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LETTER TO THE EDITOR

Dynamical scaling properties of a one-dimensional Φ^4 lattice model—comparison with mode coupling theory

S Flach and J Siewert†

Institut für Theoretische Physik, Technische Universität Dresden, Mommsenstrasse 13, D-8027 Dresden, Federal Republic of Germany

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Abstract. The dynamical scaling behaviour of the displacement–displacement correlation function of the one-dimensional Φ^4 lattice model is analysed by use of molecular dynamics simulations. The existence of a crossover temperature where relaxation times drastically increase suggests possible applicability of mode coupling theory (MCT) describing freezing processes in undercooled liquids. We find two independent dynamical scaling regions (two master functions describing the time evolution of the correlator) in accordance with MCT. A quantitative comparison of the MCT predicted scaling laws with the calculated ones for the Φ^4 model shows significant non-applicability of MCT especially for the β relaxation process.

The mode coupling theory (MCT) is considered to be a powerful tool in understanding dynamical freezing processes for a large class of structurally disordered systems ([1] and references therein). The mode coupling equations (MCE) describe the dynamics of some normalized correlators $\Phi_q(t)$ with $\Phi_q(0) = 1$, $\dot{\Phi}_q(0) = 0$. Usually the variables under consideration are density fluctuations. The essential proposals of the MCT are the prediction of some (ideal) transition from ergodic ($\Phi_q(t \to \infty) = 0$) to non-ergodic ($\Phi_q(t \to \infty) \neq 0$) states at a temperature $T = T_c^{MCT}$ and the derivation of two dynamical scaling regions for $\Phi_q(t)$ [2,3]. The applicability of MCT to real systems seems to depend on the structure of the potential landscape of the system [4].

Recently a decoupling procedure was proposed by Aksenov *et al* for a system with a second-order phase transition at $T = T_c$, namely the one-component Φ^4 lattice model [5]

$$H = \sum_{l=1}^{N} \left(\frac{1}{2} P_l^2 - \frac{1}{2} X_l^2 + \frac{1}{4} X_l^4 \right) + \frac{1}{4} \sum_{l,k=1}^{N} C_{lk} (X_l - X_k)^2. \tag{1}$$

The resulting equations for the displacement–displacement correlation function $S_{lk}(t) = \langle X_l(t) X_k \rangle$, $S_{lk} = \langle X_l X_k \rangle$ after decoupling read [5] (see also [6,7] for detailed analysis)

† Present address: Institut für Theoretische Festkörperphysik, Universität Karlsruhe, Engesserstrasse 7, Postfach 6980, D-7500 Karlsruhe 1, Federal Republic of Germany.

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$$S_q(z) = \frac{S_q}{z - TS_q^{-1}(z - M_q(z)/T)^{-1}} \tag{2}$$

$$M_{lk}(t) = 6S_{lk}^3(t) \tag{3}$$

$$A(z) = \frac{1}{\mathrm{i}} \int_0^\infty \mathrm{d}t\, \mathrm{e}^{\mathrm{i}zt} A(t). \tag{4}$$

The equations (2)–(4) are a special case of the more general MCE discussed in [1]. In general they exhibit a transition from ergodic $S_q(t \to \infty) = 0$ to non-ergodic $S_q(t \to \infty) = L_q \neq 0$ at some T_c^{MCT}. This transition is an A_2 singularity following the notations of [1], i.e. for $T = T_c^{\mathrm{MCT}}$ the $L_q(T_c^{\mathrm{MCT}}) = L_q^c$ solutions are doubly degenerate. The whole A_2 scenario of MCT applies to the dynamics of $S_q(t)$, and thus near T_c^{MCT} two different dynamical scaling laws should appear for $T > T_c^{\mathrm{MCT}}$. The normalized correlator $\Phi_q(t) = S_q(t)/S_q$ will exhibit an inflection point for $T > T_c^{\mathrm{MCT}}$ at $\Phi_q(t_{\mathrm{infl}}) \approx f_q^c = L_q^c/S_q(T_c^{\mathrm{MCT}})$. For $\delta\Phi_q(t) = \Phi_q(t) - f_q^c \ll 1$ and $\varepsilon = (T - T_c^{\mathrm{MCT}})/T_c^{\mathrm{MCT}}$ one obtains the β-scaling law [1]

$$\delta\Phi_q(t) = h_q\sqrt{\varepsilon}\, g(t/t_\varepsilon) \tag{5}$$

$$t_\varepsilon = t_0 \varepsilon^{-1/2a}. \tag{6}$$

For $\Phi_q(t) < f_q^c$ one finds the α-scaling law

$$\Phi_q(t) = F_q(t/\tau_\varepsilon) \tag{7}$$

$$\tau_\varepsilon = t_0 \varepsilon^{-1/2a - 1/2b} \tag{8}$$

$$\frac{\Gamma^2(1-a)}{\Gamma(1-2a)} = \frac{\Gamma^2(1+b)}{\Gamma(1+2b)} = \lambda. \tag{9}$$

$\Gamma(x)$ is the Gamma function. The parameter λ is model dependent. The master function $g(t)$ for the β-scaling law (5), (6) can be specified as $g(t) \sim t^{-a}$ for $g(t) > 0$ and as $g(t) \sim -t^b$ for $g(t) < 0$. The master function $F_q(t)$ for the α-scaling law cannot be given in an analytical expression in general.

The features of the potential landscape of (1) and related models were studied for different cases of interaction strength and range [8–10]. Although the model (1) has no disorder in the interaction (translational invariance) the structure of the potential landscape turns out to be very complex thus not *a priori* excluding the non-applicability of MCT from the point of view of energy barrier distributions.

The case of infinite-range interaction $C_{lk} = C_0/N$, however, brought out a complete disagreement with MCT [6,7,11] in the sense that no T_c^{MCT} or even its indication exists.

Here we want to analyse the opposite case of nearest-neighbour interaction $C_{lk} = C\delta_{l\pm1,k}$ for the one-dimensional system. Earlier investigations (see e.g. [12–15]) pointed out the existence of some crossover temperature separating displacive from order–disorder behaviour [16]. Indeed molecular dynamics simulations [17] confirmed for $C > 1$ the existence of a crossover temperature T^*, at which relaxation times and correlation lengths drastically increase. Lowering C leads to a lowering of T^*.

Thus for weak coupling $C \ll 1$ no crossover is observed [17,18]. The crossover phenomenon seems to disappear for two- and three-dimensional isotropic systems [17]. It should be noted that at T^* the correlation length of the model (1) with nearest-neighbour interaction also increases [17], so we have an unusual dependence of the static structure factor S_q on temperature near T^*. Strictly speaking up to now it is unclear whether the equations (2)–(4) lead to a non-ergodic transition using the exact q-dependent values $S_q(T)$. So it might happen that the correct treatment of the equations mentioned yields only the ergodic solutions $f_q = 0$.

In this work we performed careful calculations of the displacement–displacement correlation function $S_{ll}(t) = \langle X_l(t)X_l(0)\rangle$. Our goal is to investigate the dynamical scaling behaviour (if any observed) of the imaginary part of the normalized susceptibility

$$\chi''_{ll} = \omega \int_0^\infty \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t}\Phi_{ll}(t). \tag{10}$$

We then compare its scaling behaviour with the MCT predictions (5)–(9). We performed molecular dynamics simulations (MDS) with periodic boundary conditions and used the Verlet algorithm [19]. The total energy of the system was conserved (microcanonical simulation). The time steps were $h = 0.005$ and the system sizes varied from $N = 2000$ to $N = 8000$. We found no h- and N-dependence of our calculations; thus finite-size effects can be excluded. The energy was conserved within 0.001% during one run and the correlation function $S_{ll}(t)$ was calculated with an accuracy of 0.001. The initial values S_{ll} varied between 0.7 and 1. To make sure we have calculated the correct $S_{ll}(t)$ dependence we performed two independent runs with random initial configurations for every energy. Then we mapped both solutions onto each other. We found that the shorter the total simulation time, the shorter is the maximum correlation time up to which our two independent results $S_{ll}(t)$ reasonably agree. By lowering the energy and fixing some correlation time we found a drastic increase of the shortest necessary total simulation time. This indicates that the lower the energy, the longer the system needs to overcome all barriers in the potential landscape.

All calculations were done for $C = 4$. In this strongly coupled regime a change of C is equivalent to a rescaling of the total energy [20]. The temperature was defined via $T = \langle \dot{X}_l^2 \rangle$. From our previous studies [17] we expect a possible crossover for $T = 0.3, \ldots, 0.35$. Thus we performed different runs for temperatures $0.3 < T < 0.5$. The Fourier transformation of $S_{ll}(t)$ we performed using the FILON algorithm [21].

In figure 1 we show the time dependence of the normalized correlator $\Phi_{ll}(t)$ for various temperatures against time. It should be noted that the characteristic microscopic times of the system are of order 2π. Indeed we see a shifting of relaxation times to higher values with decreasing temperature; however, the shift is only of the order 1–2 decades if the temperature decreases from 0.5 to 0.3. The scaling analysis has to be done for the more sensitive $\chi''_{ll}(\omega)$ dependence. In figure 2(a) we show $\chi''_{ll}(\omega)$ for different temperatures from the temperature interval mentioned. We see the high-frequency microscopic excitation band. Because of the appearance of kinks separating regions with positive or negative sign of the particle displacements X for strong coupling [12,22,23], this excitation band can be described by the dynamics of one cluster chain (the cluster sizes become large with lowering T) for $T \to 0$.

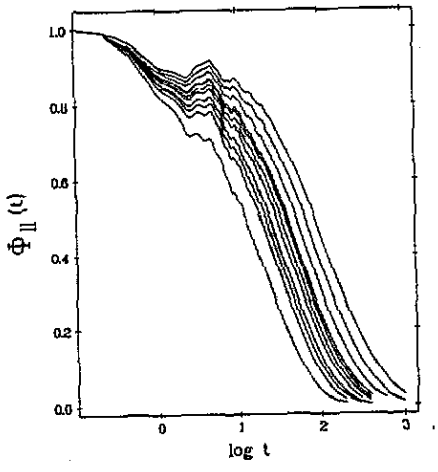

Figure 1. Normalized correlator $\Phi_{II}(t)$ against $\log(t)$ for temperatures $T = 0.331$; 0.346; 0.364; 0.379; 0.387; 0.397; 0.404; 0.42; 0.432; 0.445; 0.487. Higher temperatures correspond to smaller values of $\Phi_{II}(t)$.

A linearization of the corresponding dynamical problem yields a chain of coupled harmonic oscillators. Then a simple calculation for $\chi''_{II}(\omega)$ for $N \to \infty$ gives

$$\chi''_{II}(\omega) = \frac{T}{\sqrt{\omega^2 - 2}} \frac{1}{\sqrt{4C - (\omega^2 - 2)}} \qquad 2 \leqslant \omega^2 \leqslant 4C + 2 \tag{11}$$

$$\chi''_{II}(\omega) = 0 \qquad \text{otherwise.} \tag{12}$$

The resulting square root singularities at $\omega = \sqrt{2}$ and $\omega = \sqrt{4C+2}$ are precisely found in figure 2(*a*).

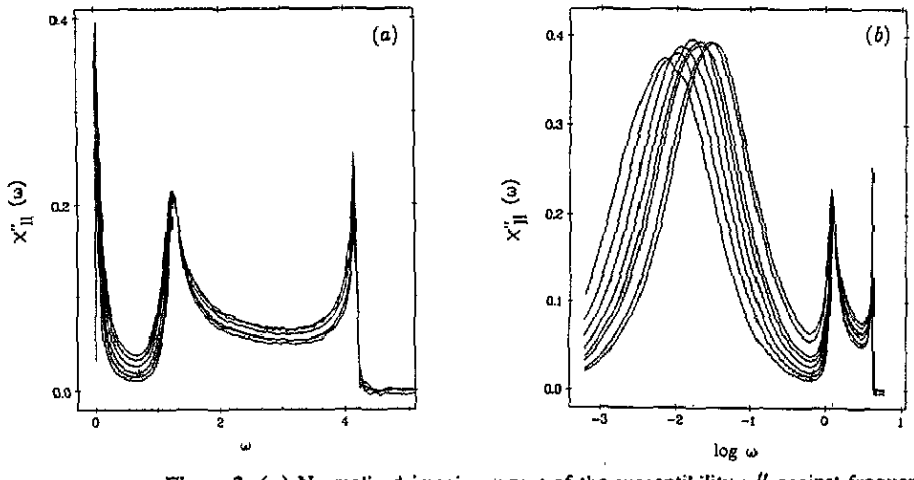

Figure 2. (*a*) Normalized imaginary part of the susceptibility χ''_{II} against frequency ω for temperatures $T = 0.331$; 0.346; 0.364; 0.379; 0.397; 0.404. Higher temperatures correspond to larger values of χ''_{II}. (*b*) χ''_{II} against $\log(\omega)$ for temperatures $T = 0.331$; 0.346; 0.364; 0.379; 0.397; 0.404; 0.432; 0.445. Higher temperatures correspond to larger values of χ''_{II} in the β'-minimum.

In figure 2(*b*) we plot $\chi''_{ll}(\omega)$ against $\log(\omega)$ to see the low-frequency behaviour. We observe a low-frequency peak denoted as the α'-peak at $\omega = \omega_{\alpha'}$ and a following minimum denoted as the β'-minimum at $\omega = \omega_{\beta'}$. The α'-peak shifts to lower frequencies as temperature is lowered. The β'-minimum *does not shift* significantly with T. Its height, however, decreases with decreasing T.

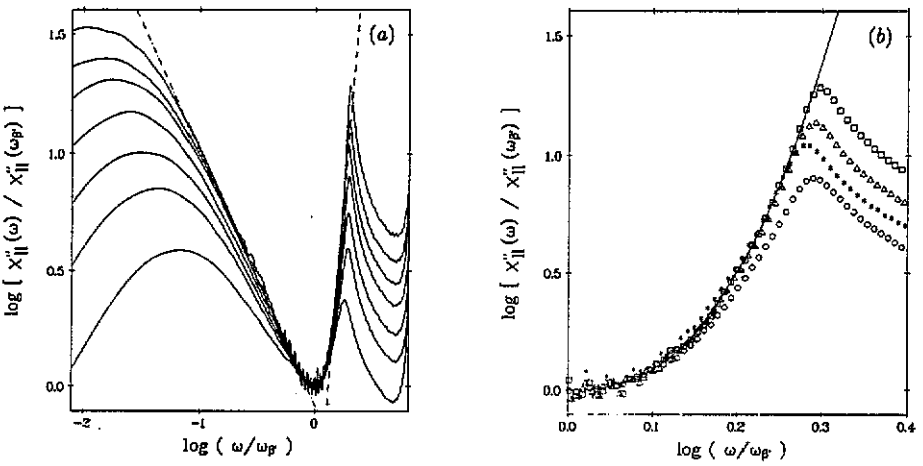

Figure 3. (*a*) Scaled $\chi''_{ll}/\chi''_{ll}(\omega_{\beta'})$ against scaled frequency $\omega/\omega_{\beta'}$ for the β'-minimum in a log–log plot. $T = 0.331$; 0.346; 0.364; 0.379; 0.404; 0.432; 0.487. Higher temperatures correspond to larger values of the scaled function outside the β'-minimum. The dashed line is a power fit $\chi''_{ll} \sim \omega^a$ with $a = 6.14$, the dashed dotted line is a power fit $\chi''_{ll} \sim \omega^{-b}$ with $b = 1.06$. (*b*) Same as figure 3(*a*) but on a stretched frequency scale. Only the right hand side of the β'-minimum is seen. Squares, $T = 0.331$; triangles, $T = 0.346$; stars, $T = 0.364$; circles, $T = 0.379$. Clearly a master function is observed. The solid line is a fit corresponding to (13).

To discuss applicability of MCT we plot in figure 3(*a*) the scaled function $\chi''_{ll,\beta'}(\hat{\omega}) = \chi''_{ll}(\hat{\omega}\omega_{\beta'})/\chi''_{ll}(\omega_{\beta'})$, $\hat{\omega} = \omega/\omega_{\beta'}$. Clearly we *see* a master function for the β'-minimum. If the MCT A_2 scenario applies then the power laws $\chi''_{ll,\beta'}(\hat{\omega} > 1) \sim \hat{\omega}^a$ and $\chi''_{ll,\beta'}(\hat{\omega} < 1) \sim \hat{\omega}^{-b}$ should be valid. From Figure 3(*a*) we find $b \approx 1.06$ (dashed dotted line in figure 3(*a*)). Thus we obtain $\lambda \approx 0.47$ (9). For the exponent a from (9) it follows that $a \approx 0.4$. In figure 3(*a*) the dashed line corresponds to a power fit of the high-frequency side of the β'-minimum with $a = 6.14$. A more confident conclusion can be drawn if one stretches the ω-scale on the high-frequency side of the β'-minimum. In figure 3(*b*) it is seen that *no* power law (linear dependence in the log–log plot) is observed. Supposing that at higher frequencies (near the β'-maximum) a power law is valid, the power exponent a would be at least $a \geqslant 6.14$. So in any case the β'-master function does not satisfy the MCT result (9). It is interesting to notice that the high-frequency side of the β'-minimum can be fitted by the expression

$$\log(\chi''/\chi''_{\beta'}) = a_1[\log(\omega/\omega_{\beta'})]^{a_2} \qquad a_1 \approx 28.24 \qquad a_2 \approx 2.5 \tag{13}$$

as shown by the solid line in figure 3(*b*).

The temperature dependence of $\chi''^2_{ll}(\omega_{\beta'})$ is shown in figure 4. While MCT predicts a linear dependence on $(T - T_c^{\mathrm{MCT}})$ (see (5)), we clearly observe no linear

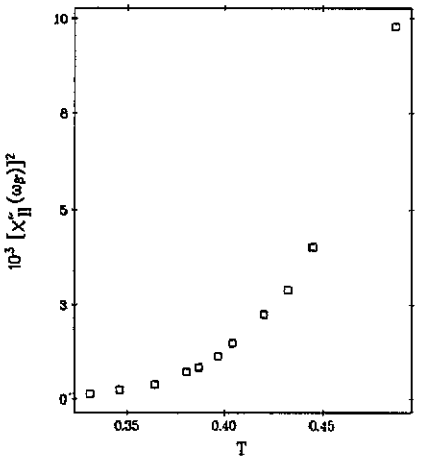

Figure 4. Squared height of the β'-minimum $\chi''^2_{\parallel}(\omega_{\beta'})$ against temperature.

dependence. The frequency of the β'-minimum $\omega_{\beta'}$ shows no temperature dependence: $\omega_{\beta'} = 0.64 \pm 0.02$ (see figure 2(*b*)). Thus no essential shift is observed in contradiction with MCT (8).

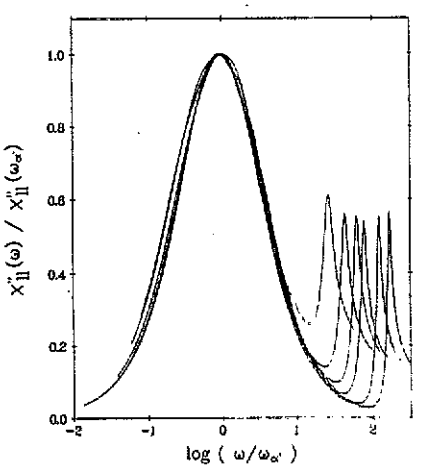

Figure 5. Scaled $\chi''_{\parallel}/\chi''_{\parallel}(\omega_{\alpha'})$ against logarithm of the scaled frequency $\omega/\omega_{\alpha'}$. $T =$ 0.331; 0.346; 0.379; 0.404; 0.432; 0.487. Higher temperatures correspond to larger values of the height of the β'-minimum.

The α'-peak scaling is shown in figure 5 for $\chi''_{\parallel,\alpha'}(\tilde{\omega}) = \chi''_{\parallel}(\tilde{\omega}\omega_{\alpha'})/\chi''_{\parallel}(\omega_{\alpha'})$, $\tilde{\omega} = \omega/\omega_{\alpha'}$. We clearly see a master function describing the α'-peak. The height of the α'-peak shows no significant temperature dependence. This is compatible with the A_2 scenario within the MCT [1]. The temperature dependence of $\omega_{\alpha'}$ is shown in figure 6. There is a decreasing of the α'-frequency scale with decreasing temperature. A fitting of this curve by MCT predictions (8) or other scaling laws seems not to be reasonable since the scale shifts only over 1–2 decades and the calculation errors are too large. It should be noted that an Arrhenius law agrees as well as a

MCT fit. Looking at the temperature dependence of viscosities of undercooled liquids approaching the glass transition [4], it is clear that distinguishing between strong and fragile glass systems is only possible with temperature variations of viscosity over five or more decades.

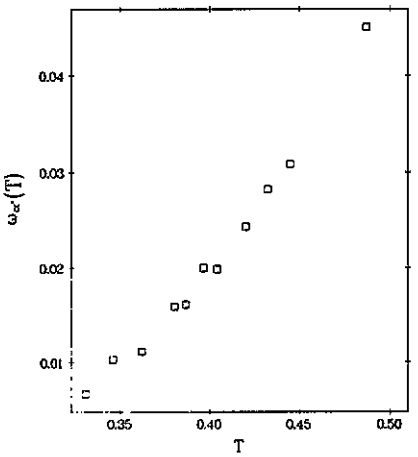

Figure 6. Position of the α'-maximum $\omega_{\alpha'}$ against temperature.

Summarizing, we found for the one-dimensional Φ^4 lattice model *two* dynamical scaling laws for the displacement–displacement correlation function near some crossover temperature. The scaling analysis brought out partially significant quantitative non-applicability of MCT in its idealized form: (i) no shift of the β'-minimum; (ii) no linear dependence of $\chi''^2_{ll}(\omega_{\beta'})$ with $(T - T_c^{MCT})$; (iii) an unreasonably high value of the expected power coefficient a; and (iv) a power law in the scaled logarithmic variables on the high-frequency side of the β'-minimum (13). On the other hand the existence of *two separated* scaling regions and the existence of a power law in the low-frequency part of the β'-minimum are well known features of an A_2 scenario of MCT. It would be difficult to understand these facts within some scenario of a suppressed phase transition due to the one-dimensional system. To our knowledge, then only *one* dynamical scaling region should appear [24].

The MCT does not deal with the critical dependence of the structure factor S_q on temperature. This seems to be significant in our case because of the drastic increase of correlation lengths approaching the crossover region [17]. Moreover, taking into account the additional relaxation processes (neglected in the idealized form of MCT [1,25,26]) one can change the previous MCT predictions essentially. Thus the applicability of a non-idealized MCT to model (1) remains an open question. Equations (2)–(4), however, cannot describe all of the dynamical features of model (1).

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