

Comment on “Mode-Coupling Theory as a Mean-Field Description of the Glass Transition”

Motivated by the interpretation of mode-coupling theory (MCT) as a mean-field theory Ikeda and Miyazaki (IM) [1] and the present authors [2] independently investigated the dependence of MCT for hard spheres, with diameter σ on the spatial dimension d , particularly in the limit $d \rightarrow \infty$. A comparison with the corresponding results from replica theory [3] has revealed serious discrepancies between both theories [1,2]. The long time limit of the self part of the van Hove function $G_{c,\infty}^{(s)}(r; d)$ is the Fourier transform of the critical self-nonergodicity parameter (NEP) $f_c^{(s)}(k; d)$:

$$G_{c,\infty}^{(s)}(r; d) = A_d r^{-(d/2-1)} \int_0^\infty dk k^{d/2} J_{d/2-1}(kr) f_c^{(s)}(k; d) \quad (1)$$

($A_d = (2\pi)^{-d/2}$). Taking $f_c^{(s)}(k; d)$ from MCT, IM show that $r^{d-1} G_{c,\infty}^{(s)}(r; d)$ has negative dips on a scale $r/\sigma = O(1)$ for $d = 4, \dots, 15$, contradicting its non-negativity. From these results IM conclude that a “reconsideration and revision of MCT from ground up is in order.” In the following we will explain why these observations are not yet sufficient to draw that conclusion.

First we show that the dips in $G_{c,\infty}^{(s)}(r; d)$ may disappear for $d \rightarrow \infty$. From our numerical approach we have found that $k^{d/2} f_c^{(s)}(k; d) \rightarrow \bar{g}_c^{(s)}(k; d) = k^{d/2} \exp[-a_d(k - k_0)/\sqrt{d}]$ ($a_\infty \cong 1.50\sigma$, $k_0 \cong 0.155\sigma^{-1}d^{3/2}$) for $d \rightarrow \infty$ (see Fig. 1 for $d = 100$).

The numerical result for $G_{c,\infty}^{(s)}(r; 100)$ (not shown) exhibits tiny negative dips. However, replacing $k^{d/2} f_c^{(s)}(k; d)$ in Eq. (1) by $\bar{g}_c^{(s)}(k; d)$ for $d \gg 1$ one obtains the analytical result $G_{c,\infty}^{(s)}(r; d) \rightarrow \bar{G}_{c,\infty}^{(s)}(r; d) = B_d/[1 + (r/a_d)^2 d]^{(d+1)/2}$ ($0 < B_d \sim d^d$). Hence $G_{c,\infty}^{(s)}(r; d)$ becomes non-negative (and a Gaussian on a scale $rd/\sigma = O(1)$) for $d \rightarrow \infty$. The same holds for the corresponding collective quantity $G_{c,\infty}(r; d)$. For $d = 100$ this also demonstrates that a small deformation of $k^{d/2} f_c^{(s)}(k; d)$ can already eliminate the negative dips even for a non-Gaussian $f_c^{(s)}(k; d)$.

A second comment is inspired by the investigation of a mean-field ϕ^4 model on a lattice with N sites [4]. It has been shown that a time scale $\tau(N) \sim N$ exists. The dynamics is nonergodic for $t \ll \tau(N)$ and ergodic for $t \gg \tau(N)$ for *all* temperatures [4]. In case that such a diverging time scale $\tau(d)$ would exist for a d -dimensional liquid, as well, both limits $t \rightarrow \infty$ and $d \rightarrow \infty$ would *not* commute. This would suggest that we investigate, e.g., the self-correlator $S^{(s)}$ in a more general scaling limit $\hat{S}^{(s)}(\hat{k}, \hat{t}; \hat{\varphi}) = \lim_{d \rightarrow \infty} S^{(s)}(d^\rho \hat{k}/\sigma, d^\eta \hat{t}; d^\kappa 2^{-d} \hat{\varphi}; d)$ with appropriate scaling exponents ρ , η and κ . This has not been done so far. In Refs. [1,2], where $\eta = 0$ is assumed the limit $t \rightarrow \infty$ has been taken first for large but *finite* d .

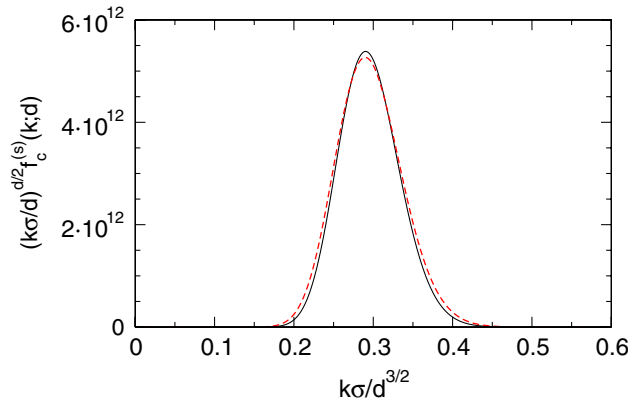


FIG. 1 (color online). k dependence of $(k\sigma/d)^{d/2} f_c^{(s)}(k; d)$ (solid line) from the numerical MCT solution and $(\sigma/d)^{d/2} \bar{g}_c^{(s)}(k; d)$ (dashed line) for $d = 100$.

The non-negativity of $G_{c,\infty}^{(s)}(r; d)$ and $G_{c,\infty}(r; d)$ for $d \rightarrow \infty$ does not imply that MCT becomes exact for $d \rightarrow \infty$. If it would turn out that MCT does not become exact for $d \rightarrow \infty$ this would imply that MCT is not a mean-field theory, at least in the conventional sense. This holds indeed for the ϕ^4 model with $\eta = 0$ [4]. Concerning $d = O(1)$, we fully agree with the existence of negative dips in $r^{d-1} G_{c,\infty}^{(s)}(r; d)$. Of course, one has to take into account that they are already strongly enhanced for $d = 15$ due to the factor r^{d-1} included by IM. Using PY theory we found that they also exist in $d = 2$ and 3 for $G_{c,\infty}^{(s)}(r; d)$ but not for $G_{c,\infty}(r; d)$. Because of the *nonlinear* structure of MCT equations this is not surprising and does not seem to affect the quality of MCT successfully tested particularly for three-dimensional liquids during more than two decades. Of course, a deeper insight, based on the removal of the negative dips or not, why MCT is so powerful in $d = 3$ and even $d = 2$ and whether it is a kind of mean-field theory or not is highly desirable.

Rolf Schilling and Bernhard Schmid
Institut für Physik
Johannes Gutenberg-Universität
D-55099 Mainz, Germany

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