Weak pseudogap behavior in the underdoped cuprate superconductors

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We report on an exact solution of the nearly antiferromagnetic Fermi liquid spin fermion model
in the limit $\pi T \gg \omega_d$, which demonstrates that the broad high energy features found in ARPES
measurements of the spectral density of the underdoped cuprate superconductors are determined by
strong antiferromagnetic (AF) correlations and precursor effects of an SDW state. We show that the
onset temperature, $T^{\ast cr}$, of weak pseudo-gap (pseudoscaling) behavior is determined by the strength,
$\xi$, of the AF correlations, and obtain the generic changes in low frequency magnetic behavior seen
in NMR experiments with $\xi(T_{cr}) \approx 2$, confirming the Barzykin and Pines crossover criterion.

74.25.-q, 75.25.Dw, 74.25.Ha

Magnetically underdoped cuprates may be distinguished from their overdoped counterparts by the presence of a maximum at a temperature $T_{cr} > T_c$ in the temperature dependent uniform susceptibility, $\chi_o(T)$. They are characterized by the occurrence of a quasiparticle peak at wave vectors close to $(\pi, \pi)$, introduced byMillis, Monien, and Pines [6] to explain NMR experiments:

$$V_{eff}^{NAFL}(\mathbf{q}, \omega) = g^2 \chi_{q}(\omega) = \frac{g^2 \chi_{Q}}{1 + \xi^2 (\mathbf{q - Q})^2 - \frac{\omega}{\omega_d}}, \quad (1)$$

where $\chi_{Q} = \alpha \xi^2$, with $\alpha$ constant, and $g$ is the coupling constant.

Since the dynamical spin susceptibility $\chi_{q}(\omega)$ peaks at wave vectors close to $(\pi, \pi)$, two different kinds of quasiparticles emerge: hot quasiparticles, located not far from the diagonals, $|k_x| = |k_y|$, feel a “normal” interaction. Their distinct lifetimes can be inferred from ARPES experiments, where a detailed analysis shows that the behavior of the hot quasiparticles is highly anomalous, while cold quasiparticles may be characterized as a strongly coupled Landau Fermi Liquid [6].

In the present communication we focus our attention on temperatures $T \geq T_{\ast}$. Our reason for doing so is that for $T > T_{\ast}$, fits to NMR experiments show that $\omega_d < pT$, the frequency equivalent of temperature. Because of its comparatively low characteristic energy the spin system is thermally excited and behaves quasistatically; the hot quasiparticles see a spin system which acts like a static deformation potential, a behavior which is no longer found below $T_{\ast}$, where the lowest scale is the temperature itself and the quantum nature of the spin degrees of freedom is essential. We find that above $T_{\ast}$, in the limit $\pi T \gg \omega_d$ it is possible to obtain an exact solution of the spin fermion model with the effective interaction, $V_{eff}^{NAFL}(\mathbf{q}, \omega)$, of Eq. (1).

Our main results are the appearance in the hot quasiparticle spectrum of the high energy features seen in ARPES, a maximum in $\chi_o(T)$ and a crossover in $63T_{1}^{T}/63T_{2G}^{T}$ for $\xi > \xi_o \approx \nu p/\Delta_o$. These are produced...
by the emergence of an SDW-like state, as proposed by Chubukov et al. Here, $v_F$ is the Fermi velocity and $\Delta_0 = \frac{\mu}{\sqrt{3}} \sqrt{\langle S^2 \rangle} \sim \frac{\pi}{2}$, a characteristic energy scale of the SDW-like pseudogap. Using typical values for the hopping elements (see below), and $\mu \approx 0.6 \text{eV}$ (determined from the analysis of transport experiments in slightly underdoped materials), we find $\xi_0 \approx 2$. For $\xi > \xi_0$, the hot quasiparticle spectral density takes a two-peak form which reflects the emerging spin density wave state, while the MMP interaction generates naturally the distinct behavior of hot and cold quasiparticle states seen in ARPES experiments.

Before discussing these results, we summarize our calculations briefly. Using the effective interaction, Eq. 1, the direct spin-spin coupling is eliminated via a Hubbard-Stratonovich transformation, introducing a collective spin field $S_\mathbf{q}(\tau)$. After integrating out the fermionic degrees of freedom, the single particle Green’s function can be written as

$$G_{\mathbf{k},\sigma}(\tau - \tau') = \langle \hat{G}_{\mathbf{k},\mathbf{k}\sigma}(\tau,\tau'|\mathbf{S}) \rangle_\mathbf{S},$$

where $\hat{G}_{\mathbf{k},\mathbf{k}\sigma}(\tau,\tau'|\mathbf{S})$ is the matrix element of

$$[G_{ok}^{-1}(\tau - \tau')\delta_{\mathbf{k},\mathbf{k}'} - \frac{g}{\sqrt{3}} S_{\mathbf{k} - \mathbf{k}'}(\tau)\delta(\tau - \tau') \cdot \vec{\sigma}]^{-1},$$

which describes the propagation of an electron for a given configuration $\mathbf{S}$ of the spin field. $\vec{\sigma}$ is the Pauli matrix vector and $G_{ok}^{-1} = -\langle \partial_\tau + \varepsilon_{\mathbf{k}} \rangle$ is the inverse of the unperturbed single particle Green’s function with bare dispersion

$$\varepsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y - \mu.$$  

In the following we use $t = 0.25 \text{eV}$ and $t' = -0.4t$ for the nearest and next nearest neighbor hopping integrals, respectively, and we adjust the chemical potential $\mu$ to maintain the constant hole concentration at $n_h = 15\%$. The average $\langle \cdots \rangle_\mathbf{S} = \frac{1}{Z_0} \int D\mathbf{S} \cdots \exp \{-S_\mathbf{S}\}$ is performed with respect to the action of the collective spin degrees of freedom:

$$S_\mathbf{S}(\mathbf{S}) = \frac{T}{2} \sum_{\mathbf{q},\nu} \chi^{-1}_\mathbf{q}(i\omega_n) S_{\mathbf{q}}(i\omega_n) \cdot S_{-\mathbf{q}}(-i\omega_n)$$

where $\omega_n = 2n\pi T$ and $Z_0$ is defined via $\langle 1 \rangle_\mathbf{S} = 1$. In using Eq. 3 we have assumed that (i) $\chi_\mathbf{q}(\omega)$ is the fully renormalized spin-susceptibility taken from the experiment and (ii) any nonlinear (higher order in $\mathbf{S}$ than quadratic) terms of the spin field can be neglected. The model which results from assumption (ii) is usually referred to as the spin fermion model.

After inversion of Eq. 3 in spin space, the average of Eq. 2 can be evaluated diagrammatically using Wick’s theorem for the spin field. In the above mentioned static limit, $\pi T \gg \omega_d$, it suffices to consider only the zeroth bosonic Matsubara frequency in $\chi_\mathbf{q}(i\omega_n)$. The remaining momentum summations are evaluated by expanding $\varepsilon_{\mathbf{k} + \mathbf{q}} \approx \varepsilon_{\mathbf{k} + \mathbf{Q}} + \mathbf{v}_{\mathbf{k} + \mathbf{Q}} \cdot (\mathbf{Q} - \mathbf{Q})$ for momentum transfers close to $\mathbf{Q}$, using $\mathbf{v}_{\mathbf{k} + \mathbf{Q}} = \partial \varepsilon_{\mathbf{k} + \mathbf{Q}} / \partial k_\alpha$. In this limit all diagrams can be summed up by generalizing a solution for a one dimensional charge density wave system obtained by Sadovskii to the case of two dimensions, and more importantly, to isotropic spin fluctuations. We find the following recursion relation for the Green’s function $G_\mathbf{k}(\omega) = G_{\mathbf{k}=0}(\omega)$, whose imaginary part determines the spectral density $A(\mathbf{k},\omega)$, seen in ARPES:

$$[G_\mathbf{k}(\omega)]^{-1} = \omega - \varepsilon_{\mathbf{k} + \mathbf{Q}} + i\frac{\nu_{\mathbf{k} + \mathbf{Q}}}{\xi} - \kappa_{l+1} \Delta_0^2 G_\mathbf{k}^{l+1}(\omega).$$

Here, $\nu_{\mathbf{k} + \mathbf{Q}} = |\mathbf{v}_{\mathbf{k} + \mathbf{Q}}|$ and $\kappa_l = (l + 2)/3$ if $l$ is odd, while $\nu_{\mathbf{k} + \mathbf{Q}} = |\mathbf{v}_{\mathbf{k} + \mathbf{Q}}|(|\cos \phi_{\mathbf{k}}| + |\sin \phi_{\mathbf{k}}|)$ and $\kappa_l = 1/3$ if $l$ is even. $\phi_{\mathbf{k}}$ is the angle between $\mathbf{v}_{\mathbf{k} + \mathbf{Q}}$ and $\mathbf{v}_{\mathbf{k}}$. The recursion relation, Eq. 4, enables us to calculate $A(\mathbf{k},\omega)$ to arbitrary order in the coupling constant $g$.

To first order in $g$, the Green’s function reduces to $G_\mathbf{k}(\omega) = \int d\Delta p(\Delta) G_{\mathbf{k} \mathbf{SDW}}(\Delta)$, where $G_{\mathbf{k} \mathbf{SDW}}(\Delta)$ is the single particle Green’s function of the mean field SDW state and $p(\Delta) \sim \Delta^2 \exp(-\frac{\Delta^2}{\Delta_0^2})$ is the distribution function of a fluctuating SDW gap, centered around $\sqrt{\frac{4}{\pi}} \Delta_0$, i.e., the amplitude fluctuations of the spins $\mathbf{S}$ are confined to a region around $\sqrt{\frac{4}{\pi}} \langle S^2 \rangle$, although in our calculations directional fluctuations are fully isotropic and spin rotation invariance is maintained. Below we show that the SDW like solution is obtained even at finite values of $\xi$.

The quantities we calculate are the single particle spectral density, $A(\mathbf{k},\omega)$ and the low frequency behavior of the irreducible spin susceptibility $\chi_{\mathbf{k}}(\omega, T)$. Our principal results are depicted in Figures 1–3. The $\xi$-dependence of the Fermi surface, shown in the inset to Fig. 1a, is similar to the results obtained by Chubukov et al. at $T = 0$; however for the experimentally relevant range of $\xi$, hole pockets around $\mathbf{k} = (\pi/2, \pi/2)$ do not form. We have used the criterion $\varepsilon_{\mathbf{k}} + \text{Re} \Sigma_{\mathbf{k}}(\omega = 0) = 0$ to determine the Fermi surface. Although strictly valid only for $T = 0$, for finite temperatures it indicates when a quasiparticle crosses the chemical potential. In the limit of very large correlation length, we find, in addition to the two broadened poles of a SDW like state, a third solution of $\omega = \text{Re} \Sigma_{\mathbf{k}}(\omega = 0) + \varepsilon_{\mathbf{k}}$, which although not visible due to the large scattering rates, ensures that even for $\xi \to \infty$ a large Fermi surface and only a pseudogap in the density of states occurs.

A comparatively sharp transition between the behavior of hot quasiparticles (located at points $a$ and $b$ on the Fermi surface of Fig. 1a) and cold quasiparticles (at $d$ and $e$) is found. For hot quasiparticles the single particle spectral density evolves with temperature as the AF correlation length increases from $\xi \approx 1$ to 5; a two
peak structure, which corresponds to a transfer of spectral weight from low frequencies to frequencies above 200 – 300 meV, develops at \( \xi_o \approx 2 \), and is quite pronounced for \( \xi \geq 3 \) (Fig. 1b). As may be seen in Fig. 1a, the shift in spectral density found for hot quasiparticles does not occur for cold quasiparticles, whose spectral density continues to be peaked at the Fermi energy.

We sum all diagrams of the perturbation series for the electron-spin fluctuation vertex function in similar fashion as the Green’s function \( G_k(\omega) \) in Eq. (6). The lack of symmetry breaking is essential for a proper evaluation of the vertex which, as long as the spin rotation invariance is intact, is reduced at most by a factor \( \approx \frac{1}{3} \) for the high energy features \([1,2]\). For lower excitation energies, this vertex is considerably enhanced for the hot quasiparticles; it is almost unaffected for the cold quasiparticles, reflecting again their qualitatively different behavior.

We combine the results for \( G_k(\omega) \) and the electron-spin fluctuation vertex function and so determine the irreducible spin susceptibility \( \tilde{\chi}(\omega) \). We find (Fig. 2) that both \( \tilde{\chi}_o(T) \) and \( \tilde{\chi}_Q(T) \) exhibit maxima at temperatures close to \( T^{cr} \) where \( \xi \approx 2 \). In these calculations we assumed that \( \xi^{-1}(T) = \frac{1}{4} + \frac{T-T^{cr}}{T^{*}} \) between \( T^{cr} = 470 \) K and \( T^{*} = 220 \) K and \( \xi^{-2}(T) = \frac{1}{4} + \frac{T-T^{cr}}{700 \text{K}} \) above \( T^{cr} \) consistent with the NMR results of Curro et al. \([3]\) for \( \text{YBa}_2\text{Cu}_4\text{O}_8 \). The behavior of \( \tilde{\chi}_o(T) \) and \( \tilde{\chi}_Q(T) \) above the maximum reflects the increasing importance of lifetime (strong coupling) effects which act to reduce both irreducible susceptibilities. Because of comparatively short correlation lengths \( \xi < 2 \), it is likely that Eliashberg calculations \([4]\) will provide a better quantitative account in this mean field regime. The fall-off in \( \tilde{\chi}_o(T) \) and \( \tilde{\chi}_Q(T) \) below \( T^{cr} \) arises primarily from the transfer of quasiparticle spectral weight to higher energies.

The determination of the full spin susceptibility \( \chi_q(\omega) = \tilde{\chi}_q(\omega)/(1 - J_q\tilde{\chi}_q(\omega)) \) requires calculating the restoring force \( J_q \), and is beyond the scope of the present work, since \( J_q \) is determined by the renormalization of the spin exchange fermion-fermion interaction through high energy excitations in all other channels. However, for \( \chi_o(T) \), with the assumption that \( J_q=0 \chi(T^{cr}) = 0.5 \), a good quantitative fit to the experimental results of Curro et al. \([2]\) between \( T^{cr} \) and \( T^{*} \) is found.

We find that both vertex corrections and quasiparticle spectral weight transfer play a significant role in determining the low frequency spin dynamics. As may be seen in the inset to Fig. 3, when both effects are taken into account, our calculated values of the spin damping \( \gamma_q = \tilde{\chi}_Q''(\omega)/\omega \big|_{\omega=0} \) display the crossover at \( T^{cr} \) anticipated by Monthoux and Pines \([13]\). A second calcu-
YBa particles, for moderate AF correlation lengths, about by the strong interaction between the planar quasi-
the appearance of SDW precursor phenomena, brought
lations apply. Strong pseudogap behavior corresponds
for states close to (π, 0) affects mostly the low frequency part of the irreducible
behavior. Because symmetry is not broken, there will
continue to be coherent states at the Fermi energy; although
their spectral weight is small one still has a large
behavior. Because symmetry is not broken, there will continue to be coherent states at the Fermi energy; although their spectral weight is small one still has a large Fermi surface. Such coherent quasiparticles, invisible in the present temperature range, are, we believe, responsible for the sharp peak for k ∼ (π, 0), observed in ARPES below the superconducting transition temperature.

The present theory cannot, of course, explain the leading edge pseudogap found below T_s, since one is then no longer in the quasistatic limit for which our calculations apply. Strong pseudogap behavior corresponds to a further redistribution of quasiparticle states lying within ≈ 30 meV of the Fermi energy. No appreciable change is seen in the high energy features found in the present calculations. It is likely that strong scattering in the particle-particle channel plays an increasingly important role below T_s, since we find above T_s important prerequisites for its appearance; an enhanced spin fluctuation vertex and a pronounced flattening of the low energy part of the hot quasiparticle states. In addition, below T_s the quantum behavior of spin excitations becomes increasingly important. This reduces the phase space for quasiparticle scattering, and leads to the sizable suppression of the hot quasiparticle scattering rate found below T_s.

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