Ferromagnetic superconductivity driven by changing Fermi surface topology

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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\textsubscript{2}. Triplett 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 magnetisation. The twin peak DOS may be derived from a tight-binding, quasi-one-dimensional bandstructure, inspired by previous bandstructure calculations.

I. INTRODUCTION

The predominance of spin singlet superconductors over their triplet counterparts has, in part, lead to the belief that superconductivity and magnetism are mutually exclusive—the upper critical field of a singlet superconductor is bounded by the Pauli paramagnetic limit. One might expect that a ferromagnet would be the natural stage for spin triplet superconductivity, where we could overcome Pauli limiting effects. But, until recently, there were no examples of ‘ferromagnetic superconductivity’ (FMSC)—the coexistence of itinerant ferromagnetism (FM) and superconductivity (SC) in a single bulk phase. This situation has changed with the observation of FMSC in UGe\textsubscript{2}, URhGe\textsubscript{2} and ZrZn\textsubscript{2}. The behaviour of these materials is an example of a more general phenomenon; the observation of a novel state on the border of magnetism at low temperatures. By suppressing magnetic order by some control parameter, be it electron/hole density or external pressure, physicists are now able to access regimes where magnetic fluctuations become quantum critical.

We choose here to concentrate on the case of UGe\textsubscript{2}, because whilst SC is only measurable in the ferromagnetic state (in common with URhGe and ZrZn), UGe\textsubscript{2} seems to possess particularly low electronic dimensionality, uniaxial magnetisation, 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\textsubscript{2}, with the Curie temperature \( T_C \) (suppressed to zero at pressure \( p_x \)) and superconducting transition temperature \( T_{SC} \) indicated. Another feature, \( T_x \), is also shown. This \( T_x \) shows up in measurements of lattice expansion\textsuperscript{4} as a jump in the low temperature \( T^2 \) component of the resistivity\textsuperscript{4} as a small enhancement in specific heat\textsuperscript{4} as a kink in resistivity\textsuperscript{4} and as a change in the character of the Fermi surface as measured in de Haas van Alphen experiments\textsuperscript{4}. Most importantly for this work, \( T_x \) also appears as a slight jump in magnetisation\textsuperscript{3} 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 a electronically three-dimensional ferromagnet, either magnetically isotropic\textsuperscript{12} or uniaxial\textsuperscript{13}. Where theoretical models have predicted an enhancement of \( T_{SC} \) in the ferromagnetic regime, their basis seems unjustified in the case of UGe\textsubscript{2}. Kirkpatrick and coworkers\textsuperscript{12} have predicted an enhancement of the superconducting \( T_{SC} \) due to the coupling of magnons to the longitudinal magnetic susceptibility. However, the ferromagnetic state of UGe\textsubscript{2} is so magnetically anisotropic that the presence of transverse magnons seems an unlikely primary explanation for the enhancement of \( T_{SC} \)—at 4.2K and an external magnetic field of 4T, the magnetisation along the easy axis.
is about 20 to 30 times that along either of the other
crystallographic axes. Other authors have drawn their
inspiration from bandstructure calculations. Bandstruc-
ture analyses of UGe$_2$ seem to indicate that low-
ering temperature sparks the evolution of a quasi-two-
dimensional majority carrier Fermi surface sheet below
$T_C$. Furthermore there is the possibility that large sec-
tions 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 (CDW or SDW) below $T_S$,
sometimes by analogy with the $\alpha$ phase of uranium.
Watanabe and Miyake have postulated that the inter-
play of CD or SD fluctuations at high wavevector will
couple to the magnetisation, $M$ in such a way as to en-
hance it at some critical value, $M_c$. However, spin
density fluctuations have yet to be observed in neutron
experiments on UGe$_2$.

We turn to the low dimensional bandstructure for a dif-
erent effect. The key idea will be that in a ferromagnet,
somewhat uniquely, the magnetisation acts as a tuning
parameter which can subtly change the topology of the
anisotropic Fermi surfaces of different spin species. By
contrast, in a rigid band picture of a paramagnetic metal,
the Fermi surface is fixed. The added topological possi-
bilities for a ferromagnet should be viewed as a useful
tool—and as a reason for observing the enhancement of
features, such as $T_S$, within the ferromagnetic phase.
This paper is planned as follows: firstly, we show that an
electronic density of states (DOS) which has two peaks
and reproducible at the two steps in the observed low tem-
perature magnetisation. We then show that the necessary
form of DOS arises naturally from a low (quasi-one-) di-

dimensional bandstructure in the bandstructure which is one-dimensional in a superconducting instability, mediated by spin fluctua-
tions.

II. MODEL

The simplest Stoner theory of magnetism is long-
known to be inadequate in describing the tempera-
ture dependence of the magnetisation even of magnet-
ically isotropic, electronically 3-dimensional ferromag-

nets, where spin fluctuations have to be taken into ac-
count. There, a fluctuation-averaged equation of state
method, in the spirit of Lonzarich and Taillefer or Ya-
mada, would be a improved model of magnetism at fi-
nite temperature, where we expect the temperature de-
pendence of $M$ to arise from the fluctuation response,
rather than just the Fermi functions included in Stoner
theory. The pronounced magnetic anisotropy of UGe$_2$
might ordinarily simplify matters, as the consequent ab-
sence of transverse spin modes will make a Stoner ap-

proach more valid, especially at low temperatures. How-
ever the reduced electronic dimensionality of UGe$_2$ will
probably heighten the importance of spin fluctuations at
finite temperatures.

We therefore circumvent finite temperature concerns by employing a zero temperature Stoner theory, with the
first aim being to reproduce the step in $M(p)$ at $p_x$. We
consider the action of pressure to be akin to that of vary-
ing the exchange energy, $I$ in a Stoner model of the one-
electron energy of separated majority (say, $\uparrow$) and minor-
ity (say, $\downarrow$) spin sheets: $E_{k\uparrow \downarrow} = \epsilon_k \pm IM$ ($\downarrow + \downarrow$). In
this description, the occupation of each spin sheet $\sigma$ is
$n_{\sigma} = \int_{e_B}^{e_B} \rho(\epsilon) d\epsilon$, where $M = \frac{2}{3} (n_\uparrow - n_\downarrow)$. Here $e_B$ is the
bottom of the band, and spin $\sigma$ occupies energy states
up to $\mu_\sigma$. The DOS is given by $\rho(\epsilon)$. We consider the total
number of spins, $n_\uparrow + n_\downarrow = N$ to be fixed. The chemical
potential, $\mu_\sigma$ of each spin sheet is therefore completely
determined by the particular magnetisation and chosen
electron number. The total energy density of the electron
system is

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

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

Most phenomenological expansions of this energy den-
sity have included terms even in $M$, up to order $M^6$. This
can give one first order transition in $M(I)$. How-

ever, we are looking for an additional transition, corre-

sponding to $p_x$, and believed to be first order. Although
there is some controversy over this. To have the possi-
bility of an additional first order transition, we need
the next even term in the Landau free energy expansion,
thus obtaining an $M^8$ theory. We now show that a
DOS with two peaks generically brings about the $M^8$ term in $F[M]$ by allowing a scenario where the global
magnetisation can change rapidly, twice. We begin by
taking a one-band DOS comprised of two Lorentzians,
normalised such that the maximum number of electrons
of each spin in the band is 1:

$$ \rho(\epsilon) = \frac{\rho_0(\epsilon)}{\int_{e_B}^{e_B} \rho_0(\epsilon) d\epsilon} \tag{2} $$

where

$$ \rho_0(\epsilon) = 1 + \frac{1}{a(\epsilon - b)^2 + 1} + \frac{1}{a(\epsilon + b)^2 + 1}, \tag{3} $$

where we can vary $a$ to adjust the sharpness of the two
humps and $b$ to adjust their position. The humps are
symmetric with respect to the zero energy and are cen-
tred on $\pm b$. We minimise $F[M]$, given by Eq. 1 with
respect to magnetisation, $M$ to obtain the variation of $M$
with respect to the Stoner exchange, $I$. In Figure 2 we
show plots of $M(I)$ for three sets of parameters $a$ and $b$,
FIG. 2: Using the twin-peak density of states given by Eqs. 2 and 3, it is possible to obtain two transitions in the magnetisation of a Stoner ferromagnet, where the exchange parameter $I$ is the varied quantity. We plot both the normalised density of states peaks sufficiently sharp and close together, to obtain two magnetic transitions, one from the paramagnetic state and another within the ferromagnetic state. If the DOS peaks are too far apart, a saturated magnetic state is favoured; if the peaks are too smooth, the transitions in $M(I)$ are weakened and if the starting paramagnetic level is too close to the half-way point between the two peaks ($N$ too close to 1) then only one transition is observed. Therefore, to observe two transitions, the paramagnetic filling level should be between the DOS peaks, but off-centre with respect to them.

### A. Bandstructure phenomenology

Having shown that a double-humped DOS is perhaps key to understanding the magnetic properties of UGe$_2$ at low temperatures, we now set about working towards a tight-binding picture of the bandstructure of this compound which can reproduce both its magnetic and superconducting properties. There have been two major efforts towards bandstructure calculations of UGe$_2$. The first, originally on a crystal structure with an incorrect space group was performed by Yamagami et al. and has since been revised. This produced spin-separated Fermi sheets that were of mixed spin type and the sheet considered by those authors as being most important for superconductivity is centred on the crystallographic $M$ point in their model. Furthermore, there was initial disagreement on the direction of the nesting vector $Q$ relative to the easy axis of magnetisation $a$ — both are ‘in-plane’, but Yamagami considered $Q \perp a$ whilst Shick found $Q \parallel a$. In summary, we take the following minimal, but key ingredients in our model:

- quasi-one-dimensional bandstructure (crucial to what follows)
- strong uniaxial magnetic anisotropy and
- spin-split Fermi sheets (even in the LDA + $U$ work, there is a large exchange splitting, of the order of 1 eV).

In our model, we utilise the interaction potential for spin fluctuation mediated pairing in the ferromagnetic state, as derived by Fay and Appel. We also follow their sign convention, namely that an attractive potential between like spins is positive. The interaction potential is heavily dependent on the Lindhard response, $\chi^{(0)}(q)$
for the bandstructure under consideration:

$$V_{\sigma\sigma}(q) = \frac{I^2 \chi_{\sigma\sigma}^{(0)}(q)}{1 - f_{\sigma}^{(0)}(q) \chi_{\sigma\sigma}^{(0)}(q)}.$$  \hspace{1cm} (5)

where $I$ is again the repulsive Hubbard-type contact interaction acting between opposite spins and $\chi_{\sigma\sigma}^{(0)}(q)$ is given by

$$\chi_{\sigma\sigma}^{(0)}(q) = \sum_k \frac{f_{\sigma}^{(0)}(k) - f_{\sigma}^{(0)}(k+q)}{\epsilon(k+q) - \epsilon(k)};$$  \hspace{1cm} (6)

$f_{\sigma}^{(0)}(k)$ being the Fermi occupation function for spin $\sigma$ which is at chemical potential $\mu_\sigma$ ($\mu_\sigma$ is defined previously). According to our chosen interaction mechanism, Eq. 3, a large $\chi_{\sigma\sigma}^{(0)}(q)$ might naively be expected to lead to an enhanced $T_{SC}$. However, the subtlety here is that the interaction potential in the ferromagnetic state mixes longitudinal susceptibilities of majority and minority spin sheets so the effect is not so clear-cut. We recall that in the free electron model, only in electronic dimensions less than two, there can be a peak in $\chi_{\sigma\sigma}^{(0)}(q)$ at non-zero $q$. In that case, we might expect that when one sheet of the Fermi surface is at optimal nesting, then perhaps $V_{\sigma\sigma}(q)$ will be highest. The problem with this argument is that a $V_{\sigma\sigma}(q)$ dominated by high-$Q$ modes would normally lead to very weak triplet pairing and in tight-binding approaches, finite $q$ peaks in $\chi_{\sigma\sigma}^{(0)}(q)$ are possible in two and three dimensions.

The approach we take is to look for density of states-driven superconductivity, where the large density of states giving rise to the magnetisation step at $M_c$ is also able to enhance superconductivity in the ferromagnetic state. In tight-binding theory in two dimensions and lower, the peak in the density of states comes from the presence of a van Hove singularity. The simplest, familiar tight-binding bandstructure for the cuprates is of the form

$$\epsilon(k) = -\alpha_x \cos k_x - \beta \cos k_x \cos k_y - \gamma \cos k_y$$  \hspace{2cm} (7)

with $\alpha_x = \alpha_y = 1$ and $\beta$ less than 1. This corresponds to equal nearest neighbour hopping in each of the two dimensions, and includes the next-nearest neighbour term, $\cos k_x \cos k_y$. This structure, as shown in Figure 3(a), has one van Hove singularity and is therefore of little use in studying the magnetic properties of UGe$_2$—as we have already found, we require two density of states peaks. However, as we will now show, if we now reduce the amplitude of the $\cos k_y$ term, we cross over into quasi-one-dimensions and begin to lift the degeneracy of the van Hove contours, giving two of them, with adjustable separation.

The most common quasi-1D bandstructure in the literature is probably

$$\epsilon(k) = -\alpha_x \cos k_x - \alpha_y \cos k_y$$  \hspace{2cm} (8)

which is used to describe some organic superconductors. Here, $\alpha_x$ is 1 and $\alpha_y$ is less than 1 and the model corresponds to nearest neighbour hopping in each of the two dimensions. This bandstructure has two van Hove contours (see Figure 3(b) and hence two density of states peaks. Thus, on tuning our magnetisation, we can observe in both spin types the transition through a van Hove singularity in the density of states at the Fermi level, provided, as stated before, that our paramagnetic Fermi level is between the two peaks in the density of states. The problem arises that when the peaks are close enough together to cause an effect in the magnetisation curves, the variation of the DOS in between them is not very rapid. This leads to a weakening of the transitions in $M(I)$ as found with a slowly varying Lorentzian DOS in the last section.

However, if we assume a quasi-one-dimensional dispersion of the form

$$\epsilon(k) = -\alpha_x \cos k_x - \beta \cos k_x \cos k_y - \gamma \cos 2k_x - \delta \cos 3k_x$$  \hspace{1cm} (9)

with $\alpha_x = 1$ and $\beta, \gamma, \delta$ all less than unit magnitude, we will be able to explore the possibility of two, first order jumps in $M(I)$.  

![Figure 3](image-url)
The higher harmonics in the principal direction $k_x$ and the next-nearest term, $\cos k_x \cos k_y$ which appear in Eq. 9, are not unreasonable in a system which we know to be strongly one-dimensional in character. The nearest neighbour term in $k_y$ has been reduced to zero. As shown in Figure 3(c), this dispersion relation yields two van Hove contours (and hence maxima in electronic density of states), and also goes through a perfect nesting scenario. We note that our choice of bandstructure is based on an extrapolation from the one point ($I = 0$) of the phase diagram calculated in Refs. [16,17,18], with the idea being that there should be strong nesting present at full magnetisation in our model, to match the bandstructure calculations. Indeed, the high energy contours of this dispersion are fairly well nested (Figure 3(d)). To achieve a magnetically saturated state which does not completely fill the band, we require less than half-filling of the band in the paramagnetic state, a requirement which is in line with the demands of the $M(I)$ profile from Section I. Our choice of bandstructure will ultimately help to link $p_x$, the maximum in $T_{SC}$ and the mass enhancement observed in de Haas van Alphen measurements. First we concentrate on the magnetisation as a function of Stoner exchange, $I$.

III. RESULTS

A. Two jumps in magnetisation from a tight-binding bandstructure

Taking the quasi-one-dimensional bandstructure given by Eq. 3 and varying parameters $\beta$, $\gamma$, and $\delta$, we obtain the variation of zero temperature magnetisation with exchange interaction $I$ as we did for Lorentzian densities of states [20]. In Figure 4, we present $M(I)$ for different total numbers of electrons, $N$ below half-filling in the case of four different sets of tight-binding parameters. In each case, the paramagnetic Fermi level sits in between the two peaks in the DOS. Initial polarisation at $I_e$ (labelled by analogy with $p_e$ in experiment) is first order—this is due to the minority sheet approaching the lower van Hove peak as polarisation commences.

There are several features to be noted from the plots in Fig. 4. Firstly, as in Fig. 3, if $N$ is below half-filling, a second magnetic transition can occur when the majority spin sheet feels the effect of the upper peak in the DOS. However, when $N$ is too close to half filling, or when the dip between the two density of states peaks is too sharp, we get only one first order transition, which can even be straight to saturation magnetisation. Once again, in order to observe the two transitions seen in UGe$_2$, one should have a paramagnetic Fermi level which is off-centre with respect to two DOS peaks. Secondly, the upper transition (which we henceforth label $I_s$ by analogy with $p_s$ from experiment), can either be to finite magnetisation (and either first order or beyond the first order critical point) or can be first order to saturation magnetisation. According to Eq. 3, a transition to saturation magnetisation would naturally kill any magnetically-mediated superconductivity due to the lack of one spin species. Thus we turn our attention to an upper transition not of saturating nature, and which could be first order, or close to first order, as the latter would allow the Fermi surface sheet configurations to be

FIG. 4: A set of phenomenological quasi-one-dimensional dispersions for UGe$_2$, where both the possibility of tuning the magnetisation through a van Hove singularity and a perfect nesting condition are present. (a), (c), (e) and (g) show the calculated density of states whilst (b), (d), (f) and (h) are the calculated graphs of magnetisation as a function of $I$, the Stoner exchange parameter for various levels of band-filling, below half-filling. The tight-binding parameters for our dispersion, $\epsilon(k) = -\cos k_x (1 + \beta \cos k_y) - \gamma \cos 2k_x - \delta \cos 3k_x$ are indicated. As in Fig. 3 two magnetic transitions are often visible.
FIG. 5: The phase diagram of our model in $N, I$ space shows a line of first order transitions at $I_c(N)$ which end in a critical point. The transitions at the Curie onset, $I_c$ are also first order. This can be seen in the behaviour of (a) the longitudinal susceptibility and (b) the resulting (approximate) phase diagram. The tight-binding parameters used here are $\beta = 0.7$, $\gamma = 0.03$ and $\delta = -0.03$, in line with what follows.

The above considerations make the second example in Fig. 6 a most useful candidate, as we have the option of the upper transition being first order or close to first order, depending on $N$, and the magnetisation does not saturate at the upper transition. Henceforth, we take $\beta = 0.7$, $\gamma = 0.03$ and $\delta = -0.03$.

Interestingly, the magnetic phase diagram in the $N, I$ plane seems to contain a line of first order transitions corresponding to $I_c(N)$. This line terminates at a critical point at a value of $N$ of about 0.76. For values of $N$ below this, the transition in $M(I)$ is smooth and can be described as close to first order. This is perhaps best seen in Figure 6(a), where we show the longitudinal susceptibility, $\chi$ as a function of $I$ for $\beta = 0.7$, $\gamma = 0.03$ and $\delta = -0.03$, taking different values of $N$. We take the longitudinal susceptibility from the Stoner forms:

$$\chi_{para} = \frac{\rho(\mu_{EF})}{1 - I \rho(\mu_{EF})},$$

$$\chi_{ferro} = \frac{2\rho(\mu_\uparrow)\rho(\mu_\downarrow)}{\rho(\mu_\uparrow) + \rho(\mu_\downarrow) - 2I\rho(\mu_\uparrow)\rho(\mu_\downarrow)}$$

in the paramagnetic (Fermi level $\mu_{EF}$) and ferromagnetic states, respectively. As seen in Figure 6(a), the susceptibility at $I_c$ grows as we move closer to the critical point; the resulting (approximate) phase diagram in $(N, I)$ space is shown in Figure 6(b).

**B. Magnetic field effects**

It has also been found that the features associated with $T_x$ and $T_b$ can be recovered at pressures above $p_x$ and $p_c$ respectively by the application of a magnetic field. In our model, this metamagnetism arises as a direct consequence of having spin-split Fermi surfaces, with the spin species being governed by number conservation and the free energy of the form given in Eq. 3. As shown in Fig. 6, turning on the magnetic field, $H$, pushes both the magnetisation jump at $I_c$ (the Curie transition) and at $I_x$ (within the ferromagnetic state) to lower values of $I$, or equivalently, higher pressures. Both the predicted $M(I)$ curves and the resulting phase diagram in $H, I$ space bear a striking resemblance to recent experimental data. We should point out that the calculated $H, I$ phase diagram was obtained by looking for the maximum in the gradient of the magnetisation for each $M(I)$ plot in field. The first order nature of both transitions is softened with decreasing $I$—corresponding to going to higher pressures. Experimentally, such softening is not observed at pressures reached this far, as can be seen from Figure 6(b). We indicate where the magnetic transition in our model is no longer first order by a dotted line on the $H, I$ phase diagram.
C. Superconductivity and the zero-temperature phase diagram

From the heavy nature of the quasiparticles alone, we expect strong coupling theory to be required to gain a true estimate of $T_{SC}$ in UGe$_2$. However, we can gain useful information on the form of the phase diagram from examining the zero temperature, weak-coupling properties of our model. We note here that, without a reliable model of $M(T)$, it is impossible to construct the usual $T_{SC}$ equation in the BCS theory in the ferromagnetic state, as here we have an example of a temperature-dependent potential—the changing magnetisation alters the spin-dependent interaction.

A reasonable estimate of the strength of triplet pairing can be gained from examining the relative magnitudes of the mass renormalisation parameter $\lambda_Z$ and interaction parameter $\lambda_\Delta$, defined as

$$\lambda_Z = \frac{\int_{FS} \int_{FS'} d^2k d^2k' V_{\uparrow\uparrow}(k-k')}{\int_{FS} d^2k},$$

and

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

where each integration is over the Fermi surface (FS) either in $k$ or $k'$ space. The term $\eta(k)$ is the angular part of the superconducting order parameter. In the above we are following the notation adopted by Monthoux and Lonzarich and restrict ourselves to examine majority spin triplet pairing, using $V_{\uparrow\uparrow}(q)$. The choice of order parameter should naturally reflect the symmetry properties of the UGe$_2$ crystal structure. Such considerations should lead us to examine non-unitary states, but here for simplicity we consider as an example the states $\Delta_k = \Delta_0 \sin(k_x)$ and $\Delta_0 \sin(k_y)$, anticipating that which state is favoured may change as the majority Fermi surface is tuned through $p_x$, making the transition from being open to being closed. The favoured state is determined by which $\eta(k)$ gives a larger positive value of $\lambda_\Delta$.

There is a caveat at this stage. The sharpness of the van Hove singularities is useful in providing the magnetisation behaviour shown in Section 11A. However, as can be readily seen from Eq. 5, it can also lead to a switching of the sign of the pair interaction from attraction to repulsion at zero $q$ if the density of states at the van Hove point is too high. This is because $\chi^{(0)}_{\sigma\sigma}(q = 0) = \rho(\mu_\sigma)$. With the presence of a strict low dimensional van Hove singularity (an infinity in the DOS) at zero temperature, the quantity $\rho(\mu_\uparrow)\rho(\mu_\downarrow)$ will be greater than 1 when the majority Fermi level reaches the van Hove point.

There are several possible routes to softening the van Hove singularity. One would be to introduce a small amount of disorder into the model. Another would be to transfer the calculation to three electronic dimensions, rather than the current two, but that is computationally time-consuming. Here we take a simpler approach, calculating all $\chi^{(0)}_{\sigma\sigma}(q)$ at a small finite temperature ($k_B T = 0.045$), retaining the original zero-temperature value of $I$ for each magnetisation examined. This procedure maintains the order of the magnetic transition at $I_x$, although it does mean that the effective density of states, $\chi^{(0)}_{\sigma\sigma}(q = 0)$ is inconsistent with that used to find $M(I)$. $\chi^{(0)}_{\sigma\sigma}(q)$ is calculated on a 40 by 40 grid for $k$ and $k'$ points in the Brillouin zone. The agreement is close away from the van Hove regions.

In order to have two first order magnetic phase transitions (see Fig. 3(b)), we take $N = 0.77$ in what follows, and examine majority sheet, spin triplet superconductivity. The final refinement to the model comes in the form of adjusting the $q$-dependence of $I$ at this stage. Until now, we have considered a $q$-independent Stoner factor which arises from on-site repulsion of like-spin electrons. However, $I$ should really convey some of the physics of electron-electron interactions at finite distances, and so, in calculations of the superconducting transition temperature, we convert to the following form:

$$I \rightarrow \frac{I}{1 + \zeta q^2},$$

which effectively reduces high-$q$ modes in the system, in line with the ferromagnetism of the real compound. This is the simplest, first approximation of such effects.

In Fig. 4 we show a measure of the superconducting interaction strength, $\lambda_{27,28}$, for various values of $\xi$, our Stoner ‘structure factor’. The term $1 + \lambda_Z$ measures the mass renormalisation—this is shown separately in Fig. 5. Of course, $\lambda_{27,28}$ is not the full story when one considers the superconducting transition temperature $T_{SC}$ should behave as a function of $I$. Roughly speaking, $T_{SC} \sim \omega_c e^{-(\xi + \lambda Z)^{-1}}$ (see, for example, Fay and Appel) and there is substantial variation of $\omega_c$, the paramagnon energy with $I$, especially when soft magnetic modes are present. The paramagnon energy can be expanded as

$$\omega_c \sim \zeta q(x^{-1} + cq^2),$$

where $\zeta$ and $c$ are temperature dependent parameters, equivalent to $\gamma$ and $c$ in the work of Lonzarich. As developed by Brinkman and Engelsberg and implemented by Fay and Appel, the $\omega_c$ prefactor will substantially reduce superconductivity at the ferromagnetic $I_c$, and the same argument should apply around the secondary transition at $I_x$, although in both cases this effect is more drastic for a second order magnetic transition (where the susceptibility diverges, i.e. $\chi^{-1} \rightarrow 0$) than for the first order cases here. What remains important, therefore, is the stable region of superconductivity in the ferromagnetic state, where $\lambda_{27,28}$ is approximately flat and high, especially for higher Stoner structure factor, $\xi$.

We might reasonably ask what it is that enhances superconductivity in the region between $I_x$ and $I_c$. In this range of $I$, the majority Fermi level sits between the two van Hove peaks, and an examination of the $q$ dependence of the interaction potential, Eq. 5 reveals that there is a
as a function of Stoner interaction strength, $I$, normalised with respect to $I_c$, the value of $I$ at the zero temperature Curie point. $I_c$, the value of $I$ for the second jump in magnetisation, akin to the pressure identified as $p$ in UGe$_2$, gives rise to the peak at $I_c/I_c \sim 1.34$. Also shown is the magnetisation, scaled down by a factor of two in the dimensionless units we are using. The inset shows the ratio $\lambda_Z$ is always less than 1, as expected. In both plots, we show the results for different values of ‘Stoner structure factor’, $\xi$ (Eq. [4]). The tight-binding parameters used here are again $\beta = 0.7$, $\gamma = 0.03$ and $\delta = -0.03$, and the number of spins, $N = 0.77$.

region of high, sustained zero $q$ pairing for $I_c < I < I_x$. At both $I_c$ and $I_x$, $V(q)$ is broad and high around $q = 0$. Outwith the region $I_c < I < I_x$, the pairing potential is smaller and more localised around zero $q$. Furthermore, in the region between $I_c$ and $I_x$, the mass renormalisation, represented by $\lambda_Z$ is also approximately flat and high. This mass enhancement, shown in Fig. 8, compares well with the high effective mass plateau found in de Haas van Alphen measurements on the ferromagnetic state between pressures $p_c$ and $p_x$.

Lastly we note that the order parameter, $\eta(k)$ favoured on tuning $I$, changes as we go through $I_x$. This makes sense from the point of view of the Fermi surface topology, as depicted in Figure 7. $\eta(k) = \sin(k_y)$ is favoured when the majority spin sheet is open—for all $I < I_x$—and the $\sin(k_x)$ order parameter becomes favoured for the closed surfaces for $I > I_x$. As already stated, these are overly simplified gap functions, so this change of symmetry may well be more gradual or masked in a non-unitary representation.

### IV. CONCLUSIONS

In this paper 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 magnetisation of the ferromagnetic state. We have constructed a model for this which illustrates how superconductivity, the tunable magnetisation features and the quasiparticle mass are related by a twin-peak density of states feature, consistent with experiment. Indeed, the twin-peak DOS feature is also apparent in the most recent LDA $+U$ calculations of the non-magnetic state.

We have first looked for an explanation of the two transitions in the low temperature magnetisation of UGe$_2$. We have shown how a density of states with two peaks as a function of energy will give rise generically to a zero temperature magnetisation which has two transitions as the ratio of Stoner exchange energy to bandwidth is tuned. We have demonstrated how this interesting
form of DOS arises when the bandstructure is quasi-one-dimensional, as is believed to be the case for UGe$_2$.

We are thus able to propose a mechanism for the asymmetry of the superconducting $T_{SC}$ with respect to the magnetic quantum phase transition associated with the Curie temperature, shifting the focus of our attention away from $p_c$ towards $p_c$ as the magnetic transition point of interest with regard to superconductivity. In our model, a large density of states at the majority spin Fermi surface is associated with the $T_c$ transition and is also driving superconductivity. This causes superconductivity to be favoured in the ferromagnetic state relative to the paramagnetic state in a natural and previously overlooked way, and could also be a reason for the enhancement of superconductivity in the ferromagnetic state of other materials. We further note that, in a real system, the presence of impurities will probably enhance further the relative tendency to formation of the superconducting state in the ferromagnetic phase.

There is also a straightforward explanation in the band magnetism scenario for the observed metamagnetic behaviour and a large, constant mass enhancement between $I_x$ and $I_c$, consistent in form with de Haas van Alphen measurements. Potentially we may have a reason for the disappearance of dHvA signal between $p_x$ and $p_c$, which would here be due to the Fermi surface becoming open. However, we should note that only one set of authors have observed such disappearance of dHvA signal.

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35. By coupling high wavevector fluctuations to the $q = 0$ mode, Watanabe and Miyake’s model is reminiscent of the spin-bag mechanism of nodeless superconductivity proposed by Schrieffer et al. in the context of the cuprates.
36. It is worth noting that, on scanning through energy in quasi-one-dimensions, optimal nesting (which is also the density of states minimum) does not coincide with the van Hove point (the density of states maximum). This is because optimal nesting in quasi-1D results from a Fermi surface consisting of parallel lines, each parallel to one axis of the Brillouin zone, as shown by the blue lines in Figure 3(c). By contrast, the optimal nesting Fermi surface of a two-dimensional square lattice in a nearest-neighbour tight-binding model is a diamond shape, with parallel surfaces at 45 degrees to the Brillouin zone axes. As shown in Figure 1(a), this Fermi surface also corresponds to the van Hove point and density of states maximum.
37. Setting $\alpha_x$ to 1 in Eq. 3 and varying $I$ is equivalent to varying the quantity $I' = I/\alpha_x$ as can be seen from the form of the free energy in Eq. 1. The effect of increasing pressure is to increase, probably most strongly, the hopping parameter $\alpha_x$. This suppresses ferromagnetism, as it reduces $I'$. We show plots of $M(I)$ since $I = I'$ here.