

Ikeda and Miyazaki Reply: In the preceding Comment [1], Schilling and Schmid (SS) criticized our recent statement that reconsideration and revision of mode coupling theory (MCT) from the ground up are in order [2]. $\varphi_{\text{mct}}(d)$ Our statement is based on the fact that the long time limit of the self-part of the van Hove function $G_{c,\infty}^{(s)}(r; d)$ exhibits unphysical negative dips in as low dimension as $d = 6$ and the depths of the dips increase with dimension [2]. Although SS agreed with the existence of the dips, they suggested that these results are not yet sufficient to verify the above statement. Their suggestion is based upon two observations: (i) The negative dip of $G_{c,\infty}^{(s)}(r; d)$ is demonstrated to decrease as d increases. It is also shown that the dips are very sensitive to the shape of the nonergodicity parameter $f_c^{(s)}(k; d)$ and that an analytic function which fits $f_c^{(s)}(k; d)$ reasonably well can eliminate the negative dip.

They also claim that such a glitch is not surprising given the nonlinear structure of MCT and may not affect the quality of the theory. (ii) The long time and large d limit should be taken with caution. Numerical studies on a long-ranged ϕ^4 -model [3] show that the limits of $t \rightarrow \infty$ and $N \rightarrow \infty$ are not commutable, where N is the number of interaction bonds which should be proportional to d for off-lattice liquids.

Regarding the point (i), we believe that our conclusion is not affected by their objection. In Fig. 1, we show $G_{c,\infty}^{(s)}(r; d)$ multiplied by r^{d-1} , or the probability density function, in much higher dimensions than those shown in Ref. [2]. Similar dips have been observed for the collective part of the van Hove function $G_{c,\infty}^{(c)}(r; d)$. It clearly demonstrates that the amplitudes of the negative dips increase as d increases. The negative dips remain noticeable even at $d = 100$ where the asymptotic scaling of the MCT critical point $\varphi_{\text{mct}}(d) \propto d^2/2^d$ is observed [2,4]). Note also that the probability density $r^{d-1}G_{c,\infty}^{(s)}(r; d)$, rather than $G_{c,\infty}^{(s)}(r; d)$, is a natural observable, because the latter, if negative or positive, becomes negligibly small for arbitrary nonzero r 's as d increases. We emphasize that both the peculiar d dependence of $\varphi_{\text{mct}}(d)$ and the pathological negative dips of $G_{c,\infty}^{(s)}(r; d)$ derive from the non-Gaussian shape of $f_c^{(s)}(k; d)$. One cannot ignore this non-Gaussianity as a minor glitch hidden in MCT, because the different scaling of $\varphi_{\text{mct}}(d)$ from the prediction of replica theory is a grave problem which may undermine the mean-field picture of the glass transition theory.

Regarding the second point (ii), we believe that our argument is irrelevant to the conclusions of Ref. [3], where the relaxation time of a long-ranged model was demonstrated to increase with the system size N and diverge in the thermodynamic limit $N \rightarrow \infty$ in the ordered phase. This thermodynamic limit should not be taken to be equivalent to the large- d limit in our MCT analysis; MCT as well as

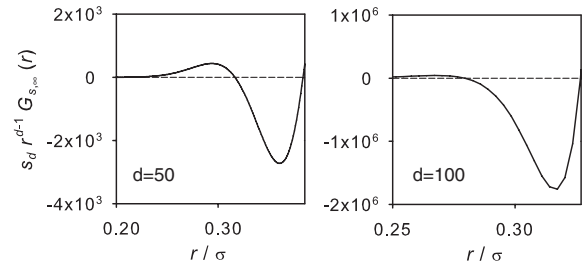


FIG. 1. $s_d r^{d-1} G_{s,\infty}(r)$ for $d = 50$ (left) and 100 (right), where s_d is the surface area of the d -dimensional unit sphere.

the replica theory are “mean-field theories” in the manner of spin glasses even in *finite* d 's.

What we have discussed in our Letter are the inconsistencies between the two theories in large but finite d 's (and not the effects of the finite-size nor finite- d in conventional critical phenomena). The reason to consider large d 's was to avoid unwanted approximations for the static parameters.

Finally, we agree with SS in that our conclusions would not imply that MCT is invalid in a certain time and temperature regime for two- and three-dimension liquids. One cannot overstate the success of MCT in predicting dynamical properties of the supercooled liquids. The question is why MCT is so powerful and robust, at least in low dimensions, despite of many uncontrolled and controversial approximations in its derivation. Another question is in what sense MCT is the mean-field theory, if there really exists a mean-field theory of the glass transition. Demonstrating the situations where MCT breaks down and fixing the breakdowns would help us to answer to these important but unanswered questions. This is the reason why we claim that “reconsideration and revision of MCT from the ground up are in order.”

Atsushi Ikeda and Kunimasa Miyazaki
Institute of Physics
University of Tsukuba
Tennodai 1-1-1, Tsukuba 305-8571, Japan

Received 17 December 2010; published 28 January 2011

DOI: 10.1103/PhysRevLett.106.049602

PACS numbers: 64.70.qj, 61.43.Fs, 64.70.pm, 66.30.hh

- [1] R. Schilling and B. Schmid, preceding Comment, Phys. Rev. Lett., **106**, 049601 (2011).
- [2] A. Ikeda and K. Miyazaki, Phys. Rev. Lett. **104**, 255704 (2010).
- [3] W. Kob and R. Schilling, J. Phys. Condens. Matter **3**, 9195 (1991).
- [4] B. Schmid and R. Schilling, Phys. Rev. E **81**, 041502 (2010).