Checkerboard-pattern vortex with the long-range Coulomb interaction in underdoped high-temperature superconductors

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Abstract. Vortex structures in high-transition-temperature superconductors are studied by solving Bogoliubov–de Gennes equations based on a model Hamiltonian with competing antiferromagnetic (AF) and d-wave superconducting orderings in the presence of a long-range Coulomb interaction. We show that transition from a checkerboard pattern to stripe structure for spin density wave (SDW), charge density wave, and d-wave orderings may occur by enhancing the strength of the on-site repulsion \( U \) in the absence of the long-range Coulomb interaction. The long-range Coulomb interaction provides an intrinsic mechanism for electron depletion inside an AF-like vortex core, and the field-induced AF order was screened and confined onto the near core region. Consequently, two-dimensional modulations or the checkerboard patterns of vortex charge distribution and SDW order recovered for underdoped samples of large \( U \) when a reasonably large long-range Coulomb interaction \( V_c \) strength had been introduced into the model Hamiltonian.

Intensive efforts have been focused on vortex structure in high-temperature superconductors (HTSCs) for the past several years. Experimental observations of a peculiar static stripe phase by Tranquada et al [1] provided a possible explanation of the long-standing mysteries associated with the doping dependence of electronic and magnetic properties at the hole doping level or the ‘1/8 anomaly’. Nuclear magnetic resonance (NMR) experiments [2] on \( \text{YBa}_2\text{Cu}_3\text{O}_{7-x} \) (YBCO) probed a strong antiferromagnetic (AF) fluctuation around vortex cores, implying possible existence of spin density wave (SDW) order outside the vortex core. In slightly overdoped

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Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$ (BSCCO), Hoffman et al [3] reported that a four-unit cell checkerboard pattern is localized in a small region near vortex cores, and Levy et al [4] observed four-fold structure that was related to the vortex-core states (VCS) [5] inside the vortex cores using low-temperature scanning-tunneling-microscopy (STM), which confirmed the coexistence of static charge modulation (or the charge density wave (CDW)) and superconductivity. Since a large on-site repulsion is assumed to induce stripe-modulation [5], the recent STM experiments for underdoped Na$_x$Ca$_2-x$CuO$_2$Cl$_2$ [6] and BSCCO [7] samples that probed the checkerboard pattern are very interesting. SDW orders with two-dimensional (2D) [8]–[10] or stripe [11, 12] modulations were theoretically proposed to explain the observed checkerboard patterns. In particular, the checkerboard pattern was attributed to a superposition of $x$- and $y$-axes-oriented stripe modulations of the CDW [13], since the SDW order modulations have to accompany the CDW modulations. We can prove that these two phases are exactly degenerated in energy only when there are no asymmetrical fluctuations in the system. This implies that an in-plane field such as a magnetic field or a dc-bias field would break down their degeneracy. Therefore, one needs to explore the physical mechanisms that would respond to the recent observations of the checkerboard pattern in underdoped samples [7].

It has been pointed out by Khomskii and Freimuth [14] that for a type-II superconductor the particle–hole symmetry breaking upon superconducting condensation can lead to charge redistribution around vortex cores. Furthermore, vortex cores are intrinsically charged-up in superconductors having a small value of $k_F$ due to Coulomb repulsion between conducting electrons, as commonly observed in a neutral superfluid system. This would screen the AF order by expelling the electrons outside the cores, and may modulate the vortex structure. Hence, it is natural to take this intrinsic mechanism for electron depletion inside an AF-like core into account in specifying vortex structure.

We investigate vortex structures for HTSCs with competing AF and d-wave superconducting (DSC) pairing by including the long-range Coulomb interaction into the model Hamiltonian. Using the method described in previous papers [15]–[17], we show that an enhancement of the on-site repulsion that is assumed to be responsible for the AF order favors essentially the stripe-like vortex structures. Indeed, for a small $U$, 2D SDW and CDW orders presented when the long-range Coulomb interaction was not considered. A transition from 2D- to stripe-modulations may occur by enlarging the on-site repulsion strength. The main effect of involving the long-range Coulomb interaction that would expel electrons outside of AF-like vortex cores seems to be to weaken the on-site repulsion $U$. Consequently, the vortex structure transition from the stripe- to 2D-modulations is likely to occur with increasing long-range Coulomb interaction strength, implying the possible existence of the DSC, SDW and CDW orders of the spatial distribution with 2D-modulation or a checkerboard-like distribution for underdoped cuprate superconductors, which seems to be consistent with the STM experiments [7].

We begin with an effective mean-field $t - t' - U - V$ Hamiltonian in the mixed state by assuming that the on-site repulsion $U$ is responsible for the AF order and the nearest-neighbor attraction $V_d$ for the wave superconducting paring and in the presence of a long-range Coulomb interaction:

$$
H = - \sum_{\langle ij \rangle, \sigma} (t_{ij,\sigma}) c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i,\sigma} (U \langle n_{i\sigma} \rangle - \mu) c_{i\sigma}^\dagger c_{i\sigma}
+ \sum_{\langle ij \rangle} (\Delta_{ij} c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger + \text{H.c.}) + \sum_{i,\sigma} \frac{V_d}{2} \sum_{\langle ij \rangle} \frac{(n_i - \bar{n})}{|\vec{r}_i - \vec{r}_j|} c_{i\sigma}^\dagger c_{i\sigma},
$$

(1)

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is the on-site repulsion that will generate an AF-like SDW order $U$
boundary conditions for
average field approximates to
whereas the pairing attraction involves only the nearest-neighbor. As to the long-range Coulomb interaction term, the sum over $l$ runs over a magnetic unit cell. The long-range Coulomb interaction strength is $V_c = e^2/(2\varepsilon_0 a^2)$ with $\varepsilon_0$, the effective dielectric constant and $a$, the lattice constant. Note added: $V_c$ in our model is a parameter and the form of the long-range Coulomb interaction is settled down (the last term in equation (1)). Fortunately, there seems some room left for the effective dielectric constant that has a general tendency of increasing with hole concentration in HTSCs [18]. Consequently, one can reasonably use a large value of $V_c$ for an underdoped sample, but a small one for the overdoped case. In the presence of a magnetic field $\tilde{H} = \nabla \times \tilde{A}$, the hopping integral can be expressed as $t_{ij} = \tilde{r} \exp[i \frac{\pi}{a} \int_{ij} A \cdot d\tilde{r}]$ with the superconducting flux quantum $\Phi_0 = \hbar c/2e$. Assume each magnetic unit cell of dimension $(N_x \times N_y)a^2 = 48 \times 24a^2$ can accommodate two superconducting vortices. The average field approximates to $B \simeq 24 T$ ($\gg H_c$). Since the internal magnetic field induced by the supercurrent around the vortex core is smaller as compared with the external magnetic field, the screen current effect can be neglected. We then choose a Landau gauge $\tilde{A} = \frac{\tilde{B}}{\tau}(-y, x, 0)$, with $x, y$ as the $x, y$ component of the position vector $\tilde{r}$.

We make use of the translation symmetry property to reduce the $M \times N$-dimensional problem. The Bogoliubov transformation can be expressed as:

$$c_{k_0}^\dagger = \sum_\alpha \left[ u_{k_0}^{\alpha \sigma}(\mathbf{k}) \gamma_{k\alpha\sigma}^+ - u_{k_0}^{\alpha \bar{\sigma}}(\mathbf{k}) \gamma_{k\alpha\bar{\sigma}}^+ \right],$$

$$c_{-k_0\sigma} = \sum_\alpha \left[ u_{k_0}^{\sigma \alpha}(\mathbf{k}) \gamma_{k\alpha\sigma} - u_{k_0}^{\bar{\sigma} \alpha}(\mathbf{k}) \gamma_{k\alpha\bar{\sigma}} \right].$$

For the translation vector $\mathbf{R} = (mN_x a nN_y a)$; here $m$, $n$ are integers; translation operation gives:

$$\Gamma(\Delta(\mathbf{r})) = \Delta(\mathbf{r} + \mathbf{R}) \rightarrow e^{i x(\mathbf{r}, \mathbf{R})} \Delta(\mathbf{r}),$$

and $(u_{k_0\sigma}, v_{k_0\sigma}(\mathbf{r} + \mathbf{R}) \rightarrow e^{i \mathbf{k}_0 \cdot \mathbf{R}}(e^{i x(\mathbf{r}, \mathbf{R})}u_{k_0\sigma}(\mathbf{r}) e^{i x(\mathbf{r}, \mathbf{R})}v_{k_0\sigma}(\mathbf{r}))$ with the phase accumulation $\chi(\mathbf{r}, \mathbf{R}) = 2\pi \tilde{A}(\mathbf{r}) \cdot \mathbf{R}/\Phi_0 - 4mn\pi$. This property sets the periodic boundary conditions for $\Delta$, $u_\sigma(\mathbf{k})$ and $v_\sigma(\mathbf{k})$, and the problem can be reduced to an $N$ dimensional one [15].

We then diagonalize Hamiltonian (1) by solving the Bogoliubov–de Gennes (BdG) equation (3) self-consistently within one magnetic unit cell.

$$\sum_j^N \left( \begin{array}{cc} \mathcal{H}_{ij\sigma} & \Delta_{ij} \\ \Delta_{ij}^* & -\mathcal{H}_{ij\bar{\sigma}} \end{array} \right) \left( \begin{array}{c} u_{ij\sigma}^n \\ v_{ij\sigma}^n \end{array} \right) = \varepsilon_n \left( \begin{array}{c} u_{ij\sigma}^n \\ v_{ij\sigma}^n \end{array} \right),$$

where

$$\mathcal{H}_{ij\sigma} = -t_{ij} + \frac{V_c}{2} \left( c_{i+\delta\sigma}^\dagger c_{j\sigma} + (c_{i+\delta\sigma}^\dagger c_{j\sigma})/\sqrt{2} \right) + \left[ U \langle n_{i\sigma} \rangle - \mu + \frac{V_c}{2} \sum_{l \neq i} \langle n_{l\sigma} \rangle \delta_{ij} \right] d_{ij}$$

and

$$\Delta_{ij} = \frac{V_c}{2} (c_{i\sigma}^\dagger c_{j\bar{\sigma}} - c_{i\bar{\sigma}}^\dagger c_{j\sigma}) - \frac{V_c}{2} (c_{i\sigma}^\dagger c_{j\bar{\sigma}}).$$

Here $\delta = \pm \mathbf{e}_x, \pm \mathbf{e}_y$, and $\mathbf{e}_{x,y}$ denotes the unit vector along the $(x, y)$ direction. The index $i + \delta$ and $i + \sqrt{2}\delta$ are the four nearest and next-nearest neighbors of the $i$th site, respectively. $V_d$ is the coupling strength that describes the electron–electron attractive interaction.

The time-reversal symmetry of equation (3) allows one to find the states in the pair: $(u_{i\sigma}^n, v_{l\bar{\sigma}}^n, \varepsilon_n) \leftrightarrow (-v_{i\bar{\sigma}}^n, u_{l\sigma}^n, -\varepsilon_n)$. Denote the $2N$ dimensional wavefunction vectors
 Samples orders less than the experimental observations of steps is less than 10 chemical potential. Each time the on-site repulsion or the long-range Coulomb interaction is in the nearest-neighbor hopping integral parameter superconductors. Coherence length, respectively, from which the vortex charge is estimated to be by a factor of TF approximation. According to their theory, the screening effect reduces the vortex charges the work of Blatter short coherence length, e.g. HTSCs, is completely neglected. To see this clearly, we refer to between conduction electrons that has shown to be more crucial for superconductors having a only in the long wavelength limit, since the short wavelength part of the Coulomb interaction the TF-type screening is dominant. As is well known, however, the TF approximation is valid the screening effect in the superconducting state of metallic superconductors and showed that screening effect such as the Thomas–Fermi (TF)-type screening should in general be carried out until the relative difference of order parameter between two consecutive iteration steps is less than $10^{-4}$ to achieve the required accuracy.

The screening effect such as the Thomas–Fermi (TF)-type screening should in general be involved in specifying the vortex charge profile in a superconductor. Fetter [19] investigated the screening effect in the superconducting state of metallic superconductors and showed that the TF-type screening is dominant. As is well known, however, the TF approximation is valid only in the long wavelength limit, since the short wavelength part of the Coulomb interaction between conduction electrons that has shown to be more crucial for superconductors having a short coherence length, e.g. HTSCs, is completely neglected. To see this clearly, we refer to the work of Blatter et al [20] who discussed the screening effect within the phenomenological TF approximation. According to their theory, the screening effect reduces the vortex charges by a factor of $(\lambda_{TF}/\xi)^2$, where $\lambda_{TF}$ and $\xi$ are the TF screening length and the superconducting coherence length, respectively, from which the vortex charge is estimated to be $(10^{-4}–10^{-5})e$ ($e$ is the electron charge), using $\xi \sim 30\AA$ and $\lambda_{TF} \sim 1\AA$. This value is unfortunately 2–3 orders less than the experimental observations of $(0.02–0.05)e$ for YBa$_2$Cu$_3$O$_7$ and YBa$_{2-x}$Cu$_x$O$_8$ samples [21], which indicates that the TF screening effect is not as important as it is for metallic superconductors.

In our calculations, the distance is measured in units of the lattice constant $a$, and the energy is in the nearest-neighbor hopping integral parameter $t$. In the extreme limits of $U/V_d \gg 1$ or $U/V_d \ll 1$, the system is in either the SDW state or the pure d-wave superconducting state; whereas the coexistence of the SDW and superconducting orders may occur at intermediate values of $U/V_d$. For concentration, we set $V_d = 1$, the ratio of $U$ to $V_d$ varies in the range of $(2.2–2.4)$. The next-nearest-neighbor hopping $t' = −0.2$ has been chosen to fit the band structure of most cuprate superconductors. The averaged charge density is chosen as $\bar{n} = 0.875$, corresponding to a slightly underdoped level $x = 0.125$. We report on the results for $V_c \sim (0–0.35)$, which corresponds to a static dielectric constant from $\varepsilon_e \rightarrow \infty$ to $\varepsilon_e \sim 15$ for doped cuprate superconductors [22].

First, we discuss the effect of the on-site repulsion $U$ without including the long-range Coulomb interaction. Our numerical results show that the transition from 2D-modulation to

\[ u_i^n = (−v_{i1}^n, u_{i1}^n) \quad \text{and} \quad v_i^n = (u_{i1}^n, v_{i1}^n) \]
stripe SDW and CDW orders occurs when $U$ varies from small to large. In figure 1, we plot the typical spatial profiles of the vortex structure for two types of vortices for $U = 2.2$ and 2.4, respectively: (a) and (d) are for DSC order parameter, (b) and (e) show the staggered magnetization of SDW order that is defined as $M^s_i = (-1)^i \Delta^{\text{SDW}} / U$, and (c) and (f) illustrate the vortex charge density. The left panels (see figures 1(a)–(c)) are for small $U (= 2.2)$. The vortex core is situated at site (12,12), where the DSC order parameter vanishes and the AF order is the strongest. Away from the vortex core the DSC order parameter is modulated. This modulation is considered to be closely related to the appearance of the field-induced AF. Clearly, the DSC, the field-induced SDW and the associated CDW orderings are 2D-modulations with fourfold symmetry, indicating that the vortex structures are 2D in this case. For large $U (= 2.4)$, however, the right panels (see figures 1(d)–(f)) illustrate a $y$-axis-oriented stripe-like structure. The DSC (figure 1(d)) and CDW (figure 1(f)) orders have a modulation period of $6a$, whereas the SDW order in figure 1(e) behaves like an almost uniform stripe oscillating along the $y$-axis with a wavelength of $12a$. The results are in qualitative agreement with the experimental [23] and theoretical [24] results. Note that the halved periodicity of the CDW modulation has been

**Figure 1.** Spatial variations of the DSC order parameter $\Delta^D_i$ ((a) and (d)), staggered magnetization $M^s_i$ ((b) and (e)), and electron density relative to the average density $\delta n = \sum_\sigma n_{i\sigma} - \bar{n}$ ((c) and (f)) in a 24 x 24 lattice. The left panels ((a)–(c)) and right panels ((d)–(f)) are for $U = 2.2$ and 2.4, respectively. The average electron density is fixed at $\bar{n} = 0.875$. 

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Figure 2. Spatial variations of the DSC order parameter $\Delta^D_i$ ((a) and (d)), staggered magnetization $M^s_i$ ((b) and (e)), and electron density relative to the average density $\delta n = \sum n_{i\sigma} - \bar{n}$ ((c) and (f)) in a $24 \times 24$ lattice. The left panels ((a)–(c)) and right panels ((d)–(f)) are for $V_c = 0.05$ and $V_c = 0.15$, respectively. The on-site repulsion and average electron density are fixed at $U = 2.4$ and $\bar{n} = 0.875$.

discussed by Emery et al [25] using the stripe model. In addition, Demler et al [26] argued that it was associated with the ‘Friedel oscillation of the spin gap’. We should mention that the periods of SDW and CDW modulations obtained from the experiments [27] are $8a$ and $4a$ for an optimally doped sample, which could be reproducible from our computations by tuning model parameters such as the on-site repulsion $U$ and/or the chemical potential $\mu$. These results indicate that there exists a critical on-site repulsion strength $U_c$ with a value between 2.2 and 2.4. For $U < U_c$, a spatial distribution with 2D-modulation or a checkerboard-like distribution is presented; whereas, the stripe phase is energetically favored for $U$ beyond $U_c$.

We then investigate the influence of the long-range Coulomb interaction on vortex structures. We checked the $U = 2.4$ case, where the vortex structure with stripe-modulation exists when $V_c \rightarrow 0$. Qualitatively, an involving of the long-range Coulomb interaction seems to weaken the effect of on-site repulsion $U$, due to the competition between the long-range Coulomb interaction term and the on-site repulsion term, as shown in the effective model Hamiltonian (3). Thus, the introduction of the long-range Coulomb interaction is expected to change the vortex structure. The left panels in figure 2 show that the DSC, SDW and CDW
orders remain a quasi-1D structure when the long-range Coulomb repulsion strength is small \( (V_c = 0.05) \). The periodicities of the stripe-modulation for the SDW and CDW orders are still 12\( a \) and 6\( a \), respectively. A close examination revealed that spatial variations for DSC, SDW and CDW orders became slightly sharper compared with those in the right panels of figure 1. For a sufficient strength of the long-range Coulomb interaction, say, \( V_c = 0.15 \), the vortex structures presented in the right panels in figure 2 are fundamentally different from those for \( V_c = 0.05 \), where the 1D stripe modulations have been removed, and a spatial distribution with 2D-modulation or a checkerboard-like distribution appear instead. Noticeably, the size of the vortex core is smaller, which implies that the AF order fluctuation has been confined to a region closer to the core center because the long-range coulomb interaction screened the AF order by expelling electrons outside of the AF-like core. The spatial variations of the staggered magnetization and the vortex charges are presented in figures 2(e) and (f), indicating indeed the ‘1D stripe to checkerboard pattern’ transition compared with those in figures 2(b) and (c). We noticed that the d-wave superconducting order was depressed and the peak charge density at the vortex core center became less in the presence of long-range Coulomb interaction. With further increase in the strength of the long-range Coulomb interaction \( V_c \), the 2D-structure or the checkerboard pattern nature remains. In order to see more clearly, figure 3 shows the 2D density plots of the 3D plots in figure 2 in a 72 × 72 lattice. These results show the possible existence of the checkerboard pattern vortex for some underdoped cuprate superconductors with strong on-site repulsion. We would like to point out that this is in no conflict with the common consensus that a strong on-site repulsion should induce an AF-like SDW with stripe modulation, since the amplitude of the AF order had been dramatically reduced due to the existence of a competing long-range Coulomb interaction. The above results seem to be consistent with the STM experiments for underdoped samples [7].

Note added: one might argue that the SDW and CDW orders with 2D-modulations or the checkerboard pattern can be attributed to a superposition of \( x \)- and \( y \)-oriented stripe phases. We can prove that these two phases are exactly degenerated in energy only when there are no asymmetrical fluctuations in the system. This implies an in-plane field such as a magnetic field or a dc-bias field would break down their degeneracy. Therefore, the observed checkerboard pattern in the STM experiments for samples [7] is most likely associated with the screening of the AF order.

In the following, we plot the local density of states (LDOS) in figure 4, which is defined by

\[
\rho_i(E) = \frac{1}{M_x M_y} \sum_{n,k}^{2N} \left( |u_i^{n,k}|^2 f'(E_n - E) + |v_i^{n,k}|^2 f'(E_n + E) \right),
\]

where \( f'(E) \) is the derivative of the Fermi distribution function. \( \rho_i(E) \) is proportional to the local differential tunneling conductance which could be measured by low-temperature STM experiments, and the summation is averaged over \( M_x \times M_y \) wavevectors in first Brillouin zone. The LDOS as a function of energy have been calculated at the vortex core center (solid line) and at the midpoint (red dashed line) between two nearest neighbor vortices along the \( x \) direction for \( V_c = 0, 0.05 \) and 0.15, respectively. As can be seen from figure 4(a), the presence of the AF order in the vortex core provides a mechanism for splitting of the zero-bias conductance peak into two local peaks at the core center. The LDOS at the midpoint between two nearest-neighbor vortices does not, however, display these features, implying that the AF order is localized around the core center [3]. Hence, the states associated with these two peaks have been referred to as the
Figure 3. 2D density plots of the 3D plots in figure 2. The DSC order parameter $\Delta^D_i$ ((a) and (d)), staggered magnetization $M^S_i$ ((b) and (e)), and electron density relative to the average density $\delta n = \sum_{\alpha} n_{\sigma i} - \bar{n}$ ((c) and (f)) in a $72 \times 72$ lattice. The left panels ((a)–(c)) and the right panels ((d)–(f)) are for $V_c = 0.05$ and $V_c = 0.15$, respectively. The on-site repulsion and average electron density are fixed at $U = 2.4$ and $\bar{n} = 0.875$.

AF-like VCS [5]. Noticeably, the peak splitting is found to decline, accompanied by somewhat weakening of the AF order inside the core, when the long-range Coulomb repulsion enhances, as shown in figures 4(b) and (c). In figure 4(c), the calculated LDOS at the vortex center (see inset) seemed to be in agreement with the STM experiments on BSCCO, regarding the VCS peak locations and energy-dependence of the LDOS [4].

In summary, the influence of the on-site repulsion $U$ and the long-range Coulomb interaction on vortex structures has been investigated by numerically studying the BdG equations based on an effective model Hamiltonian with competing AF and d-wave superconducting orders and long-range Coulomb interaction in a 2D lattice. We showed that vortex structure transition between the 2D and 1D stripe modulations can occur by tuning the on-site repulsion and the long-range Coulomb interaction strength. A large on-site expulsion seems to favor the stripe-modulation. The effect of the long-range Coulomb interaction on the
Figure 4. The LDOS as a function of energy with various strengths of long-range Coulomb interaction $V_c = 0$ (a), $V_c = 0.05$ (b) and $V_c = 0.15$ (c). The solid line is at the vortex core center, and the red dashed line is at the midpoint between two nearest-neighbor vortices along the $x$-direction. The inset is the details of the line shape near zero bias at the core center. The two arrows point to the VCS. The on-site repulsion and average electron density are fixed at $U = 2.4$ and $\bar{n} = 0.875$. The wave vectors in the first Brillouin zone are $M_x \times M_y = 24 \times 24$.

vortex structures was examined. We found that the 1D stripe-like vortex structure for large $U$ would change to the checkerboard pattern, accompanying a depressed and screened SDW order, when a sufficient strength of long-range Coulomb interaction had been involved. Consequently, experiments [4, 7] are well understood when the long-range Coulomb interaction has been taken into account.

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