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Pseudogap and the Fermi surface in the t–J model

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Abstract

We calculate spectral functions within the t–J model as relevant to cuprates in the regime from low to optimum doping. On the basis of equations of motion for projected operators an effective spin–fermion coupling is derived. The self-energy due to short-wavelength transverse spin fluctuations is shown to lead to a modified self-consistent Born approximation, which can explain strong asymmetry between hole and electron quasiparticles. The coupling to long-wavelength longitudinal spin fluctuations governs the low-frequency behavior and results in a pseudogap behavior, which at low doping effectively truncates the Fermi surface.

Keywords: D. Fermi surface

Here we concentrate on some of the experimental facts revealing the nature of quasiparticles (QP) and pseudogap in underdoped cuprates. Several quantities, in particular the uniform susceptibility, the Hall constant, the specific heat, show the (large) pseudogap scale T^* [1], consistent with the angle resolved photoemission (ARPES) revealing a spectral function $A(\mathbf{k},\omega)$ with a hump at ~ 100 meV observed in $Bi_2Sr_2CaCu_2O_{2+\delta}$ (BSCCO) near the momentum $\mathbf{k} = (\pi, 0)$ [2,3]. QP dispersing through the Fermi surface (FS) are resolved by ARPES in BSCCO only in parts of the large FS, in particular along the nodal (0,0)–(π,π) direction, indicating that the rest of the large FS are either fully or effectively gaped. Some aspects of the pseudogap have been found in the phenomenological spin–fermion models [4]. The renormalization group studies of the Hubbard model [5,6] also indicate the breakdown of the standard Fermi liquid and the truncation of the FS. That such features also emerge from prototype models of correlated electrons has been confirmed in numerical studies of spectral functions in the Hubbard [7] and in the t–J model [8–10], which both show the appearance of the pseudogap at low doping.

Our aim is to capture these features within an analytical treatment of a single band model. The most difficult aspect in the latter is inherent strong coupling between mobile fermions and spin degrees, for which it is hard to find even a proper phenomenological model. In the following, we show that such an effective spin–fermion model can be derived via equations of motion (EQM) and dividing the coupling into short and long-wavelength spin fluctuations.

We study the planar t–J model

$$H = -\sum_{i,j,s} t_{ij}\tilde{c}^{\dagger}_{js}\tilde{c}_{is} + J\sum_{\langle ij\rangle}\left(\mathbf{S}_i\cdot\mathbf{S}_j - \frac{1}{4}n_i n_j\right), \tag{1}$$

where we take into account possible longer range hopping, i.e. besides $t_{ij} = t$ for n.n. hopping also $t_{ij} = t'$ for n.n.n. neighbors on a square lattice. The latter appears to be relevant in the study as shown later. We evaluate the single-particle propagator in this model explicitly taking into account that fermionic operators are projected ones not allowing for double occupancy of sites, e.g. $\tilde{c}^{\dagger}_{is} = (1 - n_{i,-s})c^{\dagger}_{is}$. We use EQM directly for projected operators [11] and represent them in variables relevant for a paramagnetic metallic state with $\langle \mathbf{S}_i\rangle = \mathbf{0}$ and electron concentration $\langle n_i\rangle = c_e = 1 - c_h$. EQM for $\tilde{c}_{\mathbf{k}s}$ can be used to construct approximations for the electron propagator $G(\mathbf{k},\omega)$ [11–13], which can be represented as

$$G(\mathbf{k},\omega) = \frac{\alpha}{\omega + \mu - \zeta_{\mathbf{k}} - \Sigma(\mathbf{k},\omega)}, \tag{2}$$

where the renormalization $\alpha = (1 + c_h)/2$ is a consequence of a projected basis, and $\zeta_{\mathbf{k}} = -4\eta_1 t\gamma_{\mathbf{k}} - 4\eta_2 t'\gamma'_{\mathbf{k}}$ is the 'free' propagation term emerging from the EQM, with $\gamma_{\mathbf{k}} = (\cos k_x + \cos k_y)/2$ and $\gamma'_{\mathbf{k}} = \cos k_x \cos k_y$. Here $\eta_j = \alpha + \langle S^z_0 S^z_j\rangle/\alpha$ is determined by spin correlations. The central quantity for further consideration is the self-energy $\Sigma(\mathbf{k},\omega) = \langle\langle C_{\mathbf{k}s}; C^{+}_{\mathbf{k}s}\rangle\rangle^{irr}_{\omega}/\alpha$, where $iC_{\mathbf{k}s} = [\tilde{c}_{\mathbf{k}s}, H] - \zeta_{\mathbf{k}}\tilde{c}_{\mathbf{k}s}$, and only the 'irreducible' part of the correlation function

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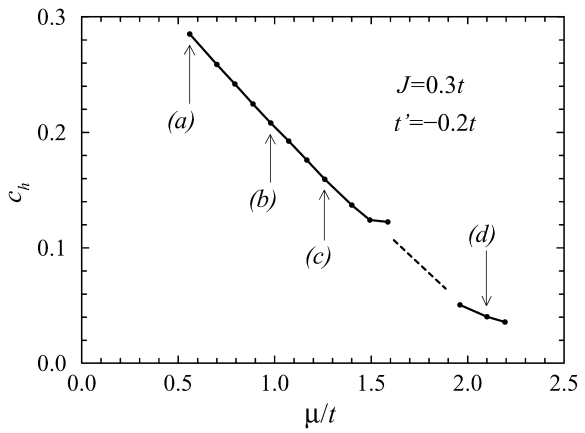

Fig. 1. Hole concentration c_h as a function of the chemical potential μ/t for $J/t = 0.3$, $t'/t = -0.2$ and $N = 32 \times 32$ sites in the Brillouin zone. Note selected cases presented further on (a) $c_h = 0.28$, (b) $c_h = 0.21$, (c) $c_h = 0.16$ and (d) $c_h = 0.04$.

should be taken into account in the evaluation of Σ. In finding an approximation for Σ, we assume that we are dealing with the paramagnet with pronounced AFM SRO with the dominant wave vector $\mathbf{Q} = (\pi, \pi)$ and the AFM correlation length $\xi > 1$ with corresponding $\kappa = 1/\xi$. EQM naturally indicate on an effective coupling between fermions and spin degrees, however, the role of short- and longer-range spin fluctuations is quite different.

In an undoped AFM system the spectral function of an added hole is quite well described within the self-consistent Born approximation (SCBA) [14–16], where the strong hole–magnon coupling induced by the hopping t-term leads to a broad background representing the incoherent hopping and a quite narrow QP dispersion determined by J. Our EQM formalism naturally reproduces SCBA in an undoped system and it is easy to generalize the equations for finite doping $c_h > 0$ where we have also electron-like QP above the Fermi energy ($\omega > 0$). In 2D the AFM long-range order is broken at $T > 0$ and $c_h > 0$, still spin fluctuations are magnon-like with a dispersion $\omega_{\mathbf{q}}$ for $q > \kappa$ and $\tilde{q} > \kappa$ where $\tilde{\mathbf{q}} = \mathbf{q} - \mathbf{Q}$. The paramagnon contribution to the self-energy can be written as

$$\Sigma_{\rm pm}(\mathbf{k}, \omega) = \frac{16t^2}{N} \sum_{q,\tilde{q}>\kappa} (u_{\mathbf{q}} \gamma_{\mathbf{k}-\mathbf{q}} + v_{\mathbf{q}} \gamma_{\mathbf{k}})^2 \times [G^-(\mathbf{k}-\mathbf{q}, \omega+\omega_{\mathbf{q}}) + G^+(\mathbf{k}+\mathbf{q}, \omega-\omega_{\mathbf{q}})], \quad (3)$$

where $(u_{\mathbf{q}}, v_{\mathbf{q}}) = (1, -\mathrm{sign}(\gamma_{\mathbf{q}}))\sqrt{(2J \pm \omega_{\mathbf{q}})/2\omega_{\mathbf{q}}}$ and $G^{\pm}$ refer to the Green's functions corresponding to electron ($\omega > 0$) and hole ($\omega < 0$) QP excitations, respectively.

We are dealing with a paramagnet without the AFM long-range order, therefore it is essential to consider also the coupling to longitudinal spin fluctuations which for $\tilde{q} < \kappa$ appear to be quite uncoupled, therefore we express the longitudinal contribution as in Refs. [11–13],

$$\Sigma_{\rm lf}(\mathbf{k}, \omega) = \frac{1}{\alpha N} \sum_{\mathbf{q}} \tilde{m}^2_{\mathbf{kq}} \int\int \frac{\mathrm{d}\omega_1 \, \mathrm{d}\omega_2}{\pi} g(\omega_1, \omega_2) \times \frac{A^0(\mathbf{k}-\mathbf{q}, \omega_1)\chi''(\mathbf{q}, \omega_2)}{\omega - \omega_1 - \omega_2}, \quad (4)$$

where $\chi(\mathbf{q}, \omega)$ is the dynamical spin susceptibility, $A^0(\mathbf{k}, \omega) = -(\alpha/\pi)\mathrm{Im}(\omega + \mu - \zeta_{\mathbf{k}} - \Sigma_{\rm pm})^{-1}$, $g(\omega_1, \omega_2) = [\mathrm{th}(\omega_1/2T) + \mathrm{cth}(\omega_2/2T)]/2$ and $\tilde{m}_{\mathbf{kq}} = 2J\gamma_{\mathbf{q}} + \frac{1}{2}(\epsilon^0_{\mathbf{k}-\mathbf{q}} + \epsilon^0_{\mathbf{k}})$ with $\epsilon^0_{\mathbf{k}} = -4t\gamma_{\mathbf{k}} - 4t'\gamma'_{\mathbf{k}}$ [13].

In $\Sigma_{\rm lf}$ only the part corresponding to irreducible diagrams should enter, so there are restrictions on proper decoupling. We use in Eq. (4), the most appropriate and simplest approximation to insert the unrenormalized $A^0(\mathbf{k}, \omega)$, i.e. the spectral function without a self-consistent consideration of $\Sigma_{\rm lf}$ but with $\Sigma_{\rm pm}$ fully taken into account. Such an approximation has been introduced in the theory of a pseudogap in CDW systems [17], used also in related works analyzing the role spin fluctuations [18,19], and recently more extensively examined in Ref. [20].

So far we do not have a corresponding theory for the spin response at $c_h > 0$ and $T > 0$, so $\chi(\mathbf{k},\omega)$ is assumed as a phenomenological input, bound by the sum rule

$$\frac{1}{N} \sum_{\mathbf{q}} \int_0^{\infty} \mathrm{cth}\left(\frac{\beta\omega}{2}\right) \chi''(\mathbf{q}, \omega)\mathrm{d}\omega = \frac{\pi}{4}(1 - c_h). \quad (5)$$

The response should qualitatively correspond to a paramagnet close to the AFM instability, so it is assumed of the form

$$\chi''(\mathbf{q}, \omega) \propto \frac{\phi(\omega, T)}{(\tilde{q}^2 + \kappa^2)(\omega^2 + \omega_\kappa^2)}, \quad (6)$$

where $\phi(\omega, T) \propto \omega$ would be appropriate for a nearly AFM Fermi liquid [4,19] or an undoped AFM in 2D. The self-consistent set of equations for G is closed with $\Sigma = \Sigma_{\rm pm} + \Sigma_{\rm lf}$. For given chemical potential, μ, the FS emerges as a solution determined by the relation $\zeta_{\mathbf{k}_F} + \Sigma'(\mathbf{k}_F, \mathbf{0}) = \mu$. We should note that at given μ, electron concentration c_e as calculated from the density of states $N(\omega) = (1/N) \times \sum_{\mathbf{k}} A(\mathbf{k}, \omega)$ integrated for $\omega < 0$, does not in general coincide with the one evaluated from the FS volume, $\tilde{c}_e = V_{\rm FS}/V_0$. Nevertheless, apart from the fact that within the t–J model validity of the Luttinger theorem is anyhow under question [21], in the regimes of large FS both quantities appear to be quite close. The position of the FS is mainly determined by $\zeta_{\mathbf{k}}$ and $\Sigma_{\rm pm}$, while in this respect $\Sigma_{\rm lf}$ is less crucial. We choose further on parameters $J = 0.3t$, $t' = -0.2t$ and $\kappa = \sqrt{c_h}$ while η_1 and η_2 are determined as a function of c_h from model calculations [22]. We use $N = 32 \times 32$ points in the Brillouin zone and broadening $\epsilon/t = 0.02$.

In Fig. 1, we present hole concentration c_h vs the chemical potential μ/t as obtained from Eq. (3). We solve the equation by iteration. With labels (a), (b) and (c) are

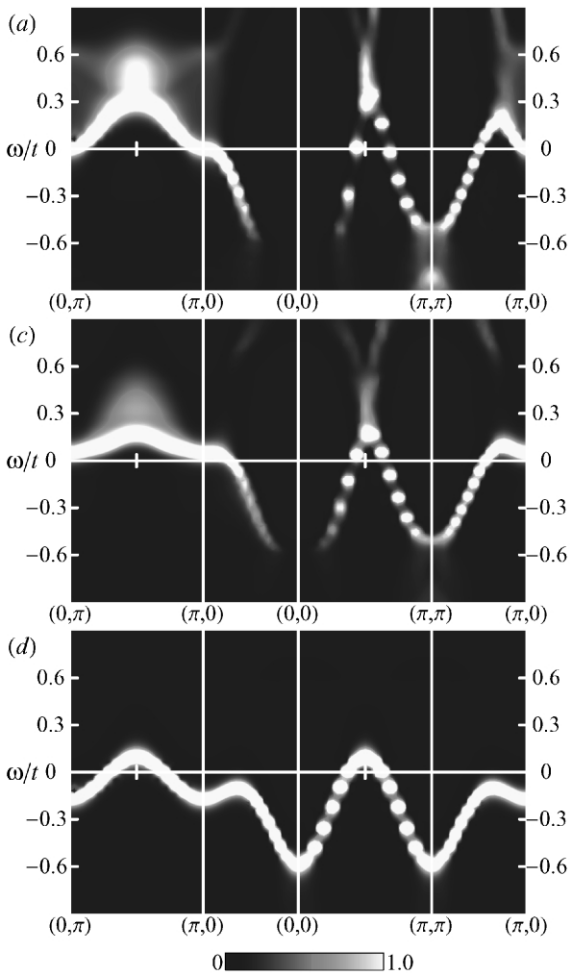

Fig. 2. Spectral functions $A(\mathbf{k},\omega)$ along principal lines in the Brillouin zone. For convenience of presentation the functions are clipped at $A(\mathbf{k},\omega)=1.0$. Labels (a), (c) and (d) correspond to selected cases in Fig. 1.

indicated special cases presented in next figures. At $c_h \sim 0.12$ we observe in the equations an instability signaled by oscillatory behavior instead of convergence and a unique solution cannot be obtained in the region indicated by the dashed line. However, at lower doping, $c_h < 0.05$, the solution converges again and a typical result is indicated with (d). The region of instability coincides with the transition from the large to a small FS, as presented below.

In Fig. 2 are presented spectral functions $A(\mathbf{k},\omega)$ along the principal directions in the Brillouin zone for Fig. 1(a), (c) and (d). It is evident that Σ_{pm} leads to strong damping of hole QP and quite incoherent momentum-independent spectrum $A(\mathbf{k},\omega)$ for $\omega \ll -J$ which qualitatively reproduces ARPES and numerical results [10]. Electron QP (at $\omega > 0$) are in general very different, i.e. with much weaker damping arising only from Σ_{pm}. At low doping $c_h < 0.05$ we find the regime of small (pocket-like) FS.

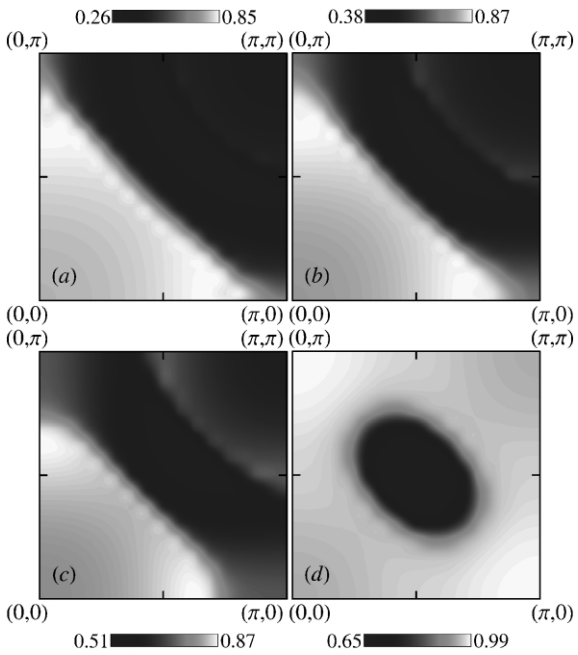

Fig. 3. Electron momentum distribution function $\tilde{n}(\mathbf{k})$ for various c_h as selected in Fig. 1.

The shape of the FS is most clearly presented with contour plot of the electron momentum distribution function $\tilde{n}(\mathbf{k}) = \alpha^{-1}\int_{-\infty}^{0} A(\mathbf{k},\omega)\mathrm{d}\omega$. Results for a characteristic development of the FS with c_h are shown in Fig. 3. At $c_h < c_h^* \sim 0.05$ solutions are consistent with a small pocket-like FS (d), whereby this behavior is enhanced by $t' < 0$ as realized in other model studies [23]. On increasing doping, the FS rather abruptly changes from a small into a large one as suggested from the results of SCBA [24,25]. The smallness of c_h^* has the origin in quite weak dispersion dominated by J and t' at $c_h \to 0$ which is overshadowed by much larger $\zeta_{\mathbf{k}}$ at moderate doping, where the FS is large and its shape is controlled by t'/t. Figures (a), (b) and (c) correspond to higher doping with common large FS topology. However, in the intermediate doping regime (b) and (c), the pseudogap is pronounced at momenta around $(\pi,0)$ point. The gap is more pronounced in (c) because of longer AFM correlation length ξ (smaller κ). In Fig. 4, the development of the PG is presented for $c_h = 0.21$ (case (b)). Here $\kappa = 0.4$ and the PG is not fully developed yet. With increasing ξ—for this doping somewhat unrealistic values—the gap opens. At lower doping, case (c) in Fig. 3 the gap is opened what also shows up the form of the FS which tends to avoid points $(\pi,0)$, $(0,\pi)$.

In conclusion, we have presented a theory for the spectral functions within the t–J model where the double-occupancy constraint is taken explicitly into account and used to derive an effective spin–fermion

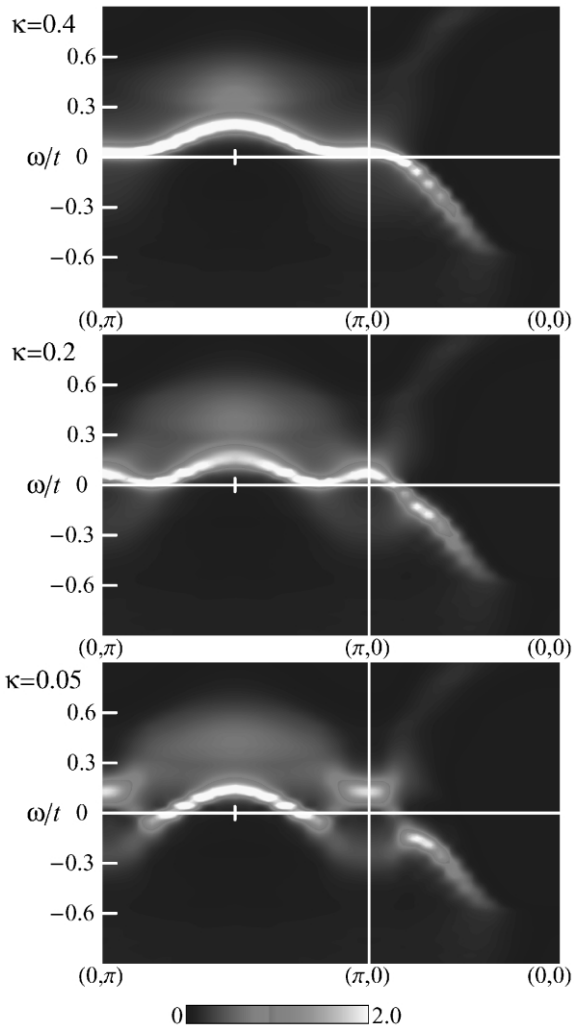

Fig. 4. Spectral functions $A(\mathbf{k},\omega)$ for $c_h = 0.21$ (Fig. 1(b)) for different κ. The functions are clipped at $A(\mathbf{k},\omega) = 2.0$. Note the opening of the gap at $\mathbf{k} = (\pi, 0)$ with decreasing κ.

coupling. The coupling to transverse AFM paramagnons is strong, nevertheless it can be well treated within a generalized SCBA. On the other hand, the coupling to longitudinal AFM fluctuations, $\tilde{m}_{\mathbf{kq}}$, is moderate near FS for low doping and leads to a pseudogap. The latter is, however, not in contradiction with the existence of a large FS, and should show up in integrated photoemission and ARPES results as well as in the uniform susceptibility and in the specific heat.

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