Induced local spin-singlet amplitude and pseudogap in high $T_c$ cuprates

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In this paper we show that local spin-singlet amplitude with $d$-wave symmetry, $\langle \Delta_d(0) \rangle^2$, can be induced by short-range spin correlations even in the absence of pairing interactions. Fluctuation theory is formulated to make connection between pseudogap temperature $T^*$, pseudogap size $\Delta_{pg}$ and $\langle |\Delta_d(0)|^2 \rangle$. 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. Calculated $T^*$ falls from a high value onto the $T_c$ line and closely follows mean-field Neél temperature $T_{N,MF}^c$. The calculated $\Delta_{pg}$ is in good agreement with experimental results. We propose an experiment in which the present scenario can be critically tested.

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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 [1] 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), [2] specific heat, [3] tunneling, [4] NMR, [5] and optical conductivity. [6] 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.

Among several theoretical proposals [1] to understand the pseudogap phenomena, the superconducting (SC) fluctuation scenario [8] of pseudogap has received much attention from the physics community. This is because some experiments such as ARPES and tunneling experiments show that the normal state pseudogap has the same angular dependence and magnitude as the SC gap and that often the only difference between the spectra in the pseudogap state and the SC state is in their linewidths. The basic idea of this scenario is that SC gap amplitude forms at $T_c$ and its phase coherence is established at $T_c$ lower than $T_{c,MF}^c$. Hence $T^* \sim T_{c,MF}^c$ and below this temperature SC fluctuations become stronger until they diverge at $T_c$. In spite of its success in explaining some features of the pseudogap, it suffers from at least three important drawbacks which were often overlooked in the past. First, just below $T^*$ there is no experimental evidence of characteristic features associated with SC fluctuations such as fluctuating diamagnetic (Meissner) effect, fluctuating superfluid density and so on. It appears that $T^*$ has nothing to do with superfluid “rigidity”. One experiment to strongly support this argument was recently carried out by Orenstein’s group [9]. In their high-frequency conductivity measurements tracking the phase-coherence time $\tau$ in the normal state, the temperature $T_\Theta^0$ where the phase-stiffness of superfluidity disappears is at most 25 K above $T_c$ for underdoped cuprates. Second, when SC correlations are treated on equal footing with antiferromagnetic (AF) correlations, which is more realistic from both theoretical and experimental points of view, $T_{c,MF}^c$ goes down to zero with decreasing doping due to the competition with the AF correlations, as shown in Fig. [1](a). Then the above scenario ($T^* \sim T_{c,MF}^c$) is inconsistent even with the doping dependence of $T^*$, which increases with decreasing doping. Apparently experimentally observed $T^*$ stays in between $T_{c,MF}^c$ and $T_{N,MF}^c$. Furthermore, in this situation the origin of the pseudogap itself is questionable, because the pseudogap appears to be caused by AF fluctuations! Third, in their recent paper Tallon and Loram [10] argued, based on experimental results, that $T^*$ falls from a high value onto the $T_c$ line instead of smoothly merging with $T_c$ in the slightly overdoped region. The above scenario for the pseudogap predicts the latter behavior of $T^*$. In this paper we demonstrate that induced local spin-singlet amplitude due to short-range spin correlations causes 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 AF and 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 $\Delta_{pg}$. Note that the present formulation below is different from standard fluctuation theory.
based on the (static) mean-field state. The mean-field result of the $t$-$J$ model will be used below solely to find the onset of leading correlations \cite{13}, and to compute mean-field AF and SC order parameters for the calculation of local spin and spin-singlet amplitudes. The mean-field $t$-$J$ Hamiltonian reads

$$H_{MF} = \sum_{\vec{k},\sigma} \varepsilon(\vec{k}) c_{\vec{k},\sigma}^\dagger c_{\vec{k},\sigma} - 2Jm \sum_{\vec{k}} (c_{\vec{k}\uparrow}^\dagger c_{\vec{k}\downarrow}^\dagger - c_{\vec{k}\downarrow} c_{\vec{k}\uparrow}) - Js \sum_{\vec{k}} \phi_d(\vec{k}) (c_{\vec{k}\uparrow}^\dagger c_{\vec{k}\downarrow} + c_{\vec{k}\downarrow}^\dagger c_{\vec{k}\uparrow}),$$

where $\varepsilon(\vec{k}) \simeq -2t(x \cos k_x + \cos k_y) - \mu$ with $x$ the hole density. $m$ and $s$ are mean-field AF and SC order parameters determined from

$$m = 1/(2N) \sum_{\vec{k},\sigma} \sigma (c_{\vec{k}\uparrow}^\dagger c_{\vec{k}\downarrow} + c_{\vec{k}\downarrow}^\dagger c_{\vec{k}\uparrow}),$$

$$s = 1/N \sum_{\vec{k}} \phi_d(\vec{k}) (c_{\vec{k}\uparrow}^\dagger c_{\vec{k}\downarrow}),$$

where $N$ is the total number of lattice sites. $\phi_d(\vec{k}) = \cos k_x - \cos k_y$ 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. 1(a)) to be interpreted as the onset of the corresponding short-range correlations. We identify $T^{MF}_{N}$ with another crossover temperature $T^0$ 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 AF and spin-singlet \cite{12} correlation functions

$$\chi_{sp}(i, \tau) = \langle T_{\tau} \sigma_z(i, \tau) \sigma_z(0, 0) \rangle,$$

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

where $\sigma_z(i) \equiv (c_{i\uparrow}^\dagger c_{i\downarrow} - c_{i\downarrow}^\dagger c_{i\uparrow}) = 2S_z(i)$ and $\Delta_d(i) = 1/2 \sum \delta g(\delta) (c_{i+\delta,\uparrow} c_{i,\downarrow} - c_{i+\delta,\downarrow} c_{i,\uparrow})$ with $g(\delta) = 1/2$ for $\delta = (\pm 1, 0), -1/2$ for $\delta = (0, \pm 1)$, and 0 otherwise. The AF and spin-singlet correlation functions are related to the local spin and spin-singlet amplitudes through the sum rules

$$\frac{T}{N} \sum_q \chi_{sp}(q)e^{-iq\nu_m} = \langle |\sigma_z(0)|^2 \rangle = n - 2(n_{\uparrow}n_{\downarrow}),$$

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

where $q = (\vec{q}, iv_m)$ and $\nu_m$ is bosonic Matsubara frequencies. $T$ is absolute temperature. These sum rules can be easily obtained by taking $\tau = 0^-$ limit and setting $i$ to the origin in Eq. (3). In terms of renormalized vertices $U_{sp}$ and $V_{pp}$, \cite{13} we approximate the AF and spin-singlet correlation functions

$$\chi_{sp}(q) = \frac{2\chi_{pp}(q)}{1 - U_{sp}\chi_{pp}(q)},$$

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

where the irreducible susceptibilities are defined as

$$\chi^{0}_{sp}(q) = \frac{T}{N} \sum_{k} G^0(k - q) G^0(k),$$

$$\chi^{0}_{pp}(q) = \frac{T}{4N} \sum_{k} \phi_d(\vec{k}) + \phi_d(\vec{q} - \vec{k}))^2 G^0(q - k) G^0(k).$$

$G^0(k)$ is the noninteracting Green’s function obtained from Eq. (1) with $J = 0$. Now two unknown vertices, $U_{sp}$ and $V_{pp}$, are determined by the sum rules Eq. (4). Hence, an increase in the local spin or spin-singlet amplitude evaluated in the interacting state over that in the noninteracting state leads to a nonvanishing positive value of $U_{sp}$ or $V_{pp}$, namely, the enhancement of the corresponding correlation function. This (non-perturbative sum rule) approach has been shown to be quite reliable \cite{13} 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. Since this method is expected to be accurate up

![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 $T = 0.2J$.](image-url)
to the intermediate coupling regime, it forces the effective bandwidth \((W = 8tx)\) to be larger than the effective interaction strength \((2J)\), which leads to \(x \geq 0.08\). In order to determine whether the pseudogap is caused by the spin-singlet or AF spin fluctuation channel, we separately consider the self-energy coming from each channel

\[
\Sigma_{sp}(k) = \frac{1}{N} \sum_{q} \chi_{sp}(q) G^0(k - q),
\]

\[
\Sigma_{pp}(k) = -\frac{1}{4} V \chi_{pp}(k) \sum_{q} \left( \phi_{d}(\vec{k}) + \phi_{d}(\vec{q} - \vec{k}) \right)^2 \chi_{pp}(q) G^0(q - k),
\]

where \(U = 2J\) and \(V = J\) from Eq. (4).

First let us begin by showing the interaction-induced local spin (dashed curve) and spin-singlet (solid curve) amplitudes (Fig. 1(b)) evaluated in the mean-field state of the \(t - J\) Hamiltonian in a region where \(s = 0\) (or \(T > T^{MF}\)). 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. [14] for more details). In fact the interaction-induced local spin and spin-singlet amplitudes (Eq. (4)) are determined most crucially by these quantities. The local spin amplitude starts to appear when short-range spin correlations begin to develop and keeps growing with decreasing doping, as can be easily expected from the mean-field phase diagram (Fig. 1(a)) itself. Quite unexpectedly, however, the local spin-singlet amplitude also increases with decreasing doping despite the fact that the mean-field SC order \(s\) is absent. The increase of local spin-singlet amplitude traces back to the growing short-range spin correlations with decreasing doping. This same feature was recently studied by the author [14] in the context of the Hubbard model.

In Fig. 2 we show the spectral functions at \(\vec{k} = \vec{k}_F\) along \((0,0) - (0,\pi)\) direction from spin-singlet (solid curve) and AF spin fluctuation (dashed curve) channels for two doping levels \(x = 0.15\) and \(x = 0.08\). For both densities the pseudogap appears first in the spin-singlet channel. This is verified even close to half-filling [17] by considering the Hubbard model \((U = 8t)\) [14], which is not shown in this paper. The reason why the pseudogap is always caused by the spin-singlet channel is that as the local spin amplitude increases with decreasing doping, the local spin-singlet amplitude also increases at the same time. Hence the feature found away from half-filling persists down to half-filling. In our calculations the pseudogap appears when the characteristic low frequency scale of the spin-singlet correlations is smaller than temperature (renormalized classical regime). [13] The pseudogap due to AF spin fluctuations starts to appear for \(x \leq 0.10\) with \(T \ll T^*\).

Based on the above results we show the pseudogap temperature \(T^*\) (filled diamonds) as a function of doping in Fig. 1(a). \(T^*\) falls from a high value onto the \(T_c^0\) line instead of sharing a common line with \(T_c\) in overdoped region. When superconductivity is suppressed by setting \(s = 0\), \(T^*\) vanishes near \(x_c\) where short-range spin correlations disappear. It is not surprising to find that \(T^*\) closely follows \(T^{MF}_c\), 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. All these features are at least qualitatively consistent with the findings by Tallon and Loram. [14] Although quantitative agreement with the Hubbard and \(t - J\) models is achieved only for very strong coupling \((U \gg t \text{ or } J \ll t)\), [10] it is instructive to compare the calculated \(T^*\) with the recent calculations obtained from the dynamical cluster approximation (DCA) for the Hubbard model by Jarrell et al. [17]. Their \(T^*\) near half-filling is about \(0.09t\) for \(U = 8t\), while ours is \(0.15 - 0.16t\) for \(U = 4t^2/J = 12t\). The reasonable agreement with the more systematic approach is encouraging in light of the drastically simple approximation used in the paper, namely, replacing the strongly correlated hopping term of the \(t - J\) model by \(tx\) and using the mean-field state to compute local correlations.

Figure 1(a) shows the pseudogap size \(\Delta_{pg}\) (filled diamonds) which is defined as half of the peak-to-peak distance in Fig. 3 by setting \(s = 0\) at \(T = 0\). In the same figure the pseudogap energy extracted from various experiments by Tallon and Loram [16] 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. 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) in the SC state, $\Delta_{tg}$, can be also calculated. $\Delta_{tg}$ at $T = 0$ is always larger than $\Delta_{pg}$ at $T = 0$ due to the additional contribution to the local spin-singlet amplitude from $s \neq 0$, which is shown in Fig. 3(b). $\Delta_{pg}$, $\Delta_{tg}$ and their relative ratio $\Delta_{pg}/\Delta_{tg}$ should be all monotonically decreasing functions of doping, as shown in the inset of Fig. 3(b). Since the SC order parameter vanishes at $T_c$ (at $T_{c}^{MF}$ in this paper), the SC gap below $T_c$ continuously evolves into the normal state pseudogap above $T_c$ with the same momentum dependence and magnitude.

In order to confirm the present scenario for the pseudogap, we propose an experiment in which long-range superconductivity is completely destroyed by a phase sensitive external perturbation such as a strong magnetic field. Or this can be also done in a vortex core with a relatively weak magnetic field. Then our scenario predicts that the underlying ground state will manifest itself as an insulator with a pseudogap or spin gap. The normal state pseudogap $\Delta_{pg}$ should be observable down to $T = 0$ for $x \leq x_c$ vanishing near $x_c$, and its size is given by Fig. 3(a). The present scenario for the pseudogap predicts that a normal state pseudogap is likely to appear when short-range spin correlations are well established and are not masked by long-range (AF or SC) order.

The pseudogap appears here only as the suppression of low frequency spectral weight in certain physical quantities which are obtained through $A(\mathbf{k}, \omega)$ or its convolution with a relevant vertex. It does not appear as a thermodynamic phase with broken symmetry. The pseudogap obtained in this paper is different from the spinon gap found in the previous slave boson (static) mean-field study of the $t – J$ model. [13] In fact the pseudogap size and temperature obtained in the latter are the same as $2J_s$ and $T_{c}^{MF}$ calculated from Eq. [3] with $m = 0$.

In the low energy sector short-range AF correlations compete with SC correlations to make $T_{c}^{MF}$ or $T_c$ go to zero near half-filling. At the same time, in the relatively high energy sector of order of $J$ (or in the short distance scale) the same AF correlations induce the local spin-singlet amplitude, which is responsible for the normal state pseudogap in the present scenario. When the spin-singlet (or AF spin fluctuation) aspect is completely neglected, the current approach reduces to the AF (or SC for $T < T_{c}^{MF}$) fluctuation scenario for the pseudogap. O(2) SC fluctuations associated with superfluid stiffness come into play below $T_{c}^{MF}$ [13] instead of $T^*$, and diverge at $T_c$. The present results are robust to variations of $t/J = 2.5 – 3.5$ [13] and small to moderate value of $t'$.

In this paper we have considered only the local spin-singlet amplitude induced by short-range spin correlations and its consequences. The complete theory of long-range $d$-wave superconductivity is beyond the scope of the present formulation. How local spin-singlets (appearing at $T_{c}^{MF}$) acquire local SC phases (at $T_{c}$) eventually establish their long-range phase coherence (at $T_c$) is a challenging problem to the theory of high temperature superconductivity.

In summary, we have shown that the local spin-singlet amplitude with $d$-wave symmetry, $\langle |\Delta_d(0)|^2 \rangle$, can be induced by short-range spin correlations even in the absence of pairing interactions. Fluctuation theory has been formulated to make connection between $T^*$, $\Delta_{pg}$ and $\langle |\Delta_d(0)|^2 \rangle$. 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 SC correlations to make $T_c$ go to zero near half-filling. Since the SC order parameter vanishes at $T_c$ (at $T_{c}^{MF}$ in this paper), the SC gap below $T_c$ is smoothly connected to the normal state pseudogap above $T_c$ with the same momentum dependence and magnitude. Calculated $T^*$ falls from a high value onto the $T_c$ line and closely follows $T_{c}^{MF}$. The calculated $\Delta_{pg}$ is in good agreement with experimental results. We have proposed an experiment in which the present scenario can be critically tested. 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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[1] T. Timusk and B. Statt, Rep. Prog. Phys. 62, 61 (1999).
[2] H. Ding, T. Yokoya, J. C. Campuzano, T. Takahashi, M. Randeria, M. R. Norman, T. Mochiku, K. Kadowaki, and J. Giapintzakis, Nature 382, 51 (1996).
[3] A. G. Loeser, Z. -X. Shen, D. S. Dessau, D. S. Marshall, C. H. Park, P. Fournier, A. Kapitulnik, Science 273, 325 (1996).
[4] J. W. Loram, K. A. Mirza, J. R. Cooper, and W. Y. Liang, Phys. Rev. Lett. 71, 1740 (1993).
[5] Ch. Renner, B. Revaz, J. -Y. Genoud, K. Kadowaki, and ØFischer, Phys. Rev. Lett. 80, 149 (1998).
[6] M. Takigawa, P. C. Hammel, R. H. Hefner, and Z. Fisk, Phys. Rev. B 43, 247 (1991).
[7] C. C. Homes and T. Timusk, R. Liang, D. A. Bonn, and W. N. Hardy, Phys. Rev. Lett. 71, 1645 (1993).
[8] V. M. Loktev, R. M. Quick, and S. G. Sharapov, Physics Reports in press and cond-mat/0002300, and references therein.
[9] J. Corson, R. Mallozzi, J. Orenstein, J. N. Eckstein, and I. Bozovic, Nature 398, 221 (1999).
[10] J. L. Tallon and J. W. Loram, Physica C, 349, 53 (2001).
[11] There exist several ways of decoupling the $t-J$ Hamiltonian. E. Cappelluti and R. Zeyher (Phys. Rev. B 59, 6475 (1999)), M. U. Ubbens and P. A. Lee (Phys. Rev. B 46, 8434 (1992)) considered $d$-wave and commensurate flux phases, while M. Inui et al. (Phys. Rev. B 37, 2320 (1988)) and M. Inaba et al. (Physica C 257, 299 (1996)) $d$-wave and commensurate AF phases. The latter decoupling particularly with AF order is used in this paper, because it appears more consistent with experiments, and more importantly the double occupancy and nearest neighbor correlations evaluated in this decoupling scheme are found to be in good agreement with quantum Monte Carlo results as demonstrated in Ref. [1].
[12] The spin-singlet correlation function (with $d$-wave symmetry) is more general than the $d$-wave pair correlation function in the sense that the spin-singlet correlations can be also induced by short-range spin correlations even in the absence of pairing interactions.
[13] Y. Vilk and A. M. Tremblay, J. Phys. I (France) 7, 1309 (1997); B. Kyung, Phys. Rev. B, 63, 14 502 (2001); B. Kyung, S. Allen, A.-M. S. Tremblay, cond-mat/0010001 and to appear in Phys. Rev. B.
[14] B. Kyung, Phys. Rev. B, 63, 214 505 (2001).
[15] Exactly at half-filling the pseudogap should be replaced by a Mott-Hubbard gap of order $U$.
[16] E. Jeckelmann, D. J. Scalapino, and S. R. White, Phys. Rev. B, 58, 9492 (1998).
[17] M. Jarrell, Th. Maier, M. H. Hettler, and A. N. Tahvildarzadeh, cond-mat/0011282.
[18] G. Baskaran, Z. Zou, and P. W. Anderson, Solid State Commun. 69, 973 (1987); G. Kotliar and J. Liu, Phys. Rev. B 38, 5142 (1988).
[19] For $t = 2.5J$ and $3.5J$, $\Delta_{pe}$’s vanish with slightly different slopes and $x_c$’s from the experimental results (in opposite ways).