Spatial modulation patterns in two-dimensional Fulde-Ferrell-Larkin-Ovchinnikov superconductivity

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Abstract. FFLO superconductivity breaks the intrinsic translational symmetry and has spatially modulated order parameters. Determining its spatial modulation patterns is one of the fundamental problems concerning FFLO superconductivity. Preceding studies based on Ginzburg-Landau expansion showed that, in isotropic two-dimensional systems, patterns such as stripe, triangle, square and hexagon, are realized depending on the temperature and the applied magnetic field. However, Ginzburg-Landau expansion is not applicable at low temperatures, and another approach is necessary. In this research, based on Bogoliubov-de Gennes equations we investigate the patterns at zero temperature. By calculating free energies, we show that many patterns tend to be degenerate in contrast to the distinct energy difference at finite temperatures.

1. Introduction
Superconductivity is a quantum condensed state of Cooper pairs, which are bound states of electrons in a metal, and can have internal degrees of freedom. Fulde and Ferrell [1] considered spin-singlet Cooper pairs with a center-of-mass momentum $q$. In usual circumstances, if Cooper pairs have a nonzero momentum $q$, a macroscopic current flows, and such a state is not an equilibrium state. However, Fulde and Ferrell [1] pointed out that, in a spin-imbalanced system, nonzero momentum states can be an equilibrium state. This is because there exist quasi-particles other than Cooper pairs, which give an opposite current canceling that given by the Cooper pairs. One way to realize a spin-imbalanced state is to apply an external magnetic field. This nonzero momentum state is called the Fulde-Ferrell state, and its pair potential has the plane-wave form $\Delta(r) \propto e^{iqr}$.

While Fulde and Ferrell treated a single plane-wave state, Larkin and Ovchinnikov [2] considered superposition of plane waves having different directions. Such a state has a spatially modulated pair potential and is called the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state. One of the purposes of their work was to determine the most stable pattern of the pair potential in an equilibrium. By comparing free energies near the critical external magnetic field at zero temperature, they showed that in the three-dimensional isotropic system one-dimensional sinusoidal states are realized: $\Delta(r) \propto \cos(q \cdot r)$.

A few decades after the FFLO theory, two-dimensional (or layered structure) superconductors were discovered in materials such as organic conductors, heavy-Fermion compounds, and high-$T_c$ cuprates. Many of them were unconventional superconductors. This stimulated researches on two-dimensional superconductivity, and also on two-dimensional FFLO superconductivity [3].
In the two-dimensional FFLO superconductors, the determination of the spatial modulation pattern is a more complicated problem. Shimahara [4] extended Larkin and Ovchinnikov’s work into two dimensions and finite temperatures, and found that, as temperature is lowered, the most stable state changes sequentially from a simple pattern to complicated ones: stripe, triangular, square, and hexagon. This tendency is also found for more complicated states than hexagonal state [5].

In the above research, Shimahara employed Ginzburg-Landau (GL) expansion. However, in the two-dimensional isotropic system at low temperatures, GL expansion is not applicable [4], and another approach is necessary. In the present study, by solving Bogoliubov-de Gennes (BdG) equations, we investigate the patterns at zero temperature.

2. Bogoliubov-de Gennes equations and pair potential $\Delta(r)$

In order to treat the above problem, we assume an electron gas interacting via point-like attractive interaction in a two-dimensional isotropic system under the magnetic field causing Zeeman effect. As the pairing symmetry, we assume s-wave and spin-signlet. We treat superconductivity in mean field theory.

BdG equations are second order partial differential equations. As the means of analyzing this partial differential equations, we employ a finite-element method (FEM). By this method, we can deal with complicated boundary conditions. Applying a FEM to the BdG equations, we obtain the following generalized eigenvalue matrix equation

$$\left[ \begin{array}{c} K - \mu M \\ D^* \\ -K + \mu M \\ \end{array} \right] - E \left[ \begin{array}{c} M \\ M \\ M \\ \end{array} \right] = 0,$$  \hspace{1cm} (1)

where matrices $K$ and $D$ correspond to the kinetic term and pair potential, respectively, and matrix $M$ reflects the form of finite element. Here, $\mu$ is electron’s chemical potential. Boundary conditions are included in these matrices. Since the pair potential is spatially periodic, the Bloch’s theorem holds, and we only need to deal with a unit cell and include phase factors at the boundary conditions. In our calculation, we impose the periodic boundary condition to reduce the computational cost. This means that we only retain the $k = 0$ state.

The pair potential $\Delta(r)$ is determined self-consistently with a gap equation. To discretize the gap equation, we use the fact that it can be obtained by minimizing the free energy with respect to the pair potential. Applying the same FEM to the free energy and minimizing it with respect to the discretized pair potential, we obtain the following discretized gap equation

$$\sum_j M_{ij} \Delta_j = U \sum_n \sum_k u_{nj} Q_{jik} v^*_nk [1 - f(E_n - h) - f(E_n + h)],$$  \hspace{1cm} (2)

where $i, j,$ and $k$ represent the nodes of elements, and $Q_{jik}$ reflects the form of finite element. Here, $U(>0)$, $h$, and $f(x)$ are the pairing interaction, the Zeeman energy, and the Fermi distribution function, respectively. $u_n$, $v_n$, and $E_n$ are eigenvectors and eigenvalues of eq. (1). To simplify calculation, we only retained diagonal elements of these matrices in the gap equation (2) as $M_{ij} \rightarrow \delta_{ij}$, $Q_{jik} \rightarrow \delta_{ij}\delta_{ik}$.

As the spatial modulation patterns of pair potential, we assume uniform state, stripe, triangular, and square ones. First, we make linear combinations of plane waves $\Delta(r) = \Delta \sum_m e^{i\mathbf{q}_m \cdot \mathbf{r}} (|\mathbf{q}_m| = q)$, which have the above symmetries. Then, starting from this pair potential, we solve the BdG equations iteratively together with the gap equation, and obtain the solutions which have the same symmetries as the starting symmetry. To preserve the symmetry numerically, we adopt quadratic triangular elements for the stripe and the square patterns, and equilateral triangular ones for the triangular pattern.

The resultant pair potential is displayed in Figs. 1-4. Here, $\Delta_0$ is the amplitude of the pair potential in the uniform state without magnetic field at the zero temperature. Figure 1 and 2
The free energy is given by

$$\Omega = \sum_{n,\sigma = \pm 1} E_n f(E_n - \sigma h) - 2 \sum_n E_n \int \mathbf{dr} |\nabla_n(\mathbf{r})|^2 + \int \mathbf{dr} \frac{\Delta(\mathbf{r})^2}{U} + \mu N_e + k_BT \sum_{n,\sigma} [f(E_n - \sigma h) \log f(E_n - \sigma h) + (1 - f(E_n - \sigma h)) \log(1 - f(E_n - \sigma h))], \quad (3)$$

where $N_e$ and $T$ are the total electron number and the temperature. However, when we calculated the free energy of uniform state as a function of pair amplitude $\Delta$, the free energy minimum does not coincide with $\Delta$ which is the solution of the gap equation. This is because the simplification in the gap equation ($M_{ij} \rightarrow \delta_{ij}$, $Q_{ijk} \rightarrow \delta_{ij}\delta_{ik}$) affects the correct value of free energy. In order to get a semi-quantitative estimate of the free energy, we adopt the following procedure. In the uniform case, according to the BCS theory, we know $\Delta$-dependence of the free energy: $-\frac{1}{2}N_F|\Delta|^2 + N_F|\Delta|^2 \log \frac{|\Delta|}{\Delta_0}$. By taking the coefficient of the term $\int \mathbf{dr} \frac{|\Delta(\mathbf{r})|^2}{U}$ in
eq. (3) as a fitting parameter (which is order of unity), we can reproduce this $\Delta$-dependence as in Fig. 5. We use this quantity as an estimate of the free energy.

The resultant free energies are summarized in Fig. 6, in which magnetic field dependence for the normal, uniform, stripe (FFLO), and square state is shown. Normal state free energy behaves as $\propto -h^2$, which is consistent with Pauli paramagnetic behavior. Uniform superconducting state is independent of the magnetic field up to $h = \Delta_0$, and its free energy is lower than the normal state up until $h \sim 0.7\Delta_0$. This is known as Pauli limit: $h_P = \Delta_0/\sqrt{2}$ [7].

Both stripe and square states have lower energies than the normal state if the amplitude of the pair potential remains finite. They are close to the normal state free energy, and at low fields their free energies become higher than the uniform state. A little above the Pauli limiting field, it can be seen that these spatially modulated states have the lowest free energy among these four states. The free energy difference between the stripe and square states is rather small compared with the finite temperature results. This might be a characteristics of low temperature behavior. At the zero temperature, many state tend to have close energies. To make this point clear, more accurate calculations are necessary.

4. Summary
In summary, we investigated two-dimensional FFLO superconductivity at the zero temperature. Based on BdG equations, we could analyze wider area in the phase diagram than by GL expansion. As a result, we showed that at the zero temperature more patterns tend to be degenerate energetically than at finite temperatures.

References
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