Antiferromagnetic correlation and the pairing mechanism of the cuprates and iron pnictides: A view from the functional renormalization group studies

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Abstract – We compare the one-loop functional renormalization group results for the cuprates and the iron pnictides. Interestingly a coherent picture suggesting that antiferromagnetic correlation causes pairing for both materials emerges.

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In the search for high-temperature superconductors two classes of materials with $T_c$ above 50 K have been found—the cuprates [1] and the iron pnictides [2]. There are striking similarities between them: i) both have layered structure, ii) the parent (non-superconducting) compound for both exhibit antiferromagnetic (AF) order (although with different ordering wave vector), iii) both materials become superconducting (SC) upon doping. On the other hand, there are also important differences. i) The parent compounds of the cuprates are Mott insulators while those for the iron pnictides are metallic. ii) The cuprates are effectively one-band [3] materials while the iron pnictides have multi bands at the Fermi energy [4–6]. iii) The gap function of the cuprates has $d_{x^2−y^2}$ symmetry [7], hence has nodes, while current theoretical studies [5,6,8–11] and experimental evidences [12,13] suggest that the iron pnictides has s-wave pairing symmetry. In addition to the above, there is another similarity between the cuprates and the iron pnictides —there is no consensus on the pairing mechanism.

Numerous attempts have been made to uncover the pairing mechanism of the cuprates. It is reasonable to expect considerable efforts will be devoted to that of the iron pnictides as well. In this paper we compare the one-loop functional renormalization group (1LFRG) results for both materials [8,14]. Interestingly, a coherent picture pointing to the involvement of the antiferromagnetic correlation in the superconducting pairing emerges.

Currently there is a lack of an ideal first-principle approach for strongly correlated systems. For example, direct diagonalization and density matrix renormalization group are limited by the small system size. Monte Carlo simulation is hindered by the fermion sign problem. Mean-field and variational wave function approach are not unbiased. The 1LFRG method used to gain the results in this paper is unbiased [15], and can be applied to infinite systems for a range of interaction strength. However it is not a systematic expansion of a small parameter. Applying this method to the cuprates, Honerkamp et al. found that effective interactions favoring both the AF order and $d_{x^2−y^2}$ pairing were generated [14]. Recently we generalized this method and applied it to iron pnictides. Interestingly, effective interaction favoring the $(\pi, 0)/(0, \pi)$ AF order, and an extended s-wave pairing with opposite sign in electron and hole packet [8] appears. In this paper we compare the results of 1LFRG for these two materials in hoping for hints for the paring mechanism for both. However, we would like to emphasize that when applying the 1LFRG to the cuprates our best hope is to describe the high-temperature superconductors on the overdoped side.

The goal of the 1LFRG is to generate an effective two-particle scattering

$$V(1, 2; 3, 4)\psi_{1s}^\dagger \psi_{1s}' \psi_{4s}^\dagger \psi_{4s}'$$

where 1, ..., 4 each stands for momentum and band index, and $s, s'$ are spin labels. In fig. 1(a) and fig. 2(a), we...
In constructing this plot the Fermi surface is discretized into 32 patches. (b) The Fermi surface of the single-band Hubbard model in ref. [14]. (c) The gap function deduced from the effective pair scattering amplitudes is plotted as a function of momentum on the discretized Fermi surface. Here we choose the parameter as \( t = 1 \text{ eV}, t' = 0.3 \text{ eV} \) and \( U = 3 \text{ eV} \).

Fig. 1: (Colour on-line) (a) The renormalized \( V(k_1, k_2, k_3, k_4) \) for the one-band Hubbard model used in ref. [14]. The momentum \( k_3 \) is fixed at the position shown in part (b), and the scattering amplitude is plotted as \( k_1 \) and \( k_2 \) go around the Fermi surface started from the place indicated by the small red arrow.

In constructing this plot the Fermi surface is discretized into 32 patches. Here we choose the parameter as \( t = 1 \text{ eV}, t' = 0.3 \text{ eV} \) and \( U = 3 \text{ eV} \).

There are two main features in these plots. First, the blue vertical and horizontal stripes in figs. 1(a) and 2(a) indicate strong positive scattering amplitudes. The momenta in the horizontal stripe satisfy \( k_3 = k_3 + Q \), and \( k_1 = k_1 - Q \), while those in the vertical stripe satisfy \( k_1 = k_3 \), and \( k_2 = k_1 - Q \). In the above \( Q \approx (\pi, \pi) \) for cuprates (fig. 1(a)) and \( Q \approx (\pi, 0) \) for iron pnictides (fig. 2(a)). Each of the scattering process \( V_1, 2, 3, 4 \) in the horizontal stripe has a corresponding process \( V_1, 2, 3, 4 \) in the vertical one. The fact that the amplitudes associated with both are strong implies that if we decompose eq. (1) into the sum of singlet and triplet channels
surprising for systems with strong short-range interactions. Having a positive amplitude, the scattering associated with the horizontal stripe tends to drive the AF order. The scattering associated with the vertical stripe would drive charge density wave (CDW) order had the amplitude been negative. With the wrong sign, as in figs. 1(a) and 2(a), CDW is not favored.

The second notable feature of figs. 1(a) and 2(a), (b) is the diagonal stripes. The momenta in these stripes satisfy $k_1 + k_2 = 0$ hence the corresponding process are Cooper scattering. While the color of the diagonal stripe changes (which represents sign change in the scattering amplitude) in fig. 1(a), it stays the same in fig. 2(a), (b). The sign changes in fig. 1(a) implies that the effective amplitude) in fig. 1(a), it stays the same in fig. 2(a), (b).

These second notable feature of figs. 1(a) and 2(a), (b) are associated with the inter-band and intra-band pair scattering, respectively. The fact that the inter-band pair scattering amplitudes are positive (fig. 2(a)) does not mean they disfavor pairing. Because a wrong (positive) sign in the inter-band Cooper scattering can always be absorbed by making the sign of the gap function opposite on the two Fermi surfaces [16].

The fact that the horizontal SDW (and the associated vertical stripe) intersects the inter-band rather than intra-band diagonal (Cooper scattering) stripes is responsible for the difference in pairing symmetry between the cuprates and iron pnictides. To understand that we first note that while a uniform positive inter-band pair scattering drives pairing, intra-band pairing requires the presence of negative pair scattering. Secondly, the scattering processes associated with the intersection of the horizontal and diagonal stripes, namely

$$\langle \bar{\psi}^{+}_{-k_1-Q,s} \psi^{+}_{k_1+Q,s'} \bar{\psi}^{-}_{-k_1,s'} \psi^{-}_{k_1,s} \rangle \neq 0$$

(4)

drive both AF and SC. Indeed, SC and AF appear as different decoupling of eq. (4), with

$$\langle \bar{\psi}^{+}_{-k_1-Q,s} \bar{\psi}^{+}_{k_1+Q,s'} \psi^{-}_{-k_1,s'} \psi^{-}_{k_1,s} \rangle \neq 0, \langle \bar{\psi}^{-}_{-k_1,s'} \bar{\psi}^{-}_{k_1,s} \rangle \neq 0$$

describing SC, and

$$\langle \bar{\psi}^{+}_{-k_1-Q,s} \psi^{-}_{-k_1,s'} \bar{\psi}^{+}_{k_1+Q,s'} \psi^{-}_{k_1,s} \rangle \neq 0, \langle \bar{\psi}^{-}_{k_1+Q,s'} \psi^{-}_{k_1,s} \rangle \neq 0$$

describing AF. Because AF correlation requires the scattering amplitudes to be positive, the sign of the Cooper scattering corresponding to the intersection is fixed (to be positive). Under this constraint, the only way that overall pairing can be favored for the one-band case (fig. 1(a)) is for the pairing interaction to change sign. Since the diagonal stripes intersect both the vertical and horizontal stripes, the pairing interaction $V_{\text{pairing}}(k,k')$ is forced to change sign four times as $k$ moves around the Fermi surface. As discussed earlier, this leads to the $d_{x^2-y^2}$ pairing. For iron pnictides the intersection corresponds to inter-band rather than intra-band pair scattering. Here there is no problem for all inter-band pair scattering amplitudes to stay positive; all that is required is for the gap function to take on opposite sign on the electron and hole Fermi surfaces. In this way, antiferromagnetic correlation naturally leads to an out-of-phase $s$-wave pairing.

In the following we shall provide more numerical evidence that the superconducting pairing is driven by the antiferromagnetic correlation. This is achieved by monitoring the growth of the SDW and pairing interaction during the RG. In figs. 3(a) and 4(a) we plot the RG flow of three pair scattering processes labeled as $P_1, P_2, P_3$. Here $P_1$ is at the intersection of the horizontal and diagonal stripes. This is the type of interaction that has the dual characteristics of being both SDW scattering and pairing interaction as discussed earlier. For fig. 3(a) $P_{2,3}$ are two other generic pairing interaction. For fig. 4(a) $P_2$ is a generic inter-band pair scattering while $P_3$ is an intra-band Cooper scattering. As one can see, in both figures the $P_1$ process (in fact the processes associated with the entire horizontal stripe) grows first. When $P_1$ gets strong, the magnitude of the other generic pairing interaction ($P_2$ and $P_3$) grows. This suggests that it is the AF correlation (i.e., strong SDW scattering) that drives SC!

As shown in fig. 2(d) the gap function of iron pnictides is quite anisotropic on the electron Fermi surface (the anisotropy is smaller on the hole Fermi surfaces.) Our results suggest that the degree of such anisotropy depends on the interaction parameters as well as doping, as shown in fig. 5. In the extreme case, the gap function can even change sign (hence exhibit nodes) on the electron Fermi surfaces.

Fig. 3: (Colour on-line) (a) The renormalization group flow of three different types of pair scattering amplitude for the single-band Hubbard model in ref. [14]. $P_1$ is the scattering process that drives both SDW and pairing. $P_2$ and $P_3$ are two other pair scattering processes which are not in the SDW channel (see fig. 1(a)). The red arrows mark the renormalization group steps at which the scattering amplitudes begin to increase rapidly. (b) Schematic representation of $P_{1,2,3}$. The red arrow represents $k_4 - k_2$ and the blue arrow denotes $k_3 - k_1$. 

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Fig. 4: (Colour on-line) (a) The renormalization group flow of three different types of pair scattering amplitude for the five-band Hubbard-Hunds model in ref. [8]. $P_1$ is the scattering process that drives both SDW and pairing. $P_2$ is a generic pair scattering processes which is not in the SDW channel. $P_3$ is an intra-packet pair scattering process. The red arrows mark the renormalization group steps at which the scattering amplitudes begin to increase rapidly. (b) Schematic representation of $P_{1,2,3}$. The red arrow represents $k_1-k_2$ and the blue arrow denotes $k_3-k_4$.

We would like to point out that the fact that eq. (4) can be “decoupled” in both the antiferromagnetic and the superconducting channels is reminiscent of the spirit of the so-called pairing decoupling of the AF exchange interaction in the “RVB” theory of the cuprates [17]. Similar pairing decoupling of the AF exchange has been made in refs. [9,10] for the iron pnictides. However, we should stress that the final effective interaction generated by the our FRG is not a simple spin-spin exchange interaction as described in ref. [10],

Before closing we would like to propose an experiment which can in principle detect the signature of the out-of-phase s-wave pairing discussed in this paper. The idea is to study the quasiparticle interference [18] using STM [19]. If the electron pocket and hole pocket have out-of-phase order parameter, the Nambu spinor associated with the quasiparticle at the electron and hole Fermi surfaces will be orthogonal. (Note that from the angle-resolved photoemission [12] the gap value for the electron pocket is almost identical to that of the larger-gap hole-pocket. As a result, scattering from electron to hole pocket is an allowed elastic process in the superconducting state.) For example, under the gauge where the order parameter is real, one of them will be $\sim \left( \begin{array}{c} 1 \\
-1 \end{array} \right)$, and the other $\sim \left( \begin{array}{c} 1 \\
0 \end{array} \right)$. As a result, a scalar impurity (which operates as $\left( \begin{array}{cc} 1 & 0 \\
0 & -1 \end{array} \right)$ in the Nambu space) can not scatter quasiparticle between two electron pockets, while can do so between the electron and hole pockets. As a result, for bias at the larger gap edge (∼12 meV), the interference peaks (rings) surrounding the reciprocal lattice vector (here we use the unit cell containing two Fe atoms) will be absent in the Fourier transformed STM spectroscopy. In contrast the peaks surrounding $(\pm \pi, \pm \pi)$ will be present. The missing peaks around the reciprocal lattice vector will recover as the bias increases from the gap edge. If such behavior is seen this is an evidence of the out-of-phase s-wave pairing.

In summary, we have shown that within the one-loop functional renormalization group approach the pairing in both the cuprates and iron pnictides are driven by the antiferromagnetic correlation. We have shown that this naturally leads to d-wave pairing symmetry for the cuprates, while the magnetic fluctuation is intra-band, and an out-of-phase s-wave pairing symmetry for the iron pnictides, where the magnetic fluctuation is inter-band. Finally, in addition to these two family of compounds there are other instances of superconductivity occurring upon exiting the antiferromagnetic phase (examples include the heavy fermion and the organic compounds [20]). It is possible that the mechanism discussed in the present paper is applicable to those as well.

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