Details of coexistence of superconducting and antiferromagnetic orders induced by a paramagnetic pair-breaking effect

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Abstract. We theoretically investigate the k-space distributions of coexisting $d_{x^2-y^2}$-wave superconducting (SC) and antiferromagnetic or spin-density-wave (SDW) orders induced by the paramagnetic pair-breaking (PPB) effect. It is shown that the SDW order develops in k-space regions near the SC nodes, where the SC order is suppressed by the PPB, and that the SC and SDW orders are enhanced with each other even in k-space owing to the sign change of the $d_{x^2-y^2}$-wave SC gap function. The field dependence of the PPB-induced SDW moment in the case with a large Fermi surface curvature is discussed based on the distributions of the SC and SDW orders in k-space.

1. Introduction
A novel superconducting (SC) phase observed in the high-field low-temperature region of the SC phase of the heavy fermion material CeCoIn$_5$ [1] has been extensively investigated recently. An ultrasound measurement [2, 3], an anomalously strong impurity effect [4, 5], and a NMR experiment [6] have suggested that the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) SC state, in which the SC order parameter is spontaneously modulated in real space owing to the strong paramagnetic pair-breaking (PPB) effect, is realized in this high-field low-temperature (HFLT) phase. On the other hand, a neutron scattering experiment [7] and the NMR experiment [6] have indicated the presence of an antiferromagnetic or spin-density-wave (SDW) order only in this HFLT phase. These results suggest that the HFLT phase is a coexistent phase of FFLO SC and SDW orders.

The SDW ordering in the HFLT phase exhibits a very anomalous behavior: a SDW order is present only in the HFLT phase, but not in the high-field normal phase [7]. This behavior is contradictory to the widely believed view that SC and SDW orders are competitive with each other. For this reason, the mechanism of this anomalous SDW ordering has attracted much interest.

In our previous studies [8, 9], it has been shown that a strong PPB induces the SDW order in the high-field region of a $d_{x^2-y^2}$-wave SC phase. The SDW susceptibility in a SC phase is represented as the sum of two contributions: the contribution of the quasiparticle excitations and that of the Cooper pair condensate. The contribution of the Cooper pair condensate enhances the SDW susceptibility as a consequence of the sign change of the $d_{x^2-y^2}$-wave gap function $w_k$ in k-space, i.e., the relation $w_{k+Q} = -w_k$, where $Q = (\pi, \pi, \pi)$ is the SDW modulation vector.
At zero field, however, the contribution of the quasiparticle excitations tends to be suppressed in the SC phase because of the SC excitation gap, and the total SDW susceptibility tends to also be suppressed in the SC phase [10, 11]. In the high field region of a SC phase with a strong PPB effect, however, the suppression of the SDW susceptibility by the SC excitation gap is diminished by the PPB. As a result, the enhancement of the SDW susceptibility due to the Cooper pair condensate becomes dominant, and the SDW ordering tends to be realized in the high-field region of the \( d_{x^2-y^2} \)-wave SC phase. The importance of the sign change of \( w_k \) in k-space for the PPB-induced SDW ordering have also been discussed by Michal et al. [12] in terms of the PPB-induced shift of the resonance peak appearing if \( w_k \) changes its sign in k-space in the manner \( w_{k+Q} = -w_k \). Besides this, it has also been found [9] that a FFLO spatial modulation of the SC order parameter parallel to the magnetic field strikingly enhances the PPB-induced SDW ordering. However, this does not imply that the SDW order favors the region in real space in which the SC order parameter vanishes. With increasing the field, the SDW order tends to favor the region in which the SC energy gap is larger [9]. Then, one may wonder how the magnetic order favoring coexistence, in real space, with the non-vanishing SC order appears in k-space. This naive question has motivated us to investigate details in k-space of this PPB-induced SDW order in the \( d \)-wave SC phase.

We need to mention that this PPB-induced SDW ordering has been also addressed by another research group [13], in which an importance of the nesting between quasiparticle pockets appearing due to the strong PPB has been stressed. The theoretical works of Refs.[8, 9, 12, 13] are based on essentially the same model, and thus, their argument might also be reflected in the results in the framework of Ref.[8, 9] if the quasiparticle pockets’ contribution is dominant. Even from this point of view, a comprehensive study on the k-space structure of these coexisting orders will be valuable.

In this study, we report results on the k-space distributions of the \( d \)-wave SC and the PPB-induced SDW orders obtained in the framework of Refs.[8, 9] to clarify the primary origin of the coexistence of the two orders.

2. Model

We start from the mean-field Hamiltonian of SC and SDW orders:

\[
\mathcal{H} = \mathcal{H}_{\text{kin}} + \mathcal{H}_{\text{SC}} + \mathcal{H}_{\text{SDW}},
\]

\[
\mathcal{H}_{\text{kin}} = \sum_{k,\sigma} (\xi_k - \hbar \sigma) c_{k,\sigma}^{\dagger} c_{k,\sigma},
\]

\[
\mathcal{H}_{\text{SC}} = \frac{|\Delta|^2}{\lambda} - \left[ \Delta \sum_k w_k c_{k,\uparrow}^{\dagger} c_{-k,\downarrow} + \text{H.c.} \right],
\]

\[
\mathcal{H}_{\text{SDW}} = \frac{m^2}{U} - \left[ m \sum_{k,\sigma} c_{k,-\sigma}^{\dagger} c_{k+Q,\sigma} + \text{H.c.} \right].
\]

Here, \( h = g \mu_B H \) is the Zeeman energy (\( g \) is the g-factor, \( \mu_B \) is the Bohr magneton, and \( H \) is the strength of the magnetic field perpendicular to the c-axis), \( \Delta \) is the SC order parameter, \( \lambda \) is the strength of the pairing interaction, \( w_k \) is the SC gap function, \( m \) is the SDW moment parallel to the c-axis, \( U \) is the strength of the Coulomb interaction, and \( Q \) is the SDW modulation vector. We use the dispersion relation \( \xi_k \) of the two-dimensional tight-binding model:

\[
\xi_k = -2t_1 (\cos(k_x) + \cos(k_y)) - 4t_2 \cos(k_x) \cos(k_y) - \mu.
\]
We assume that $Q$ is equal to $\pi(1 + \frac{1}{N}, 1 + \frac{1}{N}) = 2\pi(0.55, 0.55)$ (i.e. $N = 10$), and adjust the chemical potential $\mu$ so that Fermi surface nesting with the nesting vector $Q$ is realized.

Since the Hamiltonian (1) can be represented as a bilinear form of extended Nambu spinors of $2N$-dimension, the partition function and the free energy can easily be calculated. $\Delta$ and $m$ will be determined by numerically minimizing the free energy w.r.t. them.

In order to examine the k-space structure of the coexisting SC and SDW orders, we have chosen to calculate the following quantities:

$$ H(k) = -\sum_{\sigma} \left[ \langle c_{k,-\sigma}^\dagger c_{k+Q,\sigma} \rangle + \langle c_{k,-\sigma} c_{k,-Q,\sigma} \rangle \right]. \quad (6) $$

$$ F(k) = -\langle c_{-k,\downarrow}^\dagger c_{k,\uparrow} \rangle, \quad (7) $$

$H(k)$ and $F(k)$ correspond to the k-space distributions of the SDW and the SC orders, respectively. In fact, the gap equations for the SC and SDW orders can be written as

$$ \frac{m(r = 0)}{U} = \sum_k H(k), \quad (8) $$

$$ \frac{\Delta}{\lambda} = \sum_k w_k F(k). \quad (9) $$

Equation (8) indicates that the SDW moment $m$ is obtained by summing $H(k)$ over the k-space; therefore $H(k)$ is interpreted as the k-space distribution of the SDW order. Similarly, Eq. (9) shows that the SC order parameter $\Delta$ is represented as the sum of $F(k)$ over the k-space weighted by the pairing function $w_k$; therefore $F(k)$ is interpreted as the k-space distribution of the SC order.

### 3. Results

![Colormap plots of (a) $F(k)$ and (b) $H(k)$ in k-space.](image-url)

Figure 1. Colormap plots of (a)$F(k)$ and (b)$H(k)$ in k-space. The used parameters are $t_1/T_c = 10$, $t_2/t_1 = -0.05$, $\mu/t_1 = 0.62$, $U/T_c = 15.2$, $T/T_c = 0.1$, and $H/H_P = 0.85$, where $H_P$ is the Pauli limiting field.

Figure 1(a) and (b) show the colormap plots of $F(k)$ and $H(k)$ in k-space, respectively, in the coexistent phase of SDW and $d_{x^2-y^2}$-wave SC orders (i.e. $w_k = \cos(k_x) - \cos(k_y)$). In Fig. 1(a), it can be seen that the SC order ($F(k)$) is suppressed by the PPB in the vicinity of the SC nodes near $k = \pm(\pi/2, \pi/2), \pm(\pi/2, -\pi/2)$. In Fig. 1(b), it is shown that the major contribution to the SDW order ($H(k)$) comes from the Fermi surface areas near $k = \pm(\pi/2, \pi/2)$ because these
areas satisfy the nesting condition with the nesting vector $\mathbf{Q}$ ($\xi_{\mathbf{k}+\mathbf{Q}} \sim -\xi_{\mathbf{k}}$). Moreover, one can see that the SDW order develops in regions where the SC order is suppressed by the PPB in Fig 1 (a).

Next, we examine how the sign change of the $d_{x^2-y^2}$-wave gap function in k-space affects the coexistence of SC and SDW orders. For this purpose, we also analyzed the toy model in which the gap function $w_{\mathbf{k}} \equiv |\cos(k_x) - \cos(k_y)| > 0$ with no sign change in k-space is assumed. The excitation energy in this model is equal to that of the usual $d_{x^2-y^2}$-wave SC model, since the excitation energy $E_{\mathbf{k} \sigma} = \sqrt{\xi_{\mathbf{k}}^2 + |\Delta w_{\mathbf{k}}|^2} - h\sigma$ is not dependent on the sign of $w_{\mathbf{k}}$. Especially, the shape and the nesting condition of the quasiparticle pockets are the same between these models. Therefore, we can investigate the effect of the sign change of the gap function by comparing the results of the toy model with those of the $d_{x^2-y^2}$-wave SC model.

**Figure 2.** Plots of $F(\mathbf{k})$ (red solid line) and $H(\mathbf{k})$ (blue dashed line) along the Fermi surface (a) in the $d_{x^2-y^2}$-wave SC model and (b) in the toy model (see main text). The definition of $\theta$ is illustrated in (c). The used parameters in (a) are $t_1/T_c = 10$, $t_2/t_1 = -0.05$, $\mu/t_1 = 0.62$, $U/T_c = 7.30$, $T/T_c = 0.1$, and $H/H_F = 0.8$. The used parameters in (b) are the same as (a) except for $U/T_c = 9.87$.

Figure 2 shows $F(\mathbf{k})$ (red solid line) and $H(\mathbf{k})$ (blue dashed line) plotted along the Fermi surface (a) in the $d_{x^2-y^2}$-wave SC model and (b) in the toy model. The definition of $\theta$ is illustrated in Fig. 2(c). In the $d_{x^2-y^2}$-wave SC model (Fig. 2(a)), $H(\mathbf{k})$ is maximal not at the SC gap node ($\theta = \pi/4$) but at the points slightly away from the nodes where $F(\mathbf{k})$ has a finite value. Moreover, $F(\mathbf{k})$, which is completely suppressed near the nodes by the PPB in the absence of the SDW order, is slightly enhanced near the nodes in the presence of the SDW order. In the toy model (Fig. 2(b)), on the other hand, $H(\mathbf{k})$ is maximal near the SC gap nodes and is strongly suppressed as $F(\mathbf{k})$ is increased in the region away from each node. Furthermore, $F(\mathbf{k})$ is completely suppressed near the gap nodes in the presence of the SDW order.

It is suggested from these results that, in the $d_{x^2-y^2}$-wave SC model, SC and SDW orders are enhanced with each other in k-space, while, in the toy model, SC and SDW orders are exclusive in k-space. As a result, the PPB-induced SDW ordering is realized in the $d_{x^2-y^2}$-wave SC model even if there is no SDW order in the normal phase, while the SDW ordering in the SC phase seems to be strongly suppressed in comparison to the normal phase in the toy model. Comparing these results with each other, we conclude that $d_{x^2-y^2}$-wave SC and SDW orders are enhanced with each other in k-space owing to the sign change of the gap function in k-space, and that this mutual enhancement of these orders is crucial for the realization of the PPB-induced SDW ordering occurring only in the SC phase.

Finally, influences of a Fermi surface curvature on the field dependence of this PPB-induced SDW ordering are discussed. The Fermi surface curvature is parametrized by the next-nearest
Figure 3. Field dependence of the SC order parameter $\Delta$ (red solid line), and the SDW moment $m$ at $t_2/t_1 = -0.15$ (blue dashed line) and $t_2/t_1 = -0.16$ (purple dotted line). The used parameters are $t_1/T_c = 10$, $\mu/t_1 = 0$, $U/T_c = 0.185$, and $T/T_c = 0.1$.

neighbor hopping $t_2$; the Fermi surface curvature is increased as $|t_2/t_1|$ is increased. Figure 3 shows the field dependence of the SDW moment $m$ at $t_2/t_1 = -0.15$ (blue dashed line) and $t_2/t_1 = -0.16$ (purple dotted line). In the case with a smaller $|t_2|$ (blue dashed line), $m$ is maximal at $H_{c2}$ where the PPB effect is the most effective. In the case with the larger $|t_2|$ (purple dotted line), on the other hand, $m$ is maximal at the field slightly below $H_{c2}$. This behavior can be explained in terms of the mutual enhancement of the SC and SDW orders in k-space as follows: When the Fermi surface curvature is large, the hot spot for the SDW ordering is confined to the vicinity of the SC nodes near $k = \pm (\pi/2, \pi/2)$ owing to the deterioration of the nesting condition. At a high field near $H_{c2}$, the k-space region where the SC order is suppressed by the PPB becomes larger than the SDW hot spot, and hence, the coexistent region of the SC and SDW orders becomes quite narrower in k-space. As a result, the enhancement of the SDW ordering due to the SC order is suppressed at high fields near $H_{c2}$, so that $m$ is decreased. This indicates that the mutual enhancement of SC and SDW orders in k-space plays an important role in the PPB-induced SDW ordering.

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