Adiabatic approximation and the condition for the existence of a small polaron

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Perturbation theory, variational estimates, and numerical simulation by the Monte Carlo method have shown that adiabatic description of the interacting electrons and phonons based on the small ratio of the characteristic energy of a phonon, ω, to the kinetic energy of an electron, E_F, is impaired in the region of intermediate values of the coupling constant $\lambda \approx 1$.

It is generally assumed[1] that the small value of the adiabatic parameter

$$\omega/E_F \sim \omega/D \ll 1, \tag{1}$$

where D is the width of the electron energy band in an unstrained lattice ($\hbar = 1$), makes it possible to use familiar self-consistent equations for the self-energy part of the electron Green's function in the normal state[2] and the superconducting state[3] at arbitrarily large values of the coupling constant λ.

We have noted previously[4,5] that the classical theory of electron-phonon coupling[2,3] ignores a possible local lattice strain due to electron-phonon coupling, i.e., the corresponding polaron effect—self-trapping of an electron with an appreciable narrowing of the electron band.

Allowance for the finite width of the initial (seed) electron band D effectively reduces the width of the electron spectrum even in the standard equations for the Green's function[5] when

$$\lambda > E_F/\omega \gg 1. \tag{2}$$

This conclusion can also be inferred from the known expression[2] for the renormalized electron mass, $m^* = m(1+\lambda)$.

In the present letter we will show that the polaron collapse of the electron band occurs at much lower values of the coupling constant:

$$\lambda \approx 1. \tag{3}$$

An inequality, which is the reciprocal of inequality (1), holds in this case; in other words,

$$\omega/W \gtrsim 1, \tag{4}$$

and the standard approach based on the Migdal theorem is inapplicable. Here W is the maximum kinetic energy of a polaron. The Hamiltonian of the electron-phonon system in a lattice-site representation is

$$
\begin{aligned}
H &= H_e + H_{ph} + H_{e-ph}, \\
H_e &= -J \sum_{i,j} (c_i^+ c_{i+j} + c_{i+j}^+ c_i), \\
H_{ph} &= \sum_{q} \omega(\mathbf{q}) d_{\mathbf{q}}^+ d_{\mathbf{q}}, \\
H_{e-ph} &= \sum_{i,q} c_i^+ c_i \, [U(\mathbf{q}) d_{\mathbf{q}}^+ e^{i\mathbf{q}\mathbf{R}i} + \text{H.a.}].
\end{aligned} \tag{5}
$$

Here c_i^+ (c_i) and $d_{\mathbf{q}}^+$ ($d_{\mathbf{q}}$) are operators which create (annihilate) an electron at a site with index i and a phonon with a quasimomentum $\mathbf{q}$, respectively; J is an integral describing the transition of an electron from one site to another ($J = D/2z$ and is nonvanishing only for the nearest neighbors, whose number is z), $\omega(\mathbf{q})$ is the phonon frequency, and $U(\mathbf{Q})$ is the matrix element of the electron-phonon coupling. For $U(\mathbf{q})$ we will use a power-law parametrization:

$$
U(\mathbf{q}) = g_0 \omega_0 \frac{1}{\sqrt{N}} \frac{1}{(aq)^\gamma}, \tag{6}
$$

where g_0 is a dimensionless coupling constant, whose degree of nonlocalizability is determined by the parameter γ, and N and a are the total number of sites and the lattice constant. Here ω_0 is the maximum phonon frequency, $\omega_0 = \max \omega(\mathbf{q})$.

In the case of weak electron-phonon coupling the ground-state energy of Hamiltonian (5)in second-order perturbation theory in H_{e-ph} is

$$
E_0 = -zJ - \sum_{q} |U(\mathbf{q})|^2 [\epsilon(\mathbf{q}) + \omega(\mathbf{q}) - \epsilon(0)]^{-1}, \tag{7}
$$

where $\epsilon(\mathbf{q})$ is the dispersion relation for electrons, which corresponds to the Hamiltonian H_e. In the strong-coupling limit of the electron-phonon coupling the term H_e in the complete Hamiltonian (5) can be ignored in zeroth approximation and the following expression for the ground-state energy can be obtained by means of the standard canonical transformation[6]:

$$
E_0 = -\sum_{q} |U(\mathbf{q})|^2 / \omega(\mathbf{q}) \equiv -E_p, \tag{8}
$$

where $E_p = \lambda D$ is a polaron shift of the atomic level. Energy (8) determines the position of the polaron band, whose width W is smaller than the width of the original band D by a factor of $\exp(g^2)$. Accordingly, the effective polaron mass m^* is exponentially large compared with the seed band mass of the electron, m:

$$
m^* = m \exp(g^2). \tag{9}
$$

In the case of a simple cubic lattice a rigorous expression for g^2 is[6]

$$
g^2 = \sum_{q} |U(\mathbf{q})|^2 [1 - (\cos aq_x + \cos aq_y + \cos aq_z)/3] / \omega^2(\mathbf{q}). \tag{10}
$$

Specifically, this constant, rather than g_0^2, has a clear physical significance, since it determines the value of the renormalized carrier mass. In the case of local electron-phonon coupling with a dispersionless optical phonon mode [$\gamma = 0$, $\omega(\mathbf{q}) = \omega_0$] we

have $g^2 = g^2{}_0$, which can easily be seen by substituting expression (6) into (10). At the same time, a numerical estimate gives $g^2 = 0.11 g^2{}_0$ in the case of Fröhlich interaction ($\gamma = 1$). The effective frequency $\omega = E_p/g^2$, which is equal in order of magnitude to ω_0, is exactly equal to it only in the case $\gamma = 0$, $\omega(\mathbf{q}) = \omega_0$. In the case of Fröhlich interaction with a dispersionless mode a calculation based on Eqs. (8) and (10) gives $\omega \approx 1.73\ \omega_0$, a value which should be taken into account in the quantitative estimates of the parameters using the values obtained experimentally. In the strong-coupling limit, H_e can be incorporated in the perturbation theory in terms of the canonically transformed Hamiltonian. This approach requires a summing of many diagrams with many-phonon vertices. In the second-order in H_e, the ground-state energy with a local interaction with a dispersionless mode in a simple cubic lattice is given by (see Ref. 7)

$$E_0 = -E_p\left[1 + \frac{1}{2} z\left(\frac{J}{E_p}\right)^2\right] = -E_p\left[1 + \frac{1}{2}\left(\frac{D}{2\sqrt{z}E_p}\right)^2\right]. \tag{11}$$

This result shows that in the strong-coupling limit, the decomposition parameter is in fact $1/\lambda$. According to (11), the existence criterion for a polaron can be written as an inequality

$$\lambda = E_p/D \gg \frac{1}{2\sqrt{z}}. \tag{12}$$

For $z = 6$, for example, this inequality works well even at $\lambda \approx 1$. This estimate shows that the polaron regime sets in at relatively low values of λ ($\lambda \approx 1$), because the energy of the electron in the locally strained lattice is lower [see Eqs. (7) and (8)]. There have been many attempts to calculate the polaron characteristics in order to study the nature of the transition of a polaron from the state with a large radius (a broad band) to the state with a small radius (a narrow band). These attempts have been based largely on variational methods and have shown that the dependence of ground-state energy on λ is nonanalytical and that the renormalization of the polaron mass is discontinuous at the transition point. Emin,[8] for example, predicted the transition to occur at $\lambda = \lambda_c \approx 0.6$ in the case of a local interaction with a dispersionless mode in a simple cubic lattice, with $\omega_0/D = 0.05$. A numerical simulation using the Monte Carlo method, however, has apparently yielded the most reliable results for the same system.[9,10] In particular, De Raedt and Lagendijk[9] have observed a fairly abrupt transition between two states, suggesting a possible nonanalytic behavior near the critical value of the coupling constant. The transition region in this case was found to be the narrowest for a 3D lattice and the widest for a 1D lattice. The results reported in Ref. 9 for the case $\omega_0/D = 1/2z$ correspond to the critical values $\lambda_c \approx 0.85$ and $\lambda_c \approx 0.45$ for a 1D lattice and a 3D lattice, respectively.

The importance of the numerical calculations[9,10] is that they have shown that the numerical values of λ_c coincide, within a small error, with the estimate which was obtained by equating Eqs. (7) and (8). This circumstance makes it possible to determine λ_c relatively easily for any chosen value of ω_0/D. The results of the calculations for a local interaction ($\gamma = 0$) and the Fröhlich interaction ($\gamma = 1$) with a dispersionless phonon mode are shown in Fig. 1. In particular, it follows from this figure that at $D/\omega_0 \geqslant 5$ the values of $\lambda \gtrsim 1$ correspond to the polaron state and that the Migdal

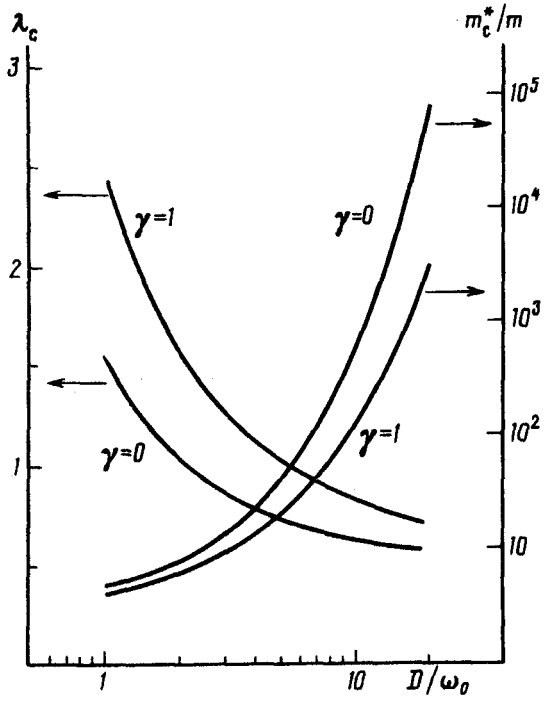

FIG. 1. The critical values of electron-phonon coupling constant λ_c and of the renormalized electron mass m_c^*/m as functions of the adiabatic parameter D/ω_0.

theorem is inapplicable. If the original band, where $D/\omega_0 \geqslant 20$, is wider, its range of application is limited to even smaller values of $\lambda (\lambda \lesssim 0.7)$.

In conclusion we note that allowance for the Coulomb interaction does not change the conclusions of this study regarding the applicability of the adiabatic approximation even at the metallic carrier concentrations, since at $\lambda \gtrsim 1$ the radius of the polaron state is on the order of the lattice constant. In the many-polaron theory of superconductivity[4] a systematic allowance for this interaction leads to a renormalization of the binding energy of the bipolaron.

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