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# On the nature of the universal properties of amorphous solids

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## Abstract

It is shown that many center excitations are responsible for the universal low energy spectral properties in an arbitrary ensemble of defect centers with an internal degree of freedom. Universality means a quasiuniform distribution of the energy and the logarithm of the tunneling amplitude together with a disappearance of the dependence on the primary defect parameters.

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1. The anomalous low-temperature properties of quite different amorphous solids demonstrate a remarkable universal behaviour. These properties are well described by the known tunneling model [1] based on an ensemble of two level systems (TLS) randomly distributed. The assumptions of the uniform TLS distribution of the level shifts  $\Delta$  and the logarithm of the tunneling amplitude  $\Delta_0$  were decisive. The first assumption seems quite natural. However the uniform distribution of  $\ln(\Delta_0)$  in the broad interval of the change of this parameter has no strong grounds in the general case. The quantitative resemblance of the properties observed in glasses also needs to be explained.

We believe that the universality of the low energy spectral properties of the amorphous solids results from the many body interaction of the defect centers with an internal degree of freedom. An inevitable appearance of these centers is linked to the local

breakdown of the spatial degeneracy. This leads to the arising of a primary system of double-well centers which, in general, should not manifest the universal spectral properties.

The analysis of the low energy spectral properties of amorphous solids caused by the interaction of the primary defect centers and the clusters of these centers is the purpose of this Letter. It will be shown that the role of many center excitations (MCE) increases with decreasing energy. The spectral properties of these MCE are independent of primary defect parameters and demonstrate practically the uniform distribution of  $\Delta$  and  $\ln(\Delta_0)$ .

It will be important that the interaction between defect centers falls off with distance as  $1/R^3$ . This interaction law is known both in amorphous insulators and metals. One should notice that recently Yu and Leggett [2] put forward the hypothesis that the  $1/R^3$  law for the interaction between defects can be

responsible for the universality of the amorphous solid properties. However the question about the nature of excitations remained open.

2. Consider an amorphous medium with double-well centers distributed randomly in space and having an arbitrary distribution of parameters. This system can be described by the standard pseudospin Hamiltonian

$$\hat{H} = - \sum_i \omega_i S_i^z - \frac{1}{2} \sum_{ij} U_{ij} S_i^z S_j^z - \sum_i \Delta_{0i} S_i^x. \quad (1)$$

Here  $\omega_i$  is a level shift of the isolated defect center  $i$ , which is distributed in the interval  $(-W/2, W/2)$ . The interaction between the centers is defined as  $U_{ij} = u_{ij}/R_{ij}^3$ . We suppose that the constants  $u_{ij}$  are uncorrelated for different pairs of centers, and their average value is zero. The average modulus  $\langle |u_{ij}| \rangle = U_0$  gives the characteristic interaction parameter. The tunneling amplitudes of the primary centers have the scale  $\Delta_{0*}$ . Let us assume that

$$\Delta_{0*} \ll U_0 n \ll W, \quad (2)$$

where  $n$  is the density of centers and therefore  $U_0 n$  is the interaction between centers on an average distance. This hierarchy of energies allows us to investigate the excitation spectrum of the Hamiltonian (1) neglecting first the tunneling. Then the tunneling will be included in the framework of the perturbation theory in  $\Delta_{0*}/W$ .

We start with the consideration of the density of states  $P(\Delta)$  neglecting the last term in Eq. (1). At zero temperature the system should be in the ground state. This means that the energies of all MCE should be positive. Such a stability requirement introduces a system of limitations which can essentially influence the density of the low energy excitations in the case of a long-range interaction. This was first demonstrated in the analysis of the Coulomb gap problem in doped semiconductors [3,4].

For the Coulomb interaction those requirements lead to the Coulomb gap in doped semiconductors [3]. For the interaction  $1/R^3$  the stability conditions turn out to be significant and they should be taken into account [4,2].

For the single particle excitations the stability requirements have the form

$$\Delta_i = \omega_i + \sum_i U_{ij} S_j^z > 0 \quad (3)$$

(it is conventionally assumed that in the ground state  $S_i^z = \frac{1}{2}$ ). For MCE including  $n$  centers the stability conditions are reduced to the inequalities

$$\Delta_{i_1, i_2, \dots, i_n} = \sum_{k=1}^n \Delta_{i_k} - \frac{1}{2} \sum_{kl} U_{i_k i_l} > 0. \quad (4)$$

3. Let us at first restrict the range of the interaction domain by the radius  $R_0$ , limited enough to consider the intercenter interaction effectively as a weak perturbation, and calculate the decrease of the density of the single particle excitations (3) caused by the stability requirements for pair excitations (4),

$$P_1(\Delta) = \frac{1}{\Omega} \sum_i \left\langle \delta(\Delta - \Delta_i) \prod_j \Theta(\Delta_{ij}) \right\rangle. \quad (5)$$

Here  $\Omega$  is the system volume. Replacing  $\Theta(\Delta_{ij})$  by  $1 - \Theta(-\Delta_{ij})$  and taking into account that this expression is not equal to unity only in a small part of the phase space one can get

$$P_1(\Delta) \sim P_0 \left( 1 - P_0 \int dR_{12} \int d\Delta_1 \times \left\langle \Theta(u/R_{12}^3 - \Delta_1 - \Delta) \right\rangle_u \Theta(R_0 - R_{12}) \right), \quad (6)$$

where  $\langle \dots \rangle_u$  denotes averaging over  $u$ . It was assumed here that the density of states for primary centers  $P(\Delta)$  has no a singularity at  $\Delta = 0$ . This allows one to replace  $P(\Delta_1)$  with  $P_0 \equiv P(0) \approx n/W$  because the main contribution to the integral (6) comes from small values of  $\Delta_1 < U_0/R_{12}^3$ .

We are interested in the density of states at the low energy

$$\Delta < U_0/R_0^3 \ll W, \quad (7)$$

where  $P_1$  proves to be independent of energy with logarithmic accuracy. Taking into account that in Eq. (6)  $u > 0$  we find

$$P_1(\Delta) \approx P_0 (1 - 2\chi\xi), \quad (8)$$

$$\chi = \pi P_0 U_0, \quad \xi = \ln(R_0/R_{\min}) \gg 1. \quad (9)$$

We assume with logarithmic accuracy that  $R_{\min}$  is defined as  $U_0/R_{\min}^3 \approx W$ .

The decrease of the density of single particle excitations (8) is accompanied by the growth of the density of many center excitations. For example, a pair excitation with low energy may arise for two centers with energy  $\Delta_{ij} = \Delta_i + \Delta_j - U_{ij} \ll \Delta_i$ ,  $\Delta_j \approx U_{ij}$ . This is already the excitation of a coupled pair cluster with only two available states which are the ground state  $S_i^z = S_j^z = \frac{1}{2}$  and the excited state  $S_i^z = S_j^z = -\frac{1}{2}$ . Let us find the contribution of pair excitations to the low energy density of states. In the leading approximation (as in Eq. (8)) we have

$$P_2(\Delta) = \frac{1}{2} P_0^2 \int d\mathbf{R}_{ij} \int d\Delta_i \int d\Delta_j \times \left\langle \delta \left( \Delta - \Delta_i - \Delta_j + \frac{u}{R_{ij}^3} \right) \right\rangle_u \Theta(R_0 - R_{ij}). \quad (10)$$

Taking into account condition (7) we find

$$P_2(\Delta) \approx P_0 \chi \xi. \quad (11)$$

From the results (8) and (11) one can easily conclude that the parameter of the perturbation theory is the product  $t = \chi \xi$ . The contribution of the primary centers decreases with increasing  $t$  and pair excitations (and, generally, MCE with  $P_n \sim t^{n-1}$ ) become significant.

4. Assuming that the inequality (2) is valid we have  $\chi \ll 1$ . At the same time the effective interaction constant increases logarithmically with  $R_0$ . If the system size is large enough then the interaction becomes strong at least at  $T \rightarrow 0$ . This is the direct consequence of the interaction law  $1/R^3$ . Under these conditions the renormalization group approach, based on the subsequent increase of the interaction range ( $R_0$ ) can be used to define the density of states  $P_n(\Delta, R_0)$  (for  $n$ -clusters, containing  $n$  initial defect centers). This approach is analogous to the one developed by Levitov [5] who analyzed the localization problem in the case of dipole–dipole interaction.

Suppose first that  $T = 0$ . The appearance with large probability of many-center excitations requires the condition  $t \sim 1$ . Since  $\chi \ll 1$  the corresponding size of the interaction range  $R^*$  is exponentially large;  $R^* \approx R_{\min} e^{1/\chi}$ . This is the scale of the dis-

tance where an arbitrary cluster finds another one to form a more complex cluster.

Let us assume that the interaction domain is limited by the radius  $R_1 \gg R_{\min}$ . Consider the evolution of the density of states when increasing the cutoff radius up to  $R_2$ , obeying the inequality  $1 \ll R_2/R_1 \ll e^{1/\chi}$ . Then  $\delta t = \chi \delta \xi = \chi \ln(R_2/R_1) \ll 1$  and the probability to form new coupled clusters is small (cf. Eq. (11)). New coupled clusters statistically occur at distances  $R \gg R_1$ . This allows us to consider the clusters as point-like objects. The shift of energy to the interval  $\Delta \sim U_0/R_2^3$  predetermines that the energies of the collective excitations of coupling clusters should be of the same order. Since other intra-cluster excitations in reality have energies  $\Delta \gg U_0/R_1^3$ , these clusters enter more complex formations as single objects. The probability of the appearance of a coupled cluster from three or more clusters will be a factor  $\chi \ln(R_2/R_1)$  smaller than two-cluster formation. Therefore, when calculating  $P_n(\Delta, R_1) - P_n(\Delta, R_2)$  we consider only pair unifications.

$P_n$  decreases with increasing interaction radius, because the number of unstable configurations increases (cf. Eq. (8)). On the other hand,  $P_n$  increases due to the unification of pairs of smaller clusters. The structure of both contributions is analogous to Eqs. (5) and (10) respectively and the general equation reads

$$P_n(\Delta, R_2) = \left\langle P_n(\Delta, R_1) \prod_{k,j} \Theta(\Delta_k + \Delta - u_{kn}/R_j^3) \right\rangle + \frac{1}{2} \sum_{k=1}^{n-1} \sum_j \left\langle \delta \left( \Delta - \Delta_k - \Delta_{n-k} + u_{k,n-k}/R_j^3 \right) \right\rangle. \quad (12)$$

Here  $\Delta_k$  is the excitation energy for the  $k$ th cluster;  $u_{km}$  is the coupling constant of the interaction between clusters  $k$  and  $m$ . The prime in the sum and the product over  $j$  means the limitation  $R_1 < R_j < R_2$ . For a small excitation energy  $\Delta < U_0/R_2^3$  the r.h.s. in Eq. (12) can be calculated in the limit  $\Delta \rightarrow 0$ . Taking into account the small difference between  $\chi \ln(R_1)$  and  $\chi \ln(R_2)$  ( $\delta t \ll 1$ ) we can use the substitution  $P_k(0, R) \rightarrow P_k(0, R_1)$  in the r.h.s.

of Eq. (12). Then making transformations analogous to those made for transitions from Eqs. (5) and (10) to Eqs. (8) and (11), respectively, we find

$$\begin{aligned}
 P_n(0, R_2) &= P_n(0, R_1) - 2\pi P_n(0, R_1) \\
 &\times \sum_{k=1}^{\infty} \langle |u_{kn}| \rangle P_k(0, R_1) \ln(R_2/R_1) \\
 &+ \pi \sum_{k=1}^{n-1} \langle |u_{k,n-k}| \rangle P_k(0, R_1) P_{n-k}(0, R_1) \\
 &\times \ln(R_2/R_1). \tag{13}
 \end{aligned}$$

Since the density of states  $P_n$  changes insignificantly for the transition from  $R_1$  to  $R_2$  we can proceed to the differential form of this equation

$$\frac{\partial \tilde{P}_n}{\partial t} = -2\tilde{P}_n \sum_{k=1}^{\infty} b_{kn} \tilde{P}_k + \sum_{k=1}^{n-1} b_{k,n-k} \tilde{P}_k \tilde{P}_{n-k}. \tag{14}$$

Here we introduced the following notations:  $\tilde{P}_n = P_n(0, R)/P_0$ ;  $b_{km} = \langle |u_{km}| \rangle / U_0$ ;  $t = \chi \xi(R)$ ;  $\xi(R) = \ln(R/R_{\min})$ . Eq. (14) has the integral of motion

$$I_1 = \sum_{n=1}^{\infty} n \tilde{P}_n(t) = 1 \tag{15}$$

(at  $t = 0$ ,  $\tilde{P}_n = \delta_{n1}$ ).

Eventually, we have to find the solution of Eq. (14) at  $R = R_{\max}$ . The limiting radius  $R_{\max}$  is the maximal size of the space domain where a cluster can find another one to form the new entity. At finite temperature  $R_{\max} = R_T$  and  $R_T$  is defined as  $U_0/R_T^3 \approx T$  (at larger distances the interaction between clusters is less than  $T$  and their excitations are independent). When  $\Delta < T$  the functions  $P_n$  do not depend on  $\Delta$ . In the opposite case,  $R_{\max}$  effectively reduces to  $R_{\Delta}$ , which can be found from the relation  $U_0/R_{\Delta}^3 \approx \Delta$ . Thus the final solution with a logarithmic accuracy takes the form  $\tilde{P}_n(t_m)$ ,

$$t_m = \chi \ln(R_{\max}/R_{\min}), \quad R_{\max} = \min(R_T, R_{\Delta}). \tag{16}$$

Here we make a remark. If one omits in Eq. (14) all clusters with  $n > 1$  then the equation obtains the form

$$\frac{\partial \tilde{P}_1}{\partial t} = -2\tilde{P}_1^2,$$

with the simple solution

$$\begin{aligned}
 P_1(R_{\max}) &= \frac{P_0}{1 + 2t_m} \\
 &= \frac{P_0}{1 + 2\pi U_0 P_0 \ln(R_{\max}/R_{\min})}.
 \end{aligned}$$

This solution coincides at  $T = 0$  with the result obtained earlier for the single particle density of states (see Ref. [4]). In a simple model when the coefficients  $u_{kn} = \text{const} = U_0$  the solution of Eq. (14) can be found directly. In the limit  $t \gg 1$  it reads

$$P_n(R_{\max}) \approx \frac{P_0}{t_m^2} \exp(-n/t_m).$$

We see the decisive role of the many-center excitations.

5. The interaction between clusters, in general, depends on the number of centers in clusters. This interaction is defined by the sum of pair interactions between centers in different clusters. Since the distance between clusters is much larger than the size of clusters then  $u_{km} \approx \sum_{i \in k, j \in m} u_{ij}$ . If constants  $u_{ij}$  are non-correlated for different pairs and  $\langle u_{ij} \rangle = 0$ , then  $\langle |u_{km}| \rangle \approx U_0 k^{1/2} m^{1/2}$ . (17)

Such a situation takes place particularly in amorphous metals. Actually, the indirect interaction between centers (RKKY interaction) changes sign already over a distance of the order of the interatomic scale  $a$ , while the distance between the centers in clusters is much larger than  $a$ . In amorphous dielectrics the validity of Eq. (17) needs a special analysis. However, it can be approximately justified by the large number (in general  $z = 6$ ) of independent components of the stress tensor for each primary center which defines the coupling between centers.

Consider the asymptotic solution of Eq. (14) with coefficients (17) at  $t \gg 1$ . It is easy to show that both  $\tilde{P}_1$  and the total density  $\tilde{P}(t) = \sum_k \tilde{P}_k(t)$  decrease with increasing “time”  $t$ . However the functions  $\tilde{P}_n(0) = 0$  at  $n > 1$ . They increase at small  $t$  as  $t^{n-1}$ . Therefore the function  $\tilde{P}_n(t)$  at some  $t_*(n)$  goes through a maximum and then decreases with increasing  $t$ . The inverse function  $n_*(t)$  describes the position of the wavefront, rapidly spreading to a large  $n$  with increasing  $t$ .

The analysis of Eq. (14) with coupling constants (17) (details will be published elsewhere) leads to a solution having the form

$$\tilde{P}_n(t) \approx 4 \times 10^{-2} \frac{1}{n^2 t} \ln(nt^\alpha), \quad \alpha \approx 0.4, \quad n < n_*. \quad (18)$$

It should be noted that the nonlinearity of Eq. (14) makes it possible to define the numerical coefficient in Eq. (18).

The conservation law of the first moment (15) can be used to estimate the wavefront position  $n_*(t)$ . Substituting the solution (18) into Eq. (15) and taking  $n_*(t)$  as the upper limit in the integral form of (15) we obtain with logarithmic accuracy

$$n_*(t) \approx \exp(\sqrt{50t}). \quad (19)$$

The numerical solution of Eq. (14) with coefficients (17) demonstrates clearly the exponential increasing of the wavefront position simultaneously with the dependence  $\tilde{P}_n(t)$  on  $n$  close to Eq. (18).

6. Let us now include into our consideration the intracenter tunneling in a primary set of defects (the last term in Eq. (1)). Suppose first that  $t < 1$ . Consider the dynamic properties of pairs of centers. The coherent amplitude connecting the excited state of a pair with its ground state is equal to

$$\Delta_{0ij} \approx \frac{1}{2} \frac{\Delta_{0i} \Delta_{0j}}{\Delta_i \Delta_j} |U_{ij}(R)|, \quad \Delta_{0i,j} < \Delta_{i,j}. \quad (20)$$

The distribution function of the parameters  $\Delta$  and  $\Delta_0$  which is the generalization of Eq. (10) can be written as

$$\begin{aligned} P_2(\Delta, \Delta_0) &= \frac{P_0^2}{2} \int d\Delta_{01} P'(\Delta_{01}) \int d\Delta_{02} P'(\Delta_{02}) \int d\Delta_1 \\ &\times \int d\Delta_2 \int d\mathbf{R}_{12} \langle \delta(\Delta - \Delta_{12}) \delta(\Delta_0 - \Delta_{012}) \rangle_u, \end{aligned} \quad (21)$$

where  $P'(\Delta_0)$  is the distribution of the tunneling amplitudes of the primary centers normalized to unity; the pair excitation energy  $\Delta_{ij}$  is defined by Eq. (4). The integration in Eq. (21) gives  $P_2(\Delta, \Delta_0) \approx P_{0\chi}/3\Delta_0$ . The tunneling amplitude of pairs  $\Delta_0$  in this expression is defined in the interval  $\Delta_{0*}^2/W <$

$\Delta_0 < \Delta_{0*}$ , where  $\Delta_{0*}$  is the characteristic scale for the distribution  $P'(\Delta_0)$ . Thus pair excitations already possess a uniform distribution of  $\ln(\Delta_0)$  at arbitrary  $P'(\Delta_0)$ . We will suppose that

$$\Delta_{0*} < W e^{-\eta/\chi}, \quad \eta \approx 1. \quad (22)$$

In this case at  $t_m \sim 1$  the tunneling amplitudes for pairs appears to be less than the effective interaction  $U_0/R_{\max}^3$ .

In general, each  $n$ -cluster has the definite coherent transition amplitude  $\Delta_{0n}$ . If this cluster results from the coupling of  $k$  and  $n - k$  clusters then  $\Delta_{0n}$  is defined by Eq. (20) with the replacement of  $\Delta_{0i}/\Delta_i$  and  $\Delta_{0j}/\Delta_j$  with  $\Delta_{0k}/\Delta_k$  and  $\Delta_{0n-k}/\Delta_{n-k}$ , respectively.

Analysis of Eq. (21) shows that the region  $\Delta_k \sim \Delta_{n-k} \sim |u_{k,n-k}|/R^3$  gives the main contribution to the integral. This allows us to write  $L_n \approx L_k + L_{n-k} + 3\xi_R$ , where  $L_k = \ln(\Delta_{0k}/W)$ . Continuing an analogous procedure for  $L_k$  and  $L_{n-k}$  we can approximately represent  $L_n$  through the primary defect tunneling amplitudes

$$L_n \approx nL_* + 3n/\chi, \quad L_* = \ln(\Delta_{0*}/W). \quad (23)$$

According to inequality (22) the second term in Eq. (23) can be neglected in comparison with the first one. Then using Eq. (18) and proceeding from the summation over  $n$  ( $n > 1$ ) to the integration we find the general distribution function at  $t_m \geq 1$ .

$$\begin{aligned} P(\Delta, \Delta_0) &= \int dn P_n(t_m) \delta(\Delta_0 - W e^{nL_*}) \\ &= 4 \times 10^{-2} \frac{P_0}{t_m} \frac{\ln(W/\Delta_{0*})}{\ln^2(W/\Delta_0)} \frac{1}{\Delta_0}, \end{aligned}$$

$$t_m = \chi \ln(R_{\max}/R_{\min}). \quad (24)$$

Here  $R_{\max}$  is defined according to Eq. (16) with the substitution  $\Delta \rightarrow \epsilon = \sqrt{\Delta_0^2 + \Delta^2}$ . The condition  $t > 1$  requires inequality (22) not only for  $\Delta_0$  but for  $\Delta$  and  $T$  as well.

7. The obtained distribution does not noticeably deviate from the uniform distribution of  $\ln(\Delta_0)$ . Since  $\chi/P_0$  does not depend on the distribution of primary centers we come to the important conclusion that the resulting distribution function is not dependent on the primary centers density. This demonstrates an

other significant aspect of the universality. It is interesting that the numerical factor in Eq. (24) predetermines also the quantitative scale of the distribution.

If one introduces the notation  $P(\Delta, \Delta_0) = P'/\Delta_0$ , then it is known that the dimensionless parameter  $\alpha = P'U_0$  has a rather universal value for quite different glasses (see Refs. [6,2]). It is remarkable that Eq. (24) predicts for this parameter a logarithmically weak dependence on the parameters of system and a numerical value close to the experimental value  $\sim 10^{-3}$ .

Thus the low energy spectral properties of MCE caused by the  $1/R^3$  law for the interaction between defect centers demonstrate a rather wide picture of universality: a quasiuniform distribution of  $\ln \Delta_0$  and  $\Delta$ ; the absence of the influence of the density and distribution of primary centers on the final distribution function; a quantitative relevance to the experimental data. The obtained results are in a favour of the hypothesis proposed in Ref. [2] about the principal role of the  $1/R^3$  interaction for the expla-

nation of the universal properties of amorphous solids.

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