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Local density of states maps of cuprate superconductors with field-induced charge order

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Using the $t-t'-U-V$ Hamiltonian, the local density of state (LDOS) maps have been numerically obtained near the optimal doping around the vortex core for several different bias energies. With proper chosen U, we show that magnetic field induces spin-density wave (SDW) and charge-density wave (CDW), which are absent at zero field, with periods $8a$ and $4a$ respectively. It is also found that the LDOS maps may not necessarily coincide with those of CDW or the d-wave superconductivity order parameter near the vortex core. This is because the LDOS measures the low lying excitations of the system while the CDW configuration is originated from its ground state. We point out that our energy dependent LDOS maps could be used to explain the STM experiments by J. Hoffman *et al.* [Science **295**, 466 (2002)] and S. H. Pan *et al.* [Phys. Rev. Lett. **85**, 1536 (2000)].

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In hole-doped cuprate superconductors, the interplay between the d-wave superconductivity (dSC) and antiferromagnetic (AF) order has been studied extensively in the literature. Inelastic neutron scattering experiments showed the presence of incommensurate spin structures in LSCO (Ref. 1) with a spatial periodicity $8a$ in the presence of a magnetic field. In addition, NMR imaging experiments on YBCO observed a strong AF fluctuation outside the vortex[2] indicating the possible existence of spin-density-wave (SDW) gap outside the vortex core. The STM experiment by Hoffman *et al.*[3] seems to confirm the coexistence of static charge modulation and superconductivity in BSCCO under a magnetic field. The authors reported that a four unit cell checkerboard pattern is localized in a small region around the vortex. All these experiments indicate that the AF fluctuations could be pinned by vortex cores and they could form static SDW/charge-density-wave (CDW)-like modulations in certain samples of cuprate superconductors. Theoretically, a number of works proposed that the observed checkerboard patterns could be explained by SDW order with the two-dimensional (2D)[4–6] or stripe[7–9] modulations. Both the 2D- and stripe-SDW orders induced by the magnetic field (B) are well known to have accompanying CDW modulations. In particular, the checkerboard pattern has been attributed to the superposition of stripe modulations of the CDW[7,10] oriented along x and y directions. In all these studies, the experimental STM spectra have been directly interpreted in terms of a CDW order pinned by the vortex cores. On the other hand, the CDW order represents the charge density configuration in the ground state while the STM spectrum or the spatial profile of the local density of states (LDOS map) is determined by the behavior of the low-energy excitations in the system. It is therefore important to understand the difference between these two quantities in the presence of vortex cores. This issue has not been addressed in the literature, and thus is the main purpose of the present paper.

Based on the phenomenological $t-t'-U-V$ model defined in a 2D lattice and the Bogoliubov–de Gennes' equations, we study the interplay between the dSC and the competing AF order in a sample close to the optimal doping. First, the phase diagrams for the coexistence between these two orders as a function of U/V in both zero and finite magnetic field B are discussed. We then use two different values of U/V (=2.39 and 2.44) to simulate the experiment of Pan *et al.*[11] in which no static charge order was detected, and the experiment of Hoffman *et al.*[3] where the checkerboard pattern was observed near the vortex core. In the presence of a strong B, the case for U/V (=2.39) will generate SDW/CDW-like modulations with four-fold symmetry while a larger U/V (=2.44) would make the induced SDW/CDW have stripe-like modulations with the periodicity $8a/4a$. When the bias energy E is below that of the vortex core state, our result for U/V (=2.39) shows that the LDOS map near the vortex core is of the "circular" symmetry, not the four-fold symmetry expected for the CDW or the dSC order parameter around a vortex core for dSC. This is consistent with the experiment in Ref. 11. Assuming the x- and y-oriented stripe modulations are both present in the time interval when the experiment is performed, our results for U/V (=2.44) are in good agreement with the observations in Ref. 3. In addition, we have predictions which will be presented near the end of the present paper.

We start with a mean-field $t-t'-U-V$ Hamiltonian in the mixed state by assuming that the on-site repulsion U is responsible for the competing AF order and the nearest-neighbor attraction V causes the d-wave superconducting pairing:

$$\mathbf{H} = -\sum_{\mathbf{ij}\sigma} t_{\mathbf{ij}} c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + \sum_{\mathbf{i}\sigma} (U\langle n_{\mathbf{i}\bar{\sigma}}\rangle - \mu) c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{i}\sigma} + \sum_{\mathbf{ij}} (\Delta_{\mathbf{ij}} c^{\dagger}_{\mathbf{i}\uparrow} c^{\dagger}_{\mathbf{j}\downarrow} + \Delta^{*}_{\mathbf{ij}} c_{\mathbf{j}\downarrow} c_{\mathbf{i}\uparrow}), \quad (1)$$

where $t_{\mathbf{ij}}$ is the hopping integral, μ is the chemical potential, and

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

where $\mathcal{H}_{\mathbf{ij}\sigma} = -t_{\mathbf{ij}} + (U\langle n_{\mathbf{i}\sigma}\rangle - \mu)\delta_{\mathbf{ij}}$ and $t_{\mathbf{ij}} = \langle t_{\mathbf{ij}}\rangle e^{i\varphi_{\mathbf{ij}}}$. The Peierl's phase factor $\varphi_{\mathbf{ij}} = \pi/\Phi_0 \int_{r_{\mathbf{i}}}^{r_{\mathbf{j}}} \mathbf{A}(\mathbf{r}) \cdot d\mathbf{r}$, with the superconducting flux quantum $\Phi_0 = hc/2e$. Within the Landau gauge $\mathbf{A(r)} = (-By, 0, 0)$, each magnetic unit cell can accommodate two superconducting vortices. The vortex carries a flux quantum Φ_0 and is located at the center of a square area containing $N_x/2 \times N_y$ sites where $N_x = 2 \times N_y$. Here, we choose the nearest-neighbor hopping $\langle t_{\mathbf{ij}} \rangle = t = 1$ and the next-nearest-neighbor hopping $\langle t_{\mathbf{ij}} \rangle = t' = -0.25$ to match the curvature of the Fermi surface for most cuprate superconductors. The exact diagonalization method to self-consistently solve BdG equations with the periodic boundary conditions is employed to get the N positive eigenvalues (E_n) with eigenvectors $(u^n_{\mathbf{i}\uparrow}, v^n_{\mathbf{i}\downarrow})$ and negative eigenvalues $(\bar{E}_n)$ with eigenvectors $(-v^{n*}_{\mathbf{i}\uparrow}, u^{n*}_{\mathbf{i}\downarrow})$. The self-consistent conditions are

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

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

$$\Delta_{\mathbf{ij}} = \sum_{n=1}^{2N} \frac{V}{4} (\mathbf{u}^n_{\mathbf{i}} \mathbf{v}^{n*}_{\mathbf{j}} + \mathbf{v}^{n*}_{\mathbf{i}} \mathbf{u}^n_{\mathbf{j}}) \tanh\left(\frac{\beta E_n}{2}\right), \tag{3}$$

where $\mathbf{u}^n_{\mathbf{i}} = (-v^{n*}_{\mathbf{i}\uparrow}, u^n_{\mathbf{i}\uparrow})$ and $\mathbf{v}^n_{\mathbf{i}} = (u^{n*}_{\mathbf{i}\downarrow}, v^n_{\mathbf{i}\downarrow})$ are the row vectors, and $f(E) = 1/(e^{\beta E} + 1)$ is the Fermi-Dirac distribution function. Since the calculation is performed near the optimally doped regime, the filling factor, $n_f = \Sigma_{\mathbf{i}\sigma} \langle c^\dagger_{\mathbf{i}\sigma} c_{\mathbf{i}\sigma} \rangle / N_x N_y$, is fixed to be 0.85, i.e., hole doping $\delta = 0.15$. Each time when the on-site repulsion U is varied, the chemical potential μ needs to be adjusted.

In the limit of $U/V \ll 1$, the system is in the state of pure dSC. In the opposite limit $U/V \gg 1$, the system is the SDW states. However, the most anomalous properties of cuprate superconductors do not correspond to these extreme limits, but are in the intermediate case where both the SDW and the SC may coexist. In order to simplify our discussion of the ratio of U to V, we set $V = 1.0$. In Fig. 1(a), in the absence of a magnetic field,the staggered magnetization $(M_{\mathbf{i}})$ or the SDW shows either the stripe modulation or the uniform distribution with $M_{\mathbf{i}} = 0$ in the background of dSC depending upon the magnitude of U. For $U > U_{c1}$, $M_{\mathbf{i}}$ exhibits the stripe modulation with periodicity of $8a$ (a is the lattice constant). On the other hand, for U less than U_{c1}, it shows the uniform distribution which is equivalent to the state of pure dSC. It should be noted that a two-dimensional (2D) SDW modulation can never be obtained for $B = 0$ in the present self-consistent calculation. The transition between the SDW-stripe modulation and the uniform distribution seems to be discontinuous. In Fig. 1(b), in the presence of a magnetic field, $M_{\mathbf{i}}$ (solid line) displays the stripe modulation, the 2D SDW, or the uniform distribution depending on U. As U is greater than U_{c1}, the stripe modulation in the zero field would be *slightly enhanced* under a magnetic field (Stripe$_{(I)}$). In the region of $U_{c2} < U \leq U_{c1}$, the field induced $M_{\mathbf{i}}$ shows a stripe modulation which disappears in the zero field (Stripe$_{(II)}$). For $B \neq 0$, the transition between stripe$_{(I)}$ and stripe$_{(II)}$ is not apparent and only the slope shows a weak discontinuity. When $U \leq U_{c2}$, the field induced AF order changes from the stripe-like to a 2D SDW. If U goes far below 2.3, the AF order could be completely suppressed both inside or outside the vortex core. The transition between the stripe modulation and the 2D SDW is sharp and appears to be of first order. Of course, it could be possible that all the transitions are of second order if more points in the transition region were calculated. Accompanying the stripe-like AF order is a CDW with the stripe modulation of the period $4a$. At the same time the dSC order parameter also acquires a CDW-like stripe modulation. In Fig. 1(b), the staggered magnetization (open circles) at the vortex core center seems to be weakly U dependent.

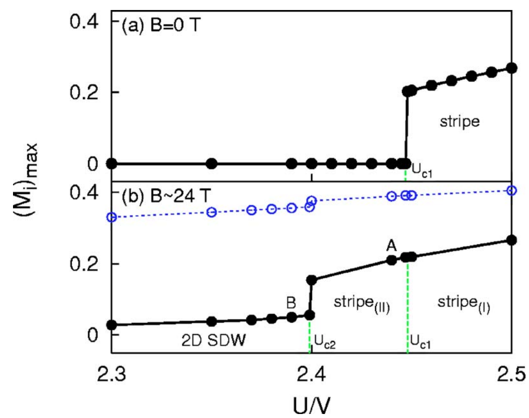

FIG. 1. (Color online) The maximum value of the staggered magnetization in the zero-field (a), and in the finite field (b). In (b), the open circle and the solid circle represent the (maximum) staggered magnetization at the center of the vortex core and away from the vortex cores, respectively. Stripe$_{(I)}$ is the region where the stripe modulations are intrinsic and stripe$_{(II)}$ corresponds to the region where the stripe modulations are field-induced. The size of the unit cell is $N_x \times N_y = 48 \times 24$ correspoding to a magnetic field $B \sim 24T$.

In the following, $U_A = 2.44$ and $U_B = 2.39$ are chosen for our study of the LDOS. Both of these U values would not generate the SDW/CDW order for nearly optimally doped cuprate superconductors when $B = 0$. In order to understand the characteristics between the two cases, we start with the LDOS formula

$$\rho_{\mathbf{i}}(E) = -\frac{1}{M_x M_y} \sum_{n,\mathbf{k}}^{2N} [|\mathbf{u}^{n,\mathbf{k}}_{\mathbf{i}}|^2 f'(E_{n,\mathbf{k}} - E) + |\mathbf{v}^{n,\mathbf{k}}_{\mathbf{i}}|^2 f'(E_{n,\mathbf{k}} + E)], \tag{4}$$

where $\rho_{\mathbf{i}}(E)$ is proportional to the local differential tunneling conductance as measured by STM experiment at zero temperature, and the summation is averaged over $M_x \times M_y$ wave vectors in first Brillouin zone.

The LDOS as a function of energy have been calculated at the vortex core center (solid line) and at site far away from the vortex (dashed line) for U_A and U_B; the results are respectively given in Figs. 2(a) and 2(b). There the spatial profiles of the field induced CDW modulations are presented in Fig. 2. For U_A, the field induced CDW has the stripe-like structure which extends over the whole magnetic unit cell with a period $4a$, while for U_B, the CDW modulation be-

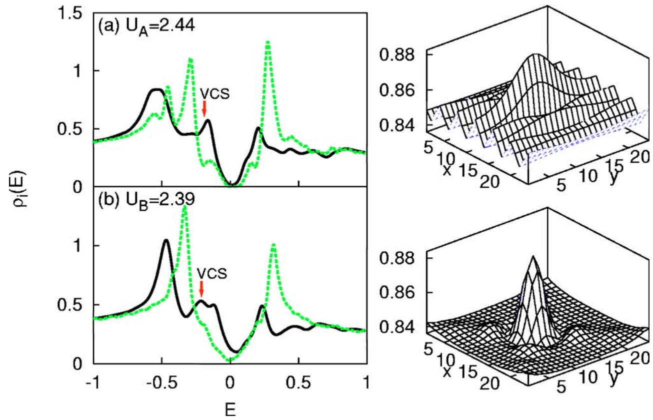

FIG. 2. (Color online) The LDOS as a function of energy, left panel, at the vortex core center for (a) $U_A=2.44$, (b) $U_B=2.39$. The solid line is at the vortex core center, and the dashed line is at the site far away from the vortex. The arrow points to the vortex core states (VCS). The spatial profiles of the corresponding CDW are shown in the right panels. The wave vectors in first Brillouin zone are $M_x \times M_y = 24 \times 24$.

comes two dimensional with four-fold symmetry. Since the SDW gap develops inside the vortex core, the resonance peak appearing in the LDOS (Ref. 13) near the zero bias in a pure dSC at the core center is suppressed and splits into two peaks.[14] This feature can be seen in Fig. 2. Furthermore, STM experiments on YBCO (Ref. 12) and BSCCO (Ref. 11) measured the double peaks structure within the maximum superconducting gap. The states associated with these two peaks have been referred to as the vortex core states. In Fig. 2, those vortex core states with negative energies are centered at $E_A=-0.19$ with a width $\Delta E_A=0.08$ and $E_B=-0.21$ with $\Delta E_B=0.04$ for U_A and U_B, respectively.

Because the energy dependence of the LDOS at the vortex center does not make any clear distinction between U_A and U_B, we examine the LDOS maps, which are the LDOS with fixed energy at each site of the magnetic unit cell, at various energies, and we look for their differences. In Fig. 3, the LDOS maps have been calculated at energies ranging from 0.0 to −0.4 with $\delta E=0.01$ decrements. For $U_A=2.44$, as the energy is far below the vortex core states (VCS) and close to the zero bias, the pattern in Fig. 3(a) shows that the stripe structure with periodicity $4a$ is strongly localized near the vortex core, and its strength drops dramatically away from the vortex. When the energy is near the VCS, such as in Fig. 3(b), the stripe modulation in the LDOS extends over the whole unit cell, similar to the feature in CDW in Fig. 2(a). If the bias voltage goes above or becomes more negative than the VCS, such as in Fig. 3(c), the stripe modulation is still extensive, but the intensities inside the vortex core are lesser than those outside the vortex core. Thus neither the STM spectra nor the LDOS maps have all the features of the CDW. For $U_B=2.39$, as the energy is far below the vortex core states (VCS) [see Fig. 3(e)], the LDOS map shows a *circular* bump with the size of a vortex core. When the energy is near the VCS, such as in Fig. 3(f), the LDOS shows a distribution with rather weak oscillations, and its feature is not quite similar to that of the CDW in Fig. 2(b). If the energy is above the VCS, such as in Fig. 3(g), the modulation pattern clearly displays four-fold symmetry.

However, the STM images obtained experimentally[3] are results of integrating the spectral density between energies E_1 and E_2, which is defined as

$$S(E_1,E_2) = \sum_{E_1}^{E_2} \rho_{\mathbf{i}}(E)\,\delta E. \tag{5}$$

There E_1 is taken to be 0 and E_2 has been set near the energy of the VCS below the chemical potential. In Fig. 3(d), the integrated spectrum $S(0.0,-0.23)$ of the LDOS maps is obtained by summing the LODS from E_1 to E_2 with an energy spacing 0.01. It shows that the intensity of the stripe modulations is predominantly concentrated near the vortex core and decays rapidly away from the vortex. This feature originates from the behaviors of the LDOS maps at energies with magnitudes smaller than those of the VCS [see Fig. 3(a)]. Since the LDOS maps display the properties of the *eigen-*

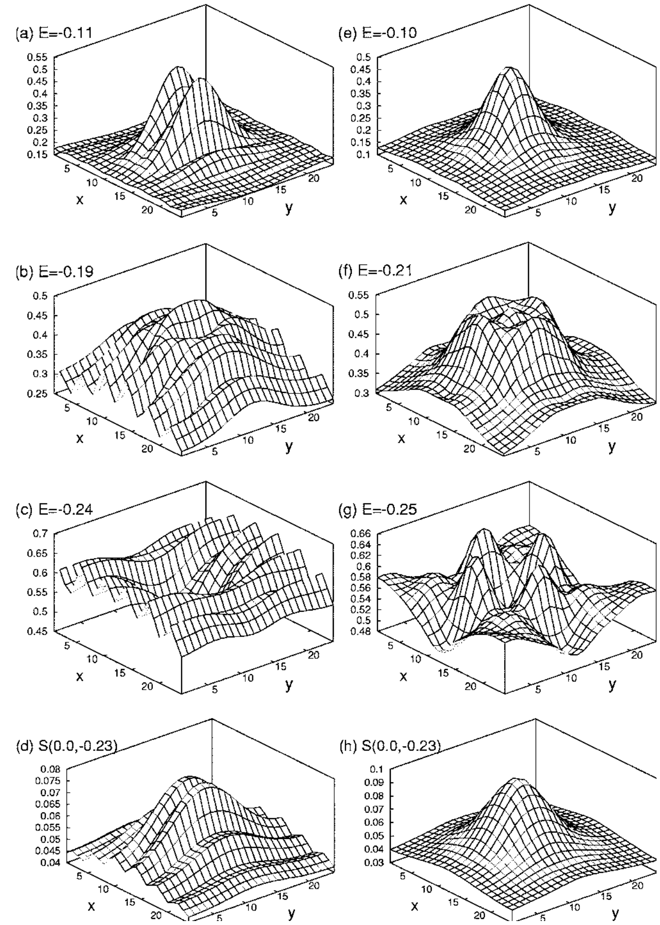

FIG. 3. The LDOS maps are at energies (a) and (e)—close to the zero bias, (b) and (f)—near the VCS, and (c) and (g)—above the VCS. The integrated spectrum of LDOS $S(E_1,E_2)$ of (d) and (h) are from the Fermi energy to the upper bound of the VCS, i.e., $S(0.0,-0.23)$. The left and right panels are for $U_A=2.44$ and $U_B=2.39$, respectively. The wave vectors in first Brillouin zone are $M_x \times M_y = 6 \times 6$.

function at the energy E, the checkerboard pattern observed by the experiments could be explained in terms of the superposition of the degenerate eigenfunctions describing the stripe modulations along x and y directions. Moreover, when the numerical calculation is performed by using the boundary condition $\exp(i\phi)$, both x- and y-oriented stripes are able to be generated. If we average the eigenfunction over randomly chosen ϕ, the checkerboard pattern is obtained. All these behaviors are in good agreement with the experiments.[3] We expected that the qualitative features obtained for U_A should still remain even if $U > U_{c1}$ and the stripe phase is intrinsic rather than magnetic field induced (see Fig. 1). In Fig. 3(h), the integrated spectrum of the LDOS maps for U_B exhibits a *circular* bump over the vortex core region which is different from that of the CDW shown in Fig. 2(b). For a sample without the stripe modulations (U_B=2.39), the integrated LDOS maps near the vortex core seem to be rather round and do not possess the strong four-fold symmetry as expected for a dSC.[14] This feature is also consistent with the STM experimental measurements[11] provided that the samples used there is different from that of Ref. 3.

Here it should be noted that our self-consistent calculation is performed on a 48×24 magnetic unit cell which is the best currently possible, and is within the limitation of theapplied simulation technique. The value of V=1 used for the attractive interaction between electrons at nearest neighboring sites may be too large; we shall look into how our results will be affected if a smaller V is chosen. In addition, the LDOS structure may also be changed by the resonant scattering of different layers[15] in the cuprate sample. All these are going to be investigated, and the results published in the future. Furthermore, the effect due to the spin fluctuations is not considered in the present mean field theory; the magnetic field induced AF long range order may not be stable and could break into short ranged AF domains.

In conclusion, two values of U are employed to calculate the LDOS maps. For U_B=2.39, the spatial profile of the CDW order around the vortex must have the four-fold symmetry. Then the question is whether this four-fold symmetry could be seen by STM experiments. The experiments in Ref. 11 detected only a "circular"-like symmetry, not the expected four-fold symmetry around the vortex with the bias energy E smaller than those of VCS. This result is consistent with our LDOS image [see Figs. 3(e) and 3(f)]. Here we predict that four-fold symmetry is observable only when a bias energy E larger than those of VCS is applied [see Fig. 3(g)]. For U_A =2.44, extended charge order induced by the magnetic field is present in the sample. If the bias energy E is smaller than those of VCS, the checkerboard pattern appears to be rather localized near the vortex core. This is consistent with the experiments in Ref. 3. We also predict that the pattern will be spreading away from the vortex core if E becomes larger than the energies of the vortex states [see Fig. 3(c)]. We further predict that the periodicity of the charge order observed by the experiments in Ref. 3 should be E independent and the STM image depends critically on E.

Note added. After the paper was submitted for publication, we noticed that in the report by Levy *et al.*,[16] the authors found that the measured peak at $(1/4a,0)\pi$ in their Fig. 4(a) does not disperse in the presence of a magnetic field. This result indicates that the charge order is induced by the magnetic field which is consistent with our present prediction.

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