

# Theory of nonergodicity of structural glasses in the quantum case

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The explicit form of the order parameter is found for the nonergodicity range of structural glasses in the quantum case. It is shown that the part of the order parameter corresponding to intervalley transitions does not exhibit quantum fluctuations. This property is used in developing a general theory of nonergodicity of structural glasses. More detailed equations are derived for the case of a small anharmonicity constant of displacive-type structural glasses. In the case of order-disorder structural glasses the explicit forms of the longitudinal and transverse dynamic susceptibilities are found for the weak tunneling case.

## 1. INTRODUCTION

A new branch of the physics of strongly disordered systems dealing with structural glasses is growing rapidly at present (see, for example, Ref. 1). Structural glasses are systems with competing interactions of different signs, exhibiting structural transitions. Structural glasses are structural analogs of spin glasses. It is known that conventional structural transitions result in ordering of a great variety of entities such as dipoles, quadrupoles, etc. Therefore, structural glasses have a great variety of forms: dipole, proton, quadrupole, orientational, Potts, etc. It is found however, that the universality typical of spin glasses is not exhibited by structural glasses. We shall therefore consider only two classes, namely dipole and proton glasses, and refer to them for brevity as structural glasses.

These classes of structural glasses are particularly interesting because the first experiments described recently demonstrated that they exhibit a strong frequency dispersion of the real part of the permittivity  $\varepsilon(\omega)$  at about several hertz. These are the frequencies that correspond to a nonzero imaginary part of  $\varepsilon(\omega)$ . Such behavior is exhibited by dipole and proton glasses<sup>2,3</sup> and in all probability is a universal property of all structural glasses.

On the other hand, precisely the same effects have been long known for spin glasses.<sup>4,5</sup> In spin glasses they form a part of a wide range of irreversible effects demonstrating that spin glasses are nonergodic (see, for example, a review by the present author in Ref. 6). In all probability, the necessary range of measurements will be made in the near future on structural glasses with the aim of detecting and investigating in detail this wide range of phenomena.

It is therefore desirable to construct a suitable theory of nonergodicity of structural glasses. This is the task of the present paper. A highly advanced theory of the molecular field in spin glasses is already available,<sup>6,7</sup> so that the question arises whether this theory can be extended also to structural glasses.

The following comments should be made. Unfortunately, conventional methods make it very difficult to go beyond the mean field approximation, so that we shall confine ourselves to this approximation. The question naturally arises whether the predictions obtained on the basis of the mean field approximation agree with real experiments. It is premature to make a detailed comparison of the molecular field theory with experiments. However, it is generally accept-

ed<sup>6,7</sup> that the molecular field theory is in qualitative agreement with experiments and can provide the language suitable for discussing the phenomena observed experimentally. However, no attempt should be made to carry out any specific quantitative fitting and the discussions have to remain qualitative.

We are hoping that this applies also to structural glasses. However, new problems appear because structural glasses are intrinsically quantum systems. We therefore face a new range of times, which are called quantum times. Moreover, there is a range of classical times and a nonergodicity range. We hope that the molecular field theory of structural glasses can provide a qualitative description of all these ranges although this can be determined definitely only by going beyond the molecular field approximation.

In extending the standard molecular field theory of spin glasses to structural glasses we are faced with a serious difficulty associated with quantum properties of structural glasses. This is due to the fact that the Parisi order parameter  $q(x)$  of quantum glasses should depend also on the Matsubara time  $\tau$ , i.e., it should be a function  $q(x, \tau)$ . A similar problem is encountered also in the case of spin glasses when the spin is  $S \sim 1$ . This problem was first pointed out in connection with the quantum properties of spin glasses.<sup>8</sup> The quantum aspect is always ignored in the modern theory of nonergodicity of spin glasses. In the case of Ising spin glasses this problem does not arise at all, whereas in the Heisenberg case it is usual to assume that  $S \gg 1$ .

In the case of structural glasses we cannot ignore the quantum properties because the quantum frequencies are as a rule of the order of the transition temperature and the quantum parameter is of the order of unity. This situation is not specific to structural glasses. It is exhibited also by conventional structural transitions (see, for example, Ref. 9). In this situation it is necessary to extend the standard theory of nonergodicity of spin glasses to structural glasses under conditions of strong quantum fluctuations. This is precisely the task of the present paper.

The derivation of the principal equations for structural glasses, similar to that given in Ref. 8 for spin glasses, shows that at first sight the function  $q(x, \tau)$  should depend on  $\tau$ . If the solution does indeed have this property, then ordinary integrals have to be replaced by functional integrals and theory would become very unhelpful. However, the main result of the treatment given below is that the molecular field equation for the order parameter  $q(x, \tau)$  (and for other quantities

representing the nonergodicity) has a solution independent of  $\tau$ . We can therefore develop in the usual way a fully helpful theory which is completely analogous to the theory of classical spin glasses. The quantum effects are then important in two cases: firstly, when the boundary conditions to the molecular field equations depend strongly on quantum fluctuations, and secondly, when the intravalley ergodic susceptibility is determined entirely by quantum effects. Therefore, it is important to point out that this susceptibility is not an order parameter and it also exists in the paramagnetic region. The quantities describing nonergodicity directly are sensitive to quantum fluctuations only via the boundary conditions to these equations.

## 2. DERIVATION OF THE PRINCIPAL EQUATIONS. ERGODIC CASE

The conventional theory of structural transitions distinguishes two cases: displacive and order-disorder transitions. A classical example of the former is  $\text{BaTiO}_3$  and of the latter is  $\text{RbH}_2\text{PO}_4$ . There is no sharp boundary between systems of these two types and many substances have intermediate properties. However, for the sake of simplicity, we shall retain this division since these extreme cases are described by the simplest model Hamiltonians.

Spin glasses are obtained when a system exhibits a competition between the ferromagnetic and antiferromagnetic interactions. A similar situation naturally occurs also in structural glasses. The competing interaction appears during the preparation of solid solutions. Such an interaction is exhibited, for example, by an alloy formed between a typical ferroelectric and a typical antiferroelectric such as  $\text{Rb}_{1-x}(\text{NH}_4)_x\text{H}_2\text{PO}_4$ .

We shall consider two characteristic Hamiltonians. The Hamiltonian of a displacive-type structural glass will be used in the form

$$H = \sum_{ik} A_{ik} x_i x_k + \sum_i \left[ \frac{M\omega_0^2}{2} x_i^2 + \frac{\lambda x_i^4}{8} + \frac{p_i^2}{2M} \right], \quad (1)$$

where  $x_i$  are the displacements,  $p_i$  are the momenta,  $M$  is the mass of an ion,  $\omega_0$  is a characteristic frequency, and  $A_{ik}$  is a random Gaussian quantity with zero average value. It is convenient to introduce dimensionless displacements and momenta:

$$x_i = m_i a, \quad p_i = r_i / a, \quad (2)$$

where  $a$  is the lattice constant. Equation (1) then becomes

$$\begin{aligned} H &= \sum_{ik} J_{ik} m_i m_k + \sum_i U(m_i, r_i), \\ U(m_i, r_i) &= m^2/2b + um^4/8 + b\omega_0^2 r^2/2, \\ u &= \lambda a^4, \quad b^{-1} = M\omega_0^2 a^2, \quad J_{ik} = A_{ik} a^2, \\ \langle J_{ik} \rangle &= 0, \quad \langle J_{ik}^2 \rangle = I_{ik}. \end{aligned} \quad (3)$$

In the classical limit we have  $\omega_0 \rightarrow 0$  and the term containing the momenta  $\omega_0^2 r_i^2$  becomes unimportant. The Hamiltonian of Eq. (3) then reduces to the well-known soft model of a spin glass (see, for example, Refs. 6 and 10–12).

The Hamiltonian structural glass of the order-disorder type has the form of the Ising model in a transverse field with random exchange<sup>13,14</sup>

$$\begin{aligned} H &= - \sum_{ik} J_{ik} S_i^z S_k^z - \Delta \sum_i S_i^x, \\ \langle J_{ik} \rangle &= 0, \quad \langle J_{ik}^2 \rangle = I_{ik}, \end{aligned} \quad (4)$$

where  $S_i^x$  and  $S_i^z$  are the spin operators for the spin 1/2.

We shall derive general expressions only for the Hamiltonian (3) and in the case of the Hamiltonian (4) we shall use specific relationships because, as demonstrated later, the general expressions are independent of the actual nature of the Hamiltonian.

It is well known that general averaging over all the realizations  $J_{ik}$  should be carried out by the replica method. In the case of the classical Hamiltonian this is a fairly simple procedure, but in the quantum case we are faced with a problem associated with the noncommutative nature of the quantum operators. A way of overcoming this difficulty was suggested in Ref. 8. We can represent the partition function  $Z$  in the form

$$Z = \text{Tr} \left\{ P \exp \left[ \int_0^{1/T} d\tau H(m(\tau), r(\tau)) \right] \right\}. \quad (5)$$

Equation (5) contains the Matsubara time  $\tau$  and the operator  $P$  is the Matsubara time-ordering operator. The quantum-mechanical operators inside the expression for  $P$  can be treated in the same way as the ordinary  $c$  numbers. Therefore, introducing replicas we can apply the standard procedure for averaging over  $J_{ik}$ . The result is

$$\begin{aligned} \langle Z^n \rangle &= \text{Tr} P \exp \left\{ \int_0^{1/T} d\tau_1 d\tau_2 \sum_{i\mu\nu} J_{i\mu\nu} m_{i\mu}(\tau_1) m_{i\mu}(\tau_1) \right. \\ &\quad \times m_{i\nu}(\tau_2) m_{i\nu}(\tau_2) \\ &\quad \left. - \int_0^{1/T} d\tau \sum_{i\mu} U[m_{i\mu}(\tau), r_{i\mu}(\tau)] \right\}, \end{aligned} \quad (6)$$

where  $\mu, \nu = 1, \dots, n \rightarrow 0$  represents replicas. The molecular field equation is obtained from Eq. (6) if the standard separation is applied to the first term. After the usual manipulations (see, for example, Ref. 6), we obtain an equation for the quantity

$$\begin{aligned} q_{\mu\nu}(\tau_1, \tau_2) &= \frac{\text{Tr} \{ P [m_\mu(\tau_1) m_\nu(\tau_2) e^{-H_c/T}] \}}{\text{Sp} \{ P e^{-H_c/T} \}}, \\ \frac{H_c}{T} &= -2I_0 \int_0^{1/T} d\tau_1 d\tau_2 \sum_{\mu\nu} q_{\mu\nu}(\tau_1, \tau_2) m_\mu(\tau_1) \\ &\quad \times m_\nu(\tau_2) + \int_0^{1/T} d\tau \sum_{\mu} U[m_\mu(\tau), r_\mu(\tau)], \\ I_0 &= \sum_k J_{ik}. \end{aligned} \quad (7)$$

Comparing Eq. (7) with the usual equation of this kind in the classical limit, we find that the principal distinction of Eq. (7) is that  $q_{\mu\nu}$  depends on the Matsubara times  $\tau_1$  and  $\tau_2$ . This dependence does not allow us to carry out further standard transformations of this equation, which would have led to the ordinary molecular field equations; this is true in the ergodic range and particularly so in the nonergo-

dic range. Therefore, at first sight it would seem that it is not possible to develop an ordinary molecular field theory for the quantum case.

However, it is found that Eq. (7) has a very simple solution, namely

$$q_{\mu\nu}(\tau_1, \tau_2) = q_{\mu\nu} + D(\tau_1 - \tau_2) \delta_{\mu\nu}, \quad (8)$$

i.e., the off-diagonal matrix elements of the operator  $q_{\mu\nu}(\tau_1, \tau_2)$  are independent of  $\tau_1$  and  $\tau_2$ . This has a very simple meaning. The off-diagonal matrix elements  $q_{\mu\nu}$  describe in fact fluctuations of frozen molecular fields. The fact that these matrix elements are independent of the Matsubara frequencies simply means that the frozen molecular fields do not exhibit quantum-mechanical fluctuations. Only the susceptibility  $D(\tau)$  has such fluctuations. Physically the picture is almost self-evident. We shall now show mathematically that Eq. (8) is indeed the solution of Eq. (7). We shall demonstrate this first in the simplest ergodic case. We then have

$$q_{\mu\nu} = q \Lambda_{\mu\nu}, \quad \Lambda_{\mu\nu} = 1. \quad (9)$$

We shall substitute Eqs. (8) and (9) into Eq. (7) for  $H_c$ . This gives

$$\begin{aligned} \frac{H_c}{T} = & -2I_0 q \int_0^{1/T} d\tau_1 d\tau_2 \sum_{\mu\nu} m_\mu(\tau_1) m_\nu(\tau_2) \\ & -2I_0 \int_0^{1/T} d\tau_1 d\tau_2 D(\tau_1 - \tau_2) \sum_{\mu} m_\mu(\tau_1) m_\mu(\tau_2) \\ & + \int_0^{1/T} d\tau \sum_{\mu} U[m_\mu(\tau), r_\mu(\tau)]. \quad (10) \end{aligned}$$

Next, we shall substitute Eq. (10) into an expression for  $q_{\mu\nu}(\tau_1, \tau_2)$  in Eq. (7), which gives

$$\begin{aligned} q_{\mu\nu}(\tau_1, \tau_2) = & \int \frac{dh}{(8\pi I_0 q)^{1/2}} \exp\left(-\frac{h^2}{8I_0 q}\right) \\ & \times \text{Tr} P \left\{ m_\mu(\tau_1) m_\nu(\tau_2) \exp\left(-\frac{1}{T} \sum_{\lambda} H_{\lambda 0}(h)\right) \right\}, \quad (11) \end{aligned}$$

$$\frac{1}{T} H_{\lambda 0}(m, r, h)$$

$$\begin{aligned} = & -h \int_0^{1/T} d\tau m_\lambda(\tau) - 2I_0 \int_0^{1/T} d\tau_1 d\tau_2 D(\tau_1 - \tau_2) m_\lambda(\tau_1) m_\lambda(\tau_2) \\ & + \int_0^{1/T} d\tau U[m_\lambda(\tau), r_\lambda(\tau)]. \end{aligned}$$

In the derivation of Eq. (11) we allowed for the fact that, as is easily demonstrated, the denominator in the expression for  $q_{\mu\nu}(\tau_1, \tau_2)$  in Eq. (7) becomes unity in the limit  $n \rightarrow 0$ . Equation (11) differs from Eq. (7) by the fact that the argument of the exponential function in Eq. (11) has a single sum over the replicas. It is important to point out that the operators corresponding to different replicas commute. Using this fact, we obtain directly the following expression in the case when  $\mu \neq \nu$ :

$$\begin{aligned} q_{\mu\nu} = q = & \int \frac{dh}{(8\pi I_0 q)^{1/2}} \exp\left(-\frac{h^2}{8I_0 q}\right) M^2(h) \quad \text{for } \mu \neq \nu, \\ M(h) = & \frac{\text{Tr} P [m \exp(-H_0(h)/T)]}{\text{Tr} P \exp(-H_0(h)/T)}. \quad (12) \end{aligned}$$

It is clear from Eq. (12) that the off-diagonal matrix elements  $q_{\mu\nu}(\tau_1, \tau_2)$  are independent of  $\tau$ . Therefore, the solution of type (8) does indeed exist. We shall now consider  $q_{\mu\mu}(\tau_1, \tau_2)$ . Obviously, we have

$$\begin{aligned} q_{\mu\mu}(\tau_1 - \tau_2) = & q + D(\tau_1 - \tau_2) = \int \frac{dh}{(8\pi I_0 q)^{1/2}} \\ & \times \exp\left(-\frac{h^2}{8I_0 q}\right) \frac{\text{Tr} P [m(\tau_1) m(\tau_2) \exp(-H_0(h)/T)]}{\text{Tr} P [\exp(-H_0(h)/T)]}. \quad (13) \end{aligned}$$

Equation (13) defines the Matsubara correlation function  $D(\tau_1 - \tau_2)$ .

### 3. NONERGODIC RANGE

We shall now consider the nonergodic range. In this range it is usual to employ the Parisi theory<sup>15</sup> of disturbed replica symmetry. However, we shall use a fully equivalent concept developed by the present author<sup>6</sup> and based directly on a pattern of an ultrametrically constructed infinite-dimensional space of objects which we shall arbitrarily call valleys.

We shall introduce  $M$  valleys which we shall label with the index  $a$  and we shall assume that the total Hamiltonian is the sum of the Hamiltonians describing each valley, i.e., we shall postulate that instead of Eq. (3), we have

$$H = \sum_{ika} J_{ik} m_{ia} m_{ka} + \sum_{ia} U(m_{ia}, r_{ia}). \quad (14)$$

Averaging then over  $J_{ik}$ , we obtain by analogy with Eq. (6)

$$\begin{aligned} \langle Z^n \rangle = & \text{Tr} P \exp \left\{ \int_0^{1/T} d\tau_1 d\tau_2 \sum_{ikab\mu\nu} I_{ik} m_{i\mu a}(\tau_1) \right. \\ & \left. \times m_{k\nu a}(\tau_2) m_{i\nu b}(\tau_2) m_{k\nu b}(\tau_2) - \int_0^{1/T} d\tau \sum_{i\mu a} U(m_{i\mu a}(\tau), r_{i\mu a}(\tau)) \right\}. \quad (15) \end{aligned}$$

Following the derivation of Eq. (7) from Eq. (6), we shall use Eq. (15) to derive the following equation:

$$\begin{aligned} q_{\mu\nu ab}(\tau_1, \tau_2) = & \frac{\text{Tr} P [m_{\mu a}(\tau_1) m_{\nu b}(\tau_2) \exp(-H_c/T)]}{\text{Tr} P \exp(-H_c/T)}, \\ \frac{H_c}{T} = & -2I_0 \int_0^{1/T} d\tau_1 d\tau_2 \sum_{\mu\nu ab} q_{\mu\nu ab}(\tau_1, \tau_2) \\ & \times m_{\mu a}(\tau_1) m_{\nu b}(\tau_2) + \int_0^{1/T} d\tau \sum_{\mu a} U[m_{\mu a}(\tau), r_{\mu a}(\tau)]. \quad (16) \end{aligned}$$

In the nonergodic range we shall assume similarly<sup>6</sup> that

$$q_{\mu\nu ab}(\tau_1, \tau_2) = q_{ab} \Lambda_{\mu\nu} + p_{ab} (1 - \delta_{ab}) \delta_{\mu\nu} + D(\tau_1 - \tau_2) \delta_{ab} \delta_{\mu\nu}. \quad (17)$$

In Eq. (17) it is postulated, by analogy with Eq. (8), that only the intravalley susceptibility  $D(\tau)$  depends on the Matsubara frequencies and this susceptibility corresponds to the

diagonal, in respect of the replicas and valleys, matrix elements  $a = b$  and  $\mu = \nu$ . The remaining matrix element  $q_{ab}$ , describing the overlap of different valleys, and  $p_{ab}$ , corresponding to the intervalley susceptibility, are independent of  $\tau$ . We shall show later that this hypothesis is indeed confirmed by Eq. (16). We note also that by substitution of Eq. (17) into Eq. (16) we can show that in the limit  $n \rightarrow 0$  the denominator of the expression for  $q_{\mu\nu ab}(\tau_1, \tau_2)$  is unity and, therefore, Eq. (16) simplifies to

$$q_{\mu\nu ab}(\tau_1, \tau_2) = \text{Tr} P[m_{\mu a}(\tau_1) m_{\nu b}(\tau_2) \exp(-H_c/T)]. \quad (18)$$

We now have to assume an ultrametric structure of the matrices  $q_{ab}$  and  $p_{ab}$ . By analogy with Ref. 6 we shall assume that we are dealing with the  $(k+1)$ th hierarchical level and that the branching of the ultrametric tree is  $j$ . It follows that each of the  $M$  valleys  $a$  can be labeled with the number  $k+1$ :

$$a_0, a_1, \dots, a_k, \quad 0 \leq a_i \leq j-1, \quad M = j^{k+1}. \quad (19)$$

Then, the matrices  $q_{ab}$  and  $p_{ab}$  can be parametrized using  $k+1$  parameters:

$$q_0, q_1, \dots, q_k, \Delta_0, \Delta_1, \dots, \Delta_k. \quad (20)$$

Next, we have to assume that

$$k \rightarrow \infty, \quad j \rightarrow \infty, \quad (21)$$

and in the final answers to have to go to the infinite limit. Following Ref. 6, we shall now assume that

$$\begin{aligned} \sum_{ab\mu\nu} q_{ab} L_{\mu a} L_{\nu b} &= q_0 \left( \sum_{\mu a_0 \dots a_k} L_{\mu a_0 \dots a_k} \right)^2 + q_1' \sum_{a_0} \left( \sum_{\mu a_1 \dots a_k} L_{\mu a_0 \dots a_k} \right)^2 + \dots \\ &+ q_k' \sum_{a_0 \dots a_{k-1}} \left( \sum_{\mu a_k} L_{\mu a_0 \dots a_k} \right)^2, \end{aligned} \quad (22)$$

$$\begin{aligned} \sum_{ab\mu} p_{ab} L_{\mu a} L_{\mu b} &= -\frac{\Delta_0'}{p_0} \sum_{\mu} \left( \sum_{a_0 \dots a_k} L_{\mu a_0 \dots a_k} \right)^2 \\ &- \frac{\Delta_1'}{p_1} \sum_{\mu a_0} \left( \sum_{a_1 \dots a_k} L_{\mu a_0 \dots a_k} \right)^2 - \dots \\ &- \frac{\Delta_k'}{p_k} \sum_{\mu a_0 \dots a_{k-1}} \left( \sum_{a_k} L_{\mu a_0 \dots a_k} \right)^2, \end{aligned}$$

$$q_i' = q_i - q_{i-1}, \quad \Delta_i' = \Delta_{i+1} - \Delta_i < 0,$$

$$p_i = j^{k-l+1}, \quad p_0 = j^{k+1} = M,$$

$$L_{\mu a} = \int_0^{1/T} d\tau m_{\mu a}(\tau).$$

Substituting Eqs. (22) and (17) into the expression for  $H_c$  in Eq. (16) and applying the Hubbard-Stratonovich transformation to all the terms except that with  $D(\tau)$ , we obtain

$$\begin{aligned} &\exp\left(-\frac{H_c}{T}\right) \\ &= \left\langle \exp\left\{\frac{1}{T} \sum_{\mu a_0 \dots a_k} H_0 [m_{\mu a}, r_{\mu a}, \xi_{\mu a_0 \dots a_{k-1}}^{(k)}]\right\} \right\rangle_{h, \xi}, \\ &\xi_{\mu a_0 \dots a_{k-1}}^{(k)} = h^{(0)} + h_0^{(1)} + \dots + h_{a_0 \dots a_{k-1}}^{(k)} + \xi_{\mu}^{(0)} \\ &\quad + \xi_{\mu a_0}^{(1)} + \dots + \xi_{\mu a_0 \dots a_{k-1}}^{(k)}, \quad (23) \\ &\langle \dots \rangle_{h, \xi} = \int \frac{dh^{(0)}}{(8\pi I_0 q_0)^{1/2}} \exp\left\{-\frac{(h^{(0)})^2}{8I_0 q_0}\right\} \\ &\quad \times \prod_{\mu} \int \frac{d\xi_{\mu}^{(0)}}{(8\pi I_0 (-\Delta_0'/p_0)^{1/2}} \exp\left\{-p_0 \frac{(\xi_{\mu}^{(0)})^2}{8I_0 (-\Delta_0')}\right\} \\ &\quad \times \prod_{a_0} \int \frac{dh_{a_0}^{(1)}}{(8\pi I_0 q_1')^{1/2}} \exp\left\{-\frac{(h_{a_0}^{(1)})^2}{8I_0 q_1'}\right\} \\ &\quad \times \prod_{\mu a_0} \int \frac{d\xi_{\mu a_0}^{(1)}}{(8\pi I_0 (-\Delta_1'/p_1)^{1/2}} \exp\left\{-p_1 \frac{(\xi_{\mu a_0}^{(1)})^2}{8I_0 (-\Delta_1')}\right\} \\ &\quad \dots \\ &\quad \times \prod_{a_0 \dots a_{k-1}} \int \frac{dh_{a_0 \dots a_{k-1}}^{(k)}}{(8\pi I_0 q_k')^{1/2}} \exp\left\{-\frac{(h_{a_0 \dots a_{k-1}}^{(k)})^2}{8I_0 q_k'}\right\} \\ &\quad \times \prod_{\mu a_0 \dots a_{k-1}} \int \frac{d\xi_{\mu a_0 \dots a_{k-1}}^{(k)}}{(8\pi I_0 (-\Delta_k'/p_k)^{1/2}} \\ &\quad \times \exp\left\{-p_k \frac{(\xi_{\mu a_0 \dots a_{k-1}}^{(k)})^2}{8I_0 (-\Delta_k')}\right\} \cdot (\dots). \end{aligned}$$

If we substitute Eq. (23) into Eq. (18), we find that

$$\begin{aligned} q_{\mu\nu ab}(\tau_1, \tau_2) &= \left\langle \text{Tr} P[m_{\mu a}(\tau_1) m_{\nu b}(\tau_2) \right. \\ &\quad \left. \times \exp\left\{\frac{1}{T} \sum_{\lambda, c} H_0 [m_{\lambda c}, r_{\lambda c}, \xi_{\lambda c_0 \dots c_{k-1}}^{(k)}]\right\} \right\rangle_{h, \xi}. \quad (24) \end{aligned}$$

Equation (24) is very similar to Eq. (11), but instead of simple integration with respect to  $h$  in Eq. (11), we find that Eq. (24) contains a path integral with respect to  $h$  and  $\tau$ . However, this does not change the basic situation. Since the operators corresponding to different replicas commute, it follows that when  $(\mu a) \neq (\nu b)$ , we find from Eq. (24) that the corresponding matrix element  $q_{\mu\nu ab}$  is independent of  $\tau$ . We can write down the explicit form of this matrix element by introducing a two-particle function representing the distribution of the molecular fields  $F_2(h_1, h_2)$ , which is discussed in detail in Refs. 6, 16, and 17. We then obtain

$$q_{\mu\nu ab} = \int dh_1 dh_2 F_2(h_1, h_2, z) M(h_1) M(h_2), \quad (\mu a) \neq (\nu b), \quad (25)$$

where  $M(h)$  is determined in Eq. (12) and  $z$  gives the ultrametric separation between the values  $a$  and  $b$  based on expressions from Ref. 6:

$$\begin{aligned} z(r_a - r_b) &= \alpha \ln |r_a - r_b|, \quad a \neq b, \\ \alpha &\rightarrow 0, \quad z \sim 1, \end{aligned} \quad (26)$$

$$\begin{aligned} r_a &= -M/2 + a_1 j^{k-1} + a_2 j^{k-2} + \dots + a_k, \\ M &= j^k, \quad a_l = 0 \dots j-1, \quad l = 1 \dots k. \end{aligned}$$

In Eq. (26) the quantity  $r_a$  defines the valley number  $a$  in the

ultrametric space, whereas  $z$  is the distance between the valleys on a logarithmic scale. We can easily show that the assumptions about the nature of the matrices of Eqs. (20) and (22) correspond to the case when  $q_{ab} = q[z(r_a - r_b)]$  and to a similar expression for  $p_{ab}$  in terms of  $\Delta(z)$ . A diagonal matrix element is described by

$$q_{\mu\alpha\alpha}(\tau_1, \tau_2) = q_{\alpha\alpha} + D(\tau_1 - \tau_2) \\ = \int dh F_1(h) \frac{\text{Tr } P[m(\tau_1)m(\tau_2)\exp(-H_0(h)/T)]}{\text{Sp } P \exp(-H_0(h)/T)}, \quad (27)$$

where  $F_1(h)$  is a one-particle distribution function of the molecular fields. Explicit equations can be written down for  $F_2$  and  $F_1$ . These are fully analogous to the corresponding equations in the classical case. The specific nature of the quantum case is that these equations contain explicitly the expression for  $M(h)$ , which naturally depends on the explicit form of  $U(m, r)$  and on quantum fluctuations, as well as on the function  $D(\tau)$ , which is defined by Eq. (27). However, neither  $F_2(h_1, h_2, z)$  nor  $q(z)$  depend explicitly on  $\tau$  and it is this fact that makes it possible to extend all the expressions and equations of the conventional theory to the quantum case. By way of example, we shall simply give the expression for  $F_1(h)$ . The equations for all the other quantities, particularly the explicit expression for the total probabilistic functional, are easily obtained following for example the treatment in Refs. 6, 16, and 17. The quantity  $F_1(h)$  is the boundary value of another function for which we have the equation

$$\frac{\partial F(z, h)}{\partial z} = 4I_0 \left\{ \frac{1}{2} q'(z) \frac{\partial^2 F(z, h)}{\partial h^2} + \frac{1}{T} \Delta'(z) \frac{\partial}{\partial h} [F(z, h) M(z, h)] \right\}, \quad (28)$$

$$F_1(h) = F(0, h), \quad F(\infty, h) = \delta(h).$$

The last equality gives the boundary condition for  $F(z, h)$ . In the case of  $M(z, h)$ , we have a similar equation

$$-\frac{\partial M(z, h)}{\partial z} = 4I_0 \left\{ \frac{1}{2} q'(z) \frac{\partial^2 M(z, h)}{\partial h^2} - \frac{1}{T} \Delta'(z) M(z, h) \frac{\partial M(z, h)}{\partial h} \right\}, \quad (29)$$

$$M(0, h) = M(h),$$

where the boundary function  $M(h)$  is defined in Ref. 12. The quantities  $q(z)$  and  $\Delta(z)$  are obtained by going to the continuous limit for  $\Delta_l$  and  $q_l$ . These topics are discussed in detail in Refs. 6 and 16. The equation for  $D(\tau_1 - \tau_2)$  is included in Eq. (27). We note that the average magnetization is  $\langle m_{\mu\alpha} \rangle = M(\infty, h)$  and not  $M(h)$ .

It is clear from Eqs. (28) and (29) that only the function  $M(h)$ , which defines the boundary conditions for  $M(z, h)$ , is sensitive to the quantum nature of the problem.

Extension of the whole theory to the case of a structural glass of the order-disorder type presents no difficulty. All that we need to do is to replace  $H_0$  of Eq. (11) everywhere with the expression

$$\frac{1}{T} H_0(S^x, S^z, h) = - \int_0^{1/T} d\tau [h S^z(\tau) + \Delta S^x(\tau)] \\ - 2I_0 \int_0^{1/T} \int_0^{1/T} d\tau_1 d\tau_2 D(\tau_1 - \tau_2) S^z(\tau_1) S^z(\tau_2). \quad (30)$$

Since in all the molecular field equations the information about the system occurs only in  $H_0$ , this defines fully all the equations.

Therefore, we now have a closed system of equations for all the quantities of interest to us. This has been possible only because  $q(z)$  and  $\Delta(z)$  are independent of  $\tau$ . If such a dependence exists, equations of this kind cannot be derived.

However, even these equations are fairly complex. We shall therefore attempt to write down simpler equations subject to certain approximations. In particular, we shall consider the intravalley susceptibility  $D(\tau)$ .

#### 4. PERTURBATION THEORY

We shall begin with a fairly simple case of a structural glass of the displacive type with a weak anharmonicity. In this case we can develop perturbation theory on the basis of the anharmonicity constant  $u$  and bypass the general theory. We shall consider only the nonergodic range so that we shall use Eq. (16).

It is clear from Eq. (16) that  $q_{\mu\nu\alpha\beta}(\tau)$  (the operator  $\hat{q}$  depends only the difference of times  $\tau = \tau_1 - \tau_2$ ) is a conventional correlation function modified somewhat to allow for the problems encountered in disordered systems and for nonergodicity. Therefore, the usual perturbation theory based on the anharmonicity constant  $u$  can be applied to this correlation function. This theory has been used in the classical limit to deal with the dynamic problem in other papers of the present author.<sup>11,12</sup> In the present case this should be the standard theory for the Matsubara correlation functions  $q_{\mu\nu\alpha\beta}(\tau)$  or their Fourier transforms (see, for example, Ref. 18):

$$q_{\mu\nu\alpha\beta}(\omega_n) = \int_0^{1/T} e^{i\omega_n\tau} q_{\mu\nu\alpha\beta}(\tau) d\tau \\ = [q_{ab}\Lambda_{\mu\nu} + p_{ab}(1 - \delta_{ab})\delta_{\mu\nu}] \frac{1}{T} \delta_{n,0} + D(\omega_n)\delta_{ab}\delta_{\mu\nu}. \quad (31)$$

The second equality follows from Eq. (17). If  $I_0 = 0$  and  $u = 0$ , we are left with a bare correlation function of a harmonic oscillator

$$D_0(\omega_n) = b\omega_0^2 / (\omega_n^2 + \omega_0^2). \quad (32)$$

In our case, we find from Eq. (16) that

$$\hat{q}(\omega_n) = \{D_0^{-1}(\omega_n)\hat{E} - 4I_0\hat{q}(\omega_n) - \hat{\Sigma}(\omega_n)\}^{-1}, \quad (33)$$

where  $\hat{q}(\omega_n)$  is the expression for the correlation function  $\hat{q}(\omega_n)$  written down in the operator form and occurring in Eq. (31), whereas  $\hat{E}$  is the unity operator. As in Refs. 11 and 12, we shall consider  $\hat{\Sigma}$  graphs of first ( $\hat{\Sigma}^{(1)}$ ) and second ( $\hat{\Sigma}^{(2)}$ ) orders in respect of the anharmonicity constant. These graphs are

$$\Sigma_{\mu\nu ab}^{(1)}(\omega_n) = -\frac{3u}{2} \delta_{\mu\nu} \delta_{ab} q_{\mu\alpha a}(\tau=0) = -\frac{3u}{2} \delta_{\mu\nu} \delta_{ab} (q+g),$$

$$q = q_{aa}, \quad g = T \sum_{\omega_n} D(\omega_n), \quad (34)$$

$$\Sigma_{\mu\nu ab}^{(2)}(\tau) = \frac{3u^2}{2} q_{\mu\nu ab}^3(\tau).$$

We can calculate  $\hat{\Sigma}$  explicitly if we allow for the fact that, as can be demonstrated on the basis of Eq. (22), each matrix element obeys  $p_{ab} \sim 1/M \ll 1$ , whereas  $q_{ab}$  and  $D$  are of the order of unity. If this is allowed for, we obtain

$$\Sigma_{\mu\nu ab}(\omega_n) = \left\{ -\frac{3u}{2}(q+g) + \frac{9u^2}{2} q^2 D(\omega_n) + \Sigma_0(\omega_n) \right\} \delta_{\mu\nu} \delta_{ab}$$

$$+ \left\{ \frac{3u^2}{2T} q_{ab}^3 \Lambda_{\mu\nu} + \frac{9u^2}{2T} p_{ab} q_{ab}^2 (1 - \delta_{ab}) \delta_{\mu\nu} \right\} \delta_{n,0}, \quad (35)$$

$$\Sigma_0(\omega_n) = \frac{3u^2}{2} T^2 \sum_{n,l} D(\omega_m) D(\omega_l) D(\omega_n - \omega_m - \omega_l)$$

$$+ \frac{9u^2}{2} q T \sum_m D(\omega_m) D(\omega_n - \omega_m).$$

It is clear from Eq. (35) that, as expected, all the terms representing nonergodicity are contained only in the term with zero frequency. Therefore, if  $n \neq 0$ , we obtain directly the following simple equation for  $D(\omega_n)$ :

$$D(\omega_n) = \left\{ D_0^{-1}(\omega_n) - 4I_0 D(\omega_n) - \left[ -\frac{3u}{2}(q+g) + \frac{9u^2}{2} q^2 D(\omega_n) + \Sigma_0(\omega_n) \right] \right\}^{-1} \quad (36)$$

We shall now consider the term with  $\omega_n = 0$  in Eq. (33). Then, as is clear from Eqs. (31) and (35), we obtain equations for

$$D(\omega_n=0) = d \quad (37)$$

and  $\Sigma(\omega_n = 0)$ . Since  $D(\omega_n)$  and  $\Sigma(\omega_n)$  are analytic in  $\omega_n$ , it follows that to find them we have to use Eq. (36) and then assume that  $\omega_n = 0$ . However, the most interesting term is nonanalytic in  $\omega_n$  and it is this term that characterizes nonergodicity.

We can write down the equations for  $q_{ab}$  and  $p_{ab}$  by noting first of all that, in the language of the variable  $z$  in Eq. (26), the hypothesis about the nature of the matrices of Eqs. (20) and (22) implies that

$$q_{ab} = q(z_{ab}), \quad p_{ab} = \frac{\alpha}{2|r|} \Delta'(z_{ab}). \quad (38)$$

We can solve our equations for the matrices  $q_{ab}$  and  $p_{ab}$  quite conveniently by the Fourier transformation in terms of the variable  $r_{ab}$ . We can easily show that

$$\sum_{r_{ab}} e^{ikr_{ab}} q_{ab} = -\frac{\pi\alpha}{|k|} q'(y),$$

$$\sum_{r_{ab}} e^{ikr_{ab}} p_{ab} = \Delta(y), \quad (39)$$

$$y = -\alpha \ln|k|.$$

Using Eq. (39), we readily find that Eqs. (33)–(35) yields

the following expressions for  $q(y)$  and  $\Delta(y)$ :

$$\left\{ 1 - \left[ \frac{4I_0}{T^2} + \frac{9u^2}{2T^2} q^2(y) \right] [Td + \Delta(y)]^2 \right\} q'(y) = 0, \quad (40)$$

$$Td + \Delta|y| = \left\{ \frac{1}{bT} - \left( \frac{4I_0}{T^2} + \frac{9u^2}{2T^2} q^2 \right) dT \right.$$

$$\left. - \frac{4I_0}{T^2} \Delta(y) - \frac{9u^2}{2T^2} \int_0^y \Delta'(z) q^2(z) dz \right.$$

$$\left. - \left[ -\frac{3u}{2T}(q+g) + \frac{1}{T} \Sigma_0(\omega_n=0) \right] \right\}^{-1}.$$

We can readily demonstrate that the boundary condition for  $\Delta(y)$  is

$$\Delta(0) = 0. \quad (41)$$

Comparing the second equation from the system (40) when  $y = 0$  with Eq. (36), we can see that Eq. (36) is satisfied for all values of  $\omega_n$ . This is of course to be expected. Next, differentiating the second equation from the system (40), we find that

$$\left\{ 1 - \left[ \frac{4I_0}{T^2} + \frac{9u^2}{2T^2} q^2(y) \right] [Td + \Delta(y)]^2 \right\} \Delta'(y) = 0. \quad (42)$$

In the classical limit ( $T \gg \omega_n$ ) all the sums over  $\omega_n$  are replaced with one term corresponding to  $\omega_n = 0$ . Then, obviously, we obtain

$$D_0(\omega_n) = b\delta_{n,0}, \quad D(\omega_n) = \frac{g}{T} \delta_{n,0}, \quad g = dT, \quad (43)$$

$$\Sigma_0(\omega_n) = \left( \frac{3u^2}{2T} g^3 + \frac{9u^2}{2T} qg^2 \right) \delta_{n,0}$$

and the usual equations for the classical soft model<sup>11</sup> then follow from Eqs. (36), (40), and (42).

We then find that the first equation of the system (40) and Eq. (42) are both degenerate and give only the relationship between  $q(y)$  and  $\Delta(y)$ :

$$\Delta(y) + Td = \left[ \frac{4I_0}{T^2} + \frac{9u^2}{2T^2} q^2(y) \right]^{-1/2} \quad (44)$$

This relationship is an expression of the well-known (in the classical case) scaling invariance.

A detailed analysis of the molecular field equations in the range of validity of perturbation theory is very interesting, but it is outside the scope of the present article.

## 5. ORDER-DISORDER STRUCTURAL GLASSES

In an investigation of the order-disorder structural glasses we have to use Eq. (16) with the Hamiltonian of Eq. (4). Our main task in this section will be to obtain explicitly the dynamic correlation function in the  $\omega$  representation in terms of quantities characterizing the nonergodicity of the system. It is this dynamic correlation function that is determined in spectroscopic experiments.

Spectroscopy of structural glasses should exhibit a range of fundamentally new phenomena. In particular, a change in any parameters of a system such as the temperature or the external electric field, should result in slow relaxation of the lines studied spectroscopically. This relaxation

is similar to slow relaxation of amplitudes of the dynamic susceptibility of spin glasses and is a very interesting effect not observed so far experimentally. Studies of these phenomena require a dynamic theory of structural glasses. This theory will be provided elsewhere. In the present paper we shall employ a static theory framework to study just the equilibrium dynamic correlation function.

The only small parameter in the Hamiltonian of Eq. (4) which can be used is a transverse magnetic field  $\Delta$ . We shall assume this parameter to be small compared with temperature and assume that the static approximation is sufficient to find it. This approximation was first suggested in Ref. 8 for the quantum spin in the paramagnetic region.

The meaning of this approximation is as follows. We have seen in the preceding section that if  $\omega_0 \ll T$ , then

$$D(\omega_n) = d\delta_{n,0}.$$

This does not mean that  $D(\omega)$  is nonanalytic in respect of the frequency. It does mean only that the characteristic frequencies are low compared with temperature and, at frequencies in the range  $\omega \sim T$  we have now a  $\delta$ -function maximum at  $\omega \ll T$ . Since the Matsubara times obey  $\tau \sim T^{-1}$ , it follows that  $D(\tau) = d$  and that it is almost independent of  $\tau$ . We can then find  $D(\tau)$  simply from the equation for  $d$ . Naturally, this equation, together with the equations for  $\hat{q}$  and  $\hat{p}$ , is valid in the static approximation. In fact, this is the classical approximation, but we are retaining the standard terminology and calling the approximation static.

In our case of an order-disorder structural glass the parameter of this approximation is  $\Delta/T$ , which we shall regard as small. However, as a result of the interaction we can have a situation when there are characteristic frequencies  $\omega \sim T$ . The behavior of the correlation function at these frequencies can be found by applying a special perturbation theory. We shall do this by taking the right-hand side of Eq. (13) and replacing  $D(\tau)$  in the exponential function simply with  $dT$  and then calculating  $D(\tau)$  on the left-hand side. This gives the following expression for the left-hand side:

$$D(\tau) = d_1 T + D_1(\tau),$$

where  $|d - d_1|T$ , and  $D_1 \ll dT$  in terms of the parameter  $\Delta/T$ . In the  $\omega$  representation we obtain correspondingly  $d_1 \delta_{n,0} + D_1(\omega_n)$  and then  $D_1(\omega)$  changes significantly at  $\omega \sim T$ . Therefore, the whole dependence at  $\omega \ll T$  occurs only via  $d$  and the dependence at  $\omega \sim T$  is calculated from perturbation theory.

It therefore follows that in the zeroth approximation with respect to the semiclassical parameter, we have

$$D(\omega_n) = d\delta_{n,0}, \quad D(\tau) = g = dT. \quad (45)$$

In the case of the parameter  $d$  we now obtain the equation valid in the nonergodic range. It corresponds to the static approximation of Ref. 8, deduced for the paramagnetic range.

We shall determine first of all the physical picture that corresponds to Eq. (45). We shall therefore discuss the following quantity:

$$Z_0 = \text{Tr } P \exp[-H_0(h)/T]. \quad (46)$$

This quantity occurs, for example, in Eqs. (12), (13), (27),

and in many other similar expressions. If the expression for  $H_0(h)$  of Eq. (11) is modified by the substitution of Eq. (45), we find that

$$Z_0 = \int \frac{dy}{(8\pi I_0 dT)^{1/2}} \exp\left(-\frac{y^2}{8I_0 dT}\right) \times \text{Tr} \exp\left[-\frac{H_1(y+h)}{T}\right] = \left\langle \text{Tr} \exp\left[-\frac{H_1(y+h)}{T}\right] \right\rangle_y, \quad (47)$$

$$H_1(h) = -hm + U(m, r).$$

It is clear from Eq. (47) that the partition function (and not its logarithm) is averaged over a certain Gaussian field  $y$ . This means that the static approximation reduces to the fact that the system now has a certain thermodynamic equilibrium Gaussian field with a variance equal to  $4I_0 dT$ , since in the presence of a thermodynamic equilibrium field the averaging procedure is applied to the partition function itself and not to its logarithm.

It follows that in the static approximation we simply have an additional stage of averaging over the equilibrium field  $y$ . For example, Eq. (12) becomes

$$q_{\mu\nu} = q = \langle M^2(h) \rangle_h \text{ for } \mu \neq \nu, \quad (48)$$

$$M(h) = \frac{\langle \text{Tr} [m \exp[-H_1(h+y)/T]] \rangle_y}{\langle \text{Tr} [\exp[-H_1(h+y)/T]] \rangle_y}$$

and similar changes occur in Eq. (13).

Similar modifications apply to all the expressions obtained for the nonergodic range. The system of equations is closed by

$$d = \int_0^{1/T} D(\tau) d\tau, \quad (49)$$

where  $D(\tau)$  is found from the modified form of Eq. (13) in the ergodic range and from a similar expression for the nonergodic range. This is clear from Eq. (24), which now can be rewritten in the form

$$q_{\mu\nu ab}(\tau_1, \tau_2) = \left\langle \text{Tr} \left\{ P \left[ m_{\mu a}(\tau_1) \cdot \prod_{\lambda, c} \left\langle \exp \left[ \frac{1}{T} H_1(m_{\lambda, c}, r_{\lambda c}, y + \xi_{\lambda c \dots c_k}) \right] \right\rangle_y \right] \right\} \right\rangle_{h, \xi}. \quad (50)$$

Separating from  $q_{\mu\nu ab}(\tau_1, \tau_2)$  the value of  $D(\tau_1 - \tau_2)$  on the basis of Eq. (17) and substituting the results in Eq. (49), we obtain a closed equation for  $d$ . Moreover, Eq. (50) gives an equation also for the matrices  $q_{ab}$  and  $p_{ab}$  that occur in Eq. (17). Therefore, the static approximation yields a closed system of equations for the matrices  $q_{ab}$  and  $p_{ab}$  and for the parameter  $d$ .

The final equations are analogous to Eqs. (28) and (29), except that the boundary condition for  $M(0, h) = M(h)$  is not described by the general expression (12), with  $H_0$  from (11), but by the simple expression for  $M(h)$  in Eq. (48). Therefore, we can see that in the static approximation the problem becomes quite simple, at least no more complex than in the classical case.

We found the form of the equations obtained in the static approximation using the example of structural glasses of the displacive type, but in the case of the order-disorder

glasses the situation is exactly the same except that  $H_1(h)$  is no longer described by Eq. (47) but becomes

$$H_1(h) = -hS^z - \Delta S^x. \quad (51)$$

Following Eq. (51), we also obtain  $M(h)$  of Eq. (48), but now instead of  $m$  in the trace we have  $S^z$ .

We shall now return to the problem posed at the beginning of this section, namely calculation of the dynamic susceptibility for an order-disorder structural glass considered in the static approximation. We shall postulate that this approximation is used in the zeroth order with respect to  $\Delta/T$  to perform the standard task in the physics of structural glasses, namely to determine  $q_{ab}$ ,  $p_{ab}$ , and  $d$ . We now know the explicit form of all the distribution functions of the static molecular field, including the single-particle function  $F_1(h)$  as well as the Gaussian distribution function of thermodynamic equilibrium fields  $y$  introduced in Eq. (47). When we know these quantities, we can calculate the dynamic susceptibility using the next order in  $\Delta/T$ .

We can easily show that in the  $\tau$  representation the longitudinal dynamic susceptibility obtained for  $q_{aa} \ll 1$  is of the form

$$D(\tau - \tau') = \int dh F_1(h) \left\langle \text{Tr } P \left\{ S^z(\tau) S^z(\tau') \right. \right. \\ \left. \left. \times \exp \left[ -\frac{H_1(h+y)}{T} \right] \right\} \right\rangle_y \left\langle \text{Tr } \exp \left[ -\frac{H_1(h+y)}{T} \right] \right\rangle_y^{-1}. \quad (52)$$

We can see that the numerator and denominator are averaged over  $y$  separately, and their ratio is averaged over  $h$ . This corresponds to the presence of static and equilibrium fields in the system. The averaging over  $y$  is carried out using Gaussian fluctuations of the distribution introduced in Eq. (47). In the denominator of Eq. (52) the symbol of ordering with respect to  $p$  is removed in exactly the same way as was used to introduce it in Eq. (5). The denominator of Eq. (52) can be calculated explicitly and the result is

$$D(\tau) = \int dh F_1(h) \frac{\langle R(h+y, \tau) \rangle_y}{\langle 2 \text{ch}[(y+h)^2 + \Delta^2]^{1/2} / 2T \rangle_y} \\ R(h, \tau) = \text{Tr } P \{ S^z(\tau) S^z(\tau') \exp[-H_1(h)/T] \}. \quad (53)$$

Calculation of  $R$  in the  $\omega$  representation yields

$$R(h, \omega_n) = \frac{\text{ch}[(h^2 + \Delta^2)^{1/2} / 2T]}{2(h^2 + \Delta^2)} \left\{ \frac{h^2}{T} \delta_{n,0} \right. \\ \left. - 2\Delta^2 \frac{(h^2 + \Delta^2)^{1/2}}{(i\omega_n)^2 - (h^2 + \Delta^2)} \text{th} \frac{(h^2 + \Delta^2)^{1/2}}{2T} \right\}. \quad (54)$$

It is clear from Eqs. (53) and (54) that if  $\Delta \rightarrow 0$ , then  $R(\omega_n) \sim \delta_{n,0}$ , as expected. Naturally, Eq. (54) is valid only if  $\Delta \ll h, T$  so that Eqs. (53) and (54) should be expanded in terms of  $\Delta^2$ , retaining the zeroth and first terms in  $\Delta^2$ . In the limit  $\Delta \rightarrow 0$  we naturally have

$$D(\omega_n) = \frac{1}{4T} \delta_{n,0}, \quad d = \frac{1}{4T}. \quad (55)$$

It is the above value of  $d$  that can be used in the averaging over  $y$  when  $\Delta^2$  is small. Therefore, for small  $\Delta$  we have to find only  $F_1(h)$ . Clearly, in the lowest order in  $\Delta^2$  we can find  $F_1(h)$  using the conventional static theory for the Ising

model. Then, if we expand all quantities in  $\Delta^2$  and retain the contribution of the zeroth order in  $\Delta^2$  in the static term ( $\sim \delta_{n,0}$ ) and the first-order contribution in the dynamic term, we find that

$$D(\omega_n) = \frac{1}{4T} \delta_{n,0} - \Delta^2 \int dh F_1(h) \\ \times \left\langle \frac{1}{h+y} \frac{\text{sh}[(h+y)/2T]}{(i\omega_n)^2 - (h+y)^2} \right\rangle_y \left\langle 2 \text{ch} \frac{h+y}{2T} \right\rangle_y^{-1}. \quad (56)$$

Therefore at low values of  $\Delta^2$ ,  $D(\omega_n)$  is given by Eq. (56) and we can find  $d$  and  $F_1(h)$  without solving the full quantum problem but simply tackling the classical Ising model. Equation (56) represents the simplest example of the application of perturbation theory based on  $\Delta^2$ , mentioned at the beginning of this section.

It is interesting to note the following. The thermodynamic equilibrium field  $y$  with the variance

$$\langle y^2 \rangle = 4I_0 d T \approx I_0 \quad (57)$$

does not disappear at all in the limit  $\Delta \rightarrow 0$ . The static term in Eq. (56) is indeed independent of  $y$ , but the dynamic term retains this dependence fully.

We must bear in mind that near the paramagnetic region we have  $\langle h^2 \rangle \ll \langle y^2 \rangle$ , so that the main broadening occurs in this region because of the scatter of  $y$ . In particular, this broadening is retained also in the paramagnetic region where  $F_1(h) = \delta(h)$ , and Eq. (56) contains only the averaging for  $y$ .

We shall now use the static approximation to calculate the transverse correlation function  $G$ . By analogy with Eq. (53), we obtain

$$G(\tau) = \int dh F_1(h) \frac{\langle K(h+y, \tau) \rangle_y}{\langle 2 \text{ch}[(h+y)^2 + \Delta^2]^{1/2} / 2T \rangle_y}, \quad (58) \\ K(h, \tau) = \text{Tr } P \{ S^x(\tau) S^x(\tau') \exp[-H_1(h)/T] \}.$$

Calculation of  $G$  and  $K$  in the  $\omega$  representation gives

$$K(h, \omega_n) = \frac{\text{ch}[(h^2 + \Delta^2)^{1/2} / 2T]}{2(h^2 + \Delta^2)} \\ \times \left\{ \frac{\Delta^2}{T} \delta_{n,0} - 2h^2 \frac{(h^2 + \Delta^2)^{1/2}}{(i\omega_n)^2 - (h^2 + \Delta^2)} \text{th} \frac{(h^2 + \Delta^2)^{1/2}}{2T} \right\}, \quad (59)$$

$$G(\omega_n) = - \int dh F_1(h) \\ \times \left\langle (h+y) \text{sh} \frac{h+y}{2T} \frac{1}{(i\omega_n)^2 - (h+y)^2} \right\rangle_y \left\langle 2 \text{ch} \frac{h+y}{2T} \right\rangle_y^{-1}.$$

The expression for  $G(\omega_n)$  given by the second equation of the system (59) is valid subject to the condition  $\Delta \ll T, y$ .

We have thus derived explicit expressions for the longitudinal and transverse correlation functions. We must stress again that the term  $\delta_{n,0}$  includes all the frequencies  $\omega \ll T$  and does not imply nonanalyticity in respect of  $\omega$ . The term with  $\omega \sim T$  in the longitudinal correlation function is small in terms of the parameter  $\Delta/T$  and therefore the use of perturbation theory in the calculation of this term is fully justified. It is interesting to note that the transverse correlation function  $G(\tau)$  depends completely on  $\tau$  when  $\Delta \ll T$ . However, this correlation function does not occur in the molecular field equation and, therefore, its significant dependence on  $\tau$



does not alter the validity of the static approximation.

We note that this behavior of  $D(\tau)$  should have the effect that in a study of longitudinal fluctuations there will be a strong central peak and a weak background greatly broadened by an amount  $\omega \sim T$ . In studies of transverse fluctuations there should be practically no central peak, but the background should be very strong for  $\omega \sim T$ . It would be interesting to check these predictions experimentally.

We shall conclude by noting that even well inside the region of existence of a structural glass phase when  $\Delta/T \ll 1$ , the condition (57) is obeyed and all the distribution functions of the type  $F_1(h)$ ,  $F_2(h_1, h_2)$ , etc. can be determined as in the case of the conventional Ising model. Therefore, expressions of the (53)–(56) type are still valid. However, if the condition  $\Delta/T \ll 1$  is not satisfied, the static approximation cannot be employed.

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