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Anti-phase superconducting domain structures in the \( t-t'-t''-J \) model

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Abstract. We study spatially modulated \( d \)-wave superconducting states in the two-dimensional \( t-t'-t''-J \) model within the Bogoliubov-de Gennes theory based on an extended Gutzwiller approximation. We find fully self-consistent solutions involving domain walls with vanishing pairing amplitudes \( \Delta \) separated by four lattice spacing when the system is about 12.5\% hole doping, while five at about 15\%. The adjacent superconducting domains are in the anti-phase patterns, that is, the relative phase difference between them is \( \pi \). The \( \Delta = 0 \) domain walls involve concentration of mobile holes due to the loss of the condensation energy. We also find that the superconducting coherence peaks at the energy of the \( d \)-wave gap in the local densities of states are strongly suppressed in these states with anti-phase superconducting domain structures.

1. Introduction
Recent STM/S experiments on Ca\(_{2-x}\)Na\(_x\)CuO\(_2\)Cl\(_2\) and Bi\(_2\)Sr\(_2\)Dy\(_{0.2}\)Ca\(_{0.8}\)Cu\(_2\)O\(_{8+\delta}\) have revealed the existence of spatially modulated structures in the local density of states (LDOS) \([1]\). Also, recent measurement of transport properties of the stripe phase in La\(_{1.875}\)Ba\(_{0.125}\)CuO\(_4\) implies that the interlayer-intrinsic Josephson coupling is suppressed in the temperature region of \( T_c < T < T_{\text{BKT}} \) \([2]\). Promptly after, this decoupling of the CuO\(_2\) layers in this material is supposed to be based on a unidirectional domain structures of \( d \)-wave superconductivity in each layer, the directions of which rotate about \( \pi/2 \) between the adjacent layers \([3]\).

Motivated by these observations, a stripe-like spatially modulated ground state again attracts theoretical attention \([11]\). Beyond the original spin stripe picture, Poilblanc and his coworkers have found that stripe-like RVB states without antiferromagnetic order cost very small energies relative to the energy of the pure \( d \)-wave superconducting states, and suggested that those states would be realized when lattice anisotropy is taken into account \([4, 5]\).

In this paper, we examine the possibility that such kinds of stripe-like states would be realized as the stable solution of a two-dimensional \( t-J \) type model with longer-range hopping terms when the partially nesting condition of Fermi surfaces \([6, 7]\) is satisfied.

2. model
The Hamiltonian of the \( t-J \) model is written as

\[
\mathcal{H} = - \sum_{\langle i,j \rangle, \sigma} P_G (t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) P_G + J \sum_{\langle i,j \rangle} S_i \cdot S_j - \mu \sum_{i, \sigma} c_{i\sigma}^\dagger c_{i\sigma} \tag{1}
\]
in the standard notation where \( \langle i, j \rangle \) means the summation over nearest-neighbor pairs. The Gutzwiller’s projection operator \( P_G \) is defined as \( P_G = \Pi(1 - n_i n_j) \). The hopping integrals \( t_{ij} \) are chosen as

\[
t_{ij} = \begin{cases} 
1.0 & \text{for the nearest neighbor sites} \\
-0.3 & \text{for the next-nearest neighbor sites} \\
0.15 & \text{for the 4th nearest neighbor sites}
\end{cases}
\]  

(2)

to reproduce the partially nested Fermi surfaces of BSCCO [6, 7].

The Bogoliubov-de Gennes (BdG) equation based on the extended Gutzwiller approximation is given as

\[
\begin{pmatrix}
H_{ij}^+ & F_{ji}^-
\end{pmatrix}
\begin{pmatrix}
\mathbf{u}_i^\alpha \\
\mathbf{v}_i^\alpha
\end{pmatrix}
= E^\alpha
\begin{pmatrix}
\mathbf{u}_i^\alpha \\
\mathbf{v}_i^\alpha
\end{pmatrix},
\]  

(3)

with

\[
H_{ij}^+ = -\sum_{\tau} \left( t_{ij}^{\text{eff}} + J_{ij}^{\text{eff}} \chi_{ij} \right) \delta_{j, i+\tau} + \sigma \delta_{ij} \sum_{\tau} h_{ij, i+\tau}^{\text{eff}} - \mu \delta_{ij}
\]

\[
F_{ji}^- = -\sum_{\tau} J_{ij}^{\text{eff}} \Delta_{ij} \delta_{j, i+\tau},
\]  

(4)

where \( \sigma = \pm 1 \), \( i + \tau \) represents the nearest neighbor sites of the site \( i \), while \( i + \nu \) the nearest, 2nd, 4th neighbor sites.

The renormalized parameters \( t_{ij}^{\text{eff}}, J_{ij}^{\text{eff}} \) and \( h_{ij}^{\text{eff}} \) are determined from cluster calculations which reproduce the variational Monte Carlo results[8]. They have the following forms:

\[
t_{ij}^{\text{eff}} = g_t(i, j) t_{ij}, \quad J_{ij}^{\text{eff}} = \frac{1}{2} g_{xy}^s(i, j) J + \frac{1}{4} g_s^z(i, j) J,
\]

\[
h_{ij}^{\text{eff}} = \frac{1}{2} g_s^z(i, j) J m_j + \frac{\partial \langle H_{ij} \rangle}{\partial m_j},
\]  

(5)

where \( g_t(i, j), g_{xy}^s(i, j) \) and \( g_s^z(i, j) \) depend on the local expectation values \( \Delta_{ij} = \frac{1}{2} \langle c_{i\sigma}^\dagger c_{j\sigma} \rangle \), \( \chi_{ij} = \langle c_{i\sigma}^\dagger c_{j\sigma} \rangle \), and \( m_j = \frac{1}{2} \langle n_{i\sigma} - n_{j\sigma} \rangle \) [9, 10]. For example,

\[
g_{xy}^s(i, j) = \left( \frac{2(1 - \bar{\delta}_{ij})}{1 - \bar{\delta}_{ij}^2 + 4 \bar{m}_{ij}^2} \right)^2 a_{ij}^{-7},
\]  

(6)

where \( \bar{\delta}_{ij} (\bar{m}_{ij}) \) is an average of hole density (AF moment) for the corresponding bond and \( a_{ij} \) is a factor close to one which depends on \( \Delta_{ij}, \chi_{ij}, \bar{\delta}_{ij} \) and \( \bar{m}_{ij} \)[8]. These somewhat complicated renormalized parameters are necessary for treating the AF and d-wave superconductivity in the same framework.

In the present calculation, we regard the 40×6 square lattice as a unit cell. We solve numerically the BdG equation and carry out an iteration until \( \Delta_{ij}, \chi_{ij}, \bar{\delta}_{ij}, \bar{m}_{ij} \) are determined self-consistently. We take \( J/t = 0.3 \) and the doping rates \( \delta \approx 0.12 \) and 0.145.

3. Anti-phase d-wave domain structures

We obtain stable self-consistent solutions of the type of site-centered anti-phase unidirectional domain structures [4] for both \( \delta \approx 0.12 \) and 0.15. First, let us look at the case \( \delta \approx 0.12 \).

Figure 1 (a) shows the spatial dependences of the hole density \( \delta \) and the superconducting gap amplitude \( \Delta^y \) along the (10) direction of the square lattice, that is, the direction perpendicular to the stripe direction. We find an anti-phase type stripe-like domain structures of \( \Delta^y \),
accompanied by the hole density modulation, quite similar to the previous theoretical results [4, 5]. However, it is worth noting here that this solution is the stable state and become unstable if we take $t''/t \leq 0.12$ in the sense of self-consistent calculations. Actually, the uniform $d$-wave superconducting state is obtained when $t''/t \leq 0.12$ as the stable self-consistent solution. This implies that the partial nesting of the Fermi surface caused by $t''$ term plays a significant role on the realization of this kind of anti-phase stripe structure as the stable state.

![Graphs showing hole density and superconducting order parameter](image)

**Figure 1.** (a),(b) Hole density $\delta_j$ and superconducting order parameter $\Delta^y_j$ plotted along the (10) direction of the square lattice. (c),(d) The local density of states (LDOS) for $\delta \sim 0.12$ and $0.145$. The thin black lines represent the LDOS for the pure $d$-wave superconducting states.

In order to see the effects of partially nested Fermi surface, next we look at the stable solution obtained for $\delta \sim 0.145$. Figure 1 (b) shows the spatial dependences of $\delta_j$ and $\Delta^y_j$ for $\delta \sim 0.145$ in the same manner as in Fig. 1 (a). Also in this case, we can clearly see that the anti-phase type structure is realized but with the period of five lattice spacings. We note here that this solution becomes unstable when $\delta \sim 0.12$ or $t''/t \leq 0.12$. Thus we conclude that the longer-range hopping term $t''$ has relevant effects on stabilizing the anti-phase stripe-like structures. Experimentally, it is occasionally observed that the periods of modulating states are deviated from 4. We speculate that those deviations are attributed to the different nesting conditions, due to the material parameters, especially the hole doping rate.
Finally we briefly look at the LDOS in these modulated states. Figure 1 (c) shows the LDOS obtained on the site-2 (blue) and -4 (red) in Fig. 1 (a), $\delta \sim 0.12$. The thin black line represents the DOS for the pure $d$-wave superconducting state. We find that the relatively small gap structure is realized at the site-2 where the $\Delta y_j = 0$. These two peaks at about $E/t = \pm 0.05$ seems are similar to those observed in the small gap regions in the inhomogeneous superconducting states, and attributed to the Andreev bound states [12]. It is also found that the noticeably asymmetric spectrum is seen at the site-2 where the amplitude of superconducting order parameter is maximum. The physical origin of this asymmetric spectrum is to be published elsewhere [13].

4. Summary and Discussions
In this paper we have shown within the Bogoliubov-de Gennes theory based on the extended Gutzwiller approximation that the anti-phase type superconducting domain structures are obtained as a stable self-consistent solution of the two-dimensional $t$-$t'$-$t''$-$J$ model when the partial nesting condition of the Fermi surface is satisfied.

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