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# Quasiparticle broadening in insulating copper oxides

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**Abstract**

We calculate the spectral function of the half-filled two-dimensional Hubbard model with realistic hopping integrals for $Sr_2CuO_2Cl_2$ within the dynamical mean-field theory at finite temperatures. It is shown that precursor effects of incommensurate spin dynamics lead to an incoherent broadening of the quasiparticle peaks on an energy scale that depends on local spin order. This might serve as an indirect method of detecting changes of local spin order under doping. 

*Keywords:* Copper-oxides; Hubbard model; Quasiparticles

Angle-resolved photoemission (ARPES) experiments on the insulating copper-oxide $Sr_2CuO_2Cl_2$, show that the measured quasiparticle dispersion can be well described within a $t$–$t'$–$t''$–$J$ model [1,2]. At the same time the quasiparticle (QP) widths obtained in experiment are of the order of $3J$, much wider than found in the Hubbard or (extended) $t$–$J$ model calculations at zero temperature, where QP peaks are normally artificially broadened [3,4]. The width of the QP peak is as large as its dispersion and poses a serious problem as there is no justification for such a heavy QP damping at present [5]. In the high-$T_c$ superconductors, where the $CuO_2$ planes are doped and become conducting, the large QP width remains. The ARPES experiments are conducted at relatively high temperatures that are of the order of the Néel temperature for this material (250 K). At these temperatures the presence of spin-waves contributes to the QP width. It was found, however, that in a $t$–$t'$–$t''$–$J$ framework the QP width for a hole moving in an antiferromagnetic (AF) background is much smaller than the observed widths [5].

We calculate the spectral function of the half-filled two-dimensional (2D) Hubbard model with realistic hopping integrals within the dynamical mean-field theory (DMFT) at finite temperatures. AF short-range order in the doped systems can be modelled by an incommensurate spin density wave (spin spiral) within a generalized DMFT. The results of this approach compare very well with quantum Monte-Carlo and exact diagonalization studies both for ground-state expectation values and for excitation spectra [6]. The competition between the kinetic and interaction terms in the Hamiltonian stabilizes a spin-spiral structure with a wave vector $\boldsymbol{Q} = \pi(1 \pm 2\eta_x, 1 \pm 2\eta_y)$, which is found by minimizing the free energy. For a half-filled system one finds the AF state ($\eta_x = \eta_y = 0$) at equilibrium.

Let us first discuss the results at $T = 0$. The obtained spectra consist of a QP peak and broad incoherent background. The calculated QP dispersion is shown in Fig. 1a for the well-accepted set of parameters [2,7] for $Sr_2CuO_2Cl_2$ and for the Hubbard model. The bandwidth of the QP is about $2J$ in both cases and its dispersion compares well with what is found in ARPES. For the Hubbard model one finds that the present method [6] reproduces the well-known QP dispersion obtained in the $t$–$J$ model [3,5,8]. The QP weight $a_k$ (Fig. 1b) obtained by integrating the low-energy part does not exceed

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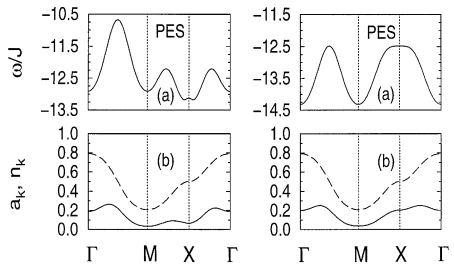


Fig. 1. Zero-temperature photoemission (PES) spectra in the main directions of the 2D BZ for $U = 12t$ ($J = t/3$): (a) QP dispersion and (b) momentum distribution $n_k$ (dashed line) and QP weight $a_k$ (full line); the special points as in Ref. [1]. Left panels: $t' = -0.28t$, $t'' = 0.18t$; right panels: $t' = t'' = 0$.

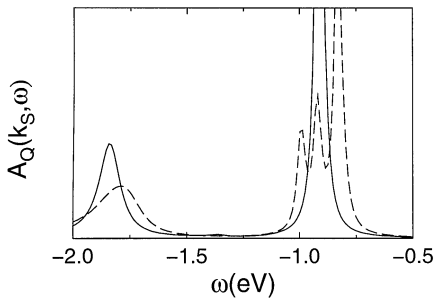


Fig. 2. Spectral function for $\boldsymbol{Q} = (\pi, \pi)$ (full line) and averaged over $\boldsymbol{Q} = [(1 \pm 0.06)\pi, (1 \pm 0.06)\pi]$ (dashed line) for the parameters as in Fig. 1 left panels, with $t = 375$ meV and artificial broadening of $0.05t$.

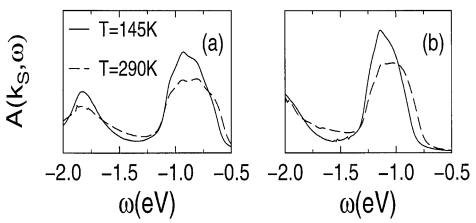


Fig. 3. Spectral function (1) at finite temperature for $\boldsymbol{k}_S = (\pi/2, \pi/2)$, with $t = 375$ meV, $U = 12t$, and: (a) $t' = -0.28t$, $t'' = 0.18t$; (b) $t' = t'' = 0$. The broadening is fully due to the finite temperature.

0.3 anywhere in the Brillouin-zone (BZ), in agreement with the results of exact diagonalization [3,4], and self-consistent Born approximation [5,8]. Due to the QP minimum which occurs for $t' = -0.28t$ and $t'' = 0.18t$ around the $X$ point, one finds there a much lower QP weight than in the $t$–$J$ model. The difference between the integrated particle density $n_k$ and the QP weight $a_k$ shows that the spectral properties are dominated by incoherent processes.

At a finite temperature there are directional fluctuations of local moments around the equilibrium position $\eta_x = \eta_y = 0$. We calculate the spectral functions $A_Q(\boldsymbol{k}, w)$ for an arbitrary pitch of the spiral $(\eta_x, \eta_y)$ and determine the averaged spectral function at finite temperature by including directional changes of the local magnetization,

$$A(\boldsymbol{k}, \omega) = \frac{1}{\Lambda}\int A_Q(\boldsymbol{k}, \omega)\, \mathrm{e}^{-\beta E(\boldsymbol{Q})}\, dQ, \qquad (1)$$

where $E(\boldsymbol{Q})$ is the internal energy, $\beta = 1/k_B T$, and $\Lambda$ is the proper normalization factor. It is found that the excitation energies of spin-spiral local configurations are of the order of $k_B T$ and can allow for considerable fluctuations in $\boldsymbol{Q}$.

At $T = 0$ only the AF state $[Q = (\pi, \pi)]$ contributes to $A(\boldsymbol{k}, \omega)$, and the QP peak is very sharp, see Fig. 2. The spiral states with shifted peak positions contribute in Eq. (1) at $T > 0$; an example of the spectral function for a 6% deviation in $Q$ from the AF state at equilibrium is shown in Fig. 2 for $\boldsymbol{k}_S = (\pi/2, \pi/2)$. Even such a long wavelength deviation has a considerable effect on the spectral function. At fixed length of the spin-spiral wave vector $\boldsymbol{Q}$ four directional deviations give rise to a three-pole structure, with the outside poles separated by an energy of about 0.24 eV. The spectral function $A_Q(\boldsymbol{k}, \omega)$ for the spin-spiral has been averaged over all energetically equivalent configurations. This explains why the averaged spectral function $A(\boldsymbol{k}, \omega)$ (1) is broadened on energy scale which is larger by one order of magnitude than the energy of thermal fluctuations (Fig. 3). For temperatures of the order of the Néel temperature one finds that the QP peak is very broad and has an asymmetric shape. This broadening is generic and is similar in the Hubbard model and for the parameters of $Sr_2CuO_2Cl_2$, but we note that the detailed shape and width of the QP peak do depend on the values of $t'$ and $t''$.

In summary, the precursor effects of incommensurate spin dynamics lead to an incoherent broadening of the QP structures which was found here at half-filling, and is expected to be similar in the doped systems as long as the local magnetic order is not destroyed. We find a width of about $3J$, a characteristic energy scale which is much larger than $k_B T$, in qualitative agreement with experiment. The unusual line shape of the QP peak is another indication that the spectrum is incoherently broadened. Therefore, the experimentally observed QP broadening and its strong temperature dependence, can, to a large extent, be attributed to spin dynamics. Our explanation of the width of the QP peak can be experimentally verified by performing photoemission experiments at low temperature ($T < 10$ K), where we predict a much smaller broadening set by the experimental resolution.

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