Anomalous specific heat jump in the heavy fermion superconductor CeCoIn$_5$

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We study the anomalously large specific heat jump and its systematic change with pressure in CeCoIn$_5$ superconductor. Starting with the general free energy functional of the superconductor for a coupled electron boson system, we derived the analytic result of the specific heat jump of the strong coupling superconductivity occurring in the coupled electron boson system. Then using the two component spin-fermion model we calculate the specific heat coefficient $C(T)/T$ both for the normal and superconducting states and show a good agreement with the experiment of CeCoIn$_5$. Our result also clearly demonstrated that the specific heat coefficient $C(T)/T$ of a coupled electron boson system can be freely interpreted as a renormalization either of the electronic or of the bosonic degrees of freedom.

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The superconductivity (SC) in CeMIn$_5$ (M=Co, Rh, Ir) heavy fermion (HF) series compounds$^{1,2}$ provides valuable information about the superconductivity nearby a possible quantum critical point (QCP) due to the excellent tunability with pressure and magnetic fields$^3$. Besides a complicated phase diagram due to a competition/interplay between the magnetism and superconductivity, the superconducting properties as well as the normal state ones around the QCP exhibit various anomalous behaviors such as non-Fermi liquid (NFL) power law of temperature in the resistivity, pseudogap behavior above the superconducting critical temperature, the continuous evolving from the second order to the first order phase transition of the superconductivity with magnetic fields, etc$^4$.

In a recent paper$^4$ we proposed the two-component spin-fermion model as a generic pairing mechanism of this series of compounds CeMIn$_5$. In this work, it is shown that some of the standard features of the d-wave superconductivity mediated by magnetic fluctuations becomes strongly modified in the vicinity of the magnetic critical point. Indeed it is very natural to expect that such a strongly coupled fermion-boson superconductivity shows various anomalies deviating from the standard weak or strong coupling theory of superconductivity$^5$.

In this paper we study anomalous property of the specific heat coefficient $C(T)/T$ in CeCoIn$_5$. Sparn et al.$^5$ measured $C(T)/T$ of CeCoIn$_5$ with varying pressure and also with applying magnetic fields. The key findings are that (1) suppressing the superconductivity with 8 Tesla fields $C(T)/T$ show $ln T$ divergence down to 0.4 K; (2) without the magnetic fields the same sample becomes superconducting at 2.3 K with the specific heat jump ratio $\Delta C(T)/C(T) \sim 5$, which is a huge jump considering $C(T_c)/T_c \sim 400mJ/K^2$mol; (3) with applying pressure $T_c$ gradually increases to 2.8 K at the pressure of 15 kbar but the jump ratio $\Delta C(T)/C(T)$ drops drastically. We think this peculiar behavior is another manifestation of the critical magnetic fluctuations mediated superconductivity. The huge specific heat jump, indicating the steep drop of the entropy below $T_c$, is actually consistent with the spin-fermion model if we consider that the critical magnetic fluctuations in this model is generated by the fermionic particle-hole excitations, which should be gapped below $T_c$. This means that below $T_c$ not only the fermions suffer the entropy drop by developing pairing correlation but also the spin fluctuations should suffer the entropy drop, which add up to make a larger specific heat jump. As will be shown below, however, this phenomena is actually very general so that it should occur even in the electron-phonon mediated superconductors. The reason why it is phenomenal in CeCoIn$_5$ is simply because the coupling of fermion-boson is strong and in particular the resulting bosonic mode is near critical. There is a recent work$^7$ addressing the same problem as in this paper, but proposing a different mechanism for the enhanced $\Delta C(T)/C(T)$.

We start with the general free energy functional of the two component spin-fermion model, which is nothing but the same form as the one for electron-phonon model$^{8-10}$.

$$\Omega_{total} = \Omega_{fer} + \Omega_{spin} + \Omega_{int}$$

$$= -\frac{T}{V} \sum_{P} [\ln(-\phi(P)) + 2\Sigma_1(P)G(P) - 2\Sigma_2(P)F(P)]$$

$$+ \left(\frac{3T}{2V}\right) \sum_{q} [\ln(-D^{-1}(q) + \pi(q)D(q))]$$

$$+ (T/V)^2 \sum_{P,P'} \alpha_{P-P'}^2 [G(P)D(P-P')G(P')]$$

$$- F(P)D(P-P')F(-P')]$$

where $P = (\mathbf{p}, i\omega_n), q = (\mathbf{q}, i\Omega_n); \omega_n = \pi T(2n+1), \Omega_n = \pi T(2n), \text{ and } G(P) = (i\omega_n - \epsilon_P + \Sigma_1(-P))/\phi(P), F(P) = -\Sigma_2(-P)/\phi(P), \phi(P) = (i\omega_n - \epsilon_P - \Sigma_1(P))(i\omega_n + \epsilon_P + \Sigma_1(-P) - [\Sigma_2(P)]^2)$, respectively. Finally, the dressed spin propagator is written as $D^{-1}(q) = D_0^{-1}(q) - \pi(q)$.

$\Omega_{fer}, \Omega_{spin}, \text{ and } \Omega_{int}$ are just apparent separation of the total free energy but the literal meaning of them is not necessarily correct as will be clear later. The notations...
are standard\textsuperscript{10}, and the one important difference is that $D_0(q)$ is not explicitly defined in the spin-fermion model in contrast to the electron-phonon case, but only the total spin propagator is defined phenomenologically as follows.

\[ D(q) = \frac{D_0}{1 - D_0 \pi(q)} = \frac{D_0}{I(T) + A(q - \tilde{Q})^2 + |\Omega_n|/\Gamma}. \]  

(3)

where $I(T)$ defines the distance from the magnetic quantum critical point (QCP) and $A$ and $\Gamma$ are the coefficients determined by the Fermi liquid parameters of the fermion sector\textsuperscript{11}. The effective spin correlation length and the relaxation energy scale are $\xi = A/I(T)$ and $\omega_{sf} = \Gamma \cdot I(T)$, respectively, and the momenta $q$ and $\tilde{Q}$ are assumed to be in the two dimensions\textsuperscript{12}. We take $\Gamma$ as the unit energy scale in our numerical calculations. The bare spin propagator $D_0$ is assumed to be trivial regarding the critical low energy behavior and taken to be a constant. As usual, the above free energy functional is constructed in such a way that it is stationary with respect to the variations of $\Sigma_{1,2}$ and $\pi$ a la Luttinger-Ward\textsuperscript{8} with the following definitions. This property of the functional is very important and utilized critically in our paper.

\[ \Sigma_1(P) = \frac{T}{V} \sum_{P'} \alpha_{P-P'}^2 G(P')D(P-P'), \quad \Sigma_2(P) = \frac{T}{V} \sum_{P'} \alpha_{P-P'}^2 F(P')D(P-P'), \]  

\[ \pi(P) = \frac{-2T}{3V} \sum_P \alpha_P^2 [G(P+q)G(P) - F(P+q)F(-P)]. \]  

(4) \hspace{1cm} (5) \hspace{1cm} (6)

Now following Ref\textsuperscript{10}, neglecting the momentum dependence of $\Sigma_{1,2}$ and using the definitions, $\Sigma_1(P) = i\omega_n(1 - Z(\omega_n))$, and $\Delta(\omega_n) = \Sigma_2(P)/Z(\omega_n)$, we obtain after the momentum integration the following.

\[ \Omega_{fer} + \Omega_{int} = -T \cdot N(0) \cdot \pi \]  

\[ \sum_{\omega_n} [Z(\omega_n) + 1) \sqrt{\Delta^2 - (i\omega_n)^2} - \frac{\Delta^2}{\sqrt{\Delta^2 - (i\omega_n)^2}}] \]  

(7)

Note that the above equation didn’t include the $\Omega_{spin}$ term yet\textsuperscript{13}. But due to the stationary property of the total free energy functional as mentioned above, the specific heat jump across the superconducting transition with the changes of $\Sigma^{(n)} \rightarrow \Sigma^{(s)}$ and $\pi^{(n)} \rightarrow \pi^{(s)}$ is solely determined by Eq.(7) with $Z(\omega_n) = Z^{(n)}(\omega_n)$ at $T = T_c$.

The Eq(7) can be written after the Matsubara frequency summation using the contour integration as

\[ \Omega_{fer} + \Omega_{int} = N(0) \int_0^\infty d\omega \frac{\Delta^2}{(\omega - Z_0)^2 + \Delta^2} \cdot \tanh\left(\frac{\omega}{2T}\right), \]  

where $\omega^2 = \epsilon^2 + \Delta^2$ and the specific heat is calculated at $T = T_c$ as

\[ C(T)/T = (Z + 1)N(0) \frac{\pi^2}{3} + \frac{ZN(0)}{T_c} \left( -\frac{\partial \Delta^2}{\partial T} \right) \]  

(9)

This is our key result in this paper and we can read the specific heat jump ratio as $\frac{C(T)}{C(T)} = \frac{2}{Z + 1} \frac{\Delta^2}{Z^2} T.\textsuperscript{13}$

We see from this formula that the jump ratio is modified with the normal self-energy renormalization factor $\frac{Z}{Z + 1}$, which is $\frac{1}{2}$ in the BCS limit with $Z = 1$ and can have a maximum value 1 in the limit of $Z(T) \rightarrow \infty$. Apparently $\frac{Z}{Z + 1} \rightarrow 1$ is the proper limit for CeCoIn\textsubscript{5} and some other heavy fermion compounds exhibiting a large $C(T)/T$ at low temperature. We summarize the consequences of this formula: (1) The jump ratio at most can be doubled to the BCS ratio assuming $\frac{Z}{Z + 1}$ is the same as the BCS limit, i.e. 9.42$T_c$; (2) Apparently the steeper slope of $\Delta(T)$ can contribute an extra enhancement to the jump ratio. And since our formula is an exact result, this formula can be utilized to estimate the temperature slope of $\Delta(T)$ at $T_c$ from the experimental $\frac{\Delta C(T)}{C(T)}$ in the limit of $\frac{Z}{Z + 1} \rightarrow 1$; (3) Finally, the interpretation of the large $C(T)/T$ and its enhanced jump ratio from the heavily renormalized fermionic quasiparticle due to the scattering from the magnetic fluctuations seems to be legitimate, if we can neglect the contribution from $\Omega_{boson}$.\textsuperscript{13}

Now in order to calculate $C_{\text{total}}(T)$ above and below $T_c$, we need to calculate $\Sigma_{1,2}^{(n)}(\omega)$ with a given $D(q)^{(n)}(\omega)$. But we found a more convenient way to proceed as follows. Adding $\Omega_{int}$ term to $\Omega_{spin}$ exactly cancels the cumbersome term $\pi(q)D(q)$ as

\[ \Omega_{spin} + \Omega_{int} = \left( \frac{3}{2} \frac{T}{V} \right) \sum_\omega \ln(-D^{-1}(\omega)). \]  

(10)

Furthermore, $\Omega_{fer}$ term alone, after the same manipulations used for Eq.(7) and Eq.(8), becomes

\[ \Omega_{fer} = -T \cdot N(0) \cdot \pi \sum_{\omega_n} [2\sqrt{\Delta^2 - (i\omega_n)^2} - \frac{\Delta^2}{\sqrt{\Delta^2 - (i\omega_n)^2}}] \]  

\[ = N(0) \int_0^\infty d\omega \cdot \frac{\Delta^2}{\omega} \cdot \tanh\left(\frac{\omega}{2T}\right). \]  

(11)

A different organization greatly simplifies $\Omega_{fer}$ so that all the renormalization effect due to the interaction miraculously drops and furthermore the explicit $\Delta(T)$ dependent term all cancels out in the final result of Eq.(11).

This amazing result is actually the consequence of the Ellashberg free energy functional built with the stationary property with respect to the variations of the self-energies. Considering that the Ellashberg free energy functional is not the exact free energy functional but a consistent approximate functional equivalent to the self-consistent Born approximation for the fermionic part and the random phase approximation (RPA) for the bosonic part, the exactness of Eq.(9) and Eq.(11) has a limited
meaning. Nevertheless, besides the accuracy of this functional the insightful reason for this result is the equivalent relation of the following.

\[
\frac{T}{V} \sum_P \left[ \Sigma_1(P)G(P) - \Sigma_2(P)F(P) \right] = -\left( \frac{3}{2N} \right) \sum_q |\pi(q)| \delta(q). 
\]

(12)

From the technical viewpoint the above relation is trivial if we consider any linked-cluster diagram obtained from the free energy expansion with \(H_{\text{int}}\). However the physical interpretation is rather revealing. Namely, the interacting free energy \(\Delta \Omega = \Omega_{\text{total}} - \Omega_{\text{bare}}\) and its derived entropy \(\Delta S\) all comes from the expansion of \(H_{\text{int}}\). Then depending on how to view or organize the same diagrams, we can view all interaction effect as the renormalization of either the fermion sector or the bosonic sector. While theoretically we have this freedom, in experiments the experimental probe itself determines how to measure the contribution of either fermionic or bosonic degree of freedom. However the thermodynamic measurement like the specific heat measures simultaneously the both degrees of freedom and it is hard to know how much contribution comes from which degree of freedom. Our analytic result clearly demonstrated that the specific heat coefficient \(C(T)/T\) of a coupled fermion-boson system can be freely interpreted as a renormalization either of the electronic or of the bosonic degree of freedom, but not for both. This point should have a far-reaching consequence to the heavy fermion experiments and its related interpretations. This important aspect will be dealt in the separate publication.

Now let us return to the calculation for the total \(C(T)\) from Eq.(10) we can calculate the entropy \(S(T)\) with the phenomenological \(D(q)\) given in Eq.(3) as follows.

\[
S = \sum_q \int_0^{\Lambda} d\omega \cdot \left( \frac{1}{4\pi} \sinh^2 \left( \frac{\omega}{T} \right) \right)^2.
\]

(13)

In real calculation, we need to fix parameters. Our unit energy scale is \(\Gamma = 1\), and we take \(\Lambda = 3\), \(A = 1.0\) and \(a = 1.0\). For the fermionic part \(\Omega_{\text{fer}}\), it is just the same form as the non-interacting fermion free energy except \(\omega = \sqrt{\epsilon_F + \Delta^2(T)}\), and therefore it develops some structure below \(T_c\) but no discontinuity at \(T_c\). Finally to fix the relative magnitude of \(\Omega_{\text{fer}}\) we need to determine the spin density of states \(N_s\) defined as \(N_s \int_0^{\Lambda} d\omega = \frac{1}{V} \sum q \cdot \omega_{\text{max}}^q \). This can be determined using Eq.(12) at normal state, which gives the following relation

\[
\frac{3}{2} TNs \sum_{\omega_n} \ln \left( \frac{I(T) + \omega_{\text{max}}^q / T + |\omega_n| / T}{I(T) + |\omega_n| / T} \right) = T N(0) \pi \sum_{\omega_n} (Z^{(n)} - 1) |\omega_n|.
\]

(14)

We assume \(\pi_n = -\frac{\omega_n}{T}\) and this in the derivation, but the above relation is not useful since both side of the equation diverges unless we introduce high frequency cut-off for \(\omega_n\) and \(\omega_n\). Since the above relation should hold for a variation of \(\delta \pi_n\), we derive another equivalent relation at \(T = 0\) as

\[
\frac{3}{2\pi} N_s \int_0^{\Lambda} d\omega \cdot \left[ I(T) + \omega_{\text{max}} + \omega_{\text{max}} \right] \frac{-\omega_{\text{max}}}{1 + \omega_{\text{max}} / T} = N(0) \int_0^\infty d\omega \cdot \left[ Z^{(n)}(\omega; \pi_n + \delta \pi_n) - Z^{(n)}(\omega; \pi_n) \right] / \delta \pi_n.
\]

(15)

A recent paper by Ref.[16] also use the similar procedure to fix the relation between \(N(0)\) and \(N_s\). Our numerical result gives \(N_s \approx 1.5 \pi \omega_{\text{max}}^2 N(0)\). Now we are ready to calculate \(C(T)\) using Eq.(11) and Eq.(13). For the calculation below \(T_c\) we need to know the temperature dependence of the gap function \(\Delta(T)\) and \(\pi_s(\Delta(T))\). For the gap function we use the generalized BCS form \(\Delta(T) = \Delta_0 \tanh(a \sqrt{T_c / T - 1})\), where \(a = 1.764\) and \(\Delta_0 = 1.74T_c\) for BCS limit, but for strong coupling superconductor these values can deviate largely from the BCS limit and we take them as parameters. Now much unclear part is the behavior of \(\pi_s(T)\) below \(T_c\). Qualitatively it should be cut off for \(\Omega < 2\lambda_0\) at \(T = 0\) and smoothly recover to the normal state form approaching \(T \to T_c\). The leading expansion of \(\pi_s(T)\) in \(\Delta^2(T)\) gives \(\pi_s = \pi_n \exp(-\Delta^2(T)/|\omega^2 + T^2|)\); but for a larger value of \(\Delta(T)\) for \(T \to 0\) this form should not be very correct.

The numerical results are shown in Fig.(1) and Fig.(2). In Fig.(1) the specific heat coefficient \(C(T)/T\) calculated from Eq.(13) are shown in unit of \(\Delta^2(0) N(0)\). For our parameter choice producing \(Z \gg 1\) (For this we need the critical spin fluctuations \(I_0 < 1\) as well as the effective coupling \(\Delta_{\text{max}}\) of \(O(1)\)), the contribution of \(C(T)/T\) from \(\Omega_{\text{fer}}\), Eq.(11) is negligibly small. Therefore we didn’t add it to \(C(T)/T\) in Fig(1) but show it separately in Fig.(2) demonstrating its qualitative features. In Fig.(1) the solid line is for the normal state \(C(T)/T\) with \(I_0 = 0\) (the spin fluctuations is at QCP), it indeed displays \(\ln T\) divergence with decreasing temperature. With SC transition at \(T_0 = 0.2\) (open square symbol) it shows the jump ratio \(\Delta(C(T)/C(T)) \sim 5\) with the choice of parameters. Then increasing \(I_0\), the \(\ln T\) divergence is quickly suppressed and at the same time the specific heat jump ratio drops with increasing \(T_c\) (\(T_c\) is increased by hand and the temperature slope of \(\Delta(T)\) is reduced accordingly as \(\Delta(T_c) / \Delta(T_c) \sim \frac{T_c}{T_c}\) ). With this rather crude phenomenological choice of parameters our numerical results reproduce the experimental features of \(C(T)/T\) in CeCoIn\(_5\) qualitatively as well as quantitatively.
In summary, starting with the general free energy functional for the coupled fermion-boson system, we derived an analytic formula of \( \Delta C(T)/C(T) \) for the general strong coupling superconductor. Then we calculate \( C(T)/T \) for the spin-fermion model and show that the salient features of \( C(T)/T \) of CeCoIn\(_5\) for both normal and superconducting states are successfully explained including its anomalous jump ratio \( \Delta C(T)/C(T) \) and the progressive reduction of it with increasing \( T_c \). Also with different organization of the Eliashberg free energy functional, which lumps all the interaction effect either into the bosonic or into the fermionic degrees of freedom, we clearly demonstrated that the effect of the interaction in the total free energy or entropy of the coupled fermion-boson system can be freely viewed as the renormalization of either the fermion sector or the boson sector. Finally, our results strongly support the idea that the two dimensional critical magnetic fluctuations plays an essential role in CeMnIn\(_5\) HF compounds in producing a large and strongly temperature dependent \( C(T)/T \) and the SC pairing itself.

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1. H. Hegger, C. Petrovic, E. G. Moshopoulou, M. F. Hundley, J. L. Sarrao, Z. Fisk, and J. D. Thompson, Phys. Rev. Lett. 84, 4986 (2000).

2. C. Petrovic, R. Movshovich, M. Jaime, P. G. Pagliuso, M. F. Hundley, J. L. Sarrao, Z. Fisk, J. D. Thompson, Europhys. Lett. 53, 354 (2001); C. Petrovic et al., J. Phys. Condens. Matter 13, L337 (2001).

3. V.A. Sidorov, M. Nicklas, P. G. Pagliuso, J. L. Sarrao, Y. Bang, A.V. Chubukov, and A.M. Finkel’stein, Europhys. Lett. 54, 488 (2001).

4. Yunkyu Bang, I. Martin, and A.V. Balatsky, Phys. Rev. B 66, 224501 (2002).

5. Ar. Abanov, A.V. Chubukov, and A.M. Finkel’stein, Europhys. Lett. 54, 488 (2001).

6. G. Sparn, R. Borth, E. Lengyel, P.G. Pagliuso, J.L. Sarrao, F. Steglich, J.D. Thompson, Physica B 312, 138 (2002)

7. S. Kos, I. Martin, and C.M. Varma, cond-mat/0302089.

8. J. M. Luttinger and J. C. Ward, Phys. Rev. 118, 1417 (1960).

9. G. M. Eliashberg, JETP 16, 780 (1963).

10. J. Bardeen and M. Stephen, Phys. Rev. 136, A1485 (1964).

11. H. Hasegawa, and T. Moriya, J. Phys. Soc. Japan, 36, 1542 (1974).

12. A. Rosch, A. Schroeder, O. Stockert, and H. v. Lovenysen, Phys. Rev. Lett. 79, 159 (1997).

13. In the electron-phonon case, the term \( \Omega_{boson} \) (in this paper \( \Omega_{spin} \)) is neglected with the argument that the change \( (\pi_+ - \pi_-) \sim \Delta^2 / E^2 \) is small\(^\text{10}\). But this argument is wrong because the change of the free energy above and below \( T_c \) is...
always $O(\Delta^2/E^2_f)$ and this small change is what makes the superconducting transition. As shown by Chester\textsuperscript{14} even before the BCS theory, the actual change of phonon kinetic energy is just the same order of magnitude as the electronic part. The correct reason why still the term $\Omega_{\text{boson}}$ can be neglected is that the contribution of the self-energy correction $\pi_{x,n}$ in $\Omega_{\text{boson}}$ exactly cancels between $\ln(-D^{-1}(q))$ and $\pi(q)D(q)$ terms for the small frequency limit. Then the actual contribution of $\Omega_{\text{boson}}$ is just the one of the un-renormalized bare boson (or phonon) propagator, so it can be dropped.

\textsuperscript{14} G. V. Chester, Phys. Rev. \textbf{103}, 1693 (1956).

\textsuperscript{15} I. Paul, and G. Kotliar, Phys. Rev. B \textbf{64}, 184414 (2001).

\textsuperscript{16} R. Haslinger, and A. V. Chubukov, cond-mat/0209600.

\textsuperscript{17} In order to compare with experiment, we should count the gap anisotropy which reduces the specific heat jump by the factor $<\Delta^2(k)>^2 / <\Delta^4(k)>$\textsuperscript{18} (for d-wave gap, this value is 0.666.). In Fig.(1), we just multiplies 0.666 to the results below $T_c$ for a better comparison with the experiment, but this artificial procedure ruins the entropy conservation.

\textsuperscript{18} T.M. Mishonov, E. S. Penev, J. O. Indenkeu, and V. L. Pokrovsky, cond-mat/0209342.