Nuclear Quadrupole Resonance in the Heavy Fermion Antiferromagnet CePt$_2$In$_7$

N apRoberts-Warren, A P Dioguardi, A C Shockley, C H Lin, J Crocker, P Klavins and N J Curro

Department of Physics, University of California, Davis, CA 95616 USA

naprobertswarren@ucdavis.edu

New $^{115}$In NQR data is presented for the 9/2 $\leftrightarrow$ 7/2 of the In(2) site transition in the heavy fermion compound CePt$_2$In$_7$. We extract the sub-lattice magnetization in the antiferromagnetic state. The spectra reveal that roughly half of the In(2) sites experience no static hyperfine field.

1. Introduction

In the conventional BCS theory of superconductivity, magnetic atoms tend to destabilize the superconducting ground state. It is therefore surprising that several new classes of superconductors, including the Heavy Fermion (HF) and High Temperature Superconducting Cuprate (HTSC) materials, exhibit phase diagrams with adjacent superconducting and antiferromagnetic (AFM) regimes. The discovery of superconductivity under pressure in cubic HF CeIn$_3$ [1,2] and the enhanced $T_c$'s in the tetragonal CeMIn$_5$ class hints at the important role of reduced dimensionality for unconventional superconductivity. In the CeMIn$_5$ family, MIn$_2$ planar squares are interleaved between the Ce-In planes. This expands the bond length c/a ratio to $\sim$1.6, reducing the dimensionality and enhancing $T_c$ by an order of magnitude. The so-called 115 materials exhibit a rich spectrum of behavior, from ambient pressure superconductivity in CeCoIn$_5$ [4] to incommensurate long-range AFM ordering in CeRhIn$_5$ [5]. Furthermore, the phase diagrams for both CeIn$_5$ and CeRhIn$_5$ reveal co-existence of superconductivity and magnetic order [6]. This proximity of superconductivity to antiferromagnetism in anisotropic crystal structures continues to attract significant attention.

CePt$_2$In$_7$ is another member of the Ce-In heavy fermion family [7,8]. It crystallizes in the $I4/mmm$ space group with unit cell parameters $a = 4.602$ Å and $c = 21.601$ Å, increasing the spacing between

![Figure 1. the unit cell of CePt$_2$In$_7$](image)
the Ce-In planes by 43% from CeRhIn₅. This material exhibits has the classic signature of a Heavy Fermion: an enhanced Sommerfeld coefficient of 450 mJ/mol ◦K at low temperature, and an effective moment μ = 2.41μ₈ consistent with Ce³⁺. At ambient pressure, CePt₂In₇ undergoes a paramagnetic to AFM phase transition at Tₐ = 5.2 K, and resistance experiments under pressure revealed clear evidence of a superconducting transition of Tc = 1 K at 2.3 GPa [8]. In this paper we present NQR data on the sub-lattice magnetization at ambient pressure.

2. Experimental Procedure

High quality crystalline samples were obtained by arc-melting the atoms Ce, Pt, and In together in the ratio 1:2:7. The resulting pellet was then wrapped in Ta foil and sealed under vacuum in a quartz ampoule. The ampoule was then placed in an oven and annealed for several days. Upon cracking the Ta envelope, regular crystallite formation was observed. The CePt₂In₇ crystallites were subjected to powder x-ray diffraction in a Siemens Diffraktometer to verify the crystal structure, and heat capacity and resistance measurements confirmed the onset of magnetic order at Tₐ = 5.2 K. No impurity peaks (such as the AFM transition for CeIn₃ at 10.2 K) were observed in the transport measurements, again verifying the high-quality of the sample (x-ray diffraction identified < 3% impurity phase).

3. ¹¹⁵In NQR

CePt₂In₇ is ideal for NQR measurements because there are three distinct crystallographic In sites. NQR spectra were obtained at the the 9.5 MHz transition of the In(2) site between 6 K and 1.5 K. Spin echoes were obtained as function of frequency, and the echo integral is plotted in Figure 3c.

The nuclear spin Hamiltonian is

$$ H = γ h \vec{H}_{\text{int}} \cdot \vec{I} + \hbar \nu_Q / 6 (3 I_Z^2 - I^2 + \eta (I_X^2 - I_Y^2)) $$

where \( \hbar \nu_Q = 3eQV_{zz}/2(2I-1) \) is the quadrupolar splitting frequency, \( V_{zz} \) is the electric field gradient (EFG) along the principal axis and \( \eta \) is the axial asymmetry parameter and \( \vec{H}_{\text{int}} \) is the static internal hyperfine field from the ordered Ce moments. For In(2), \( \nu_Q = 2.5 \) MHz and \( \eta = 0.4 \). As seen in Figure 2, the 4\( \nu_Q \) resonance is split by the presence of an internal field. The splitting looks relatively well-defined from Tₐ down to 4 K; below this significant spectral weight develops again at 9.6 MHz, in addition to the two split peaks. The upper-frequency (right-hand) remains discernible all the way to 1.7 K, and provides an estimate of internal field at the In(2) site below Tₐ (see Figure 3a). It was then fit to the function

$$ H_{\text{int}}(T) = H_{\text{int}}^0 (1 - (T/T_N))^θ $$

![Figure 2. Evolution of In(2) NQR resonance through the AFM transition with gaussian fits (solid red lines) used to assess spectral weight attached to the 1.5 K spectra.](image-url)
with values $H_{\text{int}}^0 = 332.46 \text{ Oe}$ and $\beta = 0.22$, lower then the 3D mean-field result $\beta = 0.5$ (Figure 3a) [5].

4. Magnetic Structure
Several key pieces of information can be drawn from these spectra. The fact that the splitting is symmetric about the original resonance line indicates that the internal field lies parallel to the principal EFG axis, $\vec{q}$. A priori we do not know the direction of $\vec{q}$, however in the CeMIn$_5$ materials $\vec{q}$ lies in the ab plane and points towards the center of the unit cell at the In(2) sites. We assume that $\vec{q}$, and hence the internal field at the In(2) sites in CePt$_2$In$_7$, points in the ab plane. However, without a single crystal to examine the angular field dependence of the resonance line, we conclusively cannot determine the direction of $\vec{q}$. It is important to point out, however, that the In(2) site in the 115's is analogous to the In(3), not In(2), site in CePt$_2$In$_7$.

Surprisingly, at $\sim 4$ K, a new feature emerges between the two horns of the split resonance line. The spectral weight of this feature increases with decreasing temperature and reaches 40% by 1.5 K (see Fig 3c). The origin of this three-peaked structure remains unclear, but suggests a change in the magnetic ordering wave-vector. Such a transition has been observed before in the iron-arsenides [9] but no evidence of any phase change is seen in the transport property or specific heat measurements in CePt$_2$In$_7$.

In conclusion, we have measured the sublattice magnetization in CePt$_2$In$_7$ below $T_N$. The evolution of magnetic order at In(2) suggests commensurate magnetic order, yet the anomalous re-appearence of signal in the center remains unexplained. In order to determine the magnetic structure in this crystal, high-quality single crystals are necessary, which will enable angular field-dependent studies to ascertain the principal axes of the EFG and will also enable direct neutron scattering measurements.

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Figure 3. a) internal field at In(2) site below $T_N$, b) the NQR frequencies of the AFM satellites splitting and the appearance of the central signal, and c) the normalized area of the AFM satellites and anomalous signal
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