Angular dependence of in-plane upper critical field $H_{c2}$ in $d$-wave superconductors

Jing-Rong Wang and Guo-Zhu Liu

Department of Modern Physics, University of Science and Technology of China, Hefei, Anhui 230026, P. R. China

The angular dependence of in-plane upper critical field $H_{c2}$ is widely used to identify the precise gap symmetry of unconventional $d$-wave superconductors. Apart from the well studied orbital effect of external magnetic field, $H_{c2}$ is also believed to be strongly influenced by the Pauli paramagnetic effect in some heavy fermion compounds. After calculating $H_{c2}$ in the presence of both the orbital and Pauli effects, we find that its concrete angular dependence is determined by the subtle interplay of these two effects. An interesting and unexpected result is that $H_{c2}$ may exhibit its maximal values along the nodal or antinodal directions, depending on the specific values of a number of physical parameters. We perform a systematical analysis on how the fourfold oscillation pattern of $H_{c2}$ is affected by these parameters, and then apply our results to understand the recent experiments of $H_{c2}$ in two heavy fermion compounds CeCoIn$_5$ and CeCu$_2$Si$_2$.

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I. INTRODUCTION

Unconventional superconductors usually refer to the superconductors those can not be understood within the conventional Bardeen-Cooper-Schrieffer (BCS) theory. Notable examples are high-$T_c$ cuprates, heavy fermion superconductors, organic superconductors and iron based superconductors. The unconventional superconductivity is usually driven by strong electron-electron interaction, and the electron pairing mechanism usually has a magnetic origin. In the past decades, identifying the precise gap symmetry of unconventional superconductors has attracted great theoretical and experimental efforts since such efforts may lead to important progress in seeking the microscopic pairing mechanism.

Many unconventional superconductors are believed to have a $d$-wave energy gap, which is different from that of isotropic $s$-wave superconductors. However, it is not an easy task to determine the precise $d$-wave gap symmetry. A powerful and frequently used approach is to probe the angular dependence of various observable quantities, such as upper critical field$^{10-17}$, specific heat$^{18-21}$, and thermal conductivity$^{19,23-25}$. In this paper, we are mainly interested in the behaviors of in-plane upper critical field $H_{c2}$ in heavy fermion superconductors. This issue has recently been addressed with the aim to identify the precise gap symmetry of some heavy fermion compounds, especially CeCoIn$_5$ and CeCu$_2$Si$_2$. Despite the intensive theoretical and experimental efforts, it remains unclear whether the gap symmetry of these compounds is $d_{x^2-y^2}$-wave or $d_{xy}$-wave. These two gaps are different from each other primarily in the positions of gap nodes. In principle, their positions can be clarified by measuring the angular dependence of $H_{c2}$. Unfortunately, experimental studies have not yet reached a consensus on this issue. In the case of CeCoIn$_5$, currently most of experiments suggest that the gap symmetry should be $d_{x^2-y^2}$-wave$^{20,26,27}$, however there is currently still an experimental discrepancy in the concrete angular dependence of $H_{c2}$ in CeCoIn$_5$: some experiments find that the maxima of $H_{c2}$ are along the [100] direction$^{10,28,29}$, whereas other experiment observes the maxima along the [110] direction$^{30}$. This discrepancy is still a open puzzle which need to be resolved$^{22}$. In the case of CeCu$_2$Si$_2$, many earlier experiments suggest a $d_{x^2-y^2}$-wave gap$^{31,32}$. Nevertheless, a recent measurement$^{22}$ observes the maxima of $H_{c2}$ along the [100] direction, which is argued to infer a $d_{xy}$-wave gap according the corresponding theoretical analysis$^{33}$. Apparently, more research efforts are called for to solve these puzzles, which have motivated us to revisit this issue more systematically.

Now suppose an external magnetic field is introduced to a superconductor. In principle, this field can couple to the charge and spin degrees of freedom of the electrons via the orbital and Zeeman mechanisms respectively. The former mechanism is described by the minimal coupling between the momentum of electrons and the vector potential, and can lead to the well-known Abrikosov mixed state in type-II superconductors. The latter mechanism, usually called Pauli paramagnetic or Pauli limiting effect, is known to be important in some heavy fermion compounds$^{17,33-35}$. Which one of these two effects plays a dominant role is determined by a number of physical factors. When both of them are important, novel and interesting properties may emerge.

Since the middle of 1990s, the in-plane $H_{c2}$ has been applied to identify the gap symmetry in layered unconventional superconductors$^{10-17}$. Early theoretical calculations have showed that the in-plane $H_{c2}$ exhibits a fourfold oscillation in $d$-wave superconductors$^{30,31}$. The presence of such a fourfold oscillation has already been verified in many unconventional superconductors, including high-$T_c$ cuprate superconductors$^{12,13}$, LuNi$_2$B$_2$C$^{14}$, heavy fermion compounds CeCoIn$_5$ and CeCu$_2$Si$_2$.

In the early calculations of Won et. al$^{10}$ and Takanaka et. al$^{14}$ who solely considered the orbital effect, $H_{c2}$ is found to exhibit its maxima along the antinodal directions where the $d$-wave superconducting gap is maximal. The subsequent analysis of Weickert et. al$^{16}$ includes both the orbital and Pauli paramagnetic effects, but still finds the maxima of $H_{c2}$ along the antinodal directions. A similar conclusion is drawn in a recent work$^{19}$, where
the authors also show that increasing the Pauli effect reduces the difference in \( H_{c2} \) between nodal and antinodal directions. There seems to be a priori hypothesis in the literature that a larger gap necessarily leads to a larger magnitude of \( \Delta \). However, if the maxima are observed along the direction \( H_{c2} \), the gap symmetry should be \( d_{x^2-y^2} \)-wave. To make a comparison, we show the angular dependence of \( d_{x^2-y^2} \)- and \( d_{xy} \)-wave gaps in Fig. 1.

It is necessary to emphasize that the above hypothesized connection between in-plane \( H_{c2} \) and \( d \)-wave gap, though intuitively reasonable, is actually not always correct. When there is only orbital effect, the maxima of \( H_{c2} \) and \( d \)-wave gap are along the same directions in all cases. In the presence of Pauli paramagnetic effect, however, there is indeed no guarantee that such a connection is valid. In order to clarify the detailed connection between the precise gap symmetry and the angular dependence of \( H_{c2} \), we will consider the influence of the interplay of orbital and Pauli effects on \( H_{c2} \) more systematically. This problem is important because in-plane \( H_{c2} \) has recently played a significant role in the determination of the gap symmetries of CeCoIn\(_5\) and CeCu\(_2\)Si\(_2\).

In this paper, motivated by the recent progress and the existing controversy, we analyze the angular dependence of in-plane \( H_{c2} \) and its connection with the \( d \)-wave Pauli effect by considering the interplay of orbital and Pauli effects in the contexts of heavy fermion compounds. After carrying out systematic calculations, we will show that the maxima of angle-dependent \( H_{c2}(\theta) \) are not always along the antinodal directions when both the orbital and Pauli effects are important. The concrete fourfold oscillation pattern of \( H_{c2}(\theta) \) is determined by a number of physical parameters, including temperature \( T \), critical temperature \( T_c \), gyromagnetic ratio \( g \), fermion velocity \( v_0 \), and two parameters that characterize the shape of the underlying Fermi surface. Each of these parameters can strongly affect the angular dependence of \( H_{c2} \). Among the above six relevant parameters, the temperature \( T \) is particularly interesting, due to that in any given compound \( t \) is the only free parameter and all the other parameters are fixed at certain values. If we vary temperature \( T \) but fix all the rest parameters, \( H_{c2}(\theta) \) is found to exhibit its maxima along the nodal directions at lower temperatures and along the antinodal directions at higher temperatures. This means the angle-dependent \( H_{c2}(\theta) \) is shifted by \( \pi/4 \) as temperature increases across certain critical value.

Our results can be used to clarify the aforementioned experimental puzzle about the angular dependence of in-plane \( H_{c2} \). Since \( H_{c2}(\theta) \) shifts by \( \pi/4 \) as some of the relevant parameters are changed, the seemingly contradictory experimental results reported in Refs. 16,28,29 may be well consistent. On the other hand, since the concrete behavior of \( H_{c2}(\theta) \) is very sensitive to the specific values of several parameters, one should be extremely careful when judging the gap symmetry by measuring \( H_{c2} \).

In Sec. II we derive the equation for \( H_{c2} \) after including both the orbital and Pauli paramagnetic effects. In Sec. III we present numerical results for \( H_{c2} \) in three cases, i.e., pure orbital effect, pure Pauli paramagnetic effect, and interplay of both orbital and Pauli effects. We show that \( H_{c2} \) displays complicated angle dependence due to interplay of orbital and Pauli effects. In Sec. IV we discuss the physical implications of our results and make a comparison with some relevant experiments.

II. EQUATION FOR IN-PLANE UPPER CRITICAL FIELD \( H_{c2} \)

Heavy fermion compounds are known to have a layered structure, which is analogous to cuprates. However, the inter-layer coupling is not as weak as that in cuprates. It is convenient to consider a rippled cylinder Fermi surface, schematically shown in Fig. 2. The fermion velocity has three components \( k_{x,y,z} \), where \( k_{x,y} \) denote the two components in the superconducting plane. Here, we use \( t_c \) to represent the inter-layer hoping parameter and \( c \) the

![Fig. 1: Shapes of \( d_{x^2-y^2} \)-wave and \( d_{xy} \)-wave gaps.](image-url)
unit size along z-direction, and then write the dispersion
\[ \varepsilon(k) = \frac{k_x^2 + k_y^2}{2m} - 2t_c \cos(k_z c). \] (1)

Introducing a constant magnetic field \( H \) to the system leads to fruitful behaviors. For type-II superconductors, the field \( H \) weaker than lower critical field \( H_{c1} \) cannot penetrate the sample due to the Meissner effect. As \( H \) exceeds \( H_{c1} \) and further increases, the superconducting pairing is gradually destroyed by the orbital effect. The superconductivity is entirely suppressed once \( H \) reaches the upper critical field \( H_{c2} \), which can be obtained by solving the corresponding linearized gap equation. In some superconductors, the Pauli paramagnetic effect can also close the gap by breaking spin singlet pairs, and may even be more important than the orbital effect\(^{16,17}\). In order to make a general analysis, we consider both of these two effects in the following.

To proceed, it is useful to rewrite the in-plane magnetic field \( \mathbf{H} \) in terms of a vector potential \( \mathbf{A} \). Let us choose the a-axis as x-coordinate and b-axis as y-coordinate, and then write down a vector potential
\[ \mathbf{A} = (0, 0, H(-x \sin \theta + y \cos \theta)), \] (2)
where \( \theta \) denotes the angle between a-axis and field \( \mathbf{H} \). For conventional s-wave superconductors, the gap is isotropic and the upper critical field \( H_{c2} \) is certainly \( \theta \)-independent. In the case of d-wave superconductors, however, the gap is strongly anisotropic, thus \( H_{c2} \) becomes \( \theta \)-dependent. Now the field \( \mathbf{H} \) takes the form
\[ \mathbf{H} = \nabla \times \mathbf{A} = (H \cos \theta, H \sin \theta, 0). \] (3)

One can write the generalized derivative operator as
\[ \Pi(R) = -i \nabla_R + 2e \mathbf{A}(R) = -i \partial_x e_x - i \partial_y e_y + (-i \partial_z + 2eH(-x \sin \theta + y \cos \theta)) e_z. \]

Following the general methods presented in Refs.\(^{37-44}\), we obtain the following linearized gap equation:
\[ -\ln\left(\frac{T}{T_c}\right) \Delta(R) = \int_0^{\infty} \frac{d\eta}{\sin(\pi \eta)} \int_{-\pi}^{\pi} \frac{d\chi}{2\pi} \int_0^{2\pi} \frac{d\varphi}{2\pi} \times \gamma^2 \pi(R) \left\{ 1 - \cos \left[ \eta \left( h' + \frac{1}{2} v_F \right) \right] - \Pi(R) \right\} \Delta(R), \] (4)
where \( \chi = k_z c \). The function \( \Delta(R) \) is
\[ \Delta(R) = \left( \frac{2eH}{\pi} \right)^2 e^{-eH(x \sin \theta - y \cos \theta)^2}. \] (5)

Here we do not include Landau level mixing\(^{16,17,39}\) for simplicity, which will not affect our conclusion. For the chosen Fermi surface, the Fermi velocity vector is\(^{30}\)
\[ \mathbf{v}_F(\mathbf{k}) = v_a \cos \varphi e_x + v_a \sin \varphi e_y + v_c \sin \chi e_z. \] (6)

The Fermi velocity component along the c-axis is \( v_c = 2t_c c \). The two-component in-plane velocity vector has a constant magnitude \( v_0 \), defined as \( v_0 = v_0 \sqrt{1 + \lambda \cos(\chi)} \), where \( v_0 = \frac{\hbar}{m} \) with the Fermi momentum \( k_{F0} \) being related to the Fermi energy \( \epsilon_F \) by \( k_{F0} = \sqrt{2m \epsilon_F} \). The shape of rippled cylinder Fermi surface is characterized by a velocity ratio \( v_c/v_0 = \lambda \gamma \), where \( \lambda = 2t_c c/\epsilon_F \) and \( \gamma = ck_{F0}/2 \). As will shown below, both \( \lambda \) and \( \gamma \) can strongly affect the behavior of \( H_{c2} \). Moreover, we define \( h' = -\frac{\mu_B H}{\gamma} \), where \( \mu_B \) is Bohr magneton and \( g \) is the gyromagnetic ratio. The orbital effect of magnetic field is reflected in the factor \( \mathbf{v}_F(\mathbf{k}) \cdot \Pi(R) \), whereas the Pauli paramagnetic effect is reflected in the factor \( h' \). The concrete behavior of \( H_{c2} \) is determined by the interplay of these two effects.

In Eq.\(^{(1)}\), the influence of gap symmetry is reflected in the function \( \gamma_\alpha(\mathbf{k}) \). For isotropic s-wave pairing, \( \gamma_\alpha(\mathbf{k}) = 1 \); for \( d_{x^2-y^2} \)-wave pairing, \( \gamma_d(\mathbf{k}) = \sqrt{2} \cos(2\varphi) \); for \( d_{xy} \)-wave pairing, \( \gamma_d(\mathbf{k}) = \sqrt{2} \sin(2\varphi) \).

Although the linearized gap equation Eq.\(^{(4)}\) is formally general and valid in many superconductors, its solution is determined by a number of physical effects and associated parameters. For instance, the behavior of \( H_{c2} \) may be strongly influenced by the concrete shapes of the Fermi surface. The Fermi surface has different spatial dependence in various superconductors, which naturally leads to different forms of fermion dispersion and Fermi velocity \( \mathbf{v}_F \). Such a difference certainly affects the equation of \( H_{c2} \). For spherical Fermi surface, Fermi velocity \( \mathbf{v}_F \) depends on the azimuthal angle \( \varphi \) within the basal plane and the angle between z-axis and \( \mathbf{v}_F \). Therefore,
the equation of $H_{c2}$ contains the integrations over these two variables. For cylindrical Fermi surface, the direction of vector $v_F$ solely depends on the azimuthal angle $\varphi$, so there is only the integration over angle $\varphi$ in the equation of $H_{c2}$. For rippled Fermi surface, the direction of $v_F$ depends on the azimuthal angle $\varphi$ and the coordinate $\chi$ along $z$-axis, then the integrations over $\varphi$ and $\chi$ enter into the equation of $H_{c2}$, as shown in Eq. (4).

In addition, there are two independent parameters $\lambda$ and $\gamma$ which can characterize the rippled Fermi surface in Eq. (4). Notice that once $\lambda = 0$, the rippled cylindrical Fermi surface reduces to the cylindrical Fermi surface. The influence of Fermi surface on $H_{c2}$ is rarely studied in the literature. In this paper, we adopt rippled Fermi surface and show that $H_{c2}$ can exhibit different behaviors under different parameters.

To facilitate analytical computation, we can choose the direction of field $H$ as a new $z'$-axis and define

$$
\begin{align*}
    e'_x &= e_x \sin \theta - e_y \cos \theta \\
    e'_y &= -e_z \\
    e'_z &= e_x \cos \theta + e_y \sin \theta.
\end{align*}
$$

In the coordinate frame spanned by $(e'_x, e'_y, e'_z)$, we have a new velocity vector

$$
v_F(k) = v_a \sin(\theta - \varphi)e'_x - v_e \sin(\chi)e'_y + v_a \cos(\theta - \varphi)e'_z,
$$

and a new generalized derivative operator

$$
\Pi(R) = \sqrt{\epsilon H} \left[ (a_+ + a_-) e'_x - i (a_+ - a_-) e'_y + \sqrt{2a_0} e'_z \right],
$$

where

$$
a_\pm = \frac{1}{2\sqrt{\epsilon H}} \left[ -i \sin \theta \partial_x + i \cos \theta \partial_y + \partial_z \pm 2ieH(x \sin \theta - y \cos \theta) \right],
$$

$$
a_0 = \frac{1}{\sqrt{2\epsilon H}} \left[ -i \partial_x \cos \theta - i \partial_y \sin \theta \right],
$$

which satisfy

$$
[a_-, a_+] = 1, [a_\pm, a_0] = 0.
$$

In the following analysis, we take $d_{x^2-y^2}$-wave pairing as an example and assume that $\gamma_d(k) = \sqrt{2}\cos(2\varphi)$. The results in the case of $d_{xy}$-wave pairing can be obtained analogously. It is easy to examine that the qualitative conclusion will be not changed. After averaging over the ground state $\Delta_0(R)$ on both sides of Eq. (13) and inserting the $d_{x^2-y^2}$-wave gap $\gamma_d(k) = \sqrt{2}\cos(2\varphi)$, we obtain the following integral equation for $H_{c2}$,

$$
- \ln t = \int_0^{+\infty} \frac{du}{\sinh(u)} \left\{ 1 - \cos (hu) \int_{-\pi}^{\pi} \frac{d\chi}{2\pi} \int_{-2\pi}^{2\pi} \frac{d\varphi}{2\pi} \right. \times \left[ 1 + \cos(4\varphi) \right] \times \exp \left[ -hu^2 \left( X^2 \beta^2 \sin^2(\chi) + (1 + \lambda \cos(\chi)) \sin^2(\varphi) \right) \right] \left\} ,
$$

where $t = \frac{\epsilon H}{\rho}$, $h = \frac{\rho H}{2\pi k_BT}$ and $\rho = \frac{v_e^2 eH}{8\pi^2 k_BT}$. One can analyze the detailed behavior of $H_{c2}$, especially its dependence on various physical parameters, systematically by solving this integral equation. This will be done in the next section.
Among this set of parameters, $\lambda$ and $\gamma$ are related to the shape of rippled cylinder Fermi surface. We notice that the angular dependence of in-plane effect and that of the Pauli paramagnetic effect on the $\Delta$ gap always decreases monotonously with growing temperature. Moreover, the difference $\Delta H_{c2}$ is exactly the same as that of $d$-wave gap. This is consistent with the original theoretical predictions of Won et. al.\textsuperscript{10} and Takanaka et. al.\textsuperscript{11}. An important feature that needs to be emphasized is that the positions of peaks are temperature independent, as clearly manifested in both Fig. 3 and Fig. 4.

A. Pure orbital effect

First, we consider only the orbital effect by setting the gyromagnetic factor $g = 0$. In this case, the factor $\cos(hu)$ appearing in Eq. (13) is equal to unity, $\cos(hu) = 1$. We assume that $T_c = 1K$, $v_0 = 3000m/s$, $\lambda = 0.5$, and $\gamma = 1$, which are suitable parameters in heavy fermion compounds.

After carrying out numerical calculations, we plot the angular dependence of $H_{c2}(\theta)$ in Fig. 3 at two representative temperatures $t = 0.1$ and $t = 0.9$. It is easy to see from Fig. 3 that $H_{c2}(\theta)$ exhibits a fourfold oscillation pattern. Moreover, the maxima of $H_{c2}$ are always along the antinodal directions for any values of the relevant parameters, which means the angular dependence of orbital effect-induced $H_{c2}$ is exactly the same as that of $d$-wave gap.
FIG. 7: \( t \)-dependence of \( H_{c2} \) with \( T_c = 1K, v_0 = 3000m/s, \lambda = 0.5, \gamma = 1, \) and \( g = 1. \)

**B. Pure Pauli paramagnetic effect**

We next consider the effects of pure Pauli paramagnetic effect by setting \( v_0 = 0 \), which leads to

\[
- \ln(t) = \int_{0}^{+\infty} \, du \, \frac{1 - \cos(hu)}{\sinh(u)}
\]

which is completely independent of \( \theta \). The \( t \)-dependence of \( H_{c2} \) is shown in Fig. 5. Different from pure orbital effect, \( H_{c2} \) is not a monotonous function: it rises initially with growing \( t \), but decreases as \( t \) is larger than certain critical value \( t_c \), which is roughly \( 0.5t \) under the chosen set of parameters.

**C. Interplay of orbital and Pauli effects**

We now turn to the general and interesting case in which both the orbital and Pauli paramagnetic effects are important. This case is broadly believed to be realized in several heavy fermion compounds, such as CeCoIn5 and CeCu2Si2. As aforementioned, the concrete behaviors of \( \theta \)-dependent \( H_{c2} \) are influenced by a number of parameters. In order to illustrate the numerical results and their physical implications, we vary one particular parameter while fixing all the rest parameters. In most of the following calculations, the gyromagnetic factor is taken to be \( g = 1 \). The influence of various values of \( g \) will be analyzed separately.

As shown in Fig. 6, under the currently chosen parameters, the maxima of \( H_{c2} \) locates along the antinodal directions at a relatively higher temperature \( t = 0.9 \). This behavior is very similar to that in the case of pure orbital effect. However, at a relatively lower temperature \( t = 0.1 \), the maxima of \( H_{c2} \) are along the nodal directions where the \( d_{x^2-y^2} \)-wave gap vanishes. Two conclusions can be immediately drawn: \( H_{c2} \) does not always exhibit its maxima at the angles where the superconducting gap reaches its maximal value; the fourfold oscillation curves of \( H_{c2} \) is shifted by \( \pi/4 \) as temperature grows in the range of \( 0 < T < T_c \).

From Fig. 7(a), we see that \( H_{c2} \) first arises with growing \( t \) and then decreases rapidly once \( t \) exceeds a critical value. Apparently, such a non-monotonous \( t \)-dependence of \( H_{c2} \) is a consequence of the interplay of both orbital and Pauli paramagnetic effects. On the other hand, the difference \( \Delta H_{c2} \) shown in Fig. 7(b) is positive for small values of \( t \) but becomes negative for larger values of \( t \).

Addition to temperature \( t \), the concrete angular dependence of \( H_{c2} \) is also strongly influenced by a number of other physical parameters, including critical temperature \( T_c \), fermion velocity \( v_0 \), gyromagnetic factor \( g \), and two Fermi surface factors \( \lambda \) and \( \gamma \). Indeed, different values of these parameters can lead to very different behaviors of \( H_{c2} \). In the following, we show how \( H_{c2} \) and \( \Delta H_{c2} \) are changed as these parameters are varying. To simplify the analysis, we vary one particular parameter and fix all the other parameters in each figure.

**FIG. 8: \( T_c \)-dependence of \( H_{c2} \) with \( t = 0.5, v_0 = 3000m/s, \lambda = 0.5, \gamma = 1, \) and \( g = 1. \)**
$T_c$ varies in the range of $[0, 3K]$. All the other parameters are fixed. $H_{c2}$ rises monotonously with growing $T_c$, which is obviously owing to the monotonous increase of the superconducting gap. Moreover, if $T_c$ is smaller than some critical value, $\Delta H_{c2}$ is negative, which means the maxima of $H_{c2}$ are along the antinodal directions. For larger $T_c$, $\Delta H_{c2}$ becomes positive and the maxima of $H_{c2}$ are shifted to the nodal directions. Apparently, $T_c$ has important impacts on the concrete angular dependence of $H_{c2}$. In passing, we point out that the maxima of $H_{c2}$ will be shifted back to the antinodal directions for even higher $T_c$ (not shown in the figure).

$v_0$: We then consider the influence of fermion velocity $v_0$ on $H_{c2}$ and $\Delta H_{c2}$, and show the results in Fig. 9. In the limit $v_0 = 0$, the orbital effect is actually ignored and the Pauli effect entirely determines $H_{c2}$. In such a limit, $H_{c2}$ is angle independent, so $\Delta H_{c2} = 0$. For finite $v_0$, $H_{c2}$ becomes angle dependent and exhibits fourfold oscillation, as a consequence of the interplay between orbital and Pauli effects. As $v_0$ is growing, $H_{c2}$ first increases and then decreases, which indicates that the enhancement of orbital effect does not necessarily suppress $H_{c2}$ once the Pauli paramagnetic effect is present. However, as already discussed earlier, $H_{c2}$ deceases monotonously with growing $v_0$ when the Pauli effect is completely neglected. Furthermore, $\Delta H_{c2}$ is negative for both small and large values of $v_0$, but is positive for intermediate values of $v_0$. Therefore, the concrete angular dependence of $H_{c2}$ is very sensitive to the values of fermion velocity.

$g$: We next consider the influence of the gyromagnetic factor $g$, which characterizes the effective strength of Pauli paramagnetic effect. The dependence of $H_{c2}$ and $\Delta H_{c2}$ on $g$ is given in Fig. 10. First of all, taking $g = 0$ simply leads to the known results obtained in the case of pure orbital effect presented in Sec. IIIA. Second, $H_{c2}$ decreases monotonously with growing $g$. An immediate indication of this behavior is that increasing the Pauli paramagnetic effect always tends to suppress $H_{c2}$ in the presence of orbital effect. Finally, it is easy to observe that $\Delta H_{c2}$ is negative if $g$ takes very small values and positive when $g$ becomes larger than certain critical value. Therefore, the gyromagnetic factor $g$ also plays a crucial role in the determination of the concrete angle dependence $H_{c2}$.

$\lambda$: $\lambda$ represents the ratio of inter layer coupling $2t_c$ and the Fermi energy $E_F$. If $t_c = 0$, the corresponding $\lambda = 0$, then the rippled cylindrical Fermi surface reduce to the cylindrical Fermi surface. The dependence of $H_{c2}$ and $\Delta H_{c2}$ on $\lambda$ is as depicted in Fig. 11. $H_{c2}$ deceases monotonously with the growing $\lambda$. For given values of other parameters shown in Fig. 11 the maxima of $H_{c2}$ are along the nodal directions for small $\lambda$, but along the antinodal directions for large values of $\lambda$.

$\gamma$: $\gamma$ represents the ratio of two momentum $k_{F0}$ and $1/2c$, $c$ is the unit cell size along third direction. The dependence of $H_{c2}$ and $\Delta H_{c2}$ on $\gamma$ is shown in Fig. 12. $H_{c2}$ deceases monotonously with the growing $\gamma$. For given values of other parameters shown in Fig. 12 the maxima of $H_{c2}$ are along the nodal directions for small $\gamma$, but along the antinodal directions for large values of $\gamma$.

From all these results, we see that both the magnitudes and the detailed angular dependence of in-plane $H_{c2}$ are significantly influenced by a number of physical parameters. A particularly interesting feature is the fourfold
oscillation pattern of angle dependent $H_{c2}$ can be shifted by $\pi/4$ if one varies any one of these parameters. $H_{c2}$ may exhibit its maxima along either nodal or antinodal directions, depending on the specific values of relevant parameters, which is apparently in sharp contrast in the naive notion that $H_{c2}$ always displays the same angle dependence of the $d$-wave superconducting gap.

### D. Comparison with recent experiments

As aforementioned, in the last several years the in-plane $H_{c2}$ has been widely investigated with the aim to identify the precise superconducting gap symmetry in two heavy fermion compounds CeCoIn$_5$ and CeCu$_2$Si$_2$. In this subsection, we make a comparison between our theoretical analysis and some recent experiments of $H_{c2}$. Our results are valuable to theoretical and experimental research of $H_{c2}$ in two main aspects.

First, one should be very careful when fitting theoretical calculations with experimental data. In the current literature, it is often taken for granted that the in-plane $H_{c2}$ always exhibits exactly the same angular dependence as that of the superconducting gap. In other words, the maxima of in-plane $H_{c2}$ are believed to be always along the antinodal directions where the $d$-wave gap is maximal. According to this seemingly correct relationship, the superconducting gap symmetry is simply identified as $d_{x^2-y^2}$-wave ($d_{xy}$-wave) if $H_{c2}(\theta)$ is found to exhibit its maxima at $\theta = 0^\circ$ ($45^\circ$). However, as showed in our extensive calculations, such a relationship is not always correct. In a Pauli-limited $d$-wave superconductor, the maxima of $H_{c2}$ may be along either the nodal or the antinodal direction, depending on the specific values of a number of physical parameters, as a consequence of the delicate interplay between orbital and Pauli effects. Incorrect and even incorrect conclusions might be drawn if some of these parameters are not properly chosen. In order to identify the precise gap symmetry of CeCoIn$_5$ or CeCu$_2$Si$_2$, one should first choose suitable values for all the relevant parameters before probing the angular dependence of $H_{c2}$ and deducing the gap symmetry from experimental data.

Among the above six relevant parameters, the temperature $t$ is particularly interesting, because in any given compound $t$ is the only free parameter and all the other parameters are fixed at certain values. Our extensive calculations show that there is always a $\pi/4$ difference between $H_{c2}$ and $d$-wave gap at small $t$ and that $H_{c2}$ and $d$-wave gap always exhibit exactly the same angular dependence once $t$ exceeds a certain critical value, provided that the gyromagnetic factor $g$ is sufficiently large. It appears that the impact of Pauli effect on $H_{c2}$ is much more important at low temperatures than at high temperatures. If one attempts to deduce the precise gap symmetry by fitting experiments of $H_{c2}$, it would be better to measure $H_{c2}$ at a series of very different temperatures. Otherwise, incorrect results might be obtained.

Second, our results may help to resolve some current controversies with regard to the precise gap symmetry of heavy fermion compounds. The gap symmetry of CeCoIn$_5$ has been investigated extensively by means of various experimental techniques. Settai et al. \textsuperscript{28} reported that the maxima of in-plane $H_{c2}$ are along [100] direction...
through de Haas-van Alphen oscillation signal at 40mK. The cantilever magnetometer measurements at 20mK of Murphy et al. observed that the maxima of $H_{c2}$ are along [110] direction. Bianchi et al. measured the specific heat and found the maxima of $H_{c2}$ along [100] direction at temperatures higher than 1K. After measuring the magnetic field dependence of electric resistivity at 100mK, Weickert et al. revealed that the maxima of $H_{c2}$ are along [100] direction. Obviously, there seems to be a discrepancy among the experimental results about the detailed angular dependence of $H_{c2}$, which is considered as an open puzzle and complicates the search for the precise gap symmetry.

According to our results, however, probably such a discrepancy does not exist at all, since the maxima of $H_{c2}$ may be along either [100] or [110] direction when some of the relevant physical parameters are moderately changed. In particular, the maxima of $H_{c2}$ can shift by $\pi/4$ as the temperature increases beyond certain critical value. Notice that the measurements of Ref. were performed at a temperature as low as 20mK. There is a good possibility that the position of the maxima of $H_{c2}$ are shifted from [110] direction at low temperatures to [100] direction at higher temperatures. Although this possibility needs to be further examined, it should be safe to say that the seemingly contradictory experimental results about in-plane $H_{c2}$ of CeCoIn$_5$ may be well consistent with each other. More careful and more systematical research are required to completely solve this problem.

IV. DISCUSSION AND CONCLUSION

In this paper, we have performed a detailed and systematical analysis of the unusual behaviors of in-plane upper critical field $H_{c2}$ in the contexts of Pauli-limited heavy fermion compounds. We show that the concrete angular dependence of $H_{c2}$ is determined by a delicate interplay of the orbital and Pauli paramagnetic effects. The most interesting result is that $H_{c2}$ does not necessarily exhibit the same fourfold oscillation pattern as the $d$-wave superconducting gap, which is often taken for granted in the literature. For certain values of a series of physical parameters, $H_{c2}$ may display its maxima along the nodal directions where the superconducting gap vanishes. We also have compared our theoretical analysis with some current measurements of in-plane $H_{c2}$ in two heavy fermion compounds CeCoIn$_5$ and CeCu$_2$Si$_2$.

The theoretical results presented in this paper impose an important restraint on the determination of the precise gap symmetry of Pauli limited $d$-wave heavy fermion superconductors by means of measuring the in-plane $H_{c2}$. One has to be extremely careful when trying to deduce the gap symmetry from experiments of $H_{c2}$.

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