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$t-J$ model one-electron renormalizations: High energy features in photoemission experiments on high T_c cuprates

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Abstract

Recent angle-resolved photoemission experiments on hole doped cuprates reported new and interesting high energy features which may be useful for understanding the electronic properties of these materials. Using a perturbative approach, which allows the calculation of dynamical properties in the $t-J$ model, one-electron spectral properties were calculated. A strongly renormalized quasiparticle band near the Fermi surface and incoherent spectra at high energy were obtained. Among the different current experimental interpretations, the results obtained are closer to the interpretation given by Pan et al. [Z.-H. Pan, et al., cond-mat/0610442]. The self-energy shows large high energy contributions which are responsible for the incoherent structures shown by the spectral functions and the reduction of the quasiparticle weight and bandwidth. According to the calculation, collective charge fluctuations are the main source for the self-energy renormalizations. For testing whether the self-energy obtained is compatible with transport measurement the resistivity versus temperature relation was estimated.

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The understanding of high T_c cuprates is one of the mayor challenges in solid state physics. Even with the problem unresolved, it is clear that it is not only the large value of the superconducting T_c that is anomalous. Cuprates have also in common many electronic properties which are in clear contrast with the ones expected in usual metals. One of these, which is the subject of the present paper, is the one-electron renormalization obtained by angle-resolved photoemission spectroscopy (ARPES). Some years ago ARPES studies reported a kink in the electronic dispersion, at about ∼50–70 meV, of hole doped cuprates [1–3]. This kink indicates the presence of a small energy scale in the electronic self-energy. Besides the kink, early ARPES experiments [1] reported an imaginary part of the self-energy without a sign of saturation up to energies of the order of 150–200 meV. This feature, which was recovered in further experiments (see for instance Ref. [4]), indicates that besides low energy ones, high energy excitations are also present. However, since ARPES experiments were reported only for $\omega < 300$ meV the discussion was postponed until very recently.

Recently, ARPES measurement studies [5–10] reported results up to large energy $\omega \sim -1$ eV, clearly showing the presence of high energy self-energy renormalizations contributing to the spectral functions. The extracted E-$\mathbf{k}$ dispersion from momentum distribution curves seems to show a nearly vertical "dive" [10] (also called a "waterfall"[7]) at about 350 meV. These experiments provide the opportunity for new investigations about the electronic order behind cuprate behaviors. In spite of different experiments showing similar features, the interpretation is not unique [5–10]. For instance, Xie et al. [6] argue that, near the Fermi level, the quasiparticle band breaks at about ∼−350 meV and, at higher energies, follows the dispersion predicted by band structure calculation. Graf et al. [7] interpreted their results in terms of the disintegration of the low energy Zhang–Rice singlet and the re-emergence of the band structure dispersion at high energies. Pan et al. [10] state that, at low energy, there is a strongly renormalized coherent band, while the spectra are incoherent

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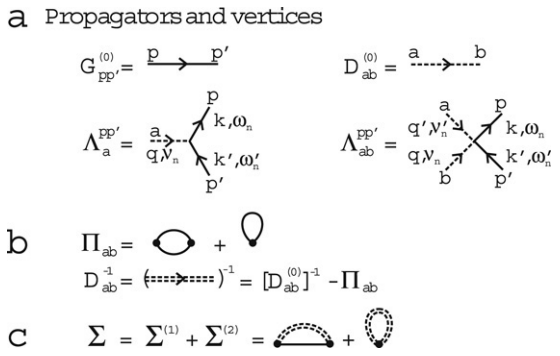

Fig. 1. (a) The solid line is the propagator, which is $O(1)$, for an electron with the dispersion E_k described in the text. The dashed line is the 6×6 boson propagator, which is $O(1/N)$, for the six-component boson field δX^a. The component δX^1 corresponds to charge fluctuations, δX^2 is introduced to fulfil the non-double-occupancy constraint, and δX^a, with a from 3 to 6, is associated with the Heisenberg coupling J. $\Lambda_a^{pp'}$ and $\Lambda_{ab}^{pp'}$ are the vertices of interaction between two fermions and one and two bosons respectively. The vertices are $O(1)$ and were obtained from the effective theory constructed under the requirement of non-double occupancy and that the Hubbard operators algebra be satisfied. Combining the order of vertices and propagators a given physical quantity can be evaluated at a given order of $1/N$. This counting means that the approach is controllable by the small parameter $1/N$. (b) The irreducible boson self-energy Π_{ab} and the renormalized boson propagator (double-dashed line). (c) Contributions $\Sigma^{(1)}$ and $\Sigma^{(2)}$ to the electron self-energy $\Sigma(\mathbf{k}, \omega)$ through $O(1/N)$. In Σ, the double-dashed line, which contains collective charge fluctuations, can be seen as the excitations that, interacting with fermions, lead to the self-energy effects and incoherent structures discussed in the text.

at high energies. In this picture the vertical "dive" can be seem as a coherent–incoherent crossover and, therefore, high energy features are not related to band structure calculations.

In this paper, electronic spectral functions and self-energy corrections are investigated in the framework of the t–J model. The results obtained are confronted with the experiments suggesting support for the scenario proposed by Pan et al. The calculation of spectral properties in the t–J model requires a controllable treatment of the non-double-occupancy constraint. While there are many calculations at mean field level, the evaluation of fluctuations above mean field level, which is of interest for understanding dynamical properties such as the electronic self-energy, is very hard. Recently we have developed a large N perturbative approach [11] (where the spin components have been generalized to N components) for the t–J model based on the path integral representation for Hubbard operators. The advantage of this approach rests on the fact that it is formulated in terms of Hubbard operators as fundamental objects and, since there is no decoupling scheme, problems that arise in other treatments are avoided, like considering fluctuations of the gauge field or the Bose condensation that appears in the slave boson approach [12]. It is not our aim to give here a detailed description of the method; it can be found in Refs. [11,13], and only a brief summary is given in Fig. 1. Using the Feynman diagrams (Fig. 1(a)), the self-energy $\Sigma(\mathbf{k}, \omega)$ can be evaluated (Fig. 1(c)) and, with it, the spectral function $A(\mathbf{k}, \omega)$ can be obtained as usual. In Ref. [13], in order to test the confidence that can be placed in our method, spectral functions were compared with those obtained using Lanczos diagonalization, finding fairly good agreement. Also

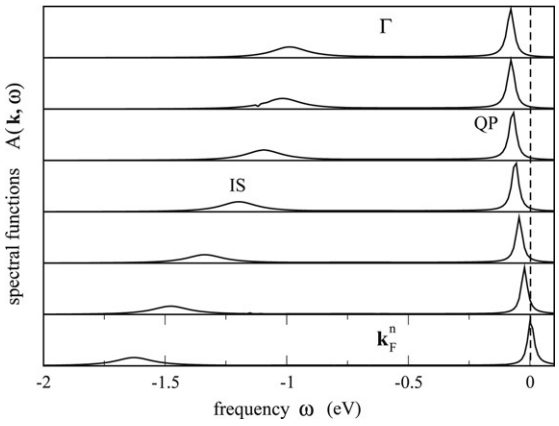

Fig. 2. Spectral functions along the nodal direction from Γ to the nodal Fermi vector $\mathbf{k}_F^n$. Close to the Fermi surface a strongly renormalized quasiparticle (QP) coherent band is obtained. For large energy (~ -1 eV) incoherent structure (IS) is observed. The vertical dashed line marks the Fermi level. All vertical scales are equal. When $\mathbf{k}$ moves from Γ to $\mathbf{k}_F^n$, while the quasiparticle peak approaches $\omega = 0$, the incoherent structure moves in the opposite direction in qualitative agreement with the experiment. See the text for discussions.

high energy self-energy excitations were identified but not compared with the new ARPES experiments [5–10] which are more recent than Ref. [13].

Once we have presented the problem and the general characteristics of the method, results for the tt'–J model are given. t and t' are the nearest and second-nearest neighbor hopping amplitudes respectively, and J is the Heisenberg coupling. In what follows we choose $t'/t = 0.35$, $J/t = 0.3$ [14] and the calculation was done in the normal state. At mean field level the electronic band obtained is $(E_k = -2(t\delta/2+\Delta)(\cos(k_x)+\cos(k_y))+4t'\delta/2\cos(k_x)\cos(k_y)-\mu)$ where $(\Delta = J/2N_s \sum_k \cos(k_x) n_F(E_k))$ and μ the chemical potential. N_s is the number of sites and n_F the Fermi function. The bare (or mean field) band E_k (which at this level is already renormalized by correlations as shown by the presence of the doping δ and J) will be dynamically dressed by $\Sigma(\mathbf{k}, \omega)$. For these parameters, in the doping range of interest for cuprates, a hole-like Fermi surface is obtained. We also choose $\delta = 0.26$ which corresponds to the highly overdoped regime where several ARPES experiments were performed [6,10]. On the other hand, as discussed in Ref. [13], our method is better for larger than for low doping. The existence of anomalous features in highly overdoped samples is very interesting because the system is far from the antiferromagnetic phase, and the pseudogap, if it is not zero, is very weak. For $\delta = 0.26$ the nodal Fermi vector is $\mathbf{k}_F^n = (0.39, 0.39)\pi/a$.

Results for the spectral functions (energy distribution curves) along the nodal direction, from $\Gamma(0, 0)$ to $\mathbf{k}_F^n$, are presented in Fig. 2 where we adopt the accepted value $t = 0.4$ eV [14]. Close to the Fermi surface a highly renormalized parabolic quasiparticle coherent band is obtained. In addition, at high energy (~ -1 eV) incoherent structures are present. For the present parameters the quasiparticle weight result is $Z = (1 - \frac{\partial \mathrm{Re}\,\Sigma}{\partial \omega})^{-1} \sim 0.4$. The remaining spectral weight lies mainly in the incoherent structure. There is also spectral weight in the form of a tail between the quasiparticle and the incoherent structure and at $\omega > 0$ (Fig. 4(a)).