The derivation of mode-coupling equations for equilibrium and non-equilibrium dynamics of a glass within the Keldysh formalism

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Abstract. The mode-coupling equations for a random glass (structural or spin-glass systems) are derived by using the Keldysh technique. For this derivation the assumption about the initial equilibrium state of the system is crucial. The glass transition corresponds to the appearance of a time-symmetry-breaking solution. Therefore the order parameter occurring below the critical temperature has a purely dynamic origin. The final dynamic equations are reduced to a model introduced by Götze and Sjögren in 1984. The other characteristic feature of the glassy state is the conservation of a slightly non-equilibrium distribution. In this quasi-equilibrium case the dynamics is described by Parisi–Sompolinsky–Zippelius equations.

1. Introduction

It is now a well established fact that in the infinite-range Ising spin glass (the model of Sherrington and Kirkpatrick (1975)) below T_c there coexist infinitely many phases (valleys) separated from each other by barriers of infinite height (see e.g. Binder and Young 1986). These states can be characterized by an overlap distribution function $P(q)$, which is directly related to the spin-glass order parameter $q(x)$ by the relation $dx/dq = P(q)$ (Parisi 1983). In terms of the mutual overlaps these states demonstrate ultrametric organization (Mèzard et al 1984). This picture does not refer to a particular mechanism providing the thermal equilibrium.

Starting from Sompolinsky and Zippelius (1982) (hereafter sz), and followed by Hertz (1983), Houghton et al (1983), De Dominicis and Young (1983) and Ginzburg (1986), a number of attempts have been made to reproduce the statistical mechanics result of Parisi (1980) within a dynamic framework. Traditionally, one assumes that in a large system but with a finite number of spins N there are inter-valley transitions, which can be described by introducing a spectrum of long relaxation times. In the limit $N \rightarrow \infty$, all times diverge and the spectrum becomes continuous. A solution obtained in this way in addition to the Parisi parameter $q(x)$ contains the new order parameter $\Delta(x)$

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representing the anomalous response. The appearance of the new independent parameter $\Delta(x)$ reflects the degeneracy of the glassy state. But an important point in the derivation of the equations for $\Delta(x)$ and $q(x)$ is the violation of the fluctuation–dissipation theorem. This is especially surprising for the finite system.

Another difficulty of the sz solution is that the dynamics includes the long-time relaxation, which is slow because of the large N. But so far it is not clear how to calculate this small parameter governing the slow relaxation. The sz approach does not, in principle, allow one to do this. Thus the question about the true dynamics of spin glass requires further study.

In the present work we study this problem by using the Keldysh formalism (Keldysh 1965, Langreth 1976). This approach has a number of advantages. First, the conventional diagrammatic representation is applicable in this technique. Secondly, this approach allows the consideration of non-equilibrium phenomena, which are an aspect of the glassy phase. Thirdly, the problem of averaging over random parameters is absent in this approach (Ginzburg 1989). This averaging problem is important for random glass transition.

Specifically, we consider the $\lambda \varphi^4$ model with random couplings. The radius of interaction and the volume of the system are assumed to be infinite. This model describes the structural-glass and spin-glass transitions in the so-called soft model of spin glass. In equilibrium we find that for the non-ergodicity parameter the standard mode-coupling equations (Götze 1991) appear, representing a purely dynamic state. Similar equations have been discussed in earlier theoretical works (Hertz 1983, Götze and Sjögren 1984). In terms of the purely thermodynamic phases, this order parameter is the long-time limit of the autocorrelation function averaged over the valleys. The corresponding dynamics describes the intra-valley transitions. We emphasize that this result has been obtained for zero external field.

In the slightly non-equilibrium case (the term 'slightly' will be specified below) sz's solution occurs, but our interpretation is different from that of sz and is completely based on the existence of similar non-equilibrium states below the glass transition. The relevance of sz's solution to a non-equilibrium situation has been previously suggested by a number of authors (Hertz 1983, De Dominicis and Young 1983).

In the following section we define the model and also derive the dynamic equations by using the Keldysh technique. In section 3 we discuss the equilibrium case and present the mode-coupling equations. Section 4 is devoted to the non-equilibrium dynamics. In the conclusion we discuss the results.

2. Model of structural glass transition and the Keldysh equations

Consider the system of N coupled anharmonic oscillators described by the following Hamiltonian:

$$H = \sum_j \varphi(x_j, p_j) + \sum_{i,j} J_{ij} x_i x_j \tag{1}$$

$$\varphi(x, p) = (1/2b)x^2 + (\lambda/8)x^4 + (b/2)\omega_0^2 p^2 \tag{2}$$

where x_j is a displacement of the jth atom in dimensionless units. In (1), J_{ij} are the elastic

constants coupling the atoms. They are assumed to be randomly distributed around zero so that

$$\langle J_{ij} \rangle = 0 \qquad \langle J_{ij}^2 \rangle = \mu^2/N \tag{3}$$

where N is the number of atoms.

The first two terms in (2) present the potential confining of an atom near its centre. For a displacive structural transition model one usually assumes

$$b > 0 \qquad \lambda > 0.$$

At high temperatures the equilibrium position of an atom is equal to zero. For strong enough interatomic coupling and weak elastic constant $1/b$, there is a critical temperature below which the sites undergo displacements. Because of the random couplings the new positions are also random. Hence we have the glass state. The last term in (2) provides the dynamics of the system.

A similar Hamiltonian is used in the soft model of spin glass. The dynamics in this case is governed by the Langevin equation

$$(\partial/\partial t)x_j = -\gamma \, \delta H/\delta x_j + \xi_j(t) \tag{4}$$

where $\xi_j(t)$ are stochastic forces with the following correlator:

$$\langle \xi_i(t_1)\xi_j(t_2) \rangle = 2\gamma T \delta_{ij}\delta(t_1 - t_2). \tag{5}$$

In the Keldysh formalism the behaviour of the system is described by the following Green matrix function (Keldysh 1965, Langreth 1976):

$$G(t_1, t_2) = \begin{pmatrix} G_{--}(t_1, t_2) & G_{-+}(t_1, t_2) \\ G_{+-}(t_1, t_2) & G_{++}(t_1, t_2) \end{pmatrix} \tag{6}$$

$$G_{\alpha\beta}(t_1, t_2) = \tfrac{1}{2}[F(t_1, t_2) - \alpha G_R(t_1, t_2) + \beta G_A(t_1, t_2)] \tag{7}$$

where $\alpha, \beta = \pm 1$, G_R is the retarded Green function

$$G_R(t_1, t_2) = -i\langle \mathrm{Sp}\{\rho_0[x_j(t_1), x_j(t_2)]\}\rangle_J \, \Theta(t_1 - t_2) \tag{8}$$

and G_A is the advanced Green function. Above, the brackets $\langle \ldots \rangle_J$ indicate averaging over the random couplings. In (8), ρ_0 is the matrix of density given in an earlier moment of time than $t_{1,2}$. It is not necessarily an equilibrium density matrix. The time dependence of the operator $x_j(t)$ is determined by the total Hamiltonian. The Green functions $G_{R,A}$ yield information about the spectrum of the system. They do not explicitly depend on the choice of ρ_0. The correlation function

$$F(t_1, t_2) = i\langle \mathrm{Sp}\{\rho_0 x_j(t_1) x_j(t_2)\}\rangle_J \tag{9}$$

additionally describes the time evolution of the distribution function.

To evaluate G perturbation theory can be used. As a free Hamiltonian we choose the harmonic part of (2). The anharmonicity in (2) and random couplings between atoms in (1) are considered as perturbations. Then in a zeroth approximation we have a system of uncoupled harmonic oscillators. In the ω representation the bare Green functions are

$$G_R^0(\omega) = b\omega_0^2/[(\omega + i0)^2 - \omega_0^2] \tag{10}$$

$$F_0(\omega) = 2i\Phi_0(\omega) \tag{11}$$
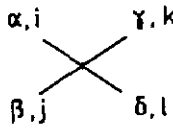
Figure 1. (a) The exact diagrammatic representation of the mass operator. (b) The structure of the bare interaction vertex.

$$\Phi_0(\omega) = [N(\omega_0) + \tfrac{1}{2}]\pi b\omega_0[\delta(\omega - \omega_0) + \delta(\omega + \omega_0)] \tag{12}$$

where $N(\omega_0)$ is the occupation number. At equilibrium $N(\omega)$ is

$$N(\omega) = [\exp(\omega/T) - 1]^{-1} \tag{13}$$

and the following relation holds:

$$F_0(\omega) = \coth(\omega/2T)[G_R^0(\omega) - G_A^0(\omega)]. \tag{14}$$

With the matrix description (6), the perturbation series can be presented by standard diagrams (Keldysh 1965). The general diagrammatic expression for the mass operator is shown in figure 1(a), where a thick line represents the whole Green function, and a circle is the total interaction vertex. The structure of the bare interaction vertex (see figure 1(b)) reads

$$\Gamma_{ijkl}^{\alpha\beta\gamma\delta} = (i\lambda/8)\delta_{\alpha\beta}(\sigma_z)_{\alpha\gamma}\delta_{\gamma\delta}\delta_{ij}\delta_{jk}\delta_{kl} + (\mu^2/N)(\sigma_z)_{\alpha\beta}(\sigma_z)_{\gamma\delta}\delta_{ik}\delta_{lj} \tag{15}$$

where the Greek characters refer to the Keldysh indices and the Roman ones are the oscillator coordinates. In a general case, the whole interaction vertex can be found from the Bethe–Salpeter equation. For large N, but not too small μ, we are able to show that *the renormalization of the vertex reduces to a factor* (see appendix). Therefore we use the bare vertex to calculate the mass operator. Using the following structure of the mass operator:

$$\Sigma_{\alpha\beta} = \tfrac{1}{2}(\alpha\beta\Omega - \alpha\Sigma_R - \beta\Sigma_A) \tag{16}$$

we find

$$-\Sigma_R(t_1, t_2) = -\mu^2 G_R(t_1, t_2) - (3\lambda i/4)\delta(t_1 - t_2)F(t_1, t_2)$$
$$+ (3\lambda^2/8)[3F^2(t_1, t_2)G_R(t_1, t_2) + G_R^3(t_1, t_2)] \tag{17}$$

and

$$-\Omega(t_1, t_2) = -\mu^2 F(t_1, t_2) + (3\lambda^2/8)\{F^3(t_1, t_2) + 3F(t_1, t_2)$$
$$\times [G_R^2(t_1, t_2) + G_A^2(t_1, t_2)]\}. \tag{18}$$

For the general case in the time representation the Dyson equations for the Keldysh Green functions read

$$G_R(t_1, t_2) = G_R^0(t_1, t_2) + \int dt_4 \int dt_3 \; G_R^0(t_1, t_4)\Sigma_R(t_4, t_3)G_R(t_3, t_2) \tag{19}$$

$$F(t_1, t_2) = F_0(t_1, t_2) + \int dt_4 \int dt_3 \; [F_0(t_1, t_4)\Sigma_R(t_4, t_3)G_A(t_3, t_2)$$
$$+ G_R^0(t_1, t_4)\Omega(t_4, t_3)G_A(t_3, t_2) + G_R^0(t_1, t_4)\Sigma_R(t_4, t_3)F(t_3, t_2)]. \tag{20}$$

Applying to both sides of these equations the following operator:

$$G_0^{-1}(t_1) = (1/b\omega_0^2)[-\partial^2/\partial t_1^2 - \omega_0^2] \tag{21}$$

and using the following properties of the bare Green functions:

$$G_0^{-1}(t_1)G_R^0(t_1, t_2) = \delta(t_1 - t_2)$$
$$G_0^{-1}(t_1)F_0(t_1, t_2) = 0$$

we obtain from (19) and (20)

$$G_0^{-1}(t_1)F(t_1, t_2) = \int dt_3 \left[\Omega(t_1, t_3)G_A(t_3, t_2) + \Sigma_R(t_1, t_3)F(t_3, t_2)\right] \tag{22}$$

$$G_0^{-1}(t_1)G_R(t_1, t_2) = \delta(t_1 - t_2) + \int dt_3 \Sigma_R(t_1, t_3)G_R(t_3, t_2). \tag{23}$$

The above with (17) and (18) is the set of equations used for further analysis. To them should be added the initial conditions. Instead of this we shall impose the relation between the Green functions.

Similar equations are valid for the spin glass where the bare retarded Green function is (Sompolinsky and Zippelius 1982)

$$[G_R^0(t)]^{-1} = [-(1/\gamma)\,\partial/\partial t + r]. \tag{24}$$

In this case the dynamics is purely dissipative. For the structural transition model, the bare Green function contains no dissipation. The dissipation is generated by the interaction term. This term provides the stability of the system in the glass state.

3. Equilibrium relaxation (mode-coupling theory)

Let us consider the equilibrium case. Then the Green functions depend on the time differences only, and the following relation between them should be valid:

$$F(\omega) = \coth(\omega/2T)[G_R(\omega) - G_A(\omega)]. \tag{25}$$

In the time representation this relation reads

$$G_R(t) - G_A(t) = -iT \int_{-\infty}^{+\infty} \frac{d\tau}{\sinh(\pi T\tau)} F(t + \tau). \tag{26}$$

For simplicity further considerations are restricted to the classical case, when temperatures are high in comparison with the characteristic frequencies. This consideration can be justified, at least, near the critical point. However, all considerations can be

extended to a quantum system on the basis of relation (26). In the classical case we can rewrite equation (26) as

$$F(t) = 2i\Phi(t)$$

$$\partial\Phi/\partial t = -T[G_R(t) - G_A(t)] = T \begin{cases} -G_R(t) & t > 0 \\ G_A(t) & t < 0. \end{cases} \tag{27}$$

Similarly, for the mass operators the following relation should hold:

$$\Omega(t) = 2im(t)$$
$$(\partial/\partial t)m(t) = T[\Sigma_A(t) - \Sigma_R(t)]. \tag{28}$$

For the model under consideration this is true since in the classical case we have from (17) and (18)

$$m(t) = \mu^2\Phi(t) + \tfrac{3}{2}\lambda^2\Phi^3(t) \tag{29}$$

$$\Sigma_R(t \geqslant 0) = -(3\lambda/2)\delta(t)\Phi(t) - (1/T)(\partial/\partial t)m(t). \tag{30}$$

In the mode-coupling theory one assumes that $m(t)$ can be rewritten as a polynomial in $\Phi(t)$ (Götze 1991)

$$m(t) = \sum_n a_n\Phi^n(t). \tag{31}$$

In accordance with (28), $\Sigma_R(t)$ should have the form

$$\Sigma_R(t > 0) = G_R(t)(\delta/\delta\Phi(t))m(t). \tag{32}$$

Such a structure of $\Sigma_R(t)$ and of $m(t)$ allows one to obtain the final equations for the general case.

Using the relations (27), (28) and (22) we can write down the closed equation for the correlation function:

$$T[G_0^{-1}(t) + (3\lambda/2)\Phi(t = 0)]\Phi(t) = \int_0^t d\tau\, \frac{\partial m(t-\tau)}{\partial\tau}\Phi(\tau)$$

$$+ \int_{-\infty}^0 d\tau\left(m(t-\tau)\frac{\partial\Phi(\tau)}{\partial\tau} + \frac{\partial m(t-\tau)}{\partial\tau}\Phi(\tau)\right). \tag{33}$$

Integrating the last term in (33), we finally obtain

$$T[\bar{G}_0(t)]^{-1}\Phi(t) + \int_0^t d\tau\, m(t-\tau)\frac{\partial\Phi(\tau)}{\partial\tau} = -\Phi(-\infty)m(+\infty) \tag{34}$$

$$[\bar{G}_0(t)]^{-1} = G_0^{-1}(t) + (3\lambda/2)\Phi(t = 0) - (1/T)m(t = 0). \tag{35}$$

Similarly from (23) we can also obtain the equation for the response function:

$$[G_0^{-1}(t) + (3\lambda/2)\Phi(t = 0)]G_R(t) = \delta(t) + \frac{1}{T}\int_0^t d\tau\, \frac{\partial m(t-\tau)}{\partial\tau}G_R(\tau). \tag{36}$$

A solution of this equation should be self-consistent with relation (27).

Now we can make the Laplace transformation. Multiplying the equations (34), (36) and (27) by $\exp(izt)$ and integrating over t from -0 to $+\infty$ we have

$$-izG_R^{-1}(z)\Phi(z) = \{G_R^{-1}(z) - [\bar{G}_0(z=0)]^{-1}\}\,\Phi(t=0) - \Phi(-\infty)m(+\infty)/T \tag{37}$$

$$TG_R(z) = \Phi(t=0) + iz\Phi(z) \tag{38}$$

$$[G_R(z)]^{-1} = [\bar{G}_0(z)]^{-1} - izm(z)/T \tag{39}$$

$$[\bar{G}_0(z)]^{-1} = (1/b\omega_0^2)(z^2 - \omega_0^2) + (3\lambda/2)\Phi(t=0) - (1/T)m(t=0) \tag{40}$$

where

$$\Phi(m) = \int_0^\infty dt\, e^{izt}\Phi(t) \qquad G_R(z) = \int_0^\infty dt\, e^{izt}G_R(t) \qquad m(z) = \int_0^\infty dt\, e^{izt}m(t).$$

These equations describe both the high- and the low-temperature phases. In the case of the soft model of spin glass, for $[G_0(z)]^{-1}$ we should use the following expression:

$$[\bar{G}_0(z)]^{-1} = -iz/\gamma + r + (3\lambda/2)\Phi(t=0) - (1/T)m(t=0).$$

The equations (34) and (37) require knowing the correlation function at $t = -\infty$,

$$p = \Phi(t = -\infty).$$

This value should be considered as a true thermodynamic order parameter. The first and simplest approach is to reproduce this order parameter from the dynamic equation (34). If we define the long-time limit of the correlation function,

$$q = \Phi(t \to +\infty) \tag{41}$$

we could expect that the following relation holds similarly to the conventional phase transition of second order:

$$p = q. \tag{42}$$

In accordance with (41) in the z representation the correlation function has a pole singularity at $z = 0$:

$$\Phi(z \to 0) = i\,q/z.$$

Extracting similar singularities from (37) and using (42), we can find the following equation for q:

$$q = [(\kappa - q)/T]^2\, m(q) \tag{43}$$

where

$$\kappa = \Phi(t=0) \qquad m(q) = \mu^2 q + \tfrac{3}{2}\lambda^2 q^3. \tag{44}$$

In accordance with (39) and (40), $\kappa = \kappa(T)$ obeys the equation

$$T/(\kappa - q) = d(\kappa, T) + m(q)/T \tag{45}$$

with

$$d(\kappa, T) = [\bar{G}_0(z = 0)]^{-1} = G_0^{-1}(z = 0) + \tfrac{3}{2}\lambda\kappa - m(\kappa)/T.$$

The response function in this case is

$$G_{R,A}(0) = (\kappa - q)/T \qquad (46)$$

and the critical temperature of glass transition is given by the equation

$$T_c^2 = [\mu\kappa(T_c)]^2. \qquad (47)$$

A solution of equation (47) exists only above some critical value μ determined by b and λ.

The equations (43)–(47) present the initial solution of Sherrington and Kirkpatrick for the thermodynamic order parameter in the glassy state. As shown by a number of authors (De Almeida and Thouless 1978, Hertz 1983), this solution appears to be unstable. Indeed, let us present the correlation function in the form

$$\Phi(t) = q + \varphi(t). \qquad (48)$$

In the long-time limit we can linearize the equation for $\Phi(t)$ over $\varphi(t)$. The requirement that $\varphi(t)$ decays with time leads to the following inequality:

$$G_R^2(+0)\,\mathrm{d}m(q)/\mathrm{d}q \le 1. \qquad (49)$$

The above solution does not satisfy this condition, at least near the critical point for $m(q)$ from (44).

This analysis means that the thermodynamics of a glassy state cannot be reproduced within this dynamic approach. In fact, in the equations (34)–(36) we have established the thermodynamic limit by setting $N = \infty$, so that the relaxation times between the ergodic components equal infinity. As a result, we cannot in this case reach the true limit $t = \infty$ to obtain the statistical mechanics quantity.

We use physical arguments to determine the parameter $p = \Phi(t = -\infty)$ in equation (34). In the absence of symmetry-breaking external fields, one expects that the parameter p is zero, owing to the averaging of variable x_j (see (9)) over the infinite interval of time (Sompolinsky and Zippelius 1982, Hertz 1983). The dynamic parameter q, however, may be non-zero because its time of averaging is always shorter than the inter-valley transition times. With these assumptions $p = 0$ and $q \ne 0$, extracting again the $1/z$ singularities from (37) and (38), we can immediately arrive at the following equation for the non-ergodicity parameter q:

$$T^2 q = \kappa(\kappa - q)m(q) \qquad (50)$$

where $\kappa = \kappa(T)$ is now given by the equation

$$d(\kappa, T) = T/(\kappa - q) - m(q)/T = T/\kappa. \qquad (51)$$

In this case, the system can be characterized by the two susceptibilities. One of them is the true static susceptibility, equal to

$$G_A(0) = \kappa/T. \qquad (52)$$

Since the parameter κ satisfying (51) does not show singular behaviour at the critical point, the static susceptibility is a continuous function of temperature near the glass transition. The other static susceptibility given by the limit $G_R(\omega \to 0)$ can be found to be

$$G_R(+0) = (\kappa - q)/T. \qquad (53)$$

It exhibits a cusp near the critical point (Hertz 1983).

The solution of (50) and (51) is already dynamically stable. Equation (50) represents the result of the mode-coupling theory (Götze 1991). The choice $m(q)$ in the form (44) corresponds to the known F_{13} model (Götze and Sjögren 1984).

4. Relaxation in non-equilibrium glass

The fluctuation–dissipation theorem used in the previous section is a consequence of the equilibrium distribution function. Since the inter-valley transition times are infinite, the non-equilibrium distribution, once created, remains infinitely long. To demonstrate this, let us take the following relation between the correlation function and the response function:

$$i\Phi(\omega) = (T/\omega)R(\omega)[G_A(\omega) - G_R(\omega)]. \tag{54}$$

Obviously, a similar solution is impossible for the high-temperature phase, except $R(\omega) = 1$. In the glassy state the present dynamic equations allow the solution with the constraint (54) for any monotonic slowly varying function of frequency $R(\omega)$. The slow frequency variation of $R(\omega)$ should be understood as the following asymptotic limit:

$$R(\omega) = f(\eta) \qquad \eta = -\alpha \ln(\omega\tau) \tag{55}$$

where $\alpha \to 0$ and τ is the microscopic relaxation time. The variable η varies over the interval $0 < \eta < \infty$. The function $f(\eta)$ is assumed to be monotonically increasing from $f(0) = 1$ to $f(\infty) = \infty$, so that the low-energy states appear to be overfilled. Note that these limitations of $f(\eta)$ do not allow inclusion in the present consideration of the equilibrium situation as a limit with $f(\eta) = 1$. Therefore, in spite of the limit $\alpha \to 0$ the constraint (54) with (55) indeed corresponds to the non-equilibrium case.

This deviation from equipartition generates the long-time relaxation. Following SZ, the Green functions can be represented in the form

$$\Phi(t) = \tilde{\Phi}(t) + q(\xi) \tag{56}$$
$$G_R(t) = \tilde{G}_R(t) - (\alpha/t)(d/d\xi)\Delta(\xi) \tag{57}$$
$$\xi = \alpha \ln(t/\tau) \tag{58}$$

where $\tilde{G}_R(t)$ and $\tilde{\Phi}(t)$ are the fast time-dependent parts. In the time representation the constraint (54) reads

$$-(d/dt)\Phi(t) = Tf(\xi)[G_R(t) - G_A(t)]. \tag{59}$$

Taking into account the weak dependence of $f(\xi)$, we can rewrite (59) in the form

$$(d/d\xi)q(\xi) = f(\xi)(d/d\xi)\Delta(\xi). \tag{60}$$

The simplest way to derive the equation for $q(\xi)$ is to use the ω representation, where the Dyson equations read

$$G_R^{-1}(\omega) = [G_R^0(\omega)]^{-1} - \Sigma_R(\omega) \tag{61}$$
$$\Phi(\omega)[G_R(\omega)G_A(\omega)]^{-1} = \Phi_0(\omega)[G_R^0(\omega)G_A^0(\omega)]^{-1} + m(\omega). \tag{62}$$

In the leading order $\alpha \to 0$ the following relations for the Fourier transforms are valid:

$$m(\omega) = (d/d\omega)m(q(\eta)) \tag{63}$$
$$(d/d\eta)\Sigma_R(\omega) = [dm(q)/dq](d/d\eta)\Delta(\eta) \tag{64}$$

which are a consequence of the identity

$$\int_{-\infty}^{\infty} dt\, q^n(\xi)\, e^{i\omega t} = \frac{\alpha}{|\omega|}\frac{d}{d\eta} q^n(\eta) \tag{65}$$

and the polynomial form of $m(\Phi)$ (see (31) and (32)). The condition $q(\infty) = 0$ is also

used in the derivation (63)–(65); it follows from the fact that $f(\infty) = \infty$. As a result, from (61) and (62), for $q(\eta)$ we obtain the Parisi–Sompolinsky–Zippelius equations:

$$(d/d\eta)q(\eta) = G_R^2(\eta)[dm(q)/dq](d/d\eta)q(\eta) \tag{66}$$

$$G_R(\eta) = [\kappa - \Delta(\eta)]/T. \tag{67}$$

Note that the explicit slowly varying dependence originates from $f(\xi)$. Therefore equations (60)–(67) can be rewritten in terms of the variable f only.

From the equations (66) and (60) it follows that for any function $f(\eta)$ (see (55)) the parameter $q(\xi)$ relaxes to zero from $q(\xi = 0) = q_0$ given by the equation

$$T^2 = (\kappa - q_0)^2(d/dq_0)m(q_0). \tag{68}$$

The parameter $\kappa(T)$ is related to the value q_0 by the previous equation

$$d(\kappa, T) + m(q_0)/T = T/(\kappa - q_0).$$

In the process of this slow relaxation the parameter $\Delta(\eta)$ determining the response of the system in the limit $\omega \to 0$ (see (67)) decreases from the value $\Delta(\eta = 0) = q_0$ to

$$\Delta(\eta = \infty) = \kappa - T/\mu = \kappa(1 - T/T_c) \tag{69}$$

so that the susceptibility increases with decreasing ω, reaching the value

$$G_{R,A}(\omega = 0) = \kappa/T_c. \tag{70}$$

The fast relaxation is determined by the marginal solution q_0 (see (68) and (49)) and does not depend on the form of $f(\eta)$.

The non-equilibrium situation can be realized by slowly cooling a system starting from the high-temperature phase (Horner 1987). We can consider this case by again introducing the slow and fast components of the Green functions. Because of the breakdown of the time homogeneity, they now depend on two times:

$$\Phi(t_1, t_2) = \tilde{\Phi}(t_1, t_2) + \varphi(t_1, t_2) \tag{71}$$

$$G_{R,A}(t_1, t_2) = \tilde{G}_{R,A}(t_1, t_2) + g_{R,A}(t_1, t_2). \tag{72}$$

Here the slow time dependence is generated by the time dependence of temperature. We shall suggest that the fast components relax to zero at any given moment of time by obeying the fluctuation–dissipation theorem. We can separate the mass operator into slow and fast parts as follows:

$$m = \bar{m} + \sigma \qquad \sigma = m(\varphi) \tag{73}$$

$$\Sigma_{R,A} = \bar{\Sigma}_{R,A} + s_{R,A} \qquad s_{R,A} = g_{R,A}n(\varphi) \qquad n(\varphi) = \delta\sigma/\delta\varphi. \tag{74}$$

After substituting (71)–(74) into (22) and (23), we can find the following equation for the slow components:

$$\varphi(t_1, t_2) = G(1)G(2)\sigma(t_1, t_2) + G(1)$$

$$\times \int dt_3 \, [s_R(t_1, t_3)\varphi(t_3, t_2) + \sigma(t_1, t_3)g_A(t_3, t_2)] \tag{75}$$

$$g_R(t_1, t_2)[1 - G(1)G(2)n(t_1, t_2)] = [G^{-1}(1) + G^{-1}(2)]^{-1}$$

$$\times \int dt_3 \, g_R(t_1, t_3)g_R(t_3, t_2)[n(t_1, t_3) + n(t_3, t_1)] \tag{76}$$

where

$$G(1) = (\kappa_1 - \varphi_1)/T_1 \qquad \varphi_1 = \varphi(t_1, t_1) \qquad T_1 = T(t_1). \qquad (77)$$

The non-ergodicity parameter φ_1 at time t_1 is again given by the marginal solution

$$G^2(1)(\delta/\delta\varphi_1)m(\varphi_1) = 1 \qquad (78)$$

where the equation for $\kappa_1 = \kappa(T_1)$ has the old form

$$d(\kappa_1, T_1) + m(\varphi_1)/T_1 = T_1/(\kappa_1 - \varphi_1). \qquad (79)$$

The equations (75) and (76) include the time dependence through $T(t)$. Therefore it is convenient to rewrite them in terms of the temperature variable. Defining

$$g_R(t_1, t_2) = -a(T_1, T_2)(d/dt_2)T(t_2) \qquad \varphi(t_1, t_2) = b(T_1, T_2) \qquad (80)$$

we have

$$a(T_1, T_2)[1 - G(1)G(2)n(T_1, T_2)] = G(1)\int_{T_2}^{T_1} dT_3\, a(T_1, T_3)a(T_3, T_2)n(T_3, T_2) \qquad (81)$$

$$b(T_1, T_2) = G(1)G(2)\sigma(T_1, T_2) + G(1)\int_{T_2}^{T_1} dT_3\, s(T_1, T_3)b(T_3, T_2)$$

$$+ G(1)\int_{T_c}^{T_2} dT_3\, [s(T_1, T_3)b(T_3, T_2) + \sigma(T_1, T_3)a(T_3, T_2)]. \qquad (82)$$

The solution of these equations can be found near the critical point by an expansion over the small parameter $\tau = (T_c - T)/T_c$ (Ioffe 1988, Freixa-Pascual and Horner 1990).

5. Conclusions

The appearance of infinitely high barriers separating the different phases forces the system to stay forever in the phase in which it was originally prepared. In other words, if we create the non-equilibrium population of these phases, this state lasts infinitely. As we have seen, the degeneracy of the order parameter revealed by SZ reflects the variety of similar non-equilibrium states below the glass transition. From this point of view the breakdown of the fluctuation–dissipation theorem for the SZ dynamic solution is natural. The infinitely small parameter α that occurs in their approach is related to this deviation from equipartition. The other characteristic feature of this deviation is its logarithmic dependence on energy. As a result, there is the slow logarithmic relaxation of the order parameter to zero. It should be emphasized that this relaxation is not a result of the inter-valley transitions. The shape of its decay is not universal, since it is determined by the non-equilibrium distribution function.

In equilibrium we have found that the dynamics obeys the mode-coupling equations. The derivation of these equations was based on the fact that in the absence of external fields the correlation function relaxes to zero over the timescales determined by the size of the system due to the inter-valley transitions, so that we always have $\Phi(t = -\infty) = 0$. The non-ergodicity order parameter occurring in the glassy state represents an intermediate asymptote of the correlation function in the whole relaxation process before

Figure 2. The diagram describing the first correction over the anharmonicity constant to the mode-coupling approximation.

inter-valley transitions happen. For the infinite system this asymptote realizes as the limit $q = \Phi(t \to +\infty)$. Therefore the non-ergodicity parameter cannot be reproduced in a thermodynamic framework.

The analysis of the dynamic equation describing the 'fast' relaxation of the correlation function or the intra-valley transitions has been done in a number of works (see e.g. Götze 1991). Depending on the model parameters, this relaxation can include exponential, power and also slow logarithmic decay (Götze and Sjögren 1989). The latter has universal character. It should be noted that the fast dynamics for the non-equilibrium case obeys the same equations. Therefore the previous mode-coupling analysis can be straightforwardly extended to this case also.

Acknowledgments

Appendix

The first diagram for the mass operator including the renormalization of vertex is shown in figure 2. With (7) and (16), its evaluation in the classical equilibrium case gives

$$m^{(3)}(t) = \frac{9}{T}\lambda^3\Phi(t)\int dt_1\ \Phi^2(t-t_1)\frac{d}{dt_1}\Phi^2(t_1). \tag{A1}$$

The function $(d/dt_1)\Phi(t_1)$ decays over large t_1 faster, at least, than $t_1^{-3/2}$. Therefore, for large t, the contribution (A1) can be approximately represented in the form

$$m^{(3)}(t) = (18/T)\lambda^3(\kappa^2 - q^2)\Phi^3(t)$$

where $\kappa = \Phi(t=0)$ and $q = \Phi(t\to\infty)$. As a result, taking into account $m^{(3)}(t)$ yields only a renormalization factor before the term $\Phi^3(t)$ in the whole expression for $m(t)$.

The previous consideration fails if $\mu = 0$. In this case $\Phi(t)$ is an oscillating function of time, the integral in (A1) diverges and we are faced with the known problem for an anharmonic oscillator.

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