A Real Space Description of the Superconducting and Pseudogap Phase

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I. INTRODUCTION

In 1957, Bardeen, Cooper, and Schrieffer published the well-known microscopic theory of superconductivity. Since then most physicists have come to believe that the superconducting state involve electron pairs bound together by the exchange of phonons (atomic lattice vibrations). In the BCS framework, it is the lattice vibrations that provides the binding energy of electrons in the Cooper pairs. This great theory has been intensively challenged by the discovery of cuprate superconductors with a critical temperature as high as 164 K, some theoretical condensed matter physicists have started to doubt the reliability of the phonon-exchange-pairing superconducting mechanism. They consider that phonons should be effectively ruled-out as the underlying cause of high-temperature superconductivity in cuprates. Consequently, many alternative quasiparticles with energies higher than the phonon frequencies have been proposed as the reason causes the loss of electrical resistance at the higher temperatures. In fact, these efforts have caused much more controversy about how can strongly repulsive electrons form a condensate that flows without resistance.

In the field of superconducting, the phenomenon of superconductivity is normally interpreted in two physical spaces: the momentum space and the real space. In our opinion, it is more reliable to discuss physical problems in the real space where electron-electron and electron-ion interactions can be illustrated in a very direct and clear manner. However, researchers seem prefer to carry out all their study in the momentum-space (dynamic screening). Besides, in order to ensure the authenticity and reliability of the physical description, there should not be any essential difference between the real-space picture and momentum-space picture. As we know, the BCS formalism was established in the momentum-space where the superconducting electrons are paired in a coherent order quantum state, while in real-space these electrons are in a disorder phase. The fundamental differences between two physical pictures of superconducting electrons reveal that the momentum-space BCS theory is not the final theory of the superconductivity. More importantly, Coulomb interaction is the elementary electrical force that causes two negative electrons to repel each other, furthermore, the random interactions between electrons and lattice ions cannot be ignored. But, from the perspective of the real-space dynamics, any small differences in force applied to each electron of a Cooper pair could lead to the breakdown of pairing correlations. So how can the real-space repulsion between electrons and the electron-ion interactions be eliminated to support the formation of the Cooper pairs? Obviously, the BCS theory of momentum-space cannot avoid this crucial challenge.

With the invention and the application of the modern experimental techniques, for example the Scanning Tunneling Microscopy (STM), researchers now can “look inside” into the superconductors and “see” the superconducting electrons. Motivated by these new results, more and more researchers have tried replace the conventional superconducting picture (dynamic screening) with a real space picture where the superconducting electrons congregate in some quasi-one-dimensional rivers of charge (or vortex lines, stripes) separated by insulating domains. Obviously, to construct a proper model and theory related to the formation of one-dimensional charge rivers will be a major challenge for those devoting themselves to crack the mystery of high-temperature superconductivity. In recent years, we have proposed a real space superconducting mechanism which provide new insights into the nature of the charge stripes.

In the present paper, we provide a complete theoretical analysis of how can the Coulomb repulsion between electrons be eliminated in favor of electron pairing and superconducting. Moreover, the physical nature of pseudogap phenomenon and d-wave pairing symmetry are also naturally understood on the basis of the short-range real space Coulomb confinement effect.
FIG. 1: According to the energy minimum principle, the charge carriers (electrons) will automatically gather in some zero-force quasi-one-dimensional spaces. The Peierls chain $u = 0$, while the periodic chain corresponds to a superconducting excited state with electron-transfer velocity $u > 0$.

II. HOW CAN THE REPULSION BETWEEN ELECTRONS BE ELIMINATED?

In the momentum space (dynamic screening), the superconducting electrons are randomly distributed in the real-space at the same time. This implies that there doesn’t exist two itinerant electrons (the so-called pairing electrons) with the exactly the same interaction environment. Hence, the Coulomb interaction between two electrons (Cooper pair) of the dynamic screening can not be completely suppressed by the other electrons and ions. Now, how can the repulsion between electrons be suppressed to support the occurrence of superconductivity? The answer lies in the quasi-one-dimensional real-space stripes, as shown in Fig. 1.

In the previous paper, we proved theoretically that a static one-dimensional vortex line (Peierls chain, or charge stripe) can be naturally formed inside the superconducting plane. The stable charge stripe is confined by the domain-walls of the positive ions (see Fig. 1). Driven by an external electric field, there will occur a charge ordering phase transition from the stable Peierls chain (the superconducting ground state of $u = 0$) to the periodic chain (the superconducting excited state of $u > 0$) in any superconductors, as illustrated in Fig. 1. For three-dimensional superconductors, the vortex lines can further self-organize into some thermodynamically stable vortex lattices with trigonal or tetragonal symmetry.

In any superconducting materials, to a very good approximation, there are mainly two kinds of Coulomb interactions on superconducting electron: (1) electron-electron repulsive interactions, and (2) electron-ion attractive interactions. In our superconducting scenarios, to maintain the zero resistance property of the superconductors it is necessary that all superconducting electrons should be in the zero-force state, or electron is the “inertial electrons”. Figure 2 shows the forces applied to one of the electrons in Fig. 1. Due to the crystal symmetry in $x$ and $z$ directions, all the forces (electron-ion interactions) in these two directions are canceled in opposite directions. This can be expressed mathematically as follows:

$$|F_x| = |F_{-x}|, \quad |F_z| = |F_{-z}|.$$  \hfill (1)

In the $y$-direction of charge stripe, the forces on the electron come from the electron-electron interactions inside the charge stripe. In our scenarios, when a superconductor enters into the superconducting state, all the superconducting electrons can be considered as the “inertial electrons” and forces on any one of them should be balanced. Hence we have

$$|F_y| = |F_{-y}|.$$  \hfill (2)

According to the symmetry of the charge stripe, it is not difficult to find that the condition above can be satisfied naturally without depending on any “glue”. Generally, for an infinite one-dimensional superconducting periodic chain with the electron-electron spacing $\delta = b/2$ and electron-transfer velocity $u > 0$ (as shown in Fig. 1). Now, let us suppose one of the electrons (marked by “0” in Fig. 3) has a small displacement in $x$-direction ($x < \delta$), if the velocity $u = 0$, the other electrons inside the stripe will repel the electron “0” through the electrostatic field. The repulsive forces from the symmetry electron pair $(l, -l)$ of Fig. 3 can be expressed as:

$$F^e(l,-l) = -e(E^e_0 + E^e_1)$$

$$= \frac{e^2 \cos \theta}{2\pi \varepsilon_0 r_1^2} i \frac{e^2 i}{2\pi \varepsilon_0 r_1^2}$$  \hfill (3)
where $\mathbf{E}_0^e$ and $\mathbf{E}_0^m$ are the electrostatic field generated by the electron $l$ and electron $-l$, respectively, and $i$ is the unit vector in $x$-direction.

When the velocity $u \neq 0$, apart from the repulsive electrostatic force, the electron $0$ will experience an attractive magnetic force exerted by the other electrons. According to electromagnetic theory, we can find that the magnetic field generated by the electron $l$ around the electron $0$ can be expressed as:

$$
B_l = -\frac{\mu_0 e u \times \mathbf{r}_l}{4\pi r_l^3}.
$$

The above magnetic field will exert on the moving electron $0$ with the following Lorentz force:

$$
F_{l}^m = -e u \times B_l = -\frac{\mu_0 e^2 u^2 x}{4\pi r_l^3} i = -\frac{\mu_0 e^2 u^2 x}{4\pi (x^2 + l^2)^{3/2}} i.
$$

Similarly, we can define a pair of magnetic force on the electron 0 as follow

$$
F_{l}^m (l, -l) = F_{l}^m + F_{-l}^m = 2F_{l}^m = -\frac{\mu_0 e^2 u^2 x}{2\pi r_l^3} i.
$$

From Eq. (3) and Eq. (6), we have the following representation:

$$
\left| \frac{F_{l}^m (l, -l)}{F_{l}^m (l, -l)} \right| = \frac{c^2}{u^2}.
$$

Because $u < c$, thus from Eq. (7) it follows that the magnetic attraction $F_{l}^m (l, -l)$ is always less than the electric repulsion $F_{l}^e (l, -l)$.

When $\delta = b/2 \gg x$, then we have $r_l \approx l\delta$. Now, combining Eq. (3) and Eq. (5), we have the total electromagnetic force on the electron:

$$
F_{Total} = \sum_{l=1}^{\infty} \left| F_{l}^e (l, -l) + F_{l}^m (l, -l) \right|
$$

$$
= \frac{e^2 x}{4\pi \varepsilon_0 b^3} \left( 1 - \frac{u^2}{c^2} \right) \sum_{l=1}^{\infty} \frac{1}{l^3}
$$

$$
= \frac{2e^2 \zeta(3)}{\pi \varepsilon_0 b^3} \left( 1 - \frac{u^2}{c^2} \right) x.
$$

where $\zeta(3)$ is a zeta function.

It can be easily found from Eq. (8), if the displacement $x \neq 0$, the $F_{Total}$ is always positive. Then from the viewpoint of energy, this repulsive force will lead directly to an increase in the system energy, which in turn decrease the stability of the superconducting state. But, it is clear that if $x = 0$, we have $F_{Total} = 0$ according to Eq. (8). This result indicates that a perfect one-dimensional charge-chain can not only reduce the energy of the superconducting state, but also eliminate completely the repulsion between the electrons inside the charge stripe.

### III. PSEUDOGAP STATE

One of the highly controversial issues in the understanding of high-temperature superconductivity is the...
origin of the normal-state gap (pseudogap). There are many theories and models attempt to describe the pseudogap phase, yet its nature remains a mystery. Here we present a new interpretation of pseudogap based on the simple real-space Coulomb confinement effect.

In the framework of the real-space approach (as discussed in the above section), the most important unit of the superconducting phase is the one-dimensional long-range correlated charge stripes that may form through long-range lattice confinement effect (electron-electron and electron-ion interactions). However, we will show that the nearest-neighbor electron-ion correlation may be responsible for the mechanism of the pseudogap. Figure 4 shows two electrons (a Cooper pair) inside a unit cell of different superconductors. For the cases of Figs. 4(a)-(c), it is not difficult to find that the “Cooper pair” will be split up due to electron-ion interactions, while the Cooper pair can survive in Fig. 4(d) in two special directions.

In what follows, we pay our attention to the case of Fig. 4(d). We try to show how can two repulsive electrons stay together inside a single plaquette and discuss the pairing symmetry of the corresponding pseudogap.

FIG. 5: The schematic plot of the confinement forces acting on the electrons. Figures (a) and (b) illustrate the eight Coulomb forces ($f_1$, $f_2$, $f_3$, $f_4$, $f_5$, $f_6$, $f_7$ and $f_8$) exerted on the electron $A$ by the ions and the repulsive force ($f_B$) inside the pair. Based on Fig. 4(a) (For the sake of simplicity, suppose $a = b$), we can get a general formula of the total confinement force $F_y$ applied to the electron $A$ in $y$-direction as:

$$F_y = f_B + F^{(1)}_y + F^{(2)}_y.$$  \hspace{1cm} (9)

The well-known Coulomb repulsion $f_B$ can be represented as

$$f_B = \frac{e^2}{4\pi \varepsilon_0 \delta^2},$$ \hspace{1cm} (10)

where $\delta$ is the electron-electron spacing which can be used to characterize the size of the Cooper pair.

$F^{(1)}_y$ is the total nearest-neighbor Coulomb force which is defined as

$$F^{(1)}_y = (f_1 + f_3) - (f_2 + f_4) = m \frac{e^2}{4\pi \varepsilon_0} \left(\frac{1}{d_1^2} - \frac{1}{d_2^2}\right),$$  \hspace{1cm} (11)

and the total next-nearest-neighbor Coulomb force $F^{(2)}_y$ can be expressed as

$$F^{(2)}_y = (f_5 + f_6) - (f_7 + f_8) = m \frac{e^2}{4\pi \varepsilon_0} \left(\frac{1}{d_3^2} - \frac{1}{d_4^2}\right).$$ \hspace{1cm} (12)
The parameters $d_1, d_2, d_3$ and $d_4$ are given by

$$d_1 = \frac{(b^2 + \delta^2)^{3/4}}{2\sqrt{2\delta}}, \quad d_2 = \frac{b^2 - \delta^2}{4\sqrt{2\delta}},$$

$$d_3 = \frac{(2b^2 + \delta^2 - \sqrt{2b\delta})^{1/4}}{4\sqrt{b - \delta}},$$

$$d_4 = \frac{(2b^2 + \delta^2 + \sqrt{2b\delta})^{1/4}}{4\sqrt{b + \delta}}. \tag{13}$$

Similarly, in $xy$-direction, we have

$$F_{xy} = f_B + F_{xy}^{(1)} + F_{xy}^{(2)}, \tag{14}$$

and the corresponding functions are defined by

$$f_B = \frac{e^2}{4\pi\epsilon_0 a^2},$$

$$F_{xy}^{(1)} = m^2 e^2 \left( \frac{1}{D_1^2} - \frac{1}{D_2^2} \right), \quad m = 1, 2, 3... \tag{16}$$

$$F_{xy}^{(2)} = n^2 e^2 \left( \frac{1}{D_3^2} - \frac{1}{D_4^2} \right), \quad n = 1, 2, 3... \tag{17}$$

The four distance parameters above are given by

$$D_1 = \frac{(b^2 + \delta^2 + \sqrt{2b\delta})^{3/4}}{2\sqrt{2b + 2\delta}},$$

$$D_2 = \frac{(b^2 + \delta^2 - \sqrt{2b\delta})^{3/4}}{2\sqrt{2b - 2\delta}},$$

$$D_3 = \frac{(2b^2 - \delta^2)}{4 \times 2\sqrt{4\delta}}, \quad D_4 = \frac{(2b^2 + \delta^2)^{3/4}}{4\sqrt{\delta}}, \tag{18}$$

where $\delta < a/\sqrt{2}$.

In the framework of our theory, whether the two electrons become paired (Characterized by the pseudogap) in Figs. 5(a) and (b) can be judged by the value of $F_y$ and $F_{xy}$, respectively. For a given superconductor with the definite structure parameters $b, Q^+ (= ne)$ and $Q^- (= -me)$, if there exist a value of $\delta$ (electron-electron spacing) which can ensure $F_y = 0$ (or $F_{xy} = 0$), then the pair can maintain it integrity in the square lattice of Fig. 5(a) [or Fig. 5(b)]. With the analytical expressions from (9) to (18), we draw in Fig. 6 and Fig. 7 the total forces $(F_y$ and $F_{xy})$ on the electron A (a discussion may be expected to be valid for the electron B) versus $\delta/b$ for the cases of the nearest-neighbor and next-nearest-neighbor interactions, respectively.

Figure 5(a) shows the relation between $F_y$ and $\Delta/b$ under the nearest-neighbor condition. As can be seen from the figure, there exist always one $\delta$ with the force $F_y = 0$. With the increasing of the charge of the ions $Q^-$ from $-e$, $-2e$ to $-3e$, the size of Cooper pair $\delta$ will decrease eventually from 0.39286, 0.33246 to 0.3015$b$, indicating a stronger confinement effect and a higher Cooper-pair binding energy. When the two electrons arranged in $xy$-direction, the forces $F_{xy}$ are always positive for any given $m$ (or $Q^-$), as shown in Fig. 6(b). This result implies that the pair along $xy$-direction can be easily destroyed due to the Coulomb interaction between the pair and ions. If we use the parameter $\delta$ as a measure of the binding energy $(E_b \propto 1/\delta)$ of the Cooper pair, it is not difficult to conclude that the pair parallel to $x$- and $y$-axis has a minimum $\delta$ that leads to a maximum binding energy in these four directions, while the binding energy may be zero when the pair in the four diagonal directions. Hence, the nearest-neighbor electron-ion interactions can directly lead to the $d$-wave pseudogap observed in the cuprate superconductors. To make this argument more convincing, we will take into account the next-nearest-neighbor interactions.

When both the nearest-neighbor and next-nearest-neighbor interactions are present in the calculation of Figs. 6 and 7, we draw in Fig. 8 the total forces $(F_y$ and $F_{xy})$ on the electron A (a discussion may be expected to be valid for the electron B) versus $\delta/b$ for the cases of the nearest-neighbor and next-nearest-neighbor interactions, respectively.

FIG. 6: Analytical confinement forces versus $\delta/b$ in two special directions. (a) Two electrons (a Cooper pair) are arranged in $y$-direction, in this case, a stable real-space Cooper pair can be formed inside the unit cell due to the existence of $F_y = 0$, (b) while two electrons in $xy$-direction, the confinement force $F_{xy} = 0$ is always positive, indicating an unstable state of the Cooper pair in this direction. These results implies a possibility pseudogap phase of $d$-wave symmetry in the superconductor.
The influence of the next-nearest-neighbor interactions on the formation of the pseudogap. (a) The adding of the next-nearest-neighbor interactions have little impact on the formation of electron pair in the y-direction, the pairing electrons can still maintain its integrity inside the single plaquette, (b) while in the diagonal xy-direction, these interactions make the pairing more difficult.

The force $F_y$ and $F_{xy}$, we find that the real-space electron pairing symmetry (Fig. 7) does not change comparing to Fig. 6 of the nearest-neighbor interactions. Figure 7(a) shows that the adding of the next-nearest-neighbor interactions almost does not affect the electron pair in the y-direction, very little difference in the size of Cooper pair $\delta$ can be observed (see the insert figure). In the case of Fig. 7(b), although significant changes were observed in the figure, but the force $F_{xy}$ can be guaranteed to be positive when considering different next-nearest-neighbor interactions ($n = 1, 2, 3$). Furthermore, the larger $F_{xy}$ indicates that the two electrons are much more difficult to be paired in the diagonal directions. These results confirm our argument that the nearest-neighbor electron-ion interactions play an important role in the origin of the pseudogap phenomenon.

From our study of the mechanism of the pseudogap based on the short-range real-space Coulomb confinement effect, the pair-pair interactions have been completely neglected. This approximation is reasonable to describe the underdoped cuprate superconductors with a small carrier concentration. Whereas for the overdoped superconductors, the pseudogap phase will be destroyed by pair-pair interactions, as shown by the experimental results. Besides, the characteristic of local nearest-neighbor interactions of our theory implies that the pseudogap phenomenon can be found from a wide variety of materials, especially those with low carrier concentrations, such as the semiconductors and some insulation materials.

IV. CONCLUDING REMARKS

In conclusion, we have shown that the Coulomb repulsion between electrons can be completely eliminated only if the charge carriers (electrons) self-organize into some quasi-one-dimensional charge stripes (vortex lines). It has been argued that the superconducting ground states are guaranteed by the energy minimum quasi-one-dimensional Peierls chains which are formed with the lattice confinement effect. In the framework of our theory, all the superconducting electrons can be considered as the “inertial electrons” at some stable zero-force positions. Furthermore, we have proved analytically that two electrons, due to the nearest-neighbor electromagnetic interactions, can be in pairing inside a single plaquette with the $d$-wave pairing symmetry. Our results suggest that the pseudogap is a common feature that can be found from a wide variety of materials, not just the cuprate superconductors.

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