Dynamics of the Structural Glass Transition and the p-Spin–Interaction Spin-Glass Model

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The mathematical structure of the dynamical theory for the soft-spin version of the p-spin–interaction ($p>2$) spin-glass model is related to that for the dynamical theories of the structural glass transition. The phase transitions predicted by both theories are discussed. The spin-glass transition predicted by the dynamical theory is related to a broken-replica-symmetry equilibrium calculation.

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A model Hamiltonian (or an effective Lagrangean) that is capable of describing relaxation processes in supercooled liquids and glasses has been difficult to obtain. In a recent paper[1] it was suggested that there may be a close connection between the dynamical theories[2-7] of the structural glass transition and exotic mean-field spin-glass models such as the Potts glass[8-11] or spin models with p-spin interactions[12] ($p>2$). The motivation for this observation was the discontinuous nature of the transition in all three models.

In this Letter this connection is made more precise. In particular, it is shown that in the ergodic phase (above the transition temperature T_g) the dynamical equations for spin fluctuations in the soft version of the mean-field p-spin–interaction ($p>2$) model are similar to Leutheusser's[2] equation for the structural glass problem. The mode-coupling approximation used to obtain an equation of motion for density fluctuations in the structural glass problem is expected to become exact as the dimensionality tends to infinity.[1] The mean-field dynamical equation satisfied by the spin fluctuations for the model proposed here is also exact when the number of spins tends to infinity. Thus the structure of the dynamical equations for the appropriate correlation functions of both the models should be viewed as identical only in the mean-field limit. Although this connection may at first seem surprising, it is in retrospect quite obvious. First, Leutheusser neglects wave-number dependence in his model. This is analogous to the use of an infinite-range mean-field Hamiltonian in the spin-glass (SG) problem. Second, the nonlinearities in the dynamical equations for the soft-three-spin–interaction model are identical in structure to the nonlinearities in the fluid dynamical equations[5,13] that lead to Leutheusser's model.

Once this connection is established we discuss the phase transition predicted by these dynamical equations. In particular, for the spin model we relate the dynamical transition, which predicts critical slowing down as the glass transition temperature, T_g, is approached from the ergodic side, to a broken-replica-symmetry equilibrium calculation.[14,15] It is important to note that a replica-symmetric (RS) solution with finite q for this model is unstable for all T, and cannot be used to locate the transition temperature. This is unlike the usual Sherrington-Kirkpatrick (SK) model[16] where RS solutions can be used to locate T_g. The essential difference is due to the discontinuous nature of the phase transition in this model. In this paper only results are quoted. More details will be given elsewhere.[17]

We start with the Hamiltonian, H, for the soft-spin version of the mean-field p-spin model ($\beta = T^{-1}$),

$$\beta H = \sum_i \left[\frac{r_0}{2}\sigma_i^2 + u\sigma_i^4\right] - \beta \sum J_{i_1\cdots i_p}\sigma_{i_1}\cdots\sigma_{i_p}, \tag{1}$$

with $-\infty < \sigma_i < \infty$. The strength of interactions[12] $\{J_{i_1\cdots i_p}\}$ are taken to be independent Gaussian random variables with variance (N=number of spins) $\sim J^2/N^{p-1}$. The relaxational dynamics for $\sigma_i(t)$ is assumed to be given by the Langevin equation,[18-20]

$$\Gamma_0^{-1}\partial_t\sigma_i(t) = -\delta(\beta H)/\delta\sigma_i(t) + \xi_i(t), \tag{2}$$

with ξ_i the usual Gaussian noise term and Γ_0 the bare kinetic coefficient.

By use of standard field-theory techniques[18-20] the average over the $J_{i_1\cdots i_p}$ can be carried out. The resulting dynamical equations for $N\to\infty$ are[17]

$$\sigma_i(\omega) = G_0(\omega)f_i(\omega) - 4uG_0(\omega)\int\frac{d\omega_1 d\omega_2}{(2\pi)^2}\sigma_i(\omega_1)\sigma_i(\omega_2)\sigma_i(\omega-\omega_1-\omega_2), \tag{3a}$$

with $G_0(\omega)$ a renormalized bare propagator,

$$G_0^{-1}(\omega)=r_0-i\omega\Gamma_0^{-1}-\frac{p(p-1)}{2}\beta^2J^2\int_0^\infty dt\, e^{i\omega t}G(t)C^{p-2}(t), \tag{3b}$$

and $f_i(\omega)$ a renormalized noise term,

$$\langle f_i(\omega)f_j(\omega')\rangle=2\pi\delta(\omega+\omega')\delta_{ij}\left[\frac{2}{\Gamma_0}+\frac{p}{2}\beta^2J^2\int_{-\infty}^{+\infty}dt\, e^{i\omega t}C^{p-1}(t)\right]. \tag{3c}$$

In Eqs. (3), $C(t)$ and $G(t)$ are the average spin-correlation function and response function, respectively. Causality yields the relation, $G(t)=-\theta(t)\dot{C}(t)$, with $\theta(t>0)=1$ and $\theta(t<0)=0$.

We treat the u terms in Eq. (3a) in the one-loop or mean-field approximation. We discuss this approximation further below. An important consequence of this approximation is that this treatment of the SG transition is restricted to models with $p=2+\epsilon$ with ϵ small (an analytic continuation to fractional p values is assumed). We will, however, be able to draw some general conclusions. It is also important to point out that the instability[21,22] usually associated with RS breaking is an $O(u^0)$ effect in the p-spin ($p>2$) model and it is a technicality (cf. below) that prevents us from treating the general p model within a small u approximation. An equation for $\hat{C}(\omega)$ ($\mathrm{Im}\omega>0$), the one-sided Fourier transform of $C(t)$, can be derived from Eq. (3b) and causality. In the ergodic phase we obtain

$$\hat{C}(\omega)=C(t=0)[-i\omega+\bar{r}_0\Gamma(\omega)]^{-1},$$

with $\mu=\frac{1}{2}p\beta^2J^2$ and

$$C(t=0)=\bar{r}_0^{-1}$$
$$=[r_0-\mu C^{p-1}(t=0)+12uC(t=0)]^{-1}.$$

$\Gamma(\omega)$ is a renormalized kinetic coefficient,

$$\Gamma^{-1}(\omega)=\Gamma_0^{-1}+\mu\int_0^\infty dt\, e^{i\omega t}C^{p-1}(t). \tag{4}$$

For $p=3$ these equations are mathematically identical to the dynamical equations for the structural glass problem.[2-7] We argue below that these equations have similar properties for any $p>2$. The equation for $C(t=0)$ is an additional equation in the SG problem that self-consistently determines the equal-time spin correlations. If we *assume*, as is effectively done in the structural glass problem, that $C(t=0)$ is continuous at T_g, then these equations predict a glass transition at $T=T_g$, and a continuous slowing down as T_g is approached. The critical parameters are[17] ($J=1$ from now on)

$$\mu_c=\bar{r}_{0c}^{p}[(p-1)/(p-2)]^{p-2}(p-1),$$
$$q_c=\lim_{t\to\infty}C(t)\,|_{T=T_g}=(p-2)/\bar{r}_{0c}(p-1)=q_{\mathrm{EA}}, \tag{5}$$

and as $T\to T_g^+$, $\Gamma(0)\sim|T-T_g|^{1.765}$. Note that the order parameter describing this phase transition, q_{EA} = Edwards-Anderson parameter, is discontinuous at T_g, unlike in the SK ($p=2$) model. The strength of the discontinuity is of $O(\epsilon=p-2)$ for small ϵ. μ_c in the equation for $C(t=0)$ gives an equation for $\bar{r}_{0c}$ which determines T_g since $\mu_c\sim T_g^{-2}$. The $\bar{r}_{0c}$ equation has a physical solution only for sufficiently small ϵ which implies that for $\epsilon\sim1$ higher-order u terms in $\bar{r}_{0c}$ are needed to correctly describe the SG transition.

We next relate the above transition to an equilibrium phase transition. First note that the crucial assumption used above, and in the structural glass theories, is that $C(t=0)$ is continuous at T_g. Although for any glass transition this seems physically well motivated, it is not clear that it is consistent with the underlying statistical mechanics of the model. In particular, it is straightforward to verify[20,22] that if we also require Eq. (3a) to be valid at T_g [this equation was not used in obtaining Eqs. (5)] then a continuous $C(t=0)$ at any critical temperature, T_g', is not consistent. Further, one can show[17] that if all of Eqs. (3) are satisfied at T_g', then the resulting description of a possible phase transition is identical to the RS equilibrium solution for the soft-spin version of Eq. (1). The RS solution is unstable everywhere, unlike in the $p=2$ model where the Almeida-Thouless line divides the region of stability. However, if one examines the possible phase transition associated with this model, then one finds that an ordered or SG phase is always unstable. The assumption that $C(t=0)$ is continuous at T_g is shown by the use of the broken-replica-symmetric solution.

So far we have shown that the dynamical equations predict a phase transition at T_g given by Eqs. (5) and that there is a continuous slowing down as $T\to T_g^+$. However, this critical temperature is not related to the RS equilibrium solution of this model. This suggests that one has to break replica symmetry to obtain a transition temperature that is related to the one predicted by the dynamical theory. To show the connection with the equilibrium theory we have used the Parisi *Ansatz* to obtain the free energy[14,15] for the soft-p-spin model. Motivated by previous work[11,12] on the Potts glass and the $p\to\infty$ model we use only one RS breaking. The order to which we work additional replica breakings seems to be irrelevant.[17] It is also convenient to consider small ϵ so that an order-parameter $q\sim O(\epsilon)$ expansion is possible. With this the Parisi free energy is given by

$$\frac{\beta F}{N}=-\frac{\beta^2C^p}{4}+\lambda_s C-\ln A_0+(1-m)\left[\frac{\beta^2q^p}{4}-\frac{q\lambda}{2}\right]+(1-m)\frac{C_0^2}{4}\lambda^2 -(1-m)\frac{C_0^3\lambda^3}{6}-(1-m)^2\frac{C_0^3\lambda^3}{6}+O(\lambda^4), \tag{6a}$$

where $C_0=A_2/A_0$ with

$$A_n=\int d\sigma\,\sigma^n\exp[-\tfrac{1}{2}(r_0-2\lambda_s)\sigma^2-u\sigma^4]. \tag{6b}$$

Here C is related to the equal-time spin-correlation function and $m=m_1$ and $q=q_1$ are the usual Parisi order parameters. We have also anticipated that[12,17] $m_0=q_0=0$. λ_s and $\lambda=\lambda_1$ are Lagrange multipliers[12] related to C and q which have been introduced to carry out spin integrals in the mean-field limit. The saddle-point solution of Eq. (6a) yields (note that $m=0$ corresponds to the RS solution)

$$1=C_0^2\mu q^{p-2}-C_0^3\mu^2q^{2p-3}(2-m), \tag{7a}$$

$$1-m=\frac{3}{C_0^3\mu^2}q^{3-2p}\left[\frac{1-p}{2p}+\frac{\mu C_0^2}{4}q^{p-2}-\frac{\mu^2C_0^3}{6}q^{2p-3}\right]. \tag{7b}$$

The critical temperature, T_g', is obtained when these equations first have a physical solution, $q>0$, $1-m>0$. At criticality $m=1$ and Eq. (7a) reduces (to the order in ϵ in which it is valid) to the equation of state that follows from the dynamical theory. However, at T_g', Eq. (7b) must also be satisfied and this additional equation leads to $T_g'<T_g$, with T_g the transition temperature according to the dynamical theory. We discuss this point further below. The solving (cf. discussion remark 4 below) of Eqs. (7) leads to a SG phase with $F_{\rm SG}>F_{\rm PM}$ for $T<T_g'$. At T_g' there is no latent heat and the specific heat is discontinuous. This SG phase is stable according to a local-replica-based stability analysis. We conclude that for T close to T_g' and for small ϵ this SG phase is the correct one on the basis of equilibrium theory. From our analysis it also follows that the equal-time spin correlations are continuous at the glass-transition temperature. This is in accord with the dynamical analysis.

We conclude with a few remarks.

(1) An important aspect of this paper is to point out that the dynamical theories for this class of models apparently lead to a T_g that is *greater* than that predicted by the equilibrium theory. According to the static solution T_g would correspond to a saddle point of F which is a maximum as a function of q but not of m. Physically, we interpret the dynamical SG phase as a phase where $F_{\rm SG}(q,m)$ is maximized with $m=1$ in the region $T_g>T>T_g'$. At T_g' there is a second SG transition specified by Eqs. (7). The requirement that $m=1$ at T_g is equivalent to the requirement that the paramagnetic and SG free energies be equal at T_g. It is also interesting to point out that a local-replica-based stability analysis leads to a marginally stable SG phase at T_g.

Technically the behavior of the dynamical theory is easy to understand. For $T>T_g$ the dynamical equation for q_c given by Eqs. (5) has the trivial solution and unphysical complex solutions. At T_g two of the complex solutions become degenerate real solutions. At T_g^- there are three real critical points of the dynamical equation that satisfy $x_{c_1}=0<x_{c_2}<x_{c_3}=q_c<C(t=0)$, with x_{c_1} and q_c stable fixed points and x_{c_2} an unstable fixed point. We then have a situation where $C(t\to\infty)=0$ and $C(t\to\infty)=q_c$ are both stable solutions but where it is impossible to reach $C(t\to\infty)=0$ because of the intervening unstable fixed point. [The only possible conclusion is that the system freezes into a SG state because it cannot reach the equilibrium state defined by $C(t\to\infty)=0$.] It is also interesting to point out that in the SK model the situation is quite different. The dynamical equation has only two fixed points and at T_g there is an exchange of stability between the fixed points.

(2) In the SG problem the effects of frustration are not obvious after averaging over the random interactions. The dynamical theories for the structural glass problem do not have frustration in them. From this one can conclude that in the SG model, frustration is not important in the ergodic phase. What is crucial in causing critical slowing down as T_g is approached from above is the nonlinearity in the dynamical equations. Below T_g, frustration effects should be important and the simple dynamical model presented here is not sophisticated enough to reflect this. It has been argued that for SG below T_g, replica methods are also needed in dynamical theories to correctly account for frustration effects.[23] The analogous argument for the structural glass problem is not clear although the ideas presented by Sompolinsky[24] in the context of the SK model may be relevant.

(3) The ideas given above allow us to speculate on the nature and the meaning of the dynamical theories of the structural glass theories.[2-7] It seems clear[1] that they are basically mean-field theories. In addition, frustration[25] leads to many equivalent stable and metastable free-energy states. In this mean-field model the free-energy

barrier between possible nonergodic phases are infinite and a true ergodic-to-nonergodic phase transition occurs. In a real glass there is no true transition and one expects finite barriers between the possible free-energy states. The transitions between states will lead to the extremely slow transport observed in real viscous liquids.[1,26]

(4) We have also examined the Ising limit ($\sigma_i^2=1$) of Eq. (1), which is obtained from the soft-spin Hamiltonian by letting $r_0 \to -\infty$, $u \to \infty$ with $u/r_0 \to$ const. For the $p=2+\epsilon$ model, $\epsilon \ll 1$, the SG transition is identical in structure [in Eqs. (7), C_0 is replaced by unity] to that for the soft model if T is close to T_g'. Near T_g' one obtains $q=\frac{3}{2}(\epsilon+t)$, $1-m=t/\epsilon$, $t=1-T/T_g'$, and $(T_g')^2 \simeq 1+\epsilon \ln \frac{3}{2}\epsilon-\epsilon$. At lower temperatures the $O(\lambda_1^4)$ term in Eq. (6a) becomes relevant and a more complicated Parisi order parameter becomes possible. This may reflect another SG transition at lower temperatures as in the Potts glass model.[11]

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