Coherent vs incoherent pairing in 2D systems near magnetic instability.

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Abstract. – We study the superconductivity in 2D fermionic systems near antiferromagnetic instability, assuming that the pairing is mediated by spin fluctuations. This pairing involves fully incoherent fermions and diffusive spin excitations. We show that the competition between fermionic incoherence and strong pairing interaction yields the pairing instability temperature $T_{\text{ins}}$ which increases and saturates as the magnetic correlation length $\xi \to \infty$. We argue that in this quantum-critical regime the pairing problem is qualitatively different from the BCS one.

In this communication we analyse the pairing problem in 2D fermionic systems near antiferromagnetic instability. Our key goal is to investigate whether or not the closeness to antiferromagnetism is in conflict with the magnetically mediated $d$–wave pairing. This problem is rather peculiar as on one hand the $d$–wave pairing amplitude increases at approaching the AFM instability due to softening of spin fluctuations \cite{1}, while on the other hand, strong spin-mediated interaction destroys fermionic coherence \cite{2,3} and therefore damages the ability of fermions to form Cooper pairs.

We demonstrate that the competition between strong pairing interaction and the destruction of fermionic coherence yields a pairing instability at a temperature $T_{\text{ins}}$ which increases and saturates when the magnetic correlation length $\xi \to \infty$. We show that under certain conditions, $T_{\text{ins}}$ is universal in the sense that it does not depend on the details of the electronic dispersion at energies comparable to the fermionic bandwidth $W$, and is determined by fermions located in a narrow region near hot spots - the points at the Fermi surface separated by the antiferromagnetic momentum $Q$. We assume in this paper that the Fermi surface does contain hot spots.

We believe that the results of our analysis may be applicable to both cuprates and heavy fermion materials. For high $T_c$ cuprates, our results may be useful for understanding of the pseudogap physics in the underdoped regime, where the data show that the temperature when the system first displays superconducting precursors saturates at the lowest dopings \cite{4}. We conject that our $T_{\text{ins}}$ may be the onset of the pseudogap behavior, while the actual superconducting transition occurs at a smaller temperature. For heavy fermion materials, our result may help understand the close correlation between the appearance of the superconductivity and an antiferromagnetic instability \cite{5}.

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The point of departure for our analysis is the spin-fermion model which describes low-energy fermions interacting with their collective spin degrees of freedom. This model can be viewed as the low-energy version of the lattice, Hubbard-type models, and is given by

\[ H = \sum_{k,\alpha} v_F (k - k_F) c_{k,\alpha}^\dagger c_{k,\alpha} + \sum_q \chi_0^{-1} (q) S_q S_{-q} + g \sum_{q,\sigma,\beta} \delta_{\sigma,\beta} c_{k+q,\sigma} \sigma S_{-q} \cdot \]  

(1)

Here \( c_{k,\alpha} \) and \( S_q \) describe fermions and collective bosonic spin degrees of freedom, respectively, and \( g \) is the spin-fermion coupling constant. The three input parameters in the model are the Fermi velocity \( v_F \), spin-fermion coupling \( g \) (which near half-filling is of order Hubbard \( U \)), and the spin correlation length \( \xi \) defined via a bare static spin susceptibility which is assumed to be peaked at the antiferromagnetic momentum \( Q \), i.e., \( \chi_0 (q) = \chi_0 \xi^2 / \left( 1 + (q - Q)^2 \xi^2 \right) \). The dynamical part of the spin susceptibility comes from the interaction with the low-energy fermions and therefore is not an input.

The model of Eq. (1) yields a spin-mediated pairing interaction which singlet component \( \Gamma (q, \beta) \), where \( \chi (q, \Omega) \) is the fully renormalized dynamical spin susceptibility. Near antiferromagnetic instability, this interaction is attractive in the \( d_{x^2-y^2} \) channel [1].

A convenient way to study whether the spin-fermion interaction gives rise to a pairing at some \( T_{\text{ins}} \) is to analyze a linearized equation for the fully renormalized \( d \)-wave pairing vertex \( F \) with zero total momentum and frequency. This vertex generally depends on relative fermionic momentum \( k \) and frequency \( \omega \), i.e \( F = F_k (\omega) \). In the ladder approximation which accuracy we discuss below, the equation for \( F_k (\omega_m) \) takes the form (see Fig 3).

\[ F_k (\omega_m) = F_k^{(0)} (\omega_m) - T \sum \frac{d^2 k'}{(2\pi)^2} F_{k'} (\omega_m') G_{k'} (\omega_m') G_{-k'} (-\omega_m') \Gamma (k - k', \omega_m - \omega_m') \]  

(2)

Here \( G_k (\omega) \) is the fully renormalized normal state single-particle Green’s function. At \( T = T_{\text{ins}} \) this equation should have a nontrivial solution even when \( F_k^{(0)} (\omega_m) = 0 \).

To analyse Eq. (3) we need to know the fully renormalized single-particle Green’s function \( G_k (\omega) \) and the pairing interaction \( \Gamma (q, \Omega) \) in the normal state. In 2D, the dimensionless coupling constant for Eq. (1) is \( \lambda = 3g^2/4\pi v_F \xi^{-1} \), where \( g = g^2\chi_0 \) is the effective spin-fermion interaction [2]. Obviously, near a magnetic instability \( \lambda \geq 1 \), and a conventional perturbation expansion is inapplicable. It turns out, however, that one can resum perturbation series and obtain a self-consistent solution for both \( G_k (\omega) \) and \( \Gamma (q, \Omega) \) [3, 4]. This solution becomes exact in the formal limit \( N \rightarrow \infty \) where \( N = 8 \) is the number of hot spots in the Brillouin zone. Two of us have checked [3] that the corrections to the spin-fermion vertex \( g \) are small by \( 1/N \) and can be safely neglected.

The key effect captured by the self-consistent solution is the appearance of the small scale \( \omega_{sf} = 9/(8\pi N) \) which separates the regions of a Fermi liquid behavior at \( \omega, T < \omega_{sf} \) and quantum-critical, non Fermi liquid behavior at \( \omega, T > \omega_{sf} \). Specifically, for electronic states near hot spots, \( k \approx k_{hs} \),

\[ \chi (q, \Omega_m) = \chi_0 \xi^2 / \left( 1 + (q - Q)^2 \xi^2 + |\Omega_m|/\omega_{sf} \right) \]
has a conventional Fermi liquid form

$$G_k^{-1}(\omega_m) = i\omega_m Z_k(\omega_m) - \epsilon_k$$  \hspace{1cm} (3)$$

where

$$Z_k(\omega_m) = 1 + \frac{\pi T\lambda}{\omega_m} \sum_n \frac{\text{sign}\omega_n}{\sqrt{1 + |\omega_m - \omega_n|} + \left(\frac{\epsilon_k + Q}{\pi T \xi}\right)}$$  \hspace{1cm} (4)$$

Here $\epsilon_k = v_k(k - k_{hs})$ and $|\mathbf{v}_F(k + Q)| = |\mathbf{v}_F(k)| = v_F$. At $T = 0$ and $k = k_{hs}$, $Z(\omega_m) = 1 + 2 \lambda/(1 + |\omega_m/\omega_{sf}|)$.

Analyzing Eq. (3) at $k = k_{hs}$, we find that at $\omega, T \leq \omega_{sf}$, $\chi(q, \Omega) \approx \chi_0(q)$, and $G^{-1}(\omega)$ has a conventional Fermi liquid form $G^{-1}(\omega) \approx \omega + i\text{sign}\omega(\omega^2 + \pi^2 T^2)/(4\omega_{sf})$. On the other hand, at $\omega, T > \omega_{sf}$,

$$\chi^{-1}(q, \Omega) \propto \tilde{\omega} \left(\frac{q - Q}{q_0}\right)^2 - i\Omega$$

$$G^{-1} \approx \omega + \left(i\pi T\lambda + (|i\omega| \tilde{\omega})^{1/2} f(T/|\omega|)\right) \text{sign}\omega$$  \hspace{1cm} (5)$$

where $\tilde{\omega} = 4\lambda^2\omega_{sf} = 9\bar{g}/(2\pi N)$, $q_0 = \bar{g}/(2\pi v_F)$, and $f(x)$ is a smooth function with $f(0) = 1$ and $f(x \gg 1) \approx -1.52v/ix$. We see that spin fluctuations behave as gapless diffusive modes and fermionic excitations are fully incoherent. This behavior is obviously a quantum-critical one. Observe in this regard that $\tilde{\omega}$ does not depend on the spin correlation length. The scale $\tilde{\omega}$ will play a central role in our further considerations.

The fermionic propagator also contains a linear in $T$ term which does depend on $\xi$. This term, however, comes from thermal spin fluctuations which contribute $n = m$ term to the frequency sum in Eq. (3). We will see that these fluctuations act as static impurities and do not affect $T_{ins}$.

We first discuss in detail the pairing problem when $\bar{g}/v_F k_F \ll 1$, i.e., when $q_0 \ll k_F$. We argue that in this case, the pairing is dominated by fermions near hot spots and is insensitive to the system behavior at energies comparable to the bandwidth. Indeed, substituting the single particle Green’s function, the spin susceptibility into Eq. (3) and estimating the momentum integral using a $d$–wave condition $F_k(\omega_m) = -F_{k+Q}(\omega_m)$, we find that typical $|Q - q|$ and $|k - k_{hs}|$ are of order $q_0$, i.e., are much smaller than $k_F$.

We also checked that for typical momenta, $Z_k(\omega)$ and $F_k(\omega)$ are weakly $k-$dependent and can be approximated by their values at a hot spot, $Z(\omega)$ and $F(\omega)$, respectively. Under these conditions, the momentum integration can be performed exactly. The $N \to \infty$ limit is particularly simple as typical momenta transverse to the Fermi surface are by a factor $1/N$ smaller than typical momenta along the Fermi surface. In this situation, the momentum integration is factorized: the one over transverse momenta affects only the fermionic Green’s functions, while the integration over momenta along the Fermi surface affects only the spin susceptibility. Performing the integration we obtain

$$F(\omega_m) = F^{(0)}(\omega_m) + \lambda\pi T \sum_n \frac{F(\omega_n)}{|\omega_n| Z(\omega_n)} \frac{\sqrt{\omega_f}}{\sqrt{\omega_{sf} + |\omega_m - \omega_n|}}$$  \hspace{1cm} (6)$$

Notice that the consequences of taking the $N \to \infty$ limit are the same as of the Migdal theorem for phonon-mediated superconductors: one can (i) explicitly integrate over momentum in the gap equation, and (ii) neglect corrections to $g$ and to ladder series. More precisely, the $1/N$ smallness of the vertex corrections appears each time when these corrections involve fermions with momenta separated by $Q$ [8]. For the spin-fermion vertex, this is always the
case, hence vertex corrections are small by $1/N$. The pairing vertex has a zero total momentum, and the ladder diagrams for this vertex, which give rise to Eq. (3), do not contain $1/N$. However, the corrections to ladder series from, e.g., crossed diagrams do involve fermions with momenta separated by $Q$, and are small by $1/N$. From this perspective, our analysis of the spin-mediated pairing is quite similar to the Eliashberg analysis for conventional superconductors [7].

We now analyse Eq. (6). First we show that classical, thermal spin fluctuations, which account for $i\pi T\lambda$ term in Eq. (6), do not affect $T_{ins}$. These fluctuations account for the scattering with zero energy transfer and therefore act in the same way as impurities. Accordingly, our argumentation parallels the one which shows that non magnetic impurities do not affect $T_c$ in conventional superconductors [8]. Introducing $\xi_m = F(\omega_m)/\eta_m$ where $\eta_m = 1 + (\lambda\pi T / Z(\omega_m)/|\omega_m|)$, we explicitly rewrite Eq. (6) as the equation for $\xi_m$:

$$\xi_m = \xi_m^{(0)} + \lambda\pi T \sum_{n \neq m} \frac{\xi_n}{|\omega_n| Z(\omega_n)} \frac{\sqrt{\omega_n}}{\sqrt{\omega_n + |\omega_m - \omega_n|}}$$

(7)

where $Z$ is the same as in Eq. (4) but without the contribution from $m = n$ term in the frequency sum. We see that Eq. (7) contains only the contributions from quantum spin fluctuations.

We next discuss the form of the kernel in the r.h.s. of Eq. (7). We see that it contains two energy scales: $\omega_{sf} \propto \xi^{-2}$ and $\xi$-independent $\bar{\omega} \gg \omega_{sf}$, which is the upper cutoff for the $\sqrt{\omega}$ behavior of the fermionic propagator. For $|\omega| > \bar{\omega}$, the kernel converges as $1/\omega^{3/2}$, i.e., the pairing problem does not extend above $\bar{\omega}$, which for $g < v_F k_F$ is still much smaller than the fermionic bandwidth.

The presence of the two energies $\omega_{sf}$ and $\bar{\omega}$ raises the question on how $T_{ins}$ depends on $\xi$. To address this issue, consider the form of the kernel in Eq. (7) at different frequencies. At $|\omega| < \omega_{sf}$, the system behaves as a Fermi liquid ($Z(\omega) \approx 1 + \lambda$). In this frequency range, the kernel reduces to a constant, i.e., the pairing problem is of BCS type, with the effective pairing coupling constant $\lambda/Z = \lambda/(1 + \lambda)$ which never becomes large. If frequencies above $\omega_{sf}$ were not contributing to pairing, $T_{ins}$ would be of order $\omega_{sf} e^{-(1+\lambda)/\lambda}$, i.e., it would scale with $\omega_{sf}$. This is similar to what McMillan obtained for conventional superconductors [8].

Consider next $|\omega| \geq \omega_{sf}$. Here the pairing interaction (the last term in the r.h.s. of Eq. (7)) becomes frequency dependent and gradually decreases compared to its zero frequency value. At weak couplings, this decrease obviously makes frequencies larger than $\omega_{sf}$ ineffective for pairing. However, at large $\lambda$ the situation is more tricky both in our case and for phonon superconductors [10]. The point is that for large $\lambda$, the mere reduction of the pairing interaction above $\omega_{sf}$ is not sufficient - one also has to neutralize the large overall $\lambda$ factor in the r.h.s. of Eq. (7). At $|\omega| < \omega_{sf}$, this overall $\lambda$ is neutralized by $Z(\omega_{m}) \approx 1 + \lambda$. However, above $\omega_{sf}$, $Z(\omega_{m})$ decreases as $Z(\omega_{m}) \sim \lambda(\omega_{sf}/|\omega_{m}|)^{1/2}$, and the effective coupling $\lambda/Z(\omega_{m})$ increases. Simple power counting shows that this increase exactly balances the decrease of the pairing interaction such that the $1/|\omega|$ form of the pairing kernel survives up to frequencies of order $\bar{\omega}$. This may sweep the pairing instability to a temperature $T_{ins} \sim \bar{\omega} \sim \bar{g}/N$.

To illustrate this point we introduce a dimensionless parameter $n_T = (\bar{\omega}/(\pi T))^{1/2}$ and consider the limit $\omega_{sf} \rightarrow 0$. In this limit, Eq. (7) simplifies to

$$\xi_m = \xi_m^{(0)} + \frac{\alpha}{2} \sum_{n \neq m} \frac{\xi_n}{\sqrt{2n - m}|\sqrt{2n + 1}|} \frac{n_T}{n_T + \sqrt{2n + 1}}$$

(8)

where $\alpha$ (= 1 in our case) is introduced for the subsequent perturbative analysis of this equation. We see that at low temperatures, i.e., large $n_T$, the kernel in Eq. (8)
has a 1/n form typical for a pairing problem. On general grounds one might expect that the pairing instability occurs at $n_T = O(1)$, i.e., at $T_{\text{ins}} \sim \bar{\omega}$ [1]. If this is the case, then the pairing is dominated by frequencies where the fermionic excitations display a fully incoherent quantum-critical behavior, i.e., the pairing is qualitatively different from that in a Fermi liquid.

The above argumentation is, however, only suggestive as it is a priori unclear whether Eq. (8) has a nontrivial solution for any $n_T$. Indeed, on one hand, the $1/\omega_n$ form of the kernel in Eq. (8) is typical for a pairing problem and gives rise to the logarithms in the ladder series. On the other hand, this kernel depends not only on the running frequency as would be the case for BCS superconductivity, but also on the frequency transferred by the interaction. This last frequency serves as a lower cutoff for the logarithmical behavior.

To get further insight into the problem we assumed that $F_m^{(0)}$ is a constant and analyzed Eq. (8) for various $\alpha$. We found that for small $\alpha$, when perturbative analysis of the logarithmical series is valid, the dependence of the kernel on the transverse frequency is crucial, and even at $T = 0$, the summation of the series of logarithms give rise to a power-law behavior $\bar{F}_m \propto \mathcal{F}^{(0)}/|\omega_m|^{(1/2)}$ rather than to a divergence. In other words, unlike BCS theory, at $\alpha \ll 1$, the logarithmical series do not give rise to a pairing instability.

We find, however, that the convergence of the perturbation theory is confined only to small $\alpha \ll 1$. Indeed, assume that at small $\alpha$, $\bar{F}_m \propto |\omega_m|^{-1/4 + \beta}$. Substituting this into Eq. (8), we obtain an equation on $\beta$: $1 = (\alpha/2)\Phi(\beta)$, where

$$\Phi(\beta) = \frac{\pi^{3/2}}{\sqrt{2}} \frac{1}{\Gamma(3/4 + \beta)\Gamma(3/4 - \beta)} \frac{1}{\cos \pi \beta - \cos \pi/4}. \tag{9}$$

For real $\beta$, $\Phi(\beta)$ is an even function of $\beta$, which increases monotonically from $\Phi(0) \approx 8.97$ and diverges at $\beta \to 1/4$ as $\Phi(\beta) \approx 1/(1/4 - \beta)$. For $\alpha \ll 1$, we find $\beta = 1/4 - \alpha/2$, i.e., $\bar{F}_m \propto |\omega_m|^{-\alpha/2}$, in agreement with the results of the summation of the logarithmical series. As $\alpha$ increases, $\beta$ becomes smaller and reaches zero at $\alpha = \alpha_{cr} = 2\Phi^{-1}(0) \approx 0.22$. At larger $\alpha$, a solution with real $\beta$ is impossible, i.e., a perturbation theory breaks down. Instead, the condition $1 = (\alpha/2)\Phi(\beta)$ yields an imaginary $\beta = i\beta^*$ i.e $\bar{F}_m \propto |\omega_m|^{-1/4} \cos (\beta^* \log |\omega_m|)$. Near $\alpha_{cr}$, we find $\beta^* \approx 1.2(\alpha - \alpha_{cr})^{1/2}$. The appearance of the oscillating solution at $T = 0$ implies that the pairing susceptibility is negative for some $|\omega_m|$. This obviously signals that the normal state at $T = 0$ is unstable against pairing. An estimate of $T_{\text{ins}}$ may be obtained from a requirement that a temperature should exceed a maximum frequency where the pairing susceptibility is negative. For sufficiently small $\beta^*$ this yields $T_{\text{ins}} \propto \bar{\omega} e^{-\pi/\beta^*}$. We see therefore that for $\alpha = 1$, when $\beta^* = O(1)$, the attraction between fully incoherent fermions is capable to produce a pairing instability at $T_{\text{ins}} \sim \bar{\omega} \sim g/N$, as we conjected above, but this result has a non perturbative origin. We also performed RG analysis of the leading $1/N$ vertex corrections and found that they only slightly, by $O(1/N)$, change $\alpha_{cr}$ which still remains much smaller than 1.

To check this analysis, we solved our original Eq. (7) with $F_m^{(0)} = 0$ numerically for various $\lambda$. The results are presented in Fig. [2]. In the limit $\lambda \to \infty$ we found $T_{\text{ins}} \approx 0.17\bar{\omega}$. It is interesting to observe that the weak dependence of $T_{\text{ins}}/\bar{\omega}$ on $\lambda$, which is an indicative of quantum critical superconductivity, persists down to $\lambda \sim 0.5$. This means that even at moderate $\lambda$ the pairing instability has a non-Fermi-liquid, quantum-critical origin.

We now discuss the momentum dependence of $\bar{F}_k(\omega_m)$ at $T_{\text{ins}}$. This momentum dependence is likely to mimic that of a pairing gap at $T < T_{\text{ins}}$ [2]. As we said above, $\bar{F}(\omega_m)$ along the Fermi surface is weakly $k$ dependent at relative deviations from a hot spot by less than $g/v_Fk_F$ which is a small parameter in the theory. We checked that at larger deviations from a hot spot, $\bar{F}(\omega_m)$ rapidly decreases, as $1/(k - k_{hs})^2$. This means that for quantum-
critical pairing, the $d$-wave pairing gap is more strongly confined to hot regions than a simple $\cos k_x - \cos k_y$ form. This result is intuitively obvious as the very fact that the pairing problem is confined to hot spots implies that the pairing state is a superposition of many eigenfunctions from the $B_{1g}$ representation with almost equal partial amplitudes. Simple manipulations with trigonometry show that in this situation, the slope of the gap near the nodes should be smaller than the one inferred from the gap value at hot points assuming $\cos k_x - \cos k_y$ dependence of the gap. Notice, however, that this effect is non-critical, i.e., the width of the gap in $k$-space remains finite even if $\xi = \infty$.

Finally, we briefly discuss the situation at large spin-fermion interaction, when $\tilde{g} \gg v_F k_F$, i.e., $q_0 \gg k_F$ (see Eq. (3)). In this limit, the momentum integration extends over the whole fermionic bandwidth, and the presence of hot spots at the Fermi surface becomes less relevant. The explicit evaluation of $T_{ins}$ is no longer possible, but the reasoning along the same lines as above shows that $T_{ins}$ is independent on $\xi$ and scales as the largest typical frequency for the pairing problem. This typical frequency is obtained from the condition that maximum $|q - Q|$ are of order $k_F$, and is obviously $J \sim (v_F k_F)^2/(N \tilde{g})$.

The analysis of the system behavior below $T_{ins}$ requires one to solve a set of three coupled integral equations for the fermionic self-energy, the anomalous vertex, and the spin susceptibility. Setting this aside for a separate publication [13], we merely argue here that the pairing state which emerges below $T_{ins}$ is highly unusual and has no analogs in BCS superconductors. Indeed, on one hand, $T_{ins}$ and hence the gap at $T = 0$ are independent on $\xi$, on the other hand, the resonance frequency of the spin mode scales as $\omega_{res} \sim v_F \xi^{-1} \sim T_{ins}/\lambda$ [3], and for $\lambda \gg 1$ is much smaller than the pairing gap. In this situation, it is tempting to conject that superconducting coherence may be destroyed by fluctuations not included in the Eliashberg treatment at $T_c < T_{ins}$, yielding a disordered region between $T_c$ and $T_{ins}$. This issue is, however, highly speculative and requires further study.

We now briefly discuss the situation in cuprates. Near half-filling, $v_F k_F$ scales with the fermionic bandwidth, while $\tilde{g}$ is of order of the Hubbard $U$, hence $J$ and $T_{ins}$ (if $\tilde{g} \gg v_F k_F$) are of order of the exchange integral of the corresponding Heisenberg model. The actual situation in cuprates probably falls into an intermediate regime $\tilde{g} \geq v_F k_F$. We emphasize however that for $\omega_{sf} \sim 10 - 20 meV$, and $\lambda \sim 1$ extracted from NMR experiments at optimal doping [14], the universal result (Fig. (2)) yields $T_{ins} \sim 10^2 - 10^3 K$ which is a reasonable estimate. The non-critical sharpening of the superconducting gap with underdoping is also consistent with the recent photoemission data [15]. More detailed analysis requires a more precise knowledge of both $\lambda$ and $\omega_{sf}$ for various doping concentrations.
Finally we discuss how our work is connected to earlier studies. The Eliashberg-type equations for magnetically mediated pairing have been analyzed several times in the literature \cite{14,16,17}, mostly using the numerical technique. In particular, Monthoux and Lonzarich \cite{17} recently solved Eliashberg equations for large $\xi$ and for the Fermi surface with hot spots. They found that for large couplings, $T_{\text{ins}}$ likely saturates at a finite value at $\xi = \infty$. This fully agrees with our result for $T_{\text{ins}}$. However, our key finding is the discovery that near antiferromagnetic instability, the pairing problem is a quantum-critical one, and is qualitatively different from the BCS pairing. We also found that in the presence of hot spots at the Fermi surface, $T_{\text{ins}}$ is universal and does not depend on the form of the pairing potential at lattice scales. This physics was not detected in earlier works \cite{14,16,17}.

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