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A mean field interpretation of critical fields in anisotropic superconductors

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Résumé. — L’anisotropie du champ magnétique critique, \( H_{c2} \), des supraconducteurs ayant des surfaces de Fermi (SF) anisotropes, est calculée en utilisant la théorie du champ moyen dans la limite propre. La théorie de Hohenberg et Werthamer est appliquée dans des calculs numériques en utilisant plusieurs pièces de SF et une sélection des fréquences de Matsubara. Les résultats de ces modèles sont comparés avec les résultats expérimentaux obtenus pour des matériaux anisotropes, en particulier les supraconducteurs organiques. Il est proposé que le comportement anormal observé pour \( H_{c2}(T) \) dans certains matériaux est dû à une combinaison des caractéristiques d’anisotropies différentes de plusieurs bandes.

Abstract. — Anisotropic magnetic critical fields \( H_{c2} \) are calculated for anisotropic Fermi surface (FS) models by use of mean field theory in the clean limit. The Hohenberg-Werthamer theory is applied numerically for selected FS pieces and Matsubara frequencies. The results are compared with experimental results on various anisotropic materials, in particular organic superconductors. It is proposed that the anomalous behaviour of \( H_{c2}(T) \) curves originates from the combination of anisotropy and multiband features.

The discovery of superconductivity in organic materials has been followed by further interest and increased number of discoveries of unusual phenomena in a whole class of organic materials [1-3]. Thus one has competing effects between superconductivity, spin-magnetism, spin or charge density waves, Peierls-type phase transitions, all within a rather wide temperature range. In addition, properties at higher temperatures such as thermal and electrical conductivity show anomalous behaviour. It is clear that these materials are very anisotropic, possibly 1-dimensional (1-D) in their properties, and it is likely that understanding of their properties needs theories founded on low dimensionality. Thus one can expect fluctuation phenomena due to the weak coupling between 1-D chains [1]. Complete knowledge about the electronic properties is very essential, but still lacking. Recent works by Grant [4] have tried to derive interaction parameters in a highly anisotropic situation. A reliable Fermi surface (FS) description for these materials, having about fifty atoms per unit cell, has to await until a full \textit{ab initio} bandstructure calculation has been undertaken. However other less complicated low dimensional superconductors are known and many of their properties resemble those of the organic superconductors. In this paper we will assume, as has been inferred from anisotropic properties, a simple anisotropic model for the FS, and calculate the anisotropies of the magnetic critical field \( H_{c2} \) using mean field theory for a discussion of the experimental data for \( (\text{TMTSF})_2X \) salts [6, 7]. As will be seen good qualitative agreement can be obtained between the model calculations and the \( H_{c2} \) data for \( X = \text{ClO}_4 \) and \( \text{PF}_6 \), assuming specific differences in their the FS anisotropies.

We will discuss two types of anisotropies when relating the Fermi velocities \( V_F \) to the direction of the magnetic field \( \vec{H} \). With directional anisotropy (DA) we mean differences in the normalized FS averages of the vectorial product \( \langle \vec{V}_F \times \vec{H} \rangle \) for different directions. With Fermi surface anisotropy (FSA), we mean the rms variation of \( \vec{V}_F \times \vec{H} \) within the FS for a given direction \( \vec{H} \). For large DA, i.e. near one and zero for two perpendicular directions respectively, the FSA will be low. On the other hand if \( \langle \vec{V}_F \times \vec{H} \rangle \) has an intermediate value, \( \sim 1/2 \), the FSA can be large so different parts of the FS have opposing contribution to the vectorial product.

For our bandstructure model we assume a tetragonal structure with \( c/a = 2 \) and \( b = c \). (In reality the \( b \) and \( c \) axes are different, but for the model calculation it is sufficient to study anisotropies between the...
Assuming large anisotropy we have for a tight binding model

\[ E(k) = E_0 + \sum_{l'} \left( \frac{2\pi}{a} k_x + \frac{2\pi}{b} k_y + \frac{2\pi}{c} k_z \right) \]

where \( t_a \gg t_b \) and the components of \( V_F \) are analytically derived as \( \lambda_{l'dE/lk_i} \) for \( i = x, y, z \). The Fermi energy \( E_F \) is assumed to coincide with the band centre \( E_c \). Later when also an ellipsoid FS in introduced we have a second band as:

\[ E(k) = E_0 + E_1 (k_x^2 + k_z^2 + \lambda \kappa^2) \]

which also have simple analytic properties (we will assume here that \( \lambda \simeq 1 \)).

In order to obtain \( H_{c2} \) one has to solve a field dependent Eliashberg equation [5]. To correct for large anisotropy we have to divide the FS into several pieces \( k \) and in short notation we have

\[ \Delta(l, k) = \frac{\pi T}{kT} \sum_{k' \Gamma} w(k') I(l') \left( \frac{\lambda_{\text{eff}}(kk' I') - \mu^*}{\omega_p Z(k' I')} \right) \Delta(l', k') \]

The gap function is \( \Delta, Z \) is the renormalization function, \( \omega_p \) is the Matsubara frequency \( 2\pi kT(2l + 1) \) and \( \lambda_{\text{eff}} \) is the effective electron-phonon coupling which depends on the phonon spectrum and \( \omega_p \). The electron-electron coupling \( \mu^* \) is here assumed constant. The FS pieces have weight factors \( w(k) \) and in order to minimize the matrix size we use only selected \( l \) values with weight factors \( I(l') \). In these calculations we use 20 Matsubara frequencies selected in rather dense mesh for low \( \omega_p \) while at larger \( \omega_p \) the mesh is more coarse. Thus effectively we have \( l_{\text{max}} = 293 \), and tests for one FS piece show only negligible errors, while the matrix size is drastically reduced. The field enters via \( V_F \times \hat{H} \) in the function \( S(k, l) \) given by Hohenberg and Werthamer [5]. For small fields and large \( S \rightarrow 1 \) while at large \( V_F \times \hat{H} \) and the first \( \omega_p \) there is a large reduction of \( T_c \) as \( S \rightarrow 0 \).

In a test calculation for a sphere the generalization \( S(l) \rightarrow S(k, l) \) using 6 weighted \( k \)-points on the irreducible FS, resulted in almost identical \( H(T) \) curves, independent of \( H \)-direction, as when using a \( S(l) \) averaged over the whole FS.

We have made several models but here we present results for just a few typical and interesting cases. For the phonon spectrum we assume a similar description as equation (1) which gives a rather normal phonon density-of-states from 0-300 K. The average of \( \lambda \) is adjusted to get a reasonable \( T_c \) in the range 0.8-2.5 K when \( \mu^* = 0.13 \).

In model I we assume one band near \( E_F \) as obtained from equation (1) for \( t_a = 10 \) \( t_b = 300 \) mRy. This gives a flat FS structure in the Brillouin-Zone. The irreducible part, \( 1/16 \) of the full FS is divided into 7 pieces and all assigned its proper \( V_F \) and weight. Since the FSA is small in this case one finds very similar results between taking the FS average of \( V_F \times \hat{H} \) before it enters \( S(l', k') \) and when the local properties of each piece is kept, i.e. the division of the FS seems unnecessary. This is not the case in model II, discussed later, or when \( H \) deviates from a symmetry direction, because the FSA are large and local variations are important.

The results for model I, assuming small variation of \( \lambda \) within the FS, are shown in figure 1. The \( H_{c2}(T) \)-curves show normal behaviour down to \( t = T/T_c \sim 0.2 \) when there seems to be a \( H_{c2} \) enhancement, but which is due to cut-off in \( \omega_p \) at \( l = 293 \). All results use the same cut-off and the results are expected to be sufficiently converged down to \( t \sim 0.2 \). The relative anisotropy for the two directions parallel and perpendicular to the \( a \)-axis is similar as found for the \( \text{CIO}_4 \) salts [6, 7]. However the \( H_{c2} \) anisotropy follows nearly the behaviour \( \langle V_F \times \hat{H} \rangle^2 \), and since the DA is nearly proportional to \( t_a/t_b \) (from model I), one derives an experimental ratio of \( t_b/t_a \) of only \( \sim \sqrt{2} \) and of \( t_b/l_c \) of \( \sim \sqrt{10} \) from the experimental data of the \( \text{CIO}_4 \)-salt by Chaikin et al. [7]. This is a considerably smaller anisotropy than found by Grant [4], but the quadratic relation between DA and \( H_{c2} \)-anisotropy tends to a linear relation as the FSA is increased. The FSA is larger as the ratio \( t_b/t_a \) is increased towards 1, or if there are other FS structures present which partly have different \( V_F \times \hat{H} \) projection.

In figure 1 is also shown the \( H_{c2}(T) \) curve when \( H \) differs from the crystallographic direction, 001. As seen, the \( H_{c2} \) decreases rapidly. Already at \( \theta^0 \) the reduction is 25 percent, at \( 17^0 \) almost 90 percent. However the shape of the \( H(T) \) curve is not change by the misalignment between the field direction and
the $z$ axis. Small misalignments ($< 10^\circ$) around the 100 axis show only negligible ($< 1\%$) increase in $H_{c2}$. The observed behaviour can partly be understood from the projected ($V_F \times H$) values given in table I. Since the FSA is small there is almost a square law between the DA and $H_{c2}$.

In model II we have added an almost spherical FS with the amplitude of $V_F$ about three times larger than the largest $V_F$ component for the tight-binding (TB) band. We assign 3 irreducible FS pieces from this structure with total weight 37\% of the total density-of-states. Now equation (3) is solved for totally 10 pieces, which depending on the field direction, gives 10 ([001]), or 20 ([100]) inequivalent pieces. The solid lines in figure 2 are the results when all FS pieces are assumed to have the same electron-phonon coupling $\lambda$. The resulting $H_{c2}$ curves are quite similar to those measured for the PF$_6$-salt [6]. The broken lines show the tailing effect for the [001]-field more evident. These results are based on the assumption that $\lambda$ for the sphere is twice that of the TB band. Further, it is assumed that there is a low coupling between the two FS structures, so that $\lambda(k, k')$, for $k$ and $k'$ being on the different FS structures, are half of the average $\lambda$.

As seen in figure 2, the field in the 001 direction creates an anomalous $H_{c2}(T)$ curve, qualitatively similar to those measured for (TMTSF)$_2$PF$_6$ salts [6]. At low fields there is almost no difference between the 001 and 100 directions, while as the field gets stronger the $H_{c2}^{001}$-curve (in contrast to the $H_{c2}^{100}$-curve which behaves normally) becomes strongly enhanced. From comparing the $\langle V_F \times \hat{H} \rangle$ values with the $H_{c2}$ values one now finds a linear or even weaker relationship between the DA and $H_{c2}$ anisotropy. This is thus very different from the case with only one very planar TB-FS considered. The different parameters can be changed substantially while still giving the anomalous behaviour of the $H_{c2}(T)$-curve. But the anomalous feature is created when there are several FS-pieces which have differences in its $V_F$-projections and $\lambda$-values. Namely, at no field all FS pieces have the same gap (if $\lambda$ is the same) and all contribute to the $T_c$. With applied field the gap on the spherical FS is quickly suppressed since its larger $V_F$ couples strongly to the field. At even higher field in the [001] direction only the TB band has a gap and with its low $V_F$ projection the field will only gradually suppress $T_c$.

The possibility of such a mechanism was already proposed by Entel and Peter [8], and small effects can be found in weak anisotropic systems as Nb [9], but in these very anisotropic organic superconductors the effects can be strong. Since the PF$_6$-salt is superconducting only under pressure, it may be difficult to obtain good alignment between the field direction and the crystallographic axis. But judging from the calculations for misaligned field in model I, it seems unlikely that the anomalous behaviour is due to misalignment.

In view of our model calculations, it seems likely that there are differences in the FS features of (TMTSF)$_2$ClO$_4$ and (TMTSF)$_2$PF$_6$ which are revealed in the $H_{c2}$ measurements. The $H_{c2}$-behaviour for the ClO$_4$ salt seems to fit with a planar TB-FS, but the ratios for the TB overlap parameter $t_o : t_e : t_e$ appears to be lower than what has been inferred and could be as low as 5 : 3 : 1. However, this is an extremely low limit since it assumes a quadratic relation between the DA and $H_{c2}$-anisotropy, while for lower DA the FSA will increase due to the warping of the FS and it will tend to be a linear relation between DA and $H_{c2}$-anisotropy. If so the TB parameters are related as 20 : 10 : 1.

For the PF$_6$-salt additional non planar FS has to be added as the one used for model II. The same effect could arise from strong warping of the edges of the TB surface. Now the FSA is considerable, the DA reduced, and the $H_{c2}$-anisotropy varies with $T/T_c$. For $T \to T_c$ there is almost no $H_{c2}$-anisotropy while at lower $T$, the ratio of $H_{c2}^{001} : H_{c2}^{001}$ tends to the ratio for the $V_F$-projections. The $H_{c2}(T)$ curve for direction [001] has a low field tail, similar to the one observed for the PF$_6$ salt [6], which would become more apparent if also $\lambda_e$ was anisotropic.

### Table I. Normalized Fermi surface averages of $\langle V_F \times \hat{H} \rangle$ for different field directions H, for the two models discussed in the text.

<table>
<thead>
<tr>
<th></th>
<th>[1, 0, 0]</th>
<th>[0, 0, 1]</th>
<th>[0.1, 0, 1]</th>
<th>[0.3, 0, 1]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model I</td>
<td>0.996</td>
<td>0.116</td>
<td>0.142</td>
<td>0.298</td>
</tr>
<tr>
<td>Model II</td>
<td>0.913</td>
<td>0.364</td>
<td>—</td>
<td>—</td>
</tr>
</tbody>
</table>

Fig. 2. $H_{c2}(T)$ curves for model II, in which an almost spherical FS piece has been added to the FS of model I. Solid lines are the curves for a constant $\lambda$. This behaviour is similar to the situation for (TMTSF)$_2$PF$_6$. Broken lines are the curves when the TB band has half as large $\lambda$ as the sphere band, and the tailing effect for the [001] direction is more evident.
While the TB part of the FS has the same $V_F$-projections as for model I, the total $V_F$-projections given in table I are different due to the spherical FS piece. Comparing with the experimental results for (TMTSF)$_2$PF$_6$ by Greene et al. [6], one can derive approximate values for the $t_a : t_b : t_c$ ratios as 20 : 6 : 1 from the low- $T$ $H_{c2}$ ratios.

At this point we should mention that in the « dirty » limit there is, assuming isotropic diffusion parameter, a linear relation between $V_F$- and $H$-anisotropy. Thus, in the dirty limit larger $t_a : t_b : t_c$ ratios can be inferred from the $H_{c2}$-anisotropies [1, 10]. Inelastic scattering processes would « wash out » FS anisotropies and lead to reduced $H_{c2}$ anisotropies. It is probably important to include such processes, leading to larger $t_a : t_b : t_c$ ratios than calculated here, when quantitative conclusions are to be drawn. But in these model calculations we restrict our interpretation to be qualitative for perfectly defined FS structures.

It is also important to note that Hohenberg-Werthamer theory was derived under the assumption of locality or of small anisotropy. But for $T \lesssim T_c$ we can apply both expressions for $S(k, w)$ and when several FS pieces are used we obtain a qualitatively similar result in both limits. An unrestricted solution of the $H_{c2}$ problem for large anisotropies and non-locality is still lacking. The conditions for a mean-field approach and the competition between superconductivity, Peierls transitions and spin-waves has been studied by Horovitz et al. [11]. Our model fulfils the conditions for the mean-field approach.

Concerning the anomalous $H_{c2}$-tail in the PF$_6$-salt it should be noted that the experimental procedure is very difficult since the measurement is performed under 11 kbar pressure [6]. The exact nature of this $H_{c2}$-tail is therefore yet somewhat uncertain. However, a qualitatively similar $H_{c2}$-curve has been observed in another low-dimensionality system, namely in (SN)$_2$ [12]. Our FS-model for the PF$_6$-salt should be applicable also to the (SN)$_2$ system. In addition we believe that FS anisotropies and multiband features ought to be discussed in the context of unusual $H_{c2}$-curves in recently reported layered materials [13] and heavy Fermion superconductors [14].

Our estimates of the $T$ overlap parameters are less anisotropic than obtained in other studies [1, 4]. However, the tails of Muffin-Tin orbitals go as $\sim R^{-(a+1)}$ where $R$ is the distance and $I$ is the angular momentum. In these organic materials it is mainly $s$ and $p$ states which are important for the electron states near $E_F$, so assuming that the angular interaction can be neglected in a simple estimation, using typical ion-ion distances, one does not expect to find strongly anisotropic overlap integrals.

Our calculations do not include spin limiting effects on $T_c$. But no unusual behaviour of measured $H_c2(T)$ curves appear compared to what is calculated, so we rule out the possibility of spin limiting effects on $T_c$.

We conclude that our model calculations, despite the approximations involved, are relevant for a mean-field interpretation of unusual $H_{c2}$-behaviour in various anisotropic materials. Thus a multiband structure, consisting of one anisotropic part and one other part having larger warping and larger Fermi velocities, leads to an anomalous $H_{c2}$-behaviour such as observed in the (TMTSF)$_2$PF$_6$ salt. A single anisotropic FS without warping leads to normally shaped $H_{c2}(T)$-curves, although the $H_{c2}$ anisotropy is very large.

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