Journal of the Physical Society of Japan
Vol. 58, No. 2, February, 1989, pp. 360-363

On the $T^3 \ln T$ Law in the Specific Heat of Spin-Fluctuation Compounds

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(Received September 5, 1988)

The effects of both the long- and shorter-wavelength spin fluctuations (SF), in particular of ferro- and antiferromagnetic SF, on the specific heat of exchange-enhanced paramagnetic metals are studied quantitatively within paramagnon theory on the basis of a uniaxially anisotropic band model. There are found different $T^3 \ln T$ laws holding in different temperature ranges. The SF model considered is shown to provide a microscopic understanding of the localised-paramagnon picture.

The study of spin-fluctuation (SF) phenomena in exchange-enhanced paramagnetic metals was revived by the observation of a $T^3 \ln T$ term in the low-temperature specific heat C_v of some heavy-fermion systems (*e.g.* UPt_3, UAl_2) and by the suggestion of SF-mediated superconducting pairing in UPt_3 ($T_c \simeq 0.5$ K).[1] As is well known, ferromagnetic (fm) SF give rise to the $T^3 \ln T$ law in C_v, whereas antiferromagnetic (afm) SF do not yield the $T^3 \ln T$ term at very low temperatures.[2] Recently, Konno and Moriya[3] have shown that localised paramagnons give rise to a $T^3 \ln T$ law in an intermediate temperature range.

In our previous papers,[4] hereafter referred to as I, we have studied the Fermi surface (FS) anisotropy and topology effects on the properties of SF compounds in the framework of RPA paramagnon theory (on the basis of the Hubbard model). We have found qualitatively novel SF phenomena as compared with the results obtained with isotropic paramagnon models and have proposed an anisotropic SF model for heavy-fermion UPt_3 which may explain the results of several relevant experiments. Our basic model is the uniaxially anisotropic quasi-particle band dispersion

$$\varepsilon_\kappa = \frac{1}{2}(k_x^2 + k_y^2) - \alpha \cos k_z, \tag{1}$$

which yields anisotropic FS of different topology characterized by the parameter $\xi = 1 + \varepsilon_F/\alpha$ (a closed FS for $0 < \xi < 2$, an open FS for $\xi > 2$). ε_F is the Fermi energy, $\alpha = 2tm_b d^2 \hbar^{-2} > 0$, where t denotes the tight-binding transfer integral between nearest neighbours on the z axis separated by d, and m_b is the effective band mass for the electron motion in the xy plane. In (1) and the following we measure the wavevector components and the energy in units of d^{-1} and $\hbar^2/m_b d^2$, respectively. As revealed by the resulting structure of the static reduced susceptibility of noninteracting quasiparticles, $\bar{\chi}_0(q) = \chi_0(q_\perp, q_{/\!/})/\chi_0(0)$ ($q_\perp^2 = (q_x^2 + q_y^2)/\alpha$, $q_{/\!/} = |q_z|$), shown in Fig. 1, the SF model describes different kinds of SF. In particular, in the FS region $1 < \xi < 2$ there is a coexistence of fm SF perpendicular to the anisotropy axis and afm SF along the anisotropy axis with wavevectors around $Q = (0, 0, \pi)$ (as observed for UPt_3). For either FS topology, in I we have found the $T^3 \ln T$ law, where the amplitude is enlarged as compared with the value obtained in the parabolic band model, and the temperature range of validity increases with FS anisotropy. In the evaluation of the SF contributions to C_v we have taken into account all types of SF simultaneously. Therefore, the origin of the $T^3 \ln T$ law in our approach has not been well clarified.

In this paper we investigate in detail the separate contributions to C_v beyond the γT term arising from both the long- and shorter-wavelength SF. We show the existence of different $T^3 \ln T$ laws and give a more microscopic basis for the localised-

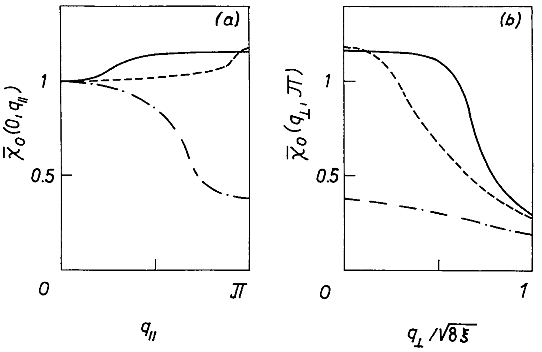

Fig. 1. The static reduced susceptibility $\bar{\chi}_0(q)$ of the model (1) for $q_\perp=0$ (a) and $q_{/\!/}=\pi$ (b). Full curve, $\xi=1.9$; broken curve, $\xi=1.1$; chain curve, $\xi=0.5$.

paramagnon model given by Konno and Moriya.[3] Our goals are (i) to study the origin and the temperature range of validity of the $T^3 \ln T$ laws and (ii) to compare our results with those of the localised-paramagnon approach. We start from the general expression (see, for example, ref. 3)

$$C_v-\gamma T=\frac{3}{\pi}\,T^3 I(T), \tag{2}$$

$$I(T)=\sum_q\int_0^\infty \mathrm{d}x x^4 n'(x)/\Gamma(q)(\Gamma^2(q)+x^2T^2), \tag{3}$$

($\hbar=k_\mathrm{B}=1$). For our model we have derived eqs. (2) and (3) in the random-phase approximation in I, where we get

$$\Gamma(q)=\bar{T}_\mathrm{F}d_{/\!/}S/4\pi^2\xi S(q)\bar{u}(q), \tag{4}$$

with

$$\bar{T}_\mathrm{F}=\varepsilon_\mathrm{F}\xi/(S-1)(\xi-1),$$
$$S(q)=S/(S-(S-1)\bar{\chi}_0(q)).$$

$S=S(0)$ is the Stoner factor, $d_{/\!/}=2\cos^{-1}(1-\xi)\theta(2-\xi)+2\pi\theta(\xi-2)$ is the maximal extension of the FS in z direction, and $n(x)=(e^x-1)^{-1}$. The function $\bar{u}(q)$ is obtained from the calculation of $\mathrm{Im}\,\chi_0(\boldsymbol{q},\omega)$ for $\omega/|\boldsymbol{q}|\ll 1$ and is well approximated by its expansion for $|\boldsymbol{q}|\ll 1$ given in I. In (3) we restrict the integration over $\boldsymbol{q}$ by a cut-off energy (ε_c) surface with the symmetry of the FS, where $\varepsilon_\mathrm{c}=q_\mathrm{c}^2\xi-1$ (the cut-off parameter q_c is used in analogy to the parabolic band case, see I). To look for the $T^3 \ln T$ law we introduce, as in I, the dimensionless quantity

$$J(T/\bar{T}_\mathrm{F})=\frac{1}{4\pi\alpha}\frac{d^3}{\Omega}\left(\frac{d_{/\!/}\bar{T}_\mathrm{F}}{2\pi\xi}\right)^3 I(T), \tag{5}$$

where Ω is the volume of the crystal. We have numerically evaluated $J(T/\bar{T}_\mathrm{F})$ for different sets of the parameters $\xi<2$, S, and q_c. For $0<T<T_\mathrm{m}$ we obtain $-J=-c(\xi;S,q_\mathrm{c})+a(\xi)\ln(\bar{T}_\mathrm{F}/T)$. Choosing, for example, $S=4$; $q_\mathrm{c}=0.05$ and $q_\mathrm{c}=2$ we obtain $T_\mathrm{m}/\bar{T}_\mathrm{F}\simeq 0.005$ and 0.04, respectively. The very low cut-off parameter $q_\mathrm{c}=0.05$ takes into consideration the contribution to C_v from only long-wavelength SF with $|\boldsymbol{q}|\simeq 0$ (including the anisotropic fm SF). This contribution gives rise to the well-known $T^3 \ln T$ law at very low temperatures. At elevated temperatures shorter-wavelength SF are excited (including the anisotropic afm SF in the case $1<\xi<2$). The total contribution from the long- and shorter-wavelength SF is obtained by taking $q_\mathrm{c}=2$ and reveals the $T^3 \ln T$ law up to higher temperatures.

Let us now separate the long-wavelength from the shorter-wavelength SF contribution. We calculate the latter one from $\Delta J=J(q_\mathrm{c}=2)-J(q_\mathrm{c}=0.05)$; our results for $-\Delta J$ with $S=4$ and different ξ-values are shown in Fig. 2 (inset). As can be seen, the shorter-wavelength SF yield a $T^3 \ln T$ law in the intermediate temperature range $0.03\bar{T}_\mathrm{F}<T<0.16\bar{T}_\mathrm{F}$. Note that in this region the slope of $-\Delta J$ versus $\ln(\bar{T}_\mathrm{F}/T)$ is somewhat smaller than the corresponding coefficient $a(\xi)$ (see above). Let us underline that this $T^3 \ln T$ law has nothing to do with the $T^3 \ln T$ contribution due to long-wavelength SF. The upper bound of the given temperature range is considerably larger than the ranges of validity of the $T^3 \ln T$ laws (T_m) arising from both the long-wavelength SF and the combined effects of long- and shorter-wavelength SF. Let us point out that our result is consistent with the fact found by Moriya[2] that afm SF do not given rise to a $T^3 \ln T$ term at very low temperatures. However, as we have shown, the afm SF yield a $T^3 \ln T$ law in an intermediate temperature range at higher temperatures.

We now compare the results of our SF model with those of the localised-paramagnon model given by Konno and Moriya.[3] This model may be obtained from (2), using (3), by

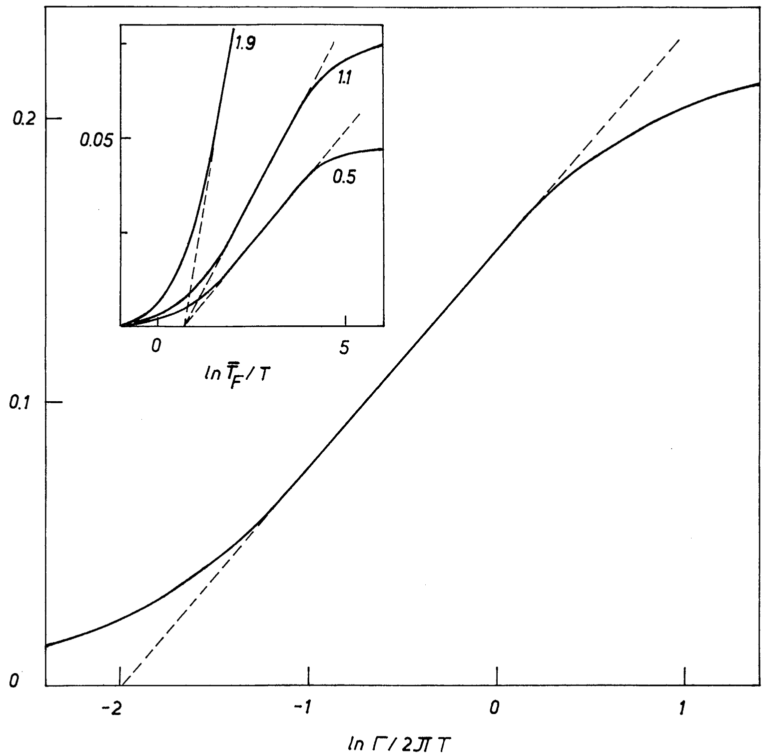

Fig. 2. The integral $-\Delta J$ obtained from (3) with $\xi=1.9$ and $S=6.5$, as described in the text. Inset: $-\Delta J$ with $S=4$; the values on the curves are of ξ.

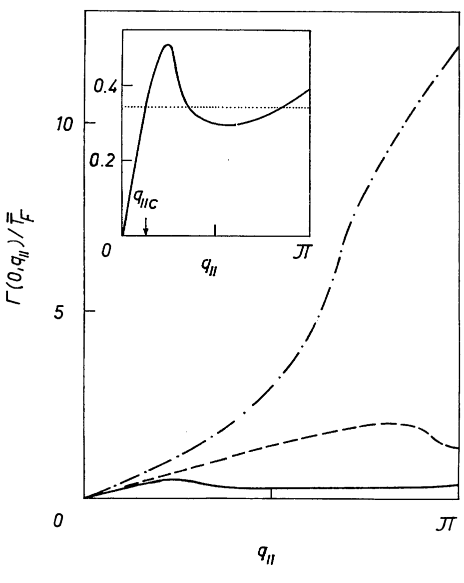

Fig. 3. The damping $\Gamma(0, q_{/\!/})$ according to (4) with $S=6.5$ for $\xi=1.9$ and $S=4$ for $\xi=1.1$, 0.5. The curves are denoted as in Fig. 1. Inset: $\Gamma(0, q_{/\!/})$ for $\xi=1.9$ on an enlarged scale; dotted line, the localised-paramagnon approximation $\Gamma(q)=0.34\bar{T}_F$.

the approximation $\Gamma(q)=\Gamma$.[4] The localised-paramagnons yield a $T^3 \ln T$ law in the intermediate temperature range $0.7\Gamma/2\pi < T < 3\Gamma/2\pi$,[3] in qualitative accord with our result for the shorter-wavelength SF contribution. For a quantitative comparison let us consider the dependence on $\boldsymbol{q}$ of $\Gamma(\boldsymbol{q})$, which is mainly determined by the structure of $\bar{\chi}_0(\boldsymbol{q})$ (Fig. 1) and is shown in Fig. 3. $\Gamma(\boldsymbol{q})$ reveals a linear increase in the small-$|\boldsymbol{q}|$ region, and the dependence on $\boldsymbol{q}$ for larger $|\boldsymbol{q}|$ is strongly affected by the FS anisotropy and the Stoner enhancement. Whereas for $\xi<1$, where only fm SF exist, $\Gamma(\boldsymbol{q})$ strongly increases with $\boldsymbol{q}$, in the coexistence region of fm and afm SF $(1<\xi<2)$ the damping shows a remarkably smaller variation with $\boldsymbol{q}$. In this region of our model it is possible to find values of ξ and S for which $\Gamma(\boldsymbol{q})$ is nearly constant in a major part of the $\boldsymbol{q}$ space. This behaviour is illustrated in Fig. 3 for the choice $\xi=1.9$ and $S=6.5$ which we use hereafter. Equating the upper bounds of the temperature ranges of validity of the $T^3 \ln T$ law due to shorter-wavelength SF (obtained from $-\Delta J$) and localised paramagnons we get $\Gamma/\bar{T}_F=0.34$. This constant is shown in Fig. 3 (inset) as a dotted line and represents a reasonable mean value of $\Gamma(q)/\bar{T}_F$ down to $q_{/\!/c}\simeq 0.39$ corresponding to $q_c=0.2$. Accordingly, we calculate $-\Delta J$ with the lower cut-off $q_c=0.2$ (instead of $q_c=0.05$) and obtain a very good agreement with the results found by Konno and Moriya,[3] as shown in Fig. 2. In particular, the temperature range for the $T^3 \ln T$ law is given by $0.8\Gamma/2\pi < T < 3\Gamma/2\pi$.

In conclusion, we have clarified the role played by arbitrary-wavevector components of SF in the different $T^3 \ln T$ contributions to C_v. Moreover, using our model we have given some microscopic understanding of the localised-paramagnon model. Note that the (almost) localised-paramagnon picture in the small-$|\boldsymbol{q}|$ region (as indicated by neutron-scattering on UPt_3) cannot be reproduced microscopically by single-band paramagnon models ($\Gamma(q)\propto|\boldsymbol{q}|$), but, maybe, by two-band models including spin-flip scattering (see discussions and references in I).

The authors are grateful to the Physical Society of Japan for financial support in publication.

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