. The simulation of such a system within the model provides a crucial test of its thermo*dynamic* behaviour. In other words the question is: does the FMD state as a function of time explore the Hilbert space according to the canonical weight?

Within Fermionic Molecular Dynamics we study the equilibration of four identical fermions enclosed in a one dimensional harmonic oscillator. The particles interact by a weak repulsive two–body potential which is neccessary to convert the integrable harmonic oscillations into chaotic motion. Figure 1 shows the time-averaged single–particle occupation numbers $p(n)$ of the oscillator shells labeled with n. Time–averaging was performed over about 2000 periods of the harmonic oscillator.

The important result is that the initial many–body state, which is far from equilibrium, approaches the canonical ensemble with Fermi–Dirac statistics in an ergodic sense. The time–averaged occupation numbers of the harmonic oscillator eigenstates (open symbols) are practically identical with the Fermi–Dirac distribution of the canonical ensemble (full line), provided the canonical ensemble is taken at the time–independent mean excitation energy of the many–body state. The temperatures in brackets refer to the canonical ensemble.

When distinguishable particles, which are described by a product–state of wave packets, are considered, the molecular dynamic equations for the parameters of the wave packets lead to a quantal Boltzmann distribution for the occupation numbers of the single–particle eigenstates.

Finally, classical thermodynamics is obtained when the many–body state is a product state and the width parameters of the single–particle gaussians are not dynamical variables anymore.

A further important result is, that the use of time averages provides us with a tool for establishing relations between well–defined quantities of a molecular dynamic model such as excitation energy and statistical quantities like temperature. This is a first step in investigating excited nuclei and for instance the nuclear liquid–gas phase transition [3] which has been of current experimental interest.

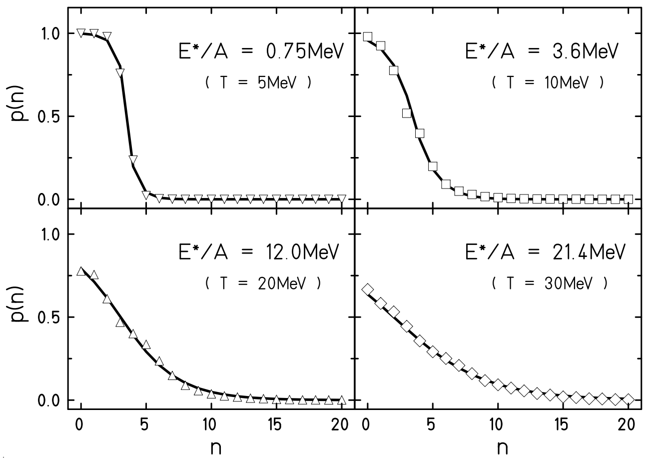

Figure 1: Occupation numbers calculated in the ergodic ensemble (symbols) compared with those calculated in the canonical ensemble (solid line).

References

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