Short-range spin correlations and pseudogap in underdoped cuprates

Bumsoo Kyung

Département de physique and Centre de recherche sur les propriétés électroniques de matériaux avancés, Université de Sherbrooke, Sherbrooke, Québec, Canada J1K 2R1 (June 22, 2001)

In this paper we show that local spin-singlet amplitude with d-wave symmetry can be induced by short-range spin correlations even in the absence of pairing interactions. In the present scenario for the pseudogap, the normal state pseudogap is caused by the induced local spin-singlet amplitude due to short-range spin correlations, which compete in the low energy sector with superconducting correlations to make $T_c$ go to zero near half-filling.

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The recent discovery of pseudogap in underdoped high $T_c$ cuprates has challenged condensed matter physicists for several years. The pseudogap behavior is observed as strong suppression of low frequency spectral weight below some characteristic temperature $T^*$ higher than transition temperature $T_c$. This anomalous phenomenon has been observed in angle resolved photoemission spectroscopy (ARPES), specific heat, tunneling, NMR, and optical conductivity. One of the most puzzling questions in pseudogap phenomena is why $T^*$ has a completely different doping dependence from $T_c$, in spite of their possibly close relation. In this paper we demonstrate that induced local spin-singlet amplitude due to short-range spin correlations can cause a normal state pseudogap with d-wave symmetry even in the absence of pairing interactions.

First of all we argue that there are two energy scales in the problem, because the pseudogap appears as a crossover phenomenon according to experiments. The low energy (or long distance) physics of antiferromagnetic (AF) and superconducting (SC) correlations is well captured by a static mean-field approach, while the relatively high energy (or short distance) physics of the pseudogap is invisible in such a study. Thus we resort to fluctuation theory in order to describe the dynamical nature of the pseudogap, and to determine $T^*$ and pseudogap size $\Delta_{pg}$.

The mean-field result of the $t - J$ model will be used below solely to find the onset of leading correlations, and to compute mean-field AF and SC order parameters for the calculation of local spin-singlet amplitude.

The mean-field $t - J$ Hamiltonian reads

$$H_{MF} = \sum_{\vec{k}, \sigma} \varepsilon(\vec{k}) c_{\vec{k}, \sigma}^\dagger c_{\vec{k}, \sigma} - 4Jm\hat{n} - J\hat{s}(\hat{s} + \hat{s}^\dagger), \quad (1)$$

where $\varepsilon(\vec{k}) \simeq -2tx(\cos k_x + \cos k_y) - \mu$ with $x$ the hole density, $\hat{n} = 1/(2N) \sum_{\vec{k}, \sigma} c_{\vec{k}, \sigma}^\dagger c_{\vec{k}, \sigma}$ and $\hat{s} = 1/N \sum_{\vec{k}} \phi_d(\vec{k}) c_{\vec{k}, \uparrow}^\dagger c_{\vec{k}, \downarrow}$ with $N$ the total number of lattice sites. $m$, $s$ are mean-field AF, SC order parameters determined from $m = \langle \hat{n} \rangle$ and $s = \langle \hat{s} \rangle$, respectively.

$\phi_d(\vec{k}) = \cos k_x - \cos k_y$ and $\vec{Q}$ is the (commensurate) AF wave vector ($\pi, \pi$) in two dimensions. In this paper we restrict ourselves to a uniform solution which is just enough for our purpose. In a mean-field approximation, mean-field order already sets in when the correlation length reaches roughly one lattice spacing. This forces the above mean-field phase line (Fig. (a)) to be interpreted as the onset of the corresponding short-range correlations. We identify $T_{MF}^N$ with another crossover temperature $T^\phi$ at which some magnetic experiments such as Knight shift show their maximum. For the parameter ($t/J = 3.0$) used in this paper, short-range spin correlations disappear at $x = x_c \simeq 0.19 - 0.20$ at low temperature.

We introduce spin-singlet correlation function

$$\chi_{pp}(i, \tau) = \langle T_\tau \Delta_d(i, \tau) \Delta_d^\dagger(0, 0) \rangle, \quad (2)$$

FIG. 1. (a) Calculated mean-field phase diagram in doping ($x = 1 - n$) and temperature ($T$) plane in the $t - J$ model for $t/J = 3.0$. $T_{MF}^N$ and $T_{MF}^c$ are mean-field AF and SC ordering temperatures, respectively. The filled diamonds are the pseudogap temperature determined from the single particle spectral function. (b) Interaction induced local spin-singlet (solid curve) and spin (dashed curve) amplitudes for $t/J = 3.0$ and $T = 0.2J$. 

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where $\Delta_d(i) = \frac{1}{2} \sum_\delta g(\delta)(c_{i+\delta,\uparrow}c_{i,\downarrow} - c_{i+\delta,\downarrow}c_{i,\uparrow})$ with $g(\delta) = 1/2$ for $\delta = (\pm 1, 0)$, $-1/2$ for $\delta = (0, \pm 1)$, and 0 otherwise. The spin-singlet correlation function is related to the local spin-singlet amplitude through the sum rule

$$\frac{T}{N} \sum_q \chi_{pp}(q)e^{-i\nu_m q} = \langle |\Delta_d(0)|^2 \rangle,$$

where $q = (\vec{q}, i\nu_m)$ and $\nu_m$ is bosonic Matsubara frequencies. $T$ is absolute temperature. In terms of renormalized vertex $V_{pp}$, we approximate the spin-singlet correlation function

$$\chi_{pp}(q) = \frac{\chi_{pp}^0(q)}{1 - V_{pp}\chi_{pp}(q)},$$

where the irreducible susceptibility is defined as $\chi_{pp}^0(q) = \frac{T}{N} \sum_k (\phi_d(\vec{k}) + \phi_d(\vec{q} - \vec{k}))^2 G^0(q - k)G^0(k)$, and $G^0(k)$ is the noninteracting Green’s function obtained from Eq. (1). Now the unknown vertex, $V_{pp}$, is determined by the sum rule Eq. (3, 4). Hence, an increase in the local spin-singlet amplitude evaluated in the interacting state over that in the noninteracting state leads to a nonvanishing positive value of $V_{pp}$, namely, the enhancement of the correlation function. This (nonperturbative sum rule) approach has been shown to be quite reliable as long as short range correlations are concerned. In our calculations, the pseudogap appears when the spin-singlet correlation length reaches about 1 lattice constant. The self-energy due to the spin-singlet correlation function is given by

$$\Sigma_{pp}(k) = -\frac{1}{4} VV_{pp} T \sum_q \left( \phi_d(\vec{k}) + \phi_d(\vec{q} - \vec{k}) \right)^2 \chi_{pp}(q) G^0(q - k),$$

where $V = J$ from Eq. (1).

First let us begin by showing the interaction-induced local spin-singlet (solid curve) amplitude (Fig. 1(b)) evaluated in the mean-field state of the $t - J$ Hamiltonian in a region where $s = 0$ (or $T > T_{MF}^c$). Since $s = 0$, the spin-singlet amplitude is entirely caused by short-range spin correlations in the absence of pairing interactions. Although in general a mean-field state is not accurate for strongly correlated electron systems, certain local and short-range static quantities such as double occupancy and nearest neighbor correlations are reasonably well captured by the mean-field state particularly with AF order (See Ref. [1] for more details). In fact the interaction-induced local spin-singlet amplitude (Eq. (3)) is determined most crucially by these quantities. Quite unexpectedly, the local spin-singlet amplitude increases with decreasing doping despite the fact that the mean-field SC order is absent. The increase of local spin-singlet amplitude traces back to the growing short-range spin correlations with decreasing doping. [13]

In Fig. 1(a) we show the pseudogap temperature $T^*$ (filled diamonds) where the single particle spectral function $A(\vec{k}, \omega)$ near $\vec{k} = (\pi, 0)$ starts to be split into two peaks. $T^*$ falls from a high value onto the $T_c (\leq T_{c}^{MF})$ line instead of sharing a common line with $T_c$ in over-doped region. It is not surprising to find that $T^*$ closely follows $T_{MF}^c = T^0$, because in our study the pseudogap is caused by induced local spin-singlet amplitude due to short-range spin correlations, which is reasonably well captured by the mean-field state with AF order. When superconductivity is suppressed by setting $s = 0$, $T^*$ vanishes near $x_c$ where short-range spin correlations disappear. All these features are at least qualitatively consistent with the findings by Tallon and Loram. [11]

Figure 2(a) shows the pseudogap size $\Delta_{pg}$ (filled diamonds) by setting $s = 0$ at $T = 0$. In the same figure the pseudogap energy extracted from various experiments by Tallon and Loram [13] is also shown as empty symbols for comparison. $\Delta_{pg}$ vanishes near $x_c$, suggesting the presence of a quantum critical point at a critical doping. The agreement between our results and experiments appears remarkable for such a simple approximation used in this paper. The linear vanishing of $\Delta_{pg}$ near $x_c$ is closely related to the corresponding behavior of the induced local spin-singlet amplitude.

The total excitation gap (or ARPES leading edge gap or SC gap) $\Delta_g$ at $T = 0$ is larger than $\Delta_{pg}$ due to the additional contribution to the local spin-singlet amplitude from $s \neq 0$, which is shown together with $\Delta_{pg}$ in Fig. 2(b). $\Delta_{pg}$, $\Delta_g$ and their relative ratio $\Delta_{pg}/\Delta_g$ are all monotonically decreasing functions of doping, as

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shown in the inset of Fig. 2(b). Since the SC order pa-
parameter vanishes at $T_c$ (at $T_{MF}^{c}$ in this paper), the SC
gap below $T_c$ continuously evolves into the normal state
pseudogap above $T_c$ with the same momentum depen-
dence and magnitude.

The pseudogap appears here only as the suppression of
low frequency spectral weight in certain physical quanti-
ties which are obtained through $A(k, \omega)$ or its convolution
with a relevant vertex. It does not appear as a ther-
modynamic phase with broken symmetry. The present
scenario for the pseudogap predicts that a normal state
pseudogap is likely to appear when short-range spin cor-
relations are well established and are not masked by long-
range (AF or SC) order. The present results are robust
to variations of $t/J = 2.5–3.5$ and small to moderate
value of $t'$. In summary, we have shown that the induced local
spin-singlet amplitude due to short-range spin correlations
causes a normal state pseudogap even in the ab-

ence of pairing interactions. $T^*$ falls from a high value
onto the $T_c$ line and closely follows $T_{MF}^{c}$. The calculated
pseudogap size is in good agreement with experimental
results. It would be interesting to see how robust are
the features found in this paper, when the no-double-
occupancy constraint is strictly imposed on the $t - J$
model and an inhomogeneous solution is used.

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