Violation of the Migdal theorem for a strongly coupled electron-phonon system

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(Submitted 3 March 1987)
Pis'ma Zh. Eksp. Teor. Fiz. **45**, No. 7, 357–360 (10 April 1987)

The classical theory of electron-phonon interaction in metals shows that in the case of strong coupling, $\lambda > 1$, allowance for the finite width of the electron band leads to its polaron collapse. The band width renormalized by the electron-phonon interaction is smaller than the characteristic phonon frequencies and the interaction becomes essentially nonadiabatic.

A large group of superconducting compounds, which are distinguished by a large coupling constant for the coupling of electrons with phonons, $\lambda > 1$ or even $\lambda \gg 1$, have now been synthesized: A15 compounds, Chevreul phases, carbides, transition-metal nitrides, $BaBiPbO_3$ ceramics, copper and lanthanum compounds, $SrTiO_3$. It is possible that in compounds with heavy fermions the f electrons are also strongly coupled to the lattice vibrations. The compounds listed above have anomalous properties in the normal and superconducting states, which cannot be described by the standard theory of electron-phonon interaction in metals.[1,2] The anomalous behavior of intermetallic compounds with $\lambda > 1$ may stem from, as was noted previously[3] (see also Ref. 4), the polaron collapse (contraction) of the electron band due to the local lattice instability, which causes the electron mass to increase sharply and the superconducting compounds to form heavy charged bipolarons of small radius.[3]

In the present letter we show that if the discrete nature of the lattice, i.e., the finite width of the conduction band D, is taken into account, the polaron collapse will occur at $\lambda > 1$ in the classical analysis of the electron phonon interaction,[1] which is based on the substantial difference between the electron energies ($\sim D$) and the characteristic phonon frequencies $\omega \ll D$. The latter inequality, as we know, allows one to ignore the vertex phonon corrections in the equation for the self-energy part Σ of the electron Green's function $G(\mathbf{k}, i\omega_n)$ (the Migdal "theorem"):

$$\Sigma(\mathbf{k}, i\omega_n) = -T \sum_{\mathbf{k}', n'} |\tilde{g}_{\mathbf{k},\mathbf{k}'}|^2 D(\mathbf{k}-\mathbf{k}', i\omega_n - i\omega_{n'}) G(\mathbf{k}', i\omega_{n'}), \tag{1}$$

where $\tilde{g}$ is the electron-phonon vertex renormalized by the Coulomb interaction, $D(\mathbf{q}, i\nu_n)$ is the exact Green's phonon function, $\omega_n = (2n+1)\pi T$, and $\nu_n = 2n\pi T (n = 0, \pm 1 \ldots)$. Using standard transformations, we can reduce Eq. (1) to the form

$$\mathrm{Re}\,\Sigma(\epsilon) = \fint_{-\infty}^{\infty} d\epsilon' N(\epsilon') \int_0^{\infty} d\Omega \alpha^2 F(\Omega) \left[\frac{n(\Omega) + f(-\epsilon')}{\epsilon - \Omega - \epsilon'} + \frac{n(\Omega) + f(\epsilon')}{\epsilon + \Omega - \epsilon'} \right], \tag{2}$$

$$\mathrm{Im}\,\Sigma(\epsilon) = -\pi \int_0^{\infty} d\Omega \alpha^2 F(\Omega) [N(\epsilon - \Omega)(n(\Omega) + f(\Omega - \epsilon)) + N(\epsilon + \Omega)(n(\Omega) + f(\epsilon + \Omega))] \,\mathrm{sign}\,(\epsilon),$$

where $\Sigma(\epsilon)$ is an analytical continuation of $\Sigma(\mathbf{k},i\omega_n)$ to the real axis $i\omega_n \to \epsilon + i\eta$; $f(\epsilon)$ and $n(\Omega)$ are the Fermi and Bose functions, respectively;

$$\alpha^2 F(\Omega) = N_0^{-1}(\xi)N_0^{-1}(\xi') \sum_{\mathbf{k},\mathbf{k}'} |\tilde{g}_{\mathbf{k},\mathbf{k}'}|^2 B(\mathbf{k}-\mathbf{k}',\Omega)\delta(\xi-\xi_{\mathbf{k}})\delta(\xi'-\xi_{\mathbf{k}'});$$

$B(\mathbf{q},\Omega)$ is the spectral density of the phonon Green's function; and $\xi_{\mathbf{k}}$ and $N_0(\xi)$ are the energy spectrum and the electronic state density of an ideal lattice (ignoring the electron-phonon interaction). Structural change in the electronic spectrum as a result of electron-phonon interaction is described by a single-particle state density $N(\epsilon)$:

$$N(\epsilon) = -\frac{1}{\pi}\int_{-\infty}^{\infty} d\xi N_0(\xi)\mathrm{Im}G(\xi,\epsilon),$$
$$G^{-1}(\xi,\epsilon) = \epsilon - \xi + \Sigma(\epsilon). \tag{3}$$

For clarity, we restrict the analysis to the Einstein model of the phonon spectrum:

$$\alpha^2 F(\Omega) = \frac{1}{2}N_0^{-1}(0)\lambda\omega\delta(\Omega-\omega) \tag{4}$$

and $T=0$. Here $N_0(0)$ is the nonrenormalized state density at the Fermi level.

In this case the system of equations (2) can be simplified considerably:

$$\mathrm{Re}\Sigma(\epsilon) = \frac{\lambda\omega}{2N_0(0)} \fint_0^{\infty} d\epsilon' \left[\frac{N(-\epsilon')}{\epsilon'+\epsilon+\omega} - \frac{N(\epsilon')}{\epsilon'-\epsilon+\omega}\right],$$

$$\mathrm{Im}\Sigma(\epsilon) = -\frac{\lambda\omega\pi}{2N_0(0)}[N(\epsilon-\omega)\theta(\epsilon-\omega)+N(\epsilon+\omega)(1-\theta(\epsilon+\omega))]\mathrm{sign}(\epsilon), \tag{5}$$

$$\theta(x) = \begin{cases} 1, & x>0 \\ 0, & x<0 \end{cases}.$$

The finite width of the conduction band D can be simulated by a Lorentzian nonrenormalized state density

$$N_0(\xi) = \frac{N_0(0)}{1+N_s}\left[\frac{D^2/4}{\xi^2+D^2/4} + N_s\right], \tag{6}$$

where N_S is a constant which corresponds in real crystals to the contribution from the broad bands, whose electrons interact weakly with the phonons. Substituting (6) into (3), we find

$$N(\epsilon) = \frac{N_0(0)}{1+N_s}\left[\frac{(|\mathrm{Im}\Sigma(\epsilon)|+D/2)D/2}{(\epsilon-\mathrm{Re}\Sigma(\epsilon))^2+(|\mathrm{Im}\Sigma(\epsilon)|+D/2)^2} + N_s\right]. \tag{7}$$

In the standard theory of electron-phonon interaction[1,2] the electronic state density is

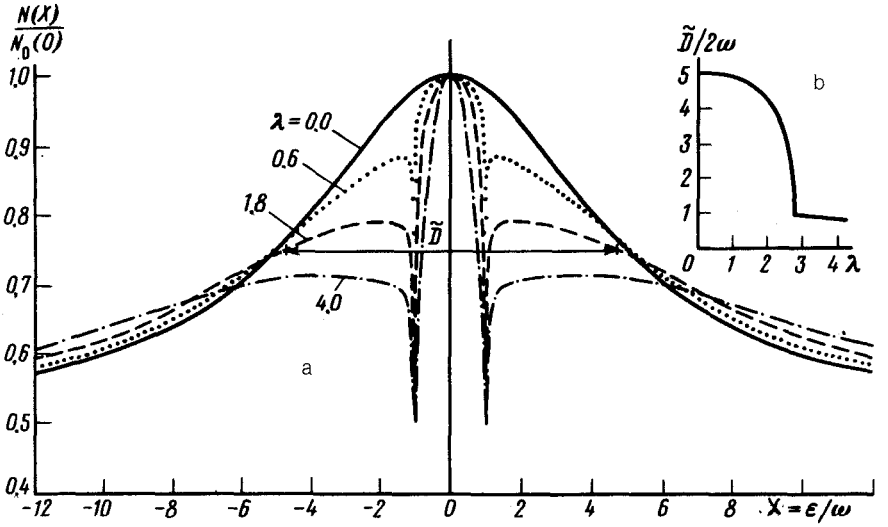

FIG. 1. Single-particle electron-state density renormalized by the electron-phonon interaction; $\tilde{D}$ is the renormalized width determined at half-maximum which depends on the energy of the component $N(\epsilon)$ ($D = 10\,\omega$, $N_S = 1$).

assumed to be independent of the energy, $N_0(\xi) = N_0(0)$, which corresponds in (6) to the limit $D \to \infty$. As can easily be seen, the electron-phonon interaction in this case does not change the state density; i.e., for any value of λ we have $N(\epsilon) = N_0(0)$.

Qualitatively, the situation is quite different for finite, though large ($\gg\omega$), values of D. The results of a numerical calculation of the system of equations (5),(7) on the basis of a simple iteration scheme are shown in Fig. 1 ($D = 10\,\omega$). Figure 1b shows the band width $\tilde{D}$ which is renormalized by the electron-phonon interaction. This band width is determined from the width of the variable component of the line $N(\epsilon)$ at half-maximum as a function of λ. Figure 1, a and b, shows that at some value of λ, $\lambda \gg \lambda^* > 1$, the band width decreases sharply to $\tilde{D} < \omega$. The kinetic energy of the electrons decreases below the characteristic phonon frequencies, so that the interaction becomes essentially nonadiabatic.

The physical reason for the polaron collapse is that at $\lambda \simeq \tilde{g}^2 N_0(0) > 1$ the depth of the polaron well,[5] $\epsilon_p \simeq \tilde{g}^2$, is greater than the kinetic energy of the electron D. Because of the normalization, we have $N_0(0) \simeq D^{-1}$, so that the strong-coupling condition $\lambda > 1$ restricts the initial width of the conduction band D and renders the approximation $N_0(\xi) = N_0(0)$ inadmissible.

Because of the nonadiabaticity of the interaction ($\tilde{D} < \omega$), the vertex phonon corrections are appreciable and Eq. (1) is, strictly speaking, inapplicable at $\lambda > 1$. A systematic analysis[3,4] of a many-electron system, which was carried out at $\lambda \gg 1$ on the basis of the theory of small-radius polaron,[5] suggests the existence of a new superconductivity mechanism based on the superfluidity of He^4.

We are deeply indebted to Academician A. B. Migdal, Academician Yu. M.

Kagan, and Professor G. M. Éliashberg for useful discussions of the problem raised in this study.

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Translated by S. J. Amoretty