The Behavior of a Triplet Superconductor in a Spin Only Magnetic Field

B. J. Powell, James F. Annett, and B. L. Györffy

H. H. Wills Physics Laboratory, University of Bristol, Tyndall Avenue, BS8 1TL, UK

Abstract. We investigate the order parameter of Sr$_2$RuO$_4$ in an exchange-only magnetic field. A Ginzburg-Landau symmetry analysis implies three possibilities: a pure $^3$He A phase, a $^3$He A$_1$ or a $^3$He A$_2$ phase. We explore the exchange field dependence of the order parameter and energy gap in a one-band model of Sr$_2$RuO$_4$. The numerical solutions show no A$_1$ phase and that the A$_2$ phase is lower in free energy than the A phase. We explore heat capacity as a function of temperature and field strength and find quantitatively different behaviors for the A and A$_2$ phases.

1 Introduction

A spin triplet superconductor should show a number of interesting magnetic-field effects which are direct consequences of the magnetic moment of the Cooper pairs. In particular, for spin-triplet superconductors the Zeeman coupling between the quasiparticle spins and an external magnetic field need not lead to Pauli limiting, unlike the case of spin-singlet superconductors. In the extreme high field limit with completely exchange-split bands we could expect single spin pairing of the majority spin Fermi surface. We may also expect possible phase transitions or symmetry changes of the order parameter in a magnetic field, which are analogous to the transitions seen in superfluid $^3$He[1,2,3]. The $^3$He B-phase is destroyed in a magnetic field in a qualitatively similar manner to a singlet superconductor. On the other hand, if the zero field ground state is one of equal-spin-pairing (ESP), then the gap function can deform continuously as a function of a Zeeman field the $^3$He A-phase evolves first smoothly into A$_2$ phase and then, via a phase transition A$_1$ phase, as it progresses from equal-spin-pairing to single spin pairing with increasing field[4].

The superconductor Sr$_2$RuO$_4$ should be an ideal candidate to examine these effects. There is strong evidence for spin-triplet pairing[5] from direct measurements of spin-susceptibility in the superconducting state[6,7]. It is has a simple and well understood Fermi surface[8], and is in the clean limit. The detailed gap function is still somewhat controversial, but is generally believed[9] to be of tetragonal $E_u$ symmetry[10], and more specifically to be a two-dimensional analogue of the $^3$He A-phase, with $d(k) \sim (\sin k_x + i \sin k_y)(0,0,1)$. This order parameter would agree with the spin-susceptibility measurements in the superconducting state[6,7], and also would lead to time-reversal symmetry breaking below $T_c[11]$. More recently, specific heat[12], penetration depth[13] and thermal conductivity[14] experiments have shown that the gap must have line-nodes
on the Fermi surface. However, for the cylindrical Fermi surface geometry\cite{8} of Sr$_2$RuO$_4$ a complete group theoretic analysis of symmetry distinct pairing states does not show any which both break time-reversal symmetry and have line-nodes\cite{10}. A possible resolution to this dilemma has been developed in the orbital dependent pairing model of Zhitomirsky and Rice\cite{15} and in a related model by Litak \textit{et al.}\cite{16}. For different reasons both groups proposed that the gap function is of the form

$$d(k) \sim (\sin k_x + i \sin k_y)(0, 0, 1)$$

(1)

on the dominant $\gamma$-Fermi surface sheet, and of the form

$$d(k) \sim \left( \sin \left( \frac{k_x}{2} \right) \cos \left( \frac{k_y}{2} \right) + i \sin \left( \frac{k_y}{2} \right) \cos \left( \frac{k_x}{2} \right) \right) \cos \left( \frac{ck_z}{2} \right)(0, 0, 1)$$

(2)

on the $\alpha$ and $\beta$ sheets. Both of these functions possess the same $E_u$ symmetry, but correspond to intra-plane and inter-plane pairing interactions respectively. This gap function has horizontal line nodes at $k_z = \pm \pi/c$ on the $\alpha$ and $\beta$ sheets, and was shown to be in good agreement with experimental temperature dependences for specific heat, penetration depth and thermal conductivity\cite{16}.

In a magnetic field Sr$_2$RuO$_4$ shows a number of unusual features. Firstly the vortex lattice is square\cite{17,18} which agrees well with the predictions of a two-component $E_u$ symmetry Ginzburg-Landau theory\cite{19,20}. Secondly there is an anomalous second feature close to $H_{c2}$, which only occurs when the field is aligned within $1^\circ$ of the a-b plane\cite{12}. At the present time the origin of this feature is uncertain. It may be a vortex lattice phase transition, or it may correspond to a change in pairing symmetry with field, perhaps analogous to the double superconducting transition in UPt$_3$\cite{21}.

In this paper we will focus specifically on the unique effects of the Cooper pair spin in a triplet superconductor. Therefore we neglect the effects of the vector potential on the quasiparticles, and instead focus solely on the Zeeman coupling of the quasiparticle spin to the magnetic field. We can justify this model by appealing to the strong Stoner enhancement in Sr$_2$RuO$_4$\cite{22,23}, and so the exchange field will be large. Alternatively, our model may be appropriate for the ferromagnetic superconductor ZrZn$_2$\cite{24}.

This paper is organised as follows. Firstly we write a simple single-band model Hamiltonian for $p$-wave pairing in the $\gamma$-band of Sr$_2$RuO$_4$. Next we examine how a spin-only magnetic field enters the corresponding $E_u$ symmetry Ginzburg-Landau theory. In section 4, we present detailed numerical results for the field dependent energy gap, and specific heat for the two relevant cases of the exchange field either parallel or perpendicular to the $d(k)$ order parameter. We show that the lower free energy state is analogous to the $^3$He $A_2$ phase. Finally, in Sec. 5 we present our conclusions.
We consider the effect of a spin-only magnetic field, $H$, on an attractive, nearest neighbour, Hubbard model. We use a one-band model, appropriate for the $\gamma$ sheet of the Sr$_2$RuO$_4$ Fermi surface. The set of interaction constants, $U^{\sigma\sigma'}_{ij}$, describe attractions between electrons on sites $i$ and $j$ with spins $\sigma$ and $\sigma'$. The Hamiltonian for this model is:

$$
\hat{H} = \sum_{ij\sigma}(\epsilon - \mu)\delta_{ij} - t_{ij}c^\dagger_{i\sigma}c_{j\sigma} - \frac{1}{2} \sum_{ij\sigma\sigma'} U^{\sigma\sigma'}_{ij} \hat{n}_{i\sigma}\hat{n}_{j\sigma} + \mu_B \sum_{i\sigma}\hat{c}^\dagger_{i\sigma}(\sigma_{\sigma\sigma'} \cdot \mathbf{H})\hat{c}_{i\sigma}
$$

(3)

where $t_{ij}$ is the hopping integral, $\epsilon$ is the site energy, $\hat{c}^\dagger_{i\sigma}$ and $\hat{c}_{j\sigma}$ are the usual annihilation and creation operators and $\hat{n}_{i\sigma}$ is the number operator. $\sigma_{\sigma\sigma'}$ are the components of the vector of Pauli matrices:

$$
\sigma = (\sigma_1, \sigma_2, \sigma_3)
$$

(4)

By making the Hartree-Fock-Gorkov approximation and taking a lattice Fourier transform the following spin-generalised Bogoliubov-de Gennes (BdG) equation can be derived from the above Hamiltonian.

$$
\begin{pmatrix}
\epsilon_k + \mu_B H_3 & \mu_B (H_1 - iH_2) & \Delta\uparrow\uparrow(k) & \Delta\uparrow\downarrow(k) \\
\mu_B (H_1 + iH_2) & \epsilon_k - \mu_B H_3 & \Delta\downarrow\uparrow(k) & \Delta\downarrow\downarrow(k) \\
-\Delta\uparrow\uparrow(-k) & -\Delta\downarrow\uparrow(-k) & -\epsilon - \mu_B H_3 & \mu_B (-H_1 - iH_2) \\
-\Delta\downarrow\uparrow(-k) & -\Delta\downarrow\downarrow(-k) & \mu_B (-H_1 + iH_2) & -\epsilon + \mu_B H_3
\end{pmatrix}
\begin{pmatrix}
\begin{pmatrix} u_{\uparrow\sigma}(k) \\ v_{\downarrow\sigma}(k) \end{pmatrix} \\
\begin{pmatrix} u_{\downarrow\sigma}(k) \\ v_{\uparrow\sigma}(k) \end{pmatrix}
\end{pmatrix} = E_\sigma(k)
$$

(5)

where $\epsilon_k$ is the (Fourier transformed) normal, spin independent part of the Hamiltonian. The order parameters $\Delta_{\sigma\sigma'}(k)$ are determined self consistently by

$$
\Delta_{\sigma\sigma'}(k) = -\frac{1}{2} \sum_{q\sigma''} U^{\sigma\sigma'}(q)(u_{\sigma\sigma''}(-q)v_{\sigma\sigma''}^*(-q) - v_{\sigma\sigma''}^*(q)u_{\sigma\sigma''}(q))(1 - 2f_{q\sigma''})
$$

(6)

where $U^{\sigma\sigma'}(q)$ is the lattice Fourier transform of $U^{\sigma\sigma'}_{ij}$ and $f_{q\sigma}$ is shorthand for the Fermi function $f(E_{q\sigma})$. It is natural to separate the spin-generalized BdG equation into triplet and singlet parts:
\[ \Delta(k) \equiv \begin{pmatrix} \Delta_{1\uparrow}(k) & \Delta_{2\uparrow}(k) \\ \Delta_{1\downarrow}(k) & \Delta_{2\downarrow}(k) \end{pmatrix} = (d_0(k) + \sigma \cdot d(k))i\sigma_2. \] (7)

\(d_0(k)\) is the (scalar) singlet order parameter and \(d(k)\) is the (vector) triplet order parameter. The singlet order parameter is symmetric under spatial inversion while the triplet order parameter is anti-symmetric under spatial inversion. Hence, the BdG equation can be rewritten as

\[
\begin{pmatrix}
\epsilon_k + \mu_B H_3 & \mu_B (H_1 - iH_2) & -d_1(k) + id_2(k) & \mu_B (H_1 + iH_2) & d_0(k) + d_3(k) \\
\mu_B (H_1 + iH_2) & \epsilon_k - \mu_B H_3 & -d_0(k) + d_3(k) & -\mu_B (-H_1 - iH_2) & d_1(k) + id_2(k) \\
-d_1^*(k) - d_2^*(k) - d_0^*(k) + d_3^*(k) & -\epsilon_k - \mu_B H_3 & d_0(k) + d_3(k) & -\mu_B (-H_1 - iH_2) \\
d_0^*(k) + d_3^*(k) & d_1^*(k) - d_2^*(k) & d_0(k) + d_3(k) & -\epsilon_k + \mu_B H_3 \\
\end{pmatrix}
\begin{pmatrix}
u_{\uparrow\sigma}(k) \\ u_{\downarrow\sigma}(k) \\ v_{\uparrow\sigma}(k) \\ v_{\downarrow\sigma}(k) \end{pmatrix}
= E_\sigma(k)
\begin{pmatrix}
u_{\uparrow\sigma}(k) \\ u_{\downarrow\sigma}(k) \\ v_{\uparrow\sigma}(k) \\ v_{\downarrow\sigma}(k) \end{pmatrix}. \] (8)

If there is no superconductivity in the triplet channel we regain the standard result for the spectrum of a singlet superconductor in a spin only magnetic field:

\[ E(k) = \pm \sqrt{\epsilon_k^2 + |d_0(k)|^2 \pm \mu_B |H|}. \] (9)

By setting the singlet order parameter to zero we find that the equivalent result for a triplet superconductor is

\[ E(k) = \pm \sqrt{\epsilon_k^2 + \mu_B^2 |H|^2 + |d(k)|^2 \pm \sqrt{\Lambda(k)}}. \] (10)

where

\[ \Lambda(k) = |d(k) \times d(k)^*|^2 + 4\epsilon_k^2 \mu_B^2 |H|^2 + 4\mu_B^2 |H \cdot d(k)|^2 + 4i\epsilon_k \mu_B |H \cdot d(k) \times d(k)^*|. \] (11)

It should be noted that this does not assume a unitary order parameter.\(^1\)

It is a relatively straightforward process to calculate thermodynamic properties for a triplet superconductor. For example the specific heat is given by

\(^1\) A unitary state is any state for which \(d(k) \times d^*(k) = 0\).
3 Ginzburg–Landau Theory of a Quasi–Two Dimensional Triplet Superconductor in a Magnetic Field

Before considering numerical solutions of the self consistent Bogoliubov–de Gennes equations, we will examine the possible results by deriving a Ginzburg–Landau theory from our microscopic theory.

Consider a quasi–two dimensional system with two orbital degrees of freedom (which we label x and y) and three spin degrees of freedom (labelled 1, 2 and 3). Hence, instead of the familiar 3 by 3 order parameter, we will examine the possible results by deriving a Ginzburg–Landau Theory of a Quasi–Two Dimensional Triplet Superconductor in a Magnetic Field described by the complex 2 by 3 matrix $A$

\[
C_V = T \frac{\partial S}{\partial T} \\
= -k_B T \frac{\partial}{\partial T} \sum_{\kappa \sigma} (f_{\kappa \sigma} \ln(f_{\kappa \sigma}) + (1 - f_{\kappa \sigma}) \ln(1 - f_{\kappa \sigma})) \\
= \sum_{\kappa \sigma} f_{\kappa \sigma} (1 - f_{\kappa \sigma}) \left( \frac{E_{\sigma}(k)}{k_B T^2} + \frac{1}{k_B T} E_{\sigma}(k) \frac{d}{dT} E_{\sigma}(k) \right) \\
= \sum_{\kappa \sigma} f_{\kappa \sigma} (1 - f_{\kappa \sigma}) \left( E_{\sigma}(k)^2 - \frac{T}{2} \frac{d}{dT} |d(k)|^2 \right)
\]

\[
F = \alpha (T - T_c) (|A_x|^2 + |A_y|^2) + \beta_1 (|A_x|^2 + |A_y|^2)^2 + \beta_2 |A_x \cdot A_x + A_y \cdot A_y|^2 \\
+ \beta_4 (|A_x \cdot A_y|^2 + \sigma^y \cdot \sigma_x)^2 + (A^*_x \cdot A_x)^2 + (A^*_y \cdot A_y)^2) \\
+ \beta_5 (2 |A_x \cdot A_y|^2 + |A_x \cdot A_x|^2 + |A_y \cdot A_y|^2) \\
+ \beta_6 (|A_x \cdot A_x|^2 + |A_y \cdot A_y|^2) + \beta_7 (|A_x|^4 + |A_y|^4).
\]

Only the first five quartic terms ($\beta_1 - \beta_5$) are required to describe $^3$He [25]. The additional two terms here ($\beta_6$ and $\beta_7$) appear because the rotational symmetry of the crystal is discrete, where as rotational symmetry is continuous in the fluid. Gradient terms can also be calculated [10, 13, 20], but we will not make use of these here.

To second order in $A$ the free energy in a finite magnetic field, $F_{H}$, is
\[ F_H = \frac{1}{\beta} \sum_{\omega_n} \int dk \ \text{tr} \left( G^0(k, \omega_n) \mathbb{A}(k) G^0(-k, \omega_n) \mathbb{A}^\dagger(-k) \right), \]  

(18)

where,

\[ G^0(k, \omega_n) = (\omega_n + \varepsilon_k - \mu + \mu_B \sigma \cdot H)^{-1} \]  

(19)

and \( \omega_n \) are the Matsubara frequencies.

Thus to all orders in \( H \)

\[ F_H = -\frac{1}{\beta} \sum_{\omega_n} \text{tr} \int dk \ (\omega_n - \varepsilon_k + \mu + \mu_B \sigma \cdot H) \]

\[ \times \left( \sigma \cdot A_x \sin k_x + \sigma \cdot A_y \sin k_y \right) \Delta \left( \omega_n - \varepsilon_k + \mu + \mu_B \sigma \cdot H \right) \]

\[ \times \left( \sigma^* \cdot A^*_x \sin k_x + \sigma^* \cdot A^*_y \sin k_y \right) \sigma_2. \]  

(20)

Hence,

\[ F_H = A_x \chi_{xx} A^*_x + A_x \chi_{xy} A^*_y + A_y \chi_{yx} A^*_x + A_y \chi_{yy} A^*_y, \]  

(21)

where,

\[ \chi^{\alpha\beta}_{ij} = -\frac{1}{\beta} \sum_{\omega_n} \int dk \sin k_i \sin k_j \]

\[ \times \text{tr} \left( \frac{\Delta(\omega_n - \varepsilon_k + \mu + \mu_B \sigma \cdot H) \sigma_\alpha \sigma_\beta}{\Delta(\omega_n - \varepsilon_k + \mu + \mu_B \sigma \cdot H) \sigma_\alpha \sigma_\beta} \right). \]  

(22)

By x–y symmetry \( \chi_{xy} = \chi_{yx} = 0 \). Some algebra then leads to

\[ F_H = (\alpha_0 + \alpha_2 |H|^2)(|A_x|^2 + |A_y|^2) + i\alpha_1 H \cdot (A_x \times A^*_x + A_y \times A^*_y) \]

\[ -2\alpha_2 |H \cdot A|^2. \]  

(23)

Where,

\[ \alpha_0 = \frac{2}{\beta} \sum_{\omega_n} \int dk \frac{\sin^2 k_x (\varepsilon_k - \mu)^2 + \omega_n^2}{\Delta(\omega_n - \varepsilon_k + \mu)^2 - |H|^2 \Delta(\omega_n - \varepsilon_k - \mu)^2 - |H|^2}, \]  

(24)

\[ \alpha_1 = -\frac{4\mu_B}{\beta} \sum_{\omega_n} \int dk \frac{\sin^2 k_x (\varepsilon_k - \mu)}{\Delta(\omega_n - \varepsilon_k + \mu)^2 - |H|^2 \Delta(\omega_n + \varepsilon_k - \mu)^2 - |H|^2}. \]  

(25)
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and

\[ \alpha_2 = -\frac{2\mu_B^2}{\beta} \sum_{\omega_n} \int \frac{dk}{[(\omega_n - \varepsilon_k + \mu)^2 - |H|^2] [(\omega_n + \varepsilon_k - \mu)^2 - |H|^2]} \sin^2 k_x. \] (26)

Clearly \( \alpha_0 \) reduces to \( \alpha \) (17) in zero magnetic field, but the \( \alpha_1 \) and \( \alpha_2 \) terms do not have an analogue in the zero field Ginzburg–Landau expansion. It is interesting to note the similarity of these extra terms to the change in the Hartree–Fock–Gorkov quasiparticle spectrum caused by the magnetic field - (11). The cross product of any complex vector with its complex conjugate is purely imaginary\(^2\) so the square root of minus one before the \( \alpha_1 \) term in the expression for the free energy is to be expected.

As we have expanded in \( A \) but not in \( H \) the above expression for the free energy is valid for small gaps at all field strengths. It is therefore valid close to \( H_c \). But, note that, since we assumed an exchange-only magnetic field we do not consider the vortex lattice here. Agterberg and Heeb\[19,20\] have discussed the vortex lattice using Ginzburg–Landau theory, but did not include the Zeeman terms of (23).

In the Ginzburg–Landau formalism the superconducting phase transition occurs when the quadratic terms go to zero. In a zero field this condition is simply

\[ \alpha(T - T_c) = 0. \] (27)

In a finite spin only magnetic field the equivalent condition is that the matrix

\[ \mathbf{\Xi} = \alpha_{ij} A_i A_j^* \] (28)

has (at least) one zero eigenvalue, but no negative eigenvalues, where the indices \( i \) and \( j \) run over both orbital and spin degrees of freedom. In this case

\[ \mathbf{\Xi} = \begin{pmatrix} \beta & 0 \\ 0 & \beta \end{pmatrix}, \] (29)

where,

\[ \beta = \begin{pmatrix} \alpha_0 + \alpha_2 |H|^2 - 2\alpha_2 H_1^2 & i\alpha_1 H_3 & -i\alpha_1 H_2 \\ -i\alpha_1 H_3 & \alpha_0 + \alpha_2 |H|^2 - 2\alpha_2 H_2^2 & i\alpha_1 H_1 \\ i\alpha_1 H_2 & -i\alpha_1 H_1 & \alpha_0 + \alpha_2 |H|^2 - 2\alpha_2 H_3^2 \end{pmatrix}. \] (30)

The condition for there being a zero eigenvalue of \( \mathbf{\Xi} \) is

\(^2\) This can easily be confirmed. Consider the cross product of the most general complex vector, \( \mathbf{v} = (a + ib, c + id, e + if) \). It is trivial to show that \( \mathbf{v} \times \mathbf{v}^* = -2i(cf - de, be - af, ad - bc) \).
\[(\alpha_0 + \alpha_2 |H|^2 - 2\alpha_2 H^2_\parallel) (\alpha_0 + \alpha_2 |H|^2 - 2\alpha_2 H^2_\perp) (\alpha_0 + \alpha_2 |H|^2 - 2\alpha_2 H^2_x) \]

\[- (\alpha_0 + \alpha_2 |H|^2 - 2\alpha_2 H^2_\parallel) \alpha^2_1 H^2_1 \]

\[- (\alpha_0 + \alpha_2 |H|^2 - 2\alpha_2 H^2_\perp) \alpha^2_1 H^2_2 \]

\[- (\alpha_0 + \alpha_2 |H|^2 - 2\alpha_2 H^2_x) \alpha^2_1 H^2_x = 0. \]

This expression can be greatly simplified by choosing our coordinate system so that \(H\) lies parallel to one of the axes. With, for example, \(H = (0,0,H)\) we find

\[
\beta = \begin{pmatrix}
\alpha_0 + \alpha_2 H^2 & i \alpha_1 H & 0 \\
-i \alpha_1 H & \alpha_0 + \alpha_2 H^2 & 0 \\
0 & 0 & \alpha_0 - \alpha_2 H^2
\end{pmatrix}.
\]

Which has at least one zero eigenvalue when

\[(\alpha_0 - \alpha_2 H^2)((\alpha_0 + \alpha_2 H^2)^2 - \alpha^2_1 H^2) = 0. \]

The eigenvectors of \(\beta\) are

\[
\begin{pmatrix}
A_{1x} \\
A_{2x} \\
A_{3x} \\
A_{1y} \\
A_{2y} \\
A_{3y}
\end{pmatrix} = \begin{pmatrix}
0 \\
0 \\
1 \\
0 \\
0 \\
1
\end{pmatrix}, \begin{pmatrix}
0 \\
0 \\
i \kappa \\
0 \\
i \kappa \\
0
\end{pmatrix}, \begin{pmatrix}
0 \\
0 \\
0 \\
1 \\
0 \\
0
\end{pmatrix}, \begin{pmatrix}
0 \\
0 \\
0 \\
i \kappa \\
0 \\
0
\end{pmatrix}, \begin{pmatrix}
0 \\
1 \\
0 \\
0 \\
0 \\
0
\end{pmatrix}, \begin{pmatrix}
0 \\
1 \\
0 \\
0 \\
0 \\
0
\end{pmatrix}
\]

Where \(\kappa\) is real. To second order in \(A\), \(\kappa\) is given by

\[
\kappa = -\frac{\alpha_0 + \alpha_2 H^2}{\alpha_1 H}
\]

Much recent work (see introduction) has suggested that \(\text{Sr}_2\text{RuO}_4\) is likely to be in an state analogous to the A-phase of \(^3\text{He}\). If the pairing interaction favours the A-phase in zero magnetic field there are three possible solutions in a magnetic field.

\[
\begin{align*}
A_x &= -i A_y = (0,0,1) \\
A_z &= -i A_y = (1,i\kappa,0) \\
A_z &= -i A_y = (-i\kappa,1,0)
\end{align*}
\]

Equation 36 is the A-phase with \(d(k)\) parallel to \(H\). Equations 37 and 38 both give the \(A_2\)-phase for \(0 < |\kappa| < 1\) and the \(A_1\)-phase for \(|\kappa| = 1\). Analogy may be drawn to the description of elliptically polarised light in optics [26]. One can
think of the three A-like phases as being described by an ellipse of eccentricity \(\sqrt{1-\kappa^2}\). The A-phase is the special case of linear polarization when the ellipse reduces to a line parallel to \(d(k)\). The \(A_1\) phase is the special case of circularly polarized light a circle which lies in the 1,2-plane. The \(A_2\) corresponds to any ellipse between these two extremes. In the \(A_1\) and \(A_2\)-phases by taking the appropriate superposition of (37) and (38) the major axis of the ellipse can be made to point in any direction in the plane perpendicular to \(H\).

4 Numerical results

To progress further we must resort to solving the self consistent Bogoliubov–de Gennes equations numerically. To do this we fit the hopping integral and site energy to the experimentally determined Fermi surface of the \(\gamma\)-sheet of \(\text{Sr}_2\text{RuO}_4\) \(^8\). The interaction potential is restricted to include nearest neighbour terms only and chosen to give the experimentally observed critical temperature (1.5K).

4.1 \(d(k)\) parallel to \(H\)

We begin by studying the first solution of the Ginzburg–Landau theory \(^{36}\), in which \(d(k)\) is parallel to \(H\). In zero field we find that the ground state of the model is a triplet state analogous to the A-phase of \(^3\text{He}\), specifically the state is

\[
d = \Delta_0 (\sin k_x + i \sin k_y) \hat{e}.
\]

(39)

Here we have defined the vector order parameter to point in the \(e\) direction. In zero field, all directions in spin space are degenerate if spin–orbit coupling is neglected. When an external field is applied the ground state has \(d(k)\) perpendicular to the field, as we will show below. However, in \(\text{Sr}_2\text{RuO}_4\) the order parameter is thought to be aligned with the c-axis \(^3\), by spin-orbit coupling. Therefore despite the low critical field along the c-axis, \(\text{Sr}_2\text{RuO}_4\) presents us with the possibility of studying a triplet superconductor with a magnetic field parallel to the order parameter. It is therefore interesting to predict what would be observed in such experiments. To do this we simply discard any A-phase like solutions with \(d(k)\) not parallel to \(H\). We then consider the remaining self consistent solution of the BdG equation with the lowest free energy.

A field applied parallel to \(d(k)\) does not cause a change in the symmetry of the gap. It follows that at zero temperature the gap is independent of magnetic field strength (see appendix). At finite temperature, a field applied parallel to the order parameter causes a change in the magnitude of the gap (see Fig. \(^3\)). It should be noted that the gap is nodeless but has minima at \(k_x = 0\) and \(k_y = 0\).

We calculate the heat capacity, magnetisation and magnetic susceptibility as functions of temperature and field strength. For an isotropic nodeless gap in zero
field it is well known\cite{3} that these properties behave as
\[ C_v, M, \chi \sim \exp(\frac{\Delta}{k_B T}). \] (40)

We find that for an anisotropic, nodeless, p-wave gap the thermodynamics have the same form, even in the presence of a magnetic field (see inset Fig. 2). We therefore define the effective gap, \( \Delta_{\text{eff}} \) ‘seen’ by the thermodynamic functions as

\[ C_v, M, \chi \sim \exp(\frac{\Delta_{\text{eff}}}{k_B T}). \] (41)

We find that \( \Delta_{\text{eff}} \) is the mean gap at the Fermi surface, \( |d(k_F)| \) in zero field and that \( \Delta_{\text{eff}} \) is a linear function of magnetic field strength (see Fig. 2). That is to say that

\[ \Delta_{\text{eff}} = |d(k_F)| - \mu_B |H|. \] (42)

4.2 \( d(k) \) perpendicular to \( H \)

Recall that the ground state of the model in zero field is

\[ d = \Delta_0 (\sin k_x + i \sin k_y)(1, 0, 0). \] (43)
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Fig. 2. $\Delta_{\text{eff}}$ (normalised to $|d(k_F)|$ at $T = H = 0$) as a function of magnetic field parallel to $d(k)$ extrapolated from heat capacity (circles), magnetisation (squares) and magnetic susceptibility (diamonds). The line is $|d(k_F)| - \mu_B H$. Inset - Logarithmic plot of heat capacity with inverse temperature at various fields. From the bottom up: H=0T, 0.28T, 0.42T, 0.71T, 0.85T, 1.13T, 1.41T, 1.76T, 2.12T, 2.47T and 2.82T.

(See Fig. 3a.) We will now examine the numerical solutions of the full BdG equations corresponding to the second solution of the Ginzburg–Landau theory (37) and (38). In a magnetic field the ground state is when the vector order parameter points perpendicular to the field. There is also a change in the pairing state to a phase analogous to the $A_2$-phase of $^3$He, where

$$d = \Delta_0(\sin k_x + i \sin k_y)(1, i\kappa, 0),$$

(44)

where $\kappa$ is a real function of temperature and field strength (Fig. 3b,c.) Physically this corresponds to the majority of the spin 1 Cooper pairs aligning themselves antiparallel to the magnetic field.

In $^3$He as the field and temperature increase $\kappa$ increases until $\kappa = 1$. This is the $A_1$ phase which is the ground state of $^3$He near to $T_C$ in finite fields. The $A_1$-phase has order parameter

$$d = \Delta_0(\sin k_x + i \sin k_y)(1, i, 0)$$

(45)

and corresponds to single spin pairing with all of the Cooper pairs aligning themselves with the magnetic field (Fig. 3d.) However, even near $T_C$ and in large fields we do not find that the $A_1$-phase is the ground state of our model. If such a transition does occur then it is certainly well above the experimentally
observed upper critical field. This is in agreement with experiment as no $A_1$-phase has been observed to date.

Due to the nodeless gap in the $A_2$ phase the specific heat has an exponential temperature dependence. Hence we can calculate the effective gap for this field orientation (Fig. 4.) We find a linear field dependence in low fields but its dependence is much weaker than for $d(k)$ parallel to $H$ and there is an upturn in large fields. There is known to be a qualitative change in heat capacity in this field orientation [12]. It remains to be seen if these are related.

5 Conclusions

We investigated the order parameter of $\text{Sr}_2\text{RuO}_4$ in an exchange-only magnetic field. A Ginzburg–Landau symmetry analysis implied three possibilities: either a $^3\text{He} A_1$ or $A_2$ phase with $d(k)$ perpendicular to the magnetic field or a pure $^3\text{He} A$ phase with $d(k)$ parallel to the magnetic field. We explored the exchange field dependence of the order parameter and energy gap in a one-band model of $\text{Sr}_2\text{RuO}_4$. The numerical solutions showed no $A_1$ phase for physically reasonable field strengths and that of the two remaining phases the $A_2$ phase is lower in free energy. We did not include the effect of spin-orbit coupling which could change
Fig. 4. $\Delta_{eff}$ (normalised to $|d(k_F)|(T = H = 0)$) as a function of $H$ perpendicular to $d(k)$ (solid line) extrapolated from heat capacity. For comparison we plot $\Delta_{eff}$ for $H$ parallel to $d(k)$ (dashed line).

the ground state for particular orientations of the magnetic field (particularly with $H$ parallel to the c-axis of the crystal.) We investigated the behaviour of the heat capacity as a function of both field and temperature for both of these solutions. We have shown that the variation of the exponential cutoff below $T_C$ as a function of $H$ is quantitatively and qualitatively different for these two phases. This makes heat capacity an excellent experimental probe of the symmetry state in a magnetic field.

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Appendix

For an A-phase triplet superconductor with $H$ parallel to $d(k)$ and $z$ the BdG equations are
\[
\begin{pmatrix}
\epsilon_k + \mu_B H & 0 & d_3(k) \\
0 & \epsilon_k - \mu_B H & 0 \\
d_3^*(k) & 0 & -\epsilon_{-k} - \mu_B H
\end{pmatrix}
\begin{pmatrix}
u_{\uparrow\sigma}(k) \\
u_{\downarrow\sigma}(k) \\
v_{\uparrow\sigma}(k) \\
v_{\downarrow\sigma}(k)
\end{pmatrix}
= E_{\sigma}(k)
\begin{pmatrix}
u_{\uparrow\sigma}(k) \\
u_{\downarrow\sigma}(k) \\
v_{\uparrow\sigma}(k) \\
v_{\downarrow\sigma}(k)
\end{pmatrix}.
\]

Hence, the eigenvalues are
\[E_{\sigma} = E_0(k) + \sigma \mu_B H\] (47)
where
\[E_0 = \sqrt{\epsilon_k + |d_3(k)|^2}\] (48)
is the spectrum in zero field. The eigenvectors are
\[u_{\sigma\sigma}(k) = \frac{d_3(k)}{\sqrt{(E_0(k) - \epsilon_k)^2 + |d_3(k)|^2}}\] (49)
and
\[v_{\sigma\sigma}(k) = \frac{E_0(k) - \epsilon_k}{\sqrt{(E_0(k) - \epsilon_k)^2 + |d_3(k)|^2}}\] (50)

Substituting these into the self-consistency condition (5) we find that the gap equation is
\[d_3(k) = \frac{1}{2} \sum_{k\sigma} U_{\sigma\sigma}(k) \frac{d_3(k)}{E_0(k)} \tanh\left(\frac{E_0(k) + \sigma \mu_B H}{2k_B T}\right)\] (51)
At \(T = 0\) this becomes
\[d_3(k) = \frac{1}{2} \sum_{k\sigma} U_{\sigma\sigma}(k) \frac{d_3(k)}{E_0(k)}\] (52)
which is independent of \(H\).

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