Energy relaxation in a $\varphi^4$-model with long range interactions

R. Németh,* R. Schilling

Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, D-55099 Mainz, Germany

Received: 18 October 1994/Revised version: 19 December 1994

Abstract. We investigate the influence of long range interactions on the relaxation behaviour of a lattice model with an on-site potential of $\varphi^4$-type and "infinite" range harmonic interactions. For finite number of particles $N$, it is shown that the autocorrelation functions $\langle \delta E_n(t) \delta E_n \rangle$ of the fluctuations of the one-particle energies $E_n(t)$ decays exponentially. The corresponding relaxation time $\tau$ is proportional to $N$ and is given by $\tau(T, N) \sim N \tau_0(T)$. The temperature dependent time scale $\tau_0$ can explicitly be related to the dynamics of a one-particle correlator of the noninteracting system. The results are derived using Mori-Zwanzig projection formalism. The corresponding memory kernel is calculated within a mode coupling approximation and by a perturbative approach. Both results agree in leading order in $1/N$.

PACS: 05.50.+q; 61.20.Lc; 63.10.+a

1. Introduction

The motivation of this paper is to investigate the dynamics of systems with long range interactions. We restrict ourselves to systems undergoing structural phase transitions usually described by a $\varphi^4$-model with harmonic interactions [1]

$$H(p, x) = \sum_{i=1}^{N} H_0(p_i, x_i) + H_1(x)$$

where $x = (x_1, \ldots, x_N)$ are the scalar displacements from a specific lattice $\{R_i\}$, $p = (p_1, \ldots, p_N)$ are the conjugate momenta, $N$ is the number of particles with mass $m$, $C_{ij}$ are the elastic constants and the on-site potential $V_0$ is of $\varphi^4$-type

$$V_0(x) = -\frac{a}{2} x^2 - \frac{b}{4} x^4$$

with $b$ positive. $a$ can be either positive or negative.

We will consider the extreme case of long range interactions which is given by

$$C_{ij} = \frac{\mu}{N}, \quad \mu > 0$$

where all displacements interact with each other with same strength of order $1/N$. Of course, such an interaction does not occur in reality. But keeping $N$ finite, some dynamical properties of model (1) with either $C_{ij}$ given by (3) or, e.g. by $C_{ij} = \exp[-|R_i - R_j|/\lambda]$ may relate to each other if the interaction range $\lambda$ is identified with $N$. On the other hand, our choice makes the mean field approach exact and accordingly the static properties at finite temperatures can easily be calculated. This was one of the reasons why Hamiltonian (1) in connection with (3) has recently attracted some attention [2, 3] and why such long range interactions have been used for spin glass models [4].

The main motivation of [2] and [3] was to check the applicability of mode coupling theory (MCT) [5, 6], since a MCT approach for model (1) but with short range interactions predicted a dynamical phase transition at a temperature $T_\ast$ from an ergodic to a nonergodic phase [7]. Because MCT involves the factorization of a higher order time dependent correlation function, it was the believe that this approximation becomes better for long range coupling like (3), where at least the static order parameter correlation functions to factorize, i.e. the fourth and higher order parameter correlation functions can be expressed by the corresponding second order correlation. However, the result for the nonergodicity parameter

$$f = \lim_{t \to \infty} S(t), \quad S(t) = \langle \delta x_n(t) \delta x_n \rangle$$

*i Present address: Institut für Statistik in der Mediain, Universität Düsseldorf, D-40001 Düsseldorf, Germany*
where \( \delta x_n = x_n - \langle x_n \rangle \), did not exhibit any transition from zero (ergodic phase) to a nonzero value (nonergodic phase) [2, 3], but remained nonzero for \( a > 0 \) and for all temperatures investigated. Here it is important to realize a difference between both contributions. In [2] the canonical averaging \( \langle \cdot \rangle \) included the mean field interaction, whereas the Newtonian time evolution of \( \delta x_n(t) \) was taken for the noninteracting system. Since \( a > 0 \) implies a double well potential, it is obvious that in this case all particles with one-particle energy smaller than the height of the potential barrier in \( V_0(x) \) are captured in their well for ever and therefore contribute to the nonzero value of \( f \). Hence, the origin of the nonergodic behaviour is not caused by a collective behaviour, but is just a single particle property. The authors of [3] integrated numerically the Newtonian equation of motion for (1)–(3)

\[ m \ddot{x}_n - a x_n + b x_n^3 = \frac{\mu}{N} \sum_{k=1}^{N} x_k \]

and found a time scale \( \tau(T, N) = \tau_0 T N \) above the critical point \( T_c \) such that \( S(t) \) relaxes to a plateau for \( 0 \leq t \leq O(1) \) and decays to zero for \( t \gg \tau \), i.e. the system is quasi-nonergodic on a time scale small compared to \( \tau \sim N \) and ergodic for \( t \gg \tau \). Considering the height of the plateau as nonergodicity parameter has led to a good agreement with \( f \) obtained for the noninteracting system [2, 3, 8]. These findings can easily be understood. Above \( T_c \) where the order parameter \( \langle x_n \rangle \) vanishes the average of the r.h.s. of (5) is zero, but its fluctuations are of order \( N^{-1/2} \), due to the central limit theorem. For \( N \) infinite these fluctuations disappear and the dynamics reduces to that of the noninteracting particles [2].

Therefore, for \( N \) finite and \( t \) small enough we expect one-particle behaviour resulting in the plateau and for \( t \) large enough the order of \( N^{-1/2} \) become active leading to the final decay of the correlation. This clearly demonstrates that the long range character of the interactions generates a time scale \( \tau \) which is \( N \)-dependent.

It is our main concern to investigate this dynamical behaviour in more detail. For \( t \) small enough, the r.h.s of (5) is practically zero. Therefore the one-particle energies \( E_n(t) = H_0(p_n(t), x_n(t)) \)

\[ \text{are almost constants of motion. On a long time scale compared to } \tau, \text{ } E_n \text{ will change significantly. Figure 1 demonstrates this behaviour for } E_1(t) \text{ obtained from a MD-simulation. The variation of } E_1(t) \text{ on a time scale of the order of } N \text{ can clearly be observed. For that reason we take } E_n(t) \text{ as the primary slow variable and calculate its relaxation behaviour. All the other quantities, e.g. the displacement } x_n(t) \text{ will have a slowly varying part induced by the slowness of } E_n(t). \]

Our paper is organized as follows. The next section presents some general properties of the energy correlator and in the third section an equation of motion in combination with a mode coupling approach will be studied for this correlator. A perturbative treatment is performed in the fourth section and compared with the MCT-results. The fifth section contains a discussion of our results and some conclusions. Finally, an appendix provides the reader with some useful technical details.

![Fig. 1. \( E_1(t) \) for \( N = 200, \mu = 0.4 \) and \( T = 3 \) in reduced units](image)

### 2. Energy correlator: general properties

The dynamics of many-particle systems is best studied by means of correlation functions [9]. As argued above the one-particles energies \( E_n \) or their Fourier transform [10]

\[ \tilde{E}_q = \sum_{n=1}^{N} E_n \omega^{qn} \]

are the primary slow variables. \( q \) takes the value \( 2\pi v/N \) for \( v = 0, 1, \ldots, N - 1 \). To investigate their dynamical behaviour we calculate the normalized energy correlator

\[ \Phi_q(t) = \frac{\langle \delta \tilde{E}_q(t) \delta \tilde{E}_q \rangle}{\langle \delta \tilde{E}_q \rangle^2} \]

where \( \delta \tilde{E}_q = \tilde{E}_q - \langle \tilde{E}_q \rangle \). \( A^* \) denotes the complex conjugate of \( A \) and \( \mathcal{L} = \mathcal{L}_0 + \mathcal{L}_1 \) with

\[ i\mathcal{L}_0 = \sum_n \left[ \frac{1}{m} p_n \frac{\partial}{\partial x_n} - V'(x_n) \frac{\partial}{\partial p_n} \right] \text{, } i\mathcal{L}_1 = \frac{\mu}{N} \sum_k \omega^{qk} \frac{\partial}{\partial p_n} \]

is the corresponding Liouvillian.

The permutation symmetry of our model leads to

\[ \langle \delta E_n(t) \delta E_m \rangle = \begin{cases} \langle \delta E_1(t) \delta E_1 \rangle, & \text{for all } n = m \\ \langle \delta E_1(t) \delta E_2 \rangle, & \text{for all } n \neq m \end{cases} \]

which implies

\[ \Phi_q(t) = \begin{cases} \Phi_0(t), & q = 0 \\ \Phi_1(t), & \text{for all } q \neq 0 \end{cases} \]

i.e. either in real or in Fourier space there exist only two independent correlation functions.

We have decomposed \( L \) into the noninteracting part \( \mathcal{L}_0 \) and the part \( \mathcal{L}_1 \) stemming from the long range interactions. Replacement of \( \frac{1}{\mu} \sum_k x_k \) in \( i\mathcal{L}_1 \) by its thermal average \( \langle x_k \rangle \) results in the Vlasov dynamics [5], where the fluctuations governing the final decay of \( S(t) \) are eliminated. Since these fluctuation effects are our main concern, it is obvious that we have to go beyond the Vlasov approximation. The decomposition of \( L \) may also suggest to treat \( \mathcal{L}_1 \) as a perturbation. In that case \( \exp[-i(L_0 + L_1)\tau] \) could be rewritten in an interaction representation like in