Dispersion and damping of zone-boundary magnons in the noncentrosymmetric superconductor CePt$_3$Si

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Abstract

Inelastic neutron scattering (INS) is employed to study damped spin-wave excitations in the noncentrosymmetric heavy-fermion superconductor CePt$_3$Si along the antiferromagnetic Brillouin zone boundary in the low-temperature magnetically ordered state. Measurements along the ($\frac{1}{2} \frac{1}{2} L$) and ($H \frac{1}{2} \frac{1}{2} - H$) reciprocal-space directions reveal deviations in the spin-wave dispersion from the previously reported model. The broad asymmetric shape of the peaks in energy signifies strong spin-wave damping by interactions with the particle–hole continuum. Their energy width exhibits no evident anomalies as a function of momentum along the ($\frac{1}{2} \frac{1}{2} L$) direction which could be attributed to Fermi surface nesting effects, implying the absence of pronounced commensurate nesting vectors at the magnetic zone boundary. In agreement with a previous study, we find no signatures of the superconducting transition in the magnetic excitation spectrum, such as a magnetic resonant mode or a superconducting spin gap, either at the magnetic ordering wavevector ($0 0 \frac{1}{2}$) or at the zone boundary. However, the low superconducting transition temperature in this material still leaves the possibility of such features being weak and therefore hidden below the incoherent background at energies $\lesssim 0.1$ meV, precluding their detection by INS.

(Some figures may appear in colour only in the online journal)

1. Introduction

Unconventional superconductivity in the noncentrosymmetric heavy-fermion superconductor CePt$_3$Si [1, 2] emerges below $T_c = 0.46$ K [3, 4] out of an antiferromagnetically (AFM) ordered metallic phase [5]. It has been suggested that the lack of inversion symmetry mixes the spin-singlet and spin-triplet superconducting pairing channels, leading to an exotic ground state with an $s + p$-wave symmetry of the order parameter [6, 7], supported by recent experimental evidence [8–10]. An intense discussion about the details of such pairing is underway, in particular concerning the relative magnitude of the singlet and triplet contributions [7], and the role of the static AFM order and spin fluctuations for superconductivity [11]. A detailed knowledge of the spin excitation spectrum is indispensable to answer these questions.

Recently, in an extensive inelastic neutron scattering (INS) study [12], it was shown that Kondo-type spin
fluctuations are found in the vicinity of the AFM ordering wavevector (0 0 1/2) in the paramagnetic state.\footnote{Here and in the following, reciprocal-space vectors (HKL) are given in dimensionless reciprocal lattice units (r.l.u.), i.e. in units of the reciprocal lattice vectors 2π/a, 2π/b and 2π/c, where a = b = 4.072 Å and c = 5.450 Å are low-temperature lattice constants, as determined during sample alignment.} Below the Néel transition temperature, T_N = 2.2 K, these fluctuations give way to damped spin waves, persisting in a wide range of momenta in the (H 0 L) plane of the reciprocal space. Their dispersion has been successfully parameterized by an effective Heisenberg-type model that involves five principal exchange integrals between localized Ce moments \footnote{Incoherent scattering intensity from the sample for different k_f, fitted with Voigt profiles.}. However, the effects of spin-wave damping via coupling to the continuum of particle–hole excitations across the Fermi level have so far been neglected.

The Fermi surface of CePt_3Si, evaluated from both band structure calculations and quantum-oscillation measurements \footnote{2. Description of the sample and experimental conditions}, suggests a possible presence of several nesting vectors \footnote{Second-order neutrons were eliminated by a cold Be-filter placed between the sample and the analyzer. To maximize the intensity, no collimation was used.} that could lead to enhanced spin-wave damping or softening of the spin excitation energies at certain nearly commensurate wavevectors at the Brillouin zone (BZ) boundary. Such anomalies, if found, could serve as a direct probe of particle–hole scattering and, hence, would shed light on the Fermi surface geometry and electron correlations in this material. This argument motivated our present study.

3. Magnons in the magnetically ordered state

In figure 3, we show a series of energy scans measured at different zone-boundary wavevectors (1/2 1/2 L), spanning the irreducible part of the BZ between L = 0 and 1/2. Panel (a) shows the raw data, whereas panel (b) results from a subtraction of the incoherent scattering background, fitted to the Voigt profile (figure 2), whose extrapolation is given by the solid line in figure 3(a). The strongly asymmetric lineshape of the resulting magnetic signal could not be well fitted by the damped harmonic oscillator model (possibly due to a resolution effect). Therefore, an empirical fit shown by solid lines in figure 3(b), which includes a constant background offset shared by all curves, was used. The resulting magnon dispersion (defined here by the positions of the peak maxima) in the (HHL) scattering plane, as shown in figure 1. The overall mosaicity of the sample, measured at half maximum of the (110) and (002) Bragg peaks, was better than 1°. We used a 3He dilution insert to cool the sample down to 80 mK. The triple-axis cold-neutron spectrometer IN14 was operated in the ‘W’-geometry in the constant-k_f mode, with focusing applied to both the monochromator and the analyzer. Second-order neutrons were eliminated by a cold Be-filter placed between the sample and the analyzer. To maximize the intensity, no collimation was used.

The energy profiles of the incoherent scattering intensity from the sample, measured at Q = (0.4 0.4 0) for three values of the final neutron momentum, k_f = 1.55, 1.3 and 1.15 Å\(^{-1}\) (figure 2), can be well fitted with the Voigt function, yielding full widths of the energy resolution at half maximum (FWHM) of 0.20, 0.10 and 0.077 meV, respectively. The Lorentzian contribution to the peak width, w_L = 0.015 meV, was found to be independent of k_f within the accuracy of the fit. Its long ‘tails’, dominating the incoherent background at low energies, led us to the choice of k_f = 1.55 Å\(^{-1}\) throughout the experiment as a compromise between the energy resolution and the signal-to-noise ratio.

Figure 1. Mounting of the single-crystalline CePt_3Si ingots for low-temperature INS measurements in the (H H L) scattering plane. The copper sample holder (bottom) is shielded with Cd foil.

Figure 2. Incoherent scattering intensity from the sample for different k_f, fitted with Voigt profiles.
Figure 3. Evolution of the magnon intensity along the $(\frac{1}{2} \frac{1}{2} L)$ BZ boundary, measured at $T = 80$ mK. (a) Raw energy scans measured in the magnetically ordered state at different wavevectors, as indicated in the legend. (b) The same after subtraction of the Voigt-shaped incoherent background. The solid lines result from a global fit to an empirical model. (c) Dispersion (top) and half width (bottom) of the peak that resulted from the fit shown in panel (b). The solid and dotted lines are guides to the eyes. The model of Fåk et al [12] is shown by the dashed line for comparison.

Figure 4. The magnon dispersion along the $(H H \frac{1}{2} H)$ direction, measured at $T = 0.8$ K. (a) Energy scans after subtraction of the Voigt-shaped incoherent background. (b) Dispersion of the peak maximum. The spin-wave model of Fåk et al [12] is shown by the dashed line for comparison. The solid lines are guides to the eyes.

and the half width at half maximum (HWHM) of the peak, related to the magnon lifetime, are shown in figure 3 (c). Here, the solid line is given by the fit of the experimental dispersion to a sum of sinusoidal functions, whereas the dashed black line shows the dispersion given by the spin-wave model of Fåk et al [12] along the same reciprocal-space direction. One can see that the latter is characterized by a somewhat smaller amplitude as compared to the directly measured one.

A similar analysis of the magnon dispersion is presented in figure 4 for the $(H H \frac{1}{2} H)$ direction, which connects the AFM ordering wavevector $(0 0 \frac{1}{2})$ with the zone boundary at $(\frac{1}{2} \frac{1}{2} 0)$. These data were measured at $T = 0.8$ K > $T_c$, but since the spin-wave spectrum is insensitive to the SC transition, these experimental conditions are practically equivalent to those in figure 3. A fit of the experimental dispersion, shown in panel (b) by a solid line, exhibits a pronounced nonmonotonic behavior that deviates from the spin-wave model of [12] (dashed line) by up to 20%.

The strong variation in measured inelastic intensity between $L = 0$ and $1/2$ in both figures results from the momentum-dependent AFM structure factor, which is maximized at the AFM ordering wavevector $(0 0 \frac{1}{2})$ and becomes strongly reduced, but not vanishing, at $(\frac{1}{2} \frac{1}{2} 0)$. This periodic intensity modulation is shown in figure 5 after subtraction of the constant background, and can be approximated with a sum of the first- and second-harmonic sinusoidal functions of $L$ (solid line).

The same structure-factor modulation can also be seen in the color maps of the INS intensity that are shown in figures 6(a) and (b) for the $(H H \frac{1}{2} H)$ and $(\frac{1}{2} \frac{1}{2} L)$ reciprocal-space directions, respectively. The fits of the experimental dispersion (the same as in figures 3 and 4) are summarized here by solid lines and compared to the
Figure 5. $L$-dependence of the background-subtracted intensity at the peak maximum along $(\frac{1}{2} \frac{1}{2} 0)$, modulated due to the AFM structure factor. The empty symbols represent the directly measured intensity at $\omega = 1.43$ meV, whereas the solid symbols result from the amplitudes of the fits presented in figure 3(b). The least-squares fit (solid line) is given by the following periodic function:

$$I(L) = I_0 \left[ 1 - 0.827 \cos 2\pi L + 0.161 \cos 4\pi L \right].$$

model of Fåk et al [12] shown by dashed lines. In spite of the apparent differences between these two fits in both directions, the disparity always remains smaller than the intrinsic energy width of the overdamped signal. These color maps also demonstrate the absence of any pronounced additional branches of paramagnon excitations in the vicinity of $(\frac{1}{2} \frac{1}{2} 0)$ that could originate from the nested sections of the normal-state Fermi surface.

4. Superconducting state

In the unconventional heavy-fermion superconductor CeCoIn$_5$ ($T_c = 2.3$ K), a pronounced magnetic resonant mode, centered at $\sim 0.6$ meV, emerges below $T_c$ out of a weak and featureless normal-state spectrum [15]. This resonance is similar to the one found in high-$T_c$ cuprates [16] and iron pnictides [17], where it serves as the hallmark of a sign-changing superconducting order parameter. However, no such resonant enhancement has been reported either in the spin-triplet p-wave superconductor Sr$_2$RuO$_4$ [18] or in the earlier experiments on CePt$_3$Si [12] close to the magnetic ordering wavevector. We have therefore performed a comparison of the inelastic signal in CePt$_3$Si above and below $T_c$ to establish the absence of resonant effects both near the zone boundary at $(\frac{1}{2} \frac{1}{2} 0)$ and at the AFM propagation vector, $(0 0 \frac{1}{2})$. This comparison is presented in figure 7. Indeed, within the statistical error, the inelastic intensity remains unchanged between 800 mK ($> T_c$) and 70 mK ($< T_c$), in agreement with a previous report [12]. This can be best seen in the difference spectra in figure 7(b), which are indistinguishable from zero within the statistical uncertainty for both high-symmetry points. The larger error bars of the $Q = (0 0 \frac{1}{2})$ data points are explained by the intense ‘tails’ of the magnetic Bragg peak that persist at this AFM wavevector in the low-energy region. This observation cannot rule out a weak magnetic resonance at extremely low energies below 0.1 meV, which is plausible taking into account that the $T_c$ of CePt$_3$Si is a factor of six lower than in CeCoIn$_5$. Such a scenario would render it practically unobservable to INS due to the high level of incoherent scattering background at these low energies. We also cannot rule out the possibility of a resonant mode located at an incommensurate wavevector not covered by the present and previous studies, although this alternative would be rather unusual.

5. Conclusions

In conclusion, our experiments revealed no additional branches of paramagnetic excitations along the $(\frac{1}{2} \frac{1}{2} L)$ direction, apart from the strongly damped spin-wave modes,
and found a nearly constant intrinsic line width of the spin-wave excitations without pronounced anomalies. These observations point to the absence of strong nesting vectors in the Fermi surface of CePt$_3$Si along the zone boundary.

The strong damping of spin-wave excitations in the magnetically ordered state results in peak widths of the order of the spin-wave energies, leading to the failure of the conventional damped-oscillator model to describe the spectral line shape appropriately. This questions the applicability of localized Heisenberg-type models for the description of the spin-wave spectrum in this metallic system, as in such a case the spin-wave energies are no longer well defined except in the immediate vicinity of the magnetic Bragg reflections.

Deviations of up to 20% in the dispersion of the peak maximum from the previously constructed Heisenberg-type model are found, but this disparity remains smaller than the intrinsic energy width of the peak.

We also found no anomalies in the INS signal across the superconducting transition, which essentially excludes the possibility of an intense commensurate resonant mode at the AFM wavevector, similar to the one found in CeCoIn$_5$ [15]. Yet, a weak resonance at an extremely low energy or at an incommensurate $Q$ vector would still be consistent with our results.

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