Gapless Fermi Surfaces in Superconducting CeCoIn$_5$?

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According to [M.A. Tanatar et al., Phys. Rev. Lett. 95, 067002 (2005)], in a multi-band d-wave superconductor CeCoIn$_5$ electrons remain partially uncondensed. Interactions must induce superconducting order on all Fermi surfaces. We calculate specific heat and thermal conductivity in a two band model in presence of defects. Superconductivity originates on one Fermi surface, inducing a smaller gap on the other. Impurities diminish the induced gap and increase the density of states, restoring rapidly the Wiedemann-Franz law for this Fermi surface. Our calculations are in agreement with experiment.

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The heavy fermion "115" materials CeMIn$_5$ (M=Ir,Co,Rh) are currently under extensive experimental scrutiny. The compounds reveal non-Fermi liquid features, the “two-fluid”, or, alternatively, two energy scales behavior in their thermodynamics and magneto-transport. These materials are d-wave superconductors (SC), and their properties in high magnetic fields testify in favor of an important role played by the Pauli spin limitation and, more generally, the involvement of magnetic mechanism.

More recent experiments on thermal conductivity and specific heat in the heavy fermion superconductor CeCoIn$_5$ have found that the variation of thermal conductivity with increased concentration of impurities (Ce$_{1-x}$La$_x$CoIn$_5$) contradicts the expected behavior of nodal quasiparticles in a d-wave superconductor. According to Ref. [4], these results favor multi-band superconductivity, with a group of light quasiparticles that remains uncondensed and coexists with superconductivity on other Fermi surfaces (FS), even in the absence of defects ($x = 0$). It was suggested that such a scenario could explain many other experimental anomalies observed in this material, such as the saturation of the penetration depth at low temperatures, the unexpectedly large difference in thermal conductivity between longitudinal and transverse field orientations in the plane with respect to the heat flow, and the apparent contradiction in the angular field dependence of thermal conductivity and specific heat.

It seems difficult to justify the idea of uncondensed electrons on separate FS in the SC state. There are no fundamental reasons why the interactions between electrons on any two given Fermi surfaces in a multi-band metal would become identically equal to zero. In other words, if the superconducting (SC) pairing takes place on one of the FS, even an arbitrary weak interaction would inevitably induce a SC order parameter on the second FS. At the same time, it is well-known that ordinary impurities may lead to gapless superconductivity in multi-band superconductors. One example is MgB$_2$, where at least two different Fermi surfaces participate in s-wave superconductivity. Another example of a multi-band case is given by surface superconductivity, where a 2D Fermi surface becomes split by the Rashba spin-orbit interaction.

The "115" CeMIn$_5$ materials (where $M = $Rh,Ir,Co) are multi-band compounds. In particular, in CeCoIn$_5$ quasi-2D Fermi surfaces coexist with small 3D ones. CeCoIn$_5$ is a d-wave superconductor.

The main assertion made in Ref. [4] is that while in the d-wave Ce$_{1-x}$La$_x$CoIn$_5$ the thermal conductivity, $κ$, must obey the so-called “universal” law, experimentally it does not, and gapless carriers are needed to explain the observed behavior.

According to the “universal” law, the zero-$T$ limit value of $(κ/T)_{T=0}$ should not depend on the concentration of defects, $x$. The argumentation given in Ref. [4] has followed the ideas of the kinetic theory. It is well known that in the absence of defects the density of states (DOS) at the d-node is zero at zero energy and increases linearly with energy. Defects would introduce a finite DOS. If the latter were proportional to $x$, specific heat would be proportional to $x$ as well. With the number of scattering centers given by the very same $x$, the concentration of defects drops out of the new relation that connects the thermal conductivity and resistivity instead of the familiar Wiedemann-Franz law.

Actually, the “universal” law has been rigorously derived only in the so-called “clean limit”. By this one means that the concentration of defects, $x$, is very small, so that one can neglect the changes in $T_c$ and in the value of the gap order parameter with $x$.

Another provision for the validity of the arguments given in Ref. [4] is that, at the same time, $x$ should be not too small, otherwise one would encounter the region...
of a well-known singularity in DOS that appears due to the presence of impurity scattering near \( x = 0 \) \(^{22}\), where the specific heat (or DOS) cannot be linear in \( x \). The range of applicability of this second provision is not well defined, and, as we show below, depends on the strength of impurity centers.

The arguments given in Ref.\(^{4}\) may look plausible in the framework of the kinetic theory, and may even be fulfilled for the Zn-doped cuprates\(^{3, 8, 23}\), are certainly not applicable for the samples of Ce\(_{1-x}\)La\(_x\)CoIn\(_5\) studied in Ref.\(^{2}\). In fact, the latter are not in the “clean limit”, as follows from Figs 1.2 of Ref.\(^{4}\), where at \( x = 0.02 \) the value of \( T_c \) is already significantly reduced \(^{4}\), and, hence, \( \tau^{-1} \sim T_c \sim \Delta \). For all the above reasons the data presented in Fig.3 of Ref.\(^{4}\) reveals the presence of a thermal conductivity component that rapidly decreases with the increased \( x \), the feature reminiscent of the \( x \)-dependence for normal phase thermal conductivity, where the Wiedemann-Franz law applies.

To accommodate this last fact, we postulate the existence of the second FS (FS\(_2\)) with a small induced SC gap, which is therefore very sensitive to scattering on defects. This FS, we suggest, becomes practically gapless already in the presence of a small amount of defects, without changing significantly SC parameters on the other, leading FS (FS\(_1\)). FS\(_1\) makes its own contributions to the specific heat and thermal conductivity. We argue that the sum of contributions from the two FS explains the characteristic \( x \)-dependence for data\(^2\), without invoking an unphysical idea of isolated and uncondensed electrons on one of the FS.

In what follows we perform calculations of the specific heat and thermal conductivity for two FS separately: first, for FS\(_2\), where one may neglect the variation of the order parameter with the concentration of defects, and, second, for FS\(_1\), where such variations must be taken into account. The model, as it is shown below, accounts well for the main feature in the experimental data\(^2\), at least qualitatively.

We use the standard weak-coupling BCS-like approach to unconventional superconductivity\(^{27, 28}\), generalized to the multi-band situation\(^{22, 26, 27, 28}\). The Fermi liquid quasiparticles in bands \( i \) and \( j \) interact via a weak short-range interaction, \( U_{ij}(r, r’) \). The Hamiltonian can be written as:

\[
H_{\text{int}} = \frac{1}{2} \sum_{i,j} U_{ij}(q) a_{i\sigma}^\dagger q a_{j\sigma}^\dagger q a_{j\sigma'} q^{-} a_{i\sigma} q a_{j\sigma'} q.
\]  

(1)

Here \( \sigma, \sigma' \) are spin indices, and the sum over all indices is written in momentum space, \( k, k', q \). The scattering potential for impurities has the form:

\[
H_{\text{imp}} = \sum_{\sigma, l} \sum_{k, q} \sum_{\alpha} e^{i(q-k) R_{\alpha}} V_{\sigma l}(q, R_{\alpha}) a_{j\sigma}^\dagger q a_{j\sigma} q.
\]  

(2)

where \( l \) and \( j \) are band indices and \( R_{\alpha} \) are the defect positions. In turn, the inverse Gor’kov matrix \( \tilde{G}^{-1} \) defining the normal (\( G \)) and anomalous (\( F, F^\dagger \)) Green’s function is:

\[
\tilde{G}^{-1} = \begin{bmatrix}
\hat{\omega}_{j,n} - \epsilon_{jk} & -\Delta_k \\
-\Delta_k & \hat{\omega}_{j,n} + \epsilon_{jk}
\end{bmatrix},
\]  

(3)

where, as usual\(^{22}\), \( \hat{\omega}_{j,n} \equiv \omega_n - \Sigma_j(\omega_n) \). In the Born approximation:

\[
\Sigma_j(\omega_n) = n_{\text{imp}} \sum_{k,l} |u_{jl}|^2 G_l(i\omega_n, k),
\]  

(4)

\( n_{\text{imp}} \) is the concentration of impurities, while the self-energy for the anomalous Green’s function \( F_j(i\omega_n, k) \) vanishes for isotropic scattering due to momentum integration, and \( |u_{jl}|^2 = \int \frac{d\Omega}{4\pi} \int \frac{d\omega}{2\pi} |V_{jl}(k_F, k'_F)|^2 \). The Gor’kov equations are then solved, along with the gap equation,

\[
\Delta_j(k) = -T \sum_{q,n,l} U_{jl}(q) F_l(i\omega_n, k - q).
\]  

(5)

We find:

\[
\Sigma_j(\omega_n) = -\sum_l \frac{i\omega_n}{2\tau_{jl}} \int \frac{d\Omega}{4\pi} \frac{1}{\omega_l^2 + |\Delta_j(k)|^2}.
\]  

(6)

where

\[
\frac{1}{\tau_{jl}} = 2\pi N_{\text{int}} n_{\text{imp}} |u_{jl}|^2.
\]  

(7)

The general analysis of the above equations when all couplings are of the same order is somewhat cumbersome\(^{13, 27}\). Neither is it necessary, since \( T_c \) depends exponentially on the coupling constant, and superconductivity will first emerge on the Fermi surface with the largest quasiparticle attraction potential (denoted FS\(_1\)) below. Even if \( |U_{11}| \gg |U_{22}|, |U_{12}| \), the superconducting gap induced by the intra-band coupling on other Fermi surfaces (FS\(_2\), FS\(_3\), etc.), although being small, has the smallness only linear (not exponential!) in \( U_{12} \). Clearly, for singlet unconventional superconductors in presence of pair-breakers the smaller gap will get completely “erased” first, resulting in a new type of superconducting state, in which almost “normal” \( (\tau_{22}^{-1} \gg \Delta_2) \) quasiparticles on the FS\(_2\) coexist with “gapped” (i.e., having the d-wave nodes) quasiparticles on the leading band.

We consider first the case when the amount of defects, while being too small to significantly change \( T_c \) and SC parameters on FS\(_1\), is sufficient to change thermodynamics and transport attributable to FS\(_2\).

The theoretical formalism is well-known (see, for instance, Ref.\(^{24}\)). However, numerical results are different for FS\(_2\) (compare, e.g., with Ref.\(^{30}\)), because \( \Delta \) for FS\(_2\) \((= \Delta_2)\) is taken as an \( x \)-independent constant.

For a better readability, we provide a brief summary of the theoretical results here. In Eq.\(^{6}\) the analytical continuation of \( i\omega_n \) from the upper energy half-plane defines
the variable $t(E)$ (in the Born approximation) as:

$$t(E) = E + \frac{i}{2\pi} \int_0^{2\pi} \frac{d\varphi}{2\pi} \frac{t}{\sqrt{t^2 - |\Delta_k|^2}}$$  \hspace{1cm} (8)

$$\Delta_k = \Delta \cos(2\varphi).$$  \hspace{1cm} (9)

The density of states is:

$$N(E) = 2N_0 \tau Im[t(E)],$$  \hspace{1cm} (10)

and for the specific heat one has:

$$C(T) = \frac{1}{4T^2} \int_0^\infty N(E) \frac{E^2 dE}{\cosh^2 \left(\frac{E}{2T}\right)}. $$  \hspace{1cm} (11)

Here $N_0$ is the normal DOS. From general expressions for the thermal conductivity, $\kappa(T, x)$ \cite{24, 25}, we need only the low temperature limit \cite{6} (see Ref. \cite{24}):

$$\kappa_{ii} = \frac{\pi^2}{3} N_0 v_F^2 T \int \frac{d\Omega}{4\pi} \frac{k_i^2}{\varepsilon_i} \left(\gamma^2 + |\Delta_k|^2\right)^{3/2}. $$  \hspace{1cm} (12)

If in Eq. (12) $\gamma \ll \Delta$, one obtains the notorious “universal” limit, i.e., $\kappa$ independent of the concentration of impurities \cite{3, 4}:

$$\kappa = \frac{2\pi}{9} N_0 v_F^2 T \Delta $$  \hspace{1cm} (13)

The formal definition of $\gamma$ is given by:

$$\gamma = Im[t(E \rightarrow 0)],$$  \hspace{1cm} (14)

however, its explicit expression strongly depends on the assumption about the strength of the scattering potential for the defects \cite{31}. At small $x$, in the Born approximation,

$$\gamma = \frac{N(0)}{2N_0 \tau} = 4\Delta e^{-\pi \tau \Delta}. $$  \hspace{1cm} (15)

In the opposite limit of strong scattering (the unitary limit \cite{31}):

$$\gamma = \sqrt{\frac{\pi \Gamma \Delta}{\ln \frac{32\Delta}{\pi^2}}}, $$  \hspace{1cm} (16)

where

$$\Gamma = \frac{n_{imp}}{\pi N_0}. $$  \hspace{1cm} (17)

The results of our calculations of the specific heat and thermal conductivity contributions from FS2 are presented in Fig. 1 for these two extreme cases. One sees that in the Born approximation a flat region (the “universal” law) in $\kappa/T$ appears at small $x$; in the unitary limit for impurity scattering this interval is practically absent, although, as it was explained above, $\Delta_2$ was kept constant. At larger $x$ $\kappa/T$ decreases, merging rapidly with the $1/x$ behavior expected from the Wiedemann-Franz law in the normal phase. No interval is seen for the linear in $x$ behavior of the Sommerfeld coefficient in the specific heat.

The same characteristics have been calculated for FS1 in and are given in Fig. 2. Unlike for FS2, now both $\Delta$ and $T_c$ decrease with $x$, as shown in the inset (the dependencies practically coincide with the results for the unitary

FIG. 1: Contribution of FS2 to the linear coefficient for the heat capacity $\gamma(T)/\gamma_N(T)$ (left axis; blue-Born approximation, green-unitary limit) and the ratio of thermal conductivity $\kappa(T)/T$ to its universal limit for FS2 (right axis) at small temperatures $T \rightarrow 0$ as a function of $1/2\tau \Delta$ in the Born approximation, or $\Gamma/\Delta$ in the unitary limit.

FIG. 2: Contribution of FS1 to the linear coefficient for the heat capacity $\gamma(T)/\gamma_N(T)$ (left axis; blue-Born approximation, green-unitary limit) and the ratio of thermal conductivity $\kappa(T)/T$ to its universal limit for FS1 (right axis; black-Born approximation, red-unitary limit) at small temperatures $T \rightarrow 0$ as a function of $1/2\tau \Delta$ in the Born approximation, or $\Gamma/\Delta$ in the unitary limit. The inset shows the dependence of $T_c$ (black) and the order parameter in the Born approximation (red) and the unitary limit (blue).
limit from Ref.[30]. Note a considerable variation of $\kappa/T$ both in the Born approximation and in the unitary limit for the scattering amplitude between $x = 0$ and $x = x_{cr}$, where $T_c = 0$ and SC is destroyed. A linear in $x$ behavior in the specific heat is seen in some $x$-interval only in the unitary limit. Above $x_{cr}$ DOS reaches its normal value, independent of $x$, and $\kappa/T$ begins to decrease as $1/x$, according to the Wiedemann-Franz law, leading to the corresponding "bump" at $x = x_{cr}$. Note that one sees such a "bump" in experimental data shown on Fig.3 of Ref.[31].

To summarize, the model of two FS with different values of SC order parameter provides an excellent qualitative interpretation of the remarkable findings in Ref.[4]. Indeed, we have shown that at smaller $x$ the $x$-dependent contribution to $\kappa/T$ in Ref.[4] can be attributed to a FS2 (such as the $\epsilon$- sheet)[18,19] "stripped" of a SC gap by strong scattering. Linear in $x$ dependence of the Sommerfeld coefficient in the specific heat at $T = 0$ seen in Ref.[4] may come from the FS1 [20].

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