Spin and Charge Order around Vortices and Impurities in High-T_c Superconductors

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A comparative study is made for the spin and charge structure around superconducting vortices and unitary impurities, by solving self-consistently an effective Hamiltonian including interactions for both antiferromagnetic spin-density wave (SDW) and d-wave superconducting orderings. Around vortices, we show the induction of an SDW two-dimensionally modulated with a period of eight lattice constants ($8a_0$) and an associated charge-density wave (CDW) with a period of $4a_0$, which explains very well recent experimental observations. In the case of unitary impurities, an SDW modulation with identical periodicity, but without an associated CDW, is also predicted.

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The main research theme of high-T_c superconducivity mechanism centers on how to establish the connection between antiferromagnetic (AF) and d-wave superconducting (DSC) orderings, i.e., whether they exclude each other, or coexist microscopically. The interplay between these two orderings can be explored by weakening the superconductivity in the optimally or slightly overdoped regime. Recent inelastic neutron scattering (INS) measurements on optimally doped $La_{2-x}Sr_xCuO_4$ (LSCO) samples by Lake and co-workers provide the first evidence of the field-induced magnetic order [1]. The field-induced spin fluctuations are found to have a spatial periodicity of $8a_0$ with the wave vector pointing along the Cu-O bond directions. The principle magnetization oscillations in the vortex state are coherent over a distance $L_M > 20a_0$, substantially longer than the superconducting coherence length ξ_0 ($\sim 5a_0$). The field-induced enhancement of the Bragg peak intensity was also observed more recently in the elastic neutron scattering (ENS) measurement on underdoped LSCO samples by Lake *et al.* [2], and on a related material, La_2CuO_{4+y} (LCO), by Khaykovich *et al.* [3], both with $L_M > 100a_0$, indicating the existence of the field-induced static AF order of $8a_0$ periodicity. Strong AF fluctuations have also been observed by Mitrovic *et al.* [4] in a high-field nuclear magnetic resonance (NMR) imaging experiment on near-optimally doped $YBa_2Cu_3O_{7-x}$ (YBCO). Complementarily, the scanning tunneling microscopy (STM) imaging by Hoffman *et al.* [5] has revealed the quasiparticle states around the vortex cores in slightly overdoped $Bi_2Sr_2CaCu_2O_{8+x}$ (BSCCO) as a Cu-O bond-oriented "checkboard" pattern with $4a_0$ periodicity. Thus, the periodicity ($4a_0$) of charge modulation is one-half of that ($8a_0$) of the field-induced spin density wave (SDW) modulation. Theoretically, Demler and co-workers proposed a phenomenological model [6] to argue that the halved periodicity of the static CDW modulation is associated with the "Friedel oscillation of the spin gap." Within the SO(5) theory [7], Hu and Zhang [8] showed that the vortex-induced AF region can be greater than ξ_0, due to the light effective mass of the dynamic AF fluctuations at optimal doping. In these two kinds of work, the $8a_0$ periodicity of the magnetic modulation is not fully understood due to the phenomenological nature of the models. Distinctly, stripe models [9–13] predict that the spin modulation of wavelength λ in cuprates should be associated with the charge modulation of wavelength $\lambda/2$. However, two-dimensional modulation is apparent in the STM imaging [5]. In this Letter, by using an effective microscopic mean-field model for the competition between the AF and DSC orderings [14,15], we present a comprehensive study of the spin/charge structure around the vortices and nonmagnetic unitary impurities in optimally doped high-T_c superconductors. We show for the first time microscopically the induction around vortices of an SDW two-dimensionally modulated with a period of $8a_0$ and an associated CDW with a period of $4a_0$. These results are in good agreement with the INS [1] and STM [5] observations. Also significantly, we predict that an SDW order modulated with identical periodicity can be induced around nonmagnetic unitary impurities. Neutron scattering experiments can directly test this prediction.

We consider a t-U- V Hubbard model defined on a two-dimensional (2D) square lattice, in which the onsite repulsion is solely responsible for the antiferromagnetism while the nearest-neighbor attraction causes the d-wave superconductivity [14]. The effective mean-field Hamiltonian can be written as

$$H = -\sum_{ij,\sigma} t_{ij} e^{i\varphi_{ij}} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i,\sigma} (U n_{i,\bar{\sigma}} + \epsilon_i - \mu) c_{i\sigma}^\dagger c_{i\sigma} + \sum_{ij} (\Delta_{ij} c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger + \Delta_{ij}^* c_{j\downarrow} c_{i\uparrow}) . \quad (1)$$

Here $c_{i\sigma}$ annihilates an electron of spin σ at the ith site. $t_{ij} = t$ and t' are the nearest and next-nearest neighbor hopping integrals, respectively. U is the strength of on-site repulsion. $n_{i\sigma} = \langle c_{i\sigma}^\dagger c_{i\sigma} \rangle$ is the electron density with spin σ. The quantity ϵ_i is the single-site potential describing the scattering from impurities. μ is the chemical potential. $\Delta_{ij} = \frac{V}{2}\langle c_{i\uparrow}c_{j\downarrow} - c_{i\downarrow}c_{j\uparrow}\rangle$ is the spin-singlet d-wave bond order parameter, where V is the strength of nearest-neighbor attraction. With the application of an external magnetic field $\mathbf{H}$, the Peierls phase factor is given by the integral $\varphi_{ij} = \frac{\pi}{\Phi_0}\int_{\mathbf{r}_j}^{\mathbf{r}_i} \mathbf{A}(\mathbf{r}) \cdot d\mathbf{r}$, where $\Phi_0 = hc/2e$ is the superconducting flux quantum and $\mathbf{A} = \nabla \times \mathbf{H}$ is the vector potential.

The above Hamiltonian can be diagonalized by solving self-consistently the Bogoliubov-de Gennes equation:

$$\sum_j \begin{pmatrix} \mathcal{H}_{ij,\sigma} & \Delta_{ij} \\ \Delta_{ij}^* & -\mathcal{H}_{ij,\bar{\sigma}}^* \end{pmatrix} \begin{pmatrix} u_{j\sigma}^n \\ v_{j\bar{\sigma}}^n \end{pmatrix} = E_n \begin{pmatrix} u_{i\sigma}^n \\ v_{i\bar{\sigma}}^n \end{pmatrix}, \quad (2)$$

subject to the self-consistency conditions for the electron density and the DSC order parameter: $n_{i\uparrow} = \sum_n |u_{i\uparrow}^n|^2 f(E_n)$ and $n_{i\downarrow} = \sum_n |v_{i\downarrow}^n|^2[1 - f(E_n)]$, where $f(E) = 1/[e^{E/k_BT} + 1]$ is the Fermi distribution function, and $\Delta_{ij} = \frac{V}{4}\sum_n(u_{i\uparrow}^n v_{j\downarrow}^{n*} + v_{i\downarrow}^{n*} u_{j\uparrow}^n)\tanh(\frac{E_n}{2k_BT})$. In Eq. (2), the single particle Hamiltonian reads $\mathcal{H}_{ij,\sigma} = -t_{ij}e^{i\varphi_{ij}} + (Un_{i\bar{\sigma}} + \epsilon_i - \mu)\delta_{ij}$. We report results below for two cases at zero temperature. For the Abrikosov vortex state, the magnetic field effects enter through φ_{ij} and no impurities are introduced ($\epsilon_i = 0$). For the effects of a single impurity, we set $\mathbf{A} = 0$ so that $\varphi_{ij} = 0$. Hereafter we measure the length in units of the lattice constant a_0 and the energy in units of t. To mimic a holelike Fermi surface, as relevant to the hole-doped cuprates, we take $t' = -0.2$. The pairing interactions are taken to be $V = 1.0$. Since both INS [1] and STM [5] experiments were performed in the optimal or slightly overdoped regime, we choose the filling factor $n_f = \sum_{i,\sigma} n_{i\sigma}/N_xN_y = 0.83$ (i.e., the hole doping $n_h = 0.17$), where N_x, N_y are the linear dimension of the unit cell under consideration. The BdG Eq. (2) is solved self-consistently with an exact diagonalization method. We have considered the values of $U = 2.2$ and 2.5. In the absence of magnetic field and impurities, we find two types of solution at $n_h = 0.17$: (i) A vanishingly small AF SDW and homogeneous DSC; (ii) A uniaxial stripe, where both the SDW and DSC are modulated along the x direction. The first configuration has the energy lower by 10^{-6}/site than the latter [16]. Therefore, we take the homogeneous DSC phase as the initial condition for iteration. This choice is consistent with the INS observation on optimally doped LSCO [1] that no zero-field AF spin signal exists at low temperatures.

Field-induced SDW and CDW.—When an external magnetic field is applied perpendicular to the 2D Cu-O plane, $\mathbf{H} = H\hat{\mathbf{z}}$ ($H_{c1} \ll H \ll H_{c2}$), an Abrikosov vortex state is formed. It is assumed that the superconductor is in the extreme type-II limit so that the screening effect from the supercurrent is negligible. Within a Landau gauge, the vector potential as given by $\mathbf{A} = (-Hy, 0, 0)$ determines φ_{ij} uniquely. By taking the strength of magnetic field, $H = 2\Phi_0/N_xN_y$, such that the flux enclosed by each unit cell is twice Φ_0, the BdG equation (2) is solved with the aid of the magnetic Bloch theorem [15]:

$$\begin{pmatrix} u_{\mathbf{k},\sigma}(\mathcal{T}_{mn}\tilde{\mathbf{r}}) \\ v_{\mathbf{k},\sigma}(\mathcal{T}_{mn}\tilde{\mathbf{r}}) \end{pmatrix} = e^{i\mathbf{k}\cdot\mathbf{R}} \begin{pmatrix} e^{i\chi(\mathbf{r},\mathbf{R})/2}u_{\mathbf{k},\sigma}(\tilde{\mathbf{r}}) \\ e^{-i\chi(\mathbf{r},\mathbf{R})/2}v_{\mathbf{k},\sigma}(\tilde{\mathbf{r}}) \end{pmatrix}. \quad (3)$$

Here $\tilde{\mathbf{r}}$ is the position vector defined within a given unit cell, the vector $\mathbf{R} = mN_x\hat{\mathbf{e}}_x + nN_y\hat{\mathbf{e}}_y$, $\mathbf{k} = \frac{2\pi l_x}{M_xN_x}\hat{\mathbf{e}}_x + \frac{2\pi l_y}{M_yN_y}\hat{\mathbf{e}}_y$ with $l_{x,y} = 0, 1, \ldots, M_{x,y} - 1$ are the wave vectors defined in the first Brillouin zone of the vortex lattice, M_xN_x and M_yN_y are the linear dimension of the whole system, and the phase $\chi(\mathbf{r}, \mathbf{R}) = \frac{2\pi}{\Phi_0}\mathbf{A}(\mathbf{R}) \cdot \mathbf{r} - 4mn\pi$. In the calculation, we consider a single magnetic unit cell of size $N_x \times N_y = 48 \times 24$. The numerics shows that each unit cell accommodates two superconducting vortices each carrying a flux quantum Φ_0, which conforms to the above prescription for the magnetic field strength. The unit cell is equally partitioned between these two vortices, each located at the center of a square area having $\frac{N_x}{2} \times N_y$ sites, indicative of a square vortex lattice. Typical results on the structure around one vortex core with $U = 2.5$ are displayed in Fig. 1, where the left column is three-dimensional plots and the right column is contour plots. As

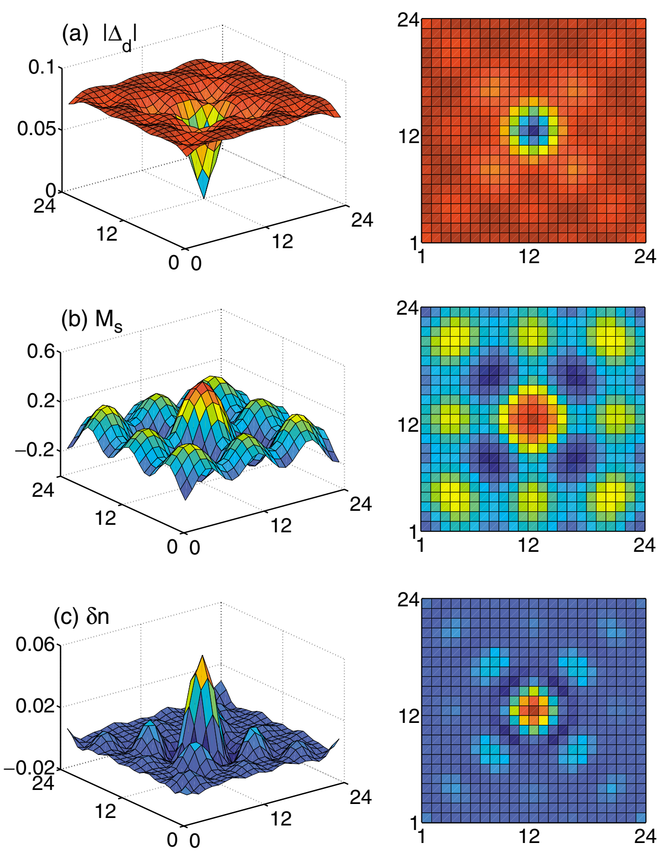

FIG. 1 (color). The spatial distribution of the d-wave SC order parameter $|\Delta_d|$ (a), the staggered magnetization M_s (b), and the electron density $\delta n = \sum_\sigma n_{i\sigma} - n_f$ (c) around one vortex located at the center of an area of 24×24 sites. The size of the whole magnetic cell is 48×24. Parameter values: $t' = -0.2$, $U = 2.5$, $V = 1$, and $n_f = 0.83$.

shown in Fig. 1(a), the DSC order parameter vanishes at the core center and approaches its zero-field value, which is about $\Delta_0 = 0.08$ for the chosen parameter values, away from the core center. The DSC order parameter is not uniform beyond the distance ξ_0 away from the core center. Instead, it is weakly modulated. The maximum modulation amplitude is less than $0.05\Delta_0$. This modulation is closely related to the appearance of the field-induced SDW, as we now discuss. Figure 1(b) displays the spatial distribution of the staggered magnetization of the local SDW order defined as $M_s = (-1)^i(n_{i\uparrow} - n_{i\downarrow})$. Clearly, the maximum strength of M_s is pinned at the vortex core center. This AF SDW order exhibits a modulation pattern with the satellite peaks and valleys regularly spaced throughout the unit cell along the Cu-O bond directions. The modulation pattern of the SDW implies a much longer magnetic correlation length as compared to ξ_0, which is consistent with the INS measurements [1]. The appearance of the SDW order around the vortex core also strongly affects the electron density $n_i = \sum_\sigma n_{i\sigma}$. As shown in Fig. 1(a), at the vortex core center, where the SDW amplitude reaches the global maximum, the electron density is strongly enhanced. In addition, the charge density also exhibits regular modulation. By comparing the spatial distribution of the DSC order parameter with the field-induced SDW as well as the associated CDW, one finds that when the absolute amplitude ($|M_s|$) of SDW reaches a local maximum, the associated CDW also reaches a local maximum, while the DSC order parameter has a local minimum. For a closer inspection of the periodicity of the SDW and associated CDW modulation, we perform a Fourier transform of these two quantities. As shown in Fig. 2(a), the strongest spectral intensity of the SDW modulation occurs at the wave vectors $\mathbf{k} = 2\pi(\frac{3}{24}, 0)$ and $\mathbf{k} = 2\pi(0, \frac{3}{24})$, which gives the period of approximately $8a_0$ along the Cu-O bond directions. To verify this point, we have performed a calculation on a unit cell of size $N_x \times N_y = 52 \times 26$, and found that the period of the SDW modulation remains $8a_0$, supporting the periodicity of the field-induced SDW modulation as an intrinsic property. For $U = 2.2$, the amplitude of the SDW is a little reduced, but the periodicity of the modulation is unchanged. Therefore, the periodicity of the SDW modulation observed in the INS measurement [1] is very well explained [17].

Impurity-induced SDW and CDW.—The d-wave superconductivity can also be suppressed locally by a strong nonmagnetic impurity. The effects of impurities on superconductors have been of theoretical and experimental interest even in their own right for some time. In view of the recent observations of the AF magnetism around the vortex core, it is important to explore whether a similar spin and charge structure can also be induced around an impurity. We perform the numerical calculation on a unit cell of $N_x \times N_y = 36 \times 36$ sites. The single-site potential is taken to be $\epsilon_0 = 100$ at the unitary impurity site and zero otherwise. Since $\varphi_{ij} = 0$ in this case, a periodic boundary condition is used. The results for the spatial distribution of the three orderings with $U = 2.5$ are displayed in Fig. 3. The DSC order parameter is depressed dramatically at the impurity site and approaches the bulk value at the scale ξ_0. Beyond this range, almost no modulation of the DSC order parameter is seen. The induced staggered moment of the

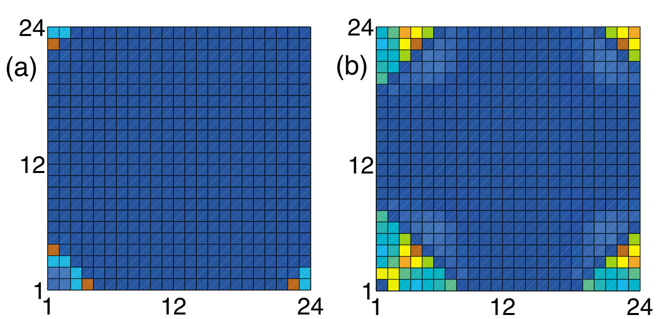

FIG. 2 (color). The Fourier spectrum of the spatial modulation of the spin-density M_s (a) and the charge-density δn (b) around the vortex. Parameter values are the same as in Fig. 1.

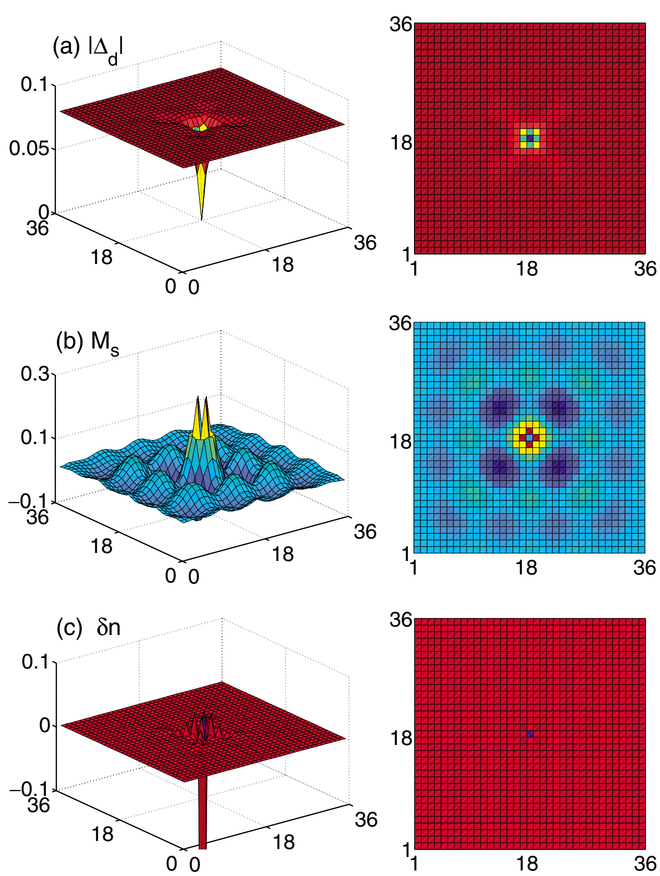

FIG. 3 (color). The spatial distribution of the d-wave SC order parameter $|\Delta_d|$ (a), the staggered magnetization M_s (b), and the electron density $\delta n = n_i - n_f$ (c) around a nonmagnetic unitary impurity ($\epsilon_0 = 100$) located at the center of the unit cell of 36×36 sites. Parameter values are the same as in Fig. 1.

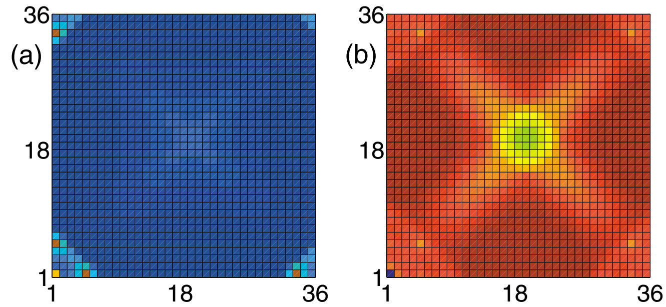

FIG. 4 (color). The Fourier spectrum of the spatial modulation of the spin-density M_s (a) and the charge-density δn (b), around a nonmagnetic unitary impurity. Parameter values are the same as in Fig. 3.

SDW is zero at the impurity site and has maxima on the four nearest-neighbor Cu sites of the impurity. Away from the impurity, the induced SDW shows a modulation very similar to the vortex case, though with a much weaker amplitude [18]. However, the electron density, which is zero at the impurity, exhibits only a Friedel-like oscillation within a limited range around the impurity. The Fourier spectrum, as shown in Fig. 4, gives a clear picture: The main modulation period of the SDW is about $8a_0$; the CDW is modulated with a period of approximately $2a_0$, which is roughly the Fermi wave length. Therefore, the correspondence between the SDW and CDW is absent in the impurity case. The reason lies in the fact that the CDW is very sensitive to the strong impurity scattering. This result is consistent with the STM measurements in BSCCO [19] that show no evidence for the CDW modulation with a period of $4a_0$ around the impurities. However, SDW appears to be a robust feature induced by the impurity, which should be observable in neutron scattering experiments. Nuclear magnetic resonance (NMR) measurements have shown that when a Cu^{2+} in the Cu-O plane is substituted by a strong nonmagnetic impurity, such as Zn^{2+}, an effective magnetic moment can be induced on the Cu sites around the impurity site [20–23]. More recent NMR measurements [23] show for the first time that near-optimal doping, the Kondo screening effect observed above the superconducting transition temperature, is strongly reduced in the superconducting state. This indicates the stabilization of the magnetic moments. Our result that the strongest staggered magnetic moment is on the four nearest-neighbor Cu sites of the impurity is consistent with the above experiment [23]. This leads us to speculate that the magnetism around vortices and around impurities may share a common origin.

In conclusion, we have studied the spin and charge order around vortices and nonmagnetic unitary impurities. In the case of vortices, the experimentally observed $8a_0$ period of the SDW modulation is explained for the first time based on a microscopic model. The correspondence between the SDW and CDW modulations has also been established. Around the unitary impurity, we have also shown the existence of the SDW modulation with a period of $8a_0$, which can be tested by neutron scattering experiments.

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