Phase structure and vortex configurations of superconductors coexisting with ferromagnetism

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Abstract. We study the Ginzburg-Landau lattice gauge model that we introduced recently for ferromagnetic superconductors, i.e., superconductors in which the p-wave superconducting (SC) order and the ferromagnetic (FM) order may coexist. We report some interesting results obtained by Monte-Carlo simulations. In particular, we have two types of coexisting states distinguished by the transition temperatures of the SC order \( T_{SC} \) and the FM order \( T_{FM} \): (i) homogeneous state for \( T_{FM}/T_{SC} > 1 \) and (ii) inhomogeneous state for \( T_{FM}/T_{SC} < 0.7 \). In (ii) the two orders appear only near the surface of the lattice as observed in ZrZn₂. We also study vortex configurations of SC order parameters. Two kinds of vortices, one for spin-up electron pairs and one for spin-down pairs show different behaviors because of the Zeeman coupling.

1. Introduction
Magnetism and superconductivity are two typical and important phenomena in condensed matter physics. The discovery of the ferromagnetic (FM) superconductor (SC) in 2000 [1] surprised many physicists because FMSC state is counter intuitive, i.e., magnetic field usually destroys SC. For this reasion, the FMSC has been of intensive interest for the last decade. Soon after its discovery, a phenomenological Ginzburg-Landau (GL) theory was proposed[2]. However, as the Cooper pair couples nontrivially to the magnetism through vector potential (i.e., gauge field) in the FMSC state, simple perturbative analysis of the GL theory such as mean-field theory does not give reliable results. That is, the FMSC state is another example of “competing orders” of strongly-correlated electron systems. In Ref.[3] we proposed a lattice-gauge-theory model for the FMSC state based on the above GL theory. In the elementary article physics, it is established that the lattice formulation of field theory is well suited for nonperturbative calculations, and, in particular, its numerical study gives very important results beyond the perturbative calculations. The mode that we proposed has just this advantage. As a result of lattice formulation, topologically nontrivial excitations such as vortices are included in a natural way as in the real materials with lattice structure. In this paper we explain the model and discuss some important results obtained by Monte Carlo simulations (MCS). In Sec.2, we review the model, and in Sec.3 we discuss the phase structure and the vortex configurations. Section 4 is devoted for the conclusion.
2. Model

The typical Ginzburg-Landau (GL) free-energy density $f_{GL}[2]$ proposed for the FMSC materials has the following form in the three-dimensional (3D) continuum space at finite $T$,

$$f_{GL} = K \sum_{\mu} (D_{\mu} \vec{\psi})^* \cdot (D_{\mu} \vec{\psi}) + (T - T_{SC}^0) |\vec{\psi}|^2 + \alpha_s |\vec{\psi}|^4$$

$$+ K' \sum_{\mu} \left( \partial_{\mu} \vec{m} \right)^2 + (T - T_{FM}^0) |\vec{m}|^2 + \alpha_f |\vec{m}|^4 + f_Z,$$

$$D_{\mu} = \partial_{\mu} - 2eA_{\mu}, \quad f_Z = -J\vec{m} \cdot \vec{S}, \quad \vec{S} = i\vec{\psi}^* \times \vec{\psi},$$

with the direction index $\mu = 1, 2, 3$. The three-component complex field $\vec{\psi} = (\psi_x, \psi_y, \psi_z)^T$ is the spin-triplet SC order parameter (the Cooper-pair field). $\vec{\psi}$ is proportional to the $\vec{d}$-vector in the spin space, $\vec{d} \propto \vec{d}$, and also the wave function of the $p$-wave SC state in the real space as a result of the spin-orbit coupling. In terms of $\vec{\psi}$, the magnetization (and angular momentum) $\vec{S}$ of Cooper pairs is expressed as in Eq.(1)[2]. The FM order is described by the magnetization $\vec{m}$ of electrons that do not participate in the SC state. $T_{SC}^0$ and $T_{FM}^0$ are the bare critical temperatures ($T$) of SC and FM transitions, respectively. Because $\vec{m}$ satisfies $\nabla \vec{m} = 0$, it can be expressed in terms of the vector potential $\vec{A}$ as $\vec{m} = \text{rot}\vec{A}$. Because the Cooper-pair field bears the electric charge $-2e$, it couples with $\vec{A}$ minimally via the covariant derivative $D_{\mu}$ reflecting the electromagnetic gauge invariance. $f_Z$ is the Zeeman coupling term between $\vec{S}$ and $\vec{m}$. It may induce the FMSC state[2], in which $\langle \vec{S} \rangle \neq 0$.

To obtain an effective lattice model, we follow the following simplifications. First, we consider the “London limit” of $\vec{\psi}$ such that $\vec{\psi} \cdot \vec{\psi} = \text{const.}$, neglecting its radial fluctuations. Second, because the Zeeman coupling $f_Z$ favors $\psi_{\uparrow\uparrow} \propto \psi_x + i\psi_y$ or $\psi_{\downarrow\downarrow} \propto \psi_x - i\psi_y$, we neglect $\psi_z = \psi_{\uparrow\downarrow}$, as in the previous studies[2]. That is we consider only the two-component complex field $(\psi_x, \psi_y)^T$ with $|\psi_x|^2 + |\psi_y|^2 = \text{const.}$. Then the GL energy density $f_r$ of the effective lattice model at the site $r$ of the 3D cubic lattice is given by

$$f_r = -\frac{c_1}{2} \sum_{\mu=1}^3 \sum_{\alpha=1}^2 (\bar{z}_{r+\mu} U_{r\mu} z_{r\alpha} + c.c.) - c_2 \bar{m}_r^2 - c_3 \vec{m}_r \cdot \vec{S}_r + c_4 (\bar{m}_r^2)^2 - c_5 \sum_{\mu} \bar{m}_r \cdot \vec{m}_{r+\mu},$$

where the Cooper-pair field $z_r$ is a two-component complex variable, $z_r = (z_{r1}, z_{r2})^T$ satisfying the CP$^1$ constraint, $|z_{r1}|^2 + |z_{r2}|^2 = 1$. It is related to $\psi_x$ and $\psi_y$ as $\psi_x \sim \sqrt{\rho} z_{r1}, \psi_y \sim \sqrt{\rho} z_{r2}$, where $\rho$ is the density of Cooper pairs per site. $U_{r\mu} = \exp(iA_{r\mu})$ is the exponentiated vector potential put on the link $(x, x + \mu)$, which is called U(1) gauge variable in lattice gauge theory. The FM order parameter $\vec{m}_r = (m_{rx}, m_{ry}, m_{rz})^T$ is the magnetic field made out of $A_{r\mu}$, $m_{r\mu} = \sum_{\nu,\lambda} c_{\mu\nu\lambda} \nabla_\nu A_{r\lambda}$, $\nabla_\nu A_{r\lambda} \equiv A_{r+\nu,\lambda} - A_{r\lambda}$. $\vec{S}_r = (0, 0, S_{rz})$ is the Ising-type spin vector of Cooper pairs made out of $z_{ra}$ as $S_{rz} \equiv i(z_{r1} z_{r2} - z_{r2}^* z_{r1}^*) \propto |\psi_{\uparrow\uparrow}|^2 - |\psi_{\downarrow\downarrow}|^2$. $f_r$ is invariant under a U(1) gauge transformation, $z_{ra} \to z_{ra}' = \exp(i\lambda_{ra}) z_{ra}$, $U_{r\mu} \to U_{r\mu}' = \exp(i\lambda_{r+\mu}) U_{r\mu} \exp(-i\lambda_r)$.

The five coefficients $c_i$ ($i = 1 \sim 5$) in (2) are real nonnegative parameters that are expected to distinguish various materials among each other. The meaning of each term in $f_r$ is the same as in the continuum case. The $c_1$-term describes coherent and gauge-invariant hopping of Cooper pairs. The $c_2$-term describes the quartic GL potential of $\vec{m}_r$ and favors a finite local magnetization $m_r^2 > 0$ (note that we take $c_2 > 0$). The $c_3$-term enhances uniform configurations of $\vec{m}_r$, i.e., a FM order with a finite magnetization, $\lim_{r \to r'} \to \infty (\vec{m}_r \cdot \vec{m}_{r'}) \neq 0$. The $c_4$-term is the Zeeman coupling, which favors parallel configurations of $\vec{m}_r$ and $\vec{S}_r$, namely the coexistence of ferromagnetism and superconductivity. The partition function $Z$ of the model at $T$ is given by the integral over the CP$^1$ site variables $z_{ra}$ and the real link variables $A_{r\mu}$,

$$Z = \int [dz][dA] \exp(-\beta F), \quad \beta = T^{-1}, \quad F = \sum_r f_r.$$
3. Results of Monte-Carlo simulations

3.1. Phase structure

In MCS, we consider the 3D lattice of the size \((2 + L)^2 \times L\), and impose the free boundary condition for \(\mu = 1.2\) and the periodic one for \(\mu = 3\). Physical quantities are calculated in the central region \(R\) of the size \(L^3\). To study the phase structure, we take \((c_1, c_2, c_3, c_4) = (0.2, 0.5, 0.2, 4.0)\). As \(\beta\) is varied, the specific heat exhibits two second-order phase transitions at \(\beta_{SC}\) and \(\beta_{FM}\). For \(c_5 = 1.0\), \(\beta_{SC} = 2.1\) and \(\beta_{FM} = 4.5\). As \(c_5\) is decreased, their order is reversed at \(c_5 \simeq 0.5\). For \(c_5 = 0.4\), \(\beta_{SC} = 5.0\) and \(\beta_{FM} = 8.3\).

To study the properties of each phase, it is useful to measure the correlation functions

\[
G_m(r - r_0) = \langle \vec{m}_r \cdot \vec{m}_{r_0} \rangle, \quad G_S(r - r_0) = \langle S_{r,z} S_{r_0,z} \rangle / \langle S_{r,z} S_{r_0,z} \rangle,
\]

where \(r_0\) is on the surface of \(R\) such as \((3, 2 + L/2, z)\). In Fig.1 we present them for \(c_5 = 1.0\) and \(c_5 = 0.4\). The SC and FM orders in the coexisting region are almost homogeneous for \(c_5 = 1.0\) throughout the lattice, while they are inhomogeneous for \(c_5 = 0.4\), the orders appearing only in the region near the surface of the lattice. The similar behavior is observed in ZrZn\(_2\) [1].

It is intriguing to draw a phase diagram in the pressure\((P)\)-\(T\) plane assuming certain phenomenological relation between \(c_5\) and \(P\). For example, one may "phenomenologically" assume

\[
P = P(c_5) = \left( \frac{c_5^*}{c_5^*} \right)^\gamma - \left( \frac{c_5^*}{c_5^*} \right)^\gamma P_c,
\]

where \(P_c\) is the critical pressure at which the FM order disappears even at \(T \to 0\) (i.e., at \(c_5 = 0\)), \(c_5^*\) is the value of \(c_5\) at which \(P = 0\), and the power \(\gamma\) is a fitting parameter. In Fig.2 we show the phase diagram drawn with certain choice of these parameters. This phase diagram has a similar structure to the experimental result of UCoGe.

**Figure 1.** Correlation functions \(G_m(r)\) and \(G_S(r)\) of (4) at various \(\beta\)'s for \((c_1, c_2, c_3, c_4) = (0.2, 0.5, 0.2, 4.0)\) and \(c_5 = 1.0\) (Left), 0.4 (Right). For \(c_5 = 0.4\) the FM and SC orders in the coexisting state are inhomogeneous; they appear only in the region near the surface of the lattice.

**Figure 2.** Phase diagrams in (a) \(c_5\)-\(T\) and (b) \(P\)-\(T\) planes with \(P_c = 1.0, c_5^* = 2.2\) and \(\gamma = 3.0\). \(c_1 - c_4\) are same as in Fig.1.
3.2. Vortex configurations

Vortices made of SC order parameters reflect the nature of SC state. In the present model, one may define the following two kinds of vortex densities $V_{x^+}$ and $V_{x^-}$ in the 1-2 plane;

$$z_{x^\pm} \equiv z_{x1} \pm iz_{x2} \equiv \rho_{x^\pm} \exp(i\lambda_{x^\pm}), \quad V_{x^\pm} \equiv \frac{1}{2\pi} [\mod(\lambda_{x+1,\pm} - \lambda_{x\pm} - \theta_{x1}) + \mod(\lambda_{x+1+2,\pm} - \lambda_{x+2,\pm} - \theta_{x+2,1}) - \mod(\lambda_{x+2,\pm} - \lambda_{x\pm} - \theta_{x2})].$$  (6)

In Fig. 3 we present snapshots of $V_{x^\pm}$ at $c_1 = c_3 = 0.2$ for fixed values of gauge potential $A_{x\mu}$ corresponding to constant magnetization, $\vec{m} = (0, 0, \pi/4)$. It shows that (i) both of the fluctuations around zero $\langle |V_{x^\pm}| \rangle$ decreases as $\beta$ increases, and (ii) $V_{x^+}$ has larger fluctuations than $V_{x^-}$ at high $T$, whereas smaller ones at low $T$. These behaviors are consistent with the Zeeman ($c_3$) term in the energy $f_r$ of (2), which distinguishes $z_{x^+}$ order and $z_{x^-}$ order, and the fact $\vec{m}$ directs to $z$-direction in the present case.

![Figure 3. Snapshots of vortex densities $V_{x^\pm}$ at $c_1 = c_3 = 0.2$ for a fixed $\vec{m} = (0, 0, \pi/4)$. (A)$V_{x^+}$ at $\beta = 3.0$, (B)$V_{x^-}$ at $\beta = 3.0$, (C)$V_{x^+}$ at $\beta = 7.0$, (D)$V_{x^-}$ at $\beta = 7.0$. The average magnitude $\langle |V_{x^\pm}| \rangle$ is (a) 0.387, (b) 0.380, (c) 0.331 and (d) 0.335. The points $V_{x^\pm} = -0.125 = -m_z/2\pi$ reflect $\vec{m}$ itself.](image)

4. Conclusion

We have explained the lattice gauge model introduced recently for the FMSC state, and shown that the model explains some experimental observations such as the phase diagram, properties of the coexisting state (homogeneous or inhomogeneous). The phase diagram and vortex configurations exhibit that the model is interesting enough and worth to study in other parameter regions in detail.

References

[1] Saxena S S et al. 2000 Nature (London) 406 587; Huxley A et al. 2001 Phys. Rev. B 63 144519; Tateiwa Net al. 2001 J. Phys. Condens. Matter 13 L17; Aoki D et al. 2001 Nature (London) 413 613; Pfleiderer C et al. 2001 Nature (London) 412 58.

[2] Machida K and Ohmi T 2001 Phys. Rev. Lett. 86 850; Walker M B and Samokhin K V 2002 Phys. Rev. Lett. 88 207001, Mineev V P 2002 Phys. Rev. B 66 134504.

[3] Shimizu A, Ichinose I and Matsui T 2011 preprint arXiv:1106.3130.