Theory of superconducting and nonsuperconducting stripe phases in the hole-doped superconductor Ca$_{2-x}$Na$_x$CuO$_2$Cl$_2$ ($x = 1/8, 1/16$)

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Based on the newly developed real-space spin-parallel pairing and superconducting theory, we explore a simple explanation for the observed checkerboard patterns in hole-doped Ca$_{2-x}$Na$_x$CuO$_2$Cl$_2$ cuprate superconductor. At a hole concentration $x = 1/8 = 0.125$, the analytical results show that there exists a phase competition between non-superconducting 4$a$ × 4$b$ (a = b) checkerboard phase and 8$a$ × 2$c$ superconducting vortex phase, where $a$, $b$ and $c$ are the lattice constants of the superconductor. At a lower hole concentration $x = 1/16 = 0.0625$, it is revealed that the metastable 4$\sqrt{2}a$ × 4$\sqrt{2}a$ checkerboard phase can reorganize itself into a more stable octahedron phase with the $4a$ × 4$a$ checkerboard symmetry.

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The hole-doped Ca$_{2-x}$Na$_x$CuO$_2$Cl$_2$ (CNCOC), with a crystal structure similar to that of La$_{2-x}$Sr$_x$CuO$_4$ (LSCO), has been studied extensively because of the simplicity of its structure. Single crystals of lightly doped CNCOC can be cleaved easily like mica, which provides an ideal surface for scanning tunneling microscopy or spectroscopy (STM and STS) studies [1,2]. At the doping level 1/8, results of STM and angle-resolved photoemission spectroscopy (ARPES) experiments on CNCOC suggest a checkerboard-like spatial modulation of electronic density of states with a periodicity of $4a$ × $4a$ [1,3], which has been shown to be a universal feature of cuprate superconductors [4,5]. Many theoretical efforts have been made to explain the non-dispersive checkerboard charge ordering patterns [1,6,7,8,9,10,11]. Even though the checkerboard pattern can be simulated numerically by adjusting different parameters in a number of proposed models, the exact causes of the checkerboard pattern in cuprate superconductors are still not conclusive.

Recently, we have proposed a real space spin-parallel mechanism [12,13,14] of superconductivity which has successfully provided coherent explanations to a number of complicated problems in conventional and nonconventional superconductors (including the new iron-based materials [13,16]). Our work marks an important step forward in unraveling the mystery of the superconductivity. In the present paper, we will show that our simple pictures of Cooper pairing and vortex lattices can lead to new understanding of the emergence of nonsuperconducting checkerboard phases and superconducting vortex phases in CNCOC superconductor.

It is well known that the formation of stripe patterns is generally attributed to the competition between short-range attractive forces and long-range repulsive forces [17]. In a superconductor with the primitive cell ($a$, $b$, $c$), at a rather low doping level, the interactions among electrons can be neglected and the superconductor behaves much like a charged random system. As more carriers are added, the effect of the competitive interactions among electrons will emerge. At a proper doping level (not too low, not too high), the electron pairs can self-organize into a low-temperature orthorhombic (LTO) phase (Wigner crystal of Cooper pairs) of $(A,B,C) = (ha,kb,lc)$, as shown in Fig. 1. Thus, the carrier density $x$ is given by

![Fig. 1: Simplified schematic unitcell of the electron-pairs (Cooper pairs) Wigner crystal in the high-$T_c$ cuprates.](image-url)
FIG. 2: The schematic interpretation of the theory of superconductivity based on the minimum energy principle in cuprate superconductors. (a), A quasi-zero-dimensional localized Cooper pair (with the electron-electron separation $\Delta_0$) located inside a square lattice of two-dimensional CuO plane. (b), A quasi-one-dimensional dimerized vortex line and a collective real-space spin-parallel confinement picture in CuO plane, where $\Delta_1$ ($<\Delta_0$) is the electron-electron separation. (c-f), Four quasi-two-dimensional vortex lattices with a uniform distribution of vortex lines. (c), LTT1(h, k, l) phase, the charge stripes have a tetragonal symmetry in XZ plane. (d), LTT2(h, k, l), the vortex lattice has a tetragonal symmetry in XZ plane with a orientation 45°. (e) and (f), The simple hexagonal (SH) phases [SH1(h, k, l) and SH2(h, k, l)]. Where $\xi_{xz}$ is the nearest neighbor stripe-separation.

$$x = p(h, k, l) = \frac{2V_{abc}}{V_{ABC}} = 2 \times \frac{1}{h} \times \frac{1}{k} \times \frac{1}{l},$$

and the corresponding charge carrier density is

$$\rho_s = \frac{2}{ABC} = \frac{2}{hklabc} = \frac{x}{abc},$$

where $h, k,$ and $l$ are integral numbers, and $V_{abc}$ and $V_{ABC}$ are the unit cell volumes of the lattice and the corresponding superlattice, respectively.

Physically, electron pairing (Cooper pair) in cuprates is an individual behavior characterized by pseudogap, while superconductivity is a collective behavior of many coherent electron pairs. To maintain a stable superconducting phase (minimum energy), first the Cooper pairs of Fig. 2 must condense themselves into a real-space quasi-one-dimensional dimerized vortex line (a charge-Peierls dimerized transition), or a Cooper pairs’s charge river in the CuO$_2$ plane of cuprate superconductor, as shown in Fig. 2a. It should be noted that this figure also illustrates a collective real-space spin-parallel confinement picture where any electron pair inside always experiences a pair of compression forces (indicated by the two big arrows). And second, in order to further minimize the system energy, the vortex lines must self-organize into four possible quasi-two-dimensional vortex lattices where a uniform distribution of vortex lines is formed in the plane perpendicular to the stripes, as shown in Figs. 2c-f. In the picture, superconducting charge stripe and the vortex line are exactly the same thing. Moreover, this scenario indicates that the superconductivity is relevant to the lattice constants, in support of a recent experiment which has shown that cuprate superconductivity can be varied by the interatomic distances within individual crystal unit cells.

In the LTT1(h, k, l) phase, as shown in Fig. 2a, the charge stripes have a tetragonal symmetry in XZ plane in which the superlattice constants satisfy

$$\frac{A}{C} = \frac{ha}{lc} = 1.$$  

Fig. 2a shows the LTT2(h, k, l), the vortex lattice has a tetragonal symmetry in XZ plane with a orientation 45° and the superlattice constants:

$$\frac{A}{C} = \frac{ha}{lc} = 2.$$  

While in simple hexagonal (SH) phases, as shown in Figs. 2c and f, the charge stripes possess identical trigonal crystal structures. In the SH1(h, k, l) phase [see Fig. 2e], the superlattice constants have the following relation

$$\frac{A}{C} = \frac{ha}{lc} = \frac{2\sqrt{3}}{3} \approx 1.15470.$$  

For the SH2(h, k, l) phase of Fig. 2, this relation is given by

$$\frac{A}{C} = \frac{ha}{lc} = 2\sqrt{3} \approx 3.46410.$$  

It is worth to emphasize that our theory of Fig. 2 is based on the most solid minimum energy principle. Physically, in a material, the dominant structural phase should be a minimum-energy state which satisfies the basic symmetry of the crystal structure. In this sense, the superconducting states are merely some minimum energy condensed states of the electronic charge carriers, or some kinds of real-space low-energy Wigner-crystal-type charge orders. We argued that the appearance of the stable vortex lattices (see Fig. 2) is a common feature of the optimally doped superconducting phases. But, for
FIG. 3: The nondispersive LTT3(4, 4, 1) superlattice of the localized electron pairs in CNCOC at doping level $x = 1/8$. (a), The $4a \times 4a$ checkerboard in the doped CuO$_2$ plane. (b), The localized Cooper pairs form a non-superconducting stabilized simple-cubic structure ($A = B \approx C$).

non-optimal doping samples we found that the vortex lattices tend to form the superconducting low-temperature orthorhombic (LTO) phase where the superlattice constants satisfy $A \neq B \neq C$.

We consider the lattice-constant-dependent schematic [Figs. 1-2 and Eqs. 1-3] as a promising approach to the checkerboard problem in CNCOC, as it can naturally explain both the longstanding puzzle of “magic doping fractions” and checkerboard pattern in LSCO [12]. In CNCOC, the experimental lattice constants are $a \approx b = 3.84\AA$ and $c = 15.18\AA$. From Eq. 1, it is clear that the nondispersive superlattices of $4a \times 4a$ in CuO$_2$ planes can be expected at $x = 1/8$ of phase LTT3(4, 4, 1) with $A = B$ (or $p(4, 4, 1)$ phase), as shown in Fig. 3a. From the structure parameters, one has $A = B = 4a(\sim 15.36\AA) \approx C = c(\sim 15.18\AA)$, this implies that it is possible for the localized Cooper pairs in CNCOC to form a non-superconducting stabilized simple-cubic structure at $x = 1/8$, as shown in Fig. 3b. Furthermore, the real space pictures of “localized hole pair” and “localized electron pair” are illustrated in the figure.

Since $A(\sim 30.72\AA) \approx C(\sim 30.36\AA)$, the $x = 1/8$ sample of CNCOC may also be possible in the LTT1(8, 2, 1) superconducting phase of Fig. 2c, where the vortex lines are formed in CuO XY-planes with a uniform spacing of $A = 8a$ while the low-temperature tetragonal vortex lattice is established in XZ plane, as shown in Fig. 4a and Fig. 4b, respectively. The formation of this superconducting phase is in competition with the predominant non-superconducting phase of Fig. 3.

Most recently, a theoretical prediction of the checkerboard pattern has been carried out with the solution of the $4\sqrt{2a} \times 4\sqrt{2a}$ superstructure in CNCOC superconductor at $x = 1/16$ [13]. However, it has been found that two different LSCO compounds ($x = 1/8$ and $x = 1/16$) can exhibit the same nondispersive $4a \times 4a$ superstruc-
The two-dimensional $4\sqrt{2}a \times 4\sqrt{2}a$ checkerboard in Fig. 5b. In fact, the doped CuO$_2$ planes of the most stable octahedron superlattice structure, as shown localized Cooper pairs have a strong tendency to form the A$_{16}$ CNCOC can be divided into “odd doped CuO$_2$ planes” and “even doped CuO planes” and there is a displacement $Q = 4a$ between them. This figure shows that though a single CuO$_2$ exhibits the $4\sqrt{2}a \times 4\sqrt{2}a$ checkerboard pattern at $x = 1/16$, the results of STM experiment on this sample may still be the $4a \times 4a$ pattern.

According to our theory, the localized Cooper pairs in the doped CuO$_2$ of CNCOC can exhibit the $4\sqrt{2}a \times 4\sqrt{2}a$ checkerboard pattern at $x = 1/16$, as shown in Fig. 5b. Due to the fact that $A = B(30.72\,\text{A}) \approx C(30.36\,\text{A})$, the localized Cooper pairs have a strong tendency to form the most stable octahedron superlattice structure, as shown in Fig. 5b. In fact, the doped CuO$_2$ planes of the $x = 1/16$ CNCOC can be divided into “odd doped CuO planes” and “even doped CuO planes” and there is a displacement $Q = 4a$ (or $4b$) between them, as indicated in Fig. 5b. This result implies that though a single CuO$_2$ exhibits the $4\sqrt{2}a \times 4\sqrt{2}a$ checkerboard pattern at $x = 1/16$, the results of STM experiment on this sample may only show the $4a \times 4a$ pattern as illustrated in Fig. 6. In other words, the theoretical expectation of $4\sqrt{2}a \times 4\sqrt{2}a$ pattern in CNCOC is experimentally unobservable.

In conclusion, the observed checkerboard patterns in hole-doped CNCOC superconductor have been well explained by the newly developed real-space spin-parallel pairing and superconducting theory. At $x = 1/8$, we show for the first time the real-space phase competition between the nondispersive $4a \times 4a$ checkerboard phase and $8a \times 2c$ superconducting low-temperature tetragonal vortex phase. At $x = 1/16$, we show that the localized Cooper pairs can organize themselves into the most stable octahedron phase with a global $4a \times 4a$ checkerboard pattern, while the theoretical expectation of $4\sqrt{2}a \times 4\sqrt{2}a$ pattern is formed within each doped CuO$_2$ plane.
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