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Striped morphologies induced by magnetic impurities in d-wave superconductors

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ABSTRACT

We study striped morphologies induced by magnetic impurities in d-wave superconductors (DSCs) near optimal doping by self-consistently solving the Bogoliubov–de Gennes equations based on the $t - t' - U - V$ model. For the single-impurity case, it is found that the stable ground state is a modulated checkerboard pattern. For the two-impurity case, the stripe-like structures in order parameters are induced due to the impurity-pinning effect. The modulations of DSC and charge orders share the same period of four lattice constants ($4a$), which is half the period of modulations in the coexisting spin order. Interestingly, when three or more impurities are inserted, the impurities could induce more complex striped morphologies due to quantum interference. Further experiments of magnetic impurity substitution in DSCs are expected to check these results.

1. Introduction

Recent studies of spatial inhomogeneous phases with stripe or checkerboard modulations in copper oxide-based compounds has received much attention. Neutron scattering (NS) experiments reveal the existence of incommensurate magnetic peaks in cuprates, which has led to discussions of a stripe phase [1–11]. Meanwhile, scanning tunneling microscopy (STM) experiments observed checkerboard-like charge-density wave (CDW) modulations [12–14], which break the square symmetry of the underlying lattice. It was proposed that the effect can be understood in terms of quasi-particle interference (QPI) due to scattering on impurities and other inhomogeneities [15–18] within the so-called 'octet' model, or in terms of static or fluctuating stripes [19]. Kohsaka et al. suggest that both dispersive and non-dispersive modulated patterns originate from different regions in momentum and energy space [14]. The well-defined states in the nodal region are responsible for the low energy QPI structure, whereas the ill-defined quasi-particle states in the antinodal regions are responsible for the non-dispersive charge order above some energy scale. On the other hand, zero-field experiments on the well ordered YBCO samples show no evidence of static broken translational symmetry in nuclear magnetic resonance or NS experiments, which leads to the proposal that the checkerboard patterns observed by STM is caused by the local disorders [20]. In brief, the physics that determines the ultimate patterns of competing orders is subtle. For instance, there are striped structures interpreted in terms of actual or incipient orders [19], or attributed to be induced by lattice distortion or impurity-pinning effect [21,20]. To date, the issue of the nature of spatial inhomogeneous phases in cuprates is still controversial.

Impurity effects have been proven to be a valuable probe to explore the fundamental properties of cuprates since it often provides important insights into the underlying physics. Experimentally, STM detection of the modulation of the local density of states by impurities was used to great advantage to probe the nature of quasi-particle states of DSCs both in the superconducting and pseudo-gap phases [22–24]. Another interesting issue is interference patterns and pinning stripes by impurities in DSCs. In general, impurity substitution causes additional slowing down of spin fluctuations and pinning of the stripes, leading to the formation of a static charge or spin order. Zhu et al. have proposed an explanation to the checkerboard pattern around a impurity or vortex cores based on an effective mean-field $t - U - V$ model [15]. For the case without an applied magnetic field, the disorder can produce a similar pinning effect of the fluctuating stripes. Andersen et al. investigate disorder-induced freezing of incommensurate spin fluctuations, which agrees qualitatively with experimental observations [25]. In the present work, we study the striped morphologies induced by magnetic impurities in d-wave superconductors (DSCs) near optimal doping. Including the competitions and coexistence among the DSC, spin-density wave (SDW), and CDW orders, the system is explored by self-consistently solving the Bogoliubov–de Gennes (BdG) equations. It is found that the local disorders can induce interesting phenomena, including checkerboard, stripe modulations, and other complex striped morphologies. We expect that these phenomena could be observed in the STM and NS experiments.

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2. Theory and calculation details

We start from the two-dimensional $t - t' - U - V$ model, which consists of two parts, $H = H_0 + H_{imp}$. The Hamiltonian H_0 and H_{imp} describe the superconductor and magnetic impurities, respectively, which can be written as

$$H_0 = -\sum_{ij\sigma} t_{ij}(c^\dagger_{i\sigma}c_{j\sigma} + H.c.) + \sum_{ij}\left(\Delta_{ij}c^\dagger_{i\uparrow}c^\dagger_{j\downarrow} + H.c.\right) + \sum_{i\sigma}(Un_{i,\bar{\sigma}} - \mu)c^\dagger_{i\sigma}c_{i\sigma},$$
$$H_{imp} = \sum_i h_{eff}(i)\left(c^\dagger_{i\uparrow}c_{i\uparrow} - c^\dagger_{i\downarrow}c_{i\downarrow}\right). \quad (1)$$

Here $c_{i\sigma}$ annihilates an electron of spin σ at the ith site. The hopping integral t_{ij} takes t between nearest-neighbor (NN) pairs, and t' between next-nearest neighbor (NNN) pairs. U is the on-site Coulomb repulsion interaction. μ is the chemical potential, which is determined self-consistently in the calculation. The local effective field $h_{eff}(i)$ is introduced to model the exchange coupling between conducting electrons and the impurity spin, where we have treated the Kondo impurity spin as a Ising-like one. Some similar model had been employed to study the effects of magnetic impurities on cuprate superconductors [26,27], which can qualitatively explain the observed impurity states well [23]. Therefore, we employed the above model in this work. The self-consistent mean-field parameters are given by $n_i = \sum_\sigma\langle c^\dagger_{i\sigma}c_{i\sigma}\rangle$, the magnetization $m_i = (1/2)\left(\langle c^\dagger_{i\uparrow}c_{i\uparrow}\rangle - \langle c^\dagger_{i\downarrow}c_{i\downarrow}\rangle\right)$, and the DSC order parameter $\Delta_{ij} = (V/2) < c_{i\uparrow}c_{j\downarrow} - c_{i\downarrow}c_{j\uparrow} >$ with V the phenomenological pairing interaction.

The Hamiltonian H can be diagonalized by solving the following BdG equations,

$$\begin{pmatrix} H_{ij,\uparrow} & \Delta_{ij} \\ \Delta^*_{ij} & -H^*_{ij,\downarrow} \end{pmatrix}\Psi_j = E\Psi_i, \quad (2)$$

where the quasiparticle wave function $\Psi_i = (u_{i\uparrow}, v_{i\downarrow})^T$. The spin-dependent single-particle Hamiltonian reads $H_{ij\sigma} = -t\delta_{i+\tau,j} - t'\delta_{i+\tau',j} + \left[\sum_{i_m}\sigma h_{eff}(i)\delta_{i,i_m} + Un_{i,\bar{\sigma}} - \mu\right]\delta_{ij}$. Here the subscripts τ and τ' denote the unit vector directing along four NN and NNN bonds respectively, and i_m is the position of the impurity site. The self-consistent parameters are given by $n_{i\uparrow} = \sum_n\left|u^n_{i\uparrow}\right|^2 f(E_n), n_{i\downarrow} = \sum_n\left|v^n_{i\downarrow}\right|^2[1 - f(E_n)]$, and $\Delta_{ij} = \frac{V}{4}\sum_n\left[u^n_{i\uparrow}v^{n*}_{j\downarrow} + v^{n*}_{i\downarrow}u^n_{j\uparrow}\right]tanh(\frac{\beta E_n}{2})$, where $f(E) = 1/(1 + e^{\beta E})$ is the Fermi-Dirac distribution function. Hereafter, the length is measured in units of the lattice constant a, and the energy in units of t. We set $U = 2.5$ and $t' = -0.2$ in this paper. The pairing interaction is chosen as $V = 1.0$ to guarantee that the superconducting order $\Delta_0 \simeq 0.08t$, comparable with the observed T_c in cuprate superconductors. We study the impurity effects on the electronic states of DSCs near optimal doping with the filling factor $n_f = \sum_{i\sigma}c^\dagger_{i\sigma}c_{i\sigma}/(N_xN_y) = 0.83$ (i.e., the hole doping $x = 0.17$), where N_x, N_y are the linear dimension of the unit cell. The BdG equations are solved self-consistently for a square lattice of 32×32 sites, and the periodic boundary conditions are adopted. The numerical calculation is performed at a very low temperature, $T = 10^{-5}$ K, to extract the low-energy physics. The local effective field is taken to be $h_{eff} = 3$ at the impurity site and zero otherwise. The DSC order parameter at the ith site is defined as $\Delta_i = (\Delta_{i,i+e_x} + \Delta_{i,i-e_x} - \Delta_{i,i+e_y} - \Delta_{i,i-e_y})/4$, and the spin order parameter is $M_i = (-1)^i m_i$.

3. Numerical results and discussion

In Fig. 1, we plot the spatial distributions of the DSC, spin, and charge orders around the impurity site. One can see that all the three orders display checkerboard modulations around the magnetic impurity. Similar to the nonmagnetic impurity case, a SDW checkerboard pattern is observed around the magnetic impurity [15,28], which coincides with the NS data [1]. However, it is noteworthy that the checkerboard pattern of the DSC order can also be

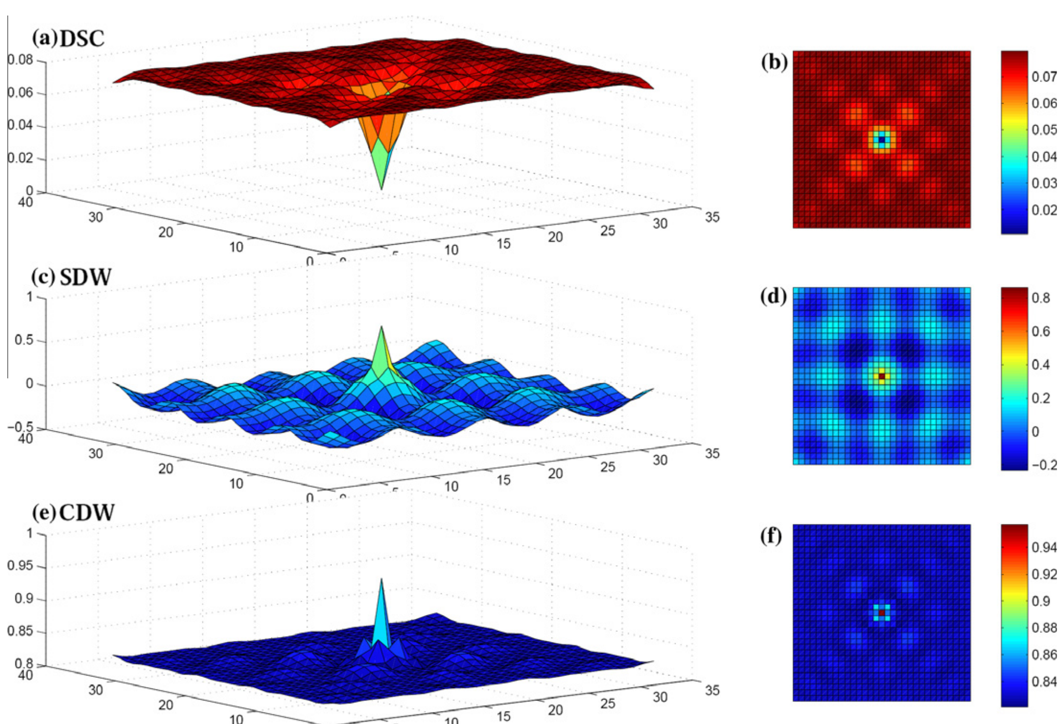

Fig. 1. The surface plots of orders around the magnetic impurity on a unit cell of size 32 × 32 sites. (a, c, and e) are the spatial distributions of the DSC, spin and charge orders. (b, d and f) are their contour plots.