Probing Onset of Coherence in CeIrIn$_5$

A C Shockley, A P Dioguardi, N apRoberts-Warren, P Klavins, N J Curro
Physics Department, University of California Davis,
One Shields Ave Davis, CA, USA, 95616
E-mail: shockley@student.physics.ucdavis.edu

Abstract. We report $^{115}$In NMR measurements in the heavy fermion superconductor CeIrIn$_5$. The Knight shift for the symmetric In(1) site displays the same behaviour as the related material CeCoIn$_5$. Our results support the phenomenological two-fluid model proposed by Nakatsuji et al. Comparison to recent DMFT calculations for CeIrIn$_5$ further strengthens our conclusions.

1. Introduction
Since the discovery of the heavy fermion class of superconductors, scientists have been trying to understand their microscopic electronic behaviour. Among families such as the CeMIn$_5$ (M = Ir, Co, Rh) class, research focuses around what drives one compound, e.g. CeRhIn$_5$, to be anti-ferromagnetic [1] and another compound, e.g. CeIrIn$_5$ or CeCoIn$_5$, to be superconducting [2,3,4] at ambient pressure. The question remains open as these materials are notoriously difficult to model theoretically. Throughout this class, however, certain normal state properties appear to be universal. Nakatsuji et al [5] (henceforth NPF) proposed that this scaling behaviour could best be explained by a two-fluid model. At a temperature $T^*$, these compounds possess itinerant behaviour; the heavy-electron itinerant component, described by an order parameter $f(T/T^*)$, scales with $T^*$. This phenomenon is best illustrated by the Knight Shift anomaly. In this paper, we present data for the Knight Shift anomaly in CeIrIn$_5$ and compare this data with the behaviour of CeCoIn$_5$.

2. Knight Shift Anomaly
The Kondo lattice can be modelled as a lattice of local f-moments embedded in a sea of conduction electrons. In the two-fluid model proposed by NPF, a fraction of the f-moments, $f(T)$, delocalize below a temperature $T^*$ to form a coherent state with the conduction electrons much like in superfluid $^4$He. The magnetic system then has one component corresponding to the localized f-moments with susceptibility $\chi_{KI}$ and one component for the itinerant heavy-electrons with susceptibility $\chi_{HF}$.

$$\chi(T) = [1 - f(T)]\chi_{KI}(T) + f(T)\chi_{HF}(T)$$  \hspace{1cm} (1)

The total spin of the system is a combination of the localized f-moments and the conduction electron spins:

$$S_{tot} = \sum_l S^f(l) + \sum_l S^c(l)$$  \hspace{1cm} (2)

Published under licence by IOP Publishing Ltd
where $r_i$ is the location of the local f-moments and $r_l$ is the location of the itinerant component [6]. The susceptibility is represented by the correlation function of the spins so that the uniform susceptibility is:

$$
\chi = \chi_{ff} + 2\chi_{cf} + \chi_{cc} \approx \chi_{ff} + 2\chi_{cf} \quad (3)
$$

where $\chi_{ff} = 1/N \langle S_f(r_i)S_f(r_i') \rangle$ and $\chi_{cf} = 1/N \langle S_f(r_i)S_c(r_i) \rangle$ are the orbital resolved susceptibilities. Since the susceptibility from the background conduction electrons is small, we omit it to obtain the NPF result. In principle, these two components may have different temperature dependences.

In general, the hyperfine couplings to these two spin components will differ [6]. We write the hyperfine Hamiltonian as:

$$
\mathcal{H}_{hyp} = \gamma h \sum_i I(r_i) \cdot A \cdot S^c(r_i) + \gamma h \sum_i I(r_i) \cdot B \cdot S^f(r_i) \quad (4)
$$

where $A$ and $B$ are temperature independent contact and transferred hyperfine couplings, respectively, and $r_i$ are the locations of the nearest neighbour 4f sites. The Knight shift is related to the hyperfine couplings by

$$
K_\alpha(T) = K_{0,\alpha} + (A_\alpha + B_\alpha)\chi_{cf}(T) + B_\alpha\chi_{ff}(T) \quad (5)
$$

where $K_{0,\alpha}$ is an offset and we have dropped the summation over the neighbouring sites for simplicity. For $T>T^*$, we assume that $\chi_{cf}(T) \sim 0$ so that we can solve for the coupling constant $B$. Below $T^*$, $K_\alpha(T)$ and $\chi(T)$ are no longer proportional. $\chi_{cf}(T)$ and $\chi_{ff}(T)$ enter into $\chi(T)$ and $K_\alpha(T)$ with different weights due to the onset of coherence.

In order to investigate the onset of coherence, we have performed NMR measurements on a single crystal of CeIrIn$_5$. A 2x2x1 mm$^3$ single crystal was grown according to the standard growth

---

**Figure 1.** NMR spectrum for the In(1) site with $H \parallel c$ for the $I=3/2 \rightarrow 5/2$ transition measured with a field of 79.351kG. Spectra are shifted to correspond to the temperature at which they were measured.

**Figure 2.** The Knight Shift (represented as circles for $H \parallel c$ and triangles for $H \parallel ab$) and the magnetic susceptibility (represented as solid lines) are plotted as a function of temperature. The data for CeIrIn$_5$ are shown as solid blue for $H \parallel c$ and purple for $H \parallel ab$. The data for CeCoIn$_5$ are shown as empty pink for $H \parallel c$ and green for $H \parallel ab$ [8].
method [7] and acid-etched to remove excess metallic indium from the surface. CeIrIn₅ has two unique crystallographic In sites (I=9/2); we measured the axially symmetric In(1) site. In a Quantum Design PPMS, we acquired field-swept spectra with the crystalline c-axis oriented both perpendicular and parallel to the applied field. As a function of temperature, we measured the shift of the I=3/2 → 5/2 transition with an applied field of 79.351 kG parallel to the c-axis shown in Fig 1 and of 66.209 kG perpendicular to the c-axis.

The onset of coherence, T*, is manifest as a breakdown in the linear relationship between K and χ (see Figs 2, 3). For the field applied parallel to the c-axis, we found a hyperfine coupling constant of 25.6 ± 0.2 kG/μν from the linear fit shown in Fig 3. The contribution Kcf can be found by subtracting our data from the linear fit shown in Fig 4. To obtain a value for T*, we compare our data to the NPF model [9]:

\[ K_{cf} = K_{cf0}(1 - \frac{T}{T^*})^3(1 + \ln \frac{T}{T^*}) \]  

where K_{cf0} is a scaling factor. According to this model, T* for CeIrIn₅ is 34.9 ± 1 K.

3. Discussions and Conclusion

Recent work by Kambe et al on the Knight shift in CeIrIn₅ matches the trend of the data presented in this paper but yields a lower hyperfine coupling constant, B [10]. They argue that the two-fluid model gives unphysical results for the magnetic fluctuations measured by the anisotropy of the nuclear spin lattice relaxation rate (SLRR). On the other hand, a two-component analysis of the SLRR in CeCoIn₅ yields new insight into the origin of superconductivity in this system [11]. Based on the similar behaviours of both these materials as presented here, we would expect that the NPF model would either physically represent both CeIrIn₅ and CeCoIn₅ or neither. Currently, this question is still open to debate. In comparison with DMFT + LDA calculations for CeIrIn₅, a slow build-up of coherence is predicted as in the NPF approach [12]. In conclusion, the key to a microscopic understanding of the CeMIn₅ materials may be found by exploiting their similarities rather than highlighting their uniqueness.
Acknowledgments
The authors thank the Yukawa Institute for Theoretical Physics at Kyoto University. Discussions during the YITP workshop YITP-W-10-12 on “International and Interdisciplinary Workshop on Novel Phenomena in Integrated Complex Sciences: from Non-living to Living Systems” were useful to complete this work. The authors would also like to thank the conference organizers as well as ICAM/I2CAM for travel funding. We also thank Yi-Feng Yang and David Pines for enlightening discussions.

References
[1] H. Hegger, et al., Phys. Rev. Lett. 84 (2000) 4986.
[2] C. Petrovic et al., Europhys. Lett. 53 (2001) 354.
[3] C. Petrovic et al., J. Phys. Condens. Matter 13 (2001) L337.
[4] R Movshovic et al., Physica B 312-313, (2002) 7-12.
[5] S Nakatsuji et al., Phys. Rev. Lett. 92, 016401 (2004).
[6] NJ Curro et al., Phys. Rev. B 70, 235117 (2004).
[7] Moshopoulou et al., Journal of Solid State Chemistry, Vol 158, Issue 1, 2001, P 25-33.
[8] NJ Curro et al., Phys. Rev. B 64, 180514(R) (2001).
[9] Yi-Feng Yang and David Pines, PRL 100, 096404 (2008).
[10] S. Kambe et al., Phys. Rev. B 81, 140405(R) (2010).
[11] Yi-Feng Yang et al., PRL 103, 197004 (2009).
[12] JH Shim, K Haule and G Kotliar, Science 318, 1615 (2007).