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Facilitated spin models, mode coupling theory, and ergodic–nonergodic transitions

Steven J. Pitts, Thomas Young, and Hans C. Andersen
Department of Chemistry, Stanford University, Stanford, California 94305

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Facilitated kinetic Ising spin models are models for cooperative relaxation in liquids. Some of them have ergodic–nonergodic transitions of the type predicted by the mode coupling theory of supercooled liquids. We discuss two mode coupling theories, that of Kawasaki and one developed by us, and compare their predictions with the properties of several facilitated kinetic spin models, including the hierarchically constrained kinetic Ising model in one dimension (the East model), the North-east model, and the class of $(a,a-1)$-Cayley tree models. We present new simulation data for the East model. For models with low dimensionality and low coordination number, there is little or no relationship between the transitions predicted by the mode coupling theories and the actual behavior of the spin systems, with the mode coupling theories generally predicting transitions for models that don't have them and attributing qualitatively incorrect properties to those transitions that do occur. The mode coupling theories describe the relaxation of the East model well for short times but fail at long times in the vicinity of the incorrectly predicted transition and for the states that are incorrectly predicted to be nonergodic. Simulation evidence is presented for scaling behavior of the relaxation for low temperatures and long times in the East model, but no extant mode coupling theory predicts this behavior correctly. An analogy between liquids and facilitated spin models is proposed, whereby the slightly supercooled liquid regime is analogous to the spin system states near the spurious mode coupling transition, and the low temperature supercooled liquid near its glass transition is analogous to the spin model states just above the actual ergodic–nonergodic transition (in the case of models that have such a transition) or in the low temperature scaling regime (in the case of models with this type of low temperature behavior). According to this analogy, the actual transition or the low temperature scaling behavior of the spin models is analogous to the behavior at or near the thermodynamic transition that is sometimes proposed as the basis for the glass transition in liquids.
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I. INTRODUCTION

Facilitated kinetic Ising spin models were originally devised by Fredrickson and Andersen[1,2] as models for cooperative slow relaxation in condensed phases and have been the subject of a considerable number of theoretical and simulation studies.[3–23] In these models, each spin is at a site on a lattice, each spin can point either up or down, and the flip rate of a spin is zero unless a certain number of its neighbors are in the up state. In the two-spin-facilitated kinetic Ising (2sfkI) model, for example, a spin can flip only if it has at least two up-neighbors and the spin flip rates satisfy a detailed balance condition. This model was originally of interest because an approximate theory for the spin autocorrelation function of this model, on hypercubic lattices with dimensions of two or higher, predicted an ergodic–nonergodic transition, similar to those predicted for liquids by the idealized mode coupling theory.[24–26] Subsequent simulation studies by Fredrickson and Brawer[3] showed that this model does not have such a transition but that it does have dynamical relaxation properties much like those of real viscous liquids. The similarity between the facilitated kinetic Ising model and real liquids is striking on two levels: the spin system and liquids have similar correlation functions for fluctuations (of spin density and particle density, respectively), as well as similar theories that predict an ergodic–nonergodic transition that does not actually take place. In the case of liquids, subsequent extensions of the mode coupling theory for liquids predicted that the singular behavior is removed when certain dynamical processes are included in the theory,[27–29] and such extensions of the theory for spin systems can also be made.[30,31]

The class of facilitated models was extended by Jäckle and co-workers, who defined models with directed constraints.[32,33] In these models, a spin can flip only if a specific set of its neighbors (not merely a specific number of them) are in the up state. One is the North-east model, a two dimensional system of spins on a square lattice in which a spin can flip only if the spin to its ''east'' and the spin to its ''north'' are both up. An even simpler model is the ''hierarchically constrained kinetic Ising model in one dimension,'' a one-dimensional system of spins with flip rates that allow a spin to flip only if the neighboring spin to the right is up. We shall refer to this, for simplicity, as the East model. (For recent work on the East model, see Refs. 34, 35.) Similar models with directed constraints were defined for spins on Cayley trees. [See below for a definition of the (a,n)-Cayley

tree models.] One reason for interest in these models is that some of them do in fact have ergodic–nonergodic transitions. For a concentration of up spins that is above a critical concentration, the system is ergodic, and at lower concentrations the system is not ergodic and cannot relax completely to equilibrium.

Ergodic–nonergodic transitions are predicted by theories with the structure of the simplified mode coupling theory,[24–26] and the relationship between the genuine dynamical transitions in these spin models and the simplified mode coupling theory as formulated for liquids became an object of investigation. Because of the difference between the dynamics of the two types of systems (stochastic irreversible dynamics for spins, and deterministic reversible dynamics for liquids), it was not at first clear how to formulate the analog of mode coupling theory for spin models. The first formulation of mode coupling theory for a spin system, by Jäckle and Sappelt,[36] was based on constructing an approximation for the second-order memory function (i.e., the memory function of the memory function) of the spin autocorrelation function that was of the same form as the approximation made for the second order memory function of the density autocorrelation function for liquids. However, this approximation led to equations for the correlation functions that gave unphysical results. Kawasaki[37,38] subsequently showed that a so-called irreducible memory function could be defined for spin systems based on the first-order memory function and that approximations constructed using the irreducible memory function had the mathematical characteristics of simplified mode coupling theory as applied to liquids. (For a further discussion of the meaning of the irreducible memory function, see Ref. 39.)

In this article we discuss several facilitated spin models with directed constraints, including the East model, the $(a,a-1)$-Cayley tree models, and the North-east model. We present simulation results for the spin autocorrelation function of the East model for various concentrations, and we discuss two types of mode coupling theory for these models, one due to Kawasaki[37] and one that we have developed using diagrammatic methods.[30,31] (For the East model, our mode coupling theory is equivalent to the ''effective medium approximation'' of Eisinger and Jäckle.[40]) The major conclusions are that (1) the two different mode coupling approximations, obtained in reasonable ways for the same system, give drastically different predictions for the ergodic–nonergodic transitions, (2) the new mode coupling approximations that we have developed work very well for the $(a,a-1)$-Cayley tree models for large a, i.e., for large coordination number, but give qualitatively and quantitatively incorrect predictions for the transition for the lowest coordination numbers. However, even for the lowest coordination number case, the East model, the approximation is a good description of the time dependence of the spin autocorrelation function above the incorrectly predicted transition at all times and below the transition for short times, and (3) the mode coupling theories of Kawaski are qualitatively incorrect in their predictions of the transition for all the Cayley tree models.

The motivation for this work is the hope that an understanding of the dynamics of cooperative relaxation and of the validity of mode coupling approximations in these simple models, which are much more amenable to detailed theoretical analysis than are realistic models of liquids, will lead to an understanding about how to improve the theory of liquids. This hope is strengthened by the many similarities between the relaxation phenomena in these models and those found in and predicted for real liquids.

II. THE EAST MODEL

A. Definition of the model and basic properties

The East model, or one-dimensional hierarchically constrained kinetic Ising model, is an Ising spin system, with N spins on a one-dimensional lattice. It was originally proposed by Jäckle and Eisinger.[32] Each spin can either point up or down. There are no static interactions between spins, but there is a difference in energy between the spin up and spin down states for each spin. The energy difference (divided by kT) determines c, the equilibrium concentration of up spins at any temperature. The thermodynamic state of the system is usually specified by the value of the single state variable c, which is the equilibrium average fraction of spins that are up and also the probability that any particular spin is up.

The dynamics are stochastic, with the time dependent probability distribution function for the states of the system being governed by a master equation. The allowed transitions are those in which a single spin flips from down to up or from up to down, but the transition probability for the flip of a particular spin is nonzero only if the neighboring spin to the right (i.e., the ''east'' neighbor) is up. The ratio of the flip rates for the two types of flips is given by a detailed balance condition that is consistent with establishment of an equilibrium distribution of states for long times. Small values of c correspond to low temperature states that relax slowly, and large values correspond to high temperature states that relax quickly.

A complete specification of the model requires a statement of a boundary condition at the far right. In the original definition by Jäckle and Eisinger, the boundary condition is provided by adding a site at the far right with a spin that is either permanently up (free boundary condition) or permanently down (blocking boundary condition). This spin determines whether or not the last of the N spins on the right can flip. Alternatively, periodic boundary conditions can be used. The correlation functions in the limit of an infinite system size are the quantities of main interest. In this limit, we presume that all sites have identical statistical properties (in the case of free and blocking boundary conditions) and that all three boundary conditions give the same correlation functions.

It is convenient to use ''occupation number'' variables rather than spin variables to characterize the state of a system. The lattice sites are labeled by an index i $(0 \leqslant i \leqslant N-1)$, with $i=0$ at the far left and $i=N-1$ at the far right, then n_i is the occupation number for site i and has the value 1 if the spin is up and 0 if it is down. The state of the entire system is specified by specifying the occupation

number for each of the N sites. The flip rate for spin i is zero unless $n_{i+1}=1$. In the case of periodic boundary conditions, the spin flip rate for spin $N-1$ is zero unless $n_0=1$.

The equilibrium average of n_i for a system of N spins, denoted $\langle n_i \rangle_N$, is c. (We use $\langle \cdots \rangle_N$ to denote an equilibrium average for a system of size N.) The fluctuation from the average is $\delta n_i = n_i - c$. The fundamental correlation function of interest is the normalized autocorrelation function of this spin fluctuation,

$$C(t) \equiv \lim_{N\to\infty} \frac{\langle \delta n_i(t)\, \delta n_i(0) \rangle_N}{\langle \delta n_i(0)^2 \rangle_N}.$$

(If this limit exists, it is clearly independent of i.) Because of the directed nature of the constraint, there are no dynamic correlations between spins on different sites,[41] so the cross correlation function of the fluctuations on different sites will not be considered. The correlation function depends on c, but this dependence has not been indicated explicitly.

Jäckle and Eisinger[32] have presented arguments, together with supporting simulation results, that assert that $C(t)\to 0$ as $t\to\infty$ for either free or blocking boundary conditions. Recently, Aldous and Diaconis[42] have proven that the spin autocorrelation function decays to zero for all $c>0$ for the infinite system.

B. Mode coupling approximations

Two approximate mode coupling theories of the East model have been presented in the literature. We shall first discuss the structure of mode coupling approximations and then discuss the two theories.

The memory function formalism of Mori[43,44] provides the context for the discussion of mode coupling theories. For situations like the current one in which there is only one correlation function of interest, $C(t)$, the memory function $M(t)$ of the correlation function is related to the correlation function in the following way:[45]

$$\tilde{C}(z) = \frac{1}{z + \alpha + \tilde{M}(z)}. \tag{2.1}$$

A tilde denotes the Laplace transform, defined by

$$\tilde{f}(z) = \int_0^\infty dt\, e^{-zt} f(t).$$

Here $\alpha = -\dot{C}(0)$ is a positive constant; its reciprocal defines the shortest time scale of the problem. Formal expressions for the memory function in terms of projection operators can be obtained for systems such as the East model that have stochastic irreversible dynamics.

In the theory of liquids a similar form is obtained for the dynamic structure factor. In this case, $\dot{C}(0)=0$ and so the α term is zero. The second-order memory function (or the memory function of the memory function) can also be defined, and this function is the starting point for theories that lead to the simplified mode coupling approximations. This procedure does not give meaningful results for the East model, however[40] [or for the North-east model and the (3,2)-Cayley tree model].[36]

Instead, the procedure that gives approximations with a character similar to those of the simplified mode coupling theory of liquids is that of Kawasaki, who introduced the irreducible memory function $M^{\rm irr}(t)$, which is related to the memory function in the following way:

$$\tilde{M}(z) = -\frac{\tilde{M}^{\rm irr}(z)}{1 + \alpha^{-1}\tilde{M}^{\rm irr}(z)}.$$

Kawasaki also obtained formal expressions for $M^{\rm irr}$ in terms of projection operators.

Mode coupling approximations are obtained by deriving or assuming that the irreducible memory function is a polynomial function of the correlator, with positive definite coefficients, i.e.,

$$M^{\rm irr}(t) = \sum_n a_n(c)[C(t)]^n, \tag{2.2}$$

where each n is a positive integer, and each $a_n \geqslant 0$ and is a smoothly varying function of c. The character of the results for $C(t)$ depends on the values of the coefficients $a_n(c)$ and is strongly affected the values of n included in the series.

Kawasaki obtained an approximation with this structure from his projection operator representation of the irreducible memory function,

$$M_K^{\rm irr}(t) = c(1-c)[C(t)]^2.$$

Here the subscript K denotes the approximation obtained by Kawasaki. Using a very different theoretical framework, Eisinger and Jäckle[40] obtained a theory that is in effect a theory for the irreducible memory function. Their result is

$$M_{\rm EJ}^{\rm irr}(t) = c(1-c)C(t),$$

which they call an effective medium approximation. We shall refer to both of these theories as ''mode coupling approximations'' since they are both of the form of Eq. (2.2).

Both of these theories predict that the East model has an ergodic–nonergodic transition. We define the nonergodicity parameter in the usual way,

$$f(c) \equiv \lim_{t\to\infty} C(t).$$

As discussed above, the correct behavior of f is that $f(c)=0$ for all $c>0$. However, the Kawasaki theory predicts that $f(c)>0$ for $c<0.2$, and the Jäckle–Eisinger theory predicts that $f(c)>0$ for $c<0.5$. In the classification of Götze,[26] the predicted singularity under the Kawasaki theory is a type-B transition; the nonergodicity parameter jumps up abruptly to a nonzero value as c is lowered through 0.2. Under the Jäckle–Eisinger theory, the predicted singularity is a type-A transition; the nonergodicity parameter rises from zero continuously as c is lowered through the transition at 0.5.

As noted above, the model actually has no transition, and this was recognized by the authors who obtained the approximations. Kawasaki regarded M_K as a better approximation because it at least predicted a lower concentration for the nonexistent transition. One of the purposes of the present

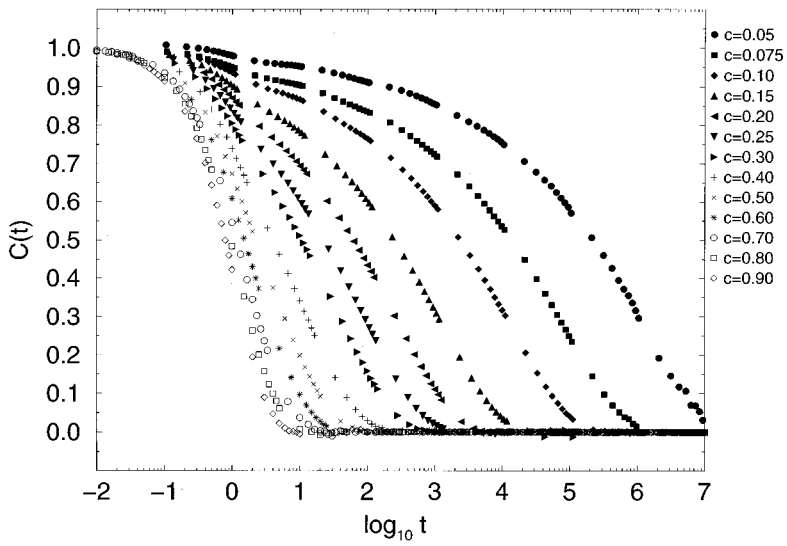

FIG. 1. The spin autocorrelation function for the East model as a function of time obtained in the present simulations. Note the logarithmic time axis.

work was to obtain simulation results so that the detailed time dependent predictions of the two theories could be tested.

C. Simulation method

We have performed computer simulations of the dynamics of the East model. All simulations were performed using periodic boundary conditions. The method of the simulations was the same as those of Reiter *et al.*[33]

The simulations used a system of 600 spins at higher c values and 1000 spins for the smaller c values. Exploratory studies with smaller systems convinced us that the system sizes we report here are large enough to give the true infinite size limiting results for the correlation functions. For each concentration studied, a variety of initial states were constructed and a chain starting with each one was constructed. For each concentration, the total duration of the simulations divided by the relaxation time (defined as the time at which the correlation function has decayed to *zero* within the noise of the simulations) is a measure of the quality of the statistics. This ratio can be taken to be a lower bound to the number of statistically uncorrelated pieces of data used to obtain each correlation function. The ratio varied from about 600 to 11 000 for $c=0.1$ and above. For $c=0.075$ and 0.05, the ratio was 207 and 14, respectively. The significantly lower quality of the data for these two lowest values of c should be taken into account in considering the results which follow. These simulation studies are more extensive than those previously reported by Jäckle and Eisinger,[32] who studied systems as large as 25 spins with simulations of much shorter duration, and by Eisinger and Jäckle.[40]

D. Results

The correlation functions for the range of concentrations studied are given in Fig. 1. Note that as c is lowered from 1 to 0.05, the time scale for the relaxation increases by 5 or 6 orders-of-magnitude, and the data suggests that it would increase even further if the concentration were lowered further. The correlation functions are nonexponential, but we can define a concentration dependent relaxation time, $\tau_r(c)$, as the time at which the correlation function reaches the value of r. The numerical values obtained depend on the choice of r, but the general trend with concentration is similar. Both $\tau_{1/10}$ and $\tau_{1/e}$ are increasing with decreasing c, for $c \approx 0.1$, at a rate that is approximately as c^{-6}. This is consistent with the result obtained by Eisinger and Jäckle[40] in similar simulations. Mauch and Jäckle[46] have argued that as $c \to 0$ the relaxation time diverges more strongly than any inverse power of c. This has been proven by Aldous and Diaconis.[42]

The correlation functions are highly nonexponential, except for high c, as can be seen in Fig. 2. In this form of plot, an exponential gives a straight line with a slope of unity, and a stretched exponential [proportional to $\exp(-(t/\tau)^{\beta})$] gives a straight line with a smaller slope. The data for low c shows persistent curvature out to the longest times for which we have data.

In Fig. 3, the simulation results are compared with the correlation functions predicted by the mode coupling approximations for a variety of concentrations. There is no unusual behavior of the correlators near $c=0.5$ or $c=0.2$, which are the locations of the ergodic–nonergodic transitions predicted by the mode coupling theories discussed above. The correlation functions decay to zero, with not even a hint of a plateau at these concentrations. The Jäckle–Eisinger (EMA) theory provides an excellent fit to the data at the higher concentrations and fits the short time data well at lower concentrations but ultimately fails because the EMA correlator does not decay to zero for $c<0.5$. The EMA correlator appears to provide an upper bound to the correlator. The Kawasaki (MCA) theory is less accurate at all concentrations, predicting relaxation that is too rapid at short times at all concentrations and then predicting a failure to relax to zero at long times for low concentrations.

It is in the limit of small c that the relaxation gets very slow and perhaps critical. To test this possibility, we have performed a scaling analysis. Figure 4 shows a plot of the correlation function vs. the log of the rescaled time

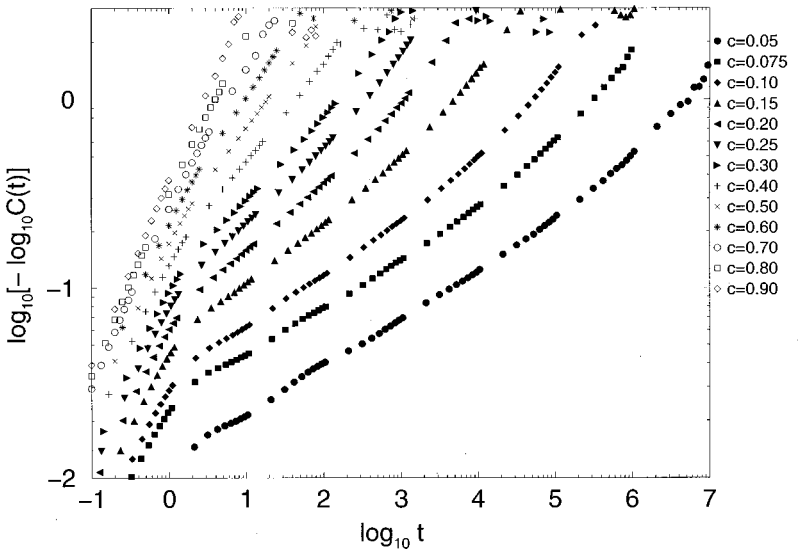

FIG. 2. A plot of $\log_{10}[-\log_{10} C(t)]$ vs $\log_{10} t$. In this type of plot, an exponential or stretched exponential would be a straight line. Note the persistent curvature of the plots at long times for low c, indicating the absence of exponential and stretched exponential behavior for the times investigated.

$\hat{t} = t/\tau_{1/10}(c)$. We have excluded the lowest concentrations, for which the data are of lesser quality. For concentrations between 0.1 and 0.3, the long time data falls on a master curve, with the data for each concentration joining the master curve as a reduced time that that decreases as c decreases. This suggests that some form of scaling law holds and suggests the possibility of a dynamical critical point at lower concentrations (presumably at $c=0$). The form of the scaling function for small reduced times is suggested by another type of scaling plot in Fig. 5, which gives $\log_{10}(1-C(t))$ as a function of $\log_{10}(t/\tau_{1/10})$. The extended region over which the consensus curve is linear suggests that

$$C(t) \approx 1 - h(t/\tau_{1/10})^b, \tag{2.3}$$

in the short time part of the scaling regime, where the value of the exponent obtained from the straight line fit is $b \approx 0.229$. Because of the lower quality of the data for $c=0.05$ and $c=0.075$, the short time part of the scaling function can't be well established. This functional form was also fit to only the $c=0.1$ data, and the result is shown as the dashed line in Fig. 4. In this fit, the exponent b is approximately 0.236. The dashed line fits the data well over a range of about three orders-of-magnitude in reduced time, during which the correlation function drops by a factor of about 2. Equation (2.3) looks superficially like a von Schweidler law as predicted by the simplified mode coupling theory of supercooled liquids, but with a nonergodicity parameter (the constant term) of unity. It is conceivable that a mode coupling theory could predict a nonergodicity parameter close to unity. But to our knowledge, no version of mode coupling theory has yet been derived that predicts a transition at very low c or at $c=0$.

In summary, the long time scaling analysis and arguments given by Jäckle and Eisinger[32] suggest the reasonable conclusion that there is dynamical critical behavior in the model as $c \to 0$, but, to our knowledge, no mode coupling theory of this model has been developed that predicts such critical behavior. Of the two extant mode coupling theories,

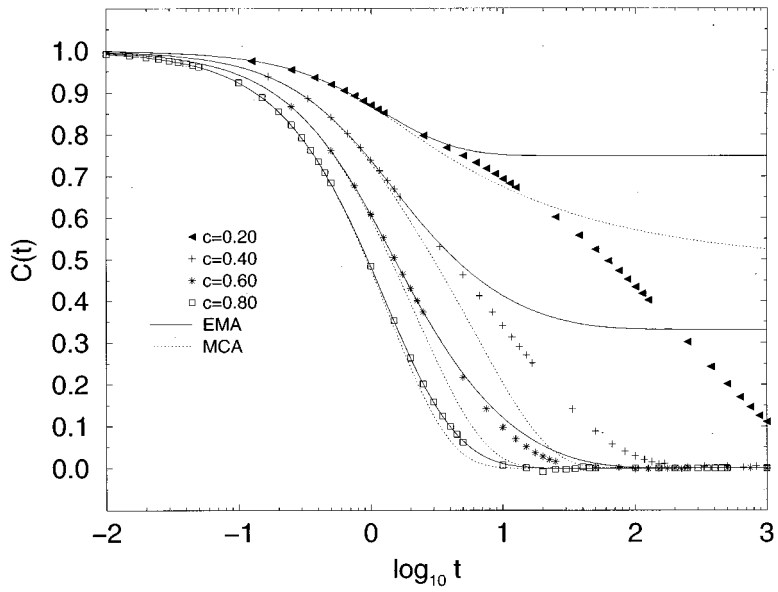

FIG. 3. The spin autocorrelation function for the East model as a function of time for various values of c and comparison with the predictions of two mode coupling theories: that of Kawasaki (dotted line: MCA) and that of Eisinger and Jäckle (solid line: EMA).

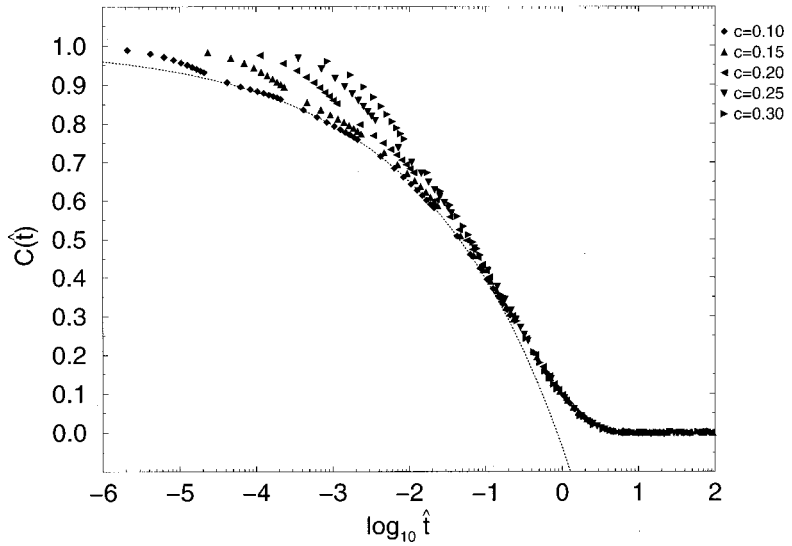

FIG. 4. The spin autocorrelation function of the East model for various low concentrations plotted as a function of the rescaled time, $\hat{t}$. See the text for the definition. The dashed curve is a power law behavior of the form of Eq. (2.3) that is fit to the data for the single concentration of $c=0.1$. The exponent b and the constant h for this fit are 0.236 and 1.04.

the EMA theory of Jäckle and Eisinger provides the more satisfactory description of the short time behavior at all concentrations and of the overall behavior above $c=0.5$, despite the fact that it predicts a spurious transition at $c=0.5$.

III. CAYLEY TREE MODELS

Reiter *et al.*[33] defined a class of kinetic spin models with directed constraints on Cayley trees for which there is a hierarchy of sites. In the (a,n)-Cayley model, each site on the Cayley tree has a neighbors, one of them being lower in the hierarchy and $a-1$ being higher. A spin can flip only if n or more of its higher neighbor spins are up. The East model is equivalent to the (2,1)-Cayley tree model.

Associated with each such model is a ''bootstrap percolation'' problem.[47,48] Imagine picking a state at random from the ensemble of states with an average up-spin concentration of c. If a spin is down but has n or more of its higher neighbors pointing up, then flip the spin up. This procedure is continued until either all spins are up or until no more can be flipped up. At high c, all spins will be flipped up for almost all states, so that the ensemble average fraction of spins left in the down state is zero in the limit of large system size. However, below the percolation threshold c^*, a nonzero fraction of the spins will be left in the down state. An appropriate choice of the order parameter for this percolation problem is the fraction of spins that have fewer than n higher neighbors in the up state after the spin flip process is over.

If the percolation problem has such a percolation threshold, the corresponding spin system cannot be ergodic below the threshold concentration. In particular, the order parameter defined above for the percolation problem at a particular value of c is equal to the fraction of the spins in the corresponding kinetic spin problem that can never flip and thus is a lower bound to the nonergodicity parameter. Simulations of the dynamics of the (3,2)-Cayley tree model[33] support the reasonable conclusion that the dynamical ergodic–

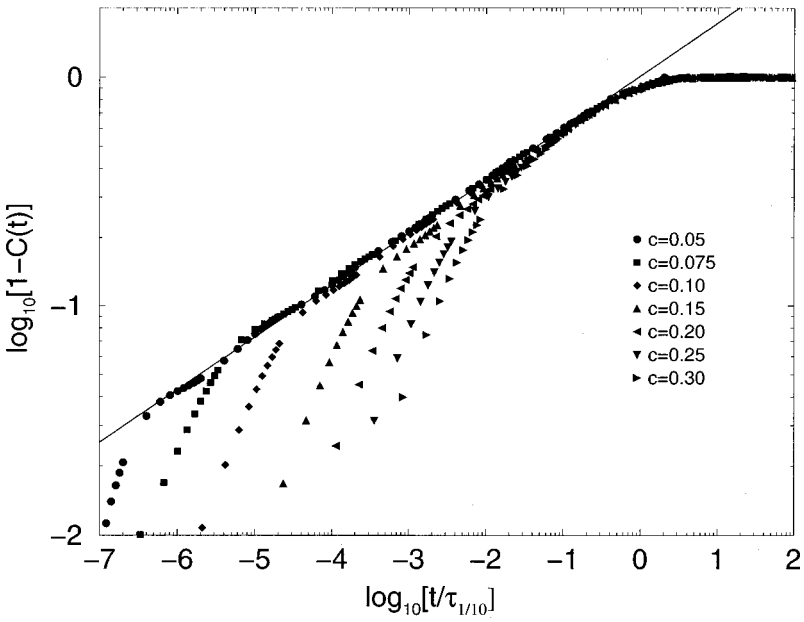

FIG. 5. The spin autocorrelation function of the East model for low concentrations plotted vs the logarithm of a reduced time. The apparently straight line seen for the consensus curve suggests power law behavior of the type in Eq. (2.3) for small values of the reduced time. The exponent b and the constant h for the straight line are 0.229 and 1.02, respectively.

nonergodic transition occurs at the same value of c as the bootstrap percolation threshold rather than at some higher c. A similar equivalence of the dynamical and percolation transitions was found for the North-east model.[36] In the following discussion, we shall assume that this is generally the case for models with directed constraints. More generally, we shall assume that, for each value of c, the order parameter for the bootstrap percolation problem is equal to the fraction of spins in the corresponding kinetic Ising model that cannot flip and hence is equal to the nonergodicity parameter.

We shall focus on the $(a,a-1)$-Cayley models and a comparison of the properties of these models with two mode coupling theories. Analysis of the bootstrap percolation problem for these models[33] indicates that these models have a percolation threshold at

$$c^*=(a-2)/(a-1), \tag{3.1}$$

that the transition is of type-A, and that the nonergodicity parameter is proportional to $|c-c^*|^1$ for c just below c^*.

Kawasaki[37] has presented a general method for deriving mode coupling approximations for this class of models and has presented the detailed results for the (3,2)-Cayley tree model. His method gives

$$M_K^{\mathrm{irr}}(t)=\sum_{k=1}^{a-1}\binom{a-1}{k}c^{2a-2-k}(1-c)^k[C(t)]^{k+1}. \tag{3.2}$$

The result for $a=3$ was given by Kawasaki, and the general result was obtained by us using his prescription. Using the standard methods of mode coupling theory,[26] it is easily shown that this implies that the long time limit of the correlation function is the largest solution of the equation

$$\frac{f}{1-f}=\sum_{k=1}^{a-1}\binom{a-1}{k}c^{-k}(1-c)^k f^{k+1}, \tag{3.3}$$

that is less than or equal to unity. (Note that $f=0$ is always a solution.)

By a diagrammatic method[30,31] that expresses the irreducible memory function in terms of diagrams, we have obtained a similar approximate result:

$$M_{\mathrm{PA}}^{\mathrm{irr}}(t)=\sum_{k=1}^{a-1}\binom{a-1}{k}c^{2a-2-k}(1-c)^k[C(t)]^k. \tag{3.4}$$

(Note that $M_K^{\mathrm{irr}}(t)=M_{\mathrm{PA}}^{\mathrm{irr}}(t)C(t)$.) This implies the following equation for the long time value of the correlation function:

$$\frac{f}{1-f}=\sum_{k=1}^{a-1}\binom{a-1}{k}c^{-k}(1-c)^k f^k. \tag{3.5}$$

Kawasaki's mode coupling theory cannot predict a type-A transition, because of the absence of a term in Eq. (3.2) that is linear in $C(t)$. [A type-A transition can take place only if $f=0$ is a double root of Eq. (3.3) for some c between 0 and 1. It is easily seen by inspection, after canceling one factor of f from both sides of the equation, that no such solution exists.] We have solved the equations for f from Kawasaki's theory for the $a=3$ model and found that it predicts a type-B transition at $c^*=0.4090$. For comparison, the model actually has a type-A transition at $c^*=1/2$.

Our mode coupling approximation, Eq. (3.4), has a linear term and predicts a type-A transition at

$$c^*=(a-1)/a,$$

cf. Eq. (3.1). [In particular, it is straightforward to show that Eq. (3.5) possesses only the trivial $f=0$ solution for $c>c^*$ and that a second solution with $f>0$ arises at and below c^*.] For $a=2$, which corresponds to the East model, it predicts a transition for $c>0$ whereas there is no transition for the model. For larger a, however, this result correctly predicts a transition with some quantitative error in the concentration. For $a=3$, it predicts a type-A transition at $c^*=2/3$. For very large a it predicts $c^*=1-a^{-1}+O(a^{-2})$, which is consistent with the exact result. Moreover, this mode coupling theory (as does any simplified mode coupling theory that predicts a type-A transition)[26] predicts an exponent of unity for the c dependence of the nonergodicity parameter just below the transition, in agreement with the exact results.

Thus, for the class of $(a,a-1)$-Cayley models for $a>2$, the mode coupling theory that is derived by Kawasaki's method gives the wrong type of transition, whereas the very similar result obtained by our diagrammatic method predicts the correct type of transition and becomes quantitatively more accurate in predicting the location of the transition as a increases.

IV. NORTH-EAST MODEL

The North-east model has been studied by computer simulation by Jäckle and Sappelt,[36] who performed a finite size scaling analysis of the results. The conclusions are consistent with the existence of an ergodic–nonergodic transition of type-A at $c^*=0.294$, which is the percolation threshold for the bootstrap percolation problem. Just below the transition, the nonergodicity parameter is proportional to $|c-c^*|^{0.25\pm0.05}$.

Kawasaki's mode coupling theory results for the North-east model are equivalent to those for the (3,2)-Cayley model, which are given by Eqs. (3.2) and (3.3) for $a=3$. Thus this theory predicts a type-B transition at $c^*=0.4090$. Our diagrammatic method,[31] when applied to the North-east model, also gives the same result as that for the (3,2)-Cayley model, namely a type-A transition at $c^*=2/3$. It predicts the usual mode coupling exponent of unity for the nonergodicity parameter.

Thus, neither of the two mode coupling theories is satisfactory for this model, which combines low coordination number with the complications that arise from being on a lattice embedded in a low-dimensional space rather than being on a Cayley tree.

V. DISCUSSION AND CONCLUSIONS

As was known from previous work, the two versions of simplified mode coupling theory for the East Model incorrectly predict an ergodic–nonergodic transition for the model. The simulation results above show that there is not even the hint of a plateau in the correlation function or other evidence of an ''avoided'' transition in concentration ranges near those for which transitions are predicted, whereas there

is evidence for critical slowing down near $c=0$, something that is not predicted by any mode coupling theory.

Simplified mode coupling theories have been derived in various ways for a variety of facilitated spin models, including the East model, the North-east model, and the $(a,a-1)$-Cayley tree models (for $a>2$), which are discussed above, and the two-spin-facilitated model in two dimensions.[1] From the literature cited above and the new results in this work, the following generalizations can be made.

(1) In the case of models that have no transition, simplified mode coupling theories can incorrectly predict a transition (e.g., Kawasaki's theory or the EMA or our theory for the East model, and the graphical theory of Fredrickson and Andersen for the 2sfkI model).

(2) For the models that have an ergodic–nonergodic transition, the simplified mode coupling theories that have been derived generally predict too high a value of c^*. [The exception is Kawasaki's mode coupling theory for the (3,2)-Cayley tree, which predicts a value of c^* lower than the correct result.]

(3) In the case of the models that have a transition of type-A, in the categorization of Götze, simplified mode coupling theories can predict type-B transitions (e.g., Kawasaki's theory for the North-east model).

(4) When a simplified mode coupling theory does predict a type-A transition, it always predicts that the nonergodicity parameter varies as $|c-c^*|^1$ for c just below the critical concentration c^*.[26]

The predicted exponent of unity is apparently correct for those Cayley tree models that have a transition. However, the North-east model has an exponent of 0.25 ± 0.05 for its type-A transition.[36] Thus, even if a simplified mode coupling theory for the North-east model were to be developed that predicts (correctly) a type-A transition, such a theory could not describe the singularity in the dynamical behavior correctly in that it would give the wrong exponent for the nonergodicity parameter.

For models with low dimensionality (East, North-east) and low coordination number [$(a,a-1)$-Cayley trees with $a=2$ or 3], the simplified mode coupling theories give qualitatively incorrect predictions for the correlation functions at long times because they incorrectly predict ergodic–nonergodic transitions or correctly predict a transition but at too large a value of c. However, for the East model, they can provide good descriptions of the dynamics for all times at high c and for short times at low c, with the EMA (equivalent to our theory) being significantly better in this regard than Kawasaki's mode coupling theory. This is analogous to the situation in liquids, in which the simplified mode coupling theories predict a transition that is eliminated by subsequent extensions of the theory. In a future article[31] we shall derive, using diagrammatic techniques, the analogs of the extended mode coupling theory that correspond to each of these simplified mode coupling theories. The extended theories will in fact eliminate the spurious transitions and extend the range of times over which the theory is accurate.

As noted in the introduction, there are many similarities between relaxation in liquids and in facilitated spin models. In particular, for liquids and low dimensionality spin models, a spurious ergodic–nonergodic transition can be predicted and then eliminated. In the spin case, the two theories that predict a spurious transition also provide a reasonably accurate description of the correlation function at short times even below the spurious transition and represent significant improvement over a naive theory that would predict simple exponential decay of the correlator. For liquids, the temperature usually identified as that of an avoided transition corresponds to the slightly supercooled regime, and the transition actually corresponds to a smooth change in the fundamental nature of the dynamics as the temperature is lowered. Our results suggest an analogy between low-dimensionality spin models and liquids. According to this analogy, the slightly supercooled regime of liquids is analogous to the range of concentrations of the spurious predicted transition in the spin models, while the deeply supercooled regime, where the laboratory glass transition takes place, corresponds to the region of the actual ergodic–nonergodic transition or the critically slow relaxation associated with the $c\rightarrow0$ limit. The actual transition or low c critical behavior is then analogous to an ''underlying'' thermodynamic transition that is sometimes postulated to exist below the laboratory glass transition. With this analogy, we see that the mode coupling approach succeeds in describing behavior in the spin models for states that correspond to the liquid and slightly supercooled liquid, but it produces spurious results for the long time scale relaxation behavior for states corresponding to the deeply supercooled liquid.

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$$\frac{dC(t)}{dt} = -\alpha C(t) - \int_0^t dt'\, M_1(t-t')C(t').$$
Note the minus signs on the right.
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