Real Space Coulomb Interaction: A Pairing Glue for FeAs Superconductors

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In this paper we present a real space pairing glue for the iron-based layered superconductors. It is shown that two static electrons embedded symmetrically in two adjacent Fe plaquettes of the superconductor can be bound due to the Coulomb interaction. The pairing mechanism favors the existence of the pseudogap in the underdoped FeAs superconductors. A criterion is introduced to distinguish whether or not the pseudogap can open in a material.

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Twenty-two years after the discovery of high-$T_c$ cuprate superconductors \cite{1, 2}, although under intensive studies, physicists do not agree on how superconductivity works in these materials \cite{8}. MgB\textsubscript{2} superconductor was discovered seven years ago \cite{4}, so far we also do not know what causes superconducting in this material. Most recently, the iron-based superconductors have been found by researchers in Japan and China \cite{5, 6} has raised the hope that the new materials will help solve the mystery of high-$T_c$ superconductors, on the contrary, researchers now need to be more confused than ever about the fundamental mechanism of superconductivity. “If it’s really a new mechanism, God knows where it will go.” says Philip Anderson \cite{7}.

As is well known, the superconductivity is indeed a rather common phenomenon in nature. There are now several thousand materials showing the superconductivity. Correspondingly, physicists have developed many theories and models on atomic level in attempts to pin down the mechanism responsible for the observed superconducting phenomena in different materials. It seems as if a new superconductor always calls for a new superconducting mechanism. But this situation should not continue like that. It is time for the condensed matter community to consider one important question: for different superconductors, there are different superconducting mechanisms, or there is only one unified mechanism? Personally, I think that the latter case is a more reasonable possibility physically and naturally. The intrinsic mechanism of the superconductivity is at base simple and determinate, it is scientists themselves who have made the problem more complex and not determinate.

Recently, we have proposed a real space spin-parallel mechanism of superconductivity which has successfully provided coherent explanations to a number of complicated problems in conventional and non-conventional superconductors \cite{8, 9, 10, 11, 12}, for example, the local checkerboard patterns and "magic doping fractions" in La\textsubscript{2−x}Sr\textsubscript{x}CuO\textsubscript{4} \cite{8}, the tetragonal vortex phase in Bi\textsubscript{2}Sr\textsubscript{2}CaCu\textsubscript{2}O\textsubscript{8} \cite{9}, the hexagonal vortex lattice and charge carrier density in MgB\textsubscript{2} \cite{12} and pressure effects \cite{10} in the new iron-based superconductors, and the $4a \times 4a$ and $4\sqrt{2}a \times 4\sqrt{2}a$ checkerboard patterns in hole-doped Ca\textsubscript{2−x}Na\textsubscript{x}CuO\textsubscript{2}Cl\textsubscript{2} \cite{11}. Although these results are in excellent agreement with experiments, disappointingly, they have been totally neglected by the community.

On the other hand, despite recent attention and greater efforts to understand the FeAs superconductors, there is no consensus on the origin of the ‘superconducting glue’ that binds electrons into superconducting pairs. It should be pointed out that most of the theoretical works are playing absolutely the same “mathematical and numerical games” which have been played intensively in cuprate superconductors. Undoubtedly, many theories about electron pairing and superconducting in the iron-based superconductors may also be on the wrong track \cite{3}. We insist that in order to have a deeper insight into the forces responsible for Cooper pairs in the superconducting materials, the framework of $k$-space weak-coupling BCS theory should be abandoned and the original configuration of Cooper pairs (antiparallel spins and opposite momenta) should be modified \cite{3}.

In the present paper, we aim to improve the suggested unified superconducting theory \cite{8, 9} and extend the application of the theory to the pairing mechanism (glue) and pseudogap phase in Fe-based superconductors.

How are two negatively charged electrons bound into Cooper pairs in the iron-based superconductors? Theoretical and numerical studies have shown that superconductivity in these materials is associated with the FeAs layer which can be further subdivided into a square Fe lattice with the Fe-Fe distance $a = a_0/\sqrt{2}$, where $a_0$ is the lattice parameter. The iron atoms are separated by arsenic atoms above and below Fe plane. As shown in Fig. 1 when two static electrons embedded symmetrically into two adjacent Fe plaquettes of the FeAs superconductor with a distance $2\Delta$, there is a long-range repulsive electron-electron Coulomb interaction

$$f_c = \frac{e^2}{4\pi\varepsilon_0(2\Delta)^2}. \quad (1)$$

Obviously, the two electrons cannot be naturally paired due to this strong repulsion. So how can repulsive
FIG. 1: The schematic plot of the pairing glue in the FeAs superconductor. (a) Two spin parallel electrons with a joint magnetic moment $M_s$ is confined inside two adjacent Fe plaquettes of the superconductor. The electron-electron ($f_c$ and $f_m$), Fe-electron ($f_1, f_2, f_3, f_4, f_5$ and $f_6$) and As-electron interactions ($f_7$ and $f_8$) are considered, when the net force $F_y = F'_y = 0$, indicating a completely suppression of the Coulomb repulsion $f_c$ and the opening of pseudogap, (b) picture of detailed illustration of As-electron interactions.

Coulomb forces exerted on electrons be eliminated so that the electrons can be in pairs? First, as shown in Fig. (a), for two spin parallel electrons with a joint paired-electron magnetic moment $M_s = m_s(1) + m_s(2) = 2m_s$ (where $m_s$ is the monoelectron spin magnetic moment), there is a magnetic dipolar attraction $f_m$ which is given by

$$f_m = \frac{3\mu_0\mu_0^2}{8\pi\Delta^2}. \quad (2)$$

Because of the short-range interaction characteristics of Eq. (2), as is usually the case $F_c \gg F_m^{\text{max}}$. It is then clear that other factors, which have the effect of weakening the long-range repulsive force $f_c$, should be taken into account. We presume that the real-space confinement effect (electromagnetic interactions) in FeAS plane (see Fig. (b) plays a central role in suppressing the influence of the Coulomb repulsion between electrons. For the purpose of a simplified case, we consider the nearest-neighbor (1 and 2) Fe-electron interactions

$$f_1 + f_2 = \frac{e^2}{\pi\varepsilon_0} \frac{\Delta}{[(a/2)^2 + \Delta^2]^{3/2}}, \quad (3)$$

next-nearest-neighbor (3, 4, 5 and 6) Fe-electron interactions

$$f_3 + f_4 = -\frac{e^2}{\pi\varepsilon_0} \frac{a - \Delta}{[(a - \Delta)^2 + a^2/4]^{3/2}}, \quad (4)$$

and

$$f_5 + f_6 = \frac{e^2}{\pi\varepsilon_0} \frac{a + \Delta}{[(a + \Delta)^2 + a^2/4]^{3/2}}. \quad (5)$$

The nearest-neighbor As-electron (7 and 8) interactions are also considered, as shown in Fig. (b), we get

$$f_7 = \frac{3e^2}{4\pi\varepsilon_0} \frac{a/2 - \Delta}{[(a/2 - \Delta)^2 + d^2]^{3/2}}, \quad (6)$$

$$f_8 = -\frac{3e^2}{4\pi\varepsilon_0} \frac{a/2 + \Delta}{[(a/2 + \Delta)^2 + d^2]^{3/2}}. \quad (7)$$
FIG. 2: Analytical total confinement force $F_y$ versus $\Delta$ in LaO$_{1-x}$F$_x$FeAs superconductor. In two special positions (blue circles), where the electrons are in the energy minimum bound states characterized by the pseudogaps.

Now we have a general formula of the total confinement force $F_y$ (or $-F_y'$) applied to the electron of the pair in $y$ direction as

$$F_y = -F_y' = \sum_{i=1}^{8} f_i \pm f_m - f_e.$$  

Physically, when $F_y$ (or $-F_y'$) is equal to zero, it indicates a completely suppression of the Coulomb repulsion between two electrons. As a consequence, the electrons will be in the energy minimum bound state. Based on the analytical expressions (1)−(7), we draw in Fig. 2 the confinement force $F_y$ versus $\Delta$ for LaO$_{1-x}$F$_x$FeAs. This figure reveals one important fact: there are two special positions ($\Delta = 0.215a$ and $0.449a$) where the localized Cooper pair (characterized by a pseudogap) can survive in the superconductor.

Now we present a brief discussion of the doping dependence of the pseudogap phenomenon. At a rather low doping level, as shown in Fig. 3(a), the interactions among electron pairs can be neglected and the pairs can maintain their integrality (pseudogap phase) at a temperature $T^*$ which is higher than the superconducting transition temperature $T_c$. With an increase in doping, the effect of the competitive interactions among pairs will emerge [see the lower right corner of Fig. 3(b)]. When the doping concentration reaches certain threshold values, the localized Cooper pairs (pseudogap phase) will be destroyed instantly due to the strong interactions among the crowded Cooper pairs, as shown in Fig. 3(b).

In an earlier article [9, we showed that the charge carrier density for a doped superconductor is given by

$$\rho_s = \frac{2}{ABC} = \frac{x}{abc}, \quad (8)$$

where $x$ is the doping level, $(a, b, c)$ and $(A, B, C)$ are the constants lattice (atoms) and superlattice (electrons) constants [9, respectively. From Eq. (8), for a bulk superconducting materials, we can define a parameter
(the average pair-pair distance $\xi$) as follows

$$\xi_{3d} = \sqrt[3]{\frac{2}{\rho_s}}.$$ (9)

For the quasi-two-dimensional layered superconductors ($c \gg a, b$), we can define

$$\xi_{2d} = \sqrt{\frac{2}{c \rho_s}} = \sqrt{\frac{2ab}{x}} \approx a \sqrt{\frac{2}{x}}.$$ (10)

The above parameters of Eqs. (9) and (10) can be used as the criteria for the existence of pseudogap phase in the superconductors. Many experimental results have indicated the existence of the pseudogap phases in the underdoped cuprate and FeAs superconductors, for example, La$_{2-x}$Sr$_x$CuO$_4$ (LSCO, $x = 0.15$) [13] and LaO$_{1-x}$Fe$_x$As (LOFFA, $x = 0.07$) [14]. However, researchers find no experimental evidence for the pseudogap in conventional and MgB$_2$ superconductors. The nature of the pseudogap phase is still highly controversial. There are many models attempt to describe the mysterious pseudogap state. Strictly speaking, none of the proposed models is completely satisfactory. As discussion above, here we present a new approach based on the simple and natural picture of the real-space confinement effect of Fig. 1, and the pseudogap is associated with the local structure and the charge carrier density in the superconductors.

According to the experimental data and Eqs. (9) and (10), the average pair-pair distances for La$_{2-x}$Sr$_x$CuO$_4$ ($x = 0.15$) and LaO$_{1-x}$Fe$_x$As ($x = 0.07$) are $\xi_{\text{LSCO}} \sim 13.88\,\text{Å}$ and $\xi_{\text{LOFFA}} \sim 15.23\,\text{Å}$, respectively. But MgB$_2$ ($a = b = 3.086\,\text{Å}$, $c = 3.524\,\text{Å}$ and $\rho_s = 1.49 \times 10^{22}/\text{cm}^3 = 1.49 \times 10^{-2}/\text{Å}^3$ [8]) superconductor has a relatively small $\xi_{\text{MgB}_2} \sim 6.17\,\text{Å}$, which indicates a much strong pair-pair interaction ($\propto \xi^{-2}$) in the system. Here, we argue that when $\xi < 10\,\text{Å}$, the pair-pair interactions are strong enough to break up the electron pairs, and eventually closes the pseudogap in the sample. Normally, the value of the average pair-pair distance satisfies $\xi < 5\,\text{Å}$ in the conventional superconductors, thus it should not be surprising about the non-pseudogap behavior in these materials.

In conclusion, it is found that the Coulombic interaction can play a key role for pairing glue for the iron-based layered superconductors. The mechanism reveals the existence of the pseudogap in a low doping FeAs sample (underdoped), which is in satisfactory agreement with recent experiment. Furthermore, we have introduced a criterion which can be applied to distinguish whether or not the pseudogap can open in a material. Finally, it should be emphasized that the suggested mechanism responsible for the pseudogap is not specific to the iron-based family and it may also be applicable to other superconducting and even non-superconducting materials.

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