Energy localization and propagation in disordered media: low-temperature thermal conductivity of amorphous materials

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The model of two-level systems with an interaction $U(R) \sim R^{-\alpha}$ is used to show that delocalized collective excitations exist in disordered media for $\alpha < 6$. The low-temperature thermal conductivity resulting from these excitations is calculated. The behavior $\kappa \sim T^{4/3}$ is found for $\alpha = 3$.

According to Anderson's theorem, elementary excitations localize in a disordered three-dimensional medium if the scale of the energy fluctuations of these excitations, N_0^{-1}, is sufficiently large in comparison with the characteristic tunneling amplitude of the excitations, M. It was shown in Refs. 1 and 2 that incorporating collective excitations lowers the localization threshold substantially in the direction of smaller values of N_0M, and under certain conditions it erases the localization completely.

Let us examine the localization and propagation of energy in the model of two-level systems with an average distance a between systems and with the customary distributions of the energy parameters E and Δ_0 (Ref. 3), of width N_0. We will show that the interaction between the two-level systems, which we chose in the form

$$U(R) = A(a/R)^{\alpha}, \quad \gamma = N_0 A \ll 1, \quad \alpha > 3, \tag{1}$$

completely erases the localization at a finite temperature and creates a new nonphonon mechanism for thermal conductivity if $\alpha < \alpha_c = 6$. We find $\kappa_{\text{nonph}} \sim T^{4/3}$ as $\alpha \rightarrow_3$ (an interaction through a strain field).

It is easy to see that "thermal" two-level systems, for which the tunneling energy and amplitude satisfy $E \approx \Delta_0 \approx T$, will play the major role in the propagation of energy. The average distance between thermal two-level systems is $R_T \approx a(N_0T)^{-1/3}$, so the characteristic energy of the interaction between these systems, (1), is

$$U_T = U(R_T) \approx T\gamma^{\alpha/3}(T/A)^{(\alpha-3)/3}. \tag{2}$$

This is a small quantity in comparison with the temperature at essentially all temperatures $(T \ll T_A = N_0^{-1}\gamma^{-3/(\alpha-3)})$.

It was shown in Ref. 4 that expression (1) characterizes both the energy shift of the excitation, E, of the two-level system and the amplitude for a flip-flop transition of the two-level systems. Working from the relation $T_T \ll T$ and Anderson's theorem, we find that in the system under consideration here $(\alpha > 3)$ single-quantum energy excitations cannot propagate over macroscopic distances.

Let us consider a pair of thermal two-level systems, one in the ground state and the other in the excited state. This pair forms a two-level cluster with a distance $E_{12} = |E_1 - E_2|$ between levels. If the resonance condition

$$M_{12} = U(R_{12}) > E_{12} \tag{3}$$

is satisfied, the eigenstates of the pair are coherent mixtures of the ground and excited states of each two-level sysetm. The concentration of resonant pairs for which the relation $M_{12} \approx M$ holds is, in order of magnitude,

$$W(M) \approx a^{-3}(N_0 T)(N_0 M)(A/M)^{3/\alpha} = R_M^{-3}. \tag{4}$$

The first factor here is the probability for $E_1 \approx T$, the second is the probability for $E_{12} \approx M$, and the third is the volume within which condition (3) holds. The average distance between such pairs is R_M, and the characteristic energy of the interaction between neighboring resonant pairs of this type, divided by the distance between the levels of the pairs, is

$$\chi_M = U(R_M)/M = (N_0^2 TA)^{\alpha/3}(A/M)^{(6-\alpha)/3}. \tag{5}$$

If $\alpha < 6$, then χ_M increases with increasing M, and for the maximum possible value $M \approx T$ we have

$$\chi_T \approx (N_0^2 AT)^{\alpha/3}(T/A)^{(\alpha-6)/3}. \tag{6}$$

This result means that the interaction between resonant pairs is weak and thereby indicates that there are no delocalized states in the system. In the case $\alpha < 6$, on the other hand, the value of χ_M increases without bound with decreasing M, so we find $\lim_{M \to 0} \chi_M = \infty$

$$\chi_M = (M_*/M)^{(6-\alpha)/3}, \quad M_* \approx T(T/A)^{2(\alpha-3)/(6-\alpha)}\gamma^{2\alpha/(6-\alpha)}. \tag{7}$$

This result is evidence that there are macroscopic clusters of strongly interacting resonant pairs in the system, with a quasicontinuous spectrum of states: The system is delocalized.

It can be shown that incorporating resonant clusters of $n \gtrsim 3$ two-level systems leaves the value $\alpha_c = 6$ and the T dependence of M_* unchanged.

If the interaction of the two-level systems falls off more rapidly than R^{-6}, the system of two-level systems is thus localized, and the localization is eliminated only to the extent that there is an interaction with phonons. In the case of a slower decrease in the interaction, the system of two-level systems, thought of as a closed system, is delocalized at a finite temperature and allows the propagation of energy excitations over macroscopic distances.

We conclude with a look at a nonphonon mechanism for thermal conductivity in a system of two-level systems with $\alpha < 6$. The relaxation of energy excitations goes most efficiently through a system of bound resonant pairs, by which we mean pairs for which the relation $M \lesssim M_*$ holds [see (7)]. Since resonant pairs are strongly coupled, the relaxation rate, i.e., the reciprocal lifetime of these pairs, is the same in order of magnitude as the distance between levels. Associated with these pairs is a heat capacity $\sim W(M_*)$ [see (4)]. The elementary energy-transfer process is a hop of an energy T from one two-level system to another over a distance determined by the size scale of the pair, $l \approx a(A/M^*)^{3/\alpha}$ [see (4)]. As a result, we find an estimate of the thermal conductivity:

$$\kappa \approx W(M_*) l^2 \tau^{-1} = a^2 A (T/A)^{(\alpha+1)/(6-\alpha)} \gamma^{2[(\alpha+1)/(6-\alpha)]} \qquad (8)$$

The calculations above could be carried out at a more rigorous level, by treating (as in Ref. 2) the self-consistent problem of the relaxation of resonant pairs of two-level systems in the fluctuating field of surrounding two-level systems and by calculating the energy flux through a unit area perpendicular to ∇T. The solution of that problem will be published separately.

As $\alpha \to 3$, we find from (8) $\kappa_{\text{nonph}} \sim T^{4/3}$; i.e., the thermal conductivity falls off more slowly with the temperature than the thermal conductivity caused by the scattering of phonons by two-level systems: $\kappa_{\text{ph}} \sim T^2$ (Ref. 3).

We would expect that as the temperature is lowered in an amorphous material, the temperature dependence of the thermal conductivity would change from a T^2 law to a softer law, as is observed in many experiments.[5]

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