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Title: ^{209}Bi NMR in Heavy-Electron System YbBiPt

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^{209}Bi NMR in Heavy-Electron System YbBiPt

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Abstract

Bismuth NMR Knight shift and spin lattice relaxation rate $1/T_1$ are reported between 35-325K in the low-carrier heavy fermion system YbBiPt. The Knight shift is strongly temperature dependent and negative. Its temperature dependence tracks the bulk susceptibility with a hyperfine coupling constant $A_{hf} = -7.88$ kOe/μB. At low temperatures $1/T_1$ exhibits a dramatic increase, such that the average $4f$ spin correlation time τ_f shows a crossover behavior at about 75K. The rate $1/\tau_f$ is proportional to temperature, but with a different proportionality constant above and below about 75K. The linear temperature dependence is consistent with non-interacting $4f$ local moments which are relaxed via Korringa-type scattering with the conduction electrons. Below 75K, we infer that the reduced thermal excitation of a higher crystal-field multiplet is responsible for the dramatic decrease in the rate of $4f$ relaxation.

Keywords: NMR, heavy fermions, spin-lattice relaxation, spin correlation

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Introduction

The discovery of a large γ in heavy-electron compound YbBiPt has attracted a number of recent investigations [1-3]. YbBiPt has a very large Sommerfeld constant (γ~8J /mole K^2) and possesses an apparent small-moment [4], spin-density wave [5] transition at 0.4K which gaps part of the Fermi surface and which arises from a low-carrier density heavy electron state. Although many interesting aspects of this compound occur at low temperatures (<1K), it is important to investigate other relevant properties at high temperatures. For example, neutron scattering data reveals a temperature dependent inelastic peak at ~ 6 meV which was attributed to a crystal-field splitting of a J = 7/2 ground state multiplet [6]. Also, muon spin relaxation data exhibit an anomalous cusp-like behavior in the vicinity of 20K [7]. The work reported here provides more microscopic information to help clarify the physics of this compound using ^{209}Bi nuclear magnetic resonance.

YbBiPt crystallizes in a cubic MgAgAs type (half-Heusler structure) with $F\bar{4}3m$ symmetry. The sample was grown in a bismuth flux as described in Ref. 2. One gram of polycrystalline material was crushed and quickly mounted in a helium cryostat to avoid sample degradation, which had been observed previously when the material came in contact with air [8]. The quality of our sample was verified by measuring the temperature dependence of the susceptibility after the NMR data were taken. No appreciable change was observed compared to a reference measurement. Extra care was also taken to avoid eddy current heating of the sample due to high voltage RF pulses from the conventional pulsed NMR spectrometer. In this regard, we observed a rather large temperature rise (as much as ~40K) for duty cycles exceeding 0.1% at 77K. This situation could have been aggravated by oxide layers that might have formed on the surface of the grains. Although the oxides would prohibit efficient thermal conduction throughout the sample and container, their microscopic effects would nevertheless be undetectable in the NMR experiment.

The NMR spectra exhibit a single Gaussian line at all temperatures measured. Since all the atoms sit in a site of cubic local symmetry, quadrupolar effects are not expected. The single line observed in the NMR spectrum is associated with the bismuth-209 nuclei (I = 9/2). The platinum and ytterbium signals are expected to be weaker by more than an order of magnitude because of their smaller spins (I=1/2 for ^{195}Pt and ^{171}Y, I=5/2 for ^{173}Y). In addition, ytterbium would have been visible as two lines corresponding to two different isotopes having relatively low natural abundance. If the observed line were due to Pt, the calculated Knight shifts would be ≈ 26% at room temperature, which is unphysically large. We note that the corrections due to demagnetization were negligible (0.04%) at fields where the Knight shifts were measured (6-9 T).

Results and Discussions

Figure 1 shows the temperature dependence of the ^{209}Bi Knight shift K in YbBiPt. The Knight shift is large, isotropic, negative and follows the Curie-Weiss behavior of the bulk susceptibility. A large shift is not unexpected for bismuth, and the negative sign is consistent with what has been observed in other rare-earth intermetallics with more than half-filled f-shells, *i.e.* $K > 0$ for $\mathbf{J} = \mathbf{L} - \mathbf{S}$ and $K < 0$ for $\mathbf{J} = \mathbf{L} + \mathbf{S}$ [9]. These facts suggest that the Knight shift is mainly due to a transferred hyperfine field from Yb 4*f*-moments. Plotting the Knight shift versus the bulk susceptibility with temperature as an implicit parameter yields a hyperfine coupling constant of $A_{hf} = -7.88(4)$ kOe/μ_B (Fig. 1). A high temperature extrapolation of these data results in a temperature independent Knight shift of –0.38(2)%. In the tight-binding limit, this can be separated into orbital and conduction electron contributions. Because the former is always positive, we assume that the measured shift originates mainly from the conduction electrons near the Fermi level, presumably due to core polarization by the unfilled Bi 6p orbitals.

The spin dynamics of YbBiPt show interesting behavior at high temperatures. In Fig. 2 we show the temperature dependence of the spin-lattice relaxation time T_1 and its inverse $1/T_1$. The relaxation rate $1/T_1$ increases monotonically as the temperature is lowered, but below about 75K increases by almost two orders of magnitude. By about 35K the T_1 value has become so short (15μs), that the NMR echo is no longer visible. The spin-spin relaxation time T_2 (not shown) behaves similarly and approaches the value of T_1 at low temperatures.

In general, the spin-lattice relaxation in paramagnetic metals is related to the imaginary part of the complex dynamical susceptibility $\chi(\mathbf{q}, \omega)$ by the relation

$$\frac{1}{T_1} = \gamma_N^2 k_B T \sum_q [A_{hf}(q)]^2 \frac{\chi''(q,\omega_0)}{\omega_0} \tag{1}$$

where $A_{hf}(q)$ is the spatial Fourier transform of the transferred hyperfine field, e.g. from Yb^{3+} ions and ω_0 is the Larmor frequency. Neglecting the wavenumber dependence of the susceptibility and assuming that the energy spectrum for spin-spin correlation is Lorentzian and the hyperfine field tensor is isotropic, $1/T_1$ can be expressed in terms of the spin correlation time τ_f of the 4f local moments. One has

$$\frac{1}{T_1} = \gamma_N^2 k_B A_{hf}^2 T \chi_f(T) \tau_f \tag{2}$$

where static f-susceptibility $\chi_f(T)$ is derived from the bulk measurements. The hyperfine field is taken from the Knight shift data of Fig. 1.

Local moments mutually interacting via exchange produce hyperfine fields at nuclear sites with a relaxation rate that is independent of temperature: $1/T_1 \sim \gamma_N^2 A_{hf}^2/\omega_e$, in the limit where the fluctuation frequency of the local moments $1/\tau_f \sim \omega_e >> \omega_o$.[Ref. 10] The observed decrease of $1/T_1$ is not consistent with this expectation and we argue th at this may then be due to the temperature dependence $1/\tau_f$. We demonstrate this in Fig. 3 where we show the temperature dependence of $1/\tau_f$ derived from T_1 data using eq. 2. Strictly speaking, the $1/T_1$ could have contributions from the conduction electrons, which we neglect for purposes of this discussion. Over the entire temperature range $1/\tau_f$ increases monotonically with temperature, but with a changeover in behavior around 75K. A Korringa-like relation ($1/\tau_f \propto T$) is observed above and below this temperature, suggesting that the interaction among 4*f* moments is dominated by scattering from the conduction electrons. The crossover behavior near 75K could be explained by the excitation of higher crystal field multiplets previously seen in inelastic neutron scattering [6]. The linear dependence above and below 75K suggests that the relaxation mechanisms are of the same origin.

In summary, we presented NMR data on heavy electron compound YbBiPt. A transferred hyperfine coupling constant of -7.88 kOe/μ_B was measured and attributed to Yb *f*-moments. An anomalous behavior of the spin-lattice relaxation rate at about 75K was attributed to crystal field effects.

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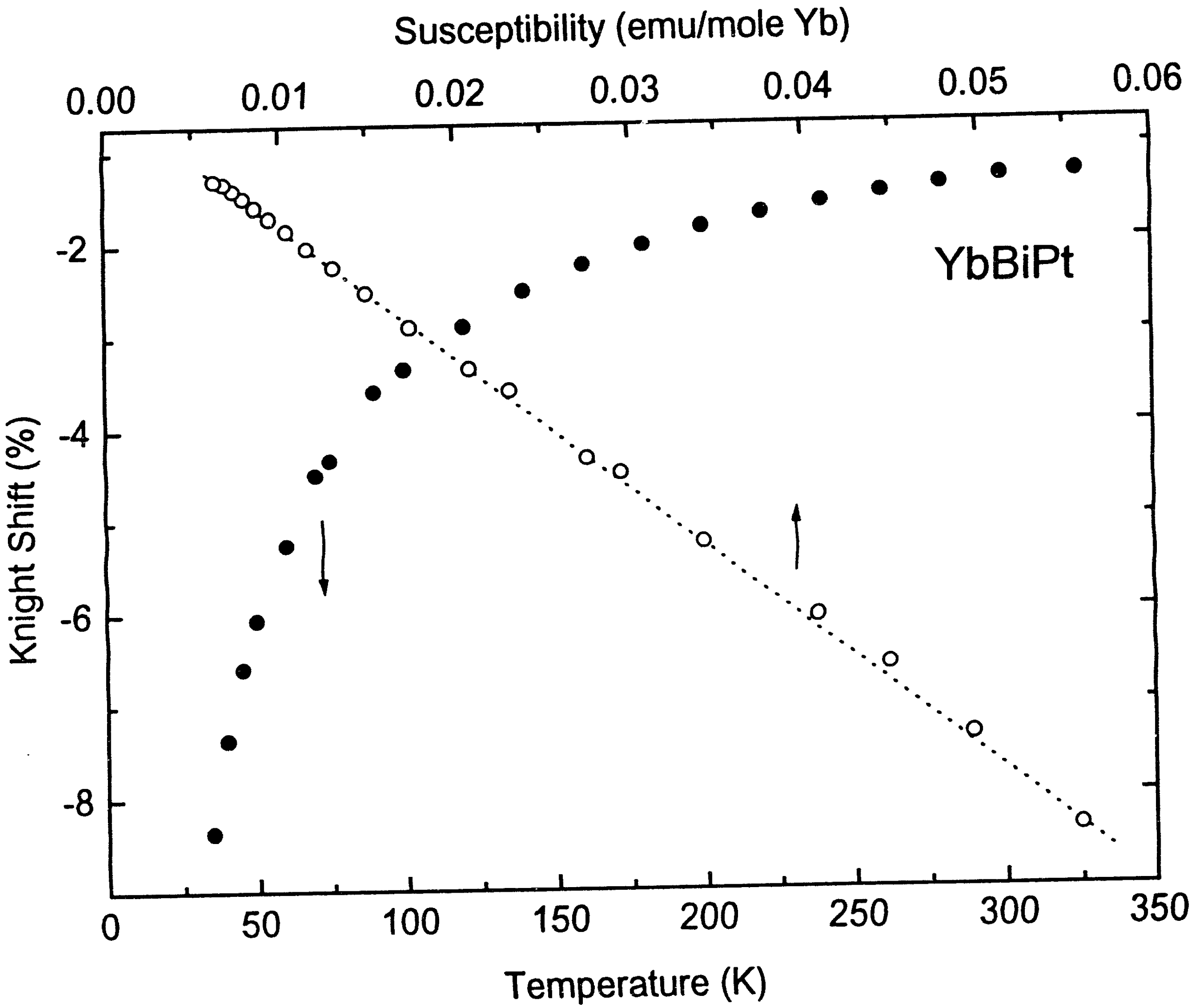
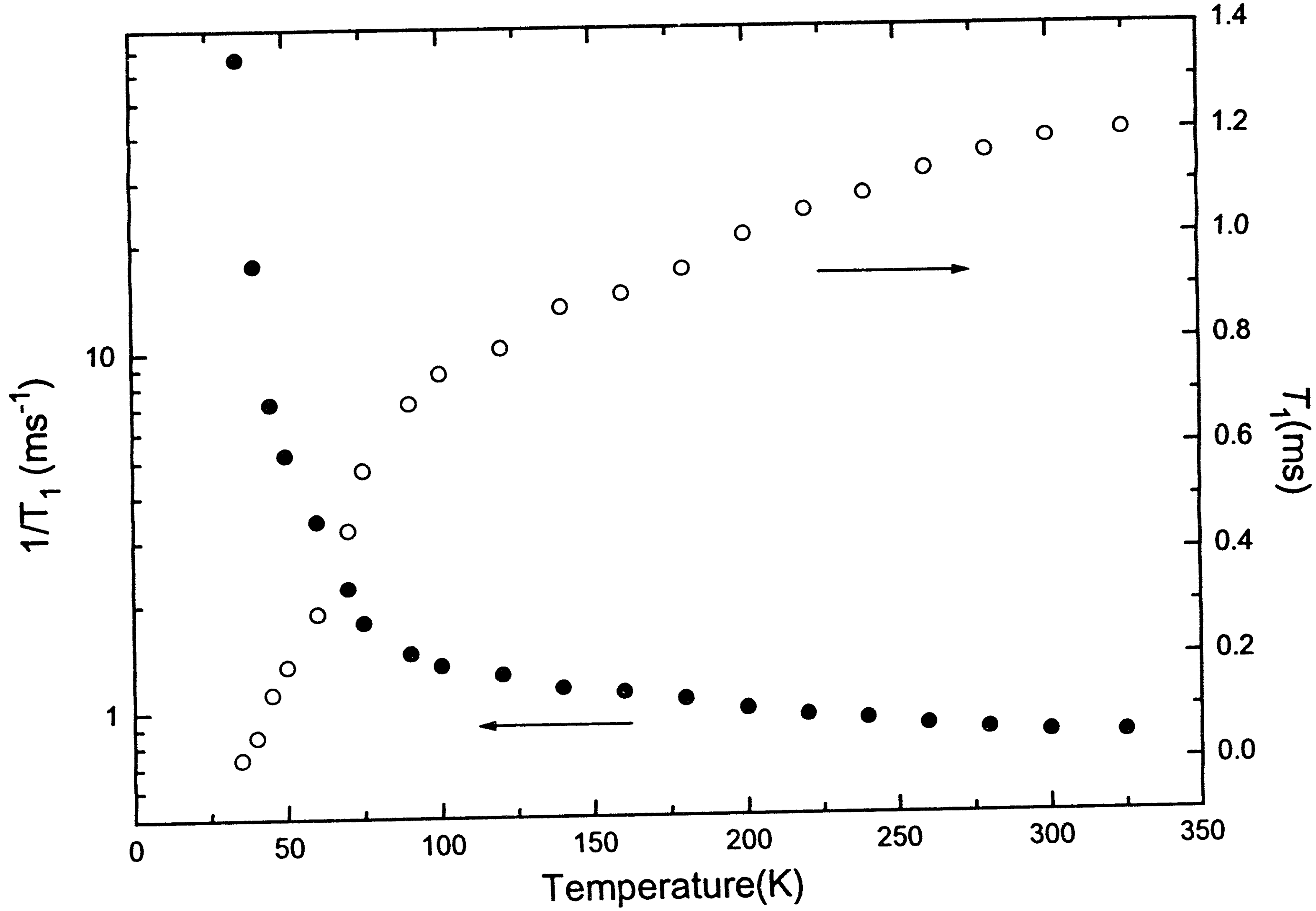
Figure Captions:

Fig. 1. Knight shift plotted against temperature (bottom scale) and against susceptibility with temperature as implicit parameter (upper scale).

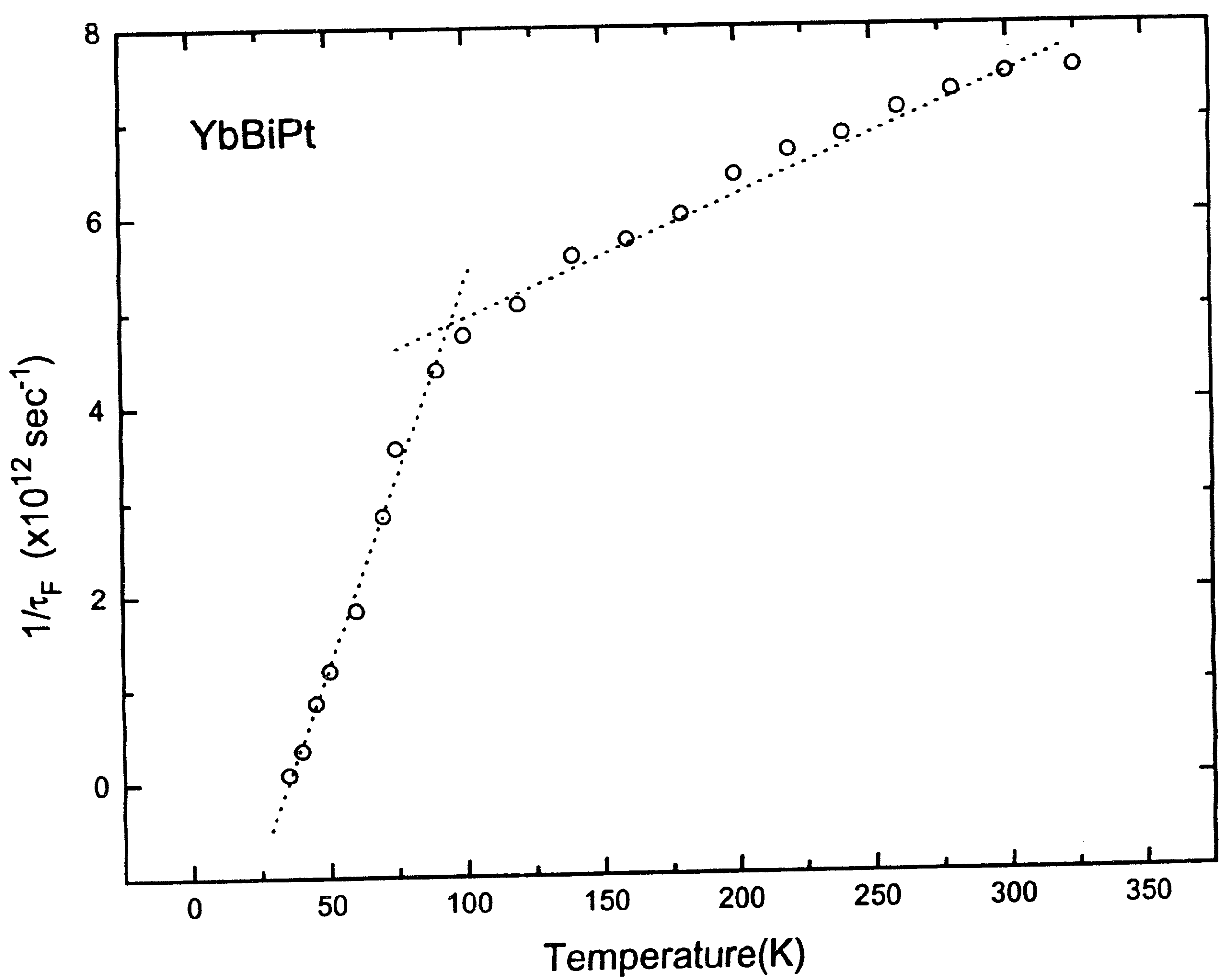
Fig. 2. Temperature dependence of spin-lattice relaxation time T_1 and rate $1/T_1$.

Fig. 3. Temperature dependence of spin correlation rate of Yb local moments.


Susceptibility (emu/mole Yb)
0.00
0.01
0.02
0.03
0.04
0.05
0.06
YbBiPt
Knight Shift (%)
-2
-4
-6
-8
0
50
100
150
200
250
300
350
Temperature (K)



1/T$_1$ (ms^{-1})
10
1
T_1(ms)
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0
50
100
150
200
250
300
350
Temperature(K)


YbBiPt
$1/\tau_F$ (x10^{12} sec^{-1})
Temperature(K)
0
2
4
6
8
0
50
100
150
200
250
300
350

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