Temperature Dependence of the Angle Resolved Photoemission Spectra in the Undoped Cuprates: Self-Consistent Approach to the t-J Holstein Model

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(Received 20 June 2007; published 30 November 2007; corrected 20 February 2008)

We develop a novel self-consistent approach for studying the angle resolved photoemission spectra (ARPES) of a hole in the t-J Holstein model giving perfect agreement with numerically exact diagrammatic Monte Carlo (DMC) data at zero temperature for all regimes of electron-phonon coupling. Generalizing the approach to finite temperatures, we find that the anomalous temperature dependence of the ARPES in undoped cuprates is explained by cooperative interplay of coupling of the hole to magnetic fluctuations and strong electron-phonon interaction.

DOI: 10.1103/PhysRevLett.99.226402 PACS numbers: 71.10.Fd, 02.70.Ss, 71.38.−k, 79.60.−i

The parent compounds of the high temperature superconductors, i.e., the undoped cuprates, turned out to be an ideal arena for studying the dynamical properties of the single polaron in an antiferromagnetic background [1]. The polaron formation is expected from the ionic nature of the parent compounds and the resulting strong electron-phonon interaction (EPI), together with the strong electron correlation as evidenced by the realized Mott insulating state. Therefore, the interplay between the magnetism and EPI is a key to resolve the quantum dynamics of the doped carrier into the cuprates.

This problem has been theoretically studied [2,3] in terms of a hole in the t-J model coupled by short-range Holstein interaction to optical phonons (t-J Holstein model). The theoretical predictions were verified experimentally [4,5], and it was shown that the real quasiparticle peak has only a tiny weight at lower binding energy compared with the involving multiphonon excitations Franck-Condon peak. The former one can hardly be observed in ARPES experiments because of tiny spectral weight while the latter broad one reproduces the dispersion of the pure t-J model.

It has been shown [2,6,7] that the polaronic effect is enhanced by the entanglement of the interactions of a hole with magnons and phonons, and this interplay is the unique feature of the cuprates. Indeed, the EPI alone is absolutely unable to explain the temperature dependence of ARPES because experimentally found temperature dependence of ARPES is considerably larger than that predicted by polaronic theory [8]. A magnetic subsystem alone is also not a suitable candidate [9] since the typical energy scale of magnons $2J \approx 0.2$ eV is even larger than that of phonons $\omega_0 \approx 0.04$ eV. Given such a desperate situation, there is a temptation to explain the temperature driven peak broadening by the destruction of the antiferromagnetic background due to the quantum or thermal fluctuations as approaching the Neél temperature. Recent studies revealed one more puzzle questioning the polaronic scenario: the temperature dependence of the linewidth is linear in the range 400 K $< T <$ 200 K [5] and extrapolates to zero linewidth at zero temperature [2,3,6]. From the theoretical point of view, it is a challenge to study the temperature dependence of the Lehman spectral function (LSF) of the single hole in the t-J Holstein model, which corresponds to the ARPES experiment in the undoped system [1], in the intermediate or strong coupling regime in a reliable way, which has never been achieved to the best of our knowledge.

In the present Letter, we solve the t-J Holstein model by a novel Hybrid Dynamical Momentum Average (HDMA) self-consistent method uniting the advantages of Momentum Average (MA) approach [10,11], keeping the essential information on the magnon dispersion, and Dynamical Mean Field (DMF) technique, properly taking into account strong but essentially local coupling to the lattice. Comparing results of the HDMA method with exact data obtained by diagrammatic Monte Carlo (DMC) approach, we show that the HDMA method provides accurate results for t-J Holstein model where quasiparticle weakly interacts with delocalized magnons and is strongly coupled to local vibrations. Making a generalization of HDMA technique to finite temperatures, we show that the basic features of anomalous temperature dependence of ARPES in undoped cuprates can be explained by mutual interplay of magnetic and lattice systems in the t-J Holstein model.

The Hamiltonian of the t-J Holstein model in the spin-wave approximation [12–14] reads

$$H = \omega_0 \sum_{k} b_k^\dagger b_k + g\omega_0 \sum_{k,q} [h_k^\dagger h_{k-q} b_q + \text{H.c.}] + \sum_{k} \omega_k a_k^\dagger a_k + \sum_{k,q} [M_{k,q} h_k^\dagger h_{k-q} a_q + \text{H.c.}] \quad (1)$$

where $h_k^\dagger$, $a_k^\dagger$, and $b_k^\dagger$ are the creation operators of a hole, a magnon, and a phonon of momentum $\boldsymbol{k}$, respectively. The hole motion is associated with the creation and annihilation of magnons of energy $\omega_{\boldsymbol{k}} = 2J\sqrt{1-\gamma_{\boldsymbol{k}}^2}$ ($\gamma_{\boldsymbol{k}} = (\cos k_x + \cos k_y)/2$) with coupling vertex $M_{\boldsymbol{k},\boldsymbol{q}} = 4t(u_q\gamma_{\boldsymbol{k}-\boldsymbol{q}} + v_q\gamma_{\boldsymbol{k}})/\sqrt{N}$ where $u_{\boldsymbol{q}} = \sqrt{(1+\alpha_q)/(2\alpha_q)}$, $v_{\boldsymbol{q}} = -\text{sgn}(\gamma_{\boldsymbol{q}})\sqrt{(1-\alpha_q)/(2\alpha_{\boldsymbol{q}})}$, $\alpha_{\boldsymbol{q}} = \omega_{\boldsymbol{q}}/2J$, and N is the number of lattice sites. The short-range interaction between the hole and local distortions due to dispersionless optical vibrations with frequency ω_0 is described by the coupling constant g. For the following, we use the corresponding experiment values $J/t = 0.3$, $\omega_0/t = 0.1$ [1], to measure all energies in units of t and assume Planck and Boltzmann constants equal to unity.

The generic features of the model (1), causing difficulties to semianalytic approaches, is the intrinsic interplay between interaction of a hole with magnons, reducing the spectral weight of its quasiparticle as well as reducing its bandwidth, and coupling to local phonons backing the self-trapping of the quasiparticle [15]. Brute force disentangling of these two contributions is impossible because the energy scales of the two processes are of the same order [15]. The only attempts which were successful so far, in quantitative description of the spectral properties of the model (1) at zero temperature, were based on numerically involved methods, such as exact diagonalization [15–17] or DMC [2] techniques. However, the results of the former method are limited to small lattices while the latter one, working in the thermodynamic limit, requires extremely extensive numerics efforts at finite temperature due to the "ill posed" nature of the analytic continuation [18].

In spite of the same energy scales involved into the hole-magnon and hole-phonon couplings, these two interactions are profoundly different since the coupling to magnons is essentially momentum dependent and always weak whereas that to phonons is local and can be strong. Indeed, since the spin $S = 1/2$ cannot flip more than one time, each site can not possess more than one magnon [19], and, thus, the weak-coupling Self-Consistent Born Approximation (SCBA) is satisfactory for small values of J/t [6,20]. To the contrary, SCBA fails for EPI even in the intermediate coupling limit [2]. Therefore, to cope with the t-J Holstein problem, it is enough to treat the essential momentum dependent coupling to magnons within the SCBA and to sum vibrational variables nonperturbatively, at least in some local approximation. Nonperturbative local approaches, valid at any coupling strength and neglecting the $\boldsymbol{k}$-dependence in the self-energy $\Sigma_{h\text{-ph}}(\boldsymbol{k},\omega)$, are DMF technique [21] and recently developed MA method [10,11]. They provide explicit form for the hole self-energy due to hole-phonon interaction in terms of a continued fraction

$$\Sigma_{h\text{-ph}}[\alpha(\omega)] = \frac{(g\omega_0)^2\alpha(\omega-\omega_0)}{1-\frac{2(g\omega_0)^2\alpha(\omega-\omega_0)\alpha(\omega-2\omega_0)}{1-\frac{3(g\omega_0)^2\alpha(\omega-2\omega_0)\alpha(\omega-3\omega_0)}{1-\ldots}}}. \quad (2)$$

The difference in DMF and MA lies in the definition of $\alpha(\omega)$ which is a function that has to be fixed by a self-consistent procedure in the DMF approach while it is identified with the $\boldsymbol{k}$-average of the bare Green's function in the MA scheme. Obviously, the MA scheme is preferable when one is interested in properties of 2D model (1) with highly anisotropic coupling $M_{\mathbf{k},q}$.

Summarizing the above considerations, a reasonable self-consistent procedure expresses the total self-energy of the hole as the sum of the self-energies caused by magnetic and phonon subsystems

$$\Sigma_{tJH}(\boldsymbol{k},\omega) = \Sigma_{h\text{-mag}}^{\text{SCBA}}(\boldsymbol{k},\omega) + \Sigma_{h\text{-ph}}[\alpha_{tJH}(\omega)]. \quad (3)$$

Weak and highly anisotropic interaction with magnons is taken into account in the SCBA

$$\Sigma_{h\text{-mag}}^{\text{SCBA}}(\boldsymbol{k},\omega) = \sum_{\boldsymbol{q}} \frac{M_{\boldsymbol{k},\boldsymbol{q}}^2}{\omega-\omega_{\boldsymbol{q}}-\Sigma_{tJH}(\boldsymbol{k}-\boldsymbol{q},\omega-\omega_{\boldsymbol{q}})+i\varepsilon}, \quad (4)$$

and the $\alpha(\omega)$-function for hole-phonon self-energy

$$\alpha_{tJH}(\omega) = \frac{1}{N}\sum_{\boldsymbol{k}} \frac{1}{\omega-\Sigma_{h\text{-mag}}^{\text{SCBA}}(\boldsymbol{k},\omega)+i\varepsilon} \quad (5)$$

is expressed in terms of momentum average of "bare" Green function whose $\boldsymbol{k}$-dependence is determined by the hole-magnon self-energy (3) in the SCBA. The Eqs. (2)–(5) constitute the self-consistent set of the HDMA approach.

The set of Eqs. (2)–(5) has the same structure as obtained in the DMF formulation of the t-J Holstein model [22,23], with the important exception that the $\alpha(\omega)$-function is determined not from the purely local self-consistent DMF condition but defined through the momentum average [10,11] of the bare Green function containing the anisotropic self-energy of two dimensional t-J model. Within the framework of DMF approach, the t-J Holstein model is indistinguishable from the t-J_z model where the hole coherent motion is suppressed [22]. To the contrary, the HDMA approach preserves coherent motion of the hole. The ground state energy, E_{GS}, and its spectral weight, $Z_{\text{GS}} = (1-\partial\Sigma_{tJH}/\partial\omega|_{\omega=E_{\text{GS}}})^{-1}$, are in good agreement with the data of numerically exact DMC approach [2], and the crossover to the strong coupling limit at

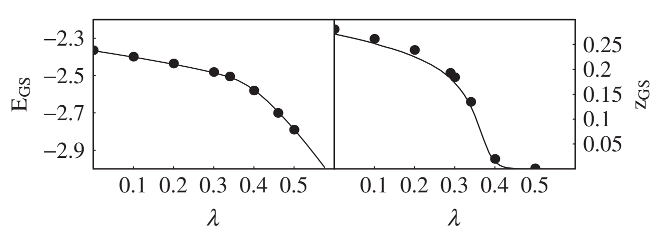

FIG. 1. The ground state energy (E_{GS}) and the spectral weight (z_{GS}) as a function of the EPI strength $\lambda = g^2\omega_0/4t$ in the DMC approach (line) and in the HDMA method (points). The error bars of the DMC data are less than the point size.

$\lambda \geq 0.4$ is perfectly reproduced (see Fig. 1). Indeed, HDMA is particularly successful in the strong coupling limit where the Franck-Condon peak inherits the dispersion of the hole interacting only with magnons [2] and, hence, the momentum dependence of the hole-magnon self-energy (3) is the only relevant **k**-dependence.

For further check of validity of the HDMA scheme, we compare the spectral function calculated on a lattice 64×64 with that obtained by the approximation-free DMC technique for pure *t-J* model ($\lambda = 0$) and *t-J* Holstein model in the weak ($\lambda = 0.1$), intermediate ($\lambda = 0.289$), and strong ($\lambda = 0.462$) coupling regimes (Fig. 2). The very good agreement of the overall shapes is observed for all coupling regimes, and mismatch of fine details can be attributed to finite size effects of 64×64 lattice [24] and the "local" approximation used in the present approach [Eq. (2)] that, at strong coupling, gives the typical oscillations with the period of phonon energy. Apart from these details, our approach is reliable in all coupling regimes and gives the spectral function with a computational effort much less than by the DMC approach.

An important advantage of our scheme is that its generalization to finite temperature is straightforward. Performing analytical continuation of $\Sigma^{\mathrm{SCBA}}_{h\text{-mag}}(\boldsymbol{k}, \omega)$ to Matsubara formalism, one gets [25,26]

$$\Sigma^{\mathrm{SCBA}}_{h\text{-mag}}(\boldsymbol{k}\omega) = \sum_{\boldsymbol{q}} \frac{M^2_{\boldsymbol{k},\boldsymbol{q}}[1 + n_b(\omega_{\mathbf{q}})]}{\omega - \omega_{\mathbf{q}} - \Sigma_{tJH}(\boldsymbol{k} - \boldsymbol{q}, \omega - \omega_{\boldsymbol{q}}) + i\varepsilon} + \sum_{\boldsymbol{q}} \frac{M^2_{\boldsymbol{k}+\boldsymbol{q},\boldsymbol{q}}[n_b(\omega_{\mathbf{q}})]}{\omega + \omega_{\boldsymbol{q}} - \Sigma_{tJH}(\boldsymbol{k} + \boldsymbol{q}, \omega + \omega_{\boldsymbol{q}}) + i\varepsilon}, \tag{6}$$

where $n_b(\omega)$ is the Bose-Einstein factor. For the generalization of Eq. (2), we followed in the following way. Since the $\alpha(\omega)$-function in Eq. (4) is reduced to a local momentum independent value, the temperature dependence of the hole self-energy can be included as follows [27,28]

$$\Sigma_{h\text{-ph}}[\alpha(\omega)] = \alpha^{-1}(\omega) - \sum_{n=0}^{\infty} \frac{(1-x)x^n}{\alpha^{-1}(\omega) - A_n(\omega) - B_n(\omega)} \tag{7}$$

where $x = \exp(-\beta\omega_0)$ and

$$A_n(\omega) = \frac{n(g\omega_0)^2\alpha(\omega+\omega_0)}{1 - \frac{(n-1)(g\omega_0)^2\alpha(\omega+\omega_0)\alpha(\omega+2\omega_0)}{1 - \frac{(n-2)(g\omega_0)^2\alpha(\omega+2\omega_0)\alpha(\omega+3\omega_0)}{1-\dots}}}$$

$$B_n(\omega) = \frac{(n+1)(g\omega_0)^2\alpha(\omega-\omega_0)}{1 - \frac{(n+2)(g\omega_0)^2\alpha(\omega-\omega_0)\alpha(\omega-2\omega_0)}{1 - \frac{(n+3)(g\omega_0)^2\alpha(\omega-2\omega_0)\alpha(\omega-3\omega_0)}{1-\dots}}}.$$

The Eqs. (3) and (5)–(7) provide a set of self-consistent equations that can be solved iteratively typically within 40 iterations. We verified the relevance of the relation (7) for our scheme checking the sum rules [10,11] and found that the first three sum rules for the LSF are satisfied at any temperature and EPI with high accuracy. Therefore, our results for peak energy and linewidth, determined mainly by the first and second sum rule, do not lose accuracy from the approximations made to obtain the HDMA self-consistent scheme.

The temperature dependence of LSF at $k = (\pi/2, \pi/2)$ at different values of EPI is shown in Fig. 3. The trends for peak position and linewidth are in agreement with experimental data [5,8,29,30]. With the increase of temperature, the binding energy [31] and width of the main broad peak increase while their intensity decreases. It is seen that all temperature driven effects are more pronounced in the *t-J* Holstein model than in the *t-J* model supporting the statement [2,6] that the entanglement of the magnetic and vibrational fluctuations is essential for cuprates and crucial for description of anomalously enhanced temperature driven effects in undoped compounds [8].

The temperature dependence of the peak width estimated through a Gaussian fitting is shown in Fig. 4. It is

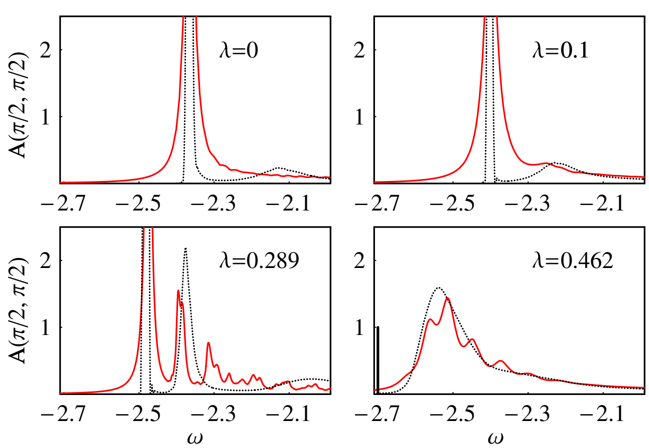

FIG. 2 (color online). The LSF $A(\pi/2, \pi/2)$ for different EPI λ in the HDMA (solid line) and DMC (dotted line) approaches. Vertical line in the panel with $\lambda = 0.462$ indicates the position of the ground state quasiparticle peak. The error bar of the ground state DMC energies is less than 10^{-4}.

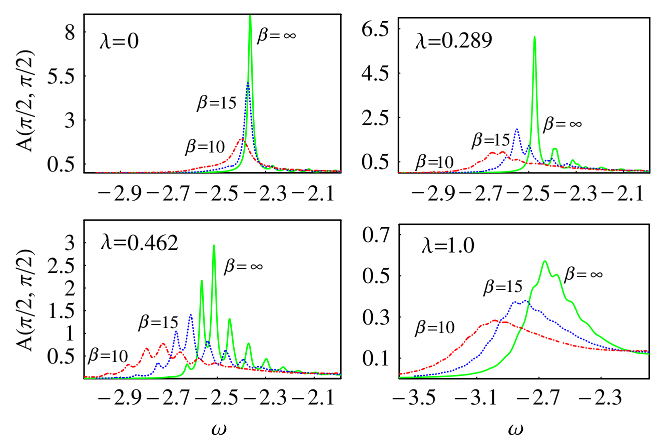

FIG. 3 (color online). The LSF ($A(\pi/2, \pi/2)$) for different EPI couplings λ and different temperatures $\beta = t/T$.

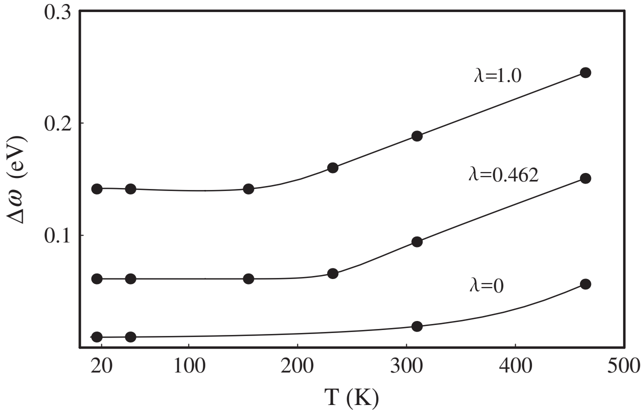

FIG. 4. The peak's width, $\Delta\omega$, as a function of the temperature, T, for the t-J model ($\lambda = 0$) and in strong EPI limit ($\lambda = 0.462$ and $\lambda = 1$). The temperature T is defined in units of Kelvin assuming $t = 0.4$ eV.

remarkable that in the strong coupling regime of the EPI, the peak width is almost constant up to $T \simeq \omega_0/2 \approx 200$ K and then, for $T \geqq \omega_0/2$, demonstrates linear dependence which, in according with experiment, can be naively extrapolated to almost zero value at zero temperature. Note, the temperature dependence is strongly enhanced in the strong coupling limit $\lambda > 0.4$ providing, in contrast with purely polaronic or purely magnetic models, correct order of magnitude of the effect, and even showing a good semiquantitative agreement with experiment [5,8,29,30]. For $\lambda = 0.462$, the peak width, in quantitative agreement with experiment [5], doubles in the range from 200 to 400 K though the absolute value of the peak width is a factor of 2 below the experimental values. On the other hand, the absolute value of the linewidth fits the experiment for $\lambda = 1$, but the enhancement of the width is a factor of 1.5 below that found experimentally [5]. The above discrepancies can be attributed to the fact that the longer range hoppings of the more realistic $tt't''$-J model and virtual charge fluctuations due to Hubbard corrections [32] are missing in the present approach, or as well to the fact that, in realistic systems, the holes are coupled to several phonon modes through the EPI of different strength [33].

In conclusion, by using a new hybrid dynamic momentum average approach to the calculation of a hole LSF in the t-J Holstein model, we have shown that the origin of the anomalously large temperature dependence of the ARPES in the undoped parent compound of high temperature superconductors originates from the constructive interplay between magnetic and strong electron-phonon interactions.

We acknowledge fruitful discussions with Professor Z. X. Shen, Dr. K. M. Shen, C. A. Perroni, and V. Marigliano Ramaglia. One of the authors (N. N.) acknowledges the financial support from the Grant-in-Aids under the Grant Nos. 15104006, 16076205, and 17105002, and NAREGI Nanoscience Project from the Ministry of Education, Culture, Sports, Science, and Technology, Japan. A. S. M. acknowledges support of RFBR No. 07-0200067-a.

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