Non-fermi liquid behaviour in uranium-based heavy-fermion compounds

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3. Experimental

A variety of experimental techniques was used to investigate the thermal, magnetic and transport properties of $\text{U}_2\text{Pt}_3\text{In}$ and related compounds. Since most of the techniques and experimental set-ups have been described in detail by others, only a short presentation is given here. General overviews of cryogenic techniques and low-temperature thermometry are given by Pobell [1], White [2] and Betts [3]. Descriptions of the particular $^3\text{He}$ system and $^3\text{He}/^4\text{He}$ dilution refrigerator used in this work are given in Refs. 4 and 5 and Refs. 6 and 7, respectively. The pressure cell used for the magnetotransport experiments is described in Section 3.3.1. Section 3.6 is devoted to the $\mu$SR technique, which is described in more detail.

3.1. Sample preparation

The preparation methods of the single crystals studied in this work will be described in Chapters 4 ($\text{U}_2\text{Pt}_3\text{In}$) and 7 (other compounds), where the corresponding experimental results are presented and discussed. Regarding $\text{U}_2\text{Pt}_3\text{In}$, it should be mentioned that it is a difficult material to prepare under normal arc-melting conditions due to In evaporation. Indium evaporation leads to the formation of a secondary phase, namely UPt. In fact, small single crystals of UPt have been grown recently out of polycrystalline $\text{U}_2\text{Pt}_3\text{In}$ by inducing complete In evaporation through annealing [8].
Traces of superconductivity at about 0.7 K have been detected in the resistivity of certain polycrystalline samples of U₃Pt₂In. A.c.-susceptibility measurements showed however that superconductivity is not a bulk property. Electron probe microanalysis (EPMA) on these samples indicate the presence of a network of UPt as an impurity phase. Upon annealing, the network is partially destroyed and the superconducting transition is suppressed. Other batches of polycrystalline U₃Pt₂In. containing UPtIn as an impurity phase, show a full superconducting resistive transition at 0.85 K. The superconducting phase has a critical field of about 1.4 T. Neither UPt nor UPtIn present a sign of superconductivity at low temperatures. The superconducting phase might be an In-rich phase precipitated at the U₃Pt₂In grain boundaries.

The single-crystalline batches of U₃Pt₂In. from which the specimens used in this work were taken, are, as far as it has been reported, the only ones prepared so far.

For general references on crystal growth of U and Ce intermetallic compounds, see e.g. Refs. 9 and 10.

The structural properties of most of the samples used were checked by means of X-ray and neutron diffraction, optical microscopy and secondary electron microscopy. The quality of the single crystals of U₃Pt₂In was also checked by means of EPMA at the FOM-ALMOS facility.

The single crystals were oriented by means of the X-ray back-reflection Laue method. Next, they were cut by spark-erosion. For the thermal-expansion measurements, the relevant surfaces of the samples were shaped plane-parallel within 5 μm by means of spark-erosion.

3.2. Magnetization

Magnetization measurements were performed by means of a commercial Quantum Design SQUID magnetometer (2 K ≤ T < 400 K, -5.5 T ≤ B ≤ 5.5 T) at the University of Lisbon.

High-field magnetization measurements up to 35 T were performed at the High-Field Facility of the University of Amsterdam [11]. Field pulses of 7, 14, 21 and 35 T were used with the magnetization measured during a 7-step field decay. After each pulse, the empty pick-up coil was measured. The magnetization of the sample plus teflon holder is then given by
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\[ M = M_{\text{sample-in}} - M_{\text{sample-out}} \]. The contribution of the teflon sample holder was measured in the same way, in order to correct the data for the diamagnetic signal of teflon.

### 3.3. Resistivity and magnetoresistance

Resistivity measurements were performed using a standard a.c. 4-probe method with a Linear Research resistance bridge (model LR-400 or LR-700). Since most of the materials used in this work are very brittle, the voltage and current leads (copper wires with thickness of 50 μm) were attached to the bar-shaped samples with silver paste. Excitation currents of 300 μA or lower were applied in order to prevent Joule heating.

High-field magnetoresistance measurements were carried out using the step-wise field decay of 7.14 and 21 T pulses. In addition, free (exponential-like) decays of 5.20 and 38 T pulses were used.

#### 3.3.1. Resistivity under pressure

Resistivity measurements were performed under hydrostatic pressures up to 2 GPa (≈20 kbar) in a 3He system. An overview of pressure techniques and pressure cells is given in Ref. 12.

A schematic view of the pressure cell used in this work is given in Figure 3.1 (after T. Naka - National Research Institute for Metals in Tsukuba, Japan). Besides a standard 4.7 kΩ RuO₂ thermometer, a cernox thermometer was mounted in order to monitor the cell and sample temperature in the temperature range 10-300 K.

The pressure cell, which can sustain pressures up to at least 2 GPa, is made primarily of CuBe. The outer and inner diameters amount to 25 and 6 mm, respectively. A short tungsten carbide piston is used to transfer the pressure to the teflon holder containing the sample. The sample is mounted on a specially designed plug and put inside the teflon holder together with the pressure-transmitting medium.
Figure 3.1 - Pressure cell for resistivity measurements.

The cell is placed in a press, in order to apply a load. The load necessary to obtain a pressure \( p \) is simply given by \( (\pi \phi_{\text{cell}}^2/4) \rho \), where \( \phi_{\text{cell}} \) is the inner diameter of the cell (\( \phi_{\text{cell}} = 6 \) mm). For \( \rho = 2 \text{ GPa} \), the load is \( 5.8 \times 10^3 \text{ kgf} \). After the load is applied, the screw head is adjusted in order to clamp the piston. In this way, the pressure is maintained when the cell is removed from the press. To change the applied pressure after the experiment, the cell has to be warmed up to room temperature. A load equivalent to the previous pressure is applied, such that the cell can be unclamped, after which a new load is applied.

The pressure medium used is liquid 3M Fluorinert. Fluorinert remains hydrostatic in the applied pressure range due to its low viscosity. Moreover, it has a low compressibility and good thermal conductivity. During solidification, hydrostaticity is conserved. In fact, the pressure medium used is a 1:1 mixture of two Fluorinerts, FC-70 and FC-77, which have glass solidifications at 248 and 163 K, respectively. This difference in solidification temperatures ensures that there are no sudden changes on the thermodynamic properties during the solidification of the pressure medium. The Fluorinerts used are chemically inactive and do not react with the components of the cell, nor with the samples, the wires or the silver paste used for placing the electrical contacts on the samples. Additionally, they have extremely small solubilities (less than 1%) for H\(_2\)O, oil, ethanol, methanol, etc.
Due to the different thermal-expansion coefficients of the pressure medium and the cell components, the pressure reduces during cooling. The pressure values presented in this work were corrected for an empirical low-temperature efficiency value of 80% obtained by T. Naka on the same cell.

### 3.4. Specific heat

Specific-heat measurements were performed using a relaxation method at low temperatures (dilution refrigerator and $^4$He system) and a semi-adiabatic method at high temperatures ($^4$He bath cryostat).

In the relaxation method, sample and addenda are connected by a weak thermal link to a heat reservoir at constant temperature $T_0$. A constant power $\dot{Q}$ is applied to a heater on the sample holder (sapphire plate) until thermal equilibrium is achieved at a temperature $T + \Delta T$. When the power is switched off, the sample and addenda will have an exponential relaxation towards the reservoir temperature $T_0$: $T(t) = T_0 + \Delta T e^{-\tau t}$. The relaxation time $\tau$ is related to the heat capacity $C$ by $C = \tau k = \tau \dot{Q} / \Delta T$ where $k$ is the thermal conductivity.

For heavy-fermion compounds, which present large specific heats, the addenda contribution at low temperatures to the total heat capacity is small and can be neglected. Special care was taken to stabilize the temperature of the sample since bad thermalization induces errors in the measured values of $\Delta T$ and the calculated values of $\tau$. The power supplied by the heater is calculated after measuring the voltage $V_{\text{ref}}$ across a reference resistance $R_{\text{ref}}$, in series with the heater, and the voltage drop over the heater: $\dot{Q} = V_{\text{heater}} I_{\text{heater}} = V_{\text{heater}} V_{\text{ref}} / R_{\text{ref}}$.

In the semi-adiabatic method, there is no deliberate thermal link between the sample and the heat reservoir. A heat pulse of energy $\Delta Q$ gives a sample temperature rise $\Delta T$ and the heat capacity is simply given by $C = \Delta Q / \Delta T$. The high-temperature specific-heat data presented in this work have been corrected for the contribution of the addenda.

A description of the used experimental set-ups is given in Refs. 6 and 13.
3.5. **Thermal expansion**

Thermal-expansion measurements were carried out with a parallel-plate capacitance method. The capacitance of a parallel-plate capacitor is $C = \varepsilon A/d$ where $\varepsilon$ is the dielectric constant of the medium between the plates, $A$ the area of the plates and $d$ the distance between the plates. Typical gap distances used are $d = 100 \mu m$. The length change of the sample as function of temperature is proportional to the change in capacitance. The uncertainty in the determination of the effective area of the capacitor plates, $\varepsilon A = 9.73 \times 10^{-16}$ Fm, gives an accuracy limit of about $3\%$ on the absolute value of the experimental data. The capacitance was measured using a sensitive three-terminal technique with an Andeen-Hagerling capacitance bridge. The maximum sensitivity of the set-up used is about $0.01 \, \AA$ for a sample of $5 \, mm$. A schematic drawing of the capacitance cell is given in Ref. 14.

The coefficient of linear thermal expansion is given by $\alpha = 1/L \, (dL/dT)$ where $L$ is the length of the sample. A heating in steps of $\Delta T$ is used. The linear thermal expansion of the sample is calculated from

$$\alpha = -\frac{1}{L} \left( \frac{\Delta d}{\Delta T} \right)_{\text{cell}} + \frac{1}{L} \left( \frac{\Delta d}{\Delta T} \right)_{\text{cell}} + \alpha_{\text{Cu}} \quad (3.1)$$

Here, the first term corresponds to the change in gap distance with the sample mounted in the cell, the second term is the corresponding change with a oxygen-free high-conductivity (OFHC) copper sample mounted in the cell (cell effect) and the third term is the correction for the linear thermal expansion of the OFHC copper of the cell. The cell effect is small at low temperatures ($\Delta d/\Delta T = -2.5 \, \AA/K$ at $T = 4.2 \, K$). However, a progressive increase is observed when the temperature is further decreased ($\Delta d/\Delta T = -9.0 \, \AA/K$ at $T = 0.3 \, K$).

The volume expansion coefficient $\alpha_V$, where $V = abc$ is the volume, is given by

$$\alpha_V = \frac{1}{V} \frac{dV}{dT} = \frac{1}{abc} \left( \frac{da}{dT} + \frac{db}{dT} + \frac{dc}{dT} \right) = \alpha_a + \alpha_b + \alpha_c \quad (3.2)$$

For general references on thermal-expansion measurements see Refs. 15-17.
3.6. Muon Spin Relaxation and Rotation

μSR is an acronym for Muon Spin Relaxation, Rotation, Resonance or even Research. μSR is a technique increasingly used in solid state physics, chemistry, and materials science because of its sensitivity to static and dynamic microscopic magnetic fields, which enables a study of relevant aspects of structural, magnetic and electronic phenomena in magnets, superconductors, semiconductors, and insulators. In the μSR technique, the positive muon, μ⁺, is used as a probe. Intense μ⁺ beams with a high spin polarization can be produced. Some properties of μ⁺ are given in Table 3.1. A general description of the μSR technique can be found in Refs. 18-20, while experimental results on some exemplary materials are given in Refs. 21-23. The μSR experiments presented in this work were carried out at the Paul Scherrer Institute (PSI) in Villigen (Switzerland), in the General Purpose Spectrometer (GPS), equipped with a gas flow ⁴He cryostat for 1.5 K ≤ T ≤ 300 K, and in the Low Temperature Facility (LTF), equipped with a top-loading dilution refrigerator with a base temperature of about 0.025 K.

<table>
<thead>
<tr>
<th>Table 3.1 - Some properties of the μ⁺ particle.</th>
</tr>
</thead>
<tbody>
<tr>
<td>mass m_µ = 206.76826(11) m_e</td>
</tr>
<tr>
<td>charge +e</td>
</tr>
<tr>
<td>spin 1/2</td>
</tr>
<tr>
<td>magnetic moment μ_µ = 8.8905981(13) μ₄</td>
</tr>
<tr>
<td>gyromagnetic ratio γ_µ / 2π = 135.53879(1) MHz/T</td>
</tr>
<tr>
<td>average lifetime τ_µ = 2.1970(4) μs</td>
</tr>
</tbody>
</table>

Because of its positive charge, the muon localizes at an interstitial site, where it probes the local magnetic environment. Since the muon has no quadrupolar electric moment (S_μ = 1/2) it does not couple to electric-field gradients. The muons produced by the decay of pions have a kinetic energy of 4.119 MeV. At this energy, muons rapidly thermalize within a sample without losing their polarization.

Once the muon is implanted in a sample, the local magnetic environment dictates the subsequent evolution of its spin vector. If the muon experiences a unique off-axis magnetic field B_µ (i.e. a magnetic field not in the direction of the muon spin), the spin precesses around the magnetic field at the Larmor frequency: ω_µ = γ_µ B_µ. However, any spatial or temporal, site to
site, variation of the magnetic field results in a dephasing or depolarization of the muon spin. This motion of precession and/or spin depolarization can be monitored due to the spatial anisotropy of the direction of positron emission when the muon decays. The decay positrons are distributed around the muon spin direction according to the probability function

\[ W(\theta) = 1 + A \cos \theta \quad \text{(3.3)} \]

where \( \theta \) is the angle between the muon spin and the direction of positron emission. The factor \( A \), called the asymmetry factor, increases monotonically with the positron energy up to a value of \( A = 1 \) for the maximum energy of 52.83 MeV. A value of \( 1/3 \) is obtained if all emitted positrons are detected with the same efficiency, irrespective of their energy. The variation of the angular probability function \( W(\theta) \) is shown in Figure 3.2 for a number of decay positron energies. The experimentally observed maximum asymmetry depends on the appropriate integration over the energy-dependent probabilities of positron emission and detection, the energy-dependent asymmetry and the solid angle of the detector. A typical experimental value for the asymmetry factor in an actual \( \mu \)SR experiment is about 0.25.

![Figure 3.2 - Angular decay positron distribution for various positron energies. After Ref. 19.](image)

The decay positrons, \( e^+ \), are monitored by means of a detector array consisting of counters placed perpendicularly to the positive and negative coordinate axes centered on the sample. The time histogram of the collected events in each counter has the form

\[ N_e(t) = N_0 e^{-t/\tau_e} [1 + AP(t)] + b_0 \quad \text{(3.4)} \]
where $N_0$ is a normalization constant, $\exp(-t/\tau_\mu)$ accounts for the muon decay. $A$ is the asymmetry. $P(t)$ is the muon depolarization function which describes the time dependence of the polarization (with $P(0) = 1$) and $b_0$ is the background contribution. The depolarization function $P(t)$ reflects the spatial and temporal distribution of the magnetic fields at the muon sites. In the case of a static magnetic field $B_\mu$ at the $\mu^+$ site, $P(t)$ is given by

$$P(t) = \int f(B_\mu)[\cos^2 \theta + \sin^2 \theta \cos(\omega_c t)]dB_\mu \ .$$

where $f(B_\mu)$ is the magnetic-field distribution function and $\theta$ the angle between $B_\mu$ and the initial muon polarization $P_\mu(0)$.

For a particular crystal structure, the possible presence of different muon stopping sites, with different magnetic environments, will be reflected in a $\mu$SR signal with different components, i.e. with different depolarization functions. Moreover, since the muons are uniformly implanted in a sample, the coexistence of different domains, characterized by different types of ground states, can also be detected by the presence of different components with distinctive functions $P(t)$, even if only one stopping site is present.

Different experimental geometries can be used with respect to the direction of an external magnetic field $B_{\text{ext}}$. In fact, each geometry corresponds to a different meaning of the acronym $\mu$SR: muon spin relaxation for zero or longitudinal field ($B_{\text{ext}} || P_\mu(0)$) and muon spin rotation for transverse field ($B_{\text{ext}} \perp P_\mu(0)$).

The muon beam at the PSI is of the continuous type (compared to beams of the pulsed type). Because each event is treated separately, the continuous beam has a good time resolution but a large background $b_0$, which limits the time window to about 10 $\mu$s. Recently, a new facility, called MORE (Muons On REQuest), has been installed at the PSI, which reduces drastically the background, increasing the time window to 16 $\mu$s. In this arrangement, a "kicker" sends a muon to the instrument only when it is required, deflecting all the other muons away from the experimental set-up. A disadvantage of MORE is however the initial dead-time (about 0.15 $\mu$s) in the histograms, which limits its usefulness to the case where there is no fast depolarization rate.
3.6.1. Zero-field $\mu$SR

The $\mu$SR technique yields the possibility to probe magnetic signals in zero external field. Its large magnetic moment makes the muon sensitive to internal fields as small as $10^{-5}$ T (which corresponds to the magnitude of fields originating from nuclear dipoles).

The zero-field (ZF) $\mu$SR technique can be used to measure the spontaneous $\mu^+$ Larmor frequencies in magnetically ordered phases and provides information about the magnetic structure and the value of the static moment. In the simplest case of a magnetic structure producing a field of well defined magnitude and direction at the $\mu^+$ sites, $f(B_{\mu})$ is represented by a $\delta$ function and the muon-depolarization function is

$$P(t) = \cos^2 \theta + \sin^2 \theta \cos(\omega_0 t)$$ \hspace{1cm} (3.6)

For a polycrystalline sample, averaging over the angular dependence results in

$$P(t) = \frac{1}{2} + \frac{1}{2} \cos(\omega_0 t)$$ \hspace{1cm} (3.7)

A static distribution of internal fields, as the one arising from static nuclear or electronic dipole fields, will produce a depolarization. Assuming that the internal fields are Gaussian distributed in their values and randomly oriented, the field distribution has zero average and no spontaneous precession frequency is observed. $P(t)$ assumes the form of a Kubo-Toyabe function [24]

$$P_{kT}(t) = \frac{1}{2} + \frac{1}{2} \left( 1 - \Delta \tau^2 \right) e^{-\Delta \tau^2}$$ \hspace{1cm} (3.8a)

where $\Delta^2 \tau^2 = <B^2>$ is the second moment of the field distribution. If the field distribution is Lorentzian then

$$P_{kL}(t) = \frac{1}{2} + \frac{1}{2} \left( 1 - \lambda \tau \right) e^{-\lambda \tau}$$ \hspace{1cm} (3.8b)

where $\lambda \tau$, represents the half width at half maximum of the distributions. For early times ($t < \Delta^{-1}$ or $t < \lambda^{-1}$), these functions approach a Gaussian and an exponential function, respectively:

$$P_{kT}(t) = P_G(t) = e^{-\Delta \tau^2}$$ \hspace{1cm} (3.9a)

$$P_{kL}(t) = P_L(t) = e^{-\lambda \tau}$$ \hspace{1cm} (3.9b)

In the case of a time-dependent Gaussian distribution of the internal fields, the Kubo-Toyabe function is modified to a dynamical Kubo-Toyabe function which cannot be expressed
analytically, except in the limiting case of slow and fast fluctuations. If $\nu$ is the fluctuation rate of the magnetic moments, the dynamical Kubo-Toyabe function becomes

$$P(t) = \frac{1}{2} e^{-2\nu t/3} + \frac{1}{2} \left( 1 - \Delta^2 t^2 \right) e^{-\Delta^2 t^2/2}$$

for slow fluctuations ($\nu \ll \Delta$). For fast fluctuations, $P(t) = P_{\nu}(t) = e^{-\lambda t}$ with $\lambda = 2\Delta^2/\nu$. In the latter case, the depolarization rate $\lambda$ describes the spin-relaxation rate and involves spin-flip transitions induced by the fluctuating magnetic field with a component perpendicular to the initial muon-polarization direction. The dynamical Kubo-Toyabe function is plotted in Figure 3.3 for several fluctuation rates (notice that the static Kubo-Toyabe function corresponds to the case $\nu=0$).

**Figure 3.3** - Dynamical Kubo-Toyabe function for several fluctuation rates $\nu$.

### 3.6.2. Longitudinal-field $\mu$SR

In the longitudinal-field (LF) configuration, an external field is applied in the direction of the initial muon polarization. In the case of a random distribution of static internal fields, the
effect of $B_{\text{ext}}$ is to gradually remove the time dependence of the polarization. Eventually, by choosing $B_{\text{ext}}$ to be stronger than the internal fields ($\gamma_{\mu}B_{\text{ext}} \gg \Delta$), the muon's "up" and "down" states are eigenstates of the Zeeman Hamiltonian and any inhomogeneous static distribution of the internal fields will not affect the time evolution of the muon polarization, which will therefore remain constant. This behaviour reflects the decoupling of the muon spin from the static internal fields. This situation is depicted in Figure 3.4 for a random distribution of static moments, where a strong longitudinal field results in local fields parallel to the muon spin, which maintains its initial polarization in the field direction.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure3.4.png}
\caption{Effect of a longitudinal external field on a random distribution of local fields. a) $B_{\text{ext}}=0$; b) when $B_{\text{ext}}$ is significantly larger than the local field at $B_{\text{ext}}=0$, the resulting field is almost parallel to $P_{\mu}(0)$. After Ref. 25.}
\end{figure}

The polarization function for a Gaussian distribution as function of applied field is shown in Figure 3.5. It assumes the analytical form [26]

\begin{equation}
P_{K\tau}(t, B_{\text{ext}}) = 1 - \frac{2\Delta}{\gamma_{\mu}B_{\text{ext}}^2} \left[ \gamma_{\mu}B_{\text{ext}} \cos \left( \gamma_{\mu}B_{\text{ext}} t \right) \right]
+ \frac{2\Delta^2}{\gamma_{\mu}B_{\text{ext}}^3} \int_0^\Delta dy \, e^{-\Delta^2 y^2} \cos \left( \gamma_{\mu}B_{\text{ext}} y \right) \left( \gamma_{\mu}B_{\text{ext}} y \right) \left( \gamma_{\mu}B_{\text{ext}} y \right)
\end{equation}

(3.11)
Figure 3.5 - Kubo-Toyabe depolarization function for a decoupling of the muon spin from a Gaussian distribution of static fields due to a longitudinal external field.

However, for fast fluctuations of the internal fields, the spin-lattice relaxation regime is recovered and induced spin-flip transitions will lead to a depolarization in longitudinal fields similar to the one observed in zero field.

Due to these differences, longitudinal-field $\mu$SR provides a powerful tool to distinguish static from dynamic distributions of internal fields (if there are no spontaneous Larmor frequencies in the static case, zero-field $\mu$SR cannot distinguish the two situations). In the static case, there is no depolarization in an external field, while in the dynamic case the depolarization function will have the same form as in the zero-field case, with a slightly reduced depolarization rate

$$\lambda = \frac{2\Delta^2/\nu}{1+(\gamma_\nu B_{\text{ext}}/\nu)^2}.$$  \hspace{1cm} (3.12)
In the transverse-field (TF) configuration, the external magnetic field $B_{\text{ex}}$ is applied perpendicular to the initial muon polarization $P_\mu(0)$. The local magnetic field at the interstitial site where the muon is implanted can be determined from the Larmor precession frequency. The measured frequency or frequencies are expressed in the form of a Knight shift:

$$K_\mu = \frac{|B_{\mu}| - |B_{\text{ex}}|}{|B_{\text{ex}}|} = \frac{\omega_0}{\omega_0} - 1,$$

where $\omega_0 = \gamma_\mu B_{\text{ex}}$. Here, we consider only metals in the paramagnetic state that are exposed to a magnetic field. The local magnetic field $B_{\mu}$ at the interstitial site where the muon comes to rest can be written as

$$B_{\mu} = B_{\text{ex}} + B_{\text{dip}} + B_{\text{con}} + A_{\text{con}} \tilde{\chi} B_{\text{ex}} + B_{\text{dia}}.$$

$B_{\text{dip}}$ represents the dipolar fields of the localized lattice spins. The third and the fourth term are called the direct and indirect hyperfine contact field, respectively, and are connected with the presence of the muon itself. The direct hyperfine contact field, $B_{\text{con}}$, results from the spin density at the muon site, which is induced by the polarization of the conduction electrons. In the paramagnetic state, this polarization is induced by an external field. $B_{\text{con}}$ is proportional to the Pauli susceptibility of the conduction electrons and is usually assumed to be temperature independent and isotropic, in contrast to the other contributions. The indirect contact field is due to the RKKY interaction between localized moments and the muon. The effective contact coupling constant, $A_{\text{con}}$, is temperature independent, so that the indirect contact field is proportional to the susceptibility tensor $\tilde{\chi}$ and the applied magnetic field. The last contribution, $B_{\text{dia}}$, is due to the diamagnetic response of the electron-cloud screening of the muon charge. The diamagnetic screening produces only a very small contribution to the local magnetic field. For materials with an enhanced effective electron mass $m^*$, the small diamagnetic contribution is reduced by a factor $m/m^*$, becoming negligible for heavy-fermion compounds.

In order to separate the different contributions to the local magnetic field, the experimental Knight shift in heavy-fermion compounds is usually compared to the calculated one. If the principal axes of the crystalline structure are chosen as the coordinate frame, the dipolar field contribution can be written as
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The dipolar tensor $\tilde{A}_{\text{dip}}$ is given by

$$A_{\text{dip}}^{ii} = \frac{1}{r_i^2} \left( \frac{3x_i x_i - \delta_i}{r_i^2} \right).$$

where the sum is over all $f$-moments at positions $r_i$ and $r = r_i - r_{\mu}$.

In order to calculate this finite sum, one can define a "Lorentz sphere" with radius $r_l$, and separate the sum into a part inside the sphere and a part outside the sphere. If one chooses the radius large enough, the summation over the outer region can be approximated with an integral. The magnetic field resulting from this integral yields the Lorentz field $B_L = \mu_0 M/3$ and the demagnetizing field $B_D = -\bar{N} \mu_0 M$, where $M$ is the magnetization and $\bar{N}$ the demagnetization tensor related to the shape of the sample (notice that for a sphere $N = 1/3$ and $B_L + B_D = 0$).

After correcting for the demagnetizing and Lorentz fields, the Knight shift is related to the diagonal susceptibility tensor according to

$$K_u = K_{\text{con}} + b \cdot (\tilde{A}_{u} \tilde{x} b).$$

where $b = B_{\text{ex}}/|B_{\text{ex}}|$ is the unit vector parallel to the applied magnetic field, $K_{\text{con}}$ the Knight shift due to the direct contact field and $\tilde{A}_u = \tilde{A}_{\text{dip}} + \tilde{A}_{\text{con}}$ the total hyperfine coupling tensor. In contrast to $K_{\text{con}}$ and $\chi_{\text{rad}}$, the contribution from the localized $f$-moments will exhibit a strong temperature dependence. $K_{\text{con}}$ can therefore be determined from the experimental data: $K_{\text{con}} = K_u(\chi \rightarrow 0)$. The elements of $\tilde{A}_u + \tilde{x}$ can be determined experimentally from the Knight shift anisotropy for the principal axes. The Knight shift is simply given by

$$K_u = A_u^{ii} \chi_u.$$  \hspace{1cm} (3.18)

With the knowledge of $\chi_u$, the tensor elements $A_u^{ii}$ can be determined from the observed Knight shift $K_u$. Because $\tilde{A}_{\text{tot}}$ is the sum of a traceless dipolar tensor and a scalar contact part, $\tilde{A}_{\text{tot}}$ can be decomposed using $A_{\text{con}} = \text{Tr}(\tilde{A}_{\text{tot}})/3$. By comparison of the experimentally determined $\tilde{A}_{\text{dip}}$ with the calculated values, it is often possible to determine the actual muon stopping site. If a sample orders magnetically and the muon stopping site is known, then it is easy to calculate from the local field in the ordered state (measured by zero-field $\mu$SR) the size of the ordered moment.
References