Ferromagnetic Superconductivity Driven by Changing Fermi Surface Topology

K. G. Sandeman,[1] G. G. Lonzarich,[1] and A. J. Schofield[2]

[1]Low Temperature Physics Group, Cavendish Laboratory, Madingley Road, Cambridge CB3 0HE, United Kingdom
[2]School of Physics and Astronomy, University of Birmingham, Edgbaston, Birmingham B15 2TT, United Kingdom

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We introduce a simple but powerful zero temperature Stoner model to explain the unusual phase diagram of the ferromagnetic superconductor, UGe_2. Triplet superconductivity is driven in the ferromagnetic phase by tuning the majority spin Fermi level through one of two peaks in the paramagnetic density of states (DOS). Each peak is associated with a metamagnetic jump in magnetization. The twin-peak DOS may be derived from a tight-binding, quasi-one-dimensional band structure, inspired by previous band-structure calculations.

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Until recently, there were no examples of "ferromagnetic superconductivity" (FMSC)—the coexistence of itinerant ferromagnetism (FM) and superconductivity (SC) in a single bulk phase—suggesting that superconductivity and ferromagnetism are mutually exclusive [1]. This situation has changed with the observation of FMSC in UGe_2 [2], URhGe [3], and $ZrZn_2$ [4]. The behavior of these materials is an example of a more general phenomenon; the observation of novel states on the border of magnetism at low temperatures (e.g., Refs. [5,6]). Here we consider the case of UGe_2, because while SC is only measurable in the ferromagnetic state (in common with URhGe and $ZrZn_2$), UGe_2 seems to possess particularly low electronic dimensionality, uniaxial magnetization, and revealing features in the temperature-pressure phase diagram which we now review.

In Fig. 1, we show the temperature-pressure phase diagram for UGe_2, with the Curie temperature T_C (suppressed to zero at pressure p_c) and superconducting transition temperature T_{SC} indicated [2,7,8]. Another feature, T_x, is also shown. This T_x shows up as an anomaly in measurements of lattice expansion [10], resistivity [2,8], specific heat [8], and as a change in the character of the Fermi surface as measured in de Haas–van Alphen experiments [11]. Most importantly for this work, T_x also appears as a slight jump in magnetization [8] which is sharpened at lower temperatures such that the low temperature moment has a step at pressure p_x in addition to the step at the quantum phase transition pressure, p_c (see Fig. 1). Furthermore, we note the close proximity of the $T_x(p)$ line to the peak in T_{SC}.

Most theories which describe ferromagnets close to a quantum phase transition have predicted that the superconducting transition temperature, T_{SC}, should be at least as high in the paramagnetic state as it is in the ferromagnetic state. These theories have considered an electronically three-dimensional ferromagnet, either magnetically isotropic [12] or uniaxial [13]. Kirkpatrick and co-workers [14] have predicted an enhancement of the superconducting T_{SC} in the ferromagnetic regime from the coupling of magnons to the longitudinal magnetic susceptibility. However, the ferromagnetic state of UGe_2 is highly anisotropic—at 4.2 K and an external magnetic field of 4 T, the easy-axis magnetization is 20 to 30 times that along either of the other crystallographic axes [15]—so transverse modes seem unlikely to explain the exclusively ferromagnetic superconductivity in this material. Mechanisms favoring *s*-wave superconductivity in the ferromagnet [16–18] need also to account for the exchange splitting being 2 orders of magnitude larger than the gap [19]. Other authors have drawn their inspiration from band-structure calculations [19,20] of UGe_2 which seem to indicate that a quasi-two-dimensional majority carrier Fermi surface sheet evolves at temperatures below T_C. Furthermore, there is the possibility that large sections of the quasi-two-dimensional Fermi surface may be parallel, making it almost one dimensional. Until now, this low-dimensional magnetism has pushed authors in the direction of postulating the existence of a charge- or spin-density-wave state below T_x [2,7], sometimes by analogy with the α phase of uranium. Watanabe and Miyake [21] have postulated that the interplay of CD or

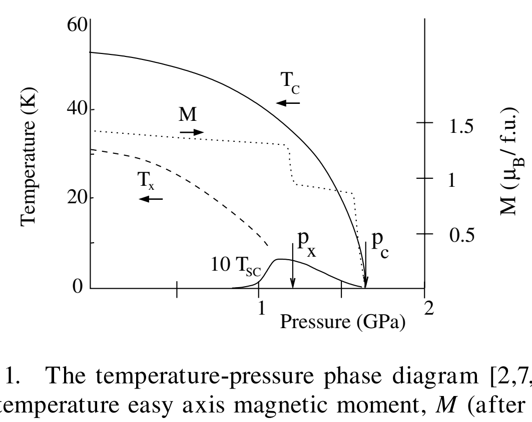

FIG. 1. The temperature-pressure phase diagram [2,7,8] and low temperature easy axis magnetic moment, M (after [9]) of UGe_2. T_{SC} is the superconducting transition temperature, scaled by a factor of 10 for clarity. T_C denotes the Curie temperature. T_x is a feature in the FM state seen in various properties including magnetization, as described in the text.

SD fluctuations at high wave vector will couple to the magnetization, M, in such a way as to enhance it at some critical value, M_x [22].

We turn to the low-dimensional band structure for a different effect. The key idea will be that, in a ferromagnet, the magnetization acts as a tuning parameter which can subtly change the topology of the *anisotropic* Fermi surfaces of different spin species. In contrast to a paramagnetic metal, the added topological possibilities for a ferromagnet should be viewed as a useful tool—and as a reason for observing the enhancement of features, such as T_{SC}, within the FM phase. This Letter is planned as follows: First, we show that an electronic density of states (DOS) which has two peaks can reproduce the two steps in the observed low temperature magnetization. We then show that the necessary form of DOS arises naturally from a low (quasi-one-)dimensional part of the band structure and that the magnetization resulting from this band structure has a jump in the ferromagnetic state which is coincident with the maximum in a superconducting instability, mediated by spin fluctuations.

We circumvent concerns over the accurate calculation of magnetization at finite temperature [24,25] by employing a *zero* temperature Stoner theory, with the first aim being to reproduce the step in $M(p)$ at p_x. While laboratory pressure is likely to have a very minor effect on the bare parameters in a microscopic model (e.g., bandwidth W and quasiparticle interaction strength I_0), in a heavy fermion compound such as UGe_2, effective energy scales can be very small, amplifying its effect. We use a phenomenological approach where we fix the bandwidth and vary an effective Stoner exchange parameter for quasiparticles, I (notionally $\sim I_0/\tilde{W}$), where many-body effects enhance the role of pressure through a renormalized bandwidth, $\tilde{W}$. The one-electron energy of separated majority (say, $\uparrow$) and minority (say, $\downarrow$) spin sheets is then $E_{k\sigma} = \epsilon_k \pm IM$ ($-\uparrow, +\downarrow$). In this description, the occupation of each spin sheet σ is $n_\sigma = \int_{\epsilon_b}^{\mu_\sigma} \rho(\epsilon)\, d\epsilon$, where $M = \frac{1}{2}(n_\uparrow - n_\downarrow)$, so states occupy the dimensionless DOS, $\rho(\epsilon)$, from the band edge ϵ_b up to μ_σ. We fix the total number of spins, $n_\uparrow + n_\downarrow = N$, and the total energy density is thus

$$F[M] = \int_{\epsilon_b}^{\mu_\uparrow} \rho(\epsilon)\, d\epsilon + \int_{\epsilon_b}^{\mu_\downarrow} \rho(\epsilon)\, d\epsilon + I\left(\frac{N^2}{4} - M^2\right) - g\mu_B HM, \qquad (1)$$

where we have included a term for the presence of an external magnetic field, H.

We are looking for two magnetic transitions, corresponding to p_x and p_c, both believed to be first order [9], although there is some controversy over that at p_x [26]. We now show that a two-peak DOS generically allows for both transitions. In terms of an expansion of $F[M]$ in even powers of M, this DOS brings about the required M^8 term [27]. We begin with a one-band DOS comprised of two Lorentzians, normalized to 1: $\rho(\epsilon) = \rho_0(\epsilon)/\int_{\epsilon_B}^{\epsilon_T} \rho_0(\epsilon)\, d\epsilon$, where $\rho_0(\epsilon) = 1 + [a(\epsilon - b)^2 + 1]^{-1} + [a(\epsilon + b)^2 + 1]^{-1}$ and a and b adjust the width and centering of the peaks, respectively. Minimizing $F[M]$ with respect to M gives $M(I)$. In Fig. 2(a), we show an example of $M(I)$ for $a = 10$, $b = 0.5$, and different levels of band filling. The bottom and top, ϵ_B and ϵ_T, of the band are set at -2 and $+2$, respectively.

In each case, the paramagnetic Fermi level is off center with respect to the two DOS peaks so, as the spin sea is polarized by increasing I, the majority and minority spin Fermi levels feel the effect of the DOS peaks at different I. The result is that, by making the DOS peaks sufficiently sharp and close together, *we can obtain two first order magnetic transitions, one from the paramagnetic state and another within the ferromagnetic state.*

Having shown that a double-humped DOS is perhaps key to understanding the magnetic properties of UGe_2 at low temperatures, we now reproduce the above effect in a tight-binding picture of the band structure of this compound which will predict both its magnetic and superconducting properties. We focus on electronic quasi-one-dimensionality, as only below two dimensions can we have two peaks in the tight-binding DOS, due to the presence of two Van Hove singularities.

We consider a simple quasi-1D tight-binding band structure of the form

$$\epsilon(\mathbf{k}) = -\alpha_x \cos k_x - \beta \cos k_x \cos k_y - \alpha_y \cos k_y - \gamma \cos 2k_x - \delta \cos 3k_x, \qquad (2)$$

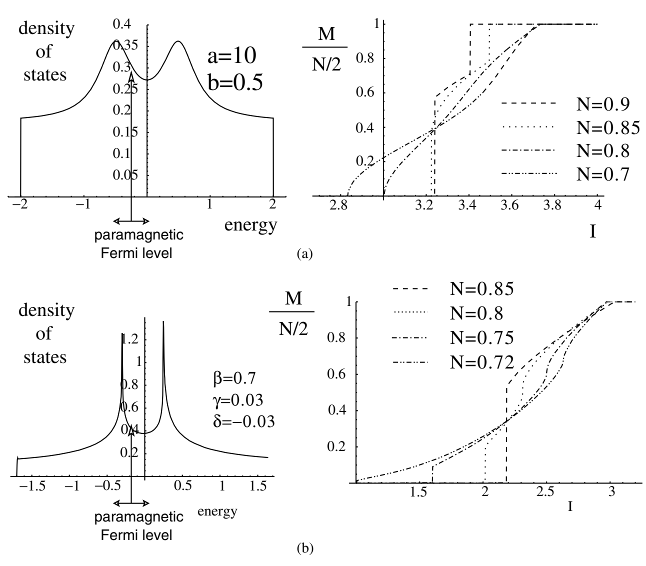

FIG. 2. DOS and resultant $M(I)$ plots for various levels of band filling, below half filling in the case of (a) the twin-Lorentzian DOS and (b) the quasi-one-dimensional dispersion for UGe_2 given in the text. Two magnetic transitions are visible. Reference [28] contains examples for further DOS parameters.

with $\alpha_x = 1$ and all other parameters less than unit magnitude. We find that we require α_y to be zero and δ and γ to be nonzero for the variation of the DOS between to the two Van Hove peaks to be sufficiently rapid for two first order transitions in $M(I)$ to be observed—see Fig. 2(b) and Ref. [28]. These parameter choices are not unreasonable in a system containing a one-dimensional band. As before, the paramagnetic Fermi level sits in between the two peaks in the DOS.

It has also been found that the features associated with T_x and T_c can be recovered at pressures above p_x and p_c, respectively, by the application of a magnetic field. This metamagnetism arises straightforwardly from the present model. As shown in Fig. 3, turning on the magnetic field, H, pushes both the magnetization jump at I_c (the Curie transition) and at I_x (within the ferromagnetic state) to lower values of I or, equivalently, higher pressures. The predicted phase diagram in H, I space bears a striking resemblance to that from recent experimental data [9].

Our choice of band structure is an extrapolation from the one point ($T = 0$, $p = 0$) of the phase diagram calculated in Refs. [19,20], such that there should be strong nesting present at full magnetization. This particular choice will now help to link p_x, the maximum in T_{SC}, and the mass enhancement observed in de Haas–van Alphen measurements. We use the interaction potential for spin fluctuation mediated pairing in the ferromagnetic state, as derived by Fay and Appel [12]. We also follow their sign convention, namely, that an attractive potential between like spins is positive. The interaction potential,

$$V_{\sigma\sigma}(\mathbf{q}) = \frac{I^2 \chi^{(0)}_{-\sigma-\sigma}(\mathbf{q})}{1 - I^2 \chi^{(0)}_{\sigma\sigma}(\mathbf{q}) \chi^{(0)}_{-\sigma-\sigma}(\mathbf{q})}, \qquad (3)$$

is written in terms of the Lindhard response, $\chi^{(0)}_{\sigma\sigma}(\mathbf{q})$, given by $\chi^{(0)}_{\sigma\sigma}(\mathbf{q}) = \sum_{\mathbf{k}} \{[f^{(0)}_\sigma(\mathbf{k}) - f^{(0)}_\sigma(\mathbf{k}+\mathbf{q})]/[\epsilon(\mathbf{k}+\mathbf{q}) - \epsilon(\mathbf{k})]\}$; $f^{(0)}_\sigma(\mathbf{k})$ being the Fermi function for spin σ at chemical potential μ_σ.

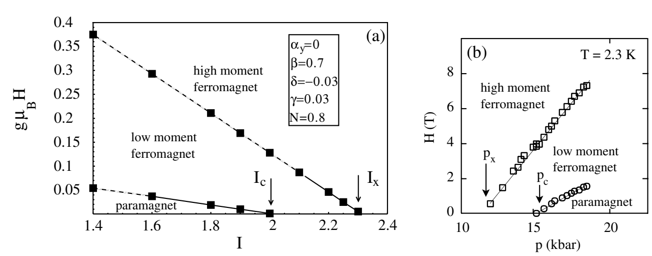

FIG. 3. (a) Predicted H, I phase diagram and (b) the experimental H, p phase diagram (after Ref. [9]). Both show tunable metamagnetic transitions corresponding to the Curie point (I_c or p_c) and the transition in the FM state (I_x and p_x). In (a), we indicate where the magnetic transition in our model is no longer first order by a dotted line on the H, I phase diagram. This crossover is not yet observed at the highest experimental pressures. The tight-binding parameters are also shown.

We now explore how the DOS peak giving rise to the magnetization step at I_x can enhance superconductivity in the ferromagnetic state. According to Eq. (3), a transition to saturation magnetization would kill any magnetically mediated superconductivity due to the lack of one spin species. Thus, we consider a transition at I_x not of saturating nature and take $\beta = 0.7$, $\alpha = 0$, $\gamma = 0.03$, and $\delta = -0.03$ with $N = 0.77$ in what follows.

Calculating the value of T_{SC} is notoriously difficult and the heavy nature of the quasiparticles indicates that a strong-coupling theory is required. A full numerical study of the Eliashberg equations near magnetic instabilities in anisotropic materials has recently been undertaken [29]. There it was found that a McMillan formula of the form $T_{SC} \sim \omega_c e^{-(1+\lambda_Z)/\lambda_\Delta}$ (relating T_{SC} to the spin fluctuation scale ω_c, the mass renormalization parameter λ_Z, and the pairing interaction parameter λ_Δ) did not appear to be valid. Nevertheless, the trends in the evolution of T_{SC} and the leading instabilities were demonstrated by considering λ_Δ.

To estimate the strength of majority spin, triplet pairing we therefore calculate the static pairing interaction parameter

$$\lambda_\Delta = \frac{\int_{FS} \int_{FS'} d^2k\, d^2k'\, V_{\uparrow\uparrow}(\mathbf{k}-\mathbf{k}')\eta(\mathbf{k})\eta(\mathbf{k}')}{\int_{FS} d^2k\, \eta^2(\mathbf{k})}, \qquad (4)$$

where each integration is over the majority spin Fermi surface (FS) either in $\mathbf{k}$ or $\mathbf{k}'$ space. The term $\eta(\mathbf{k})$ is the angular part of the superconducting order parameter. Similarly, the mass renormalization parameter λ_Z is calculated using Eq. (4) with $\eta(\mathbf{k})$ set to unity. In the above, we are following the notation adopted in Ref. [29]. The symmetry properties of the UGe_2 crystal structure should lead us to examine nonunitary order parameters [30,31], but here for simplicity we consider as an example the states $\Delta_{\mathbf{k}} = \Delta_0 \sin(k_x)$ and $\Delta_0 \sin(k_y)$. The favored state is determined by which $\eta(\mathbf{k})$ gives a nonzero value of λ_Δ, as dictated by Fermi surface topology [28]. In calculating the superconducting properties of our model, we transfer $I \to I/[1 + \xi q^2]$, where ξ is a "Stoner structure factor" [32]. This conveys some of the physics of electron-electron interactions at finite distances and reduces high-$\mathbf{q}$ modes in the system, in line with the ferromagnetism of UGe_2.

In Fig. 4, we show λ_Δ, for various values of ξ. This exhibits a sharp maximum around I_x consistent with very recent specific heat measurements showing bulk superconductivity to be much more narrowly confined to pressures near p_x than the resistive transition would suggest [33]. In the region between I_c and I_x, both λ_Δ and the mass enhancement, λ_Z, are approximately flat and high. This compares well with the high effective mass plateau found in de Haas–van Alphen measurements in the ferromagnetic state between pressures p_c and p_x [11]. In contrast to the experiment, we also find a tendency to pair for

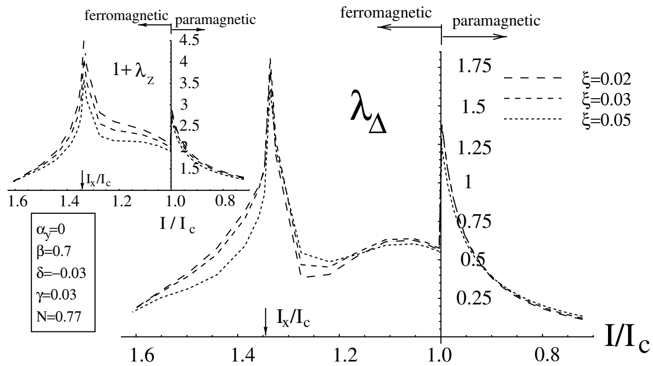

FIG. 4. A measure of the strength of superconductivity: λ_Δ as a function of the ratio of Stoner exchange to its value at the zero temperature Curie point. The inset shows the mass renormalization factor, $1 + \lambda_Z$. All points are calculated at a small finite temperature to prevent the sharpness of the Van Hove singularity from reversing the sign of the pair interaction. The tight-binding parameters are indicated.

$I < I_c$—though it falls rapidly. However, this is separated from the magnetic region by a first order transition, the size of which is underestimated by this model. Moreover, if one were to assume a McMillan formula for T_{SC}, the relevant scale ω_c for $I < I_c$ will be unrelated to that in the ferromagnetic state and could be much smaller.

In this Letter, we have proposed that the unusual phase diagram of UGe_2 is a result of a novel tuning of the Fermi surface topology by the magnetization of the ferromagnetic state. We have constructed a model for this which illustrates how superconductivity, the tunable magnetization features, and the quasiparticle mass are related by a twin-peak density of states, consistent with experiment and with the electronic quasi-one-dimensionality already proposed for this material. In particular, the T_x transition is associated with a large density of states at the majority spin Fermi surface which thus causes superconductivity to be favored in the ferromagnetic state relative to the paramagnetic state.

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