# DENSITY OF STATES OF INTERACTING TWO-LEVEL SYSTEMS IN AMORPHOUS SOLIDS IN THE MEAN RANDOM FIELD APPROXIMATION

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The mean random field approach [1,2] is generalized to the case of random (with certain distribution) values of tunneling matrix elements and double-well potential asymmetries and applied to account for the dipole interaction between two-level systems in glasses. The obtained mean random field distribution function is used to calculate the interaction-modified density of states of the two-level system ensemble. Taking the realistic values of phenomenol-ogical parameters, only a minor correction to the low-energy density of states is found.

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#### **1. INTRODUCTION**

In the sub-Kelvin temperature range nonmetallic glasses display a variety of universal physical properties, which are usually attributed to the specific low-energy excitations, present in all amorphous solids. A model of tunneling systems (TS) is very popular for description of a variety of interesting phenomena, related to thermal, dielectric and acoustic properties of glasses in this temperature range [3]. Though the microscopic origin of TS in glasses remains not completely clear (see however, results of the recent simulations [4]), it is assumed that in glasses they are present with a low (about  $10^{-6}$ ... $10^{-4}$  per atom) concentration due to the possibility of realization of two (or more) spatial configurations in a group of several atoms, with the mean variation of bond length  $\Delta a \leq 0.1\overline{a}$ ( $\overline{a}$  being the mean bond length) and bond angle  $\Delta \phi \leq 10^{\circ}$  in the group. It is also assumed that these structure configurations are separated by the low potential barriers  $V/k_B \le 100 \,\mathrm{K}$  ( $k_B$  being the Boltzmann's constant) and that the differences of energies in the potential minima of these configurations  $|U_{\min i} - U_{\min j}| \ll V$ . At

low temperatures only the ground states in each potential minimum are relevant. In this way, in the simplest case a TS can be introduced as an effective particle moving in a double-well (W) potential, in which in the temperature range  $k_BT \leq V$  the quantum tunneling transitions between the potential minima are dominant. That is why the TS ensemble is governed by the Gibbs statistics in the whole temperature range if the characteristic time of perturbation change is greater then the inverse value of the minimal tunneling frequency.

Due to the overlap of the ground-state (GS) wavefunctions in two wells the GS energy level splits into a doublet with a gap, which in the quasiclassical approximation (see e.g. [5]) equals to:

$$U = \sqrt{\Delta^2 + J^2} , \qquad (1)$$

where

$$J = \frac{\hbar\omega_0}{\pi} \exp(-\lambda) \tag{2}$$

and

$$\lambda \approx l\sqrt{2mV}/\hbar, \qquad (3)$$

 $\Delta$  is a difference of the GS energies in two wells; J is a tunneling matrix element between GS's in two wells;  $\omega_0$  is a frequency of GS oscillations (of the order of Debye frequency),  $\lambda$  is an overlap phase; m is an effective TS mass; V is a height of potential barrier above the GS energy level; l is a width of classically inaccessible region between the potential minima.

The introduced above quantum system is usually called a two-level system (2LS). The 2LS concept for amorphous solids was introduced by Phillips [6] and Anderson et el. [7] to account for their low-temperature anomalous behavior.

Due to the difference of relative spatial locations of (at least partially) ionized particles, corresponding to the 2LS states in minima of a W-potential, these states can be assigned to the eigenvalues of 2-state electric dipole moment operator (pseudospin-1/2).

Due to the structural disorder on the atomic scale in glasses the 2LS parameters  $\Delta$  and  $\lambda$  are believed to have a wide distribution.

The 1-particle distribution function over the parameters  $\Delta$  and  $\lambda$  for non-interacting 2LS is usually considered as uniform in the whole range (see e.g. [3]):

 $P_0^{1}(\Delta,\lambda) = \overline{P}\Theta(\Delta_{\max} - \Delta)\Theta(\Delta)\Theta(\lambda_{\max} - \lambda)\Theta(\lambda - \lambda_{\min}), \quad (4)$ which after transformation to variables ( $\Delta$ , J) takes the form:

$$P_0^{1}(\Delta, J) = \frac{P}{J} \Theta(\Delta_{\max} - \Delta) \Theta(\Delta) \Theta(J_{\max} - J) \Theta(J - J_{\min}), \quad (5)$$

where  $\overline{P}$  is a material constant,  $\Theta(x)$  is a step function.

The 2LS volume concentration n is related to the distribution function (5) in the following way:

$$n = \int_{0}^{\Delta_{\max}} d\Delta \int_{J_{\min}}^{J_{\min}} dJ P_0^1(\Delta, J) = \overline{P} \Delta_{\max} \ln \frac{J_{\max}}{J_{\min}} .$$
(6)

The non-interacting 2LS model in the temperature range  $T \ge 100 \text{ mK}$  is satisfactory to describe most of the phenomena occurring in cold glasses, e.g. the linear term in the temperature dependence of heat capacity, the minimum (maximum) in the temperature dependence of dielectric susceptibility (sound velocity), the electro-

magnetic and ultrasound absorption, polarization echoes, relaxation processes, etc.

However, the recent experiments displayed some discrepancies with the predictions of non-interacting 2LS model in the temperature range  $T \le 100 \text{ mK}$ . For example, the temperature dependence of both the low-frequency dielectric susceptibility and the sound velocity after passing the extremum towards low temperatures is less steep, with a tendency to saturation at ultralow temperatures [8]. The temperature dependences of internal friction and of decay time of spontaneous polarization echo are also unexplainable from these grounds. Even more surprising, there was found a sort of phase transition in amorphous BaO-Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub> at the temperature dependence of dielectric constant [9].

It is natural to try to account for the discrepancies mentioned above by considering dipole-dipole (electric or elastic) interaction in the 2LS ensemble. The effect of dipole interaction on TS density of states was first considered in the pair approximation by M. Klein [10] for a set of randomly distributed symmetric TS with equal tunneling amplitudes, the model which is applicable for the case of off-center impurities in crystals. It was found that strong interaction between a pair of TS gives rise to low-energy excitations with the gap of order  $E \approx J^2/U$ , J and U being the tunneling matrix element and the interaction energy respectively. Later A. Burin [11] considered interaction in the ensemble of 2LS obeying distribution Eq. 5 with random spatial distribution and found a decrease in the low-energy DOS, the so-called *pseudogap* effect. A. Würger [12] used the Bloch's equations for 2LS polarization components to consider the interactioninduced collective excitations in the 2LS ensemble. The interaction effect is shown to decrease the resonant and to increase the relaxation part of susceptibility. This result is consistent with the data for temperature dependence of dielectric constant (see e.g. a review paper Ref. [8]).

However, both Klein's [10] and Würger's [12] approaches have a common shortcoming of considering only the symmetric 2LS, the assumption inapplicable to glasses. The Burin's work [11] employs the approach elaborated for disordered Coulomb systems. These systems also allow the description in terms of two-state variables (corresponding to the occupied and empty state of a site), but there the conception of tunneling matrix elements is meaningless. And the way of taking interaction into account is similar to that of Klein [10] in using the pair approximation (see Eq. (19) in Ref. [11]). So, the result for DOS obtained there is really applicable to the non-tunneling 2LS, which is not a good approximation for glasses. It would be useful to perform calculations of DOS in the pair approximation [10] for the case of random asymmetries and tunneling matrix elements.

The present work employs the approach developed for description of systems undergoing orientation glass transition (see [13,14] and refs. therein). It uses the method of mean random field (MRF) [1,2], elaborated for crystals with off-center impurities. The distribution function is constructed for the random fields, induced by the dipole moments of the neighboring 2LS at a site of arbitrary chosen 2LS, averaged over the distribution (5) and over the uniform and independent spatial and orientation distribution of 2LS. Then the selfconsistency condition is applied, i.e. the distribution function is taken to be the same for all 2LS in the ensemble. The obtained MRF distribution function is subsequently used to calculate the renormalized 2LS DOS.

Though the application of this method to orientation glasses finds numerous objections due to neglecting interaction-induced mutual orientation correlations of spins (see e.g. Ref. [14] and refs. therein), we apply it here to the 2LS ensemble for the next reason. As it was mentioned above, even non-interacting 2LS in glasses have random asymmetries of W potentials and hence each 2LS has random static polarization at any finite temperature. It means that the 2LS ensemble has a property of *initially randomly broken symmetry*. That is why this system does not possess a critical point of orientation glass transition, as the off-center impurities or dilute spin systems do, but rather demonstrates a continuous increase of interaction energy as the temperature is decreased (see Fig. 1 below). So, the critical point, which is thought to be sensitive to interaction-induced orientation correlations, is avoided here. For the case of randomfield 3D Ising model this result is confirmed in Ref. [16].

Below we consider the case of electric dipole-dipole interaction. Since the elastic interaction between 2LS can be included in the same formal way [3], the generalization of our approach is straightforward.

### 2. MEAN RANDOM FIELD DISTRIBUTION FUNCTION

Consider a set of N+1 2LS randomly distributed over the volume V of weakly polarizable medium.

The Hamiltonian of arbitrarily chosen 2LS with number i may be represented as a sum of non-interacting term and the term due to interaction with neighboring 2LS:

$$\hat{H}_i = \hat{H}_{0i} + \hat{H}_{\text{int}\,i} \,.$$
(7)

The explicit form of Hamiltonian (7) in the pseudospin-1/2 representation is:

$$\hat{H}_{0i} = \frac{1}{2} \sigma_z^i \Delta_{0i} + \frac{1}{2} \sigma_x^i J_{0i}, \ \hat{H}_{int_i} \approx \frac{1}{2} \sigma_z^i \Delta_{dip_i},$$
(8)

where

$$\Delta_{\operatorname{dip}_{i}} = 2 \left( \frac{\partial \Delta_{i}}{\partial \mathbf{e}} \Big|_{\mathbf{e}_{i}=0} \cdot \mathbf{e}_{i} \right) \equiv 2 (\mathbf{d}_{i} \cdot \mathbf{e}_{i}), \tag{9}$$

 $\mathbf{d}_i$  being the electric dipole moment of 2LS *i*;  $\mathbf{e}_i$  being the strength of electric field, induced by all the other 2LS at the site of 2LS *i*.

In Eq. (8) we neglected the effect of interaction on the off-diagonal elements of 2LS Hamiltonian, because in most cases  $|\partial J / \partial \mathbf{e}| << |\partial \Delta / \partial \mathbf{e}|$ . This means that diagonal elements of the dipole momentum operator in the coordinate representation have much greater absolute values compared to the off-diagonal ones:

$$\left|\int \Psi_{i}^{*}\mathbf{r}\Psi_{i}d\mathbf{r}\right| \gg \left|\int \Psi_{i}^{*}\mathbf{r}\Psi_{j}d\mathbf{r}\right|, \ i, j = R, L,$$

the fact which follows from the condition of small overlap of single-well wavefunctions:

$$\left|\int \Psi_i^* \Psi_i d\mathbf{r}\right| >> \left|\int \Psi_i^* \Psi_j d\mathbf{r}\right|, \ i, j = R, L.$$

Hamiltonian (7) may be rewritten as:

$$\hat{H}_i = \frac{1}{2}\sigma_z^i \Delta_i + \frac{1}{2}\sigma_x^i J_{0i} , \ \Delta_i = \Delta_{0i} + 2(\mathbf{d}_i \cdot \mathbf{e}_i).$$
(10)

In the energy representation Hamiltonian (10) takes the form:

$$\hat{H}_{i} = \frac{1}{2} \sigma_{z}^{i} U_{i}, \ U_{i} = \sqrt{\left(\Delta_{0i} + 2(\mathbf{d}_{i} \cdot \mathbf{e}_{i})\right)^{2} + J_{0i}^{2}} \ . \tag{11}$$

Using (11), the single-particle free energy of 2LS may be written as:

$$F_{i} = -k_{B}T \ln\left(2\cosh\left(\frac{U_{i}}{2k_{B}T}\right)\right).$$
(12)

The expression for 2LS polarization may be obtained by differentiation of the free energy (12) with respect to the electric field strength (see e.g. [15]):

$$\mathbf{p}_i = -\frac{\partial F_i}{\partial \mathbf{e}_i},\tag{13}$$

or in the explicit form:

$$\mathbf{p}_{i} = \frac{\mathbf{d}_{i} (\Delta_{0i} + 2(\mathbf{e}_{i} \cdot \mathbf{d}_{i}))}{U_{i}} \tanh\left(\frac{U_{i}}{2k_{B}T}\right).$$
(14)

Then the expression for thermodynamic average of the electric field strength, induced by the dipoles of neighboring 2LS at the site  $\mathbf{r}_i$  has the form:

$$\mathbf{e}_{i} = \sum_{j \neq i} \frac{b}{r_{ij}^{3}} \left[ \mathbf{p}_{j} - 3 \left( \mathbf{p}_{j} \cdot \hat{\mathbf{r}}_{ij} \right) \hat{\mathbf{r}}_{ij} \right].$$
(15)

Here  $r_{ij}$  and  $\hat{\mathbf{r}}_{ij}$  denote the distance between 2LS *i* and *j* and the unit radius-vector between them respectively;  $b = 1/\varepsilon_0 \varepsilon_m$  stands for the constant of Coulomb interaction in a given medium.

Suppose that 2LS coordinates are distributed over the volume V randomly and independently. Then the Nparticle 2LS coordinate distribution function can be represented as:

$$\Gamma^{N}(\{\mathbf{r}\}) = V^{-N} \tag{16}$$

and the normalized to unity *N*-particle distribution function of dipole moments, potential asymmetries and tunneling matrix elements has the form:

$$P_{0 norm}^{N}(\{\mathbf{d}, \Delta_{0}, J\}) = \left(\frac{\overline{P}}{4\pi Jn}\delta\left(|\mathbf{d}| - \mathbf{d}\right)\right)^{N}, \qquad (17)$$

where the factor of  $4\pi$  in the denominator means that the vectors **d**, which have equal absolute values *d*, have a uniform angular distribution.

Given the definite values of parameters of all the neighboring 2LS  $\{\mathbf{e}, \mathbf{d}, \mathbf{r}, \Delta_0, J\}$ , the induced field  $\mathbf{e}_0(\{\mathbf{e}, \mathbf{d}, \mathbf{r}, \Delta_0, J\})$  at the site  $\mathbf{r}_0$  is a definite value and may be calculated with the formula (15).

In this case the distribution function of induced fields has the form:

$$f_0(\mathbf{e}) = \delta \left( \mathbf{e} - \sum_{j \neq 0} \frac{b}{r_{0j}^3} \left[ \mathbf{p}_j - 3 \left( \mathbf{p}_j \cdot \hat{\mathbf{r}}_{0j} \right) \hat{\mathbf{r}}_{0j} \right] \right).$$
(18)

To calculate the self-consistent (averaged over the 2LS ensemble) distribution function of induced random fields  $f(\mathbf{e})$  one has to take into account that at transition between different 2LS the parameters  $\{\mathbf{e}, \mathbf{d}, \mathbf{r}, \Delta_0, J\}$  of neighboring 2LS change as random values, obeying the distribution function:

$$P(\lbrace \mathbf{e}, \mathbf{d}, \mathbf{r}, \Delta_0, J \rbrace) = \Gamma^N(\lbrace \mathbf{r} \rbrace) P_0^N_{norm}(\lbrace \mathbf{d}, \Delta_0, J \rbrace)(f(\mathbf{e}))^N,$$
(19)

where  $f(\mathbf{e})$  is the sought distribution function of induced mean random fields.

Then, by averaging Eq. (18) over the distribution function (19) and also applying the standard representation of Dirac  $\delta$  -function in the form of Fourier integral

$$\delta(\mathbf{x}) = \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} \exp(i\mathbf{x} \cdot \boldsymbol{\rho}) d\boldsymbol{\rho} ,$$

one obtains an integral equation for the self-consistent mean random field distribution function:

$$f(\mathbf{e}) = (2\pi)^{-3} \int_{(\mathbf{p})} d\mathbf{p} \cdot \exp(i\mathbf{p} \cdot \mathbf{e}) \left( \frac{\overline{P}}{4\pi V n} \int_{V} d\mathbf{r} \int_{(\mathbf{d})} d\mathbf{d} \delta \left( |\mathbf{d}| - d \right)^{\Delta_{\max}} \int_{0}^{J_{\max}} d\Delta_{0} \int_{J_{\min}}^{J_{\max}} \frac{dJ}{J} \int_{(\mathbf{e}')} d\mathbf{e}' \exp\left( -i\frac{b}{r^{3}} \left[ (\mathbf{p} \cdot \mathbf{p}) - 3(\mathbf{p} \cdot \hat{\mathbf{r}}) (\mathbf{p} \cdot \hat{\mathbf{r}}) \right] \right) \cdot f(\mathbf{e}') \right)^{N}.$$
(20)

The procedure of obtaining Eq. (20) from Eq. (18) is called the mean random field (MRF) approximation. Consider Eq. (20) in the form:

$$f(\mathbf{e}) = (2\pi)^{-3} \int_{(\mathbf{\rho})} d\mathbf{\rho} \cdot \exp(i\mathbf{\rho} \cdot \mathbf{e}) \left(1 - \frac{N(\mathbf{\rho})}{N}\right)^{N} , \qquad (21)$$

where

$$N(\mathbf{p}) = \frac{\overline{P}}{4\pi} \int_{V} d\mathbf{r} \int_{(\mathbf{d})} d\mathbf{d}\delta \left( |\mathbf{d}| - d \right) \int_{0}^{\Delta_{\max}} d\Delta_{0} \int_{J_{\min}}^{J_{\max}} \frac{dJ}{J_{(\mathbf{e}')}} \int_{(\mathbf{e}')} d\mathbf{e}' \left( 1 - \exp\left(-i\frac{b}{r^{3}} \left[ (\mathbf{p} \cdot \mathbf{p}) - 3(\mathbf{p} \cdot \hat{\mathbf{r}})(\mathbf{p} \cdot \hat{\mathbf{r}}) \right] \right) \right) \cdot f(\mathbf{e}') .$$
(22)

Assume  $\rho$  to be the direction of axis *z*. Let  $\theta$ ,  $\theta'$ ,  $\theta''$  be the angles between **r** and  $\rho$ , **p** and  $\rho$ , **p** and **r** respectively.

Then, according to [1], the angles  $\theta, \theta', \theta''$  obey the relation:

$$\cos\theta'' = \cos\theta \cos\theta' + \sin\theta \sin\theta' \cos(\varphi - \varphi').$$
(23)  
Let

$$F(\theta, \theta', \phi - \phi') = -\frac{1}{2} [(1 + 3\cos 2\theta)\cos\theta' + 3\sin 2\theta\sin\theta'\cos(\phi - \phi')].$$
(24)

We introduce the new variables:

$$z = \left| F(\theta, \theta', \varphi - \varphi') \right| p b \rho \cdot r^{-3}, \qquad (25a)$$

$$z_{1} = \left| F(\theta, \theta', \phi - \phi') \right| bp \rho \cdot R_{1}^{-3}, \qquad (25b)$$

$$z_0 = \left| F(\theta, \theta', \varphi - \varphi') \right| bp \rho \cdot R_0^{-3}.$$
(25c)

Here  $R_0$  is the minimal distance allowed between 2LS,  $R_1$  satisfies  $V = 4/3\pi R_1^3$ .

Then, using (23) - (25), one obtains from (22):

$$N(\mathbf{p}) = \frac{\overline{P}b\rho}{12\pi} \int_{-1}^{1} d\cos\theta \int_{0}^{2\pi} d\phi \int_{-1}^{1} d\cos\theta' \int_{0}^{2\pi} d\phi' \int_{0}^{\Delta_{\max}} d\Delta_{0} \int_{J_{\min}}^{J_{\max}} \frac{dJ}{J} \int_{(\mathbf{e})} d\mathbf{e}' \int_{z_{1}}^{z_{0}} dz \left(\frac{1-\cos z+i \operatorname{sgn}(F) \sin z}{z^{2}}\right) \times \left|F(\theta, \theta', \phi - \phi')\right| p(\Delta_{0} + (\mathbf{e}' \cdot \mathbf{d}), J) f(\mathbf{e}').$$

$$(26)$$

Since

$$\int_{0}^{\pi} \sin\theta d\theta \int_{0}^{2\pi} d\phi \left| F(\theta, \theta', \phi - \phi') \right| \cdot \operatorname{sgn}(F) = 0, \qquad (27)$$

and

$$\lim_{z_1 \to 0} \int_{z_1}^{z_0} \frac{\sin z}{z^2} dz \sim -\ln z_1 \sim \ln R_1 \to \infty, \qquad (28)$$

the value of  $\text{Im} N(\mathbf{p})$  in Eq. (26) is ambiguous, depending on the order of integration. If one first integrates over the angles, and then allows  $R_1 \rightarrow \infty$ , then  $\text{Im} N(\mathbf{p}) = 0$ , in the opposite case  $\text{Im} N(\mathbf{p}) \neq 0$ . We consider the next physical reasons. The value of integral (27) may be considered (neglecting the constant factor) as an average value of function (24) with respect to the arguments  $(\theta, \phi)$ . Consider an ensemble of finite number *N* of 2LS. For this ensemble the condition  $\lim_{N \to \infty} N^{-1} \sum_{i=1}^{N} F(\theta_i, \theta'_i, \phi_i - \phi'_i) = 0$  will hold. And the mean square fluctuation of this value over the ensemble will be

$$\sqrt{\frac{1}{N^2}\sum_{i=1}^N F(\theta_i, \theta_i', \varphi_i - \varphi_i')}\sum_{j=1}^N F(\theta_j, \theta_j', \varphi_j - \varphi_j') \sim \frac{1}{\sqrt{N}} \sim \frac{1}{R_1^{\frac{3}{2}}} \cdot$$

Taking this value as an upper limit of (27) and multiplying it by (28), one obtains in the limit  $R_1 \rightarrow \infty$ zero. That is why Im  $N(\mathbf{p}) = 0$ .

Now we let  $V \to \infty$ ,  $N \to \infty$ . Taking into account that  $\lim_{v \to \infty} z_1 = 0$ , we obtain from Eq. (21)

$$f(\mathbf{e}) = (2\pi)^{-3} \int df \, \ddot{\mathbf{z}} \exp(if \, \ddot{\mathbf{z}} \mathbf{e})$$

$$\times \exp\left(-\frac{\rho b}{12\pi} \int_{(\mathbf{e}')} d\mathbf{e}' f(\mathbf{e}') \langle p(\mathbf{e}') \rangle \int_{0}^{\pi} \sin\theta d\theta \int_{0}^{2\pi} d\phi \int_{0}^{\pi} \sin\theta' d\theta' \int_{0}^{2\pi} d\phi' |F(\theta, \theta', \phi - \phi')| \int_{0}^{\rho p(\mathbf{e}')bn_{0} \cdot |F|} \left(\frac{1 - \cos z}{z^{2}}\right) dz\right),$$
(29)

where  $n_0 = R_0^{-3}$  and

$$\left\langle p(\mathbf{e}')\right\rangle = \overline{P}d \int_{0}^{\Delta_{\max}} \frac{dJ}{J} \frac{\left|\Delta_{0} + e'd\cos\Theta\right|}{\sqrt{\left(\Delta_{0} + e'd\cos\Theta\right)^{2} + J^{2}}} \tanh\left(\frac{\sqrt{\left(\Delta_{0} + e'd\cos\Theta\right)^{2} + J^{2}}}{2k_{B}T}\right). \tag{30}$$

Here  $\vartheta$  is an angle between  $\mathbf{e}'$  and  $\mathbf{d}$ . Let us introduce the next notation:

$$g(t) = \int_{0}^{t} \frac{1 - \cos z}{z^{2}} dz = \frac{\cos t - 1}{t} + \sin t , \qquad (31)$$

where we denote  $\sin t \equiv \int_{0}^{t} \frac{\sin y}{y} dy$ .

As the next approximation we substitute the argument of function g in Eq. (29) by infinity:

$$g(\rho p(\mathbf{e}')bn_0 \cdot |F|) \to g(\infty) = \frac{\pi}{2}.$$
(32)

This is reasonable for  $\frac{p(\mathbf{e}')n_0}{\langle p(\mathbf{e}')\rangle} \sim \frac{n_0}{n} >> 1$ , since

function g in Eq. (31) significantly depends on its argument only in the vicinity of zero and at  $\rho > (bn_0 p(\mathbf{e}')|F|)^{-1}$  is close to its limit value  $g(\infty) = \pi/2$ . Approximation (32) fails at  $\rho < (bn_0 p(\mathbf{e}')|F|)^{-1}$ , i.e. at the field strength  $e > bn_0 p(\mathbf{e}')|F|$ , which occurs for the close  $(r \sim R_0)$  positions of 2LS. In this way, by using (32), we neglect such configurations.

Then we introduce notations:

$$\langle F \rangle = \frac{1}{4\pi} \int_{0}^{\pi} d\theta' \sin\theta' \int_{0}^{2\pi} d\phi' \int_{0}^{\pi} d\theta \sin\theta \int_{0}^{2\pi} d\phi |F(\theta, \theta', \phi - \phi')| \quad (33)$$

and

$$D(T) = \frac{\pi}{6} b \langle F \rangle \int_{(\mathbf{e}')} f(\mathbf{e}') \langle p(\mathbf{e}') \rangle d\mathbf{e}' .$$
(34)

It is worth noting that, though the direction of vector **p** may differ from that of **d**  $(\mathbf{p} \uparrow \downarrow \mathbf{d})$  when

 $\Delta_0 + (\mathbf{d} \cdot \mathbf{e}) < 0 \text{ for a given 2LS and, consequently, the spatial distribution of vectors$ **p**may not, in principle, be isotropic, as it (by the model assumption) does for vectors**d** $, it nevertheless may be, with a good accuracy, taken to be isotropic, since the result of integration over <math>\theta', \phi'$  in Eq. (33) weakly depends on the type of distribution over these variables because  $\langle F(\theta') \rangle = \int_{0}^{\pi} d\theta \sin\theta \int_{0}^{2\pi} d\phi |F(\theta, \theta', \phi - \phi')|$  weakly depends on  $\theta'$  [1].

Then, using Eqs. (30)-(34), and performing integration over  $\rho$ , one is able to rewrite Eq. (29) in the form:

$$f(\mathbf{e}) = \frac{1}{\pi^2} \frac{D(T)}{\left(e^2 + D^2(T)\right)^2} \,. \tag{35}$$

Eq. (35) is the sought distribution function of induced mean random field **e**. Since it depends only on the absolute value of **e**, the distribution obtained is spherically symmetric (isotropic).

From Eq. (35) one can see that the value D(T) plays a role of characteristic width of distribution of induced mean random field and is a measure of dipole interaction in 2LS ensemble at a given temperature.



Fig. 1. The plot of D(T) at  $d = 10^{-29.5} \text{Q} \cdot \text{m}$ ,  $J_{\text{min}} = 10^{-6} \text{ K}$ ,  $J_{\text{max}} = 1 \text{ K}$  and  $\overline{P}\Delta_{\text{max}} = 10^{22} \text{ m}^{-3}$ 

The plot of interaction strength D(T) at two different

sets of values  $(\overline{P}, \Delta_{\max})$ , such as  $\overline{P}\Delta_{\max}$  = const (which corresponds to the constant volume density of 2LS, see Eq. (6)), is given in Fig. 1:

From Fig. 1 one can see that the temperature of cooperativity onset strongly depends on the value of W potential asymmetry dispersion in the 2LS ensemble. And the low-temperature saturation value of interaction strength is mainly determined by the volume concentration of dipoles, being comparatively weakly sensitive to the W potentials' asymmetries.

From Eq. (35) it is possible to obtain the distribution function of the mean random field projections  $e_z$  on the arbitrary chosen axis z:

$$f(e_z) = \frac{1}{\pi} \frac{D(T)}{\left(e_z^2 + D^2(T)\right)}.$$
 (36)

#### **3. INTERACTION-MODIFIED DOS**

Interaction in the 2LS ensemble should lead to the change of its density of states (DOS) (4).

We shall calculate the 2LS DOS (4), modified by the interaction in the mean random field approximation using the MRF projection distribution function Eq. (36), calculated in the previous section.

The normalized to unity one-particle DOS for noninteracting 2LS (4) in the limit  $N \rightarrow \infty$  can be represented as:

$$P_{0 norm}^{1}(\Delta, \lambda) = P_{0}^{1}(\Delta, \lambda) \cdot (\Delta_{\max} \cdot (\lambda_{\max} - \lambda_{\min}))^{-1} = \overline{P} N^{-2} \sum_{j=1}^{N} \delta(\Delta - \Delta_{j}) \sum_{k=1}^{N} \delta(\lambda - \lambda_{k}).$$
(37)

To account for the interaction, one should consider the additional induced asymmetry of the double-well potential  $d \cdot e_z$ , obeying the distribution function (36). Then, by analogy with (37), one obtains:

$$\widetilde{P}^{1}_{norm}(\Delta,\lambda,T) = \overline{P}N^{-2}\sum_{j=1-\infty}^{N} \delta\left(\Delta - \Delta_{0j} - d \cdot e_{zj}\right) \cdot f\left(e_{zj},T\right) de_{zj}\sum_{k=1}^{N} \delta\left(\lambda - \lambda_{k}\right) = \overline{P}\left(\Delta_{\max} \cdot (\lambda_{\max} - \lambda_{\min})\right)^{-1} \int_{-\frac{\Delta_{\max}}{2d}}^{\frac{\Delta_{\max}}{2}} f\left(\frac{\Delta - \frac{\Delta_{\max}}{2} - \Delta_{0j}}{d}\right) d\left(\frac{\Delta_{0j}}{d}\right) \int_{-\frac{\lambda_{\max} - \lambda_{\min}}{2}}^{\frac{\lambda_{\max} - \lambda_{\min}}{2}} \delta\left(\lambda - \lambda_{\min} - \frac{\lambda_{\max} - \lambda_{\min}}{2} - \lambda_{k}\right) d\lambda_{k} = (38)$$

$$\overline{P}\left(\pi\Delta_{\max} \cdot (\lambda_{\max} - \lambda_{\min})\right)^{-1} \cdot \left(\arctan\left(\frac{\Delta}{d \cdot D(T)}\right) - \arctan\left(\frac{\Delta - \Delta_{\max}}{d \cdot D(T)}\right)\right),$$

or, after transformation to variables (U,J):

$$\widetilde{P}^{1}_{norm}(U,J,T) = \frac{\overline{P}}{\pi \Delta_{\max} \cdot (\lambda_{\max} - \lambda_{\min})} \cdot \frac{U}{J\sqrt{U^{2} - J^{2}}} \cdot \left(\arctan\left(\frac{\sqrt{U^{2} - J^{2}} + \Delta_{\max}}{d \cdot D(T)}\right) - \arctan\left(\frac{\sqrt{U^{2} - J^{2}} - \Delta_{\max}}{d \cdot D(T)}\right)\right). (39)$$

The plot of 2LS DOS, given by Eq. (38), for two different values of interaction strength  $d \cdot D(T)$ , is shown in Fig. 2. Due to the "smearing" by the induced random fields, the values of asymmetries of W potentials allowed belong now to the interval  $(-\infty;\infty)$ . This

result can be qualitatively understood in the next way. The distribution function of  $\Delta$ 's for noninteracting 2LS is a step, which begins at  $\Delta = 0$  and ends at  $\Delta = \Delta_{max}$ .

Including the interaction between 2LS leads to the smearing of the step's edges by the characteristic value

 $d \cdot D(T)$ . This causes the emergence of non-zero DOS at  $\Delta < 0$  (it corresponds to the DOS of W potentials which change their asymmetry sign due to interaction) and at  $\Delta > \Delta_{\text{max}}$ , and within the range  $0 \le \Delta \le \Delta_{\text{max}}$  DOS decreases due to the normalization condition Eq. (6).



Fig. 2. Plot of 2LS DOS vs.  $\Delta$ , Eq. (38), in the limits of high  $(d \cdot D(\infty) = 0)$  and low  $(d \cdot D(0) = 0.057 \text{ K})$  temperature

From Eq. (39) one can see that the 2LS excitation spectrum is practically insensitive to the interaction in the MRF approach, provided that

$$\Delta_{\max} - \sqrt{U^2 - J^2} \ll d \cdot D(T).$$
<sup>(40)</sup>

The condition given by Eq. (40) is satisfied (for the standard value  $\Delta_{\text{max}} \approx 1 \text{ K}$ ) for any thermal 2LS in the temperature range  $T \leq 100 \text{ mK}$ , where the discrepancies with the standard 2LS model are found.

So, we conclude that the ultra-low-temperature deviations of some physical properties of glasses from predictions of the standard 2LS model can not be accounted for by including mutual dipole interaction, at least in the static MRF approach.

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## ПЛОТНОСТЬ СОСТОЯНИЙ ВЗАИМОДЕЙСТВУЮЩИХ ДВУХУРОВНЕВЫХ СИСТЕМ В АМОРФНЫХ ТВЕРДЫХ ТЕЛАХ В ПРИБЛИЖЕНИИ СЛУЧАЙНОГО СРЕДНЕГО ПОЛЯ

## А.А. Борисенко

Метод случайного среднего поля [1, 2] обобщен для случайных (с определенной функцией распределения) величин туннельных матричных элементов и асимметрий двухямных потенциалов и применен для учета дипольного взаимодействия между двухуровневыми системами в стеклах. Найденная функция распределения случайного среднего поля использована для расчета модифицированной взаимодействием плотности состояний ансамбля двухуровневых систем. При использовании реалистичных величин феноменологических параметров найденная поправка к низкоэнергетической плотности состояний является весьма малой.

## ЩІЛЬНІСТЬ СТАНІВ ДВОРІВНЕВИХ СИСТЕМ, ЩО ВЗАЄМОДІЮТЬ В АМОРФНИХ ТВЕРДИХ ТІЛАХ В НАБЛИЖЕННІ ВИПАДКОВОГО СЕРЕДНЬОГО ПОЛЯ

#### О.О. Борисенко

Метод випадкового середнього поля [1, 2] узагальнено для випадкових (з певною функцією розподілу) величин тунельних матричних елементів та асиметрій двоямних потенціалів та застосовано для врахування дипольної взаємодії між дворівневими системами в стеклах. Знайдену функцію розподілу випадкового середнього поля застосовано для розрахунку модифікованої взаємодією щільності станів ансамблю дворівневих систем. При використанні реалістичних величин феноменологічних параметрів знайдена поправка до низькоенергетичної щільності станів є вельми малою.