On formation of a barrier in two-dimensional self-localization

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The possibility of a small polaron formation within the microscopic model of the local electron-phonon interaction is considered. It is shown that in the 2D case the solution of the Schrödinger equation on a discrete lattice in the adiabatic approximation gives evidence for the presence of a barrier that separates self-localized polaron and delocalized electron states. The polaron stability and metastability regions are found. The possibility of polaron formation in high-T_c superconductors is discussed.

The discovery of high-T_c superconductivity stimulated a great number of theoretical treatments of this problem. The antiferromagnetic order observed in the CuO_2 planes at low carrier concentration indicates that the magnetic subsystem is important in the formation of the superconducting state.[1] Structural phase transitions as well as a number of other experiments[2] give evidence for the important role of the electron-phonon interaction. The reports concerning the direct observation of polarons in the dielectric phase with carrier doping[3] and a small but nonzero isotope effect[4] lead to the same conclusion. The recent work of Mott[5] and Auerbach and Larson[6] is also noteworthy. It has been shown[6] that a magnetic polaron in the CuO_2 planes has a lower ground-state energy than any other known magnetic phase. Note that magnetic polaron formation must be accompanied by the usual polaronic effect.[5]

In this connection a recent series of experiments on measurement of the optical conductivity seems of great importance.[7–9] In the insulating state the conductivity $\sigma(\omega)$ shows no absorption in the region $\omega < 1.5$–2 eV. For $\omega > 2$ eV, $\sigma(\omega)$ has a large step that corresponds to a "charge-transfer gap" in the excitation spectrum. If some carriers are introduced into the CuO_2 plane by doping, a Drude-like peak appears and its weight grows with the carrier concentration. Two peaks in $\sigma(\omega)$ occur for ω lying inside the "charge-transfer gap" at $\omega = 0.07$–0.1 eV and $\omega = 0.8$–1 eV. The effective total carrier concentration N_{eff}, defined as the integra of $\sigma(\omega)$ over the charge-transfer gap, increases faster than one could expect from the doped carrier concentration. A qualitative interpretation of these experiments within the small polaron model was proposed by Mihailovic.[10] The mid-infrared structure of the optical conductivity corresponds to the excitation of the polaron into delocalized states with energy on the order of the Frank–Condon shift.

In the present work the possibility of a small-size polaron (SSP) formation in the 2D cases is analyzed within the model of the strain interaction between an electron and dispersionless phonons. It is shown that taking into account the finite bandwidth leads to self-localization with barrier formation (see Ref. 11). Nonadiabatic corrections to the energy of the SSP are calculated in the 2D case.

In order to treat the problem of SSP formation, we consider the following model: an electron interacts locally with a single disperionless phonon mode Ω_0. The Lagrangian of this system is

$$L = \sum_i \left[\frac{1}{2\Omega_0} (\partial_\tau \phi_i)^2 - \frac{\Omega_0}{2} \phi_i^2 + i\bar{\Psi}_i \partial_\tau \Psi_i - \sqrt{2}g\Omega_0 \bar{\Psi}_i \Psi_i \phi_i \right]$$

$$- t\sum_{(i,j)} \bar{\Psi}_i \Psi_j \,, \tag{1}$$

where $\bar{\Psi}_i$ (Ψ_i) is the fermion fields describing creation (annihilation of an electron at the site i, ϕ_i is the scalar field corresponding to a local displacement at the site i,

$$\phi_i = \frac{1}{\sqrt{2}} (b_i^+ + b_i),$$

b_i^+ (b_i) being the local phonon creation (annihilation) operator, t is the hopping integral, and g is the dimensionless electron-phonon coupling. Note that $\phi \propto M^{1/4}$, $g \propto M^{1/4}$ and $\Omega_0 \propto M^{-1/2}$ (M is the ion's mass). Since the parameter $g^2\Omega_0$ is independent of M, it is possible to use the adiabatic approximation.

Since the Lagrangian (1) is quadratic in the fermion fields, we can perform explicitly the functional integration over these fields. Formally the problem is reduced to calculating the fermionic determinant in an arbitrary field ϕ. As a result of this procedure, we obtain the effective boson action, its minimum in ϕ bring the phonon vacuum. Note that the effective action is not merely a classical quantity, since it involves quantum fluctuations arising from the fermionic determinant. Below we apply the method used widely in the theory of non-zero least action. The main idea of this approximation is to substitute the Schrödinger wave functions for the fermion fields ψ_i:[12]

$$\exp(iS_{eff}) \approx \sum_{n_r} \tilde{C}(n_r) \exp[iT(E_{cl}(\phi) + \sum_{n_r} n_r \varepsilon_r)] \,, \tag{2}$$

where $\tilde{C}(n_r)$ is a combinatorial factor, $E_{cl}(\phi)$ is the classical energy of the field ϕ_i, n_r is the occupation number, and ε_r is the eigenvalue of the Schrödinger equation in the field ϕ.

Applying the variational procedure in ϕ to (2), one can obtain the following set of equations:

$$\phi_i = -\sqrt{2}g\sum_r |\psi_i|^2 n_r, \tag{3}$$

$$t\sum_l \psi_{i+l}^{(r)} + \sqrt{2}g\Omega_0 \psi_i^{(r)}\phi_i = \varepsilon_r \psi_i^{(r)}. \tag{4}$$

The equations (3) and (4) give the polaron energy and are written in the approximation $\partial\phi/\partial\tau = 0$ (adiabatic approximation[11]). Note that similar equations have been derived in Ref. 6 for a magnetic polaron in an antiferromagnetic background. Equation (4) contains no spatial derivatives, since the bare phonon subsystem is supposed to be dispersionless.

Assuming that a single fermion mode is excited, the solution of Eqs. (3) and (4) can be written as a power series in $t/(g^2\Omega_0)$ $(2g^2\Omega_0 \gg t)$:[11]

$$\psi_0(0) = 1 - z\frac{t^2}{8}(g^2\Omega_0)^2, \quad \psi_0(1) = -\frac{t}{2}g^2\Omega_0, \quad (5)$$

$$\varepsilon_0 = -2g^2\Omega_0. \quad (6)$$

The total energy of the system is the sum of the electronic energy ε_0 in the strain field ϕ and the energy of the field ϕ itself:

$$E_{tot} = \varepsilon_0 + \sum_i \frac{\Omega_0}{2}\phi_i^2 = \varepsilon_0 + g^2\Omega_0\sum_i |\psi_i|^4$$

$$\approx -g^2\Omega_0 - \frac{zt^2}{g^2\Omega_0}. \quad (7)$$

Note that the correction to E_{tot} is of order t^2 and consistent with the result obtained by summation of a definite set of diagrams with noncrossing phonon lines.[13] Equations (3) and (4) have the extended solution

$$\psi_i = \frac{1}{\sqrt{N}}\exp(i\mathbf{ki}),$$

which reaches the minimum at the point $\mathbf{k} = (\pi,\pi)$ of the Brillouin zone and corresponds to the absence of a self-localized state.

For the 1D case in the limit $g^2\Omega_0 \gg t$ the solution of Eqs. (3) and (4) is given by expressions (5) and (6) with $z = 2$. In the opposite limiting case $g^2\Omega_0 \ll t$ one can obtain the following exact solution:[14]

$$\psi(x) = \sqrt{\frac{|\varepsilon + 2t|}{g^2\Omega_0}}\cosh^{-1}\left(x\sqrt{\frac{|\varepsilon + 2t|}{ta^2}}\right),$$

$$\varepsilon = -2t - \frac{g^4\Omega_0^2}{4t}. \quad (8)$$

The results of numerical analysis of Eqs. (3) and (4) are represented in Fig. 1. As can be seen from Fig. 1, a self-trapped state exists for all g of interest. If we have $g^2\Omega_0 < t$ the radius of this self-trapped state is restricted to the lattice constant. Further decrease of electron-phonon coupling g leads to an increase in the radius. Thus in the 1D case a smooth transition from a SSP with energy $E_p \propto g^2$ to a large-size polaron with energy $E_p \propto g^4$ takes place and self-localization occurs without barrier formation.

In the 2D case the situation changes drastically (Fig. 1). The bound states of Eqs. (3) and (4) arise for $g^2 > g_{c1}^2$ ($g_{c1}^2 = 2.85t/\Omega_0$ in 2D). However, the polaron energy is greater than the energy of delocalized state. For

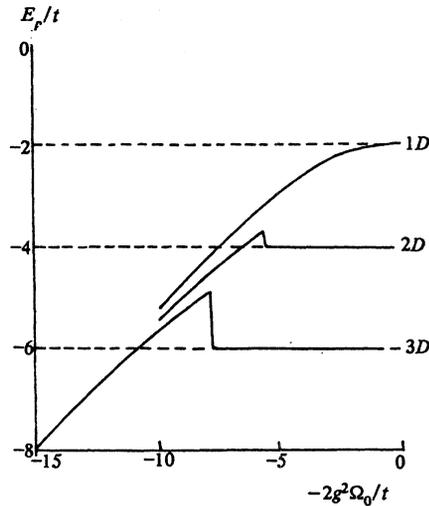$$g_2 > g_{c2}^2 \approx \left(z - \frac{1}{2}\right)\frac{t}{\Omega_0},$$

FIG. 1. Energy of the self-localized state versus coupling $g^2\Omega_0$. Dashed lines correspond to the energy of the delocalized states.

the SSP becomes the ground state of the system. Thus the formation of a self-localized state in the 2D case is accompanied by the formation of a barrier that separates the self-localized and delocalized states. Note that the formation of the barrier is associated with a finite bandwidth. Numerical study of Eqs. (3) and (4) in the effective mass approximation indicates that self-localization occurs without barrier formation. This is attributed to the fact that as the polaron size decreases the kinetic energy and the strain energy increase in proportional to $1/R^2$, where R is the radius of the self-localized state.[15] However,[11] self-localization takes place within the interatomic space, and the finite bandwidth (lattice discreteness) plays a major role. It means that the kinetic energy scaling[15] is broken. The dependence of energy on the polaron radius is shown in Fig. 2. For $g_{c1} < g < g_{c2}$ the SSP is metastable. For $g > g_{c2}$ the SSP has lower energy than the delocalized state. Note that for

$$g_{c2} < g < g_{c3} = \sqrt{2\pi t/\Omega_0}$$

the delocalized state is metastable. In the 3D case lattice discreteness has no qualitative effect on the results. Note
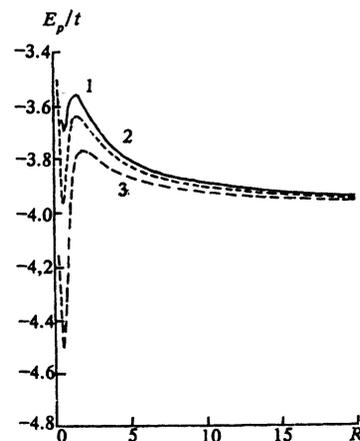

FIG. 2. Energy versus polaron radius for various $g^2\Omega_0$ value: 1 — $g_{c1} < g < g_{c2}$, 2—$g = g_{c2}$, 3—$g_{c2} < g < g_{c3}$.

that these results are in good agreement with the Monte-Carlo calculations.[16] These results show the region of g value where the self-localized solution is metastable in the $2D$ and $3D$ cases.

The set of equations (3) and (4) and their solutions (5) and (6) correspond to the adiabatic approximation in the polaron theory. The calculation of fluctuation corrections in the vicinity of the classical phonon vacuum results in nonadiabatic corrections to the SSP energy. As a result, new phonon frequencies will be present in the Lagrangian.

For this purpose we expand the effective action $S_{\text{eff}}(\phi)$ in fluctuations

$$\delta\phi_i = \phi(i, \tau) - \phi_0(i). \tag{9}$$

Keeping in mind that the minimum of the action $S_{\text{eff}}(\phi)$ is realized in the phonon vacuum ϕ_0, we calculate the corrections to S_{eff} corresponding to the one-loop approximation:

$$\delta S = ig^2\Omega_0^2 \sum_{i,j} \delta\phi_i(\Omega)\delta\phi_j(-\Omega)G_{i,j}(\omega)G_{j,i}(\omega + \Omega), \tag{10}$$

where

$$G_{i,j}(\omega) = \frac{\psi_0(i)\psi_0^*(j)}{\omega - \varepsilon_0 + \mu} + \sum_k \frac{\psi_k(i)\psi_k^*(j)}{\omega - \varepsilon_k + \mu}$$

is the Green's function describing the motion of an electron in the vacuum field $\phi_0(i)$, $\psi_0(i)$ is the wavefunction corresponding to the ground state energy ε_0,

$$\varepsilon_k = 2t\sum_{i=1}^d \cos k_i,$$

$\psi_k(i)$ is the wavefunction of an electron corresponding to the energy ε_k, and $\delta\phi_i(\Omega)$ is a fluctuation in the field $\phi_0(i)$. Direct evaluation of (9) gives the expression for δS to lowest order in $t/g^2\Omega_0$:

$$\delta S = \frac{\Omega_0 z t^2}{8(g^2\Omega_0)^2} |\delta\phi_0(\Omega)|^2, \tag{11}$$

where the subscript 0 refers to the centre of the polaron. The additional contribution from (11) leads to the renormalized phonon mode (see Refs. 11, 17):

$$\Omega = \Omega_0[1 - \frac{zt^2}{2}(g^2\Omega_0)^2]^{1/2}. \tag{12}$$

Also note that the expression (12) differs from the similar one obtained in Ref. 17 which is likely to be valid for $\Omega_0 \gg t$ (antiadiabatic approximation).

The evaluation of the functional integral over $\delta\phi_i(\Omega)$ yields a nonadiabatic correction to the ground-state energy of the SSP:

$$\Delta E = -\frac{1}{8}\frac{zt^2\Omega_0}{(g^2\Omega_0)^2}. \tag{13}$$

In the region of the coupling g where the delocalized solution is the most favorable $(\phi_0(i) = 0)$ the corresponding nonadiabatic correction is well-known:[18]

$$\Delta E = -g^2\Omega_0^2/\pi^2 t^2. \tag{14}$$

To summarize, we have shown in the $2D$ case within the model of local electron-phonon interaction that the formation of a polaron is accompanied by the formation of a barrier attributed to the finite electronic bandwidth (lattice discreteness). In addition, lattice discreteness has no influence on the qualitative picture of self-localized state formation in the $1D$ and $3D$ cases.

In the $2D$ and $3D$ cases the criterion for the formation of a SSP has the following form in the notation of:[17]

$$\lambda = \frac{g^2\Omega_0}{D} > \lambda_c, \tag{15}$$

where D is the bandwidth $(D = zt)$ and $\lambda_c \approx 1$.

Note that within this model the discontinuous transition to the delocalized state occurs at $\lambda = \lambda_c$. The criterion (15) differs from the similar one $\lambda_c^* \approx 1/\sqrt{2z}$ obtained in Refs. 13, 18. This criterion determines a small value of the hopping corrections to the polaronic shift. However, the transition to the delocalized state occurs before these corrections become large. The self-trapped state is formed at $\lambda = \lambda_c^*$, but it is metastable.

The $1D$ case is essentially different from the $2D$ and $3D$ ones. The self-trapped state is the ground state of the system at any value of the electron-phonon coupling. For $\lambda > \lambda_c^*$ the radius of this state is determined by the value of the lattice constant (SSP). The radius grows rapidly for $\lambda < \lambda_c^*$ $[r \sim a/\lambda$ if $\lambda \ll 1$; see Eq. (8)]. Thus, unlike the $2D$ and $3D$ cases in the $1D$ case the transition from the polaron state to the delocalized electronic state is continuous.

The criterion (15) for the formation of SSP is rather strict. The estimate of g^2 for $D \sim 0.5$–1 eV and the most favorable value of $\Omega_0 \sim 0.1$ eV is equal to 5–10. This value implies that the effective mass of the polaron is strongly renormalized and means that it is practically localized. However, correlation effects play a major role in high-T_c superconductors and lead to the effective narrowing of electronic bandwidth[19] and even to the formation of magnetic polarons.[5,6,20] These effects may change the criterion (15) substantially. In addition, the formation of magnetic polarons must enhance the standard polaronic effects.[5] In this connection it is worth mentioning that the isotope effect has been observed in all high-T_c superconductors.[4] This fact indicates that the phonon subsystem is of great importance for the transition to superconducting state.

It is also interesting to note that intermediate-size polarons are supposed to be formed in high-T_c superconductors.[21] In that case the increase of the radius of such a polaron causes a decrease in its effective mass. Within our model the formation of an intermediate-size polaron is impossible. For this reason in our case the only way to decrease the effective mass is to decrease the initial bandwidth and electron-phonon coupling simultaneously, keeping their ratio λ constant.

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