

Superconductivity in a ferromagnetic layered compound

Hiroshi Shimahara and Satomi Hata*

Department of Quantum Matter Science, ADSM, Hiroshima University, Higashi-Hiroshima 739-8526, Japan

(Received 7 July 2000; revised manuscript received 11 September 2000)

We examine superconductivity in layered systems with large Fermi-surface splitting due to coexisting ferromagnetic layers. In particular, the hybrid ruthenate-cuprate compound $\text{RuSr}_2\text{GdCu}_2\text{O}_8$ is examined on the coexistence of the superconductivity and the ferromagnetism. We calculate critical fields of the superconductivity taking into account the Fulde-Ferrell-Larkin-Ovchinnikov state in a model with realistic Fermi surfaces the shapes of which are similar to those obtained by a band calculation. It is shown that the critical field is enhanced markedly due to nearly flat areas of the Fermi surfaces and the van Hove singularity points in the momentum space. The result of the critical field is very large for realistic parameters, and seems to support the coexistence in a microscopic scale. We also clarify the direction of the spatial oscillation of the order parameter, which may be observed by scanning tunneling microscope experiments.

I. INTRODUCTION

Recently, the coexistence of superconductivity and ferromagnetism (due to canted antiferromagnetism) has been reported in the hybrid ruthenate-cuprate compounds $R_{1.4}\text{Ce}_{0.6}\text{RuSr}_2\text{Cu}_2\text{O}_{10-\delta}$ ($R = \text{Eu}$ and Gd) and $\text{RuSr}_2\text{GdCu}_2\text{O}_8$.¹⁻⁴ These compounds have similar crystal structures to the high- T_c cuprate superconductor $\text{YBa}_2\text{Cu}_3\text{O}_7$ except that layers of CuO chains are replaced with ruthenate layers. Experimental and theoretical studies indicate that the ruthenate layers are responsible for the magnetic long-range order,^{3,5} while the cuprate layers for the superconductivity.³ Recently, it was found in some experiments⁴ that the ferromagnetism is due to canted antiferromagnetism, but large exchange interactions exist between the spins and the carriers.⁶

One of the remarkable features of these compounds is that the superconducting transition occurs at a temperature well below the (weak) ferromagnetic transition temperature unlike most of the other ferromagnetic superconductors. For example, in $\text{RuSr}_2\text{GdCu}_2\text{O}_8$, the superconducting transition was observed at $T_c \sim 46$ K, whereas the ferromagnetic transition at $T_M \sim 132$ K.¹ Therefore, the magnetic order can be regarded as a rigid background which is not modified very much by the appearance of the superconductivity. This picture was also supported by experimental observations.¹⁻⁴

For the coexistence of the superconductivity and the ferromagnetism, the possibility of an inhomogeneous superconducting state that is called a Fulde-Ferrell-Larkin-Ovchinnikov (FFLO or LOFF) state⁷ was discussed by Pickett *et al.*⁵ In this paper, we examine the FFLO state taking into account a realistic Fermi-surface structure, and clarify some conditions which stabilize the superconductivity at high fields.

First, we discuss a possibility of the FFLO state in the $\text{RuSr}_2\text{GdCu}_2\text{O}_8$ systems. In the presence of a ferromagnetic component of magnetic order on the ruthenate layers, exchange fields mediated by electrons displace Fermi surfaces of up and down spin electrons on the cuprate layers. Thus, they play a role like magnetic fields which act only on the

spin degrees of freedom but do not create Lorentz force. On the other hand, real magnetic fields created by the ordered spin moment are weak on the cuprate layers, according to the first-principles calculations of Pickett *et al.*⁵ Thus, we assume that they do not affect the superconductivity significantly. Therefore, the situation in the present systems is very similar to a quasi-two-dimensional type-II superconductor in magnetic fields nearly parallel to the layers.

Such a Fermi-surface splitting causes pair breaking as a splitting due to a parallel magnetic field. Therefore, it is unusual that the superconductivity survives in large exchange fields due to a ferromagnetic order. The magnitude of the exchange field in $\text{RuSr}_2\text{GdCu}_2\text{O}_8$ may exceed the Pauli paramagnetic limit (Chandrasekar-Clogston limit), which is an upper limit of the superconducting critical field due to the spin pair-breaking effect, unless the ferromagnetism is too weak.

The Pauli paramagnetic limit H_P at $T=0$ is roughly estimated from the zero-field transition temperature $T_c^{(0)}$ by a simplified formula $\mu_e H_P = 1.25 T_c^{(0)}$, where μ_e denotes the electron magnetic moment. For $\text{RuSr}_2\text{GdCu}_2\text{O}_8$, since the exchange field exists in practice, $T_c^{(0)}$ of isolated cuprate layers is not known. However, it would be appropriate to assume an upper bound as $T_c^{(0)} \lesssim 90$ K from the transition temperature of $\text{YBa}_2\text{Cu}_3\text{O}_{7+\delta}$ at the optimum hole density. Inserting this upper bound of $T_c^{(0)}$ into the formula of H_P , we obtain an upper bound of the Pauli paramagnetic limit $\mu_e H_P \lesssim 110$ K at $T=0$.

On the other hand, the band calculation gives an estimation $\mu_e B_{\text{ex}} = \Delta_{\text{ex}}/2 \sim 25$ meV/2 ~ 107 K,⁵ which is the same order as the upper bound of H_P estimated above. Therefore, there is a possibility that the Pauli paramagnetic limit is broken in the present compounds.

Here, however, we should note that both B_{ex} and H_P must be much smaller than these estimations actually. For the former, the value of Δ_{ex} must be smaller in practice, because the conventional ferromagnetic order was assumed in the band calculations. On the other hand, for the latter, the value of $T_c^{(0)}$ must be smaller in practice, since the hole density is

far away from the optimum value. The $\text{RuSr}_2\text{GdCu}_2\text{O}_8$ system is probably electron doped (not hole doped). However, $\text{RuSr}_2\text{GdCu}_2\text{O}_8$ has a high transition temperature ($T_c \approx 46$ K) in spite of the presence of the strong exchange fields. Thus, the above estimations are very crude. It depends on the magnitude of the ferromagnetic component of the canted antiferromagnetic structure whether the Pauli paramagnetic limit is broken in practice.

If the Pauli paramagnetic limit is broken in $\text{RuSr}_2\text{GdCu}_2\text{O}_8$ compounds, we need some extra mechanism to stabilize the superconductivity. If the superconductivity is due to the triplet pairing of parallel spin pairing, the Fermi-surface splitting does not contribute to pair breaking. However, from their crystal structures and high transition temperatures, it is plausible that the present compounds are categorized as high- T_c cuprate superconductors and the superconductivity is due to an anisotropic singlet pairing with line nodes, which is conventionally called a d -wave pairing. For the singlet pairing, the FFLO state is a candidate of the mechanism as well as the strong spin-orbit coupling.

On the possibility of the FFLO state, Pickett *et al.*⁵ pointed out that there are nearly flat areas in the Fermi surfaces in $\text{RuSr}_2\text{GdCu}_2\text{O}_8$, which favor the FFLO state. It is known that the FFLO critical field diverges at $T=0$ in one-dimensional models. However, if the Fermi surfaces are too flat, a nesting instability to a spin density wave (SDW) or a charge density wave (CDW) is favored for realistic interaction strengths. For the present compound, even the flattest areas are not flat enough to induce the nesting instabilities, but the small curvature should enhance the FFLO state.⁸

It is also known that even in the absence of the flat areas, the critical field is enhanced in the two-dimensional (2D) systems in comparison to the three-dimensional systems.^{9,8,10,11} Further, when the Fermi-surface structure of the system satisfies a certain condition, the critical field can reach several times the Pauli limit even in the absence of nearly flat areas.¹² Such a Fermi-surface effect can be regarded as a kind of nesting effect analogous to that for an SDW and a CDW.^{8,11,12}

Direct evidence of the FFLO state may be obtained by scanning tunneling microscope (STM) experiments. For a comparison with experimental results, the spatial structure of the order parameter should be predicted theoretically. In particular, the direction of the modulation of the order parameter is important. It may appear that the modulation must be in the direction perpendicular to the flattest areas of the Fermi surface, because then the spatial variation is minimized. However, in some 2D models, it is not perpendicular to the flattest areas,^{11,12} at least just below the critical field. Only explicit calculations which take into account the Fermi-surface structure could clarify the direction of the modulation.

Therefore, we estimate the critical field and find the direction of the spatial oscillation of the order parameter of the FFLO state in this paper. We examine a tight-binding model with Fermi surfaces the shapes of which are similar to those of $\text{RuSr}_2\text{GdCu}_2\text{O}_8$, because the quantities that we are calculating are sensitive to the Fermi-surface structure.

Recently, the FFLO state has been studied in a tight-binding model with only nearest-neighbor hopping.^{12,13} It was found that ratio of the FFLO critical field and the Pauli

limit is small near the half filling. Zhu *et al.* have discussed that hence the coexistence of the superconductivity and the ferromagnetic order is difficult except in the vicinity of the ferromagnetic domains near the half filling.^{13,14} However, some experimental results indicate coexistence on a microscopic scale and a bulk Meissner state.^{1,15} Here, we should note that the tight-binding model with only nearest-neighbor hopping cannot reproduce the shapes of the Fermi surfaces of $\text{RuSr}_2\text{GdCu}_2\text{O}_8$. By taking into account the realistic Fermi-surface structure, we will show below that the critical field is enhanced markedly and thus coexistence on a microscopic scale is possible in this compound.

In Sec. II, we define the model and show a formulation to estimate the critical fields including possibility of the FFLO state. We fit a realistic Fermi surface obtained by band calculations⁵ with a tight-binding model. In Sec. III, we solve the equation numerically, and show a physical interpretation of the results. The last section is devoted to a summary and discussion.

II. MODEL AND A FORMULATION

First, we define the tight-binding model

$$H_0 = \sum_{p\sigma} \epsilon_{p\sigma} c_{p\sigma}^\dagger c_{p\sigma}, \quad (1)$$

with a dispersion relation

$$\epsilon_{p\sigma} = -2t(\cos p_x + \cos p_y) - 4t_2 \cos p_x \cos p_y - \mu + h\sigma, \quad (2)$$

where h denotes the exchange field, which is written in terms of the corresponding magnetic field B by a relation $h = \mu_e B$. We use units with $t=1$ and lattice constant $a=1$ in this paper.

Here, it should be noted that Eq. (2) is used only as a fitting function to describe a realistic electron dispersion near the Fermi surface mathematically. It does not necessarily mean that a tight-binding picture holds in the present system, even if Eq. (2) produces the realistic Fermi-surface structure very well. If a tight-binding picture does not hold in the compounds under consideration, the hopping constants t and t_2 are only fitting parameters, which do not have the physical meaning of hopping energies. However, we may use Eq. (2) practically as a fitting function, as far as we are interested in electrons near the Fermi surface.

We take the value of the fitting parameter $t_2 = -0.6t$, which gives shapes of the Fermi surfaces similar to the symmetric CuO_2 barrel Fermi surfaces obtained by Pickett *et al.*⁵ at $n=1.1$ as shown in Fig. 1.¹⁶ Here, n is the electron number per a site. Pickett *et al.* did not take into account the canted antiferromagnetic order, but the influence of the antiferromagnetic order on the Fermi-surface structure is large only in limited areas in the momentum space, that is, only near the boundary of the half Brillouin zone. Therefore, we use the result of Pickett *et al.* as an approximation.

We calculate the critical field in the ground state for $n = 0.92 \sim 2$, applying a formula developed in our previous papers.^{11,12} For anisotropic pairing

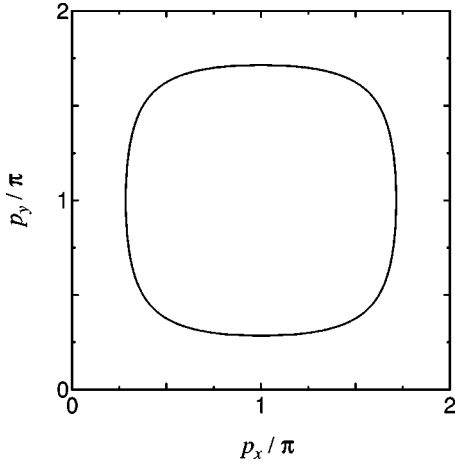


FIG. 1. Fermi surface of the present model Hamiltonian for $t_2 = -0.6$ and $n = 1.1$.

$$\Delta(\hat{\mathbf{p}}, \mathbf{r}) = \Delta_\alpha \gamma_\alpha(\hat{\mathbf{p}}) e^{i\mathbf{q} \cdot \mathbf{r}} \quad (3)$$

($\hat{\mathbf{p}} \equiv \mathbf{p}/|\mathbf{p}|$), due to the anisotropic pairing interaction

$$V(\mathbf{p}, \mathbf{p}') = -g_\alpha \gamma_\alpha(\hat{\mathbf{p}}) \gamma_\alpha(\hat{\mathbf{p}}'), \quad (4)$$

the second-order transition field of the superconductivity is calculated as follows. The gap equation at the second-order transition point is written as

$$\Delta_\alpha = g_\alpha \Pi_\alpha \Delta_\alpha, \quad (5)$$

with

$$\begin{aligned} \Pi_\alpha &= \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} \frac{1}{N} \sum_{\mathbf{p}} [\gamma_\alpha(\mathbf{p})]^2 \\ &\times \frac{1}{-\omega - i \operatorname{sgn}(\omega) \delta - \epsilon_{\mathbf{p}\downarrow}} \frac{1}{\omega + i \operatorname{sgn}(\omega) \delta - \epsilon_{\mathbf{p}+\mathbf{q}\uparrow}}. \end{aligned} \quad (6)$$

A momentum-dependent density of states $\rho_\perp(\epsilon, p_\parallel)$ is introduced by a replacement

$$\frac{1}{N} \sum_{\mathbf{p}} (\dots) = \int_{-\omega_c}^{\omega_c} d\epsilon \int \frac{dp_\parallel}{2\pi} \rho_\perp(\epsilon, p_\parallel) (\dots),$$

where p_\parallel denotes a momentum point on the equienergy surface, and ω_c is the energy cutoff of the pairing interactions. For small ω_c , we can put $\epsilon = 0$ in ρ_\perp . Performing frequency and energy integrations, we obtain a formula in the weak-coupling limit

$$h_c = \max_{\mathbf{q}} \left[\frac{\Delta_{\alpha 0}}{2} \exp \left(- \int \frac{dp_\parallel}{2\pi} \frac{\rho_\perp^\alpha(0, p_\parallel)}{N_\alpha(0)} \ln \left| 1 - \frac{\mathbf{v}_F \cdot \mathbf{q}}{2h_c} \right| \right) \right], \quad (7)$$

with $h_c = \mu_e H_c$, where $\Delta_{\alpha 0} \equiv 2\omega_D \exp[-1/g_\alpha N_\alpha(0)] \approx 1.76k_B T_c$ and $\rho_\perp^\alpha(0, p_\parallel) \equiv \rho_\perp(0, p_\parallel) [\gamma_\alpha(\hat{\mathbf{p}})]^2$. An effective density of states, $N_\alpha(0)$, for anisotropic pairing is defined by $N_\alpha(0) \equiv N(0) [\langle [\gamma_\alpha(\hat{\mathbf{p}})]^2 \rangle]$, with an average on the Fermi surface:

$$\langle \dots \rangle = \int \frac{dp_\parallel}{2\pi} \frac{\rho_\perp(0, p_\parallel)}{N(0)} (\dots) |_{|\mathbf{p}|=p_F(p_\parallel)}, \quad (8)$$

where $N(0)$ is the density of states at the Fermi level.

In the above equations, the vector \mathbf{q} is the center-of-mass momentum of Cooper pairs of the FFLO state. From the symmetry of the system, there are four or eight equivalent optimum vectors (\mathbf{q}_m 's), depending on whether \mathbf{q} is in a symmetry direction or not, respectively. Actually, an arbitrary linear combination of $\exp(i\mathbf{q}_m \cdot \mathbf{r})$ gives the same second-order transition field, and the degeneracy is removed by the nonlinear term of the gap equation below the critical field.^{7,17} However, regarding the critical field and the optimum direction of the oscillation of the order parameter near the critical field, it is sufficient to take a single \mathbf{q} as in Eq. (3).

For d -wave pairing, we use a model with $\gamma_d(\hat{\mathbf{p}}) \propto \cos p_x - \cos p_y$, where p_x and p_y are the momentum components on the Fermi surface in the directions of $\hat{\mathbf{p}}$. In our previous papers, it was shown that the qualitative and semiquantitative results are not sensitive to details of the form of $\gamma_d(\hat{\mathbf{p}})$.^{11,12}

The Pauli paramagnetic limit H_P for anisotropic pairing superconductivity is calculated as follows in the absence of the FFLO state. For the pairing interaction given by Eq. (4), the gap equation at $T=0$ is written as

$$\begin{aligned} 1 &= g_\alpha N(0) \left[\langle [\gamma_\alpha(\hat{\mathbf{p}})]^2 \rangle \ln \frac{2\omega_c}{\Delta_\alpha} \right. \\ &\left. + \left\langle [\gamma_\alpha(\hat{\mathbf{p}})]^2 \ln \left(\frac{1}{|\gamma_\alpha(\hat{\mathbf{p}})|} \right) \right\rangle \right]. \end{aligned} \quad (9)$$

Hence, we have

$$\Delta_\alpha = \frac{1}{\gamma_\alpha} \Delta_{\alpha 0}, \quad (10)$$

with

$$\frac{1}{\gamma_\alpha} = \exp \left(\frac{\langle [\gamma_\alpha(\hat{\mathbf{p}})]^2 \rangle \ln [1/|\gamma_\alpha(\hat{\mathbf{p}})|]}{\langle [\gamma_\alpha(\hat{\mathbf{p}})]^2 \rangle} \right), \quad (11)$$

at $T=0$.

The Pauli paramagnetic limit is the magnetic field at which the condensation energy balances the loss in the spin polarization energy. Thus, we have

$$\frac{1}{2} N_\alpha(0) |\Delta_\alpha|^2 = \frac{1}{2} \chi H_P^2, \quad (12)$$

where χ is the susceptibility in the normal state. If we can ignore the internal field enhancement, we may simply put $\chi = 2N(0)$. Therefore, we obtain a result

$$\mu_e H_P = \frac{\sqrt{\langle [\gamma_\alpha(\hat{\mathbf{p}})]^2 \rangle} \Delta_{\alpha 0}}{\bar{\gamma}_\alpha \sqrt{2}}. \quad (13)$$

The estimation of H_c by Eq. (7) does not have the physical meaning of a critical field if the Pauli paramagnetic limit is larger than H_c . For example, in the case of isotropic pair-

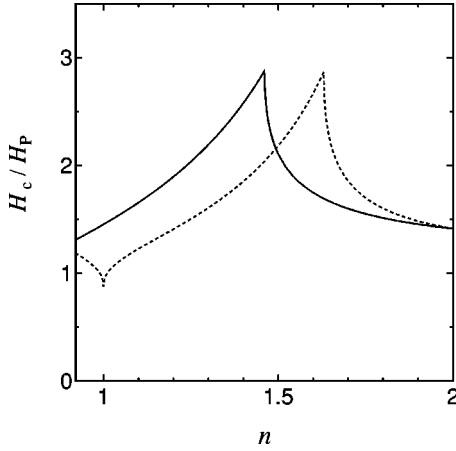


FIG. 2. Critical fields of the FFLO state of the s -wave pairing for $n=0.92\sim 2$ at $T=0$. Solid and dashed lines show the results for $t_2=-0.6$ and $t_2=0$, respectively.

ing $\gamma_\alpha=1$, if we put $\mathbf{q}=0$ in Eq. (7), we obtain $h_c = \Delta_{\alpha 0}/2$, which is smaller than $\mu_e H_P = \Delta_{\alpha 0}/\sqrt{2}$. Then, the first-order transition at the Pauli paramagnetic limit H_P is the real critical field. However, when we consider a possibility of the FFLO state ($\mathbf{q}\neq 0$), the second-order transition field H_c may exceed the Pauli paramagnetic limit H_P . Then, the FFLO state occurs at fields below H_c , at least above H_P . In order to find whether the upper critical field is determined by the second-order transition to the FFLO state ($\mathbf{q}\neq 0$) or the first-order transition to the BCS state ($\mathbf{q}=0$), we need to explicitly solve Eq. (7), optimizing \mathbf{q} .

However, if the critical field with $\mathbf{q}\neq 0$ exceeds H_P only slightly, it is not practical to consider that the FFLO state occurs in real materials. In that case, only a slight enhancement of the internal field [$\chi > \chi_0 = 2N(0)$] can suppress the FFLO state in practice,^{18,8,9,11} where χ_0 denotes the susceptibility of the free electron system. Since the Zeeman energy is enhanced by a factor χ/χ_0 , the real second-order transition field is χ_0/χ times the solution of Eq. (7). On the other hand, it is obvious from Eq. (12) that the real Pauli paramagnetic limit is $\sqrt{\chi_0/\chi}$ times H_P of Eq. (13). Thus, the enhancement of the internal field reduces the ratio H_c/H_P by a factor $\sqrt{\chi_0/\chi}$. The short-range repulsive Coulomb interactions between electrons, which are considered to be strong in the cuprate superconductors, enhance the internal field. Therefore, in the above estimations before the internal field enhancement is considered, we need to obtain a larger value of H_c/H_P than $\sqrt{\chi/\chi_0}$ for the FFLO state to occur in a finite region of the magnetic field.

III. RESULTS AND A PHYSICAL INTERPRETATION

Figures 2 and 3 show numerical results of the critical fields for $t_2=-0.6$ (solid and dashed lines) with our previous results for $t_2=0$ (Ref. 12), (dotted lines). It is found that the critical fields are markedly enhanced near the electron densities $n\approx 1.46$ and 1.20 for s -wave and d -wave pairings, respectively. At the electron density $n=1.1$, which is appropriate for $\text{RuSr}_2\text{GdCu}_2\text{O}_8$, the ratios of the critical field to the Pauli paramagnetic limit are approximately equal to 1.66 and 3.19 for s -wave and d -wave pairings, respectively. These

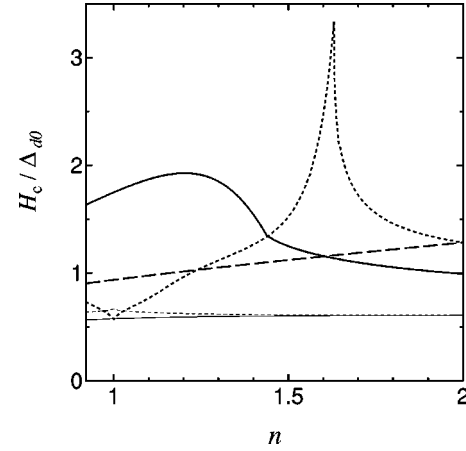


FIG. 3. Critical fields of the FFLO state of the d -wave pairing for $n=0.92\sim 2$ at $T=0$. Solid and dashed lines show the results for $\varphi_{\mathbf{q}}=\pi/4$ and $\varphi_{\mathbf{q}}=0$, respectively, when $t_2=-0.6$. The dotted line shows the result for $t_2=0$. Thin solid line and thin dotted line show the Pauli paramagnetic limits in the unit of Δ_{d0} for $t_2=-0.6$ and 0 , respectively.

values, especially the latter, seem to be large enough to make coexistence possible in the present compound. For example, the FFLO state survives against the internal field enhancement up to $\chi/\chi_0 \sim (H_c/H_P)^2 \sim 10.2$ at $T=0$ for d -wave pairing.

In Fig. 3 for d -wave pairing, both the critical fields for $\varphi_{\mathbf{q}}=\pi/4$ and $\varphi_{\mathbf{q}}=0$ are shown, but the highest one is the final result of the critical field given by Eq. (7). Here, $\varphi_{\mathbf{q}}$ is the angle between the optimum \mathbf{q} and one of the crystal axes. It is shown by a numerical calculation that the critical fields for the other values of $\varphi_{\mathbf{q}}$ are lower than the higher one of the critical fields for $\varphi_{\mathbf{q}}=\pi/4$ and 0 . Thus, the direction of the optimum wave vector \mathbf{q} jumps from $\varphi_{\mathbf{q}}=\pi/4$ to $\varphi_{\mathbf{q}}=0$ at $n\approx 1.63$. On the other hand, for s -wave pairing, $\varphi_{\mathbf{q}}=\pi/4$ is the optimum in the whole region of the electron density. These behaviors are different from that for $t_2=0$, in which $\varphi_{\mathbf{q}}=0$.¹²

For $t_2=-0.6$, a cusp is seen in Fig. 2 for s -wave pairing, whereas it does not appear in Fig. 3 for d -wave pairing (the solid and dashed lines). The physical origin of the cusp at $n\approx 1.46$ for s -wave pairing is that the Fermi-surface structure satisfies a certain condition there, which was explained in our previous paper for $t_2=0$.¹² The condition is related to how the two Fermi surfaces (for up and down spin electrons) touch by the translation by the optimum \mathbf{q} . In the present case ($t_2=-0.6$ and $n\approx 1.46$), the Fermi surfaces touch in the (110) direction, but for d -wave pairing, because of the nodes of the order parameter, the ‘‘nesting’’ is less efficient than for s -wave pairing. Therefore, a cusp does not appear for d -wave pairing, and the critical field even decreases near $n\approx 1.46$.

In spite of the absence of cusp behavior, the critical field is very large for d -wave pairing near half-filling. The value $H_c/H_P=3.19$ obtained here is much larger than the values obtained in the isotropic two-dimensional models (about 1.41 and 1.81 for s -wave and d -wave pairings, respectively) and the value in the model with $t_2=0$ at the same electron density (about 1.21 at $n=1.1$). This marked enhancement originates from a Fermi-surface effect explained as follows.

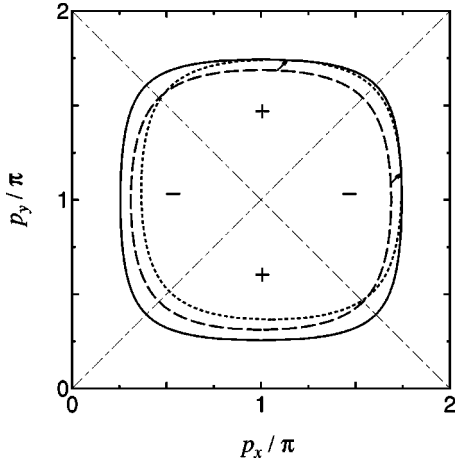


FIG. 4. Fermi-surface nesting for the FFLO state and the optimum wave vector \mathbf{q} of the FFLO state at the critical field ($h_c = 1.87\Delta_{d0}$) at $n = 1.1$. Solid and dashed lines show the Fermi surfaces of the up and down spin electrons, respectively. The dotted line shows the Fermi surface of the down spin electrons shifted by \mathbf{q} . Small arrows show the wave vector \mathbf{q} . They are placed at the momenta at which the two Fermi surfaces touch. Dot-dashed lines show the nodes of the d -wave order parameter. From the numerical calculations, we have $q = 0.805h_c/t$ and $h_c = 1.87\Delta_{d0}$. In this figure, we used a large value of $\Delta_{d0} = 0.3t/1.87$ (i.e., $h_c = 0.3t$) in order to make the displacement visible.

Figure 4 explains the nesting behavior of the Fermi surfaces at $t_2 = -0.6$ and $n = 1.1$. The direction of the optimum vector \mathbf{q} is $\varphi_{\mathbf{q}} = \pi/4$, and the Fermi surfaces touch at two points (i.e., two lines in $p_x p_y p_z$ space), $(p_x, p_y) \approx (1.113\pi, 1.713\pi)$ and $(1.713\pi, 1.113\pi)$. Since $\varphi_{\mathbf{q}} = \pi/4$ is also the direction of a node of the d -wave order parameter, it may appear that this direction is less favorable. However, in actuality the critical field is markedly enhanced for this “nesting” vector \mathbf{q} , since it gives two nesting lines which are far away from the nodes but near the flattest areas, as shown in Fig. 4. In addition, they are near both the maxima of the d -wave order parameter and the van Hove singularities, which also enhance the critical field. As the electron density increases, the two nesting lines approach the line node of the order parameter, and thus the critical field decreases.

IV. SUMMARY AND DISCUSSION

We have calculated the critical fields of the FFLO state and the optimum wave vector of the FFLO state in a model which simulates a realistic Fermi-surface shape of the $\text{RuSr}_2\text{GdCu}_2\text{O}_8$ system. A marked enhancement of the FFLO state has been found for realistic electron densities, and a physical reason for the enhancement has been explained.

The enhancement is due to that the nearly flat areas of the Fermi surfaces are placed near the van Hove singularity points in momentum space and the maxima of the d -wave order parameter at the same time. Since the $\text{RuSr}_2\text{GdCu}_2\text{O}_8$ system has this feature of the Fermi surfaces, the appearance of the FFLO state is hopeful, at least in sufficiently strong parallel magnetic fields. The wave vector of the FFLO state is not perpendicular to the nearly flat areas of the Fermi

surfaces as usually considered, but is oriented to a (110) direction in spite of the nodes of the d -wave order parameter.

This mechanism of enhancement is very different from those studied so far.^{11,12} Hence, the behavior of the critical field is quite different from that obtained in our previous paper.¹² For $t_2 = 0$ or for s -wave pairing, the enhancement occurs with a cusp behavior as a function of the electron density. On the other hand, in the present system with $t_2 = -0.6t$ (for d -wave pairing), the enhancement occurs in a wider range of the electron density, but a cusp behavior does not occur.

If the ferromagnetic component of the canted antiferromagnetic order is small, the exchange fields between spins and carriers are weak, although it might be inconsistent with experimental results.⁶ If the exchange fields are too weak, the superconductivity must be a BCS state with $\mathbf{q} = 0$, not an FFLO state. However, if we apply magnetic fields parallel to the layers, they would easily change the cant angle of the magnetic structure and could increase the exchange fields. We might be able to attain a strong exchange field experimentally at which the FFLO state is stabilized.

The direction of the optimum wave vector \mathbf{q} of the FFLO state is important for future observations of order parameter structures. Since the optimum direction $\varphi_{\mathbf{q}} = \pi/4$ is in a symmetry line, there are four equivalent directions, that is, $\varphi_{\mathbf{q}} = \pm \pi/4$ and $\pm 3\pi/4$. Therefore, symmetric linear combinations such as

$$\Delta(\mathbf{p}, \mathbf{r}) \propto \cos(qx'),$$

$$\Delta(\mathbf{p}, \mathbf{r}) \propto \cos(qx') + \cos(qy')$$

are good candidates to be considered, where $x' = (x + y)/\sqrt{2}$ and $y' = (x - y)/\sqrt{2}$. In particular, the latter 2D structures are favored at high fields.¹⁷

For the FFLO state to appear, the temperature needs to be lower than the tricritical temperature T^* of the FFLO, BCS, and normal states. T^* is generally equal to about $0.56T_c^{(0)}$ in simplified models such as Eq. (4). If we apply this to the present system $\text{RuSr}_2\text{GdCu}_2\text{O}_8$, $T^* \geq T_c \approx 46$ K requires $T_c^{(0)} \geq 82$ K, if we assume the superconductivity below 46 K is the FFLO state.

This condition for $T_c^{(0)}$ is relaxed by taking into account a mixing of order parameters of different symmetries, which increases T^* .^{19,20} The FFLO state is sensitively enhanced by subdominant triplet pairing interactions due to a mixing effect.

On the other hand, the internal field enhancement reduces the ratio H_c/H_P in practice by the factor $\sqrt{\chi_0/\chi}$ as we have discussed above. The region of the magnetic field where the FFLO state occurs disappears if the ratio H_c/H_P becomes less than 1 due to this factor. The large value $H_c/H_P \approx 3.19$ obtained here means that a region of the magnetic field exists unless there is an extremely strong enhancement of the internal field $\chi \geq 10.2\chi_0$.

In conclusion, our results seem to support the conjecture that the superconductivity and magnetic order could coexist in a microscopic scale in the $\text{RuSr}_2\text{GdCu}_2\text{O}_8$ system even if the magnetic order create very large exchange fields on the cuprate layers. If the exchange fields due to the magnetic order are sufficiently large, the superconductivity observed

near 46 K is expected to be an FFLO state. Even if not, the $\text{RuSr}_2\text{GdCu}_2\text{O}_8$ system can be an FFLO superconductor in some appropriate conditions discussed above, for example, at high external fields. A calculation for finite temperatures remains for a future study.

ACKNOWLEDGMENT

This work was supported by a grant for Core Research for Evolutionary Science and Technology (CREST) from Japan Science and Technology Corporation (JST).

*Present address: Semiconductor Energy Laboratory Co., Ltd., Atsugi-shi Hase, Kanagawa 243-0036, Japan.

¹C. Bernhard *et al.*, Phys. Rev. B **59**, 14 099 (1999).

²D.J. Pringle, J.L. Tallon, B.G. Walker, and H.J. Trodahl, Phys. Rev. B **59**, R11 679 (1999).

³I. Felner, U. Asaf, Y. Levi, and O. Millo, Phys. Rev. B **55**, R3374 (1997).

⁴O. Chmaissem *et al.*, Phys. Rev. B **61**, 6401 (2000); J.W. Lynn *et al.*, *ibid.* **61**, 14 964 (2000); J. Akimitsu *et al.* (private communication).

⁵W.E. Pickett, R. Weht, and A.B. Shick, Phys. Rev. Lett. **83**, 3713 (1999).

⁶J. F. McCrone, J. R. Cooper, and J. L. Tallon, J. Low Temp. Phys. (to be published).

⁷P. Fulde and R.A. Ferrell, Phys. Rev. **135**, A550 (1964); A.I. Larkin and Yu.N. Ovchinnikov, Zh. Éksp. Teor. Fiz. **47**, 1136 (1964) [Sov. Phys. JETP **20**, 762 (1965)].

⁸H. Shimahara, Phys. Rev. B **50**, 12 760 (1994).

⁹H. Burkhardt and D. Rainer, Ann. Phys. (Leipzig) **3**, 181 (1994).

¹⁰N. Dupuis, Phys. Rev. B **51**, 9074 (1995).

¹¹H. Shimahara, J. Phys. Soc. Jpn. **66**, 541 (1997).

¹²H. Shimahara, J. Phys. Soc. Jpn. **68**, 3069 (1999); J. Supercond. **12**, 469 (1999).

¹³J.-X. Zhu *et al.*, Phys. Rev. B **62**, 11 369 (2000).

¹⁴C. W. Chu *et al.*, Phys. Rev. B (to be published).

¹⁵C. Bernhard, J.L. Tallon, E. Brücher, and R.K. Kremer, Phys. Rev. B **61**, 14 960 (2000).

¹⁶For the reason that we have explained above, this does not mean that the present compound has such a large next-nearest-neighbor hopping energy actually.

¹⁷H. Shimahara, J. Phys. Soc. Jpn. **67**, 736 (1998); **67**, 1872 (1998); Physica B **259-261**, 492 (1999).

¹⁸S. Takada and T. Izuyama, Prog. Theor. Phys. **41**, 635 (1969).

¹⁹S. Matsuo, H. Shimahara, and K. Nagai, J. Phys. Soc. Jpn. **63**, 2499 (1994).

²⁰H. Shimahara, Phys. Rev. B **62**, 3524 (2000).