SPECTRAL FUNCTIONS AND PSEUDOGAP IN A MODEL OF STRONGLY CORRELATED ELECTRONS

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Abstract. The theoretical investigation of spectral functions within the single-band t-J model, as relevant for superconducting cuprates, is presented. For spectral functions the method of equations of motion is used, where for the self energy the decoupling of spin and single-particle fluctuations is performed. Longer-range spin fluctuations induce a pseudogap showing up at low doping in the effective truncation of the Fermi surface and in reduced electron and quasiparticle density of states at the Fermi level.

Key words: Cuprates, Superconductivity, t-J Model, Strong Correlations, Pseudogap, Spectral Functions, Fermi Surface, ARPES, Spin Fluctuations

1. Introduction

One of the central questions in the theory of strongly correlated electrons is the nature of the ground state and of low energy excitations. Experiments in many novel materials with correlated electrons reveal even in the 'normal' metallic state striking deviations from the usual Fermi-liquid universality as given by the phenomenological Landau theory involving quasiparticles (QP)(1). The attention in the last decade has been increasingly devoted to the underdoped cuprates, where experiments reveal characteristic 'pseudogap' temperatures $T > T_c$, which show up crossovers where particular properties change qualitatively. There seems to be an indication for two crossover scales T^* and T_{sg}. T^* scale (2) shows up clearly as the maximum of the spin susceptibility $\chi_0(T = T^*)$, the kink in the in-plane resistivity $\rho(T)$, in the anomalous Hall constant $R_H(T < T^*)$ and in the specific heat $\gamma = C_V/T$ (1). It seems plausible that the T^* crossover is

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related to the onset of short-range antiferromagnetic (AFM) correlations for $T < T^*$, since this is clearly the case for an undoped AFM.

The single-particle spectral function $A(\mathbf{k}, \omega)$ and its properties are of crucial importance. In recent years there has been an impressive progress in the angle-resolved photoemission spectroscopy (ARPES) experiments, in particular for cuprate materials, which in principle yield a direct information on $A(\mathbf{k}, \omega)$. In most investigated $Bi_2Sr_2CaCu_2O_{2+\delta}$ (BSCCO) (3) ARPES shows quite well defined large Fermi surface in the overdoped and optimally doped samples at $T > T_c$. On the other hand, in the underdoped materials the quasiparticles (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 (4, 3), indicating that the rest of the large FS is truncated (5). At the same time near the $(\pi, 0)$ momentum ARPES reveals a hump at ~ 100 meV (4), which is consistent with large pseudogap scale T^*.

The prototype single-band model relevant for cuprates which takes explicitly into account strong correlations is the t-J model,

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

where fermionic operators are projected ones, $\tilde{c}^{\dagger}_{is} = (1 - n_{i,-s}) c^{\dagger}_{is}$. We consider besides $t_{ij} = t$ for the n.n. hopping also $t_{ij} = t' < 0$ for the n.n.n. hopping on a square lattice.

There have been so far numerous analytical and numerical studies of the t-J model and related Hubbard model on a square lattice. The importance of AFM spin correlations for the emergence of the (large) pseudogap was found in some of these numerical studies (6, 7, 8) and in phenomenological model calculations (9, 10).

First, we describe some evidence for the pseudogap within the t-J model obtained via finite-size studies using the finite-temperature Lanczos method (FTLM) (8). A most straightforward evidence for a pseudogap appears in the uniform static spin-suceptibility $\chi_0(T)$. The maximum T^* being related to the AFM exchange $T^* \sim J$ in an undoped AFM gradually shifts to lower T with doping and finally disappears at 'critical' $c_h = c_h^* \sim 0.15$. Obtained results are qualitatively as well as quantitatively consistent with experiments in cuprates (1). Another quantity relevant for comparison with the anaytical approach is the single-particle density of states (DOS) $\mathcal{N}(\omega)$, which shows at smallest dopings a pronounced pseudogap at $\omega \sim 0$ which closes with increasing $T \sim J$. This again indicates the relation of this pseudogap with the AFM short-range correlations which dissolve for $T > J$. On the other hand, the pseudogap closes also on increasing doping being barely visible even at $c_h \sim 0.12$.

2. Spectral functions: Equation-of-motion approach

In our anaytical approach we analyse the electron Green's function for projected fermionic operators,

$$G(\mathbf{k},\omega) = \langle\langle \tilde{c}_{\mathbf{k}s}; \tilde{c}^{\dagger}_{\mathbf{k}s} \rangle\rangle_{\omega} = -i \int_0^{\infty} e^{i(\omega+\mu)t} \langle \{ \tilde{c}_{\mathbf{k}s}(t), \tilde{c}^{\dagger}_{\mathbf{k}s} \}_+ \rangle dt. \tag{2}$$

In an equations-of-motion (EQM) method one uses relations for general correlation functions $\omega\langle\langle A; B\rangle\rangle_{\omega} = \langle\{A, B\}_+\rangle + \langle\langle [A, H]; B\rangle\rangle_{\omega}$, applying them to the propagator $G(\mathbf{k},\omega)$ (11),

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

We notice that the renormalization $\alpha = (1 + c_h)/2 < 1$ is already the consequence of the projected basis, while $\zeta_{\mathbf{k}}$ represents the new 'free' propagation term

$$\zeta_{\mathbf{k}} = \frac{1}{\alpha} \langle \{ [\tilde{c}_{\mathbf{k}s}, H], \tilde{c}^{\dagger}_{\mathbf{k}s} \}_+ \rangle - \bar{\zeta} = -4\eta_1 t \gamma_{\mathbf{k}} - 4\eta_2 t' \gamma'_{\mathbf{k}}, \tag{4}$$

where $\eta_j = \alpha + \langle \mathbf{S}_0 \cdot \mathbf{S}_j \rangle / \alpha$ and $\gamma_{\mathbf{k}} = (\cos k_x + \cos k_y)/2$, $\gamma'_{\mathbf{k}} = \cos k_x \cos k_y$.

The central quantity for further consideration is the self energy

$$\Sigma(\mathbf{k},\omega) = \langle\langle C_{\mathbf{k}s}; C^{+}_{\mathbf{k}s} \rangle\rangle^{irr}_{\omega} / \alpha, \qquad iC_{\mathbf{k}s} = [\tilde{c}_{\mathbf{k}s}, H] - \zeta_{\mathbf{k}} \tilde{c}_{\mathbf{k}s}, \tag{5}$$

where only the 'irreducible' part of the correlation function should be taken into account in the evaluation of Σ. We express EQM in variables appropriate for a paramagnetic metallic state

$$\begin{aligned} [\tilde{c}_{\mathbf{k}s}, H] &= [(1 - \tfrac{c_e}{2})\epsilon^0_{\mathbf{k}} - J c_e] \tilde{c}_{\mathbf{k}s} + \\ &+ \tfrac{1}{\sqrt{N}} \textstyle\sum_{\mathbf{q}} m_{\mathbf{k}\mathbf{q}} [s S^z_{\mathbf{q}} \tilde{c}_{\mathbf{k}-\mathbf{q},s} + S^{\mp}_{\mathbf{q}} \tilde{c}_{\mathbf{k}-\mathbf{q},-s} - \tfrac{1}{2} \tilde{n}_{\mathbf{q}} \tilde{c}_{\mathbf{k}-\mathbf{q},s}], \end{aligned} \tag{6}$$

where $\epsilon^0_{\mathbf{k}}$ is the bare band energy, $\tilde{n}_i = n_i - c_e$ and $m_{\mathbf{k}\mathbf{q}}$ is the effective spin-fermion coupling,

$$m_{\mathbf{k}\mathbf{q}} = 2J\gamma_{\mathbf{q}} + \epsilon^0_{\mathbf{k}-\mathbf{q}}. \tag{7}$$

One important achievement of EQM method is that it naturally leads to an effective coupling between fermionic and spin degrees of freedom, which are essential for the proper description of low-energy physics in cuprates. Such a coupling is e.g. assumed as input in phenomenological models (9, 10) as the spin-fermion model. The essential difference in our case is that $m_{\mathbf{k}\mathbf{q}}$ is strongly dependent on $\mathbf{k}$ just in the vicinity of most relevant 'hot' spots.

We assume that spin fluctuations remain dominant at the AFM wavevector $\mathbf{Q}$ with the characteristic inverse AFM correlation length $\kappa = 1/\xi_{AFM}$.

It is sensible to divide spin fluctuations into two regimes with respect to $\tilde{\mathbf{q}} = \mathbf{q} - \mathbf{Q}$: a) For $\tilde{q} > \kappa$ spin fluctuations are paramagnons, they are propagating like magnons and are transverse to the local AFM ordering. b) For $\tilde{q} < \kappa$ spin fluctuations are critically overdamped and the deviations from the long range order are essential.

For $\tilde{q} > \kappa$ the decoupling of spin and fermion degrees of freedom reproduces for an undoped AFM the evaluation of $\Sigma(\mathbf{k},\omega)$ within the self-consistent Born approximation (12) which we generalise within the linearized magnon theory into a paramagnon contribution at finite doping (at $T = 0$), (13)

$$\Sigma_{\rm pm}(\mathbf{k},\omega) = \frac{1}{N}\sum_{q,\tilde{q}>\kappa}[M^2_{\mathbf{kq}}G^-(\mathbf{k}-\mathbf{q},\omega+\omega_{\mathbf{q}}) + M^2_{\mathbf{k+q,q}}G^+(\mathbf{k}+\mathbf{q},\omega-\omega_{\mathbf{q}})], \tag{8}$$

where $G^{\pm}(\mathbf{k},\omega)$ refer to the electron ($\omega > 0$) and hole-part ($\omega < 0$) of the propagator, respectively. We are dealing with a strong coupling theory due to $t > \omega_{\mathbf{q}}$ and a selfconsistent calculation of $\Sigma_{\rm pm}$ is required.

At $c_h > 0$ besides the paramagnon excitations also the coupling to longitudinal spin fluctuations becomes crucial. The latter restore the spin rotation symmetry in a paramagnet and EQM (6) introduce such a spin-symmetric coupling. Within a simplest approximation that the dynamics of fermions and spins is independent, we get (13)

$$\Sigma_{\rm lf}(\mathbf{k},\omega) = \frac{1}{\alpha}\sum_{\mathbf{q}}\tilde{m}^2_{\mathbf{kq}}\int\int\frac{d\omega_1 d\omega_2}{\pi}g(\omega_1,\omega_2)\frac{\tilde{A}(\mathbf{k}-\mathbf{q},\omega_1)\chi''(\mathbf{q},\omega_2)}{\omega-\omega_1-\omega_2}, \tag{9}$$

where $g = (1/2)[\mathrm{th}(\beta\omega_1/2) + \mathrm{cth}(\beta\omega_2/2)]$ and χ is the dynamical spin susceptibility. Quite analogous treatment has been employed previously in the Hubbard model (14) and more recently within the spin-fermion model (9, 10).

If we want to use the analogy with the phenomenological spin-fermion model the effective coupling parameter $\tilde{m}_{\mathbf{kq}}$ should satisfy $\tilde{m}_{\mathbf{k,q}} = \tilde{m}_{\mathbf{k-q,-q}}$ therefore we use instead the symmetrized coupling $\tilde{m}_{\mathbf{kq}} = 2J\gamma_{\mathbf{q}} + (\epsilon^0_{\mathbf{k-q}} + \epsilon^0_{\mathbf{k}})/2$. In contrast to previous related studies of spin-fermion coupling (9, 10), $\tilde{m}_{\mathbf{kq}}$ is strongly dependent on $\mathbf{k}$, but also quite modest along the AFM zone boundary ('hot' spots), here determined solely by J and t'. For $\tilde{A}$ we first insert the unrenormalized A^0, i.e. without $\Sigma_{\rm lf}$.

In the present theory spin response $\chi(\mathbf{q},\omega)$ is taken as input. The system is close to the AFM instability, so we assume the overdamped form

$$\chi''(\mathbf{q},\omega) \propto \frac{\omega}{(\tilde{q}^2+\kappa^2)(\omega^2+\omega_\kappa^2)}. \tag{10}$$

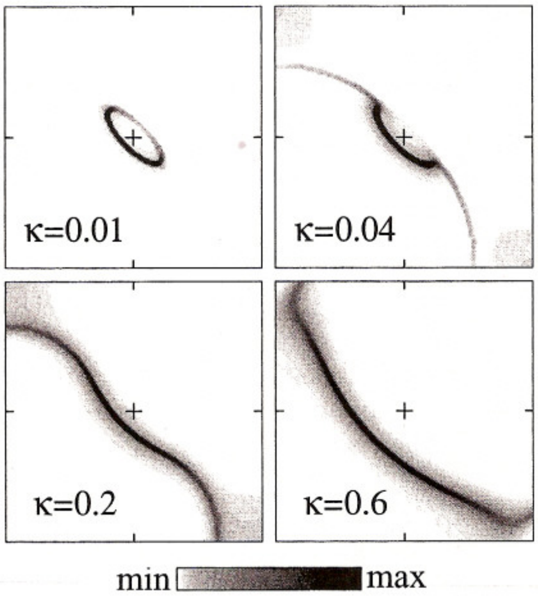

Figure 1. Contour plot of spectral functions $A(\mathbf{k}, \omega = 0)$ at $T = 0$ for various κ in one quarter of the Brillouin zone.

of $Z_F \ll 1$ the QP velocity v_F is not diminished within the pseudogap. In fact it is even enhanced, as seen in in Fig. 2 where the contour plot of $A(\mathbf{k}, \omega)$ is shown. Again, it is well evident in Fig. 2 that QP are well defined at the FS, while they become fuzzy at $\omega \neq 0$ merging with the solutions $E^{\pm}_{\mathbf{k}}$, respectively, away from the FS. The effect can be only explained with crucial $\mathbf{k}$ dependence of $\Sigma'(\mathbf{k}, \omega)$ (13). Assuming that $\mathbf{k}$ enters only via $\epsilon(\mathbf{k})$ we can express v_F renormalization as

$$\frac{v_F}{v^{\mathrm{ef}}_{\mathbf{k}}} = (1 + \frac{\partial \Sigma'}{\partial \epsilon}) \frac{Z_F}{Z^{\mathrm{ef}}}. \qquad \frac{\partial \Sigma'}{\partial \epsilon}\Big|_{\omega=0} \sim \frac{\Delta^2}{w(\omega_\kappa + w)}, \tag{13}$$

While $Z_F/Z^{ef} \ll 1$, $\partial \Sigma'/\partial \epsilon$ compensates or even leads to an enhancement of v_F. In the case $\omega_\kappa w \ll \Delta^2$ we get $v_F/v^{\mathrm{ef}}_{\mathbf{k}} \sim \omega_\kappa/w \sim 2J/v_{\mathbf{k}}$. Final v_F is therefore not strongly renormalized, since $2J$ and $v^{\mathrm{ef}}_{\mathbf{k}}$ are of similar order. Furthermore, $\tilde{v}_F$ is enhanced near $(\pi, 0)$ point. The situation is thus very different from 'local' theories where $\Sigma(\mathbf{k}, \omega) \sim \Sigma(\omega)$ and the QP renormalization is governed only by Z_F.

From $A(\mathbf{k}, \omega)$ we can calculate the DOS $\mathcal{N}(\omega)$. The contribution will come mostly from FS arcs near the zone diagonal while the gapped regions near $(\pi, 0)$ will contribute less due to $Z(\mathbf{k}_F) \ll 1$. As expected the DOS

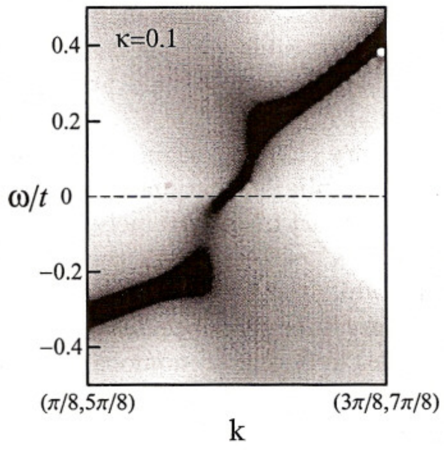

Figure 2. Contour plot of spectral functions $A(\mathbf{k}, \omega = 0)$ across the FS in the pseudogap regime.

decreases with decreasing κ, i.e. approaching an undoped AFM, consistent with experiments in cuprates (15, 16). We can as well define the QP DOS $\mathcal{N}_{QP} \propto \oint dS_F/v(\mathbf{k})$. It is quite important to notice a decreasing κ leads also to a decrease of $\mathcal{N}_{QP}$. This is consistent with the observation of the pseudogap also in the specific heat in cuprates (17), since $\mathcal{N}_{QP} \propto \gamma$. We note here that such a behavior is not at all evident in the vicinity of a metal-insulator transition. Namely, normally in a Fermi liquid one would drive the metal-insulator transition by $Z_{\rm av} \to 0$ and within an assumption of a local character $\Sigma(\omega)$ this would lead to $v_F \to 0$ and consequently to $\mathcal{N}_{QP} \to \infty$.

It is also important to understand the role of finite $T > 0$. The most pronounced effect is on QP in the pseudogap regime. The main conclusion is, that weak QP peak with $Z_F \ll 1$ at $T = 0$, as seen e.g. in Fig. 2, is not just broadened but entirely disappears (becomes incoherent) already by very small $T > T_s \ll J$ (13).

4. Conclusions

We have presented our results for spectral functions and pseudogap within the t-J model, which is the prototype model for strongly correlated electrons. The physics of the t-J model at lower doping is determined by the interplay of the magnetic exchange and the itinerant kinetic energy of fermions. At intermediate doping the system is frustrated, the effect showing up in large entropy, pronounced spin fluctuations, non-Fermi liquid effects etc. Evidently, this is one path towards the metal-insulator transition, but definitely not the only one possible. In our case, fermionic and spin degrees of freedom coexist but are coupled and both active and relevant for low-energy properties.

Within the present theory (13) the origin of the pseudogap feature is in the coupling to longitudinal spin fluctuations near the AFM wavevector **Q**. It is important to note that apart from extremely small κ we are still dealing with large FS. Still, at $\kappa \ll \kappa^* \sim 0.5$ parts of the FS in the nodal direction remain well pronounced while the QP weight within the pseudogap (zone corners) region of the FS are strongly suppressed. QP within the pseudogap have small weight $Z_F \ll 1$ but due to nonlocal character of $\Sigma(\mathbf{k},\omega)$ not diminished (or even enhanced) v_F. This gives an explanation for a well known theoretical challenge that approaching the magnetic insulator both electron and QP DOS decrease and vanish.

We presented results for $T = 0$, however the extension to $T > 0$ is straightforward. Discussing only the effect on the pseudogap, we notice that it is mainly affected by κ. So we can argue that the pseudogap should be observable for $\kappa(c_h, T) < \kappa^* \sim 0.5$. This effectively determines the crossover temperature $T^*(c_h)$ approximately as $T^* \sim T_0^*(1 - c_h/c_h^*)$ where $T_0^* \sim 0.6J$ and $c_h^* \sim 0.15$.

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