Incommensurate Magnetism around Vortices and Impurities in High-\(T_c\) Superconductors

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By solving self-consistently an effective Hamiltonian including interactions for both antiferromagnetic (AF) and \(d\)-wave superconducting (DSC) phases controlled by the doping—At low temperatures, the AF order of the parent compounds is replaced by a DSC order upon doping. The main theme of high-\(T_c\) superconductivity research centers on how to establish the connection between these two kinds of orderings, i.e., whether they exclude each other, or coexist microscopically. In one of the strategies, the interplay between the AF and DSC ordering is explored by weakening the superconductivity in the optimally or slightly overdoped regime. The inelastic neutron scattering (INS) measurements on both optimally doped and underdoped La_{2−x}Sr_xCuO_4 (LSCO) samples by Lake and co-workers provide the first evidence of the field-induced magnetic order. The field-induced spin fluctuations have a spatial periodicity of 8\(a_0\) 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 \(\xi_0\) (\(≈ 5a_0\)).

The field-induced enhancement of the Bragg peak intensity was also observed by Khaykovich et al. in the elastic neutron scattering (ENS) measurement on a related material, La_2CuO_4+y (LCO), but with \(L_M > 100a_0\), indicating the existence of the field-induced static AF order of 8\(a_0\) periodicity. Strong AF fluctuations have also been observed by Mitrovic et al. in a high-field nuclear magnetic resonance (NMR) imaging experiment on near-optimally doped YBa_2Cu_3O_{7−x} (YBCO). More recently, the scanning tunneling microscopy imaging by Hoffman et al. has revealed the quasiparticle states around the vortex cores in slightly overdoped Bi_2Sr_2CaCu_2O_{8+\delta} (BSCCO) a Cu-O bond-oriented “checkboard” pattern with 4\(a_0\) periodicity. The periodicity (4\(a_0\)) of charge modulation is one half of that (8\(a_0\)) of the field-induced SDW modulation. Theoretically, Demler and co-workers, by focusing their attention on the far-field regions outside the vortex core, proposed a phenomenological model that when the superconductivity is weakened by the circulating currents caused by the vortices, a coexisting SDW plus DSC phase appears surrounding the core; more recently they also argued that the halved periodicity of the static CDW modulation is associated with the “Friedel oscillation of the spin gap”. As an extension of earlier work within the SO(5) theory, originally suggesting an AF insulating region inside the core, Hu and Zhang showed that the vortex-induced AF region can be greater than \(\xi_0\), due to the light effective mass of the dynamic AF fluctuations at optimal doping. In these two cases, the 8\(a_0\) periodicity of the magnetic modulation is not fully understood due to the phenomenological nature of the models. Distinctly, stripe models predict that the spin modulation of wavelength \(λ\) in cuprates should be associated with the charge modulation of wavelength \(λ/2\). However, two dimensional modulation is apparent in the STM image.

One of us and C.S. Ting have applied an effective microscopic mean-field model accounting for the competition between the AF and DSC orderings to successfully explain the peak-split structure around the Fermi surface in the local density of states (LDOS) at the vortex core center. Nevertheless, due to the use of the simplest band structure parameter values, the spin and charge modulation is too weak for the determination of the periodicity. In this work, using realistic model parameter values, 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 find, for the first time, microscopically: (i) For the vortex case, the oscillation periods of the SDW and the associated CDW are indeed 8\(a_0\) and 4\(a_0\), respectively, in good agreement with the INS and STM experiments. (ii) Around the nonmagnetic unitary impurity, the modulation of the SDW order still ex-
hibits $8a_0$ periodicity. However, the charge density shows only the Friedel oscillation with a period of the Fermi wavelength due to the strong potential scattering from the impurity.

Consider a minimal model defined on a two-dimensional (2D) lattice square, in which the on-site repulsion is solely responsible for the antiferromagnetism while the nearest neighbor attraction causes the $d$-wave superconductivity \[1\]. With the application of an external magnetic field and/or in the presence of nonmagnetic impurities, the effective mean-field Hamiltonian can be diagonalized by solving self-consistently the Bogoliubov-de Gennes equation \[15\]:

$$
\sum_j \left( \mathcal{H}_{ij,\sigma} - \Delta_{ij} \right) \begin{pmatrix} u^n_{ij\sigma} \\ v^n_{ij\sigma} \end{pmatrix} = E_n \begin{pmatrix} u^n_{ij\sigma} \\ v^n_{ij\sigma} \end{pmatrix}.
$$

(1)

Here $(u^n_{ij\sigma}, v^n_{ij\sigma})$ is the quasiparticle wavefunction corresponding to the eigenvalue $E_n$, the single particle Hamiltonian $\mathcal{H}_{ij,\sigma} = -t_{ij} e^{i\phi_{ij}} + (m_{ij} + \epsilon_i - \mu)\delta_{ij}$, where $t_{ij} = t$ for the nearest neighbor hopping while $t_{ij} = t'$ for the next-nearest neighbor hopping, $\epsilon_i$ is the single site potential describing the scattering from impurities, and the Peierls phase factor $\phi_{ij} = \frac{x}{2} \int_{0}^{t} A(x) \cdot dr$ with $\Phi_0 = hc/2e$ the superconducting flux quantum in the presence of an externally applied magnetic field. Notice that the quasiparticle energy is measured with respect to the Fermi energy. The self-consistency conditions read:

$$
m_{\uparrow\uparrow} = U n_{\uparrow\uparrow} = U \sum_n |u^n_{\uparrow\uparrow}|^2 f(E_n),
$$

(2a)

$$
m_{\uparrow\downarrow} = U n_{\uparrow\downarrow} = U \sum_n |v^n_{\uparrow\downarrow}|^2 [1 - f(E_n)],
$$

(2b)

and

$$
\Delta_{ij} = \frac{V}{4} \sum_n (u^n_{i\uparrow} v^n_{j\downarrow} + v^n_{i\downarrow} u^n_{j\uparrow}) \tanh \left( \frac{E_n}{2kB T} \right),
$$

(3)

where $U,V$ are the strength of the on-site repulsion and the nearest neighbor attraction, respectively, and the Fermi distribution function $f(E) = 1/(e^{E/k_B T} + 1)$. Here the summation is over the eigenstates with both positive and negative eigenvalues \[13\]. We report results below for two cases at zero temperature. For the Abrikosov vortex state, the magnetic field effects enter through the Peierls phase factor $\phi_{ij}$ and no impurities are introduced ($\epsilon_i = 0$). For the effects of a single impurity, we set $A = 0$ so that $\phi_{ij} = 0$. Hereafter we measure the length in units of the lattice constant $a_0$ and the energy in units of the hopping integral $t$. To mimic a hole-like Fermi surface, as relevant to the hole-doped cuprates, we take $t' = -0.2$. As a model calculation, the on-site repulsion and pairing interactions are taken to be, $U = 2.5$ and $V = 1.0$. In addition, the filling factor $n_f = \sum_n n_{n\sigma}/N_x N_y$ is fixed to be 0.84, which corresponds to an optimal hole doping $n_h = 1 - n_f = 0.16$. Here $N_x,N_y$ are the linear dimensions of the unit cell under consideration. We use an exact diagonalization method to solve the BdG equation \[1\] self-consistently. In the absence of magnetic field and impurities, we recover all results reported in \[14\]. In the optimal doping regime ($n_h = 0.16$), the AF SDW order is absent while the DSC order is homogeneous. When the DSC is weakened by the application of an external magnetic field or by introducing impurities, the AF SDW will be nucleated in the region where the DSC order is depressed.

**Field-induced SDW and CDW.** When an external magnetic field is applied perpendicular to the 2D Cu-O plane, $\mathbf{H} = H\mathbf{z}$ ($H_{c1} \ll H \ll H_{c2}$), an Abrikosov vortex state is formed. As the vortex core is approached, the DSC order parameter vanishes topologically due to the circulating supercurrent surrounding the core. It is assumed that the superconductor is in the extreme type-II limit where the Ginzburg-Landau parameter $\kappa = \lambda_0/\xi_0$ goes to infinity so that the screening effect from the supercurrent is negligible. We choose a Landau gauge to write the vector potential as $\mathbf{A} = (-Hy,0,0)$, where $y$ is the $y$-component of the position vector $\mathbf{r}$, so that the Peierls phase factor $\phi_{ij}$ is uniquely determined. By taking the strength of magnetic field, $H = 2\Phi_0/N_x N_y$, such that the flux enclosed by each unit cell is twice $\Phi_0$, we solve self-consistently the BdG equation \[1\] with the aid of the magnetic Bloch theorem as given by Eq. (3) in Ref. \[13\]. For the calculation, we consider the magnetic unit cell of size $N_x \times N_y = 48 \times 24$, which gives a square vortex lattice. The numerics shows that each unit cell accommodates two superconducting vortices each carrying a flux quantum $\Phi_0$, 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 area $\frac{\sqrt{2}}{2} \times N_s$ sites. Typical results on the structure around one vortex core are displayed in Fig. 1, where the left column is three-dimension plots and the right column is contour plots. As shown in Fig. 1(a), the DSC order parameter vanishes at the core center (dark-blue site) and approaches its zero-field value, which is about $\Delta_0 = 0.08$ for the chosen parameter values, away from the core center. Notice that the DSC order parameter is not uniform beyond the distance $\xi_0$ 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 will be discussed immediately. Fig. 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 (yellow spots) and valleys (dark-blue spots) 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 $\xi_0$, which is consistent with the INS measurements \[.\] 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(c), 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, the field-induced SDW as well as the associated CDW, one finds that as long as the absolute amplitude $|M_s|$ of SDW reaches a local maximum (both yellow and dark-blue spots in Fig. 1(b)), the associated CDW also reaches a local maximum (green spots in Fig. 1(c)), that is, a local minimum in the hole density, while the DSC order parameter has a local minimum (shallow red spots in Fig. 1(a)). The one to one correspondence between the SDW and associated CDW orderings at zero field, was discussed in the context of stripes [11, 12, 13, 14, 16]. To make 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 unambiguously the period of $8a_0$ along the Cu-O bond directions. To verify this point, we have performed a calculation on the unit cell of different size $N_x \times N_y = 52 \times 26$, and found that the period of the SDW modulation remains $8a_0$, indicating convincingly that the periodicity of the field-induced SDW modulation is an intrinsic property. Therefore, our result explains very well the INS measured value of the SDW modulation [1]. We notice that, in the optimal doping regime, the circulating supercurrent around the vortex, which favors the isotropy between $x$ and $y$ directions, overcomes the one-dimensionality of stripes. In the underdoping regime, the stripe behavior becomes dominant [2].

**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 its own right for a long time. In view of the recent observations of the AF magnetism around the vortex core, it is important to see whether a similar magnetic 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 $\varepsilon_0 = 100$ at the unitary impurity and zero on other sites. Since $\varphi_{ij} = 0$ in this case, the conventional Bloch theorem is used. The results on the spatial distribution of the three orderings is displayed in Fig. 3. The DSC order parameter is depressed dramatically at the impurity site and approaches the bulk value at the scale $\xi_0$. Out of this range, almost no modulation of the DSC order parameter is seen. The induced staggered moment of the 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, although with a much weaker amplitude. However, the electron density, which is zero at the impurity, only exhibits a Friedel-like oscillation within a limited range around the impurity. The Fourier transform, as shown in Fig. 4.
The main modulation period of the SDW is 8\(a_0\) gives a clear picture: The main modulation period of the SDW is 8\(a_0\); the CDW is modulated with a period of 2\(a_0\), which is roughly the Fermi wavelength. Therefore, the correspondence between the SDW and CDW is absent in this 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 \[21\] that show no evidence for CDW modulation 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 \[22, 23, 24, 25\]. 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 of the strongest staggered magnetic moments on the four nearest-neighbor Cu sites of the impurity is consistent with the above experiment \[25\]. This leads us to speculate that the magnetism around vortices and around impurities may share a common origin.

In conclusion, we have studied the magnetism around vortices and nonmagnetic unitary impurities. In the case vortices, the experimentally observed 8\(a_0\) 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 8\(a_0\). The existence of such modulation can be tested by neutron scattering experiments.

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FIG. 3: The three-dimensional (left column) and contour (right column) display of the amplitude 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 \(\times\) 36 sites. Parameter values are the same as in Fig. 1.

FIG. 4: The Fourier transform of the spatial modulation of the spin density \(M_s\) (a) and the charge density \(\delta n\) (b), around a nonmagnetic unitary impurity. Parameter values are the same as in Fig. 3.
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