Magic doping: From the localized hole-pair to the checkerboard patterns

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Intensive experiments have revealed that the superconductivity of the hole-doped cuprates can be strongly suppressed at the so-called magic doping fractions. Despite great research efforts, the origin of the ‘magic doping’ remains mysterious. Recently, we have developed a real-space theory of high-temperature superconductivity which reveals the intrinsic relationship between the localized Cooper pair and the localized hole pair (arXiv:1007.3536). Here we report that the theory can naturally explain the emergence of non-superconducting checkerboard phases and the magic doping problem in hole-doped cuprate superconductors. It clearly shows that there exist only seven ‘magic numbers’ in the cuprate family at $x = 1/18$, $1/16$, $2/25$, $1/9$, $1/8$, $2/9$ and $1/4$ with $6a \times 6a$, $4a \times 4a$, $5a \times 5a$, $3a \times 3a$, $4a \times 4a$, $3a \times 3a$, and $2a \times 2a$ checkerboard patterns, respectively. Moreover, our framework leads directly to a satisfactory explanation of the most recent discovery [M. J. Lawler, et al. Nature \textbf{466}, 347 (2010)] of the symmetries broken within each copper-oxide unit in hole-doped cuprate superconductors. These findings may shed new light on the mechanism of superconductivity.

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The ‘1/8 anomaly’ \cite{1}, one of the long-standing puzzles of superconducting physics, is believed to be a key to understanding the mechanism of high-$T_c$ superconductivity. Later, a number of experiments have indicated that the anomalous suppression of superconductivity can be observed in the hole-doped ($p$-type) cuprates at other ‘magic’ hole densities, for example, $1/16$ \cite{2,3} and $1/9$ \cite{2}. Great efforts have been made to determine these ‘magic numbers’. The SO(5) theory predicts a series of magic doping fractions at $x = (2m + 1)/2^n$, where $m$ and $n$ are integers \cite{4}, while Feng \textit{et al.} \cite{5} obtained a single-parameter expression as $x = (2 + n^2 - 4m)/n^2$, where $n = 4, 5, 6, \cdots$. These interpretations imply the possibility of an infinite magic doping fractions in $p$-type cuprate superconductors, which is obviously inconsistent with the experimental facts. In addition, the physical meanings of the integers $n$ and $m$ are not very clear in these results. In our opinion, these theoretical results cannot be expected to be physically correct and reasonable.

Recently, we have proposed a universal mechanism for the superconductivity which offers a new way of looking at the superconducting phenomenon \cite{6,7}. In particular, we have introduced a new model for $d$-wave pairing in hole-doped high-$T_c$ superconductors which is able for the first time to satisfactorily describe the pseudogap related phenomena, such as the Fermi pocket (or Fermi arc), the two pseudogap behavior and the linear relationship between the pseudogap temperature $T^*$ and the hole doping level $x$ in these compounds \cite{8}.

In the present paper, based on the new theory and model, we aim to uncover the underlying relationship between the ‘magic numbers’ and the nature charge ordering of ‘checkerboard’ as suggested by neutron and STM experiments \cite{9,11}. Seven magic numbers and the corresponding checkerboard structures are analytically and uniquely determined for the $p$-type cuprates. One will easily find that our results are completely different from those obtained through quantum theory and quantum field theory \cite{4,5}. Finally, we will show that the suggested model can explain the recent experiments of the rotational symmetry breaking of the pseudogap phases in hole-doped cuprate superconductors \cite{12,13}.

\section{1. LOCALIZED COOPER PAIR AND HOLE PAIR}

The hole-doped cuprates have been intensively investigated because of the relatively high superconducting transition temperature and a rich phase diagram. However, the question of what causes the loss of electrical resistance in these materials is still one of the major unsolved problems in physics. We have argued that the main reason for this situation is that researchers are confused about some fundamental ideas of modern physics. For example, what is the ‘hole’? As emphasized by Hirsch \cite{14}, using the language of ‘holes’ rather than ‘electrons’ in fact obscures the essential physics since these elec-

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure1.png}
\caption{The relationship between the localized Cooper pair and the localized hole pair in the hole-doped cuprates. (a) Two electrons arranged along the $x$-direction, (b) two electrons aligned in the $y$-direction. If $a = b$, we have proved analytically that the repulsive interactions among Cooper pairs have been completely suppressed with the appropriate $\delta \approx 0.3068$ \cite{8}.}
\end{figure}
trons are the ones that ‘undress’ and carry the supercurrent (as electrons, not as holes) in the superconducting state.

In our scenario model [3], a hole is a real-space ‘quasiparticle’ which is composed of some well-known electrons and ions. For the hole-doped cuprates, a localized hole-pair is a cluster of two electrons (a localized Cooper pair), four \( O^{-1} \) and four \( Cu^{2+} \) inside the Cu-O plane, as illustrated in Fig. 1. According to the classical electromagnetic theory, it is very easy to prove that the direct and strong electron-electron repulsion can be entirely excluded if two electrons are aligned in \( x \)-direction [Fig. 1(a)] or \( y \)-direction [Fig. 1(b)] within each copper-oxide unit with the Cooper-pair size \( \delta \approx 0.396b \) (when \( a = b \)). More importantly, we have shown analytically and numerically that the nearest-neighbor electron-\( O^{-1} \) repulsive interactions play the key role of the ‘pairing glue’ for the real-space localized Cooper pair. The simply picture of Fig. 1 could yield a pairing and superconducting scenario that has the potential to resolve the pseudogap and the high-\( T_c \) superconducting puzzles in the hole-doped cuprates. In our series of studies, we will show that the ‘hole’ pictures (Fig. 1) are considered to be the most basic structural units of the hole-doped cuprates, which can further self-assemble into some superconducting electron states and non-superconducting pseudogap and checkerboard phases. All the related physical properties, such as vortex lattices, Meissner effect, London penetration depth, Hall effect, \( d \)-wave symmetry, checkerboard patterns, magic doping fractions, Fermi pocket (or Fermi arc), two pseudogap behavior and rotational symmetry breaking, can be perfectly interpreted by our framework.

II. NON-SUPERCONDUCTING CHECKERBOARD PATTERNS

The question remains open as to why is the superconductivity suppressed in the cuprates at the magic doping levels? In our opinion, the suppression of superconductivity is caused by a electronic structure phase transition from a superconducting state to a localized state. It is most likely that the charge carriers are pinned via Coulomb interaction with their associated ions. From the perspective of symmetry breaking, the electrons in the localized state must have a higher symmetry than that of the superconducting state. Two high symmetry non-superconducting Wigner crystals of localized Cooper pair of Fig. 1 are suggested and shown in Fig. 2.

Figs. 2(a) and (b) represent the tetragonal phase, where the \( na \times na \) checkerboard pattern can form in all doped planes [see Fig. 2(a)]. If one of \( m \) planes in the layered superconductor are doped, then the corresponding doping level is given by

\[
x = p_1(n, n, m) = 2 \times \frac{1}{n} \times \frac{1}{n} \times \frac{1}{m} = \frac{2}{n^2 m}. \tag{1}
\]

For the case of the octahedral phase of Figs. 2(c) and (d), the checkerboard shows \( \sqrt{2}na \times \sqrt{2}na \) structure in each doped plane [see Fig. 2(c)]. It is easy to obtain the doping level for this phase as follows

\[
x = p_2(n, n, m) = 2 \times \frac{1}{\sqrt{2}n} \times \frac{1}{\sqrt{2}n} \times \frac{1}{m} = \frac{1}{n^2 m}. \tag{2}
\]

Evidently, such commensurate stripes are unmovable and should be insulating. Note from Fig. 2 that when \( C = A = B \), the tetragonal and octahedral phases will transit into the more stable cubic and regular octahedral phases, respectively. In the following section we will show that the perfect cubic and regular octahedral phases can be found in \( Ca_{2-z}Na_zCuO_2Cl_2 \) at \( x = 1/8 \) and \( 1/16 \), respectively.

III. CHECKERBOARD AND MAGIC DOPING

Fig. 3 shows the purely electronic description of the \( 4a \times 4a \) checkerboard in hole-doped \( CuO_2 \) plane, where the structural relationship between the localized hole pair (the geometry of a cluster of two electrons, four \( O^{-1} \) and four \( Cu^{2+} \)) and the localized Cooper pair is clearly illustrated. In a previous paper [3], we proved analytically that the localized Cooper pair is a pure nearest-neighbor confinement effect of the four nearest-neighbor \( O^{-1} \), as indicated in Fig. 1. Moreover, it has been evidently shown that a localized Cooper pair is stable only when the two electrons aligned in \( x \)- or \( y \)-directions, supporting the \( d \)-wave pairing symmetry. The nearest-neighbor character of the pairing mechanism implies that the localized Cooper pairs (pseudogap) are likely to survive in insulating...
or nonmetallic materials, as was reported recently by Stewart et al. [15].

It is now well accepted that the 1/8 anomaly is always accompanied by the appearance of the 4a × 4a checkerboard in the hole-doped cuprates [9]. In fact, equations (1) and (2) imply the existence of some sort of connection between the magic doping fractions and the checkerboard patterns. According to equation (1), when all CuO planes are doped (m = 1), the 4a × 4a checkerboard pattern of Fig. 3 can selforganize into a periodic nondispersive superlattices due to the real space Coulomb confinement effect.

![4a×4a checkerboard](image)

**Figure 3:** The 4a × 4a checkerboard in hole-doped CuO plane at doping level x = 1/8. A pure electron picture of the localized hole pairs, where the localized hole pairs of Fig. 1 can selforganize into a periodic nondispersive superlattices due to the real space Coulomb confinement effect.

| Phase     | Tetragonal phase | Octahedral phase |
|-----------|------------------|------------------|
| x         | 1/8              | 1/8              |
|           | 2/9              | 1/8              |
| 1/8       | 25               | 1/8              |
| 1/9       | 49               | 1/8              |
| 1/16      | 18               | 1/8              |
| 1/3       | 25               | 1/8              |
| 1/4       | 16               | 1/8              |
| 2/25      | 25               | 1/8              |
| 1/25      | 25               | 1/8              |
| 1/25      | 25               | 1/8              |
| 1/41      | 25               | 1/8              |
| 1/81      | 25               | 1/8              |
| 1/161     | 25               | 1/8              |
| 1/325     | 25               | 1/8              |
| 1/659     | 25               | 1/8              |
| 1/1317    | 25               | 1/8              |
| 1/2634    | 25               | 1/8              |
| 1/5268    | 25               | 1/8              |
| 1/10536   | 25               | 1/8              |
| 1/21072   | 25               | 1/8              |
| 1/42144   | 25               | 1/8              |
| 1/84288   | 25               | 1/8              |
| 1/168576  | 25               | 1/8              |
| 1/337152  | 25               | 1/8              |
| 1/674304  | 25               | 1/8              |
| 1/1348608 | 25               | 1/8              |
| 1/2697216 | 25               | 1/8              |
| 1/5394432 | 25               | 1/8              |
| 1/10788864| 25               | 1/8              |
| 1/21577728| 25               | 1/8              |

Table I: The possible magic doping fractions x for p-type cuprates when all the Cu-O planes are doped (m = 1).

It is immediately seen that in our framework the magic doping fractions are closely correlated with the local checkerboard patterns. Based on equations (1) and (2), one can obtain all the relevant magic doping fractions for hole-doped cuprate superconductors with the full-doped CuO planes (m = 1), as shown in Table I. As we all know, the Tc of hole-doped cuprates has a dome-like shape as a function of hole concentration ranged from x ≈ 0.05 to 0.27, under this restriction, only seven ‘magic numbers’ (x = 1/18, 1/16, 2/25, 1/9, 1/8, 2/9 and 1/4) are possible in the cuprate family. Clearly, our conclusions are different from those drawn from other theories which suggest an infinite number of magic doping fractions in the superconductors [4, 5].

For the tetragonal phases of x = 1/18, 2/25, 1/8 and 2/9, the 6a × 6a, 5a × 5a, 4a × 4a and 3a × 3a checkerboard patterns can be easily determined from Fig. 2 and equation (1), respectively. While for the octahedral phases of x = 1/16, 1/9 and 1/4, the experimental results of checkerboard structures must be 4a × 4a, 3a × 3a and 2a × 2a, respectively, which are different from those proposed by Fig. 2. This is nothing to be surprised about as the checkerboard structures of the

![4√2a×4√2a checkerboard](image)

**Figure 4:** The 4√2a × 4√2a nondispersive checkerboard in hole-doped CuO plane. For 3D superconductors, this checkerboard pattern is experimentally unobservable, as discussed in the text.
find that the results of their experiments are rough to some extent, more sophisticated experiments may reveal that the peaks of 0.06 and 0.09 are in fact double degenerate. According to our theory, the 0.06 peak corresponds to two adjacent magic doping fractions of $1/18 \approx 0.0556$ and $1/16 \approx 0.0625$, while the 0.09 peak may be contributed by $2/25 \approx 0.080$ and $1/9 \approx 0.111$. Furthermore, in our framework, the number of $3/16$ is not the magic number in cuprates. Let us pay attention to the experimental results of Fig. 2b in Komiya et al. paper [19], which clearly show a stronger peak around $x = 0.22$ (apparently different from the suggested $x = 3/16 = 0.1875$) consistent with our prediction of $x = 2/9 \approx 0.222$. For the largest magic number $x = 1/4 = 0.25$, the corresponding non-superconducting $2a \times 2a$ checkerboard phase is more unstable because of a much stronger pair-pair interaction inside the superconductor. Consequently, the suppression of $T_c$ at $x = 1/4$ can only be observed at a much lower temperature.

It is worth noting that all the available experimental data of the ‘magic numbers’ are included in our theory. However, for exactly the same question, two researcher groups [4,5] have derived two totally different expressions indicating ‘infinite magic numbers’ in the $p$-type superconductors, while at the same time some typically ‘magic numbers’ (such as $1/9$ and $1/18$) have been excluded from their expressions. Hence, it is reasonable to argue that they may also be on the wrong track.

### IV. ROTATIONAL SYMMETRY BREAKING

Broken symmetries have been detected in many hole-doped high-temperature superconductors when they undergo a phase transition [12]. The nature of the broken symmetry in the non-superconducting pseudogap phase is a central problem in the effort to understand the pseudogap in the high-$T_c$ copper oxide superconductors. Recently, it has been experimentally confirmed that the breaking of $90^\circ$-rotational symmetry may occur within every $CuO_2$ unit cell in underdoped $Bi_2Sr_2CaCu_2O_8$, which can be regarded as the best support for the model of Fig. 1.

The localized hole pairs (see Fig. 1) are the intra-unit-cell states of the pseudogap phase with an intrinsically broken of the four-fold rotational symmetry within single $CuO_2$ unit cell. This apparent broken symmetry may be the key to understanding the pseudogap phase of copper-oxide superconductors [8]. Similar to the liquid crystals, the significant ultra short-range anisotropic orientational structure of Fig. 1 may eventually lead to the long-range orientational order in the superconductors, as shown in Fig. 4. Since we assume $n_x > n_y$, the macroscopic four-fold rotational symmetry of the checkerboard patterns of Fig. 2 are broken. In addition, it is not difficult to find from Fig. 6 that the polarized Cooper pairs (or localized hole pairs) can self-organize into some minimum-energy quasi-one-dimensional Peierls chains. For the special case of $n_x = 1$, the localized Cooper pairs form some periodic orders (quasi-two-dimensional vortex lattices) of the most compact Peierls chains, which we considered as the superconducting ground states [4]. By applying an external field on the superconductor along $y$-direction, there is a charge or-

![Figure 5: The tetragonal phase with $4a \times 4a$ checkerboard in hole-doped cuprates at doping level $x = 1/16$.](image-url)
V. CONCLUSIONS

We have shown for the first time the intrinsic relation between the magic doping fractions and checkerboard patterns in hole-doped cuprates. It has been proved theoretically that there exist merely seven magic doping fractions numbers ($x = 1/18, 1/16, 2/25, 1/9, 1/8, 2/9$ and $1/4$) in the superconductors, which are completely different from those of quantum field theory, suggesting the existence of an infinite magic doping fractions in the systems. In our view, the phenomenon of the completely destruction of superconductivity is a macro-reflection of the localization of all the micro paired electrons in the superconductor. Physically, the pinning of a huge amount of electrons must always accompanied by the appearance of a high symmetry localized electronic state which is characterized by a definite and periodic checkerboard pattern. For the seven magic doped samples, all of the checkerboard structures have been uniquely determined in this study. Our theoretical framework supports the new finding of the symmetries broken within one copper-oxide unit in the superconductors. We are confident that a ‘new window’ to the mysterious world of superconductivity has been opened.

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