Relaxation of two-level systems and sound absorption in metallic glasses

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A general theory of relaxation of two-level systems in an amorphous metal, with allowance for the tunneling-induced electron polaron effect, is developed. The anomalous behavior of the absorption of a low-frequency sound resulting from the transition to the superconducting state, which was observed in Refs. 1 and 2, is explained.

1. Recent experimental studies of the absorption of a low-frequency sound in metallic glasses in the normal and superconducting states[1,2] have shown that the interaction of two-level systems with conduction electrons is extremely nontrivial. At first glance, this experimental result contradicts the standard description of such systems, which is the principal assertion of these studies.

A meaningful analysis of the problem requires a suitable theory for the relaxation of two-level systems in amorphous metals, which goes beyond the scope of the existing simplified results (see the review by Black[3]). In an effort to develop such a theory, we will use the recently obtained general solution of the problem of tunneling of heavy particles in a metal[4] (below cited as I), where the electron polaron effect is important (see Refs. 5 and 6; a similar problem in the case of interaction with phonons was analyzed in detail in a review by Leggett *et al.*[7]). The results obtained for a two-well potential, which are general in nature, can be used to describe tunneling along an arbitrary collective coordinate with an effective heavy mass, without the knowledge of the true microscopic nature two-level systems.

2. Situated in a separate well for a time τ_i, a heavy "particle" forms a many-electron wave function which is generated by virtual electron-hole pairs with an energy in the range from $\nu_i = \tau_i^{-1}$ to $\sim \epsilon_F$. We see from I that if the "particle" is tunneled with a characteristic frequency ω, the excitations with an energy $\omega < \epsilon \ll \epsilon_F$ follow the particle adiabatically, causing a renormalization of the potential relief. The slow excitations, $\nu_i < \epsilon < \omega$, cannot keep track of the particle, and the wave function corresponding to them, which remains in the well, is responsible for the electron polaron effect. This function can be constructed as an eigenstate $\psi_n^{(i)}$ of a single-well Hamiltonian,

$$H^{(i)} = H_p^{(i)} + H_{el} + V^{(i)}, \qquad V^{(i)} = V_\omega^{(i)} - V_{\nu_i}^{(i)} \qquad (i = 1, 2), \tag{1}$$

where

$$V_\alpha^{(i)} = \sum_{\mathbf{k},\mathbf{k}',\sigma}^{\alpha} V_{\mathbf{k},\mathbf{k}'}^{(i)} \hat{a}_{\mathbf{k},\sigma}^{+} \hat{a}_{\mathbf{k}',\sigma} \tag{2}$$

is the interaction of the "particle" with electron-hole pairs with an energy $|\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'}| < \alpha$. In the $\psi_n^{(i)}$ representation, the effective Hamiltonian of the two-level system is

$$H_{eff} = {}^1/_2\xi\sigma_z + {}^1/_2\Delta_{coh}\sigma_x + {}^1/_2\widetilde{V}\sigma_z + {}^1/_2\Delta_0(\hat{\Lambda} - \langle\hat{\Lambda}\rangle)\sigma_x\,; \qquad \Delta_{coh} = \Delta_0\langle\hat{\Lambda}\rangle; \qquad \widetilde{V} = V^{(1)}_{\nu_1} - V^{(2)}_{\nu_2} \tag{3}$$

Here Δ_0 is the amplitude of the transition in the absence of interaction with electrons, ξ is the relative level shift in the wells ($\Delta_0, \xi \ll \omega$), and $\hat{\Lambda}$ is the polaron operator, whose matrix elements $\Lambda_{nm} = \langle\psi_n^{(1)}|\psi_m^{(2)}\rangle$ determine the overlap integral.

The infrared divergence characteristic of the electron polaron effect determines, in the limit $|\epsilon_k - \epsilon_{k'}| \to 0$, the peculiar behavior of the tunneling amplitude Δ_{coh} diagonal in the excitations. A direct determination of $\langle\hat{\Lambda}\rangle$, with allowance for the interaction cutoff in (1) at low frequencies, gives the following expression for the case $\xi = 0(\nu_1 = \nu_2 = \tau^{-1})$:

$$\Delta_{coh} = \Delta_0 \exp\left\{ -b \iint_{-\omega}^{\omega} d\epsilon d\epsilon' \frac{n_\epsilon(1-n_{\epsilon'})}{(\epsilon-\epsilon')^2}\Big(1 - \cos(\epsilon-\epsilon')\tau\Big)\right\}$$

$$= \Delta_0 \exp\left\{ -b\int_0^{\omega} \frac{dy}{y} \coth\frac{y}{2T}(1-\cos y\tau)\right\} = \widetilde{\Delta}_0(T)\exp\{-b\ln(\sinh\pi T\tau)\}; \tag{4}$$

$$\widetilde{\Delta}_0(T) = \Delta_0 \exp\{-b\ln{}^{\omega}/_{\pi T}\}; \qquad b = \rho^2(\epsilon_F)\overline{|V^{(1)}_{\mathbf{k}\mathbf{k}'} - V^{(2)}_{\mathbf{k}\mathbf{k}'}|^2} \tag{5}$$

In (4) we introduced the cutoff factor $1 - \cos(\epsilon - \epsilon')\tau$. Here the superior bar denotes averaging over the Fermi surface. The expression for b corresponds to the Born approximation in V. (If this approximation breaks down, but the scattering is determined by a single partial channel, we can establish a correlation between $b \leqslant 1/2$ and the corresponding phase of the electron scattering.[8]) At

$$\Omega_T\tau \gg 1, \qquad \Omega_T = 2\pi bT \tag{6}$$

the amplitude Δ_{coh} is exponentially small, $\Delta_{coh} \sim \exp(-\Omega_T\tau/2)$, and the coherent tunneling channel in (3) can generally be ignored. The dynamics of a two-level system in this case is determined by the last term in (3) and is descibed by the probability for the transition from well 1 to well 2 with excitation of the system [see Eq. (5.8) in I]:

$$W(\xi, T) = {}^1/_2 \frac{\widetilde{\Delta}_0^2(T)\Omega_T}{\xi^2 + \Omega_T^2}\sqrt{\pi}\,\frac{|\Gamma(1 + (\Omega_T + i\xi)/2\pi T)|^2}{\Gamma(1 + \Omega_T/2\pi T)\Gamma({}^1/_2 + \Omega_T/2\pi T)}\,e^{\xi/2T} \tag{7}$$

This relation is valid for any value of the parameters if

$$(\Omega_T, \xi)_{max} \gg \widetilde{\Delta}_0(T). \tag{8}$$

Determining from (7) the quantity $\tau^{-1} = W$, we find that $\Omega_T\tau \gg 1$ and that Δ_{coh} is indeed exponentially small. The last assertion is always valid, even when $\xi > \tilde{\Delta}_0 > T$, if inequality (8) holds.

The term with Δ_{coh} in (3) and the dissipation-free transition become important only when $(\Omega_T,\xi)_{max} < \tilde{\Delta}_0$. Since the lifetime of the particle in a separate well in this case is $\sim \Delta_{coh}^{-1}$, we find from (4) a self-consistent equation for determining Δ_{coh}

$$\Delta_{coh} \approx \Delta_0[\pi T/(\omega \sinh \pi T/\Delta_{coh})]^b; \quad \Delta_{coh}(T=0) \equiv \Delta_* \approx \Delta_0(\Delta_0/\omega)^{b/1-b} \tag{9}$$

The overlap integral $\langle\hat{\Lambda}\rangle$ has been erroneously linked to $\tilde{\Delta}_0(T)/\Delta_0$ and therefore it was assumed to increase with increasing T, in accordance with (5). According to (4) and (9), the actual behavior has nothing in common with this assertion.

3. The inverse relaxation time of a two-level system, γ, is determined, if condition (8) holds in the limit $\Delta_{coh} \to 0$, by probability (7), to which it is related by the simple relation

$$\gamma = (1 + \exp(-\xi/T))\, W(\xi, T) \tag{10}$$

To determine γ in the region where inequality (8) is violated, we assume that $b \ll 1$, leaving $b \ln \omega/\Delta_*$ arbitrary. We introduce an intermediate frequency $\Delta_* \ll \tilde{\omega} \ll \omega$, such that $b \ln \tilde{\omega}/\Delta_* \ll 1$. We replace the cutoff frequency ν_i in (1) by $\tilde{\omega}$ and likewise in the interaction $\tilde{V}$ in (3). If T, Ω_T, $\xi \ll \tilde{\omega}$, and if the relationship between these parameters and Δ_* is arbitrary, the amplitude

$$\Delta_{coh} \approx \Delta_0 \exp\{-b \ln {}^{\omega}/_{\tilde{\omega}}\} \approx \Delta_*$$

retains the value it has in (9). Here the interaction $\tilde{V}$ in (3) can be incorporated in accordance with perturbation theory, and the problem described by Hamiltonian (3) is isomorphic to the problem of tunneling relaxation of a two-level system as a result of interaction with the phonons, which was analyzed in Ref. 9. Using the results of Ref. 9 [see Eqs. (4.10) and (4.11)], we can immediately write the result in the form

$$\gamma = \Delta_*^2 \tilde{\Omega} / (\tilde{\epsilon}^2 + \Omega_T^2); \qquad \tilde{\epsilon} = (\Delta_*^2 + \xi^2)^{1/2}, \tag{11}$$

$$\tilde{\Omega} = p \sum_{nm} \rho_n \, |\tilde{V}_{nm}|^2 \delta(E_n - E_m - \tilde{\epsilon})^1/_2 (1 + \exp(-\tilde{\epsilon}/T)) = \tfrac{1}{2}\Omega_T \tilde{\epsilon}/T \coth \tilde{\epsilon}/2T.$$

Since the ranges of application of Eqs. (10) and (11) overlap when $b \ll 1$ over a broad interval of the parameters $\tilde{\omega} \gg (\Omega_T,\xi)_{max} > \Delta_*$, we can write a general expression which is valid for the entire range of variation of T, Ω_T, and ξ

$$\gamma(\epsilon, T) = (1 + \exp(-{}^{\epsilon}/_T))\, W(\epsilon, T), \qquad \epsilon = (\Delta_{coh}^2(T) + \xi^2)^{1/2} \tag{12}$$

At ξ, $T \ll \Delta_*$ $|\Gamma(1 + b + i\epsilon/2\pi T)|^2 \sim (\epsilon/\pi T)^{2b} \approx (\Delta_*/\pi T)^{2b}$ in an asymptotic manner and the square amplitude $\tilde{\Delta}_0(T)$ is replaced by Δ_*^2 in the expression for $W(\epsilon,T)$ [expression (7)].

Over a broad range where (8) holds, expression (12) remains valid for an arbitrary value of b upon transformation to (7) and (10). Furthermore, at $b = 1/2$ expression (12) leads to a T- and ϵ-independent result:

$$\gamma(\epsilon, T) = {}^{\pi}/_{2}\Delta_{*}, \qquad \Delta_{*} = \Delta_0^2/\omega,$$

indicating that the results are exact (see the analytical study by Guinea *et al.*[10]). Expression (12) is thus an approximate expression only for the intermediate values of b ($b \lesssim 1/2$) if condition (8) is violated.

Expressions (7) and (12) differ appreciably from the results obtained previously for the relaxation rate of a two-level system in metallic glasses,[3] which are valid only for $\epsilon \gg \Omega_T$ and only if the electron polaron effect is ignored.

4. For a superconductor, expressions (7) and (12) can be generalized directly by the BCS theory. We present here only the results with clear physical nature.

In the limit $T \to 0$, the infrared divergence characteristic of the electron polaron effect is now cut off below at the scale $(\Delta_*, 2\Delta_c)_{\max}$, where Δ_c is the superconducting gap at $T=0$. If $\Delta_* > 2\Delta_c$, $\Delta_{\rm coh}(0)$ has the same value of Δ_* as in (9) and the transitions give rise to free production of electron-hole pairs ($\epsilon_{\min} = \Delta_* > 2\Delta_c$) and account for the fact that all results found for a normal metal are the same.

If $2\Delta_c > \Delta_*$, the cutoff occurs at $2\Delta_c$. We can now write

$$\tilde{\Delta}_0(T) = \Delta_0((\pi T, 2\Delta_c)_{max}/\omega)^b; \quad \Delta_{coh}(0) \equiv \Delta_*^c = \Delta_0(2\Delta_c/\omega)^b > \Delta_*. \quad (13)$$

The freezing-out of the normal excitations takes effect when $\epsilon < 2\Delta_c(T)$ and at the same time at $T < \Delta_c(T)$. We assume $T \gtrsim \epsilon$. The quantity $\gamma(\epsilon, T)$ will then be the same as in (7) and (12) if $\Delta_0(T)$ is understood to mean (13) and Ω_T^c is substituted for Ω_T (see Refs. 11 and 12):

$$\Omega_T^c = 2\Omega_T(1 + \exp(\Delta_c(T)/T))^{-1}. \quad (14)$$

This result effectively corresponds to a reduction of the parameter b and the applicability of the perturbation theory for $\tilde{V}$ in (3). The expression for Ω_T^c as it appears in (14) is correct above and below T_c.

5. The damping of low-frequency sound, ω_0, in glasses, for which the dominant mechanism is the relaxation of a two-level system, is characterized by the absorption

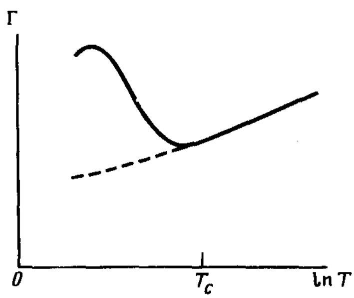

FIG. 1.

factor Γ, which can be written in general form[3] (see also Ref. 13)

$$\Gamma \sim \int (\xi/\epsilon)^2 \, (T\cosh 2\epsilon/2T)^{-1} \frac{\omega_0/\gamma(\epsilon, T)}{1+[\omega_0/\gamma(\epsilon, T)]^2} P(\xi, \ln\Delta_0) d\xi d\ln\Delta_0 \, . \tag{15}$$

The averaging in (15) over the parameters of a two-level system is carried out with the distribution function $P(\xi, \ln \Delta_0)$ which is usually assumed to be constant. That the distribution in ξ is uniform is beyond doubt. We see from (15) that all two-level systems wtih $\xi \approx \epsilon \sim T(\Delta_* \ll T$; see the discussion below) contribute to the absorption. With regard to the P independence of $\ln \Delta_0$, there is, in our view, in general, no physical basis for such an assumption. We assume that the function $P(\ln \Delta_0)$ has a smooth peak near a typical tunneling amplitude J_0

$$P = P_0\left(1 - \alpha \ln^2 \Delta_0/J_0\right), \qquad \alpha \ll 1. \tag{16}$$

The extremal value of the integrand in (15), $\omega/\gamma \sim 1$, determines the characteristic value of $\Delta_0^{\rm eff}$, near which the integral in (15) accumulates. Using (7) and (12), along with the parameters (13) and (14), we find the approximate result

$$(\Delta_0^{eff})^2 \approx \omega_0 T(1 + \exp(\Delta_c(T)/T))\,(\omega/(\pi T, 2\Delta_c)_{max})^{2b}/2\pi b. \tag{17}$$

At $T \sim 1$ K and $\omega_0 \sim 10^2$–10^3 Hz we have $\Delta_0^{\rm eff} \sim 10^{-3}$–$10^{-4}$ K in the normal state. Such values of $\Delta_0^{\rm eff}$ allow us to assume that $\Delta_0^{\rm eff}$ is found in the interval to the left of J_0. It follows from (16) and (17) that in a normal metallic phase we have $\Delta_0^{\rm eff} \sim T^{1/2-b}$ and the factor Γ decreases slowly with decreasing T. Transition to the superconducting state is accompanied by an exponential increase of $\Delta_0^{\rm eff} \approx e^{\Delta c/2T}$. As a result, after going through a minimum, Γ increases rapidly as T is lowered, which does not occur if the magnetic field destroys the superconductivity (see Fig. 1). This situation was observed experimentally in Refs. 1 and 2. Rejection of the assumption $P = \text{const}$ does not change the results for the heat capacity.

[1]H. Neckel, P. Esquinazi, G. Weiss, and S. Hunklinger, Solid State Commun. **57(3)**, 151 (1986).
[2]P. Esquinazi, H. M. Ritter, H. Neckel, G. Weiss, and S. Hunklinger, Preprint 1986 (in press).
[3]J. L. Black, in Metallic Glasses, ed. by H. J. Güntherodt, Springer-Verlag, New York, 1981.
[4]Yu. Kagan and N. V. Prokof'ev, Zh. Eksp.Teor. Fiz. **90**, 2176 (1986) [Sov. Phys. JETP **63**, 1276 (1986)].
[5]J. Kondo, Physica **84(B+C)**, 40 (1976); **126(B+C)**, 377 (1984).
[6]K. Yamada, Progr. Theor. Phys. **72**, 195 (1984).
[7]A. J. Leggett, S. Chakravarty, A. T. Dorsey, M. P. A. Fisher, A. Garg, and W. Zwerger, Rev. Mod. Phys., 1986 (in press).
[8]K. Yamada, A. Sakurai, S. Miyazima, and H. S. Hwang, Progr. Theor. Fiz. **75(5)**, 1030 (1986).
[9]Yu. Kagan and L. A. Maksimov, Zh. Eksp. Teor. Fiz. **79**, 1363 (1980) [Sov. Phys. JETP **52**, 688 (1980)].
[10]F. Guinea, V. Hakim, and A. Muramatsu, Phys. Rev. **32B**, 4410 (1985).
[11]J. L. Black and P. Fulde, Phys. Rev. Lett. **43**, 453 (1979).
[12]A. I. Morozov, Zh. Eksp. Teor. Fiz. **77**, 1471 (1979) [Sov. Phys. JETP **50**, 738 (1979)].
[13]Yu. M. Gal'perin, V. L. Gurevich, and D. A. Parshin, Zh. Eksp. Teor. Fiz. **86**, 1900 (1984) [Sov. Phys. JETP **59**, 1104 (1984)].

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