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Mode coupling approximation in a model of structural phase transitions with infinite range interaction

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The long-time value of the displacement-displacement correlation function and the mean square displacements are calculated within the ϕ^4-lattice model with infinite range interaction by use of a mode coupling approximation. Their temperature dependence is compared with exact results. While the mean square displacements (zero decoupling times) agree with exact results except the low temperature range for weak coupling, the long time correlations from MCA (infinite decoupling times) are wrong. Even a separation of the displacement function into two parts representing the two different time scales is of no use since the distribution function doesn't separate.

1. Introduction

There exist several approaches of explanation of a narrow central peak (CP) in the scattering function near structural phase transitions out-side in the critical region [1–2]. Especially a possible appearance of long-time values of the displacement-displacement correlation function (without any defects) due to nonlinearities was discussed in [3] as a reason for such an effect. The calculation of the long time correlations (LTC) in [3] was based on a mode coupling approximation (MCA) for a scalar lattice Φ^4-lattice model with finite range interaction, where no exact results of the dynamical problem are known. The main predictions are: *i)* there can exist LTC (depending on the model parameters); *ii)* there exists a temperature T_g separating regions with vanishing and nonvanishing LTC; *iii)* the temperature dependence of LTC can be calculated and *iv)* in the vicinity of $T_g \left(\left|\frac{T-T_g}{T_g} \ll 1\right|\right)$ one can apply exact results of the mode coupling theory of Götze [4] calculating the low frequency dynamics of the system. Especially *ii)* implies a connection to such interesting questions as nonmixing, nonergodicity and equipartition threshold.

In the case of infinite range interaction the temperature dependence of LTC can be calculated numerically exactly [5]. In this case it follows that besides prediction *i)* all other MCA predictions seem to fail (see also [6]). Especially prediction *iv)* was studied in [7] by molecular dynamical simulations of finite Φ^4-systems with infinite range interaction. The analysis of relaxation properties clearly demonstrate problems of MCA for finite systems too.

Here we want to discuss the results of a MCA in the infinite range interaction case by solving the MCA equations for zero decoupling times (calculating the mean square displacements (MSD)) and for infinite decoupling times (calculating the LTC). We hope that the discussion of our results will help in more understanding of the problems and advantages of MCA in our case. Of course more realistic systems have finite range interactions. We want mention here the molecular dynamics simulations of one- and two-dimensional (isotropical and anisotropical) Φ^4-systems in [8] indicating some interesting 'MCA-like' results in the case of strongly correlated one- and quasi-one-dimensional systems. However in the present paper only infinite range interaction is considered. In Sect. 2 the model is introduced and equations of motion are derived. In Sect. 3 the MCA is applied to our case. Section 4 contains results and discussion.

2. Model, equations of motion and long time correlations

We study the scalar Φ^4-lattice model used to simulate structural phase transitions (see e.g. [1]):

$$H=\sum_l \left(\frac{P_l^2}{2}-\frac{1}{2}X_l^2+\frac{1}{4}X_l^4\right)+\frac{1}{4}\sum_{l,k} f_{lk}(X_l-X_k)^2 \qquad (2.1)$$

X_l and P_l are canonically conjugated particle displacements and momenta. Index 1 runs over all unit cells, f_{lk} is the harmonical interaction. All variables are dimensionless (see [5]). In the case of infinite range interaction

$$f_{lk}=\frac{f_0}{N}, \quad N \equiv \textit{number of unit cells} \tag{2.2}$$

model (2.1) reduces to an effective one-particle problem with a mean field [1] for $N \to \infty$:

$$H(P, X)=\frac{P^2}{2}-\frac{1}{2}(1-f_0)X^2+\frac{1}{4}X^4-f_0\langle X\rangle X, \tag{2.3}$$

$$\langle\ldots\rangle=\frac{1}{Z}\int \mathrm{d}\Gamma\, \mathrm{e}^{-\beta H(P,X)}\cdot\ldots, \quad Z=\int \mathrm{d}\Gamma\, \mathrm{e}^{-\beta H(P,X)},$$

$$\mathrm{d}\Gamma=\mathrm{d}P\cdot\mathrm{d}X, \quad \beta=\frac{1}{T}.$$

We want to mention that (2.3) is valid only if we first perform the $N \to \infty$ limit and solve the dynamical problem afterwards. As it was shown in [7] the corresponding N-particle system is ergodic at all temperatures (and obeys no phase transition) where the corresponding relaxation process takes place on a time scale τ_N: $\tau_N(N \to \infty) \to \infty$.

Since we restrict our interest to the high symmetry phase ($T > T_c$, $T_c \equiv$ *phase transition temperature*) it follows $\langle X\rangle=0$ in (2.3).

Using the theory of linear response [9] one can calculate the static susceptibility χ_{ll}^T via the mean square displacements $\langle X_l^2\rangle$:

$$\chi_{ll}^T=\beta\langle X_l^2\rangle \tag{2.4}$$

$$\langle X_l^2\rangle=\frac{\int \mathrm{e}^{-\beta V(X)}X^2\,\mathrm{d}X}{\int \mathrm{e}^{-\beta V(X)}\,\mathrm{d}X},$$

$$V(X)=-\tfrac{1}{2}(1-f_0)X^2+\tfrac{1}{4}X^4. \tag{2.5}$$

Finally the long time value of the displacement-displacement correlation function

$$S_{lk}(t)=\langle X_l(t)\,X_k(0)\rangle \tag{2.6}$$

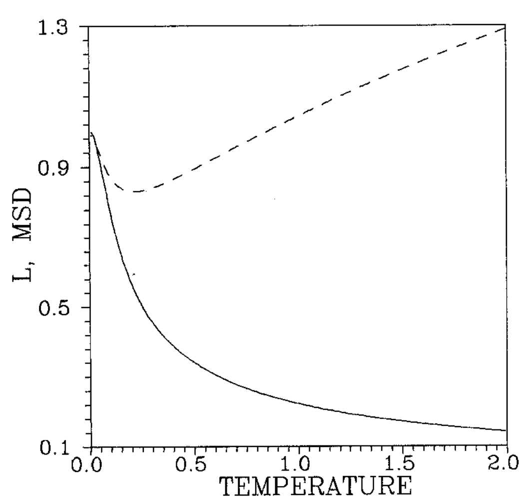

Fig. 1. Mean square displacements (dashed line) and L (solid line) versus temperature for $f_0=10^{-4}$ (from [5])

$$L_{lk}=\lim_{t\to\infty}\langle X_l(t)\cdot X_k\rangle \equiv \lim_{\tau\to\infty}\frac{1}{\tau}\int_0^\tau \mathrm{d}t\,\langle X_l(t)\cdot X_k\rangle \tag{2.7}$$

can be calculated numerically [5]. The results are shown in Fig. 1.

Since $L \neq 0$ holds for all temperatures in the case $f_0<1$ we get a $L\cdot\delta(\omega)$-component in the Fourier-transformed spectrum of the correlation function $S_{ll}(t)$ and thus a CP in the scattering function [3, 5]. For $f_0>1$ no LTC appear at arbitrary temperatures [5].

3. Mode coupling approach

The basic idea of the mode coupling approach used by Aksenov et al. [3] is a decoupling procedure of higher order correlation functions appearing in a hierarchy of equations of motion using a projection operator technique of Tserkovnikov [10] (which is equivalent to the Mori projection technique, however the kind of projections is different).

For that it is useful to start with the Laplace transform of $S_q(t)$ ($A_q=\sum_l \mathrm{e}^{iql}A_l$):

$$S_q(z)=\frac{1}{i}\int_0^\infty \mathrm{d}t\,\mathrm{e}^{izt}S_q(t), \quad \mathrm{Im}(z)>0. \tag{3.1}$$

Using the standard equations of motion of Greens functions (see e.g. [11]) one gets [3]:

$$S_q(z)=\frac{T\chi_q^T}{z-\dfrac{1/\chi_q^T}{z-M_q(z)/T}} \tag{3.2}$$

with

$$M_q(z)\equiv((X_l^3|X_k^3))_q^{(2)}(z) \tag{3.3}$$

$$((A|B))_q^{(2)}(z)$$
$$=((A|B))_q^{(1)}(z)-((A|P))_q^{(1)}(z)\frac{1}{((P|P))_q^{(1)}(z)}((P|B))_q^{(1)}(z)$$

$$((A|B))_q^{(1)}(z)=((A|B))_q(z)$$
$$-((A|X))_q(z)\frac{1}{((X|X))_q(z)}((X|B))_q(z) \tag{3.4}$$

$$((A|B))_q(z)=\frac{1}{i}\int_0^\infty \mathrm{d}t\,\mathrm{e}^{izt}\langle A(t)\,B(0)\rangle_q.$$

Now one can express L_q from (2.7):

$$L_q=\lim_{z\to i0} z\cdot S_q(z)=\frac{\chi_q^T\cdot\Pi_q}{1/\chi_q^T+\Pi_q/T} \tag{3.5}$$

where Π_q is the pole of the relaxation kernel $M_q(z)$:

$$\Pi_q=\lim_{z\to i0} z\cdot M_q(z). \tag{3.6}$$

The standard mode coupling approximation decouples all higher order correlations functions in (3.3) into products of lower order correlation functions. Due to the special character of the projections in (3.4) the result looks very simple [3]:

$$M_{lk}(t) \approx \gamma \cdot (S_{lk}(t))^3. \tag{3.7}$$

Parameter γ was assumed to be equal to 6 in [3] (this value corresponds to decoupling rules of harmonical systems with $\langle X^{2n} \rangle = 1 \cdot 3 \cdot \ldots \cdot (2n-1) \langle X^2 \rangle^n$). Here however we want to use γ as a fit parameter since it is evident that e.g. in the case of decoupled X^4-oscillators one yields

$$\langle X^{2n} \rangle = \langle X^2 \rangle^n \cdot \frac{\Gamma((2n+1)/4)}{\Gamma(1/4)} \cdot \left[\frac{\Gamma(1/4)}{\Gamma(3/4)}\right]^n, \tag{3.8}$$

$$\langle X^2 \rangle = 2 \cdot \frac{\Gamma(3/4)}{\Gamma(1/4)} \cdot \sqrt{T}. \tag{3.9}$$

With (2.7), (3.5), (3.6), (3.7) one gets assuming infinite range interaction

$$L_{ll} = \frac{\langle X_l^2 \rangle \cdot \gamma L_{ll}^3}{T^2 / \langle X_l^2 \rangle + \gamma \cdot L_{ll}^3}. \tag{3.10}$$

Equation (3.10) is the result of a MCA at infinite decoupling times in (3.7). Since (3.10) leads to two positive solutions besides the trivial one ($L=0$) we calculated only the largest one. All others can be considered as unphysical ones [4]. At a temperature T_g both positive solutions disappear leaving the zero solution as the physical one.

To obtain an expression for $M_{ll}(t=0)$ we use the Mori-representation for the relaxation kernel [12]:

$$M_{ll}(t) = \langle \hat{Q} \ddot{X}_l e^{i\hat{Q}\hat{L}\hat{Q}t} \hat{Q} \ddot{X}_l \rangle \tag{3.11}$$

with

$$\hat{Q}A = A - \frac{\langle \dot{X} A \rangle}{\langle \dot{X}^2 \rangle} \cdot \dot{X} - \frac{\langle X A \rangle}{\langle X^2 \rangle} \cdot X$$

where $\hat{P} = 1 - \hat{Q}$ being the projection operator onto the X, P-subspace and $\hat{L}$ being the Liouville-operator: $i\hat{L}A = \dot{A}$. Using the Kubo-identity [12] we obtain

$$\langle \dot{X}_l^2 \rangle = T = \langle X_l \cdot \ddot{X}_l \rangle \tag{3.12}$$

$$\langle \ddot{X}_l^2 \rangle = T \cdot (-1 + f_0 + 3 \langle X_l^2 \rangle) \tag{3.13}$$

and thus for $M(t=0)$:

$$M_{ll}(t=0) = T \cdot (-1 + f_0 + 3 \langle X_l^2 \rangle) - T / \chi_{ll}^T. \tag{3.14}$$

Now we are able to write down an equation for $\langle X_l^2 \rangle$ using the MCA in (3.7) at zero decoupling times:

$$\gamma \cdot \langle X_l^2 \rangle^3 / T + T / \langle X_l^2 \rangle - (-1 + f_0 + 3 \langle X_l^2 \rangle) = 0. \tag{3.15}$$

The next steps are: first we calculate L_{ll} from (3.10) using the exact solution of $\langle X_l^2 \rangle$ [5] and compare with the exact solution from [5]. Then we calculate $\langle X_l^2 \rangle$ from (3.15) and compare it with the exact solution $\langle X_l^2 \rangle$.

4. Results and discussion

The $L_{ll}(T)$-dependence from (3.10) for different values of γ is shown in Fig. 2 for $f_0 = 0.0001$. It is clearly seen, that no agreement with the exact results can be found. The absence of a dynamical transition $L = \emptyset \leftrightarrow L \neq 0$ at a temperature T_g as predicted by MCA (Fig. 2) and moreover the absence of a plateau in the $L(T)$-dependence is evident. The agreement of the $L(T)$-dependence for $T \to 0$ is independent on the concrete MCA in (3.7), only $M \neq 0$ is a necessary condition (this comes from the divergency of $\chi_{ll}^T(T \to 0)$). These conclusions are correct for all $f_0 < 1$.

In Figs. 3 and 4 the T-dependence of $\langle X_l^2 \rangle$ from Eq. (3.15) is shown. We get good agreement of the MCA-result with the exact one for strong coupling $f_0 > 1$ and also for weak coupling $f_0 \ll 1$ if $T \geqq 4$. It should be noted here that from the quartic equation (3.15) we get always a second positive solution at higher values which can be adressed to a higher susceptibility and thus to a more unstable phase.

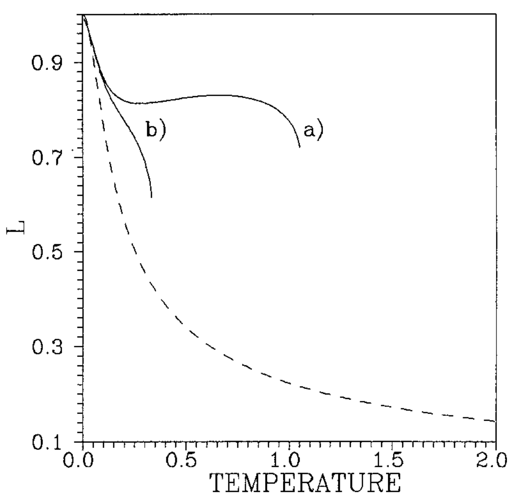

Fig. 2. L from MCA versus temperature ($f_0 = 10^{-4}$) **a** $\gamma = 6$ **b** $\gamma = 1.5$; dashed line: exact result [5]

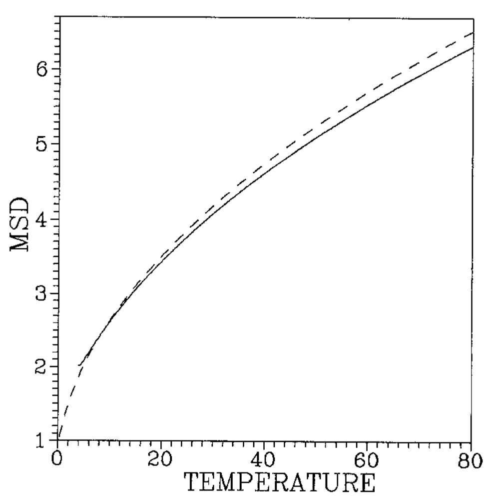

Fig. 3. $\langle X_l^2 \rangle$ from MCA versus temperature for $f_0 = 10^{-4}$, $\gamma = 1.5$; dashed line: exact result [5]

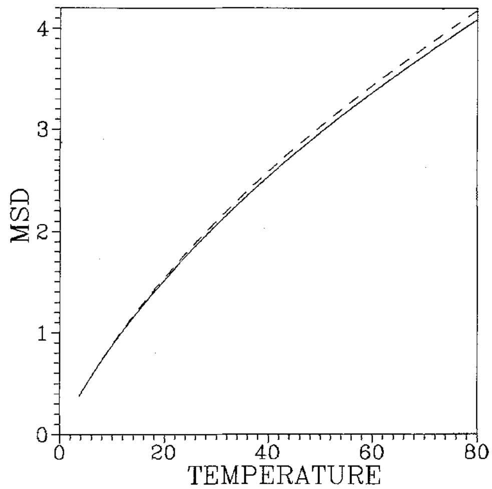

Fig. 4. $\langle X_l^2 \rangle$ from MCA versus temperature for $f_0=10$, $\gamma=2$; dashed line: exact result [5]

Thus we can conclude the MCA being a quite good approximation for zero decoupling times and high enough temperatures. This is not surprising since for high enough temperatures the particle feels only the X^4-term in potential (2.5) and then Gauss-like decoupling procedures like MCA are correct for static fluctuations (see (3.8), (3.9)). For infinite decoupling times the MCA leads to incorrect results in the case of a Φ^4-model with infinite range interaction (except the statement that $L \neq 0$ can appear).

To proceed in the finding of reasons for such a behaviour we tried to take into account the two-time character of the displacement function $X(t)$ (a fast component $\bar{\bar{X}}(t)$ representing the fluctuations around a metastable mean displacement and a slow component $\bar{X}(t)$ representing the fluctuations of the mean displacements). Thus we define

$$X = \bar{X} + \bar{\bar{X}}$$

$$\langle \bar{X}^2 \rangle = L, \quad \langle \bar{X} \rangle = \langle \bar{\bar{X}} \rangle = \langle \bar{X} \cdot \bar{\bar{X}} \rangle = 0. \tag{4.1}$$

An exact and comprehensive introduction of this separation using projection techniques [12] leads also to the properties

$$\lim_{t\to\infty} \langle \bar{X}(t) \cdot \bar{X}(0) \rangle = \langle \bar{X}^2 \rangle \tag{4.2}$$

$$\lim_{t\to\infty} \langle \bar{X}(t) \cdot \bar{\bar{X}}(0) \rangle = \lim_{t\to\infty} \langle \bar{\bar{X}}(t) \cdot \bar{\bar{X}}(0) \rangle = 0. \tag{4.3}$$

If $\lim_{t\to\infty} S(t)$ exists then one can use the property

$$\lim_{t\to\infty} \left(\frac{\mathrm{d}}{\mathrm{d}t}\right)^n \langle X(t) X \rangle = 0 \qquad n > 0$$

deriving

$$\lim_{t\to\infty} \langle X(t) \cdot X^3 \rangle = (1 - f_0) \cdot L. \tag{4.4}$$

Now we make a nontrivial assumption about the separation of the distribution function

$$\mathrm{e}^{-\beta V(X)} / \int \mathrm{e}^{-\beta V(X)} \, \mathrm{d}X \equiv \rho(X, T) \equiv \rho(\bar{X}, \bar{\bar{X}}, T) \tag{4.5}$$

of both variables $\bar{X}$ and $\bar{\bar{X}}$ into a product of two functions $\rho(\bar{X}, \bar{\bar{X}}, T) = \bar{\rho}(\bar{X}, T) \cdot \bar{\bar{\rho}}(\bar{\bar{X}}, T)$ each depending only on one of both variables (4.1). The result of (4.4) is

$$\langle \bar{X}^4 \rangle + 3 \langle \bar{X}^2 \rangle (\langle X^2 \rangle - \langle \bar{X}^2 \rangle)$$
$$= (1 - f_0) \cdot \langle \bar{X}^2 \rangle. \tag{4.6}$$

This equation is definitely wrong at high temperatures where $\langle X_l^2 \rangle$ is an increasing function of temperature $\langle X_l^2 \rangle \sim \sqrt{T}$ (see (3.9)) since there exist only one term of leading order in $\langle \bar{X}^2 \rangle \langle X^2 \rangle$ and we exclude the possibility $\langle \bar{X}^4 \rangle \sim \langle \bar{X}^2 \rangle^\alpha$, $\alpha > 1$ (because of $L < 1$, $|x(E)| < 1$ [5] ($x(E) \equiv$ averaged position of $x(t, X, P)$ for a fixed energy E) and thus $\langle \bar{X}^4 \rangle < L < 1$). It is not difficult to see one reason of failure of (4.6). Calculating the left side of (4.4) directly in the case of infinite range interaction in the same manner as L in [5] it is seen that replacing the impulse integration in (4.4) by an energy integration only energies below the barrier maximum of the potential (2.5) contribute. However making the assumption of separability of the distribution function $\rho(\bar{X}, \bar{\bar{X}})$ one gets Eq. (4.6) where in the average $\langle X^2 \rangle$ all energies contribute, i.e. for high temperatures arbitrary high energies contribute, whereas they cancel in the exact solution. Thus it is evident that just for high temperatures (high energies) disagreement will appear.

Summarizing we conclude for infinite range interaction that

i) the simple mode coupling approximation leads to good agreement with exact results for zero decoupling times i.e. for the static correlation function at high enough temperatures due to dominant Gauss-like contributions in $\langle X^2 \rangle$;
ii) the mode coupling approximation leads to false results for infinite decoupling times especially since it predicts a transition temperature

$$T_g\colon \; L(T \leq T_g) \neq 0, \qquad L(T > T_g) = 0;$$

iii) the possibility of a separation of the displacement $X(t)$ into two parts representing the two different time scales cannot be used in a decoupling procedure since the distribution function $\rho(X)$ doesn't separate.

These conclusions, especially *iii)* are not in contradiction to the results of [13] where a double well potential was found leading to a distribution function being equal to the sum of two Gauss-distributions. Then there exists a possibility of separating the displacement into two components and the separability of the distribution function is exact in that case. However this 'Ising-like' part has nothing to do with the long-time correlations of $\langle X(t) X \rangle$ since it represents only the position of the minima of the double well potential thus being T-independent in contrast to the $L(T)$-dependence. This conclusion comes from a fitting procedure of the distribution function (4.5) by the one from [13] (where the potential is temperature dependent) using the width of one Gauss distribution and the distance between both ones as parameters. Then the result of this fitting procedure to a Φ^4-model is the distance between the Gauss-distributions (the 'Ising'-like part) being equal to the (temperature independent) distance of the minima of the Φ^4 double well potential for all temperatures.

Finally we want to point to the rightness of our results only in the case of infinite range interaction where no energy fluctuations between the particles are allowed. There are indications that for one-dimensional strongly correlated Φ^4-systems with next neighbour interaction the situation can be changed drastically and MCA-predictions may be correct also for infinite decoupling times [8].

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