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2009 J. Phys.: Condens. Matter 21 322203

(http://iopscience.iop.org/0953-8984/21/32/322203)

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J. Phys.: Condens. Matter **21** (2009) 322203 (3pp) doi:10.1088/0953-8984/21/32/322203

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The effects of anisotropy and Yb–Yb interactions on the low-field electron spin resonance in $Yb_2Rh_2Si_2$ and $YbIr_2Si_2$

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Received 5 June 2009, in final form 10 June 2009
Published 23 July 2009
Online at stacks.iop.org/JPhysCM/21/322203

Abstract
The effect of anisotropy on the low-field electron spin resonance in the Kondo lattice compounds $YbRh_2Si_2$ and $YbIr_2Si_2$ is assessed. It is shown that the g-shift in $YbRh_2Si_2$ is a consequence of the anisotropy in the Yb–Yb interactions as mirrored in the molecular field parameters characterizing the resonant susceptibility. It is also pointed out that the large residual linewidth for $YbIr_2Si_2$ results from the modification of the Korringa contribution that occurs when the Curie susceptibility of the isolated ion is replaced by the resonant susceptibility with an experimentally determined molecular field parameter.

1. Introduction

The discovery of low-temperature electron spin resonance (ESR) in the heavy fermion metal $YbRh_2Si_2$ is important because it was the first observation of the ESR of a Kondo ion (Yb^{3+}) below the Kondo temperature (T_K) in a Kondo lattice system [1]. Subsequent studies have explored various aspects of the resonance including the effects Ge doping [2], the role of the residual linewidth [3], the local and itinerant properties of the ESR [4], and the anisotropy in the linewidth [5]. More recent studies have focused on field-dependent collective modes and the bottleneck-like behavior of the ESR spectra [6, 7].

The current theoretical situation can be summarized as follows. Krellner *et al* have pointed out that ESR in Kondo lattice systems is associated with the presence of ferromagnetic correlations [8]. Two alternative approaches to understanding the ESR have been developed. Abrahams and Wölfle based their analysis on a semi-phenomenological Fermi liquid description [9], whereas Schlottmann utilized a Kondo lattice model [10]. Experimental studies carried out in fields up to 8 T indicate that the Fermi liquid theory is applicable at high fields for experiments carried out above 2 K, whereas at low fields, $B < 1$ T, the Fermi liquid model breaks down above 2 K [11].

The theory outlined in [9] is based on a scalar interaction between the conduction electron spin and the fluctuating field that models the spin–lattice relaxation, whereas in [10], the interaction between the conduction electrons and the Kondo ions involves the scalar product of the electron spin and the pseudospin of the ground doublet. In contrast, the analysis in this work takes into account the anisotropies of the static and dynamic susceptibilities. The approach is based on an earlier theory of electron paramagnetic resonance in anisotropic magnets [12], which, in turn, is an application of a general approach to collective motion in many-particle systems developed by Mori [13].

2. Analysis

In this section, we apply the general theory developed in [12] to the case of a uniaxial system. We consider only the low-field limit where the magnetization is proportional to the applied field. When the static field is perpendicular to the c-axis, the corresponding g-factor, $g_\perp$, is expressed as

$$g_\perp(T) = g_c^0(\chi_\perp^{\mathrm{R}}(T)/\chi_\parallel^{\mathrm{R}}(T))^{1/2} \quad (1)$$

whereas when the static field is parallel to the c-axis we obtain the result

$$g_\parallel(T) = (g_a^{02}/g_c^0)(\chi_\parallel^{\mathrm{R}}(T)/\chi_\perp^{\mathrm{R}}(T)). \quad (2)$$

In equations (1) and (2) the symbols g_a^0 and g_c^0 designate the parameters that characterize the microscopic g-tensor and the superscript R refers to the resonant component of the static susceptibility. By resonant component, the contribution from the pseudospin doublet in resonance with the rf field is meant. At low temperatures, the contribution from the ground state doublet is often the dominant term. In situations where this is not the case, the resonant contribution must be separated out. Apart from a multiplicative factor, the resonant susceptibility along the direction of the rf field can usually be obtained by integration over the absorption line; in situations where the form of the non-resonant contribution is known, e.g. a constant, the resonant susceptibility can also be inferred by fitting the measured static susceptibility to the resonant term plus a constant. Specializing to a situation where the resonant static susceptibilities are of the antiferromagnetic, molecular field form, $\chi^R \sim C/(T+\theta)$, equation (1) reduces to

$$g_\perp(T) = g_c^0(C_\perp/C_\parallel)^{1/2}(1-(\theta_\perp-\theta_\parallel)/(T+\theta_\perp))^{1/2} \approx g_c^0(C_\perp/C_\parallel)^{1/2}(1-0.5(\theta_\perp-\theta_\parallel)/(T+\theta_\perp)) \quad (3)$$

assuming that the fractional shift is $\ll 1$. For $g_\parallel$ we find

$$g_\parallel(T) = (g_a^{02}/g_c^0)(C_\parallel/C_\perp)(1+(\theta_\perp-\theta_\parallel)/(T+\theta_\parallel)). \quad (4)$$

Equations (3) and (4) show that the shift in the g-factor is proportional to the resonant susceptibility along the direction of the applied field multiplied by a factor proportional to $\theta_\perp-\theta_\parallel$. Hence, it is a consequence of the anisotropy, vanishing in the limit of cubic symmetry. It is also evident that the shift in $g_\parallel$ is in the opposite direction from the shift in $g_\perp$, so when $\theta_\perp > \theta_\parallel$ the shift in $g_\perp$ is negative while the shift in $g_\parallel$ is positive.

The theory outlined in [12] also addresses the linewidth. At low fields, the linewidth $\Delta\omega$ ($\Delta\omega = g\mu_B\Delta B/\hbar$) with the static field perpendicular to the c-axis is the average of the zero-field rate along the c-axis and the zero-field rate in the basal plane; when the static field is along the c-axis, the linewidth is equal to the zero-field rate in the basal plane, i.e.

$$\Delta\omega_\perp = (1/2)(\Gamma_a+\Gamma_c) \quad (5)$$

$$\Delta\omega_\parallel = \Gamma_a. \quad (6)$$

From these equations, we see that the ratio $\Delta\omega_\parallel/\Delta\omega_\perp$ satisfies the inequality $0 < \Delta\omega_\parallel/\Delta\omega_\perp < 2$.

According to the general theory [13], the zero-field decay rates appropriate to the relaxation of the magnetization involve integrations over time of the relaxation functions for $\mathrm{d}M_a/\mathrm{d}t$ and $\mathrm{d}M_c/\mathrm{d}t$ divided by $T\chi_\perp^R$ and $T\chi_\parallel^R$, respectively. In the standard treatment of the Korringa linewidth for an impurity spin, the Curie susceptibility is appropriate. When Yb–Yb interactions are significant, the Curie susceptibility is replace by the molecular field susceptibilities, and the zero-field rates take the form

$$\Gamma_a^K = (\theta_\perp+T)f_a \quad (7)$$

and

$$\Gamma_c^K = (\theta_\parallel+T)f_c \quad (8)$$

where f_a and f_c are assumed to be temperature independent.

The analysis of the linewidth in uniaxial systems presented in [12] dealt only with the situations where the static field is parallel or perpendicular to the c-axis. An estimate of the width in the intermediate case, $\Delta\omega(\phi)$, can be obtained, giving the limiting frequencies $\omega_\perp$ and $\omega_\parallel$ small imaginary parts $\mathrm{i}\Delta\omega_\perp$ and $\mathrm{i}\Delta\omega_\parallel$. The width is then identified with the imaginary part of the expression

$$[(\omega_\perp+\mathrm{i}\Delta\omega_\perp)^2\sin^2\phi+(\omega_\parallel+\mathrm{i}\Delta\omega_\parallel)^2\cos^2\phi]^{1/2}$$

where ϕ is the angle between the static field and the c-axis. The resulting interpolation formula for $\Delta\omega(\phi)$ takes the form

$$\Delta\omega(\phi) = \frac{g_\perp\Delta\omega_\perp\sin^2\phi+g_\parallel\Delta\omega_\parallel\cos^2\phi}{(g_\perp^2\sin^2\phi+g_\parallel^2\cos^2\phi)^{1/2}}. \quad (9)$$

3. $YbRh_2Si_2$ and $YbIr_2Si_2$

The shift in the g-factor of $YbRh_2Si_2$ was analyzed in [7]. The approach followed was to fit the experimental susceptibility $\chi_\perp$ to the form const + $C_\perp/(\theta_\perp+T)$ over the temperature range 2 K $< T <$ 14 K. The value obtained for $\theta_\perp$, 1.48 K, which agrees with the value obtained from the temperature dependence of the integrated intensity in [5], was used in a two-parameter fit to the g-factor data using equation (3), with $\theta_\parallel$ and an overall multiplicative factor, $g_\perp^0$, as adjustable parameters. An excellent fit to the ESR data over the temperature range 4.2 K $< T <$ 14 K was obtained with the values $\theta_\parallel = 1.09$ K and $g_\perp^0 = 3.66$. As pointed out in [6], the g-shift reported in [1] is also proportional to the resonant susceptibility and should be characterized by equation (3) with a similar value of $\theta_\perp-\theta_\parallel$.

At low temperatures, the ESR linewidth in $YbRh_2Si_2$ is of the form [5]

$$\Delta B(T) = \Delta B_0 + bT + c\Delta/(\exp[\Delta/T]-1) \quad (10)$$

where ΔB_0, b, c and Δ are constants. The third term on the right-hand side of (10) reflects relaxation involving an excited crystal field doublet at an energy $\cong$10 meV above the ground doublet. The second term, linear in T, has the Korringa form appropriate to an isolated impurity. We hypothesize that the first term is also associated with the Korringa mechanism and is determined by the molecular field parameter θ appearing in equations (7) and (8). With the static field perpendicular to the c-axis, one has

$$\Delta B_0/b = \tfrac{1}{2}(\theta_\parallel+\theta_\perp) \quad (11)$$

taking the T-dependent term to be isotropic as found experimentally [5]. With the values of θ inferred above, the right-hand side of (11) is 1.3 K. This value is smaller than the ratio $\Delta B_0/b \approx 2.2$ K obtained from the linewidth data in [1] and $\Delta B_0/b \approx 3.6$ K from the data in [6], possibly indicating a contribution to ΔB_0 associated with inhomogeneous broadening. Since it has not been possible to observe the resonance with the static field parallel to the c-axis, we are unable to compare the angular dependence of the linewidth with the prediction given by equation (9).

Electron spin resonance in $YbIr_2Si_2$ has many points in common with ESR in $YbRh_2Si_2$ with the important difference

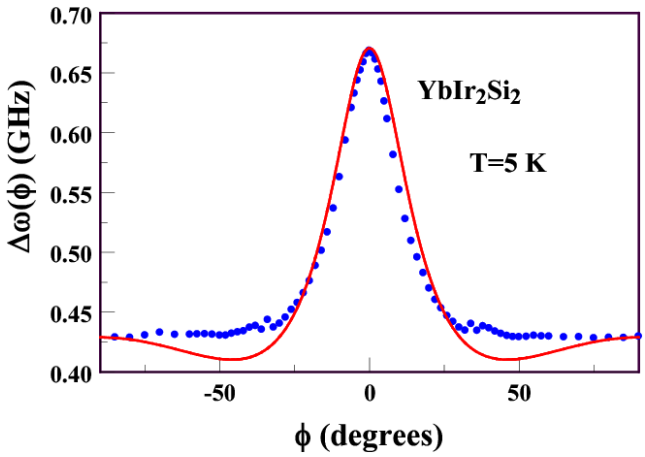

Figure 1. Angular dependence of the ESR linewidth in $YbIr_2Si_2$ at 5 K. The symbol ϕ denotes the angle between the static field and the c-axis. The solid curve is the prediction of equation (9), evaluated with $g_\perp = 3.36$, $g_\parallel = 0.85$, $\Delta\omega_\perp = 0.42$ GHz and $\Delta\omega_\parallel = 0.67$ GHz. The data points are from [14].
(This figure is in colour only in the electronic version)

that it is possible to cover the entire range from B perpendicular to the c-axis to B parallel to the c-axis [14]. The linewidth with the static field perpendicular to the c-axis can also be fit to the form shown in equation (10) [14]. It is found that $\delta B/b_0 = 14$ K, which is close to the molecular field temperature characterizing the integrated intensity above 5 K. This result suggests that the anomalously large residual linewidth in $YbIr_2Si_2$ arises primarily from interactions between Yb ions.

Since both the parallel and perpendicular g-factors and linewidths are known for this compound, one can compare the prediction of equation (9) with the measurements of [14]. The results of such a comparison are shown in figure 1. In this figure, it is evident that the interpolation equation captures the general features of the experimental data reasonably well, except for the shallow minima at approximately $\pm 45°$. It is worth pointing out that shallow minima in the linewidth in the neighborhood of $\pm 45°$ were found in $YbRh_2Si_2$ at 5 K [5].

The behavior of the linewidth below 5 K is also interesting. The width with the static field parallel to the c-axis appears to decrease while the width in the perpendicular direction remains approximately constant [14]. In the parallel direction, according to equation (6), the linewidth is inversely proportional to the transverse resonant susceptibility which, as noted, shows an anomalous increase below 5 K relative to the molecular field value. It is plausible that the increase in $\chi_\perp^R$ is the cause of the decrease in the linewidth. Why there is not a similar but weaker anomaly in the perpendicular linewidth is not understood but it may have some connection with a suppression of the 'critical' fluctuations when the static field is in the basal plane.

4. Discussion

The purpose of this note has been to point out that various features associated with the low-temperature ESR in $YbRh_2Si_2$ and $YbIr_2Si_2$ reflect the anisotropy in the resonant susceptibility and the presence of Yb–Yb interactions. In particular, the temperature dependence of the g-shift is determined by the temperature dependence of the ratio $\chi_\perp^R/\chi_\parallel^R$, while the Korringa contributions to the linewidths are modified by the factor $\chi^0(T)/\chi^R(T)$, where $\chi^0(T)$ denotes the Curie ($\sim 1/T$) susceptibility.

Acknowledgments

We would like to thank Carlos Rettori for stimulating our interest in ESR in Kondo lattice systems, Pedro Schlottmann for helpful discussions on the interpretation of the phase diagram of $YbRh_2Si_2$, and Jörg Sichelschmidt for helpful comments and for providing the numerical data shown in figure 1.

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