Anderson localization in crystals with heavy isotopic impurities

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The vibration spectrum of a harmonic crystal with heavy impurities is shown to consist of two branches, separated by a gap. Bordering the gap on each branch is a frequency interval corresponding to localized modes. The localization thresholds, the frequency dependence of the diffusion coefficient, and that of the phonon localization radius are all derived.

The anomalous behavior of the low-temperature properties of amorphous insulators stems from the particular nature of the low-frequency elementary excitations, in particular, the presence of localized modes of a two-level system[1] or fractions.[2] The excitation of two-level systems results from a tunneling, while fractions arise in percolation systems with ruptured bonds. It was hypothesized in Ref. 3 that localized excitations might arise under far less stringent conditions, specifically, in harmonic lattices with heavy defects. In the present letter we examine this idea in detail.

We begin with a scalar model of the vibrations of a cubic harmonic crystal with isotopic impurities. We consider the square of the retarded Green's function, $P_{ij} = [G_{ij}^{+}(t)]^2 = G_{ij(t)}^{+} G_{ji}^{-}(-t)$, where $G_{ij}^{\pm}(t) = \mp i\theta(\pm t) < [u_i(t), u_j]$, and the u_i are the displacement operators for an atom at site i. We have the following expression for the Fourier transform of P_{ij}, averaged over the positions of the defects:

$$P(\mathbf{k}, \Omega) = \int \frac{d\omega}{2\pi} \sum_{\mathbf{pp}'} \Phi_{\mathbf{pp}'}; \quad \Phi_{\mathbf{pp}'} = \overline{G^{+}_{\mathbf{p}_+, -\mathbf{p}'_+}(\omega_+) G^{-}_{\mathbf{p}'_-, -\mathbf{p}_-}(\omega_-)}, \tag{1}$$

where $\mathbf{p}_\pm = \mathbf{p} \pm \mathbf{k}/2$, $\omega_\pm = \omega \pm \Omega/2$, and the superior bar means an average over the positions of the impurities. Using the version of the cross technique proposed in Ref. 3, we find the following expression for $\Phi_{\mathbf{pp}'}$:

$$\Phi_{\mathbf{pp}'} = G^{+}_{\mathbf{p}_+}(\omega_+) G^{-}_{\mathbf{p}_-}(\omega_-) (\delta_{\mathbf{pp}'} + \sum_{\mathbf{p}''} W_{\mathbf{pp}''} \Phi_{\mathbf{p}''\mathbf{p}'}), \tag{2}$$

where $G^{\pm}_{\mathbf{p}_\pm}(\omega_\pm) = [\omega^2_\pm - \mathbf{p}^2_\pm - \Sigma_{\mathbf{p}_\pm}(\omega \pm i0)]^{-1}$, $\Sigma_{\mathbf{p}}(\omega \pm i0) = \Delta_{\mathbf{p}}(\omega) \mp i\Gamma_{\mathbf{p}}(\omega)$ is the eigenenergy, $W_{\mathbf{pp}'} = W_{\mathbf{pp}'}(\mathbf{k}, \Omega, \omega)$ is an irreducible vertex, and the other parameters of the ideal crystal (the mass of the atom, the lattice constant, and the sound velocity) are all assumed to be equal to unity.

We rewrite Eq. (2) in the equivalent form

$$(2\omega\Omega + 2\mathbf{pk} + \Sigma_{\mathbf{p}_+}(\omega_+) - \Sigma_{\mathbf{p}_-}(\omega_-)) \Phi_{\mathbf{pp}'} = \Delta G_{\mathbf{p}} (\delta_{\mathbf{pp}'} + \sum_{\mathbf{p}'} W_{\mathbf{pp}''} \Phi_{\mathbf{p}'\mathbf{p}''}), \tag{3}$$

where $\Delta G_{\mathbf{p}} = G^{+}_{\mathbf{p}_+}(\omega_+) - G^{-}_{\mathbf{p}_-}(\omega_-)$.

In the dipole approximation (Ref. 4, for example) we can write

$$\sum_{\mathbf{p}'} \Phi_{\mathbf{pp}'} = 2\pi i \Delta G_{\mathbf{p}} / \tilde{\omega} (\Phi_0 + 3\mathbf{p}\hat{\mathbf{k}}/\tilde{\omega}\Phi_1), \quad \Phi_{0,1} = \Phi_{0,1}(k, \omega, \Omega), \tag{4}$$

where $\tilde{\omega} = [\omega^2 - \Delta_0(\omega)]^{1/2}$, $\hat{\mathbf{k}} = \mathbf{k}/|\mathbf{k}|$, and $\Sigma_0(\omega + i0) = \Delta_0(\omega) - iT_0(\omega)$ is the momentum-independent eigenenergy calculated by ignoring interference effects[3] [see also expression (12) below]. From (3) we then find the algebraic system

$$-\omega\Omega\Phi_0 + k\Phi_1 = -i\tilde{\omega}/4\pi, \tag{5'}$$

$$-\omega\Omega\Phi_1 + k\omega^2\Phi_0/3 - iM\Phi_1 = 0, \tag{5''}$$

$$M = \Gamma(\omega) + 3\pi\tilde{\omega}^{-3} \sum_{\mathbf{pp}'} \Delta G_{\mathbf{p}}(\mathbf{p}\hat{\mathbf{k}}) W_{\mathbf{pp}'} \text{ where } \Delta G_{\mathbf{p}'}(\mathbf{p}'\hat{\mathbf{k}}) \tag{6}$$

is a memory function. In deriving (5'), we used the Ward identity

$$\Sigma^{+}_{\mathbf{p}_+}(\omega_+) - \Sigma^{-}_{\mathbf{p}_-}(\omega_-) = \sum_{\mathbf{p}'} W_{\mathbf{pp}'} \Delta G_{\mathbf{p}'},$$

which is valid for our model of the crystal. From (4) and (5) we find for Φ_0 the expression which is usually derived in the interacting-mode theory:[5]

$$\sum_{pp'} \Phi_{pp'} \approx \Phi_0 = \frac{\tilde{\omega}/4\pi\omega}{-i\Omega + k^2/3\,\dfrac{(\tilde{\omega}/\omega)^2}{-i\Omega + M/\omega}} \approx 1/4\pi\,\frac{\tilde{\omega}/\omega}{-i\Omega + Dk^2}\,, \tag{7}$$

where $D = \tilde{\omega}^2/(3\omega M)$ is a diffusion coefficient.

To calculate the memory function M, we use the approximation of fan diagrams,[6] making use of the results of Ref. 3:

$$M \approx \Gamma_0(\omega) + \frac{8\pi^2\Gamma_0(\omega)}{\tilde{\omega}^2\,\omega} \sum_q \frac{\theta(\Gamma_0(\omega) - \tilde{\omega}q)}{-i\Omega + D_0(\omega)\,q^2}, \quad q = |p + p'|, \tag{8}$$

where $D_0(\omega) = \tilde{\omega}^2/(3\omega\Gamma_0(\omega))$.

Using (7) and (8), we find for the phonon diffusion coefficient an expression which is of the same form as the corresponding expression in the theory of weak localization of electrons:[6]

$$D = D_0(\omega)\Big(1 - \frac{12\pi\Gamma_0(\omega)}{\tilde{\omega}^3} \int \frac{\theta(\Gamma_0(\omega) - \tilde{\omega}q)}{q^2 - \dfrac{i\Omega}{D_0(\omega)}}\, q^2\, dq\Big). \tag{9}$$

In the limit $\Omega \to 0$ we have

$$D = D_0(\omega)\,(1 - 12\pi(\Gamma_0(\omega)/\tilde{\omega}^2)^2). \tag{10}$$

This expression is meaningful as long as the attenuation $\Phi_0(\omega)$ is sufficiently small; the localization threshold is determined by the finite value $\Gamma_0(\omega) = (12\pi)^{-1/2}\tilde{\omega}^2$ in this case. In the localization region, in which expression (10) is no longer meaningful, we can make use of the self-consistent localization theory proposed by Vollhardt and Wolfle[4] to replace $D_0(\omega)$ by D in the integrand in (9). Solving the resulting self-consistent equation, we find

$$D \approx -i\Omega R_c^2, \quad R_c = \frac{6\pi^2\Gamma_0(\omega)\tilde{\omega}^2}{12\pi(\Gamma_0(\omega)/\tilde{\omega}^2)^2 - 1}. \tag{11}$$

To calculate the quantity $\Gamma_0(\omega)$ in (10) and (11), we use the self-consistent expression for the free energy which was derived in Ref. 3:

$$\Sigma_0(\omega + i0) = \frac{n\omega^2(m^{-1} - 1)}{m^{-1} + (m^{-1} - 1)/\omega^2\big((3/4\pi^4)^{1/3} + i(\omega^2 - \Sigma_0(\omega + i0)/4\pi)^{1/2}\big)}, \tag{12}$$

Here m and n are respectively the mass and concentration of the impurity. The density of states in this system is given by[3]

$$g(\omega) = \omega/2\pi\,\mathrm{Re}[\omega^2 - \Sigma(\omega + i0)]^{1/2}. \tag{13}$$

Ignoring the imaginary part of the denominator in (12), and substituting the result into (13), we find that the expression in square brackets is negative in the frequency

interval (ω_0, ω_*) [here $\omega_0 = (4\pi^4/3)^{1/6} \times (m-1)^{-1/2}$ is the quasilocal frequency corresponding to the pole of expression (12), at $\omega_* = \omega_0(1 + n(m-1))^{1/2}$]. Consequently, there is a gap in this interval.[7] In the interval $(0,\omega_0)$ the vibration spectrum is acoustic, with $\omega = (1+nm)^{-1/2}k$ and

$$\Delta_0(\omega) \approx -\frac{n\omega^2(m-1)}{1-(\omega/\omega_0)^2}, \quad \Gamma_0(\omega) \frac{n\omega^4(m-1)^2(\omega^2 - \Delta_0(\omega))^{1/2}}{(1-(\omega^2/\omega_0^2))^2}. \tag{14'}$$

In the interval $\omega_* < \omega \ll \omega_D$ the vibration spectrum takes the form of an optical branch, with $\omega^2 = \omega_*^2 + k^2$ and

$$\Delta_0(\omega) \approx \omega_*^2; \quad \Gamma_0(\omega) = \omega_*^4 \tilde{\omega}/n. \tag{14''}$$

Using (10)–(14), we find the following expressions for the diffusion coefficient:

$$D = D_0 \begin{cases} 1-(\omega/\omega')^6, & \omega \ll \omega_0; \quad \omega' \approx ((1-m)^2 n)^{1/3}, \\ 1-(\omega/\omega'), & \omega \lesssim \omega_c'; \quad \omega_c' \approx \omega_0(1-n^{1/3}) \text{ for } mn \ll 1, \\ & \qquad \omega_c' \approx \omega_0(1-n^{1/2}m^{1/4}) \text{ for } mn \gg 1, \\ 1-(\tilde{\omega}_c''/\tilde{\omega}), & \omega \gtrsim \omega_*; \quad \omega_c'' \approx \omega_*(1+\pi^3((m-1)^{-1}+n)^3/n). \end{cases} \tag{15}$$

The acoustic modes are thus localized in the interval (ω_c', ω_0); the localization radius is $R_c' \sim (\omega - \omega_c')^{-1}$. The optical modes are localized in the interval (ω_*, ω_c''), with a localization length $R'' \sim (\omega_c'' - \omega)^{-1}$. In contrast with the analysis of the present paper, the analysis by Akkermans and Meynard[8] ignored the singularities of the vibration spectrum near the quasilocal frequency, and the sole localization threshold found for acoustic modes in Ref. 8 was erroneously identified with the quantity ω' [see (15)], which always lies above the boundary of the acoustic branch, ω_0 (i.e., in the gap). In Ref. 8, however, there was no discussion at all of the existence of a gap, the existence of an optical branch, or the properties of its modes.

Manzheliĭ has recently reported[9] observing a strong dependence of the low-temperature thermal conductivity of solid hydrogen on the concentration of heavy impurities (Ne, Ar). We believe that those experiments can be understood in light of the results of the present letter.

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