Charged vortex structure in high-temperature superconductors*

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By using a model Hamiltonian with competing antiferromagnetic (AFM) spin density wave (SDW) and d-wave superconductivity orders, the effect of next-nearest-neighbour (nnn) hopping on spin and charge structures in high-temperature superconductors is investigated at finite temperatures. For an optimally doped sample, we find that the AFM order magnitude in the vortex core is firstly enhanced and then suppressed, accompanied with a "positively $\rightarrow$ negatively $\rightarrow$ positively" charged vortex structure transition with increasing nnn hopping strength, which implies that the AFM order is unnecessarily bounded to an electron-rich vortex core. In addition, a charge ordering pattern with four negatively charged peaks localized in a small region is also found around the vortex core centre without net charge. Recent scanning-tunneling-microscopy experimental observations of the checkerboard structure are hopefully understood.

Keywords: vortex charge, next-nearest-neighbouring hopping, Bogoliubov-de Gennes equation

PACC: 7420M, 7460E

1. Introduction

Intensive efforts have been focused on the vortex structure in high-temperature superconductors (HTSCs) for the past several years. Neutron scattering experimental observations of a peculiar static stripe phase in $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$ by Tranquada *et al.*[1] supported that spatial modulations of spin and charge density are related to superconductivity. Nuclear magnetic resonance (NMR) experiments on $YBa_2Cu_3O_{7-x}$ (YBCO) probed a strong antiferromagnetic (AFM) fluctuation around vortex cores, implying the possible existence of spin density wave (SDW) order outside the vortex core.[2] Recently, a striking feature has been revealed in the scanning-tunneling-microscopy (STM) experiments by Hoffman *et al.*,[3] where a Cu–O bond-oriented four-unit-cell checkerboard pattern is localized in a small region near vortex cores in slightly overdoped $Bi_2Sr_2CaCu_2O_{8+x}$ (BSCCO), which confirmed the coexistence of static charge modulation (or the charge density wave (CDW)) and superconductivity. Howald *et al.*[4] reported that the similar vortex-induced checkerboard modulations can survive even at zero magnetic field. In particular, the suppressions of the thermal conductivity of $La_{2-x}Sr_xCuO_4$ single crystals may be relevant to the field-enhanced charge and spin ordering.[5] Theoretically, SDW orders with two-dimensional (2D)[6−8] or stripe[9,10] modulations have been presented to understand checkerboard patterns observed experimentally. It was also found that the effects of magnetic impurities[11] and the Peierls instability due to d-wave pairing[12] can lead to the inhomogeneous phase with stripe and checkerboard modulations. In particular, the checkerboard pattern was attributed to a superposition of x- and y-axes-oriented stripe modulations of the CDW, 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. So, one needs to explore the physical mechanisms that would respond to the recent observations of the checkerboard pattern.

In addition, the charged vortex in superconductors[13−25] has attracted considerable attention. In general, it was recognized that spatially inhomogeneous chemical potential in connection with superconducting condensation can result in a charge redistribution around vortex cores, that is, vortex cores are charged up.[13,14] Kumagai *et al.* reported the experimental evidence for the presence of vor-

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tex charges in $YBa_2Cu_3O_7$ and $YBa_2Cu_4O_8$ high-temperature superconductors (HTSCs) by NMR and nuclear quadrupole resonance methods.[15] Various methods, such as the Ginzburg–Landau theory,[16] coupled Bernoulli and Poisson equations,[17] the Bogoliubov-de Gennes (BdG) model[18−23] were then presented to understand the experimental results. An effective mean-field Hubbard model without considering the next-nearest-neighbour (nnn) hopping effect has been proposed by Chen *et al.*[18] and they had predicted that the vortex charge is mainly determined by the competition of AFM order with d-wave superconducting (DSC) order. A negatively charged vortex for optimally doped samples is predicted due to the AFM order contribution,[18] whereas positive vortex charges for underdoped samples can be observed even through the AFM order which remains strong due to the nnn hopping effect.[23] Therefore, it is necessary to demand a deeper understanding of the correlation between the AFM order and the electronic structure of the vortex core.

In view of these points, together with the facts that (i) in the Hubbard model, or the closely related t-J model, which is believed to describe well the low-energy physics of cuprates, the electron–hole asymmetry can be understood by taking into account the finite nnn hopping,[26−28] and, (ii) the ratio between nearest- and next-nearest-neighbour hopping is a main electronic parameter characterizing different cuprate families,[29,30] we introduce the nnn hopping in the effective model Hamiltonian for HTSCs with competing DSC and AFM orders in this work, and investigate the effect of nnn hopping on the spin and charge structures in optimally doped HTSCs at finite temperature T by numerically solving the Bogoliubov-de Gennes equations. We find that the AFM order magnitude in the vortex core is firstly enhanced and then suppressed, accompanied by a "positively → negatively → positively" charged vortex transition with increasing nnn hopping strength. We believe that the AFM order is unnecessarily bounded to an electron-rich vortex core. In addition, around the vortex centre without net charge, an interesting charge ordering pattern with four negatively charged peaks localized in a small region is found.

The rest of the paper is organized as follows. In Section 2 we present our theoretical model and give the necessary formalism. The effect of nnn hopping on the spin and charge structures in optimally doped HTSCs is discussed in Section 3. Our results are summarized in Section 4.

2. Theoretical approach

We use 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 competing AFM order and the nearest-neighbour attraction V for the DSC pairing

$$\begin{aligned} H = & -\sum_{\langle ij\rangle,\sigma} t_{ij}\exp(\mathrm{i}\varphi_{ij})c^{\dagger}_{i\sigma}c_{j\sigma} \\ & +\sum_{i,\sigma}(U\langle n_{i\bar{\sigma}}\rangle-\mu)c^{\dagger}_{i\sigma}c_{i\sigma} \\ & +\sum_{\langle ij\rangle}(\Delta_{ij}c^{\dagger}_{i\uparrow}c^{\dagger}_{j\downarrow}+\Delta^{*}_{ij}c_{j\downarrow}c_{i\uparrow}), \end{aligned} \tag{1}$$

where $t_{ij}=t$ and t' are the nearest and next-nearest neighbour hopping integrals, respectively; $c_{i\sigma}$ ($c^{\dagger}_{i\sigma}$) is destruction (creation) operator for electron of spin σ, $n_{i\sigma}=c^{\dagger}_{i\sigma}c_{i\sigma}$ is the number operator, and μ is the chemical potential determining the averaged electron density $\bar{n}=(1/N_xN_y)\sum_{i,\sigma}\langle n_{i\sigma}\rangle$ ($N_x\times N_y$ with $N_x=2\times N_y$ is the linear dimension of the unit cell of the vortex lattice). Our study is confined to the hole-doped system ($\bar{n}<1$), i.e., the hole doping $\delta=1-\bar{n}$. The Peierl's phase factor is given by $\varphi_{ij}=\pi/\Phi_0\int_{r_i}^{r_j}\boldsymbol{A}(\boldsymbol{r})\mathrm{d}\boldsymbol{r}$ with the superconducting flux quantum $\Phi_0=hc/2e$. We choose the Landau gauge $\boldsymbol{A}(\boldsymbol{r})=(-By/2,Bx/2,0)$, and assume each magnetic unit cell can accommodate two superconducting vortices. The SDW and DSC orders have the following definitions respectively: $\Delta^{\mathrm{SDW}}_{i}=U\langle c^{\dagger}_{i\uparrow}c_{i\uparrow}-c^{\dagger}_{i\downarrow}c_{i\downarrow}\rangle$ and $\Delta_{ij}=V\langle c_{i\uparrow}c_{j\downarrow}-c_{i\downarrow}c_{j\uparrow}\rangle/2$. Using Bogoliubov transformation, $c_{i\sigma}=\sum_n[u^n_{i\sigma}\gamma_{n\sigma}-\sigma v^{n*}_{i\sigma}\gamma^{\dagger}_{n\bar{\sigma}}]$, the mean-field Hamiltonian (1) can be diagonalized by solving the resulting Bogoliubov-de Gennes (BdG) equations self-consistently,

$$\sum_{j}^{N}\begin{pmatrix}\mathcal{H}_{ij\sigma} & \Delta_{ij}\\ \Delta^{*}_{ij} & -\mathcal{H}^{*}_{ij\bar{\sigma}}\end{pmatrix}\begin{pmatrix}u^n_{j\sigma}\\ v^n_{j\bar{\sigma}}\end{pmatrix}=E_n\begin{pmatrix}u^n_{i\sigma}\\ v^n_{i\bar{\sigma}}\end{pmatrix}, \tag{2}$$

where $\mathcal{H}_{ij\sigma}=-t_{ij}+(U\langle n_{i\bar{\sigma}}\rangle-\mu)\delta_{ij}$. With the periodic boundary conditions we can obtain the N positive eigenvalues (E_n) with eigenvectors ($u^n_{i\uparrow},v^n_{i\downarrow}$) and negative eigenvalues ($\bar{E_n}$) with eigenvectors ($-v^{n*}_{i\uparrow},u^{n*}_{i\downarrow}$). The self-consistent conditions are

$$\langle n_{i\uparrow}\rangle=\sum_{n=1}^{2N}|\boldsymbol{u}^n_{i}|^2f(E_n), \tag{3}$$

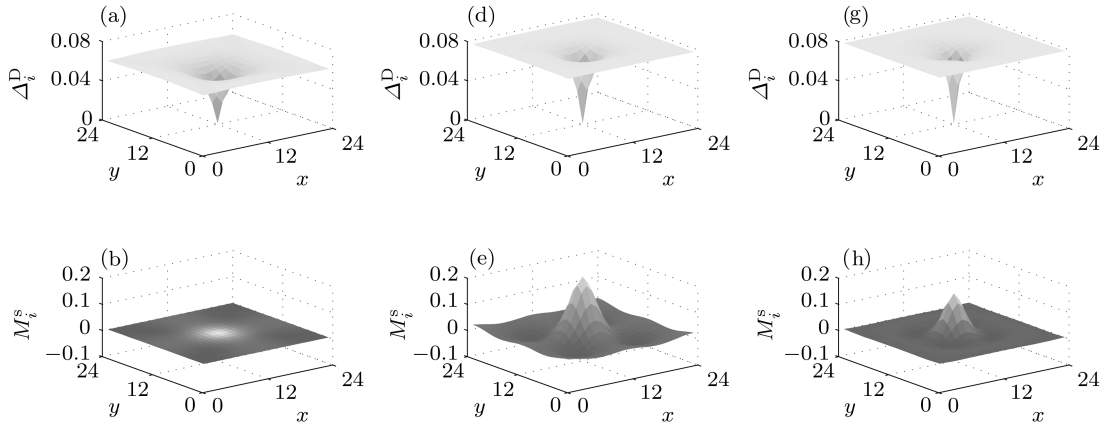
$$\langle n_{i\downarrow}\rangle=\sum_{n=1}^{2N}|\boldsymbol{v}^n_{i}|^2[1-f(E_n)], \tag{4}$$

$$\Delta_{ij} = \sum_{n=1}^{2N} \frac{V}{4} (\boldsymbol{u}_i^n \boldsymbol{v}_j^{n*} + v_i^{n*} u_j^n) \tanh\left(\frac{E_n}{2k_{\rm B}T}\right), \quad (5)$$

where $u_i^n = (-v_{i\uparrow}^{n*}, u_{i\uparrow}^n)$ and $v_i^n = (u_{i\downarrow}^{n*}, v_{i\downarrow}^n)$ are the row vectors, and $f(E) = (\mathrm{e}^{E/k_{\rm B}T} + 1)^{-1}$ is the Fermi–Dirac distribution function. The DSC order parameter is defined at site i as $\Delta_i^{\rm D} = (\Delta_{i+e_x,i}^{\rm D} + \Delta_{i-e_x,i}^{\rm D} - \Delta_{i,i+e_y}^{\rm D} - \Delta_{i,i-e_y}^{\rm D})/4$, where $\Delta_{ij}^{\rm D} = \Delta_{ij} \exp[\mathrm{i}\pi/\Phi_0 \int_{r_i}^{(r_i+r_j)/2} \boldsymbol{A}(\boldsymbol{r}) \mathrm{d}\boldsymbol{r}]$, and $\boldsymbol{e}_{\boldsymbol{x},\boldsymbol{y}}$ denotes the unit vector along the (x, y) direction. In our calculation, the distance is measured in units of the lattice constant a, and the energy is in the nearest-neighbour hoping integral parameter t. The related parameters are chosen as $V = 1.0$, and $N_x \times N_y = 48 \times 24$ which corresponds to the average field $B \approx 24$ Tesla ($\gg H_{\rm c1}$).

3. Numerical results

First we choose the parameter values, $U = 2.0$, $T = 0.03$, and an optimal doping $\delta = 0.15$. Figure 1 plots the spatial profiles of the DSC order parameter [(a), (d) and (g)], staggered magnetization [(b), (e) and (h)] and electron density [(c), (f) and (i)] in a 24×24 lattice. Here, the staggered magnetization of the induced AFM or SDW order is defined as $M_i^{\rm s} = (-1)^i \Delta_i^{\rm SDW}/U$. The vortex centre is situated at site (12,12), where the DSC order parameter vanishes. The left panels in Fig. 1 [Fig. 1(a) to 1(c)] are for the nnn hopping integrals $t' = 0$, where the AFM order is extremely weak ($|m| < 10^{-4}$) and the vortex charge is positive (hole-rich). The middle panels in Fig. 1 [Fig. 1(d) to 1(f)] are for $t' = -0.15$. The AFM order is enhanced remarkably around the vortex cores, which expulses the holes from the vortex core into the bulk of the superconductor and the vortex becomes negatively (electron-rich) charged. In contrast to the case for $t' = 0$, the SDW order exists both inside and outside the vortex cores, and exhibits a weak oscillating behaviour with the wavelength $8a$ along both x and y directions. The periodicity of the field-induced SDW modulation can be closer inspected using a Fourier transform.[6] We should mention that the period ($8a$) of SDW modulation could be obtained from our computations by tuning model parameters such as the on-site repulsion U and/or the chemical potential μ. Interestingly, further increasing nnn hopping strength $|t'|$ ($= 0.3$) the AFM order which exists both inside and outside the vortex core decreases slightly, and the size of the AFM core is smaller [see Fig. 1(h)], impliying that the AFM order fluctuation has been confined to a region closer to the core centre because a stronger nnn hopping effect may screen the AFM order by expelling electrons out of the AFM core. Consequently, the core charge changes sign from negative to positive despite that the AFM order magnitude remains strong [see Fig. 1(i)], which is in agreement with our previous studies[23] for the underdoped sample where the experimental observations[15] of a positively charged vortex may be understood. So, we believe that the AFM order is unnecessarily bounded to an electron-rich vortex core. In addition, the temperature effect on the charged vortices is also briefly examined (not shown here). In contrast with the middle panels of Fig. 1, we can draw the same conclusion that the transition of "negatively → positively" charged vortex can occur with increasing T even though the AFM order remains large. Noticeably, compared with Fig. 1(h), the modulation and the core size of the AFM order in Fig. 1(e) are almost unchangeable with increasing T except that the AFM order magnitude becomes smaller.



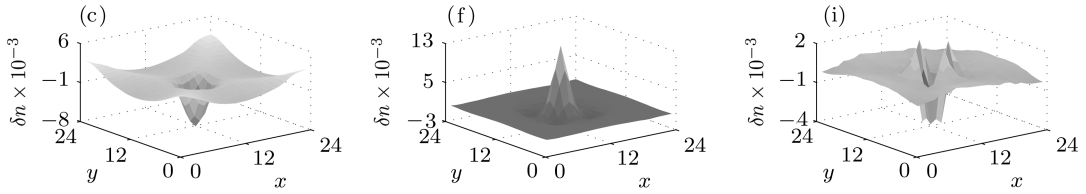


Fig. 1. Spatial variations of the DSC order parameter $\Delta_i^{\rm D}$ [(a), (d) and (g)], staggered magnetization $M_i^{\rm s}$ [(b), (e) and (h)] and electron density relative to the average density $\delta n = \sum_\sigma n_{i\sigma} - \bar{n}$ [(c), (f) and (i)] in a 24×24 lattice. The left panels [(a)–(c)], middle panels [(d)–(f)] and right panels [(g)–(i)] are for $t' = 0$, –0.15 and –0.3, respectively. The averaged electron density is fixed at $\bar{n} = 0.85$, and the strength of the on-site repulsion $U = 2.0$, and $T = 0.03$.

In Fig. 2, we present the local density of states (LDOS) spectra corresponding to Fig. 1. The LDOS of the energy E at the position i can be written as

$$\rho_{\boldsymbol{i}}(E) = -\sum_{n=1}^{2N}[|\boldsymbol{u}_{\boldsymbol{i}}^n|^2 f'(E_n - E) + |\boldsymbol{v}_{\boldsymbol{i}}^n|^2 f'(E_n + E)], \tag{6}$$

where $f'(E)$ is the derivative of the Fermi distribution function, $\rho_{\boldsymbol{i}}(E)$ is proportional to the local differential tunneling conductance which could be measured by low-temperature STM. The LDOS as a function of energy has been calculated at the vortex core centre (solid line) and at the midpoint (dot-dotted line) between two nearest-neighbour vortices along the x direction for t'=0 (a), –0.15 (b) and –0.3 (c). As can be seen from Fig. 2(a), when $t' = 0$ for which the extremely weak AFM order is induced, the LDOS at the core centre shows a single resonant peak around the Fermi energy, which is similar to that reported in Ref. [31]. When $|t'|$ is sufficiently large (= 0.15) so that the AFM gap develops inside the vortex core, the resonant peak near the zero bias is suppressed and splits into two weak peaks [see Fig. 2(b)], which agrees qualitatively with the result of Ref. [32]. The LDOS at the midpoint between two nearest-neighbour vortices does not, however, display these features, implying that the AFM order is localized around the core centre. Noticeably, the peak splitting is found to decline, accompanied by weakening of the AFM order inside the core, when the nnn hopping strength is further increased, as shown in Fig. 2(c).

Note added: The absence of the zero-bias peak in the scanning tunneling spectrum at the core centre has also been explained by the properties of the c-axis tunneling matrix elements for a particle–hole symmetric system.[33] It was shown that the pseudogap feature of the tunneling conductance at the core centre is mainly due to the suppression of the tunneling current of low-energy quasiparticles by the anisotropic c-axis hopping integral.

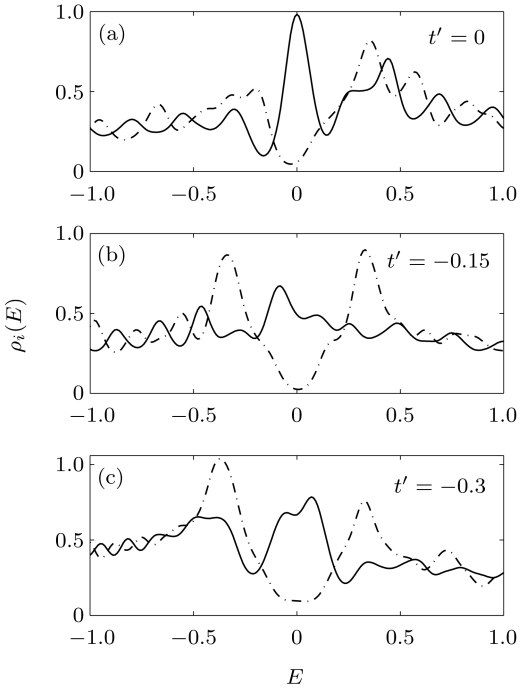


Fig. 2. The LDOS as a function of energy with various strengths of nnn hopping $|t'| = 0$ (a), 0.15 (b) and 0.3 (c). The solid line is at the vortex core centre, and the dot-dotted line is at the midpoint between two nearest-neighbour vortices along the x-direction. The other parameter values are the same as Fig. 1.

From the spatial profiles of the DSC order in Figs. 1(a), 1(d) and 1(g), we notice that the vortex size is reduced with increasing nnn hopping strength. Meanwhile, four negatively charged satellite peaks show up around the positively charged vortex core in Fig. 1(i). Next we perform the calculation for $U = 2.1$, $t' = -0.35$, $T = 0.05$, and the spatial variations the left panels as well as the contour plots the right panels of the electron density [(a) and (b)] and staggered magnetization [(c) and (d)] are presented

in Fig. 3. It is clear that a charge ordering pattern with four negatively charged peaks also appears [see Fig. 3(a)], whereas there exist no net charges in vortex centre [see Fig. 3(b)]. We also checked the case for $t' = -0.15$, and a negatively charged AFM core [similar to Figs. 1(e) and 1(f)] is exhibited (not shown here). For the stronger $|t'| = 0.35$, the AFM order is frustrated and sharpened [see Figs. 3(c) and 3(d)]. We believe that an increased nnn hopping strength can suppress and screen the AFM order, which can lead to the electron depletion inside the vortex core. Hence, the single negatively charged peak of charge order changes to four lower negatively charged peaks with four-fold symmetry which are localized in a small region around the vortex core. Our results can provide a clue to interpret the recent STM experimental observations[3] regarding the checkerboard structures in HTSCs.

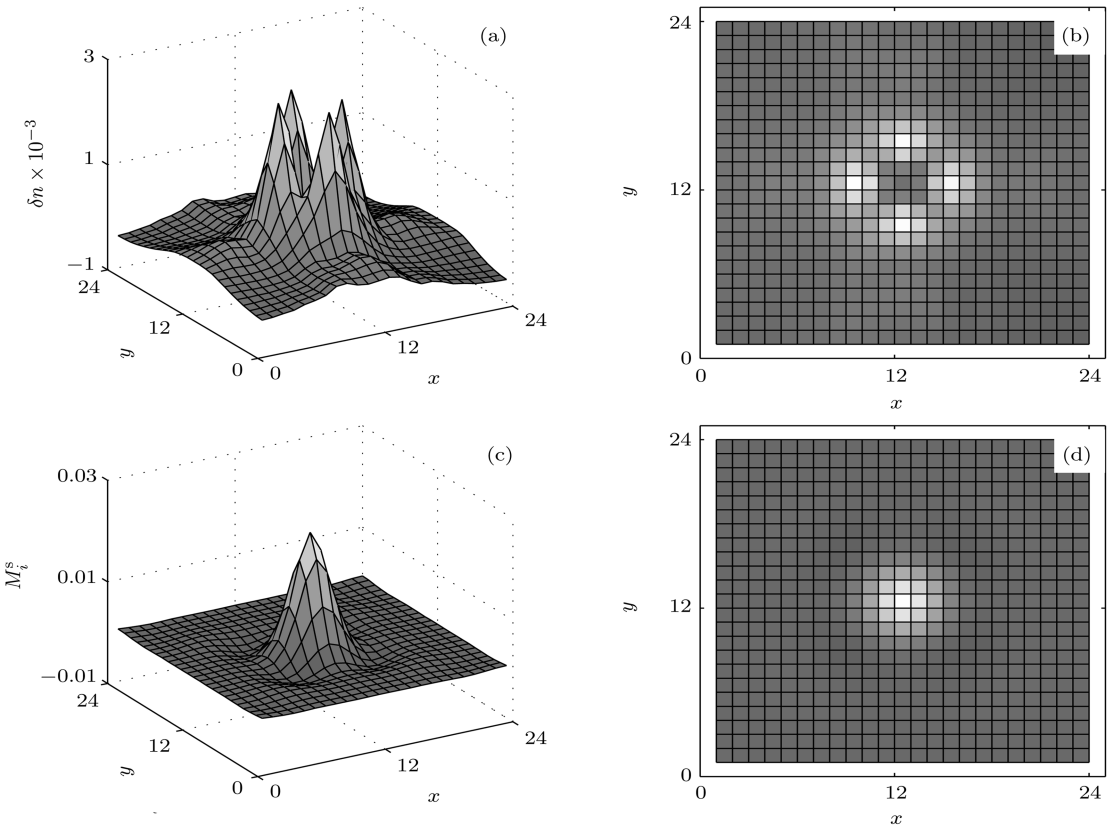


Fig. 3. Spatial variations and contour plots of the electron density relative to the average density $\delta n = \sum_\sigma n_{i\sigma} - \bar{n}$ [(a) and (b)] and staggered magnetization [(c) and (d)] in a 24×24 lattice. The parameter values are: $\bar{n} = 0.85$, $U = 2.1$, $T = 0.05$ and $t' = -0.35$.

4. Conclusions

In conclusion, the influence of the nnn hopping on the spin and charge orders around superconducting vortices for optimally doped HTSCs at finite T has been investigated by numerically solving the Bogoliubov-de Gennes equations based on an effective model Hamiltonian with competing AFM and DSC interactions. We showed that the AFM order magnitude in the vortex core is firstly enhanced and then suppressed, accompanied by a "positively → negatively → positively" charged vortex transition with increasing nnn hopping strength. We believe that the AFM order is unnecessarily bounded to an electron-rich vortex core. In addition, around the vortex centre without net charge, it was found an interesting charge ordering pattern with four negatively charged peaks localized in a small region. The recent STM experimental observations regarding the checkerboard structures are hopefully understood when the nnn hopping effect is taken into account.

Finally, we would like to emphasize that the effect due to the spin fluctuations is not considered in the present mean-field theory. The magnetic field induced AFM long range order may not be stable and could

break into short ranged AFM domains. Although our self-consistent BdG calculation tends to overestimate the stability of the SDW phase, the qualitative features of our results should still be valid, particularly in view of their favorable comparisons with experiments.

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