Self-localization of composite spin-lattice polarons

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Self-localization of holes in the Holstein t-J model is studied in the adiabatic limit using exact diagonalization and the retraceable path approximation. It is shown that the critical electron-phonon coupling λc decreases with increasing J and that this behavior is determined mainly by the incoherent rather than by the coherent motion of the hole. The obtained spin correlation functions in the localized region can be understood within a percolation picture where antiferromagnetic order can persist up to a substantial hole doping. These results restrict the possibility of self-localization of holes in lightly doped cuprates.

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The interplay of strong electronic correlations and electron-phonon (EP) interactions in the formation of dressed quasi-particles is one of central puzzles of high-Tc superconductors. Recent ARPES experiments in underdoped cuprates were interpreted in terms of strong EP coupling giving rise to self-localization of holes. Similar effects can be expected in the manganites in the colossal magnetoresistance regime, where polarons are not only dressed by spin and lattice excitations but also polarize the orbitals in the neighborhood of the holes. The properties of composite polarons are subtle and not well understood, as the different mechanisms involved may support or compete with each other.

Electronic motion in weakly doped Mott insulators is determined by the constraint of no double occupancy of sites which renders the motion of holes predominantly incoherent with an energy scale t, the bare hopping energy of electrons. In addition, the antiferromagnetic (AF) exchange interaction J allows for spin flips leading to coherent hole motion at the bottom of the band with a dispersion characterized by J. In the presence of strong EP coupling the spin polaron transforms into a spin-lattice polaron. The formation of this composite polaron affects in general both the coherent translational as well as the internal incoherent motion. In recent studies of Holstein t-J models appropriate for cuprates, it has been found that the effect of EP-interaction on spin-polarons is strongly enhanced as compared to polarons in uncorrelated systems. In particular, the critical EP-coupling λc for self-localization of composite polarons is significantly reduced, and in the regime λ < λc the coherent polaron mass is strongly enhanced as compared to the uncorrelated case.

In spite of several studies there are important open questions, which we address in the following: (i) Is the critical EP coupling λc for self-localization determined by the coherent bandwidth or rather by the incoherent hole motion? (ii) What is the dependence of λc on J? (iii) Furthermore, is the observed low doping concentration x ~ 0.02 for the destruction of AF long-range order in cuprates compatible with self-localized polarons?

To answer the above questions we investigate the Holstein t-J model in the adiabatic limit where the kinetic energy of the lattice can be neglected:

\[ H = - \sum_{<ij>} t_{ij} (\tilde{c}^+_{i\sigma} \tilde{c}_{j\sigma} + h.c) + J \sum_{<ij>} (S_i S_j - \frac{1}{4} n_i n_j) - g \sum_i u_i n_i^+ + \frac{K}{2} \sum_i u_i^2. \]  

(1)

The first two terms in Eq. 1 represent the Hamiltonian \( H_{t-J} \) of the t-J model. The transfer matrix elements \( t_{ij} \) include both nearest and next-nearest neighbor hoppings \( t' \), respectively. The third term describes the lattice potential \( H_{sp} \) proportional to the EP coupling constant \( g \), the local displacement fields \( u_i \), and the hole density operator \( n_i^h = 1 - n_i = 1 - \sum_{\sigma} \tilde{c}^+_{i\sigma} \tilde{c}_{i\sigma} \). In high-Tc cuprates this term reflects the breathing motion of oxygen ions around the hole and the subsequent change of the Zhang-Rice singlet energy due to the local lattice distortion. The last term is the elastic energy \( H_{ph} \) with force constant \( K \). In the adiabatic limit displacements \( u_i \) can be treated classically and are in the equilibrium determined by \( u_i = (g/K) < n_i^h > \). At vanishing and weak EP-coupling \( H \) exhibits coherent (delocalized) quasi-particles with bandwidth \( \sim J \). Nevertheless, we will show in the following that many features of \( H \) can be very well represented by the simpler Holstein t-J model in the retraceable path approximation (rpa), where the motion of carriers is entirely incoherent. It is convenient to express results in terms of the dimensionless EP coupling parameter \( \lambda = g^2/8Kt \). For noninteracting electrons we have then \( \lambda_c \sim 1 \). In the following we also put \( t = K = 1 \).

The Hamiltonian Eq. 1 is solved by exact diagonalization (ED) of small planar systems with a square lattice. The determination of the critical EP coupling is straightforward, namely, it separates ground states with...
homogeneous and inhomogeneous lattice displacements $u_i$ corresponding to a delocalized and a self-localized polaron solution, respectively. Since the itinerant ground state for a hole in the $t$-$J$ model is at $k_0 = (\pi/2, \pi/2)$, the ground state is degenerate. This degeneracy leads in general to inhomogeneous $u_i$ which spoil the interpretation \[5, \overline{6}\]. We avoid this problem by choosing twisted boundary conditions which lift the degeneracy. For fixed $u_i$ we find then the ground state using ED for systems with $N = 18$ and 20 sites, whereby the equilibrium is reached by the iteration of the self-consistency relation $\lambda < \lambda_c$. 

The $t$-$J_2$ Holstein model is solved within rpa, which excludes loop motion and thus neglects a very small coherent bandwidth that arises at small $J_2$ from loop trajectories \[\overline{11}\]. Using a Bethe lattice the expectation value of the electronic energy, namely, $\langle H_{el} \rangle + \langle H_{ep} \rangle$, is given by the lowest energy eigenvalue $\lambda_0$ of the symmetric matrix $H_{lt}$ with the elements

$$H_{00} = J_z - gu_0, \quad H_{ii} = \left(\frac{3}{2} + l\right)J_z - gu_i \quad \text{for} \quad l = 1, 2,.. \quad (2)$$

$$H_{0l} = -2t, \quad H_{ll+1} = -\sqrt{3}t \quad \text{for} \quad l = 0, 1, .. \quad (3)$$

Here $l = 0, 1, 2..$ denotes the shell of l-th nearest neighbors consisting of $N_l$ ions with $N_0 = 1$ and $N_1 = 4 \cdot 3^{l-1}$ for $l = 1, 2,..$, and $u_i$ is the displacement of one of the equivalent ions in the shell $l$. The expectation value of the density at the ion $i$, $\langle n_i^e \rangle$, is equal to $|e(0, l)|^2/N_l$, where $e(0, l)$ is the normalized eigenvector belonging to the lowest eigenvalue $\lambda_0$ and $l$ is the shell index of the ion $i$. Finally, the total energy $\lambda_0 + \langle H_{ph} \rangle$ is minimized with respect to the displacements $\{u_l\}$.

Fig. [1]a) shows the electronic energy $E_{el} = \langle H_{el} \rangle + \langle H_{ep} \rangle$ and the total energy $E_{tot} = E_{el} + \langle H_{ph} \rangle$ as a function of $\lambda$ for the Holstein $t$-$J$ model and $J = 0.1, 0.3$ and 0.5. The results were obtained by ED for one single hole and clusters with $N = 20$ sites. For $\lambda \gg 1$ the hole is completely localized yielding $E_{el} = 2E_{tot} \sim -8t/\lambda$. In the limit $\lambda \to 0$ the well-known single-hole energies $E_{el}^0$ of the $t$-$J$ model are reproduced. For $J \to 0$ the energy is close to the rpa result $E_{el}^0 \sim -2\sqrt{3}t$ (Note that we avoid in the ED studies very small values for $J$ where the ground state is Nagaoka-type ferromagnetic with $E_{el}^0 \sim -4t$). For a finite $J$ $E_{el}$ increases because the itinerant hole weakens the antiferromagnetic bonding. Using ED results for spin correlation functions this increase is about $4.72J$ which agrees well with Fig.1a). For $\lambda < \lambda_c$ the homogenous solution with $E_{el}^0$ is stable (the small slope appearing in Fig.1a) is a finite size effect since $u_i \sim 1/N$). For $\lambda > \lambda_c$ the localized solution has the lowest total energy approaching the linear behavior at large $\lambda$. Due to the first-order transition between itinerant and localized solutions the ED data exhibit a small jump in $E_{el}$ and a change in slope in $E_{tot}$ at $\lambda_c$.

FIG. 1: (color online) Electronic and total energies $E_{el}$ and $E_{tot}$, respectively, as a function of $\lambda$ for (a) the Holstein $t$-$J$ model using ED and (b) the Holstein $t$-$J_2$ model using rpa. The inset explaining the curves in (a) also holds for (b).

Fig. [1]b) shows the same quantities as in Fig. [1]a) but calculated for the Holstein $t$-$J_2$ model using rpa. The curves are nearly identical with those of Fig. [1]a). The main difference is the absence of a well defined transition, at least in the cases $J = 0.3$ and 0.5. For $J = 0.1$ $E_{tot}$ and, to a lesser degree, $E_{el}$ are practically constant up to $\lambda \sim 0.4$. While for small $J$ $E_{tot}$ decreases gently with increasing $\lambda$ $E_{el}$ shows a sudden decrease at $\lambda \sim 0.5$ before reaching its asymptotic linear behavior. Similar features are seen in the curve for $J = 0.1$ in Fig. [1]a) obtained by ED. In the limit $J \to 0$ $E_{tot}$ and $E_{el}$ are identical and equal to $-\sqrt{12t}$ up to a critical coupling $\lambda_{el}^{(0)} \sim 0.580$. For $\lambda > \lambda_{el}^{(0)}$ there exist two solutions of the extremal equation. One is the homogenous solution where $E_{tot}$ and $E_{el}$ are identical and independent of $\lambda$. The second solution describes a localized polaron where $E_{tot}$ exhibits an upward jump by about 0.4 and $E_{el}$ a downward jump by about 0.6 at $\lambda_{el}^{(0)}$. This means that the localized solution is unstable in the interval $[\lambda_{el}^{(0)}, \lambda_c]$, where $E_{tot}$ of the localized solution crosses $E_{tot}$ of the homogenous solution at $\lambda_c \sim 0.662$. With increasing $J$ the jumps are replaced by cross-overs with decreasing absolute changes until for $J > 0.06$ there exists only one solution of the extremal equation describing a crossover from an extended to a localized polaron.

Fig. [2] shows ED data (circles and squares) for $\lambda_{el}$ as a function of $J$. The dashed curve represents data for $t' = -0.3$, i.e., a case with a larger and more dispersive coherent part than for $t' = 0$. As a result, the dashed curve lies above the ED data for $t' = 0$, showing, that
decreasing the mass $M$ for the coherent motion leads to an increase in $\lambda_c$ as expected. Increasing $J$ also decreases $M$ but Fig. 2 implies that in this case $\lambda_c$ decreases and does not increase. This is unexpected, since an interpretation in terms of an opposite trend $\lambda_c \sim J$ has been given in a study of the Holstein $t$-$J$ model [7].

In order to understand the dependence of $\lambda_c$ on $J$ we have estimated $\lambda_c$ using the rpa and the Born approximation. For $J < 0.06$ the rpa leads to a first-order transition between a localized and delocalized ground state, the resulting $\lambda_c$'s are shown as crosses in Fig. 2. In order to find a sharp transition at larger values of $J$ the energy of the homogeneous solution has to be compared with the localized one. An estimate for the loss of coherent kinetic energy in the localized state is $\Delta E_{kin} = \epsilon - \epsilon(k_0) \sim 0.65J$ where $\epsilon(k)$ is the quasiparticle dispersion and $\epsilon$ its average value. $\lambda_c$ then follows from the rpa result via the relation $\Delta E_{kin} = E_{tot}(0) - E_{tot}(\lambda_c)$. The resulting values (crosses for $J \geq 0.1$ in Fig. 2) give the right trend but cannot reproduce quantitatively the strong decrease of $\lambda_c$ with $J$ of the ED results. Modifying the Born approximation [6] to take inhomogenous local potentials into account while retaining the homogenous self-energy we have determined the smallest value of $\lambda$ where a localized solution exists and identified this value with $\lambda_c$. The resulting diamonds in Fig. 2 are rather near to the ED data.

The above results may be interpreted in simple physical terms as follows: At $J = 0$ the hole motion is entirely incoherent and determined by the energy scale $t$. The rpa solution in this region a sharp transition at $\lambda_c$ from a very localized polaron to a very extended object. The obtained critical value $\lambda_c \sim 0.6$ is somewhat reduced compared to the free case $\sim 0.85$. For larger $J$ the transition in rpa evolves into a pronounced crossover in $E_{tot}(\lambda)$ as is evident from Fig. 2b), where the crossover value $\lambda^*$ moves to lower $\lambda$'s due to the reduced polaron radius. Although the sharp transition finally involves $\Delta E_{kin} \propto J$, $\lambda_c$ is effectively governed by the incoherent solution and its $\lambda^*$. The decrease of $\lambda_c$ with $J$ reflects a smooth transition from the large energy scale $t$ characteristic for the incoherent motion to the scale $J$ relevant for the coherent part. This picture may also explain ED data showing that $\lambda_c$ actually increases with $J$ at large $J \sim t$ where the incoherent part is small compared to the coherent one. Fig. 3(a) shows the hole density at the center of the localized state, denoted by $n_0$, as a function of $\lambda$.

FIG. 3: (color online) (a) Density $n_0$ in the center of the polaron as a function of $\lambda$. Results obtained by ED for the $t$-$J$ model (symbols) are compared with rpa results for the $t$-$J_z$ model (lines). (b) Log-linear plot of displacement fields $u_l$ of the Holstein $t$-$J_z$ model versus distance $l$ showing the exponential decay of hole distribution in the self-localized regime. The symbols are results from the ED of clusters with $N = 20$ sites in the localized region, the lines correspond to the rpa. $n_0 = 1$ corresponds to a completely localized and $n_0 = 1/N$ to an extended state. The agreement between both results in Fig. 3(a) is excellent, showing, that the degree of localization of the polaron is to a very good approximation determined by the incoherent part of the hole motion described well by the rpa. In the limit $J \to 0$ the rpa yields a curve for $n_0$ which is zero for $\lambda < \lambda_c^{(0)}$, jumps to about 0.65 at $\lambda_c^{(0)}$, and then smoothly approaches the $J = 0.1$ curve. The crossover value $\lambda^*$ is clearly visible in Fig. 3(a) and can be identified as the inflection point in the $n_0(\lambda)$ curves. Fig. 3(b) illustrates the qualitative change
of the displacements $u_l$ at $\lambda_c$, i.e., for $\lambda > \lambda_c$ $u_l$ decays exponentially with distance $l$.

An important consequence for magnetism follows from self-localization of holes in weakly doped high-$T_c$ superconductors. It is well known that AF long-range order vanishes in hole-doped cuprates at quite low doping concentration $x_{AF} \sim 0.02 - 0.04$. This small value is due to the incoherent motion of holes which destroys the AF order; on the other hand a percolative model based on static holes and broken AF bonds leads to much larger critical concentrations $x_{AF} \sim 0.5$. Self-localization at strong EP coupling $\lambda > \lambda_c$ would hinder the incoherent motion of holes and preserve the antiferromagnetic order.

The strong enhancement of AF correlations in the self-localized regime $\lambda > \lambda_c$ is displayed in Fig. 4 which shows ED data for the first ($d^2 = 1$) and third ($d^2 = 4$) nearest-neighbor spin correlation function (SCF) of the $t$-$J$ model. For the undoped Heisenberg antiferromagnet the corresponding SCF values are -0.116 and 0.067, correspondingly. For $\lambda >> \lambda_c$, the hole is totally localized and one expects a decrease of these values due to the four broken bonds yielding a reduction factor of 16/18 for 18 sites. The resulting values -0.103 and 0.059 agree quite well with the numerical data at large $\lambda$ in Fig. 4 suggesting the applicability of a simple percolation picture at large $\lambda$. The figure also illustrates that for a given type of neighbors the SCF become independent of $J$ well above $\lambda_c$ which reflects the fact that the localizing EP coupling and not the string potential $J$, Eq. (2), determines the extension of the polaron. The slight decrease of SCF’s with decreasing $\lambda$ in the localized region can be understood in the rpa. With decreasing $\lambda$ the hole explores more and more neighboring sites producing hereby an increasing number of broken bonds which reduce the SCF. Such a picture reproduces for $\lambda > 0.6$ quantitatively the ED data for SCF in the Ising, and to a good degree, also in the Heisenberg case. This suggests that for the considered doping $x \sim 0.05$ long-range AF order persists throughout the localized region and that immobile holes reduce mainly the magnitude of the SCF’s but not their spatial decay.

In conclusion, we have shown that the critical EP coupling $\lambda_c$ for self-localization in the Holstein $t$-$J$ model decreases with $J$ and that the crossover between basically incoherent (coherent) motion of the hole at small (large) $J$ is responsible for this decrease. Exact diagonalization results for $\lambda_c$, the density and displacement distribution as well as spin correlation functions have been obtained and successfully interpreted in the localized regime within the retraceable path approximation. Our results suggest that for dopings $x \sim 0.05$ self-localized holes cannot suppress sufficiently antiferromagnetic correlations to explain the observed absence of long-range order in the cuprates at this doping level. We therefore believe that holes in lightly doped cuprates are not self-localized, and that their EP coupling is below the critical value $\lambda_c \sim 0.25$ for $J = 0.3$. Our conclusions are consistent with the observation of a sharp quasi-particle peak in ARPES experiments of 3 % doped LaSrCuO$_4$[11], and also agree with the explanation of transport and optical data in lightly doped La$_2$CuO$_4$ in terms of holes bound to impurities at low but delocalized at high temperatures [12, 13].

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