Anisotropic quantum critical behavior in $CeCoGe_{3-x}Si_x$

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The intermetallic compound $CeCoGe_{2.25}Si_{0.75}$ has an antiferromagnetic transition at $T_N = 5.5$ K. Hydrostatic pressure decreases the Neel temperature and drives this system to a quantum critical point (QCP). We characterize this approach to the QCP using electrical resistivity measurements. For $T < T_N$ the resistivity is dominated by electron-magnon scattering and this allows to obtain the pressure variation of the spin-wave gap and of the spin-wave velocity. We find that for a significant range of pressure close to the QCP, the gap and the Neel temperature decrease with pressure while the velocity remains constant. We obtain the relevant magnetic parameters from the electrical measurements and discuss the implications of our results within a model that emphasizes the importance of two-dimensional fluctuations.

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I. INTRODUCTION

Much progress has been made in understanding the properties of metallic systems near a quantum critical point (QCP).[1,2] Most of the recent investigations have concentrated on the non-Fermi liquid regime, with the system just at the QCP. In this case the temperature dependence of several physical quantities is obtained and compared with the predictions of different models. These studies have revealed that in a surprising number of heavy fermions, two-dimensional fluctuations play an important role in determining the quantum critical behavior.[3] On the other hand, studies in the long-range ordered magnetic phase have been limited to obtain the shape of the critical Neel line, as a function of pressure, close to the QCP. A common strategy is to choose a system with small Neel temperature and apply pressure to drive it to the QCP. This allows for a determination of the shift exponent ψ, defined through, $T_N \propto |\delta|^{\psi}$, where $\delta = P - P_c$ with P_c the critical pressure. The usual signatures of the importance of two-dimensional fluctuations are: a critical line that vanishes linearly close to the QCP, i.e., $\psi = 1$, and a specific heat, $C/T \propto \ln T$ at $P = P_c$.[3]

In this Report we shall concentrate on the region to the left of the QCP, i.e., on the magnetic long-range ordered part of the Doniach phase diagram. Despite there being clear indication for scaling behavior in this magnetic side, as illustrated in Fig. 1,[4] no systematic study has been performed in this region. Our aim here is to obtain and follow the modifications on the nature of the spectrum of magnetic excitations in the ordered antiferromagnetic phase as T_N is reduced by the pressure. In order to carry out this program we rely on electrical transport measurements under pressure. The present analysis is possible since electron-magnon scattering is the basic mechanism responsible for the temperature dependence of the resistivity of our compound.[5] Through the fits of the resistance vs temperature, $R(T)$ curves, we are able to determine the main parameters of the magnon spectrum. In our system, and quite generally for antiferromagnets, this assumes the *relativistic* form,[6]

$$\omega = \sqrt{\Delta^2 + D^2 k^2}. \tag{1}$$

The quantity Δ is the spin-wave gap, which arises from anisotropy either in the magnetic interactions, or of the single-

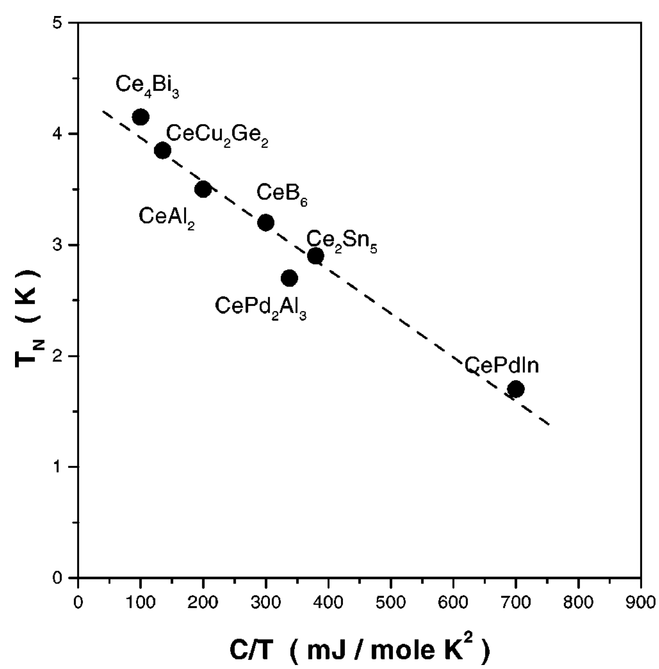

FIG. 1. The ordering temperature T_N versus the coefficient C/T of the linear term of the specific heat for some heavy fermions. As T_N decreases, C/T increases. The line is a guide to the eyes. The data is taken from Ref. 4.

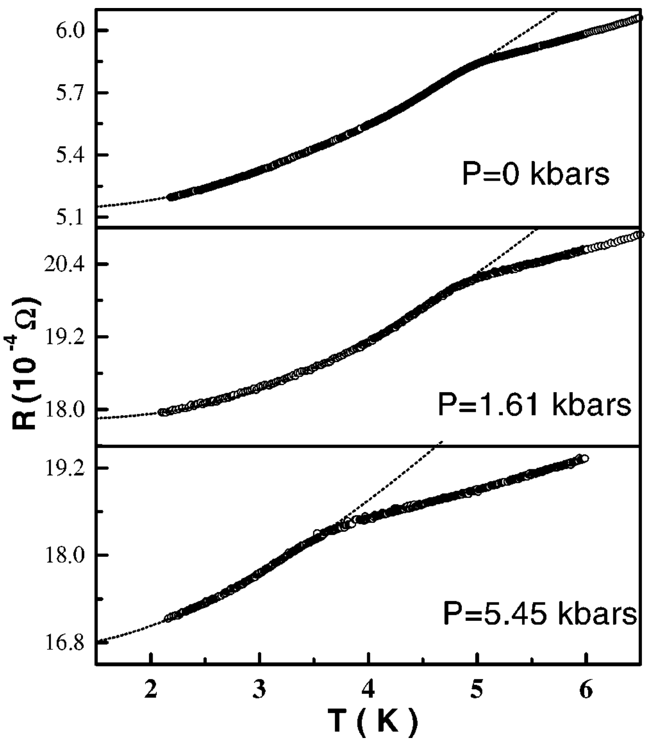

FIG. 2. Low-temperature resistance curves of $CeCoGe_{2.25}Si_{0.75}$ at different pressures. The lines correspond to fits using the expression given in the text and data for $T<0.65T_N$. For $P=8.5$ kbars the resistance varies linearly with temperature in the range investigated suggesting that for this pressure the systems is at or above the critical pressure.

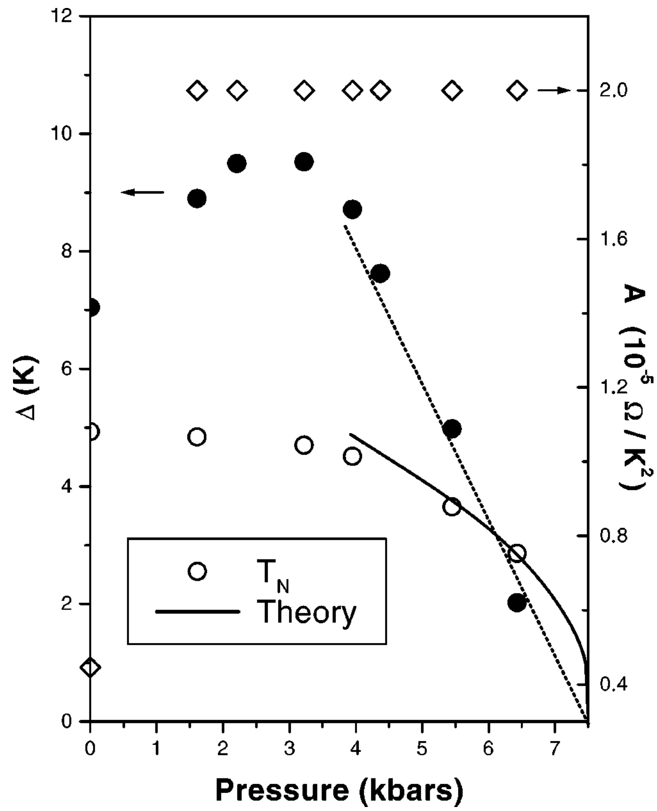

FIG. 3. Parameters obtained from the fits of the resistance curves at different pressures. Δ is the spin-wave gap, the quantity $A \propto (1/D^3)$, where D is the spin-wave velocity and T_N the Neel temperature. All these quantities are extracted from the transport data. The solid theoretical curve for T_N is obtained from the behavior of the gap described by the linear dashed line and Eq. (4) with $\Gamma/k_B=3.9$ K taken as constant.

ion type and D is the spin-wave velocity. Note that in the absence of the gap, the spectrum is linear in wave vector.

II. EXPERIMENTAL RESULTS AND ANALYSIS

$CeCoGe_{2.25}Si_{0.75}$ is an antiferromagnet with a Neel temperature, $T_N=5.5$ K.[7] This is a *layered* compound with tetragonal lattice parameters (for $x=0$), $a=4.319$ Å and $c=9829$ Å [Ref. 8] and we may expect that two-dimensional (2D) magnetic fluctuations play an important role in this system. The $R(T)$ curves of this compound for different pressures are shown in Fig. 2.[5] These measurements allow for a straightforward determination of the critical Neel temperatures. These show up as a break in the resistance curves or, more precisely, as a minimum in the second derivative, (d^2R/dT^2). The dashed lines in Fig. 2, represent theoretical fits using the equation,[5]

$$R(T)=R_0+A\Delta^{3/2}T^{1/2}e^{-\Delta/T}\left[1+\frac{2}{3}\left(\frac{T}{\Delta}\right)+\frac{2}{15}\left(\frac{T}{\Delta}\right)^2\right].$$

This expression is based on the scattering of conduction electrons by antiferromagnetic magnons with the dispersion relation given by Eq. (1). It holds for temperatures smaller than the spin-wave gap, i.e., $k_BT<\Delta$ and although only data below $\approx 0.65T_N$ has been used to determine the parameters of the fit, it describes the data in all the temperature region below T_N. This is not the case if we consider just a power-law dependence for $R(T)$. The coefficient A in the equation above is related to the spin-wave velocity D by, $A \propto 1/D^3$ or $A \propto 1/\Gamma^3$, where Γ is an effective magnetic coupling between the Ce ions. From the fit of the resistance curves for different pressures we can extract the three parameters $R_0(P)$, $A(P)$, and the spin-wave gap $\Delta(P)$. The last two are shown in Fig. 3, together with $T_N(P)$ also obtained from the transport data.

We point out that the contribution of the antiferromagnetic magnons, which scatter the conduction electrons, to the specific heat can also be easily calculated. It is given by, $C_{mag}=C\Delta^{7/2}T^{1/2}e^{-\Delta/T}[1+(39/20)(T/\Delta)+(51/32)(T/\Delta)^2]$ where the constant $C \propto 1/D^3$. This expression together with a linear temperature-dependent contribution due to the heavy electrons, i.e., $C/T=\gamma+C_{mag}/T$, fits very well the low temperature, $T \leqslant 0.65T_N$, specific heat data of Eom *et al.*[7] for the same compound, with $x=0.75$ and for that with $x=0.9$ as shown in Fig. 4. In particular the spin-wave gap for $x=0.75$, extracted from the specific heat data, $\Delta/k_B=7$ K is in excellent agreement with that obtained from the resistance.[5] For $x=0.9$, we get, $\Delta/k_B=8.9$ K.[5] Notice that this increase of the gap for the $x=0.9$ with respect to the $x=0.75$ compound is consistent with the results in Fig. 3, as the former system corresponds to the latter in an applied pressure that we estimate to be $P_{equiv}\approx 4$ kbars (see Fig. 3).

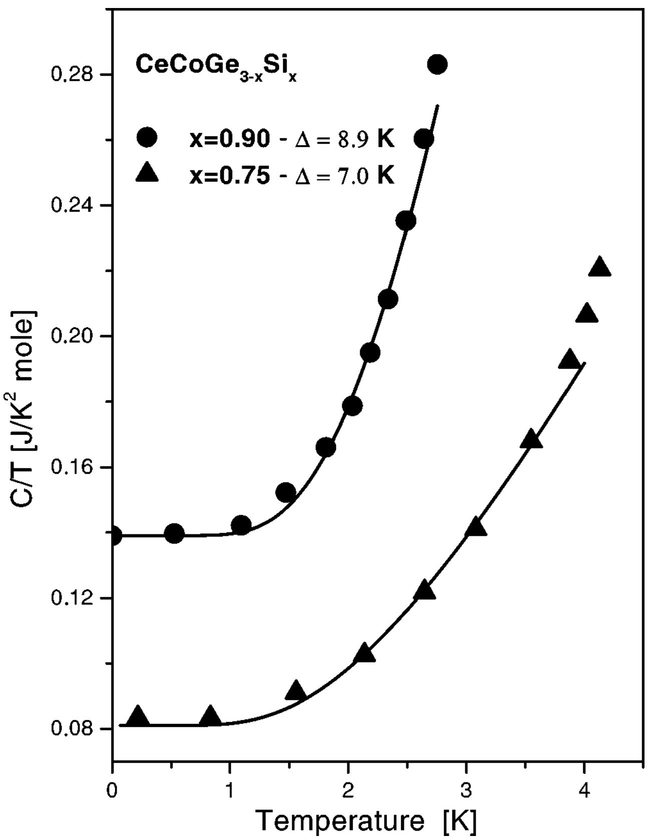

FIG. 4. Specific heat data of Eom *et al.*[7] for the $x=0.75$ and $x=0.9$ compounds and the fits using the equation for the specific heat given in the text. For $x=0.75$, $T_N=5.5$ K, $\gamma=81$ mJ/mole K^2 and for $x=0.9$, $T_N=4.0$ K, $\gamma=139$ mJ/mole K^2 (see text and Ref. 7).

III. DISCUSSION

Figure 3 reveals some unexpected results. As the critical Neel temperature is reduced by pressure, the quantity A remains nearly constant while the gap above a certain pressure has a pronounced decrease with pressure. This behavior seems to imply that the reduction of the Neel temperature with increasing pressure is correlated to that of the spin-wave gap . Within a spin-wave theory, for an antiferromagnet with magnons described by the dispersion relation, Eq. (1), it is easy to show that the critical temperature is given by

$$\frac{(S+1/2)\Gamma}{k_B T_N}=\frac{1}{N}\sum_k \frac{1+\alpha}{\alpha^2+2\alpha+(1-\gamma_k^2)}, \tag{2}$$

where Γ is an effective coupling between local moments of spin S, directly proportional to the velocity D. For a 3D cubic system with nearest-neighbor interactions we obtain, $\Gamma=\sqrt{3}(D/a)$ where a is the nearest-neighbor distance. The quantity α is essentially the ratio between the part of the Hamiltonian that leads to a magnetic stiffness and the anisotropy responsible for the gap. It is given by

$$1+\alpha=\sqrt{1+\left(\frac{\Delta}{\Gamma}\right)^2}.$$

The k-dependent term, $\gamma_k=(1/r)\Sigma_k e^{i\vec{k}\cdot\vec{\delta}}$, where r is the effective number of neighbors.

For a $3D$ system and $S=1/2$, a straightforward calculation leads to

$$k_B T_N=\frac{\Gamma}{2\sqrt{1+\left(\frac{\Delta}{\Gamma}\right)^2}\left[1-\frac{\sqrt{3}}{\pi}\frac{\Delta}{\Gamma}\arctan\left(\frac{\pi\Gamma}{\sqrt{3}\Delta}\right)\right]}. \tag{3}$$

Note that even in the absence of anisotropy, $\Delta=0$, there is a finite Neel temperature, $k_B T_N=(1/2)\Gamma$.

It will turn out important for our analysis to consider also the two-dimensional case in view of the layered structure of our compound. For a $d=2$ system there is long-range order at finite temperatures only in the presence of a spin-wave gap. The critical temperature is given by

$$k_B T_N=\frac{2(S+1/2)\Gamma}{\sqrt{1+(\Delta/\Gamma)^2}\ln\left[1+\frac{\pi^2}{2(\Delta/\Gamma)^2}\right]}, \tag{4}$$

where for a square lattice, $\Gamma=\sqrt{2}(D/a)$, with a the nearest-neighbor distance. Notice that as $\Delta\rightarrow 0$, the Neel temperature vanishes, as expected for an isotropic system in $d=2$.

We have used Eqs. (3) and (4) to calculate the effective coupling Γ, above approximately 4 kbars, in the following way. We obtain the gap ($\Delta/k_B=5.0$ K) and Neel temperature ($T_N=3.7$ K) from the transport measurements at a given pressure ($P=5.5$ kbars), and using Eqs. (3) and (4), we determine $\Gamma/k_B=3.9$ K for the 3D case and $\Gamma/k_B=4.4$ K in 2D where we took $S=1/2$. These turn out to be physically reasonable values for the effective magnetic coupling in this compound and do not allow to discriminate between the 2D or 3D results. Note that, since we have found the velocity D to be pressure independent, the effective coupling $\Gamma\propto(D/a)$ in fact increases with pressure since the average nearest-neighbor distance decreases with pressure.[7] This increase is consistent with Doniach's phase diagram for heavy fermions and the approach to the QCP, although our results indicate that the variation of Γ is small[9] to account for any significant variation of T_N as given by Eqs. (4) and (3). In particular if the trend in the pressure dependence of the quantities, $A(P)$ and $\Delta(P)$ is maintained up to the quantum critical point, the simple spin-wave expression for T_N in the 3D case, can never account for the vanishing of the critical temperature at the quantum critical point. This is not the case if the system is governed by two-dimensional fluctuations. The critical behavior in this case is controlled by that of the spin-wave gap and even if the effective coupling increases, the Neel temperature decreases as the gap vanishes with increasing pressure.

For the $d=2$ case, the shape of the critical line close to P_c can be obtained using the expression for the gap corresponding to the dashed straight line in Fig. 3, which is described by the equation $\Delta(P)=2.25(P_c-P)$ (in Kelvins), with $P_c=7.5$ kbars. Using this expression for the gap and the previous, fixed value for Γ, in Eq. (4), we obtain the theoretical critical line shown in Fig. 3 for the two-dimensional case.

Note that we get a very sharp, nonalgebraic, drop of the critical line close to P_c, since $T_N(P) \propto 1/|\ln \Delta| \propto 1/|\ln(P_c - P)|$. If we fit the results for $T_N(P)$ with a power law, either with the mean-field exponent $\psi = 1/2$ or $\psi = z/(d+z-2) = 2/3$ as expected for a 3D nearly antiferromagnetic metal, we get values for P_c much larger than that for which the gap extrapolates to zero. Since the collapse of the critical line in the present approach is much faster than a power law, the present mechanism of a soft gap and two-dimensional spin-wave excitations is a candidate to account for the behavior of $T_N(P)$ in $CeRh_2Si_2$ [Ref. 10] and other antiferromagnetic heavy-fermion systems where the drop of T_N close to P_c is very abrupt.

For completeness let us point out that at a pressure of 8.6 kbars, the resistance varies linearly with temperature down to the lowest temperatures of our experiments indicating that at this pressure the system is or has gone through the quantum critical point.

Notice that the present analysis assumes that the local moments of the Ce ions remain unquenched down to the QCP. This assumption is supported by studies in another heavy fermion that show that local moments persist even at the QCP.[11]

Equations (3) and (4) were used on the analysis of the parameters obtained from the resistance data for pressures above ≈ 4 kbars. Below this pressure the behavior of these parameters is anomalous. In particular the sharp rise of the quantity A in Fig. 3 may be related to a pressure effect on the two magnetic transitions existing in the parent compound that merge close to the concentration of the material studied here.[7,8] Note also that the increase in the gap at low pressures is consistent with the specific heat data of Fig. 4. In case 3D fluctuations are dominant at these pressures, it is possible to reconcile this small increase of the gap at low pressures without an accompanying variation of the critical temperature.

IV. CONCLUSIONS

The temperature dependence of the resistance of the compound $CeCoGe_{2.25}Si_{0.75}$ is determined by electron-magnon scattering. From the transport measurements it is possible to obtain the variation with pressure of the Neel temperature, the spin-wave velocity and the gap in the spectrum of these modes. Above a certain pressure we find that the gap decreases with pressure and this is accompanied by a reduction of the critical temperature even though the effective coupling $\Gamma \propto (D/a)$ is increasing due to the decrease of the lattice parameters. This correlation between the Neel temperature and the spin-wave gap suggests that, in the pressure range close to the QCP, the system is dominated by two-dimensional fluctuations and it is the presence of the gap that guarantees the existence of long-range magnetic order close to P_c. The approach presented here raises several important questions. First, how close to the QCP does the spin-wave theory holds? Second, which is the mechanism that makes two-dimensional fluctuations so crucial while at the same time the system becomes more isotropic, in the sense of the softening of the gap, as the QCP is approached. We hope further studies will be able to elucidate these intriguing questions.

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[1] See *Proceedings of the 1999 Conference on Strongly Correlated Systems (SCES-99), Nagano* [Physica B **281&282** (2000)].

[2] See *Proceedings of the Symposium on Strongly Correlated Systems (SCES-2000)* [J. Mag. Magn. Mater. (to be published 2001)].

[3] N.D. Mathur, F.M. Grosche, S.R. Julian, I.R. Walker, D.M. Freye, R.K.W. Haselwimmer, and G.G. Lonzarich, Nature (London) **394**, 39 (1998).

[4] B. Coqblin, J. Arispe, J.R. Iglesias, C. Lacroix, and K. Le Hur, J. Phys. Soc. Jpn. **65**, Suppl. B, 64 (1996).

[5] S.N. Medeiros, M.A. Continentino, M.T.D. Orlando, M.B. Fontes, E.M. Baggio-Saitovitch, A. Rosch, and A. Eischler, Physica B **281&282**, 340 (2000).

[6] F. Keffer, in *Encyclopedia of Physics*, edited by S. Flügge (Springer-Verlag, Berlin, 1966), Vol. XVIII, Pt. 2, p. 162.

[7] D. Eom, M. Ishikawa, J. Kitagawa, and N. Takeda, J. Phys. Soc. Jpn. **67**, 1998 (2495).

[8] V.K. Pecharsky, O.-B Hyun, and K.A. Gschneidner, Jr., Phys. Rev. B **47**, 11 839 (1993).

[9] The variation of the lattice parameter with pressure is given by, $\Delta a/a = \Delta P/(3\kappa^{-1})$ with $\kappa^{-1} \approx 1$ Mbar [J.D. Thompson and J. M. Lawrence, in *Handbook on the Physics and Chemistry of Rare Earths*, edited by K.A. Gschneider, Jr., L. Eyring, G.H. Lander, and G.R. Choppin (Elsevier Science, 1994), Vol. 19, Chap. 133, p. 383].

[10] R. Movshovich *et al.*, Phys. Rev. B **53**, 8241 (1996).

[11] A. Schröder, G. Aeppli, R. Coldea, M. Adams, O. Stockert, H.v. Löhneysen, E. Bucher, R. Ramazashvili, and P. Coleman, Nature (London) **407**, 351 (2000).