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Optical conductivity of spin/lattice polarons in underdoped copper oxides

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ABSTRACT

Optical and spectral properties of carriers in the presence of strong antiferromagnetic correlations and interacting with optical phonon modes are analyzed using Dynamical Mean Field Theory. We interpret the mid-infrared band in $\sigma(\omega)$ in term of mixed spin lattice polaronic excitations which arise from the stabilization of the lattice polaron due to the antiferromagnetic correlations. We compare our results with experimental data in NCCO showing that the doping and temperature dependences of the optical conductivity in this compound is naturally reproduced within a spin/lattice polaronic model.

1. Introduction

In this work we study the formation of spin/lattice polarons in underdoped cuprates focusing mainly on *n*-doped compounds. The phase diagram of *n*-doped cuprates shows similarities and differences with that of *p*-doped. The major similarity is the existence of an antiferromagnetic (AF) phase at half filling which is suppressed upon doping in favor of a superconducting phase as well as of the presence of a pseudogap phase at high temperature. Among the differences we note a stronger stabilization of the AF phase in the *n*-doped samples compared to *p*-doped and a relative depression of the superconducting phase. If we associate the underdoped phase with the presence of AF correlation we see that this phase is much more extended in *n*-doped.

Let us consider the underdoped region which is wider in *n*-doped materials. An interesting and comprehensive study was carried out by neutron scattering by Motoyama et al. for NCCO [2]. The underdoped region consists of a “normal” phase at high temperature, a pseudo gap (PG) phase at intermediate temperatures and an AF phase at low temperature. These phases are characterized by increasing spin correlations. The pseudogap phase boundary was determined by optical measurements by Onose et al. [11] which will be further discussed in the paper. In the underdoped samples at the PG temperature there is the onset of magnetic correlation showed by an increase of magnetic correlation length as far as the temperature decreases [2]. Finally a phase with long-range magnetic order is established at a much lower temperature. Clearly magnetic interactions are important in this region but we also concentrate our attention to the interplay between magnetic and charge–lattice interactions.

Recently isotope effects were found in the “kink” feature of the ARPES dispersion curves pointing to a phononic origin of such a feature [3]. Also for *n*-doped cuprates signatures of interaction with a bosonic degree of freedom were found e.g. in the ARPES measurements by Schmitt et al. [12] on NCCO sample at optimal doping. They show an anisotropic electron-phonon (e-ph) coupling with intermedium/strong strength. However such value of e-ph couplings are in general not sufficient to produce a definite lattice polaronic state by itself. We may also notice that in view of strong correlations effects the estimate of e-ph coupling is not trivial [16,4]. In the underdoped samples, signatures of polaron formation can be deduced by the ARPES data [5,6] characterized by a low-energy coherent peak with very low spectral weight and by a higher-energy peak which shows a dispersion related to AF background. The width of such high-energy peak is not Lorentzian, whereas it can be fitted with a Gaussian which resembles an incoherent feature related to the dressing of a particle by a large number of oscillator states, which is precisely what happen in a polaronic system.

2. Spin/lattice polarons from DMFT

We consider the t–J Holstein model which we analyze for a single particle (at low density). This model contains the basic features characteristic of the underdoped phase of the cuprates. In this model an electron moving in an AF background interacts with an optical phonon mode schematized by Einstein oscillators through

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the Hamiltonian

$$H = \frac{t}{2\sqrt{z}}\sum_{\langle ij\rangle}(h_j^\dagger h_i a_j + h.c.) + \frac{\tilde{J}}{2}\sum_i a_i^\dagger a_i + g\sum_i h_i^\dagger h_i (b_i + b_i^\dagger) + \omega_0 \sum_i b_i^\dagger b_i, \quad (1)$$

where z is the coordination number, $a^\dagger$ and $b^\dagger$ are the creation operators for boson spin defects and phonons respectively, and $h^\dagger$ is the single spinless charge operator. A local el-ph coupling constant $\lambda = g^2/\omega_0 t$ can be defined as the polaron energy in units of the half-bandwidth t. The parameter $\tilde{J}$ is an effective exchange interaction. It is linked to the microscopic J by the relation $\tilde{J} = Jm$, where m is the average on-site magnetization which, in the $z \gg 1$ limit, is governed by the Curie–Weiss equation $m = \tan h(\beta Jm/4)$ with Néel temperature $T_N = J/4$.

Evidences of both a coherent quasiparticle peak at low-energy and incoherent dispersive peak at higher energy for moderate value of the e-ph coupling were found at zero temperature in this model [7]. Noticeably the dispersion of the higher energy broad feature is of magnetic origin in the sense that its dispersion resembles that of an electron (hole) in the t–J model without e-ph coupling and has a minimum at $(\pi/2, \pi/2)$. We are going to describe by our theory the optical signature which comes from incoherent excitations at non zero temperature.

The Holstein t–J model can be solved exactly for a single electron (hole) by Dynamical Mean Field Theory at non zero temperature. The solution is given analytically in terms of a self-consistent solution for the Green's function. The AF is treated at the mean field level where magnons are dispersionless and have a characteristic temperature dependent energy $\tilde{J}/2$ [8]. The analytical solution can be used in a phenomenological theory (described in details later) by assuming that the main effect of electron or hole doping is to destroy antiferromagnetism thus allowing for a doping dependence of the effective local field [13]. This effect can be seen e.g. in the measurements of the magnetic moment by Wakimoto et al. as a function of doping in LASCO [9]. The DMFT solution has some important drawbacks basically related to the fact that it enforces a t–J_z model and consequently neglects coherent propagation of the electron (hole). However we are interested in incoherent feature of optical conductivity as well as some local features of the polaronic state which have a spin/lattice entangled origin and can be accessed by DMFT. Despite the reduction to t–J_z the spin polaron incoherent processes are still retained by DMFT: an electron or hole moves in a classical AF background leaving a defects string behind. This motion has an energy cost thus producing a real localization. Quantum fluctuations of the AF background prevent a truly localized state. However the local structure of the spin polaron is still present in this formalism in strict analogy with the localized Landau–Pekar description of the lattice polaron [1]. Adding e-ph interaction will add also lattice–charge correlations which are localized due to the localized nature of the solution even when the quantum fluctuations of phonon are retained in our theory. As for a pure lattice polaron these local features are well described in our localized formalism. Following Ref. [1] we can calculate several properties which indicate the formation of polaron having spin, lattice of both spin/lattice character. Using these features we can draw the phase diagram shown schematically in Fig. 1 at $T = 0$. Two crossover lines are relevant in the phase diagram of Fig. 1.

(i) A large to small lattice polaron crossover (red solid line) that locates the points at which the contribution of the one phonon state in the ground state exceeds that of the vacuum.
(ii) A large to small spin polaron crossover (blue dashed line) which is the locus of the points at which the mean number of spin defects around the spin/lattice polarons becomes less that one half [1].

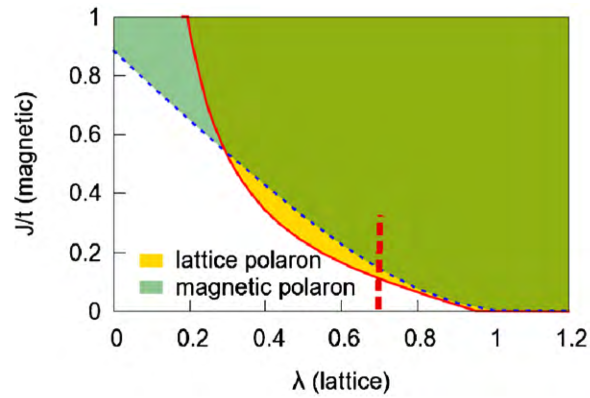

Fig. 1. The phase diagram of the model at $T = 0.0$ for $\omega_0/t = 0.1$. Solid red line marks the large to small lattice polaron crossover. Dashed blue line marks the large to small spin polaron crossover. Bold red dashed line indicates pictorially how a variation of J due to doping and temperature can intersect the polaron crossover. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Both small spin and lattice polaron are stabilized by increasing λ. In similar way an increase of J at moderate value of $\lambda (\lambda < 1)$ favors the formation of lattice polaron. It is essential for our scenario of underdoped cuprates that the lattice polaron can be tuned by antiferromagnetic correlation and can be stabilized by them even when no lattice polaron exists in the absence of magnetic interactions.

3. Optical properties and comparison with experiments

Within the context of DMFT the optical conductivity (OC) can be evaluated by means of the Kubo formula. Although DMFT neglects vertex corrections, they seem not to affect much the system when a lattice polaron state is well established as can be shown by direct comparison with exact diagonalization results [10,8].

The main outcomes from our DMFT analytical solution of the model of Eq. (1) can be summarized in two items [8].

- First, the OC gap closes as the energy scale J goes to zero. On the contrary as J increases the optical conductivity shows a polaronic feature which is J independent. The nature of the peak in the OC changes thus smoothly from a magnetic origin at small J (peak at $J/2$) to a lattice origin for large J with a peak located around the polaron energy $E_p = \lambda t$.
- Second, a gap filling occurs when the temperature increases in a way similar to what occurs for a purely lattice polaron, but at lower value of λ.

We compare our theory with a comprehensive set of optical data available for NCCO and published in the work by Onose et al. [11]. We have analyzed both doping and temperature dependence for 4 dopings ($\delta = 0.05$, 0.075, 0.10, 0.125). First of all no signature of long-range AF ordering is found in the temperature evolution of the optical data at the Néel temperature. Instead an optical gap forms at a higher temperature T^* which is related to the onset of local AF correlations. Both gap closing and gap filling behaviors are present in the data of Ref. [11] respectively at low temperature decreasing the doping, and at given doping e.g. increasing the temperature.

To compare with experimental data we choose J in our model as a measure of (local) AF correlation. A *doping dependent J* is derived by the pseudogap temperature by equating the Néel temperature *of the model* to the *experimental* optical pseudogap temperature

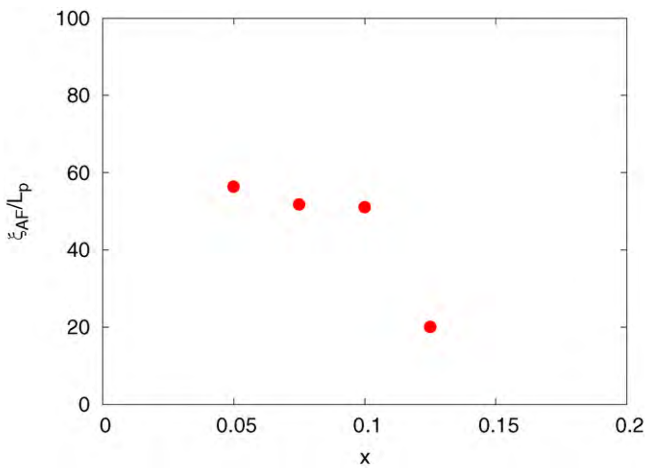

Fig. 2. The AF correlation length at T_{PG} derived for the analytic formula (Eq. (2)) of Ref. [2] divided by our estimates of the polaron extension from Refs. [1,8] as a function of doping.

T^*. Then we set the phonon frequency ($\omega_0 = 70$ meV) and the half-bandwidth parameter (t = eV) to a typical values in cuprates. Finally we fix the value of λ (assumed doping independent) by fitting the OC at the lowest value of temperature/doping available. We get $\lambda = 0.7$ which compares well with measurements at optimal doping [12]. For the chosen values of the parameters the polaron crossover is intersected along the dashed line shown in Fig. 1 while the effective $\tilde{J}$ varies with doping.

The model Eq. (1) explicitly assumes that the charge is moving in an AF background, therefore to use it to describe the optical absorption in the PG phase we must have that the local antiferromagnetic correlations have an extent larger than that of the spin/lattice polaron which is formed once the e-ph interaction is taken into account. To check that the polaron radius is lower that the AF correlation length we can estimate the AF correlation length at T_{PG} from the data of Ref. [2]. Using the procedure described in [1] we estimate the polaron radius at the same temperature obtaining the data shown in Fig. 2.

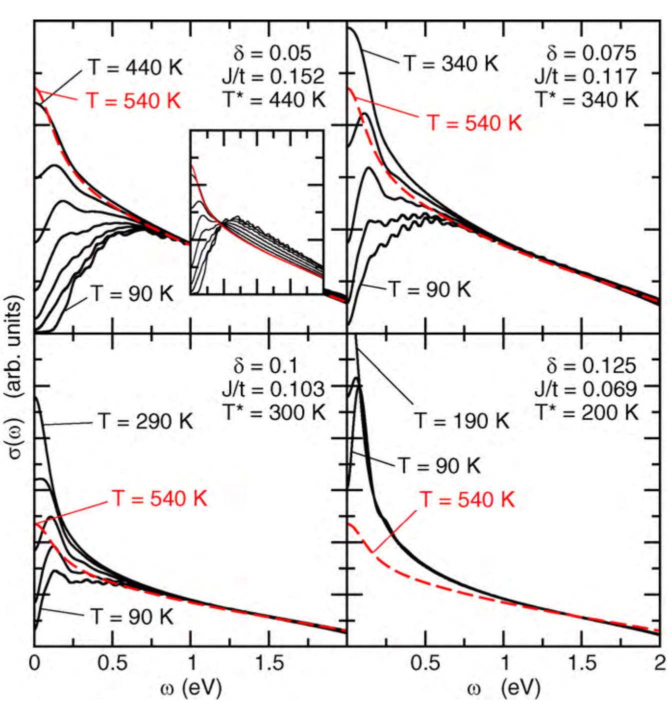

Fig. 3. (From Ref. [13]) Temperature evolution of the optical conductivity $\sigma(\omega)$ for different exchange couplings (dopings) and for (($T \leq T^*$): T = 90, 140, 190, 240, 290, 340, 390, 440 K). Also shown is the optical conductivity at T = 540 K in the normal state (dashed red line). Inset: optical conductivity for $\delta = 0.05$ normalized by its total spectral weight. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Fig. 3 shows the results for optical conductivity for the 4 data sets analyzed. Both the gap-closing with doping and the gap-filling with temperature are recovered in our analysis. However it can be seen in experimental data a sort of conservation of optical spectral weight in the mid-infrared frequency window 0.12–1.4 eV. If we implement such a conservation in our data we can also get the isosbestic (equal absorption) point shown for the lowest doping $x = 0.05$ [13].

4. Conclusions

Using DMFT it is possible to access the incoherent features of optical conductivity $\sigma(\omega)$ which are related to the internal structure of the polaron, disregarding coherent motion which should be reflected in the Drude-like peak. We have shown that magnetic and electron–phonon interactions sustain each other in establishing a polaronic regime where a small polaron can be formed even at intermediate value of e-ph coupling ($\lambda \simeq 0.7$). Such a mixed spin lattice polaronic excitation is responsible of the mid-infrared band (MIR) in $\sigma(\omega)$. Within such polaronic scenario the optical pseudogap as well as its doping and temperature dependence can be naturally explained. When the e-ph coupling is intermediate, AF correlations tune the formation of the lattice polaron which is responsible for the MIR absorption edge. As far as the AF correlations are depressed upon hole doping, the polaronic character of the carriers is lost leading to a closing of the MIR band in $\sigma(\omega)$. On the other hand an increase of temperature leads to a filling of the MIR band. We have compared our results with experimental data in NCCO showing that the doping and temperature dependences of the optical conductivity in these compounds are naturally reproduced within a spin/lattice polaronic model.

As a last remark we stress the difference between our interpretation and that of Mishchenko and coworkers [14,15] about the same subjects. In our view the magnetic correlations crucially determine the possibility of spin/lattice polaron formation. They are depressed by increasing doping or temperature leading to a disappearance of optical polaronic features. In Refs. [14,15] instead the variation of e-ph coupling with doping having a fixed value of magnetic interaction leads to the progressive loosing of polaronic signatures while doping increase.

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