PHYSICAL REVIEW B, VOLUME 63, 180506(R)

Spectral functions and the pseudogap in the t-J model

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(Received 23 October 2000; published 6 April 2001)

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, which at low doping effectively truncates the Fermi surface, in particular near the $(\pi,0)$ point in the Brillouin zone.

DOI: 10.1103/PhysRevB.63.180506 PACS number(s): 74.20.De, 71.27.+a, 71.10.Fd, 72.15.−v

In recent years underdoped cuprates are in the center of experimental and theoretical investigation, offering possibly a clue to the understanding of anomalous normal-state properties and the mechanism of superconductivity in these compounds. Here we concentrate on some experimental facts revealing the nature of quasiparticles (QP) and the pseudogap. Several quantities, in particular the uniform susceptibility, the Hall constant, and the specific heat, show the (large) pseudogap scale T^*,[1] consistent with the angle resolved photoemission (ARPES) revealing a hump at ~ 100 meV observed in $Bi_2Sr_2CaCu_2O_{2+\delta}$ (BSCCO) near the $(\pi,0)$ momentum.[2] At the same time 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 $(0,0)-(\pi,\pi)$ direction, indicating that the rest of the large FS is either fully or effectively gapped. On approaching the optimal doping the T^* scale merges with T_c and the large FS becomes well defined. All these phenomena are naturally associated with the antiferromagnetic (AFM) short-range order (SRO) in cuprates, since the scale T^* approaches the AFM exchange J in undoped materials. This is less clear for the lower spin-gap scale T_{sg} (not the subject here), not found in all cuprates.

While these facts allow for a qualitatively consistent scenario, the consensus on necessary prerequisites and moreover a satisfactory theoretical analysis are still missing. The renormalization group studies of the Hubbard model[3] indicate on the breakdown of the standard Fermi liquid and on 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[4] and in the t-J model,[5,6] which both show the appearance of the pseudogap at low doping. Some aspects of the pseudogap have been found in the spin-fermion models[7] and studied phenomenologically in the Hubbard model.[8]

Our aim is to capture these features within an analytical treatment of a single band model. In the following we show that an effective spin-fermion model can be derived via equations of motion (EQM) and dividing the coupling into short- and long-wavelength spin fluctuations an approximation for the electron self-energy can be found.

We study the planar t-J model

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

where we take into account possible longer range hopping, i.e., besides $t_{ij}=t$ for nearest-neighbor hopping also $t_{ij}=t'$ for next-nearest neighbors on a square lattice. We evaluate the single-particle propagator in this model explicitly taking into account that fermionic operators are projected ones not allowing for the double occupancy of sites, e.g., $\tilde{c}^{\dagger}_{is}=(1-n_{i,-s})c^{\dagger}_{is}$.

We use EQM directly for projected operators[9] and represent them in variables appropriate for a paramagnetic metallic state with $\langle\mathbf{S}_i\rangle=0$ and electron concentration $\langle n_i\rangle=c_e=1-c_h$,

$$[\tilde{c}_{\mathbf{k}s},H]=\left[\left(1-\frac{c_e}{2}\right)\epsilon^0_{\mathbf{k}}-Jc_e\right]\tilde{c}_{\mathbf{k}s}+\frac{1}{\sqrt{N}}\sum_{\mathbf{q}}(2J\gamma_{\mathbf{q}}+\epsilon^0_{\mathbf{k}-\mathbf{q}})\times\left[sS^z_{\mathbf{q}}\tilde{c}_{\mathbf{k}-\mathbf{q},s}+S^{\mp}_{\mathbf{q}}\tilde{c}_{\mathbf{k}-\mathbf{q},-s}-\frac{1}{2}\tilde{n}_{\mathbf{q}}\tilde{c}_{\mathbf{k}-\mathbf{q},s}\right], \tag{2}$$

where $\epsilon^0_{\mathbf{k}}=-4t\gamma_{\mathbf{k}}-4t'\gamma'_{\mathbf{k}}$ is the bare band energy on a square lattice and $\gamma_{\mathbf{k}}=(\cos k_x+\cos k_y)/2$, $\gamma'_{\mathbf{k}}=\cos k_x\cos k_y$.

EQM for $\tilde{c}_{\mathbf{k}s}$ can be used to construct approximations for the electron propagator $G(\mathbf{k},\omega)$,[9,10] which can be represented as

$$G(\mathbf{k},\omega)=\frac{\alpha}{\omega+\mu-\zeta_{\mathbf{k}}-\Sigma(\mathbf{k},\omega)}, \tag{3}$$

where the renormalization $\alpha=(1+c_h)/2$ is a consequence of the projected basis, μ is the chemical potential, and $\zeta_{\mathbf{k}}$ is the ''free'' propagation term emerging from the EQM,

$$\zeta_{\mathbf{k}}=\frac{1}{\alpha}\langle\{[\tilde{c}_{\mathbf{k}s},H],\tilde{c}^{\dagger}_{\mathbf{k}s}\}_+\rangle-\bar{\zeta}=-4\eta_1t\gamma_{\mathbf{k}}-4\eta_2t'\gamma'_{\mathbf{k}}, \tag{4}$$

where $\eta_j=\alpha+\langle\mathbf{S}_0\cdot\mathbf{S}_j\rangle/\alpha$ and $\bar{\zeta}$ is a constant. 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 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 $\kappa=1/\xi$. We first note that EQM, Eq. (2), naturally indicate on an effective coupling between fermions and spin degrees. However, the role of short-range and longer-range spin fluctuations is quite different.

In an undoped system AFM the spectral function of an added hole is quite well described within the self-consistent Born approximation (SCBA),[11] where the strong hole-magnon coupling induced by the hopping t term leads to a broad background representing the incoherent hopping and a narrow QP dispersion governed predominantly by J. If we assume as a starting point an undoped Néel state as well as $J<t$ EQM, Eq. (2) directly reproduce the coupling equivalent to the holon-spin coupling within the SCBA. Note that within the Néel (Ising) state we have $\eta_1=0$, $\eta_2=1$, $S_i^z=\pm 1/2$, and a nontrivial coupling comes from transverse $S_{\mathbf{q}}^{\mp}$ which can be represented via magnon excitations. Therefore by performing the decoupling of fermion and spin degrees in Σ and by using the identity $\tilde{c}_{js}=\tilde{c}_{j,-s}S_j^{\mp}$, we recover the standard SCBA equations.

Our EQM formalism thus naturally leads to the SCBA in an undoped system. Still we note that in an isotropic AFM $\eta_1\neq 0$ (but $|\eta_1|\ll 1$) which slightly modificate SCBA results. Since the SCBA accounts well for properties of a single QP in an AFM, we are not trying here to improve it. Within our approach we generalize the equations for finite doping $c_h>0$ where we have electronlike QP above the Fermi energy ($\omega>0$). In two-dimensional (2D) the AFM long-range order is absent due to $T>0$ and $c_h>0$, still spin fluctuations are magnonlike, i.e., propagating and transverse to the local AFM SRO, with a dispersion $\omega_{\mathbf{q}}$ for $q>\kappa$ and $\tilde{q}>\kappa$ where $\tilde{\mathbf{q}}=\mathbf{q}-\mathbf{Q}$. Hence the paramagnon contribution to the self energy can be written as

$$\Sigma_{\rm pm}(\mathbf{k},\omega)=\frac{16t^2}{N}\sum_{\tilde{q},\tilde{q}>\kappa}(u_{\mathbf{q}}\gamma_{\mathbf{k}-\mathbf{q}}+v_{\mathbf{q}}\gamma_{\mathbf{k}})^2 \times[G^-(\mathbf{k}-\mathbf{q},\omega+\omega_{\mathbf{q}})+G^+(\mathbf{k}+\mathbf{q},\omega-\omega_{\mathbf{q}})], \tag{5}$$

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. So far equations are written for $T=0$, however, in $\Sigma_{\rm pm}$ the role of finite but low $T>0$ is not pronounced. Note that analogous to the SCBA t' does not enter directly the coupling but remains in the ''free'' propagation term $\zeta_{\mathbf{k}}$. Here we stress two features of our generalized SCBA: (a) we are dealing with a strong coupling theory due to $t>\omega_{\mathbf{q}}$ hence a self-consistent calculation of Σ is required, and (b) resulting spectral functions $A(\mathbf{k},\omega)$ are very asymmetric with respect to $\omega=0$, since G^+ has less weight and consequently the scattering of electron QP is less pronounced.

We are dealing with a paramagnet, therefore it is essential to consider also the coupling to longitudinal spin fluctuations. Note that the EQM (2) naturally introduces a coupling between fermion and spin operators which is isotropic in the spin space as appropriate in a paramagnetic state. In fact analogous form as in Eq. (2) would emerge also from a spin-fermion Hamiltonian with the coupling parameter $m_{\mathbf{kq}}=2J\gamma_{\mathbf{q}}+\epsilon^0_{\mathbf{k}-\mathbf{q}}$. The effective Hamiltonian should be Hermitian, i.e., the coupling should satisfy the condition $\tilde{m}_{\mathbf{k},\mathbf{q}}=\tilde{m}_{\mathbf{k}-\mathbf{q},-\mathbf{q}}$, therefore we use further on the symmetrized $\tilde{m}_{\mathbf{kq}}=2J\gamma_{\mathbf{q}}+\frac{1}{2}(\epsilon^0_{\mathbf{k}-\mathbf{q}}+\epsilon^0_{\mathbf{k}})$.

Fermions and longitudinal spin fluctuations with $\tilde{q}<\kappa$ appear to be quite uncoupled, therefore we express the longitudinal contribution as in Refs. 9 and 10,

$$\Sigma_{\rm lf}(\mathbf{k},\omega)=\frac{1}{\alpha N}\sum_{\mathbf{q}}\tilde{m}^2_{\mathbf{kq}}\int\int\frac{d\omega_1 d\omega_2}{\pi}g(\omega_1,\omega_2) \times\frac{A^0(\mathbf{k}-\mathbf{q},\omega_1)\chi''(\mathbf{q},\omega_2)}{\omega-\omega_1-\omega_2}, \tag{6}$$

where $\chi(\mathbf{q},\omega)$ is the dynamical spin susceptibility, $A^0(\mathbf{k},\omega)=-(\alpha/\pi)\mathrm{Im}(\omega+\mu-\zeta_{\mathbf{k}}-\Sigma_{\rm pm})^{-1}$ and $g(\omega_1,\omega_2)=[\mathrm{th}(\omega_1/2T)+\mathrm{cth}(\omega_2/2T)]/2$. In $\Sigma_{\rm lf}$ only the part corresponding to irreducible diagrams should enter, so there are restrictions on proper decoupling. We are mostly dealing with the situation with a pronounced AFM SRO where longitudinal spin fluctuations are slow, with a characteristic frequency $\omega_\kappa\ll J$ which is the case of a quasistatic $\chi(\mathbf{q},\omega)$. Therefore we in Eq. (6) as the simplest approximation 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 charge density wave systems,[12] used also in related works analyzing the role of spin fluctuations,[13,14] and recently more extensively examined in Ref. 15.

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

$$\frac{1}{N}\sum_{\mathbf{q}}\int_0^\infty\mathrm{cth}\left(\frac{\beta\omega}{2}\right)\chi''(\mathbf{q},\omega)d\omega=\frac{\pi}{4}(1-c_h). \tag{7}$$

The response should qualitatively correspond to a paramagnet close to the AFM instability, so we assume the form

$$\chi''(\mathbf{q},\omega)\propto\frac{\phi(\omega,T)}{(\tilde{q}^2+\kappa^2)(\omega^2+\omega_\kappa^2)}, \tag{8}$$

where $\phi(\omega,T)\propto\omega$ would be appropriate for a nearly AFM Fermi liquid[7,14] or an undoped AFM in 2D at any $T>0$. On the other hand, in cuprates at intermediate doping more consistent with model results for $T>0$ seems to be the marginal Fermi-liquid behavior with $\phi(\omega,T)\propto\mathrm{th}(\omega/2T)$.[16,1,6]

Equations (5) and (6) for $\Sigma=\Sigma_{\rm pm}+\Sigma_{\rm lf}$ represent the self-consistent set of equations for G. Parameters κ,η_1, and η_2 are mainly dependent on c_h and are known from model calculations.[17,1] At $T=0$ and given c_h we determine μ such that the density of states $\mathcal{N}(\omega)=(2/N)\Sigma_{\mathbf{k}}A(\mathbf{k},\omega)$ integrated

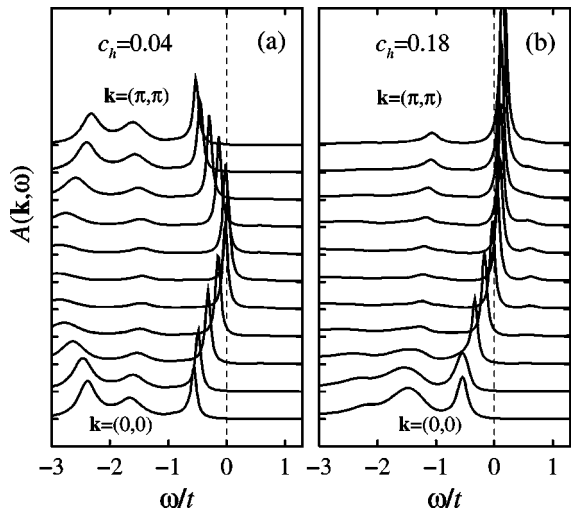

FIG. 1. $A(\mathbf{k},\omega)$ along the $(0,0)-(\pi,\pi)$ direction for $J=0.3t$ and $t'=-0.2t$. (a) $c_h=0.04$, $\eta_1=0.02$ and (b) $c_h=0.18$, $\eta_1=0.2$.

for $\omega<0$ reproduces c_e. At the same time FS is given by the relation $\zeta_{\mathbf{k}_F}+\Sigma'(\mathbf{k}_F,0)=\mu$. Full numerical analysis of self-consistent equations will be presented elsewhere. Here we concentrate on some key aspects of the theory. One is that $\Sigma_{\rm pm}$ allows for a meaningful behavior in the limit $c_h\to 0$, which has been the deficiency of most phenomenological theories so far. In this limit our results for $A(\mathbf{k},\omega)$ at $T\sim 0$ are essentially equivalent to results within the SCBA approach.[11] For $c_h\gtrsim 0$ we have a finite contribution from electron QP $A^0(\mathbf{k},\omega>0)$ and the corresponding QP density evolves as $\propto c_h$.

We choose further on parameters $J=0.3t, t'=-0.2t$, and $\kappa=2\sqrt{c_h}$. In Fig. 1 we present typical results for $A(\mathbf{k},\omega)$ along the $(0,0)-(\pi,\pi)$ direction. Since at low doping $\eta_2\sim 0.9$ main doping dependence arises from $\eta_1(c_h)$, which varies from $\eta_1\sim -0.18$ at $c_h\to 0$ to $\eta_1\sim\alpha$ for large doping. In calculation we use η_i close to values emerging from spin correlations found numerically.[17]

As presented in Fig. 1 $\Sigma_{\rm pm}$ leads to a strong damping of the hole QP and quite incoherent momentum-independent spectrum $A(\mathbf{k},\omega)$ for $\omega\ll -J$ which qualitatively reproduces ARPES and numerical results.[6] Electron QP (at $\omega>0$) are in general very different,i.e., with much weaker damping arising only from $\Sigma_{\rm pm}$. We should note that at given μ, c_e calculated from the density of states 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 the validity of the Luttinger theorem is anyhow under question,[18] in the regimes of large FS both quantities appear to be quite close.

Results for a characteristic development of the FS with c_h are shown in Fig. 2. At $c_h<c_h^*\sim 0.08$ solutions are consistent with a small pocketlike FS, whereby this behavior is enhanced by $t'<0$ as realized in other model studies.[19] On increasing doping $c_h>c_h^*$ the FS rather abruptly changes from small into a large one. 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

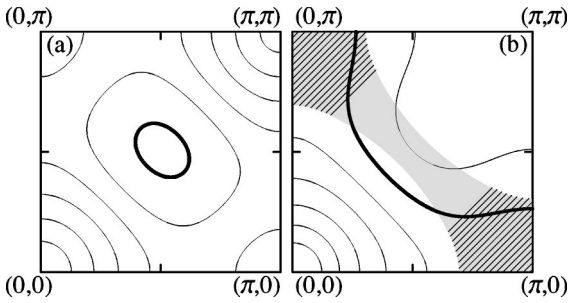

FIG. 2. Fermi surface corresponding to results presented in Fig. 1. (a) Small FS, $c_h=0.04$ and (b) large FS, $c_h=0.18$. Contour lines represent QP energy levels in increments of $0.1t$. The region with a developed pseudogap ($w/\Delta<1$) is line shaded while the gray shaded region represents the region where the pseudogap is smeared out ($w/\Delta>1$).

doping, where the FS is large and its shape is controlled by t'/t. Nevertheless, the relevance of obtained FS should be considered in connection with a coexistent pseudogap discussed further on.

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. Results for $\Sigma'_{\rm pm}(\mathbf{k},\omega=0)$ can be well parameterized in the form obtained within the SCBA for a single hole.[11] Similarly one can present also the full effective QP dispersion, $\epsilon_{\mathbf{k}}^{\rm ef}=\zeta_{\mathbf{k}}+\Sigma'(\mathbf{k},\omega=0)-\mu$, and the QP residue $Z_{\mathbf{k}}$. The simplest approximation to discuss the pseudogap is the quasistatic approximation which is meaningful for $\omega_\kappa\ll t$. Assuming also $\kappa\ll 1$ simplifying $g\chi''(\mathbf{q},\omega)\sim\pi\delta(\mathbf{q}-\mathbf{Q})\delta(\omega)/4$, as well as a single-pole form $A^0(\mathbf{k},\omega)=\alpha Z_{\mathbf{k}}\delta(\omega-\epsilon_{\mathbf{k}}^{\rm ef})$ near the FS, we obtain from Eqs. (3) and (6)

$$G(\mathbf{k},\omega)=\frac{\alpha Z_{\mathbf{k}}(\omega-\epsilon_{\mathbf{k}-\mathbf{Q}}^{\rm ef})}{(\omega-\epsilon_{\mathbf{k}-\mathbf{Q}}^{\rm ef})(\omega-\epsilon_{\mathbf{k}}^{\rm ef})-\Delta_{\mathbf{kQ}}^2},\tag{9}$$

where the gap function is given by $\Delta_{\mathbf{kQ}}^2=Z_{\mathbf{k}}Z_{\mathbf{k}-\mathbf{Q}}\tilde{m}_{\mathbf{kQ}}^2/4$. From resulting branches $E^{\pm}$ it is evident that a gap opens on the AFM zone boundary, so that the relevant pseudogap energy is $\Delta_{\mathbf{k}}^{PG}=|\Delta_{\mathbf{k}_{\rm AFM}}|\sim Z_{\mathbf{k}}|2J-4t'\cos^2 k_x|/2$. For $t'<0$ the gap is largest at $(\pi,0)$ point, as observed in experiments.[2] Since within the same $\mathbf{k}$ region the QP dispersion is also smallest the effect is even more pronounced. If $\omega=0$ is in the regime of the gap, then naturally we are dealing (in this approximation) with a truncated FS. For parameters as above we present in Fig. 2(b) the pseudogap region where the states and FS near the $(\pi,0)$ momentum are strongly suppressed.

Going beyond the quasistatic and $\kappa\sim 0$ treatment one can discuss also the QP states within the pseudogap. To study the general structure of the SF in this region it is enough to follow the development with $\epsilon=\epsilon_{\mathbf{k}}^{\rm ef}$ crossing the pseudogap perpendicular to the AFM zone boundary. It is essential to take into account $\kappa>0$ so that the averaging over $\tilde{\mathbf{q}}$ leads to an effective smearing of the delta function $A_{\mathbf{k}-\mathbf{Q}}^0$ into a broader $\bar{A}(\epsilon,\omega)$. So we have qualitatively to deal (at $T=0$) with the self-energy

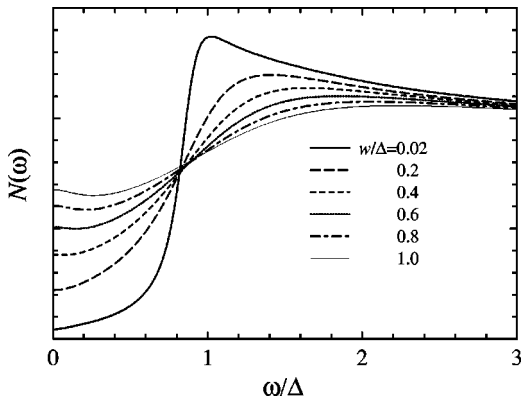

FIG. 3. Density of states $\mathcal{N}(\omega)$ as a function of ω/Δ for $\omega_\kappa = 0.2\Delta$.

$$\Sigma''(\epsilon,\omega) \propto \int_0^\omega \chi''(\omega-\omega')\overline{A}(\epsilon,\omega')d\omega', \tag{10}$$

where the simplest assumption for $\overline{A}(\epsilon,\omega)$ is a Lorentzian with the width $w = v_{\mathbf{k}_F}\kappa$. Analogous equations have been already studied in Ref. 13 and lead to the pseudogap of the order of $\Delta = \Delta_{\mathbf{k}}^{PG}$, pronounced in QP spectra and clearly in $\mathcal{N}(\omega)$. Results for the case with the gap centered at $\omega = 0$ are shown in Fig. 3, where the depletion is most evident for $w \ll \Delta$, while the pseudogap fills up for $w > \Delta$. Looking at corresponding spectral functions directly, we notice that for a developed pseudogap with $w \ll \Delta$ [in Fig. 2(b) (line-shaded)] there are still QP crossing the FS, although with small $Z_{\mathbf{k}} \ll 1$, while their velocity is not diminished. On the other hand if $w > \Delta$ the pseudogap is smeared out and consequently not effective, hence the FS is fully recovered. At intermediate doping this typically happens near the zone diagonal as shown in Fig. 2(b) (gray shaded).

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 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, fully developed near the $(\pi,0)$ point. The pseudogap is 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. More elaborate analysis of the proposed theory will be presented elsewhere.

One of the authors (P.P.) wishes to thank T.M. Rice, G. Khaliullin, and M. Imada for helpful discussions, and acknowledges the support of the Japan Society for the Promotion of Science, as well as the Institute for Theoretical Physics, ETH Zürich, the Institute for Materials Research, Sendai, and ISSP, the University of Tokyo, Kashiwa, where part of this work has been done.

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