Antiferromagnetic order in the FFLO state

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Abstract. We investigate the antiferromagnetic (AF) order in the $d$-wave superconducting (SC) state at high magnetic fields. A two-dimensional model with on-site repulsion $U$, inter-site attractive interaction $V$ and antiferromagnetic exchange interaction $J$ is solved using the mean field theory. For finite values of $U$ and $J$, a first order transition occurs from the normal state to the FFLO state, while the FFLO-BCS phase transition is second order, consistent with the experimental results in CeCoIn$_5$. Although the BCS-FFLO transition is continuous, the Néel temperature of AF order is discontinuous at the phase boundary because the AF order in the FFLO state is induced by the Andreev bound state localized in the zeros of FFLO order parameter, while the AF order hardly occurs in the uniform BCS state. The spatial structure of the magnetic moment is investigated for the commensurate AF state as well as for the incommensurate AF state. The influence of the spin fluctuations is discussed for both states. Since the fluctuations are enhanced in the normal state for incommensurate AF order, this AF order can be confined in the FFLO state. The experimental results in CeCoIn$_5$ are discussed.

The FFLO superconducting state at high magnetic fields was predicted in 1960’s by Fulde and Ferrel [1] and Larkin and Ovchinnikov [2]. In addition to the U(1)-gauge symmetry the spatial symmetry is broken by the modulation of the SC order parameter. After nearly 40 years of fruitless experimental search for FFLO states recent experiments appeared to give first evidences for such a phase [3]. Moreover, the FFLO phase enjoys growing interesting in other related fields such as in cold atomic gases [4] and in high-density quark matter [5].

Extensive studies of the FFLO state had been triggered by the discovery of a novel SC phase in CeCoIn$_5$ [6, 7]. Although several experimental results suggest the emergence of a FFLO state here [8, 9, 10, 11], some NMR and neutron scattering data rather indicate the presence of AF order [12, 13]. In this paper we theoretically examine the possibility of the coexistence of AF order and FFLO superconductivity.

Our theoretical analysis is based on the following model,

$$H = \sum_{k, \sigma} \varepsilon(k)c_{k \sigma}^\dagger c_{k \sigma} + U \sum_i n_{i \uparrow} n_{i \downarrow} + V \sum_{<i,j>} n_i n_j + J \sum_{<i,j>} \vec{S}_i \vec{S}_j - 2H \sum_i \vec{S}_i^z,$$

(1)

where $\vec{S}_i$ is the spin operator and $n_i$ is the number operator at site $i$. In order to describe the quasi-two-dimensional electronic structure of CeCoIn$_5$ we assume for simplicity a square lattice. The bracket $<i,j>$ denotes the summation over the nearest neighbor sites. The on-site repulsive interaction is given by $U$, and $V$ and $J$ stand for the attractive interaction and antiferromagnetic exchange interaction, respectively, between nearest neighbor sites. $V$ stabilizes the $d$-wave SC state and $J > 0$ takes into account the antiferromagnetic correlation in CeCoIn$_5$. 

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It has been experimentally shown that CeCoIn$_5$ is close to the quantum critical point (QCP) of AF order $\mathbf{Q}$. The other candidate materials for FFLO superconductivity are also close to the QCP of AF order $[14, 15, 16]$. These features, namely the $d$-wave superconductivity and AF correlation, can be described using the FLEX approximation for the simple Hubbard model [17]. But here, we assume the interactions $V$ and $J$ to describe the FFLO superconductivity near the QCP within the mean field theory. With the last term in eq. (1) we include the Zeeman coupling due to the applied magnetic field parallel to the $ab$-plane.

We adopt the following tight-binding model,

$$
\varepsilon(\mathbf{k}) = -2t(\cos k_x + \cos k_y) + 4t' \cos k_x \cos k_y - \mu,
$$

where the unit of energy is $t = 1$ and we fix $t'/t = 0.25$. The chemical potential enters as $\mu = \mu_0 + \frac{1}{2}Un_0$ where $n_0$ is the number density for $U = V = J = 0$. The stable AF ordered state depends on the parameter $\mu_0$ which determines the electron number. The commensurate AF order with $\mathbf{Q} = (\pi, \pi)$ appears for $\mu_0 = -0.8$ while an incommensurate AF state with $\mathbf{Q} = (\pi \pm \delta, \pi)$ or $\mathbf{Q} = (\pi, \pi \pm \delta)$ is obtained for $\mu_0 = -0.95$.

We examine the model (1) within the Bogoliubov-deGennes (BdG) theory by taking into account the Hartree-term arising from $U$ and $J$. The Hartree-term due to the attractive interaction $V$ is ignored because this term does not have any spin dependence as is essential for the following results. We first determine the phase diagram for the normal, uniform BCS and FFLO states and later examine the magnetic instability in these states. It is necessary to include both the on-site repulsion $U$ and antiferromagnetic $J$ in order to reproduce the experimental results in CeCoIn$_5$ [3]. For our choice of the parameters $U \sim 1$ and $J \sim 0.6$, the first order phase transition occurs from the normal state to the FFLO state, while the BCS-FFLO transition is second order, consistent with the experimental results [3, 4, 11]. The FFLO state is suppressed for $T < T_c$ if we assume $J = 0$, while the normal-to-FFLO phase transition is second order around the tricritical point for $U = 0$. This is incompatible with the phase diagram of CeCoIn$_5$ indicating that the phase diagram of FFLO superconductivity is significantly affected by the electron correlation.

\begin{figure}[h]
\begin{center}
\includegraphics[width=\textwidth]{phase_diagram.png}
\end{center}
\caption{Phase diagram for (a) $\mu_0 = -0.8$, $U = 1$ and $J = 0.6$ and (b) $\mu_0 = -0.95$, $U = 1.15$ and $J = 0.65$. Blue lines show the first order phase transition to the SC state while red lines show the second order BCS-FFLO transition. Black lines show the Neél temperature. We fix $V = -0.8$.}
\end{figure}

Figures 1(a) and 1(b) show the results for $\mu_0 = -0.8$ and $\mu_0 = -0.95$, respectively. For both cases AF order occurs in the FFLO and normal states, but is absent in the uniform BCS state. The Neél temperature $T_N$ of the AF order shifts discontinuously at the phase boundary between FFLO and normal state as well as between FFLO and uniform BCS state. The discontinuity at the former phase boundary is simply owing to the jump of SC order parameter at the first order phase transition. The latter discontinuity seems more surprising because that phase boundary is second order. The key lies in the appearance of Andreev bound states around the spatial nodes of the modulated SC order parameter in the FFLO state which introduce $\pi$-phase shifts in the SC order parameter as shown in the upper panel of Fig. 2. The continuous phase transition from the uniform BCS to FFLO state is associated with the nucleation of these domain walls like structures as shown in Fig. 2(a). The Andreev bound states localized around such domain
walls lead to the large quasiparticle density of states at the Fermi energy and induce the AF instability. The lower panel of Fig. 2 shows that the AF staggered moment is indeed localized around the domain walls. Because the coupling between the neighboring domain walls is weak, the Neél temperature is almost independent of the density of walls. Since the DOS is suppressed by the SC order parameter without $\pi$-phase shift, the AF order is absent in the uniform BCS state. Therefore, the $T_N$ is discontinuous although the averaged magnetic moment is continuous at the phase boundary between the uniform BCS state and FFLO state.

![Figure 2](image)

**Figure 2.** Upper panel: Spatial dependences of $d$-wave SC order parameter $\Delta(\vec{r})$ for the modulation vector of FFLO state, (a) $\vec{q}_F = (0.02\pi, 0)$, (b) $\vec{q}_F = (0.04\pi, 0)$, (c) $\vec{q}_F = (0.06\pi, 0)$ and (d) $\vec{q}_F = (0.08\pi, 0)$ at the phase boundary between the FFLO and FFLO+AF states. Lower panel: Spatial dependences of AF moment $M_{AF}(\vec{r}) = (-1)^{i+j}M(\vec{r})$ where $M(\vec{r})$ is the magnetic moment in the vicinity of the AF instability. We choose $\mu_0 = -0.8$ so that the commensurate AF order is favored. Note that $\Delta(\vec{r})$ and $M_{AF}(\vec{r})$ are independent of $y$. The other parameters are the same as in Fig. 1(a).

The discontinuity of $T_N$ at the normal-FFLO transition is qualitatively different between the commensurate AF order and the incommensurate AF order. As shown in Fig. 1, the AF order is slightly enhanced (suppressed) by the FFLO order in case of the incommensurate (commensurate) AF order. The two dimensional spatial dependence of incommensurate AF moment is depicted in Fig. 3. The parameters $H$ and $T$ are chosen so that the FFLO modulation vector is (a) $\vec{q}_F = (0.06\pi, 0)$, (b) $\vec{q}_F = (0.08\pi, 0)$, (c) $\vec{q}_F = (0.031\pi, 0.031\pi)$ and (d) $\vec{q}_F = (0.039\pi, 0.039\pi)$. It is reasonable to assume the FFLO modulation vector parallel to the magnetic field $\vec{q}_F \parallel \vec{H}$ because the vortex lattice favors this configuration [19]. Therefore, Figs. 3(a,b) and 3(c,d) show the AF moment for the magnetic field along [100] direction, and [110] direction, respectively. It is shown that the incommensurate structure along the nodal plane of FFLO order parameter is favored in both cases. We examined the possibility of incommensurate AF order perpendicular to the nodal plane, in which the $\pi$ phase shift of AF order parameter is pinned by the FFLO modulation. However, this AF state is less favorable than the AF state shown in Fig. 3 within the mean field theory.

Next we discuss the experimental results for CeCoIn$_5$ [12, 13]. The AF order observed at high magnetic fields and low temperatures might be considered as the coexistent state of FFLO superconductivity and AF order. However, according to our result this would imply the existence of AF order in the normal state too, in contrast to the experimental observation. While this discrepancy could be resolved using a more realistic electronic band structure of CeCoIn$_5$, we propose a scenario based on specific fluctuations of the AF wave vector $\vec{q}$. We assume that the spin susceptibility is enhanced at the incommensurate wave vector $\vec{q} = (\pi, \pi) - \vec{\delta}$ with a negligible
Figure 3. Spatial dependences of AF moment $M_{AF}(\vec{r})$ for $\mu_0 = -0.95$ which favors the incommensurate AF order. The FFLO modulation vector in each figure is given in the text. The other parameters are the same as in Fig. 1(b).

anisotropy in the small $\delta$. Such directional fluctuations are suppressed in the FFLO phase due to the anisotropy introduced by the FFLO nodal planes. On the other hand, the spin fluctuations are enhanced in the FFLO state because of the reduced effective dimensionality. Consequently, the realization of AF long range order in the FFLO phase depends on a subtle balance. If the directional fluctuation plays an quantitatively important role, the AF order in the normal state is suppressed. The idea of directional fluctuation of the incommensurate AF correlation could be tested by neutron scattering measurements. The way AF order and FFLO superconductivity coexist can be experimentally examined by the pressure measurements because the AF order is likely suppressed by the pressure in analogy with the case of CeRhIn$_5$ [20].

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References
[1] Fulde P and Ferrel R A 1964 Phys. Rev. 135 A550
[2] Larkin A I and Ovchinnikov Yu N 1964 Zh. Eksp. Teor. Fiz. 47 1136
[3] Matsuda Y and Shimahara H 2007 J. Phys. Soc. Japan 76 051005 and references there in
[4] Zwierlein M W et al. 2006 Science 311 492; Partridge G B et al. 2006 Science 311 503
[5] Casalbuoni R and Nardulli G 2004 Rev. Mod. Phys. 76 263
[6] Radovan H A et al. 2003 Nature 425 51
[7] Bianchi A et al. 2003 Phys. Rev. Lett. 91 187004
[8] Watanabe T et al. 2004 Phys. Rev. B 70 020506(R)
[9] Kakuyanagi K et al. 2005 Phys. Rev. Lett. 94 047602; Kumagai K et al. 2006 Phys. Rev. Lett. 97 227002
[10] Mitrovic V F et al. 2006 Phys. Rev. Lett. 97 117002
[11] Miclea C F et al. 2006 Phys. Rev. Lett. 96 117001
[12] Young B F et al. 2007 Phys. Rev. Lett. 98 036402
[13] Kenzelmann M et al. 2008 Science Express
[14] Uji S et al. 2006 Phys. Rev. Lett. 97 157001
[15] Lortz R et al. 2007 Phys. Rev. Lett. 99 187002
[16] Shimagawa J et al. 2007 Phys. Rev. Lett. 98 147002; Yonezawa S et al. 2008 Preprint arXiv:0801.0484
[17] Yanase Y 2008 J. Phys. Soc. Japan 77 063705
[18] Bianchi A et al. 2002 Phys. Rev. Lett. 89 137002; Tayama T et al. 2002 Phys. Rev. B 65 180504
[19] Adachi H and Ikeda R 2003 Phys. Rev. B 68 184510
[20] Kitaoka Y et al. 2005 J. Phys. Soc. Japan 74 186.