Upper critical field as a probe for multiband superconductivity in bulk and interfacial STO

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We investigate the temperature dependence of the upper critical field $H_{c2}$ as a tool to probe the possible presence of multiband superconductivity at the interface of LAO/STO. The behaviour of $H_{c2}$ can clearly indicate two-band superconductivity through its nontrivial temperature dependence. For the disorder scattering dominated two-dimensional LAO/STO interface we find a characteristic non-monotonic curvature of the $H_{c2}(T)$. We also analyse the $H_{c2}$ for multiband bulk STO and find similar behaviour.

Multiband superconductivity provides an intrinsically interesting extension of superconductivity. Shortly after the publication of BCS theory an earliest idea of multiband superconductivity was proposed. It is characterised by having more than one band in which Cooper pairs form. Thus two different superconducting gaps may appear. Apart from the theoretical interest, multiband superconductivity also has practical consequences. For example, some of the highest temperature superconductors are multiband superconductors. These are magnesium diboride (MgB$_2$) with a transition temperature of 39 Kelvin and the iron-based superconductors with a maximal critical temperature of about 56 Kelvin. Additionally, multiband superconductivity may lead to a higher upper critical magnetic field $H_{c2}$ that is also attributable to the interplay between the two gaps. Indeed, in the realm of technology applications, it has been speculated that due to these properties many future high magnetic field superconducting magnets, such as those found in MRI scanners, will be made of multiband superconductors.

Unambiguous detection of multiband superconductors requires advanced techniques. Currently the main probes available are scanning tunneling spectroscopy, heat transport, and specific heat. Multiband superconductivity manifests itself through the occurrence of more than one quasiparticle coherence peak in tunneling spectroscopy. However, short quasiparticle lifetimes may smear these peaks and thus make them unobservable. Heat transport may also be used to probe multiband superconductivity through its anomalous magnetic field dependence. A single band superconductor shows a strong suppression of heat transport all the way up to temperatures very close to the critical temperature. In contrast, in multiband superconductors one of the gaps may be disproportionately suppressed by a magnetic field, thus allowing that band to transport heat effectively. These techniques helped determine that e.g. MgB$_2$ and PrOs$_4$Sb$_12$ are multiband superconductors.

The recent discovery of superconductivity at the LaAlO$_3$/SrTiO$_3$ (LAO/STO) interface has made the discussion of the nature of the superconducting state and possible multiband effects relevant. In this paper we wish to put forward the temperature dependence of the upper critical field as a probe for whether SrTiO$_3$ (STO) and particularly the interface between LaAlO$_3$ (LAO) and STO is a single or multiband superconductor. The temperature dependence of the upper critical field may show characteristic behaviour inherent to multiband superconductivity.

STO has long been a material of interest. It was the first oxide which was found to be superconducting. Moreover, it was also the first material to show two-band superconductivity, through the presence of two quasiparticle coherence peaks. STO can be tuned between single band and multiband superconductivity by changing the level of doping and recently there have even been indications that, for certain doping levels, the material may be a three-band superconductor. However, despite this evidence STO is still not unanimously accepted as a multiband superconductor. Since 2004 attention has shifted to a metallic interface between LAO and STO. The system is remarkable since both LAO and undoped STO are insulators. Interest grew even further in 2007 when superconductivity was discovered at the interface.

One of the most pertinent questions now concerns the origin of the superconducting state at the interface. One suggestion is that the metallic layer and thus the superconductivity is simply a consequence of surface doping at the interface. However, in addition to the doping effects it was suggested that multiorbital effects and multiband effects are important and in fact enable multiband superconductivity. The latter proposal, that the superconductivity is a direct descendant of superconductivity from the bulk STO, is supported by the fact that other interface layers apart from LAO also give rise to a metallic and superconducting surface state of STO. Apart from the proposal of "descendant" superconductivity at the LAO/STO interface, the alterna-
tive suggestions were made that the superconductivity at the surface is of an entirely different origin, resulting from a polar catastrophe and possibly spin orbit coupling that is a unique property of the interface and has no analog in bulk STO. The ongoing debate underscores the importance of an unambiguous test that would clarify the nature of the superconducting state. The investigation of $H_{c2}(T)$ is one of these tests.

In this paper we aim to propose a direct test of the hypothesis of two-band superconductivity in bulk STO and the LAO/STO interface. We consider the perpendicular upper critical magnetic field in order to see whether its behaviour can indicate whether the material is a single band or multiband superconductor. We concentrate on the upper critical magnetic field since it is a quantity readily accessible to experiments. Some of the probes, like specific heat and heat transport, are not practical for LAO/STO interfaces, thus making the temperature dependence of $H_{c2}$ one of the few available tools to further investigate superconducting states in these materials. In doing so, we also aim to clarify the relationship between the superconductivity in the bulk and the interface system. One can directly test both the multi-gap nature and pairing symmetry of bulk STO and the LAO/STO interface. We therefore focus on the $H_{c2}$ behaviour in the clean and dirty limit for the parameters relevant to STO.

We first investigate the dirty limit behaviour of the system. This is appropriate if the mean free path is shorter than the superconducting coherence length $\xi \approx 70\text{nm}$ for interface systems this is likely to be the relevant situation. Depending on doping, it is also a realistic scenario for bulk STO, particularly at optimal doping. However, if there are two superconducting gaps, two coherence lengths and mean free paths are possible. Subsequently we address what is expected in a clean system. In principle one could be in a regime where one band is dirty and the other is clean. This regime would require a complicated analysis and is outside the scope of this paper. We focus on either the disorder dominated regime or the clean case, where all bands are in same transport regime. Our work expands and adds to earlier work that focused on $H_{c2}$, but only considered the clean limit.

The paper addresses both the case of bulk STO and LAO/STO interfaces. The possible regimes include four cases: clean and disordered (in the sense of the ratio of the coherence length to the mean free path) in bulk and interface STO. In practice the dominant regime is the disordered case, see however the extreme low doping regime in Ref.13. We start with the case of $H_{c2}$ in bulk STO in the presence of disorder in Section II. We also analyze the case of clean bulk STO in Section III. Results for the interface are presented in Section IV.

I. UPPER CRITICAL FIELD FOR BULK STO IN THE PRESENCE OF DISORDER

At a quasi classical level the physics of a dirty superconductor can be described by the Usadel equation. These give an accurate description of the physics when disorder scattering is strong, such that anisotropies of the Fermi surface are averaged out. In this section we solve the Usadel equations in the limit where the gaps $\Delta$ are very small. This describes the region very close to the transition from superconductor to normal metal and the Usadel equations may be linearised, simplifying their solution. By solving the equations as a function of an applied magnetic field and temperature we thus obtain the temperature dependence of the upper critical magnetic field.

In our approach we closely follow the approach developed in Ref.[5]. We start with the linearised Usadel equations.

\[
2\omega f_1 - D_{i\alpha}^{\beta} \Pi_{\alpha} \Pi_{\beta} f_1 = 2\Delta_1 \tag{1.1}
\]

\[
2\omega f_2 - D_{i\alpha}^{\beta} \Pi_{\alpha} \Pi_{\beta} f_2 = 2\Delta_2 \tag{1.2}
\]

where $f_i, i = 1, 2$, is the Green’s function of the system and in general depends on the momenta, position, and the Matsubara frequency $\omega = 2\pi T(2n + 1)$. $D_{i\alpha}^{\beta}$ is the diffusivity tensor within a band. is defined as $\Pi = \nabla + 2\pi i \hat{A}/\phi_0$, $\phi_0$ is the flux quantum. By assuming the diffusivity tensor to be given by $D_{m} = \delta_{\alpha\beta} D_m$ and the vector potential to be given by $\hat{A} = H x \hat{y}$, we can write these equations as

\[
2\omega f_m - D_m \left( \nabla_x^2 + \nabla_y^2 + \nabla_z^2 + \frac{4\pi i H x}{\phi_0} \nabla_y \right. \\
- \frac{4\pi^2 H^2 x^2}{\phi_0^2} \left. \right) f_m = 2\Delta_m \tag{1.3}
\]

Since this equation only depends on $x$, we now assume that $f_m$ is independent of $y$ and $z$ ($m \in \{1, 2\}$). Eq. (1.3) can now be solved for $\Delta_m$ and $f_m$ using the ansatz $f_m = h_m \Delta_m(x)$ and one obtains the solution

\[
f_m(x, \omega) = \frac{\Delta_m}{\omega + \pi H D_m / \phi_0} \tag{1.4}
\]

\[
\Delta_m(x) = \tilde{\Delta}_m e^{-\pi H x^2 / \phi_0} \tag{1.5}
\]

with $\tilde{\Delta}_m$ being a constant. The solutions for $f$ and $\Delta$ can be inserted into the gap equation for the two-band
and divide out the factor \( e \)

We can convert this into a 2x2 system of equations for \( \tilde{\Delta} \)

\[
\ln \gamma = \frac{U}{\pi T} \approx \frac{1}{2} \pi H D \eta \phi_0
\]

Since \( \eta = D_2/D_1 \) correspond to different ratios of the diffusivities.

\( \omega_0 \) is the Debye frequency and \( \lambda_{mm'} \) the superconducting coupling constants for the different bands. In the last line we have used the equality

\[
2\pi T \sum_{\omega > 0} \frac{1}{\omega + \lambda_{m'} \omega_0} = \ln \frac{2\gamma \omega D}{\pi T} - U \left( \frac{HD_{m'}}{2\pi T} \right) \tag{1.19}
\]

with \( U(x) = \psi(x + 1/2) - \psi(1/2) \) and where \( \psi \) is the digamma function. In \( \gamma \approx 0.577 \) is the Euler constant. We can convert this into a 2x2 system of equations for \( \Delta \) and divide out the factor \( e^{-\pi H x^2/\phi_0} \) and thereby replace \( \Delta \) with \( \Delta \).

\[
\begin{pmatrix}
(l - U(h)) \lambda_{11} - 1 & (l - U(\eta h)) \lambda_{12} \\
(l - U(h)) \lambda_{21} & (l - U(\eta h)) \lambda_{22} - 1
\end{pmatrix}
\begin{pmatrix}
\tilde{\Delta}_1 \\
\tilde{\Delta}_2
\end{pmatrix} = 0
\]

\[
M_0
\tag{1.10}
\]

Here \( l = \ln \frac{2\omega_0^2}{\pi^2} \) and \( \eta = D_2/D_1 \).

Since these equations resulted from a linear expansion of the Usadel equations, they are valid for small, or infinitesimal \( \Delta \). Since \( \Delta \) is infinitesimal at \( H = H_c \), these equations have a non-trivial solution at \( H = H_c \). We thus need to find the solution to the equation \( \det M_0 = 0 \).

After some manipulation one arrives at the expression

\[
a_0(\ln t + U(h))(\ln t + U(\eta h)) + a_1(\ln t + U(h)) + a_2(\ln t + U(\eta h)) = 0 \tag{1.11}
\]

with \( t = \frac{T}{T_c} \). Here the equation for \( T_c \) in a two-band superconductor has also been used in order to replace \( \omega_D \) with \( T_c \) (eq. (22) in ref[9]). The coefficients \( a_i \) depend of the coupling constants as follows

\[
a_0 = \frac{2(\lambda_{11} \lambda_{22} - \lambda_{12} \lambda_{21})}{\lambda_0} \tag{1.12}
\]

\[
a_1 = 1 + \frac{\lambda_{11} - \lambda_{22}}{\lambda_0} \tag{1.13}
\]

\[
a_2 = 1 + \frac{\lambda_{22} - \lambda_{11}}{\lambda_0} \tag{1.14}
\]

\[
\lambda_0 = \sqrt{\lambda_{11}^2 + \lambda_{22}^2 + 4\lambda_{12} \lambda_{21} - 2\lambda_{11} \lambda_{22}}. \tag{1.15}
\]

It is now relatively straightforward to solve numerically for the roots of equation (1.11) as a function of \( H_{c2} \) and \( t = T/T_c \). Figures 1 and 2 show \( H_{c2} \) for two different coupling constants which are found in the literature, and also for different ratios of the diffusivities in the two different bands. For equal diffusivities the results are identical to those for a single band superconductor[23]. Nontrivial behaviour only starts to emerge for strongly different values of the diffusivities. Moreover, the shape of the curves also strongly depends on the values of the coupling constants. For the set of coupling constants given in reference[23] it is much easier to discern non-trivial behaviour than for the set in reference[23].

We thus find that depending on what set of diffusivities and which of the two coupling constants are realised in real STO, two band superconductivity might be inferred from the shape of the \( H_{c2}(T) \) curve. This observation can provide guidance for the search of multiband superconductivity in STO. On the other hand, a seemingly trivial
behaviour of the $H_{c2}(T)$ curve does not imply that STO
is a single band superconductor. It has been argued that
unconventional $H_{c2}$ behaviour could be expected even for
a single band systems, as long as the single band is highly
anisotropic. However, for STO this is not expected to
be the case, and an unconventional behaviour of $H_{c2}$
can be taken to be good evidence for multiband super-
conductivity.

II. $H_{c2}$ FOR CLEAN DOPED BULK STO

For completeness we also present the case of clean bulk
superconducting STO. Away from optimal doping, bulk
STO may enter a regime in which the mean free path is
larger than the superconducting coherence length. In
this regime a calculation for the clean system is more
appropriate. We therefore briefly present the results
obtained from the quasi-classical Eilenberger equations.
The critical field for a three-dimensional clean two-band
superconductor is given by the solution of equation (76)
in Ref. 13

$$
I_\beta = \int_0^\infty ds s \ln(\tanh(st)) \langle \mu_{c,\beta} e^{-\mu_{c,\beta}s^2h_c} \rangle_\beta.
$$

(2.2)

$\langle \ldots \rangle_\beta$ is an average over the Fermi surface associated
with the band $\beta \in \{1, 2\}$ and $\mu_c = (v_1^2 + v_2^2)/v_0$ with
$v_0 = (2E_F^2/(\pi^2\hbar^3N_\beta))^{1/3}$. For isotropic bands $v_0 = v_F$.
$N_\beta$ is the density of states at the Fermi surface in band $\beta$. Since
the bands are expected to be roughly isotropic, we will replace the average
over $\mu_{c,\beta}$ with just a single (band dependent) value $\mu_\beta$. This we will vary, in order
to explore the different types of behaviour. $\alpha_{ii}$ are nor-
malised coupling constants. They are normalised to the
value of an effective coupling constant $\alpha_0$ whose value
would determine the superconducting gap and hence $T_c$
if the system were a single band superconductor. $\alpha_0$ is thus given by

$$
\alpha_0 = \left(-\ln \frac{\pi \gamma T_c}{2\hbar \omega_D} \right)^{-1}
$$

(2.3)

where $\ln \gamma$ is again the Euler constant and $\omega_D$ is the
Debye frequency. $\alpha_{11}$ and $\alpha_{22}$ are accordingly given by

$$
\alpha_{11} = \lambda_{11}/\alpha_0
$$

(2.4)

$$
\alpha_{22} = \lambda_{22}/\alpha_0.
$$

(2.5)

For different values of the parameter $\mu_{c,\beta}$ we have plotted
the temperature dependence of $H_{c2}$ in figures 3 and 4. This is done again for
two different values of the coupling constants found in the literature
(23,24). We can see that these curves by and large do not give a clear indication
of the presence of two-band superconductivity, at least

FIG. 3. (Color online) Temperature dependence of the upper
critical field in the clean limit for the coupling constants $\lambda_{11} = 0.14$, $\lambda_{22} = 0.13$, $\lambda_{12} = 0.023$ (the same as in Fig. 1). We have
set the parameter $\mu_2 = 1$ and vary the remaining parameter $\mu_1$.

FIG. 4. (Color online) Same as Fig. 3 but for the coupling
constants $\lambda_{11} = 0.3, \lambda_{22} = 0.1, \lambda_{12} = 0.015$ (the coupling
constants are the same as in Fig. 3).

for the temperature range which might be accessible to experiments. Therefore, it seems that the upper critical field can only be used to identify multiband supercon-
ductivity in STO in the dirty limit.

III. $H_{c2}$ FOR THE LAO/STO INTERFACE

The interface between LAO and STO is closer to the
disordered limit than bulk doped STO. The mean free
path in such a system has been estimated to be 25 nm as opposed to approximately 60 nm
for the bulk system at optimal doping. Therefore a calculation for the dirty system becomes necessary in this case, as opposed to the clean calculation that was performed previously. In the following we compute what is expected for an electron gas
confined to a layer of thickness $d_c$. From this we can then
estimate the behaviour of the interface system under an applied magnetic field perpendicular to the superconducting gap is expected to be on the order of $\Delta$. We point out though, that the expected second superconductivity is consistent with the single band effect.

The calculation for the finite thickness in $z$ direction proceeds in much the same way as the three-dimensional calculation, apart from the fact that we now need to retain the term $\nabla_z^2$ in equation (1.3). If we include this term we need to modify the ansatz to $f_m = h_m \Delta_m^x(x) \Delta_m^z(z)$. This leads to an additional eigenvalue equation for $\Delta_m^z$:

$$-\nabla_z^2 \Delta_z = \chi^2 \Delta_z.$$  \hspace{1cm} (3.1)

It has the lowest eigenvalue $\chi^2 = \left(\frac{\pi}{d}\right)^2$ if we require $\Delta_z(z)$ to vanish at $z = 0, d$. If the coherence length $\xi$ is smaller than the electron layer thickness $d_e$, then $d = d_e$. On the other hand, if $d_e < \xi$ then the length scale over which $\Delta$ varies cannot be given by $d_e$, but can only be dictated by $\xi$. So in this case $d = \xi$, $H_{c2}(T)$ exhibits a characteristic behaviour which is qualitatively different from that of single band superconductors. Experiments may thus be able to use this property to confirm that STO is indeed a two-band superconductor. We therefore see that a finite thickness of the superconducting layer effectively shifts the magnetic field by a positive amount. By redefining the quantity $h$ as

$$h = \frac{H D_1}{2 \phi_0 T_c} + \frac{D_1 \pi}{4 d^2 T_c},$$  \hspace{1cm} (3.3)

we can again obtain the temperature dependence of $H_{c2}$ from eq. (1.11). When the thickness parameter $f_P = \pi D_1/(4d^2 T_c)$ is appreciable, it can lead to a suppression of the characteristic two-band temperature dependence, as shown in figure 5. This is because effectively the low field behaviour (or alternatively high-temperature behaviour) is cut out. Since experiments indicate that the critical temperature is not much decreased in the interface system as compared to the bulk system, we can assume that the finite thickness parameter is at most on the order unity or smaller. The overall shape of the curves, and in particular the qualitative behaviour, is thus the same in the two-dimensional and in the three-dimensional case. A simple estimate of the parameter $f_P$ gives $f_P = 1.5$, where $D = l v_F$ was used and the parameters $\xi = 70nm$, $l = 25nm$, $v_F = 15km/s$ and $T_c = 0.3K$ were chosen. This is maybe a factor of three or four larger that what we expect from the experimentally only modest decrease in $T_c$, but within the accuracy that might be expected from such a simple estimate.

Recent experiments by Richter et al seem to indicate the presence of only one set of coherence peaks in planar tunneling into LAO/STO, at $\Delta_1 \sim 60\mu eV$. The correct implication hence was made that the interface superconductivity is consistent with the single band effect. We point out though, that the expected second superconducting gap is expected to be on the order of $\Delta_2 \sim 25\mu eV$ and would be below the observed lifetime broadening on the order of $\Gamma \sim 30 - 40\mu eV$. We therefore suggest that this proposed study of $H_{c2}(T)$ would be a useful alternative probe to detect multiband superconductivity.

IV. CONCLUSION

In this paper we investigated the temperature dependence of the upper critical field in two-band superconductors, with a view to finding an experimental criterion for the presence of two-band superconductivity. We have found that, in particular in the disordered regime, $H_{c2}(T)$ exhibits a characteristic behaviour which is qualitatively different from that of single band superconductors. Experiments may thus be able to use this property to confirm that STO is indeed a two-band superconductor. This tool is particularly useful for the investigation of the superconductivity at the interface between LAO and STO as it will help to relate it to the superconductivity in bulk STO.

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