Non-local composite spin-lattice polarons in high temperature superconductors

G. De Filippis1, V. Cataudella1, A. S. Mishchenko2,3, and N. Nagaosa2,4

1Coherentia-CNR-INFM and Dip. di Scienze Fisiche - Università di Napoli Federico II - I-80126 Napoli, Italy
2CREST, Japan Science and Technology Agency (JST) - AIST - 1-1-1 - Higashi - Tsukuba 305-8562 - Japan
3RRC "Kurchatov Institute" - 123182 - Moscow - Russia
4CREST, Department of Applied Physics, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113, Japan
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The non-local nature of the polaron formation in t-t′-t″-J model is studied in large lattices up to 64 sites by developing a new numerical method. We show that the effect of longer-range hoppings t′ and t″ is a large anisotropy of the electron-phonon interaction (EPI) leading to a completely different influence of EPI on the nodal and antinodal points in agreement with the experiments. Furthermore, nonlocal EPI preserves polaron’s quantum motion, which destroys the antiferromagnetic order effectively, even at strong coupling regime, although the quasi-particle weight in angle-resolved-photoemission spectroscopy is strongly suppressed.

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It is a matter of long debates whether electron-phonon interaction (EPI) plays an essential role in the formation of the puzzling properties of high temperature superconductors [1]. Early theoretical studies of the angle resolved photoemission spectroscopy (ARPES) of undoped cuprates were based on the t-t′-t″-J model, where doped holes into an antiferromagnetic (AFM) material are characterized by exchange constant J and hoppings up to 3rd near neighbors(NN) with amplitudes t, t′ and t″. This approach successfully described the dispersion of the experimentally observed peak [2,3] and appeared to exclude strong EPI. However, there was a strong contradiction between the theoretical and experimental line-shapes: in contrast with the very broad peak in experiments [1] the theory predicted a sharp peak [2,3,4]. This contradiction was resolved under assumption that the undoped parent compounds are in the strong coupling regime (SCR) of the EPI. In the simplest case of t-t′-t″-J model, where a hole interacts with dispersionless optical phonons through on-site local coupling, it was shown that at SCR the spectral weight of the quasiparticle is almost completely transferred to the broad Franck-Condon shake-off peak which inherits the dispersion of the hole when it does not interact with phonons [4]. Furthermore, the inheritance of the dispersion of the non-interacting quasiparticle by the Franck-Condon peak was shown to be a property of a broad class of models with EPI [5]. Recently, the relevance of the t-J-Holstein model for cuprates has been rather convincingly questioned [8]. It has been shown that SCR leads to a picture of a localized static hole with 4 broken bonds about it. In this case the percolative model predicts that AFM order survives up to critical concentration x ≈ 0.5 in contradiction with the experimental value x ≈ 0.02 – 0.04. Another problem of the t-J-Holstein model is the very large effective mass in the whole SCR [6] contradicting transport and optical properties of lightly doped cuprates [7].

The above arguments, in favor or against the SCR in undoped cuprates, suggest that the answer must be found in a class of more realistic t-t′-t″-J models where EPI, as it is in cuprates [10], is nonlocal. Besides of the particular relevance of the above models in the physics of high temperature superconductivity, there is a general inquiry asking whether long-range interaction can introduce profound qualitative difference compared with t-J-Holstein model. However, study of the t-t′-t″-J model with nonlocal EPI by exact diagonalization (ED) and Diagrammatic Monte Carlo (DMC) methods is hindered by their limitations. ED method has been restricted to only small two-dimensional systems [8,11] and the nonlocal effects have not been studied so far. On the other hand the study of the incoherent motion of the hole requires transformation of the DMC method [6] into the direct space where DMC encounters the sign problem [5].

In this Letter we apply recently introduced coherent state basis approach [12] to the t-t′-t″-J model with nonlocal EPI, and develop a Coherent States Lanczos (CSL) method which is able to provide a reliable description of the ground state properties of two-dimensional systems up to 64 sites. We validate it by successfully comparing the results with exact DMC data. We find that in the t-t′-t″-J model with local Holstein EPI, in contrast with t-J-Holstein model, the influence of the EPI on the properties of nodal k = (π/2,π/2) and antinodal k = (π,0) points is significantly different introducing a considerable anisotropy driven by long-range hole hoppings: the antinodal states are in the SCR with nearly zero quasiparticle weight whereas the quasiparticles in the nodal point are only weakly dressed by phonons in a very broad range of EPI. We also show that nonlocal EPI qualitatively changes the basic features of the composite spin-lattice polarons. First, according to general result [12], effective mass in the SCR of nonlocal EPI is considerably lighter than that of a model with local EPI. Second, the motion of the hole over the NN is not strongly suppressed by nonlocal EPI and, thus, the ten-
dency toward robust AFM order up to high doping levels, found in t-J-Holstein model, does not survive in the more realistic t-t’-t"-J model with nonlocal EPI.

The minimal Hamiltonian for t-t’-t"-J model with extended EPI is a sum of t-t’-t"-J Hamiltonian \( H_{tt’t"} \) \[3, 4, 5\], EPI Hamiltonian \( H_{ph} \), and Hamiltonian of dispersionless phonons \( H_{ph} = \omega_0 \sum_i c_i^\dagger c_i \) \((c_i^\dagger \) is the creation operator of a phonon at site \( i \) with frequency \( \omega_0 \)). In the spin wave approximation the t-t’-t"-J Hamiltonian reads

\[
H_{tt’t"} = \sum_{\vec{q}} \left[ \Omega_{\vec{q}} \left( a_{\vec{q}}^\dagger a_{\vec{q}} + b_{\vec{q}}^\dagger b_{\vec{q}} \right) + \epsilon_{\vec{q}} \left( h_{\vec{q}}^\dagger h_{\vec{q}} + f_{\vec{q}}^\dagger f_{\vec{q}} \right) \right] + \\
\sum_{\vec{q}} \sum_{\delta} \left( \sum_{i \in A} M_{\vec{q},i} f_{i+\delta} h_i^\dagger + \sum_{i \in B} M_{\vec{q},i} f_{i+\delta} h_i^\dagger + h.c. \right),
\]

where \( A \) (\( B \)) is the sublattice with spin up (down) and \( a_{\vec{q}}^\dagger \) \((b_{\vec{q}}^\dagger)\) is the operator creating magnon in the \( A \) (\( B \)) sublattice with dispersion \( \Omega_{\vec{q}} \). The operator in the direct space \( f_i^\dagger \langle h_i^\dagger \rangle \) creates a spinless hole on the site \( i \) of the sublattice \( A \) (\( B \)). The bare hole dispersion is \( \epsilon_{\vec{q}} = 4t \cos(q_x) \cos(q_y) + 2t’ \cos(2q_y) + \cos(2q_y) \) and the hole-magnon coupling is \( M_{\vec{q},i} = t\sqrt{2/N} \left( u_\vec{q} e^{i\vec{q} \cdot \vec{R}_i} + v_\vec{q} e^{i\vec{q} \cdot \vec{R}_i+i} \right) \), where \( u_\vec{q} \) and \( v_\vec{q} \) are the Bogoliubov factors, \( \delta \) is a unitary vector connecting \( NN \) sites, and \( N \) is the number of lattice sites. The sum over \( \vec{q} \) is restricted inside the magnetic Brillouin zone. The EPI Hamiltonian

\[
H_{ph} = \omega_0 \sum_l g(l) \sum_{i \in A} f_i^\dagger f_i \left( c_{i+l}^\dagger + c_{i+l} \right) + \\
\omega_0 \sum_l g(l) \sum_{i \in B} h_i^\dagger h_i \left( c_{i+l}^\dagger + c_{i+l} \right)
\]

in defined in terms of Holstein, \( g(0) = g \), and nonlocal coupling to the \( NN \) lattice displacements \( g(\delta) = g_1 \). Below we set \( h = 1 \) and \( t = 1 \).

In order to study the ground state of this model, we use CSL procedure based on the Lanczos recursion method that, starting from the hole in the quantum Neel state without excited magnons, \( \langle 0 \rangle^{(m)} \), generates the subspace spanned by the basis

\[
|j, \mu_1, ..., \mu_N, q_1, ..., q_l, l\rangle = |h\rangle_j \prod_i |\mu_i\rangle |q_1, ..., q_l, l\rangle,
\]

where \( |h\rangle_j \) indicates the state with the hole on the site \( j \), and \( i \) runs over the lattice sites. The notation \( |q_1, ..., q_l, l\rangle \) labels the standard Bonfim-Reiter L-magnon states which are sufficient to reproduce the results of self-consistent Born approximation (SCBA) \[13\]. These states are given in terms of an ordered product of \( a_{\vec{q}}^\dagger \) and \( b_{\vec{q}}^\dagger \) operators acting on the magnon vacuum state \( |q_1, ..., q_l, l\rangle = a_{\vec{q}_1}^\dagger b_{\vec{q}_2}^\dagger ... |0\rangle^{(m)} \langle q_1, ..., q_l, l\rangle = b_{\vec{q}_1}^\dagger b_{\vec{q}_2}^\dagger ... |0\rangle^{(m)} \).
sis\cite{2} is over-complete. Naturally, particular realization of the CSL approach requires a truncation. Actually only few CS are enough to reproduce the ground state properties of the composite spin-lattice polaron. Comparison with exact DMC data shows that the following truncation scheme minimizes the computational efforts with high accuracy for results. A finite number \( M_{ph} \) of CS is chosen, characterized by real values \( h_\alpha \ (\alpha = 0, ..., M_{ph} - 1) \) equidistant in the range \([0, 1]\), and only the phonon states \( \Pi_{i=1}^{N} |h_\alpha, i\rangle \) with \( \sum_{i=1}^{N} \alpha_i \leq M_{c, ph} \) are included into the basis. Besides, taking advantage of the fact that the hopping and EPI are restricted to 3rd NN and NN respectively, we restrict the states with nonzero parameters \( h \) to 3rd NN from the hole. Comparison (Fig. 1) of CSL results for t-J-Holstein model on \( 8 \times 8 \) lattice with approximation-free result by DMC in the thermodynamic limit\cite{3} shows that our method at \( M_{ph} = 4 \) and \( M_{c, ph} = 3 \) is valid for all ranges of EPI\cite{1}. The small differences in the weak EPI regime are mainly due to finite size effects. At large dimensionless couplings \( \lambda = g^2 \omega_0 / 4t \) the polaron size becomes small and the agreement becomes excellent. Our method perfectly reproduces crossover between weak and strong coupling regimes at critical value \( \lambda_c \approx 0.4 \) where i) the spectral weight goes to zero, indicating suppression of the coherent motion; ii) the lattice distortions rapidly increase; and iii) the size of magnetic polaron reduces.

First, we extend t-J-Holstein model with local EPI adding next NN, \( t' \), and next next NN, \( t'' \), hoppings. Comparing physical properties of these models we observe that the longer-range hoppings introduce a strong anisotropy. Physical properties of the states in the nodal \((\pi/2, \pi/2)\) and antinodal \((\pi, 0)\) points are very similar in the t-J-Holstein model but considerably different in the \(tt't''\)J-Holstein model (Fig. 2 and 3), as it is evident comparing \( Z\)-factor (Fig. 2a and 2c), mean kinetic energy (Fig. 2b and 2d), and average number of phonons (Fig. 3a and 3c). There is a wide range of the EPI strengths from the weak to intermediate coupling regime where the hole is a heavily dressed polaron in the antinodal point but an almost free particle in the nodal one. Comparing spectral weights and kinetic energies of the two models we conclude that the longer-range hoppings reinforce coherent motion in the nodal point and suppress it in the antinodal one. To characterize the anisotropy induced by \( t' \) and \( t'' \) we calculate the phonon probability distributions function (PPDF) \( P(x) = \langle \Psi_{GS} | x | \Psi_{GS} \rangle \), where \( \Psi_{GS} \) is the wave function of the ground state and \( x \) is the lattice distortion of the site where the hole is, just below the crossover into the SCR (Fig. 3b and 3d). We find that for the t-J-Holstein model both nodal and antinodal points display a bimodal structure characteristic of the intermediate coupling regime, where the ground state of the system is a quantum mixture of localized and delocalized states\cite{18}. To the contrary, in the \( tt't''\)J-Holstein model the antinodal point has bimodal PPDF while that at the nodal point displays the maximum at small lattice distortions \( x \), characteristic of weak coupling regime. The resulting picture of the anisotropic EPI, considerably stronger near the antinodal point than at the nodal one, is expected to be qualitatively similar in the case of an underdoped system and is in line with experimental findings. The explanation of the vertical dispersion of the ARPES near the antinodal points requires large \( Z \) (weaker coupling) along the nodal direction and much smaller \( Z \) (stronger coupling) along the antinodal ones\cite{19}. To study the role of nonlocal EPI we compare the properties of the \( tt't''\)J-Holstein model with that including nonlocal coupling to the NN lattice displacements \( g_1 = g/2 \ (\text{Eq.}\ 1) \). In both cases the decrease of the \( Z\)-factor (Fig. 4a) indicates the suppression of hole ground

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig2.pdf}
\caption{The spectral weight (a and c) and the mean kinetic energy (b and d) as function of \( \lambda \) for nodal (circles) and antinodal (triangles) points. The parameter values are: \( J/t = 0.4, \omega_0/t = 0.2, g_1 = 0, N = 64. \)}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig3.pdf}
\caption{(Color online) Average number of phonons (a and c) for nodal (circles) and antinodal (triangles) points; PPDF (b and d) for nodal (solid lines) and antinodal (dashed lines) points. The parameter values are: \( J/t = 0.4, \omega_0/t = 0.2, g_1 = 0, N = 64. \)}
\end{figure}
state contribution to ARPES. However, the increase of the EPI range slightly enhances (reduces) the suppression of the Z-factor at $\lambda < \lambda_c$ ($\lambda > \lambda_c$). On the contrary, when EPI is non local the polaron effective mass, that is a measure of the coherent motion, becomes larger in the weak coupling regime and smaller in the SCR. In the latter case, the mass for nonlocal EPI at $\lambda = 1.1\lambda_c$ is one order of magnitude lighter: diagonal $m_d$ (along $k_x = k_y$) and transverse $m_t$ (along $k_x = -k_y$) masses for local EPI are $m_d = 71.4$ and $m_t = 65.7$ whereas for nonlocal EPI their values are $m_d = 7.1$ and $m_t = 7.5$, respectively, in units of the bare effective masses ($g = g_1 = 0$). Similar effects have been discussed in a number of different models [13, 20].

Figure 4b and 4c show the dependence of spin deviation and the contribution to the kinetic energy arising due to magnon assisted NN hoppings, $K_t$, on the dimensionless coupling constant $\lambda$. Spin deviation, $SD = (S_{AFM} - (S_{NN}))/S_{AFM}$, measures how much the neighboring spin to the hole, $S_{NN}$, deviates from its value in an ideal antiferromagnet ($S_{AFM}$). Absolute value of $K_t$ and $SD$ are the measure of the intensity of the NN hopping and include both coherent and incoherent contributions. The decrease of the two above quantities, (Fig. 4b and 4c), signals on the suppression of the motion over NN as expected in presence of hole-phonon interaction. However, by increasing the EPI range, the motion of the hole on NN is suppressed by the nonlocal EPI much less effectively than it is in the case of the Holstein coupling. This effect is one of the main results of this work. It can be easily interpreted in the SCR where the notion of the adiabatic potential makes sense. For the Holstein local coupling the self-consistent adiabatic potential for the hole is a deep $\delta$-function, preventing, thus, the hole from the motion over the NN. To the contrary, the motion of the hole in case of a long-range EPI is not restricted to a single site, preserving, thus, the motion over the NN even at SCR. This allows an effective reduction of AFM order also in presence of strong hole-phonon interactions.

In conclusion, we demonstrated the important role played by the long range interactions in the problem of hole-phonon coupling for the physics of high temperature superconductors. Long-range electron hoppings lead to a strong anisotropy of the EPI which is possibly observed in the angle resolved spectroscopy of cuprates. The most important results are that the non-local EPI makes polaron lighter and occurs to be not effective in the suppression of the motion of the hole over the NN making, thus, the models with strong nonlocal EPI justified for description of weakly doped high temperature superconductors.

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