Fermi surface topology and ferromagnetic superconductivity in UGe$_2$

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We consider a Stoner ferromagnet in presence of a quasi-one dimensional Fermi surface in its spin majority band. Assuming a twin $\delta$-function peaked density of state due to the low dimensionality, we computed the single particle self-energy. There appears an additional divergence in the self-energy and hence in the effective mass inside the ferromagnetic phase (besides the standard logarithmic divergence at the Stoner critical point). Since such an effect is purely due to density of states, it might correspond to a first order phase transition making the ferromagnetic phase into two distinct phases. This result is in qualitative agreement with the recent specific heat capacity measurement. We also discuss its relevance to the superconducting state in UGe$_2$.

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Superconductivity (SC) and ferromagnetism (FM) are two very different cooperative phenomena and the question regarding their coexistence is very important theoretically as well as experimentally. Due to their antagonistic character, it was believed that they mutually act against each other. But the recent discovery of FMSC in UGe$_2$ [1], URhGe [2] and ZrZn$_2$ [3] has ruled out this possibility. The behaviour of these materials is an example of a more general phenomenon where a novel state appears on the boarder of magnetism at low temperature. In what follows, we concentrate on the material UGe$_2$, where SC is entirely covered within the FM phase and disappears in the paramagnetic (PM) region.

UGe$_2$ is an itinerant FM [4] with a Curie temperature of $T_c = 52$ K at ambient pressure. Upon increasing pressure, it becomes SC with a maximum transition temperature of $T_s \sim 0.8$ K in the pressure range of 1 GPa to 1.7 GPa. Furthermore, there appears an additional phase line $T_x$ [4] inside the FM phase (see Fig.1) dividing it into two distinct phases (FM1 and FM2). This has been inferred from the strong anomaly seen in the resistivity measurements [4], a small enhancement in the specific heat capacity [5], lattice expansion [6] and a change in the character of the Fermi surface measured in the de Haas van Alphen experiments [7]. This might be thought to be associated with the formation of charge and spin density waves (CSDW) since the band structure calculations [8,9] indicate that this material is prone to nesting. Until now, no density fluctuations has been observed in the neutron scattering measurements.

It is already known that in an itinerant weak FM, the magnetic fluctuations are enhanced in the vicinity of the quantum phase transition and it gives rise to triplet SC [10]. The standard phase diagram proposed in such a formalism is the appearance of SC dome both in the PM as well as FM phases close to the Curie transition. The SC transition temperature estimated in such a formulation is comparable in both the phases. Recently, similar results have been obtained by solving the Eliasberg equations rigorously [11]. However, it has also been pointed out that SC in the FM region can be enhanced at least 50 times than that of the PM phase [12]. This can be understood due to the mode coupling among transverse magnons and longitudinal spin fluctuations in the FM phase which is absent in the PM region. However, the FM state of UGe$_2$ is so magnetically anisotropic that the presence of magnons seems an unlikely explanation for the enhancement of SC in the system. Furthermore, inspired from the band structure calculations [8,9], Watanabe and Miyake [13] postulated the existence of CSDW inside the FM phase, in analogy with the $\alpha$-phase of uranium. In such a formalism, CSDW fluctuations at high wave vector couple to the magnetization in such a way that it yields a mass enhancement near CSDW transition. It also provides a pairing mechanism for SC in this system.

![FIG. 1. Schematic T-P phase diagram in UGe$_2$ showing the $T_x$ phase line which separates the two magnetic phases FM1 and FM2.](image)

Very recently, the pressure dependence of magnetization measurement at low temperature by Pfleiderer et al., [14] indicates that the two transitions (Curie as well as the transition between FM1 and FM2) are of first or-
der in nature. They further pointed out that even if the low temperature uniform longitudinal susceptibility undergoes a large change between FM1 and FM2, it becomes almost pressure independent within each phase. This suggests that the SC is not driven due to its proximity to a FM quantum critical point; rather, it could be associated with a sharp spike in the electronic density of states (DOS). This could also be responsible for the low pressure magnetic transition. Keeping this in mind, Sandeman et al. [15] studied the zero temperature Stoner model in presence of a two Lorentzian peaked DOS phenomenologically. They minimised the total energy density of the system with respect to the magnetization and obtained the magnetization-Stoner exchange energy density of the system with respect to the magnetization, 

\[ \rho(\epsilon) \]

where, the residue \( Z \), contains informations about the quasiparticle properties (which has to be less than one for well-defined quasiparticles as in the framework of Fermi liquid theory). The incoherent part of the Green function \( G_{inc} \), which describes the high energy processes, is a smooth function of \( \omega \) and \( k \). In such a situation it can only renormalize the properties at the Fermi surface without introducing any new physics. Such a liquid has two types of low energy collective spin excitations: transverse magnons and longitudinal spin fluctuations. For \( \text{UGe}_2 \), due to the large magnetic anisotropy, we consider only the latter in what follows. The relevant expression for the longitudinal spin fluctuation [17,18] is given as,

\[ \chi_l(q, \omega) = \frac{\rho(0)}{\eta + Aq^2 + \frac{\omega^2}{\eta}}. \]  

Here, \( \rho(0) \) is the DOS at the Fermi level in the PM state, \( \eta = (\lambda - 1) \sim \frac{\Delta_F}{\epsilon_F} \), \( \lambda = U\rho(0) \), \( A \) and \( C \) are the parameters related to \( \epsilon_F \) and \( \rho(0) \). Now, using the standard many body technique [19], one can calculate the single particle self-energy in the spin majority band as,

\[ \Sigma(k, \omega) = \frac{\lambda^2}{\beta} \sum_{p, i\omega_n} G^0(k + p, i\omega_n + ip_n)\chi_l(p, ip_n), \]  

where \( i\omega_n \) represents Matsubara frequencies. At this stage of the calculation, we would like to point out that the wave vector sum in the above equation can be performed by using the DOS of the FM state. The standard way to get a proper form of the DOS is to analyze the band structure data. We do exactly this for the present case. It has already been noted from the band structure calculations [8,9] that the Fermi surface in \( \text{UGe}_2 \) is quasi-cylindrical. In presence of exchange splitting, the minority electron surface contracts while the majority spin counterpart expands towards the boundary of the Brillouin zone and gets cut-off by the zone wall on both sides. This produces two large and roughly parallel sheets reminiscent of a quasi-one dimensional system. It has been known from text books that in a perfectly one-dimensional tight binding system, the DOS has square root singularity and it diverges at both the band edges. One can show that by including the higher order harmonics in the dispersion, it is possible to get double peak

\[ \frac{Z}{\omega - \epsilon_{k, \sigma} + i\delta} + G_{inc}, \]  

where \( (-W/2) \) is the bottom of the band and spin \( \sigma \) occupies energy states up to \( \mu_\sigma \). The DOS here is given by \( \rho(\epsilon) \). We also consider the total number of spins, \( N = n_\uparrow + n_\downarrow \), to be fixed. Thus, the chemical potential \( \mu_\sigma \) of each spin band is completely determined by the particular magnetization and the electron number.
structure in the DOS as has been shown by Sandeman et al [15].

To make the $p$-sum tractable analytically in equation (3), we assume a following form of DOS, which has double $\delta$-function peaked structure, written as,

$$\rho(\epsilon) = \rho(0)[1 + a(\delta(\epsilon - b) + \delta(\epsilon + d))].$$  \hspace{1cm} (4)

Here, ‘$a$, ‘$b$’ and ‘$d$’ are the parameters which determine the strength and the positions of the DOS. These parameters can be determined from the band structure calculations. Moreover, it should be noted that the energy $\epsilon$ in the DOS is measured with respect to the Fermi energy of the spin majority band ($\epsilon_{F+}$). In what follows, we show that this hidden quasi-one dimensional character associated with the large electron sheet of the majority spin Fermi surface which yields the above DOS (4), will have profound consequences.

Now, by performing the Matsubara frequency summation as well as the $p$-sum by using the above form of the DOS, one obtains,

$$\Sigma(k_F, \omega) = -\frac{\lambda^2}{4} \omega \left[ \frac{1}{P} \ln |1 + \frac{P}{\eta}| + Q \left( \frac{1}{\eta + Ab} + \frac{1}{\eta - Ad} \right) \right]$$

where $P = Ak_F^2$ and $Q = a/\epsilon_F$ are the dimensionless variables. Here, $A = P/\epsilon_F = Ak_F^2/\epsilon_F$. By differentiating the real part of the self-energy, one can compute the effective mass, which turns out to be,

$$\left( \frac{m^*}{m} - 1 \right) = -\frac{\partial}{\partial \omega} \text{Re}(\Sigma(k_F, \omega)|_{\omega = \epsilon_F} = gZ$$

$$= \frac{\lambda^2}{4} \left[ \frac{1}{P} \ln |1 + \frac{P}{\eta}| + Q \left( \frac{1}{\eta + Ab} + \frac{1}{\eta - Ad} \right) \right].$$ \hspace{1cm} (6)

This is the central result in the manuscript. Recalling the weak itinerant FM, it is known that the effective mass as well as the specific heat capacity diverges logarithmically near the Stoner critical point ($\eta \to 0$). This is exactly the first term in the above expression whereas the next two terms are due to the double $\delta$-function peaked DOS. It is obvious from the last term in the above equation that there is an algebraic divergence for finite $\eta$, which causes a phase transition inside the FM phase. This corresponds to the FM1-FM2 transition which has been discussed earlier. The specific heat capacity measurement by Tateiwa et al., [5] shows that the value $C/T$ increases approximately to 95 mJ/mole $K^2$ at pressure about 1.15GPa which is nearly the pressure where FM1-FM2 transition occurs. This causes an enhancement of the the effective mass as much as three times than that at ambient pressure. We can obtain such a mass enhancement from the above equation by considering suitable parameters. In the present formulation, since the enhancement in the effective mass is with respect to the dimensionless coupling parameter ($\eta$), we don’t go for a quantitative fit because the experiments are done with respect to pressure. We would like to further make some comments on the second term in equation (6). From the pressure dependence of magnetization, it is clear that even the Stoner transition is first order. In a standard weak Stoner FM, the PM-FM transition is second order. Thus, we can make a choice, $b = 0$ in the equation (6) so that both the first and the second term in the above equation cause mass divergence at at the same point, $\eta = 0$. Thus, one of the peak in the DOS should lay exactly at the Fermi level of the spin majority band ($\epsilon_{F+}$) (see Fig.2).

![FIG. 2. Single particle DOS whose one of the peak coincides exactly at the Fermi level of the spin majority band ($\epsilon_{F+}$).](image)

Next, let us consider the effect of such a twin peak DOS on SC. Due to the strong magnetic anisotropy in UGe2, it is believed that SC in this system is not only equal spin pairing (ESP) but also non unitary [20]. Following Fay and Appel [10], we can write down the self-consistent gap equation as,

$$\Delta_{\sigma,\sigma'}^\ast(k, i\omega) = \frac{1}{\beta} \sum_{p, \nu} V_{\sigma,\sigma'}^\ast(k, i\omega; p, \nu)$$

$$G_{\sigma}(p, i\nu)G_{\sigma'}(-p, -i\nu)\Delta_{\sigma,\sigma'}^\ast(p, i\nu),$$ \hspace{1cm} (7)

where $V_{\sigma,\sigma'}$ is the irreducible pairing potential. For a general $l$-state ESP case, one can define a BCS type pairing parameter $g_{ll'}^\sigma$ as, $g_{ll'}^\sigma = \rho_\sigma(0)V_{l,l'}^\ast\sigma$, with

$$V_{l,l'}^\ast\sigma = \int_0^{2k_F} \frac{dq}{2k_F} P_l \left( 1 - \frac{q^2}{2k^2_F} \right) V_{l,l'}^\ast\sigma(|q|, \omega = 0).$$ \hspace{1cm} (8)

Here, $q = \bar{k} - \bar{p}$ with $|\bar{k}| \approx |\bar{p}| \approx k_F$ and $(\bar{k} \cdot \bar{p}) = k_F^2 \cos \theta$, $q = 2k_F |\sin (\theta/2)|$. We can compute the pairing potential $V_{l,l'}^\ast\sigma$ due to longitudinal spin fluctuations. For the case of ESP, the ladder diagram will be absent due to the Pauli exclusion principle and the contribution to $V_{l,l'}^\ast\sigma$ will only be given by summing the odd number of bubble diagrams. Within RPA, one obtains,
where $\chi^{\sigma\sigma}$ is the particle-hole bubble for a particular spin projection $\sigma$. Computing $V^{\sigma\sigma}$ for a weak itinerant FM as has been done earlier [10], one can calculate the BCS parameter $g_{1}^{\sigma}$ by doing angular integration. Moreover, in the present case, we can compute $g_{1}^{\sigma} = g_{1s}$ (we drop the $\sigma$ index since we work in a spin majority band, the subscript ‘1’ represents the angular momentum $l = 1$, and ‘$s$’ for the SC state) in presence of a double peaked DOS, which turns out to be,

$$g_{1s} = \frac{\lambda^{2}}{4} \left[ \frac{1}{P_{s}} \ln |1 + \frac{8 P_{s}}{\eta}| + Q_{s} \left( \frac{1}{\eta} + \frac{1}{\eta - A_{s}d} \right) \right],$$

(10)

where $P_{s} = \lambda/6$, $Q_{s} = 2a/5\epsilon_{F}$ and $\tilde{A}_{s} = \lambda/15\epsilon_{F}$. Now, one can solve the self-consistent gap equation within the standard BCS approximation which yields,

$$k_{B} T_{s} = 1.14 \omega_{c} \exp[-1/g_{eff}],$$

(11)

where $g_{eff} = g_{1s}/(1 + g_{2})$, is the effective coupling and $\omega_{c}$ is the cut-off due to longitudinal spin fluctuations. It has been shown earlier by Brinkman and Engelsberg [21] that $\omega_{c}$ is in fact proportional to $\eta$. Of course, the derivation of the SC transition temperature is admittedly not very satisfactory due to the fact that the effective pairing interaction and the self-energy in an weakly FM system are energy dependent. However, the weak coupling BCS like formulation provides a qualitative understanding which is presented above.

It is clear from equation (6) and (10) that the effective mass ($g_{2}$) as well as the BCS coupling parameter ($g_{1s}$) for $l = 1$ ESP behaves exactly in the similar way, i.e., they are peaked at the Stoner threshold (though $\eta = 0$) and at the FM1-FM2 transition ($\eta \sim \tilde{A}_{s}d$). Furthermore, the effective coupling parameter ($g_{eff}$) also has similar feature as that of $g_{2}$ and $g_{1s}$ but the absolute magnitudes are different. This indicates that the factor $\exp[-1/g_{eff}]$ also attains a maximum at $\eta = 0$ and $\eta \sim \tilde{A}_{s}d$. However, due to the presence of the cut-off as a prefactor in the expression for $k_{B} T_{s}$, the SC transition temperature vanishes at the Stoner threshold while it becomes maximum near the FM1-FM2 transition. This is what is exactly observed in the material UGe$_{2}$. Thus, as far as the transport and the SC is concerned, the present formulation qualitatively explains the experimentally observed spectrum.

To conclude, we summarize the main results of the present work. We study the role of hidden quasi-one dimensional Fermi surface in the spin majority band of a weak Stoner FM. This was inferred from the band structure calculations in the material UGe$_{2}$. To make the calculations analytically tractable, we assume a double $\delta$-function peaked DOS and computed the single particle self-energy. We showed that the effective mass and hence the specific heat capacity acquires an additional divergence besides its standard logarithmic divergence at the Stoner critical point. This ultimately divides the FM phase into two distinct phases. Since this is purely due to the DOS effect, one might argue this transition to be of first order in nature. It is also shown that such a DOS yields maximum SC transition temperature at a point at which the specific heat capacity gets enhanced. This is in qualitative agreement with the phase diagram obtained for UGe$_{2}$.

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