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Inelastic magnetic neutron scattering in $CePd_3$

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Abstract

We have performed time-of-flight neutron scattering measurements on a single crystal of the intermediate valence compound $CePd_3$. At 10 K, a Kondo-esque inelastic magnetic scattering peak occurs near $\Delta E = 60$ meV with maximum intensity for momentum transfer Q near the $(\frac{1}{2}, \frac{1}{2}, 0)$ zone boundary. Spectral weight is transferred to lower energy as Q varies until at zone center the intensity at 60 meV is considerably weaker. These results are in qualitative accord with predictions of the Anderson lattice. The Q-dependence may resolve an older controversy concerning the low-temperature scattering. We discuss the relationship of these results to our recent results in $YbAl_3$.

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Keywords: Intermediate valence; Neutron scattering

There is a controversy concerning the inelastic magnetic scattering in the intermediate valence compound $CePd_3$. Murani et al. [1] argue that there is simply a broad Kondo-like feature near 60 meV, which is essentially the Kondo energy of this compound. Shapiro et al. [2] argue that there is a broad inelastic feature centered near 15 meV plus a quasielastic feature near 3–5 meV but no peak and only weak scattering at 60 meV.

In calculations [3] for the Anderson lattice, a (renormalized) energy gap due to hybridization of the 4f and conduction electrons arises at low temperature. The scattering across this hybridization gap has an energy scale equal to the Kondo temperature and is highly Q-dependent, having the greatest intensity for interband scattering at the indirect threshold. This occurs when $Q = Q_{BZ}$, i.e. the maximum intensity is for zone boundary Q.

We recently [4] observed this for the scattering near $\Delta E = 50$ meV in the intermediate valence compound $YbAl_3$. This energy scale is indeed the same as the Kondo temperature of that compound, and additionally, the intensity shows considerable variation with Q, having a maximum on the $K = \frac{1}{2}$, $L = \frac{1}{2}$ zone boundary face. Hence we believe that the spectra reflect threshold interband scattering across the hybridization gap.

In their $CePd_3$ experiments, Murani et al. utilized time-of-flight techniques, mostly on polycrystals, with broad Q-integration; hence the Q-dependence of the scattering was averaged over the Brillouin zone, for which the k-space volume would be heavily weighted near the zone boundary. Shapiro et al. used a triple axis spectrometer and a single crystal, but included essentially only one reduced Q-vector, (0.1, 0.1, 0), near zone center. Hence, the difference between their results may reflect Q-dependence of a similar origin as in $YbAl_3$.

To show this we measured time-of-flight spectra for a 20 g single crystal of $CePd_3$ (grown by the Czochralski method) on MAPS at the ISIS spallation source at

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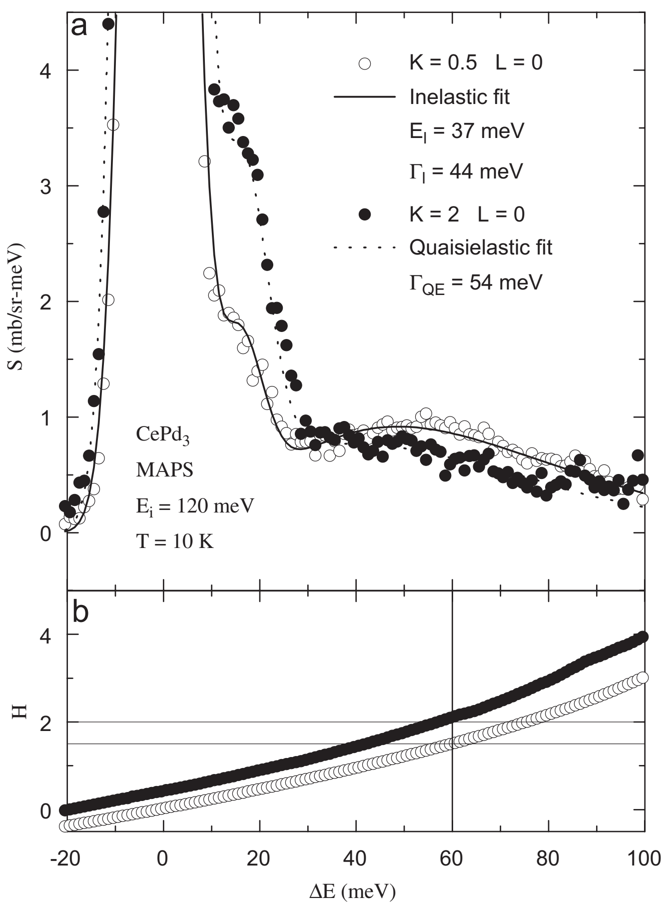

Fig. 1. The scattering intensity at 10 K in $CePd_3$ versus energy transfer at two values of (K, L), measured on MAPS using an initial energy of 120 meV. The Miller index H varies with energy transfer as shown. The lines are fits, as discussed in the text, with the parameters of the magnetic Lorentzian given in the plot.

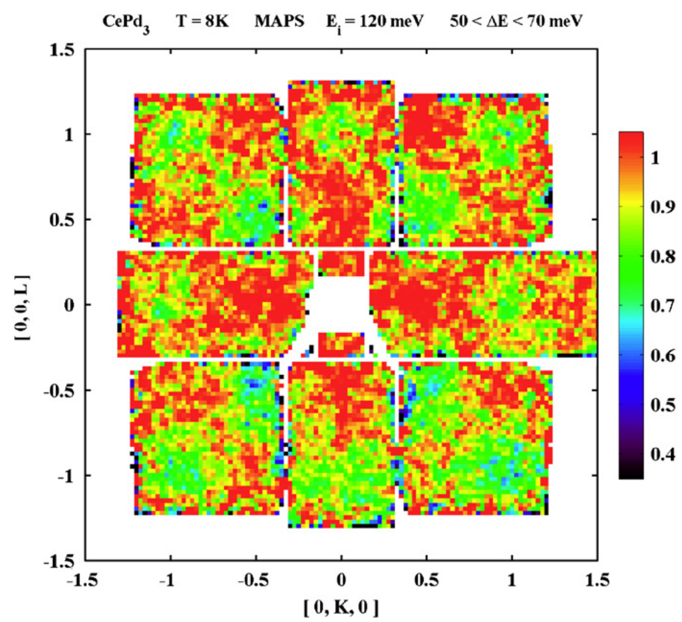

Fig. 2. Intensity versus reduced wavevector (K, L) for energy transfers in the range $50 < \Delta E < 70$ meV for data taken on $CePd_3$ at $T = 8$ K, using MAPS with $E_i = 120$ meV.

the Rutherford Appleton Laboratory. Fig. 1a shows the spectra for two scattering angles. For Miller indices $K = 0.5$, $L = 0$, the scattering exhibits an inelastic maximum near 60 meV that is very similar in shape and magnitude to that seen by Murani et al. [1]. For $K = 2$, $L = 0$, however, there is a transfer of spectral weight to lower energy. Fig. 2 shows that the scattering near 60 meV is modulated in the (K, L) plane, with maximum intensity near $K = 0.5$, $L = 0$. In these measurements the Miller index H varies with energy transfer as shown in Fig. 1b; for $\Delta E = 60$ meV, $(H, K, L) = (\frac{3}{2}, \frac{1}{2}, 0)$ for the open circles and (2, 2, 0) for the closed circles. Hence the scattering near 60 meV is strongest at the $(\frac{3}{2}, \frac{1}{2}, 0)$ zone boundary, and suppressed at the (2, 2, 0) zone center.

We have investigated the transfer of spectral weight from high to low energy in more detail by fitting the data as the sum of a Gaussian elastic peak, a single Gaussian peak centered near 17 meV with approximate width 5 meV representing the phonons [5], and a Lorentzian magnetic peak with the parameters Γ and E for the width and position as shown in the plot. On changing scattering condition from $K = 0.5$, $L = 0$ to $K = 2$, $L = 0$, the Lorentzian changes from inelastic to quasielastic. This transfer of spectral weight from higher to lower energy transfer is similar to the shift from the inelastic peak near 60 meV seen in the data of Murani et al. to the stronger low energy scattering seen in the data of Shapiro et al. While these results need to be improved using constant Q scans on a triple axis spectrometer, they clearly indicate that the reason for the discrepancy between the older results is the significant Q-dependence in the ground state magnetic scattering.

We also stress the similarity to the Q-dependence of the 50 meV peak seen in $YbAl_3$ [4]: in both cases, the Kondo-esque peak exhibits an intensity maximum at a zone boundary point. Hence, this appears to be a common feature of intermediate valence metals. It has also been observed in intermediate valence semiconductors (the so-called "Kondo insulators"); e.g. in YbB_{12}, the Kondo-esque scattering is maximal at the $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ zone boundary [6]. These results are clearly in qualitative accord with the predictions of the Anderson lattice, suggesting that the renormalized hybridization gap is an essential ingredient for understanding intermediate valence metals, as well as Kondo insulators.

Acknowledgments

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[4] A.D. Christianson, et al., Phys. Rev. Lett. 96 (2006) 117206.
[5] C.-K. Loong, et al., Phys. Rev. B 38 (1988) 7365 Given our energy resolution, the three optic phonons in the 15–20 meV range are modelled as a single phonon at 17 meV.
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