Can μSR access the phase of the longitudinal spin density wave - a parameter inaccessible by neutron diffraction?

V.Pomjakushin

Laboratory for Neutron Scattering, ETHZ & PSI

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Elastic scattering of polarized neutrons

$$\frac{d\sigma}{d\Omega} = \frac{m^2}{4\pi^2\hbar^4} Sp\{\rho_\sigma V^+ V\} = W_1 + W_2 + W_3 + W_4$$

$$V = V_{nucl} + V_{mag}$$

Pure nuclear scattering

Cd

$$W_1 \propto \delta(\vec{q} - \vec{\tau}) \left| \sum_j A_j \exp(i\vec{q}\,\vec{\rho}_j) \right|^2$$

Magnetic non-polarized scattering

$$W_2 \propto \left| \sum_\nu P_\nu(q) e^{i\vec{q}\,\vec{R}_\nu} \vec{M}_\nu \right|^2 \propto \left| \sum_{jn} \vec{Q}_{\mathbf{K}} P_j(q) e^{i(\vec{q}+\vec{K})\vec{r}_n} e^{i(\vec{q}+\vec{K})\vec{\rho}_j} e^{i\varphi} \right|^2$$

$$\vec{M}_\nu = \vec{S}_\nu - (\vec{e}\,\vec{S}_\nu)\vec{e} \qquad \propto \delta(\vec{q} - (\vec{\tau} + \vec{K})) \sum_j Q_{\mathbf{K}}^2 P_j(q) e^{i(\vec{q}+\vec{K})\vec{\rho}_j}$$

$$\vec{S}_\nu = \sum_{\vec{K}} \vec{Q}_{\mathbf{K}} e^{i\vec{K}\vec{R}_\nu + i\varphi}$$

Nucl/magnetic interference

$$W_3 \propto \sum_{\nu,l} A_l P_\nu(q) e^{-i\vec{q}\,\vec{R}_l} e^{i\vec{q}\,\vec{R}_\nu} (\vec{M}_\nu\,\vec{p}_0) \propto \sum_{\nu,l} A_l P_\nu(q) (\vec{Q}_{\mathbf{K}}\,\vec{p}_0) e^{-i\vec{q}\,\vec{R}_l} e^{i(\vec{q}+\vec{K})\vec{R}_\nu} e^{i\varphi}$$

=0

k ≠0

Additional pure magnetic

$$W_4 \propto \sum_{\nu\nu'} P_\nu(q) P_{\nu'}(q) e^{-i\vec{q}\,\vec{R}_\nu} e^{i\vec{q}\,\vec{R}_{\nu'}} \left(\left[\vec{M}_\nu \times \vec{M}_{\nu'} \right] \vec{p}_0 \right)$$

Scattering of non-polarized neutrons

$$\boxed{\underbrace{R}_{\text{Scattering amplitude}} = \underbrace{a}_{\text{Nuclear}} \underbrace{\pm}_{\text{polarization}} \underbrace{f_m}_{\text{Magnetic}}}$$

$$\boxed{\frac{d\sigma}{d\Omega} = R^2 = a^2 + f^2 \pm \cancelto{0}{2af_m}}$$

(17) $I_{\bar{\kappa}=\bar{\tau}\mp\bar{K}} = \dfrac{(p_0\langle\mu\rangle)^2}{4}\left|\sum_{\nu} f_{\nu}(\bar{\kappa})e^{\pm i\varphi_{\nu}}e^{i\bar{\tau}\bar{r}_{\nu}}\right|^2 [1+(\hat{\bar{\kappa}}\cdot\hat{\zeta})^2]$. Thus the spiral intensity varies with the factor $1 + \cos^2\psi$, where ψ is the angle between the reflecting plane and the planes of magnetic moments.

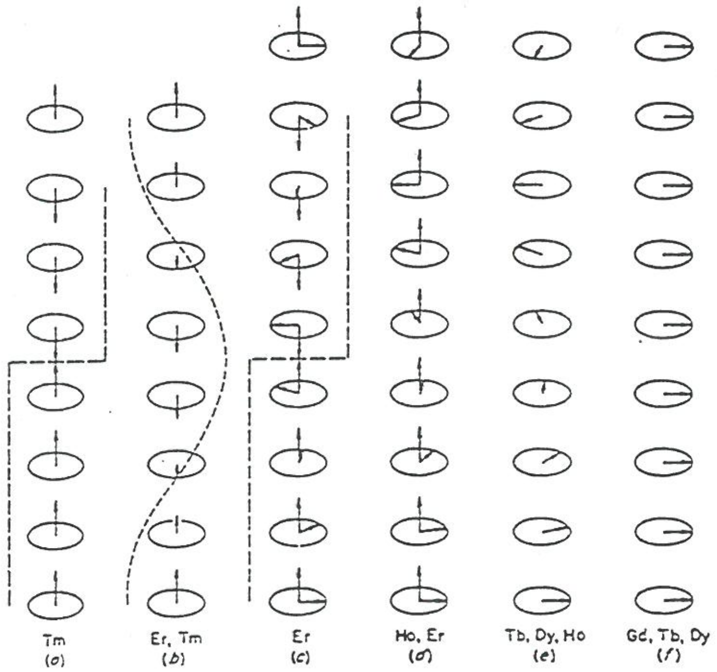


Fig. Magnetic structures of heavy lanthanide metals [after Koehler (1972)].

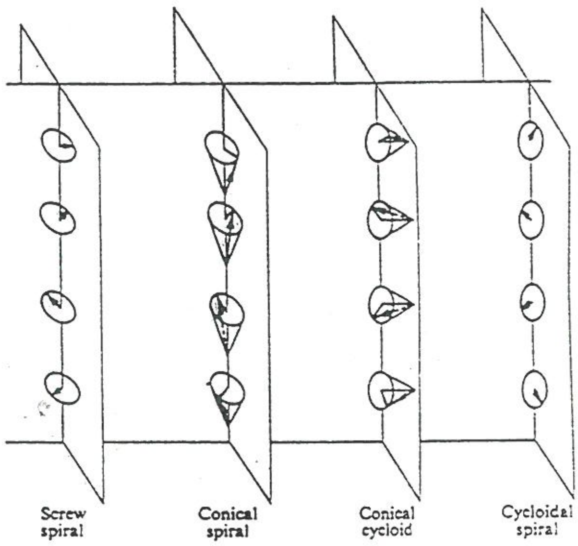


FIG. Types of spiral.

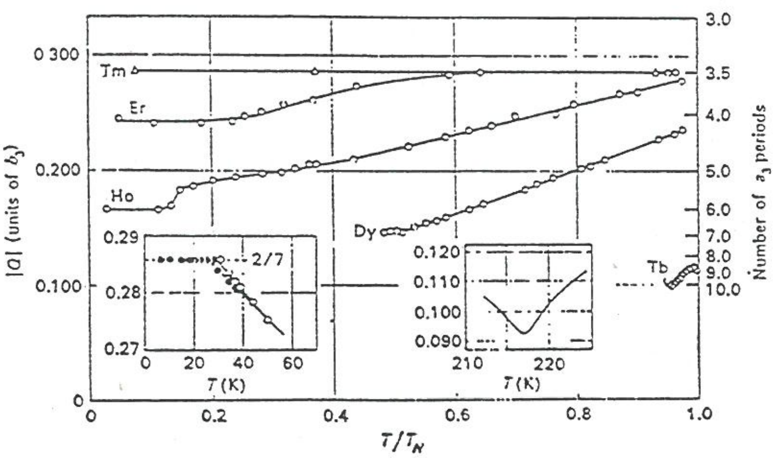


Fig. Variation of q_m with reduced temperature for the heavy rare earths. Inserts show details of data for Tm (Brun et al., 1970) and Tb (Dietrich and Als-Nielsen, 1967) on left and right hand sides respectively [after Koehler (1972)].

Ternary intermetallic compounds e.g.

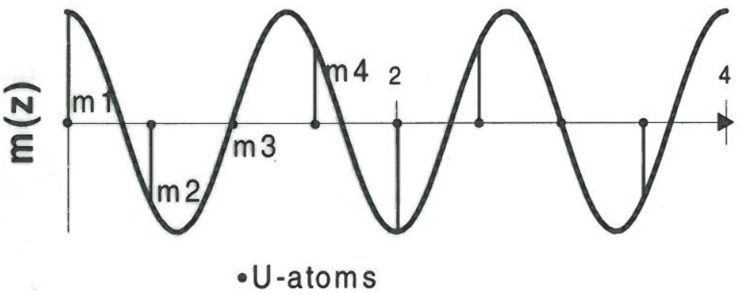
UNi_2Si_2 *H.Lin, et al PRB43, 12323, (1991)*

UPd_2Ge_2 *G.Andre, et al ' 96 SSC97, 923, (1996)*

LSDW $\quad m_U \parallel c$

$$m_U = m_0\cos(2\pi kz+\varphi) \quad k=3/4$$

1. $\varphi = 0$

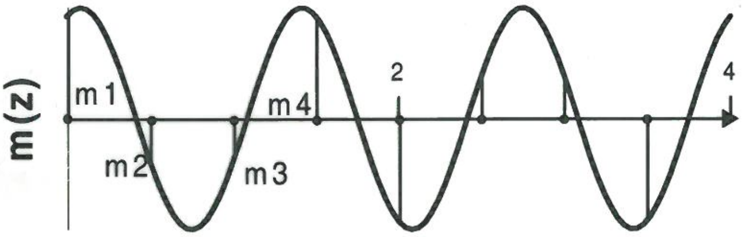


$m_1 = m_0$

$m_2 = m_0 \cdot \cos \dfrac{3\pi}{4}$

$m_4 = m_2$

2. $\varphi = -\dfrac{\pi}{8}$



$m_1 = m_0\cos \dfrac{\pi}{8}$

$m_2 = m_0\cos \dfrac{5\pi}{8}$

$m_3 = m_2$

More sophisticated examples *J.Rodriguez-Carvajal,*
$CsMnF_4$, $TbMn_6Ge_6$
two - $\vec{k}$: $TbGe_3$

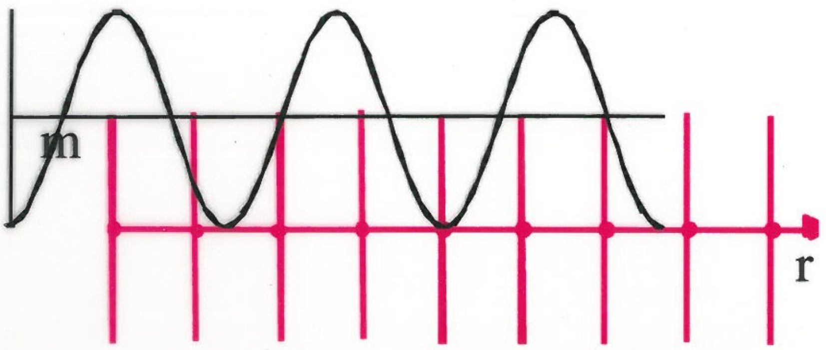
Modulated structures

- Spiral structures
  $\mathbf{m(r)} = m_0[\boldsymbol{\zeta} \cos(2\pi\mathbf{kr}+\varphi) + \boldsymbol{\eta} \overset{\sin}{\cancel{\cos}}(2\pi\mathbf{kr}+\varphi)]$,

- Spin density wave (SDW)
  $\mathbf{m(r)} = \mathbf{m}_0 \cos(2\pi\mathbf{kr}+\varphi)$
  e.g. transverse SDW $\mathbf{m}_0 \perp \mathbf{k}$,
  or longitudinal SDW $\mathbf{m}_0 \parallel \mathbf{k}$

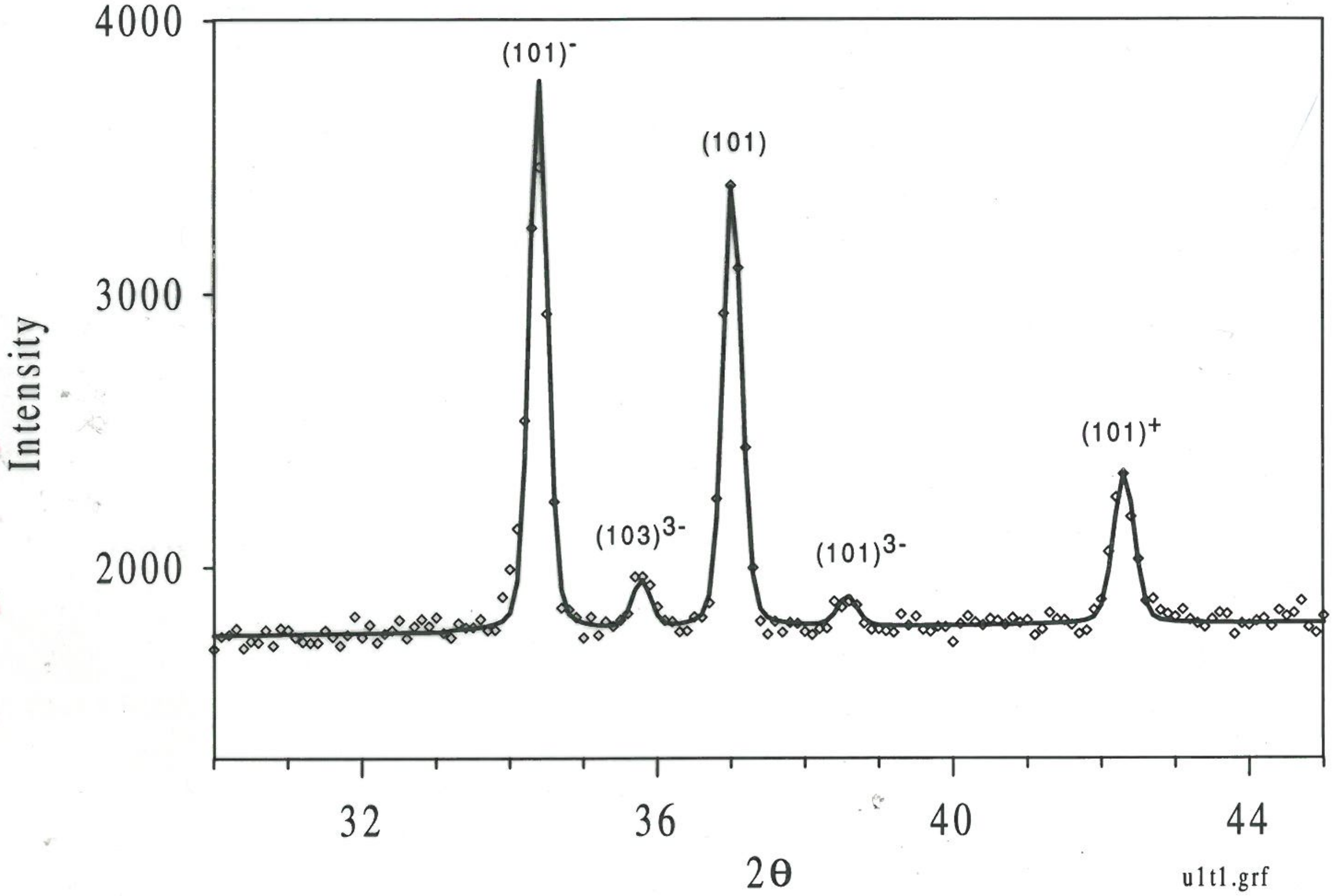
➢ Incommensurate $k \neq (m/n)$:
φ has no sense

➢ Commensurate SDW with rational $k = (m/n)$:
φ affects the true magnetic moments on the atoms!



$U(Pd_{0.99}Fe_{0.01})_2Ge_2$, T=1.5K

LLB, G4.1, λ=2.43 A

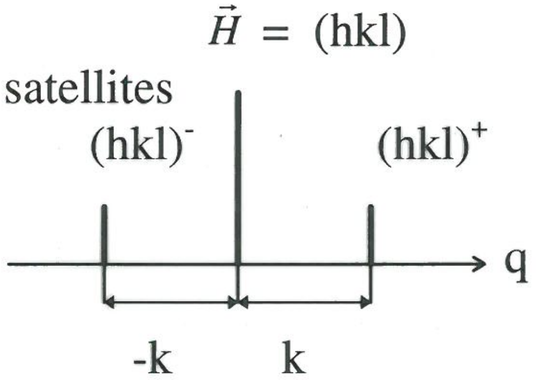


$$\vec{m}(\vec{R}) = 1/2 \sum_{(\vec{k}, -\vec{k})} e^{-(i\vec{k}\vec{R}+\varphi_k)} \vec{m}_k$$

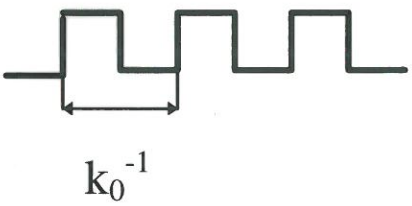
$$= \sum_{\vec{k}} \cos(\vec{k}\vec{R} + \varphi_k) \cdot \vec{m}_{\vec{k}}$$

$$\frac{dr_0}{d\Omega} \sim \left[m_k{}^2 - \left(\frac{\vec{q}}{q} \vec{m}_k \right)^2 \right] \cdot \delta\left(\vec{H} + \vec{k} - \vec{q}\right) + \ldots \delta\left(\vec{H} - \vec{k} - \vec{q}\right)$$

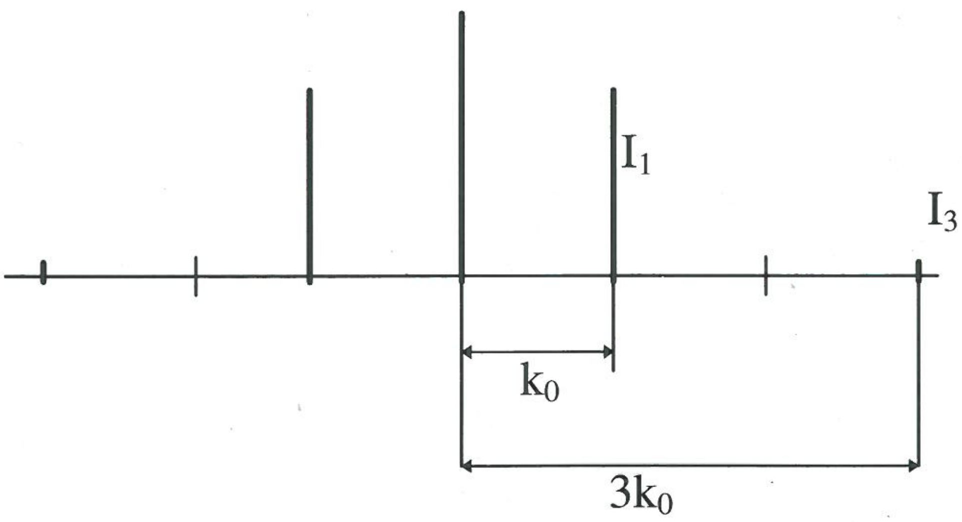
1. cos - modulation



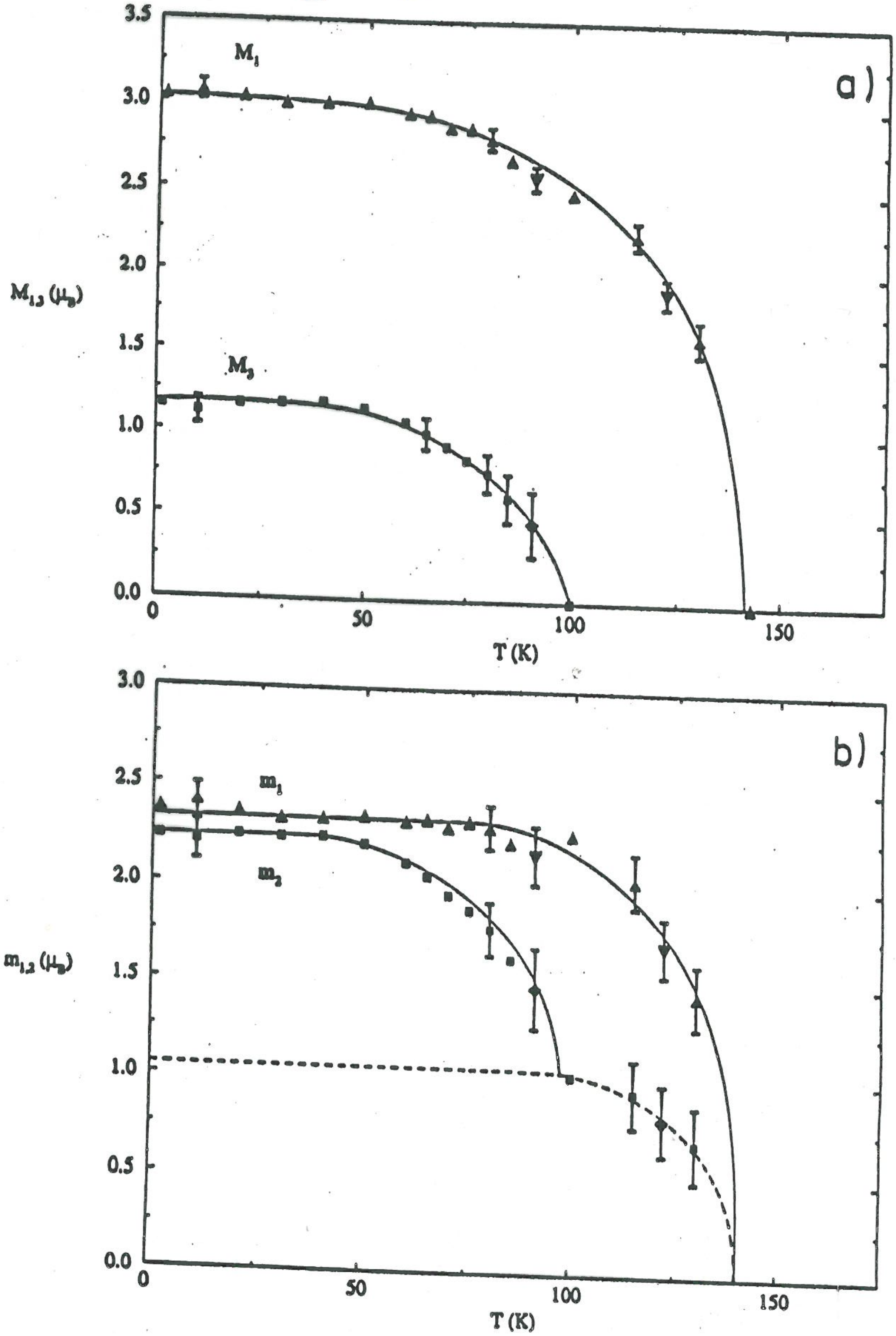
2.



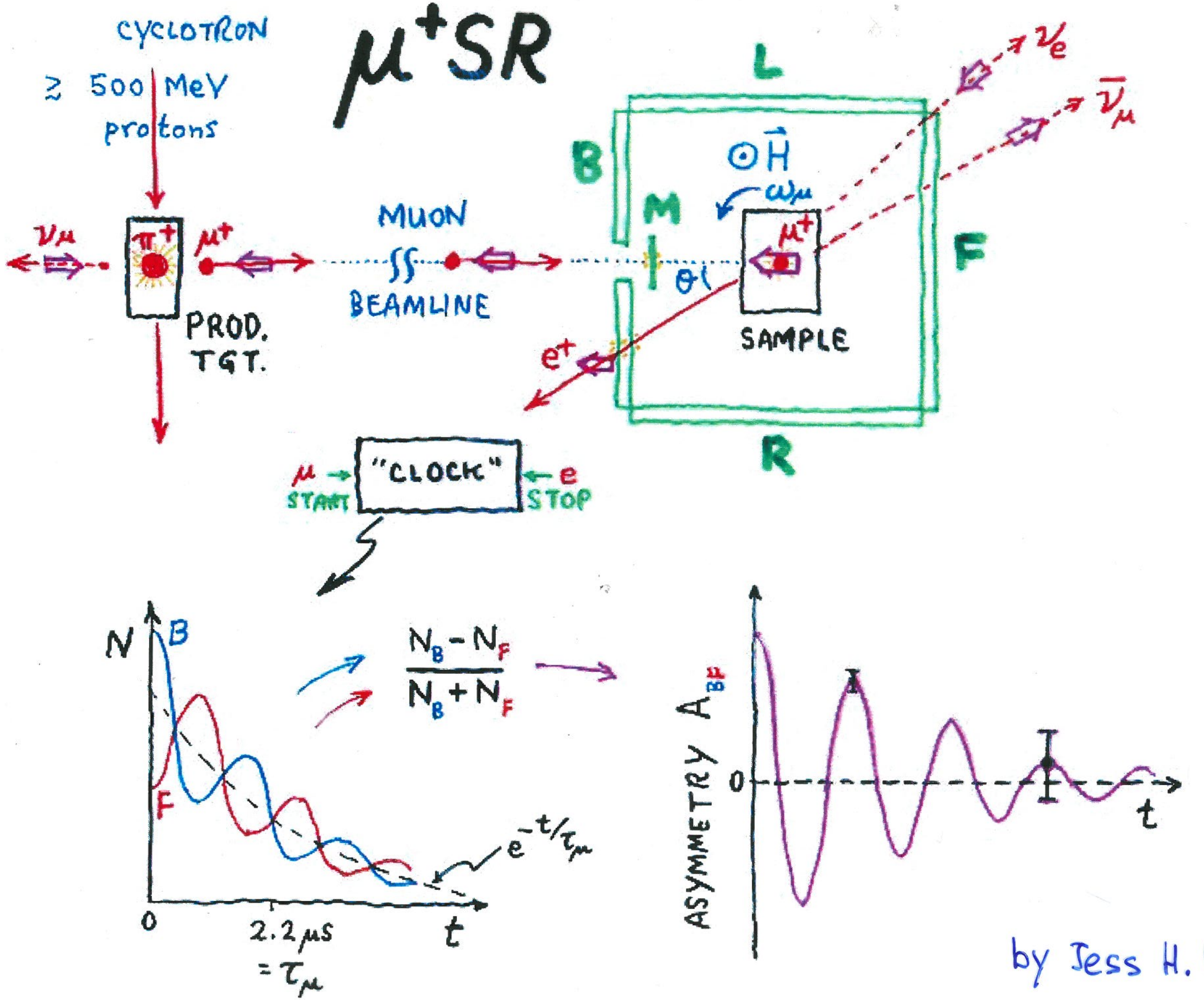
$$= \frac{4}{\pi} \left[\cos k_0 x - \frac{1}{3} \cos 3k_0 x + \frac{1}{5} \ldots \right]$$



UPd_2Ge_2



G. André, F. Bourée, et al, SSC 97, 923, (1996)



by Jess H. Brewer

Local magnetic field in an (anti)ferromagnet

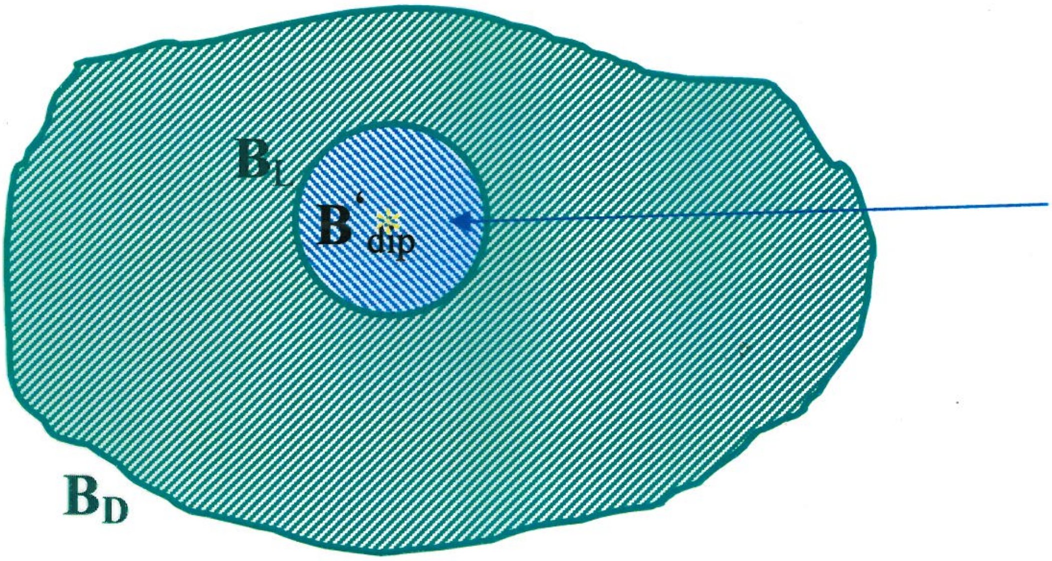
Dipole **Contact**

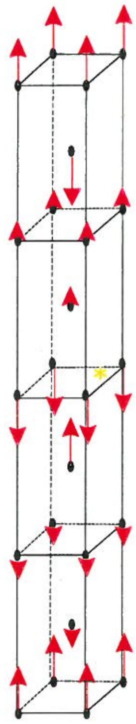
$$\mathbf{B}_{loc}(r) = [\mathbf{B}_{dip} + \mathbf{B}_L + \mathbf{B}_D] + \mathbf{B}_c$$

Discrete

Continuous (Lorentz+Demag)

$$\mathbf{B'}_{dip} = \sum_{\mathbf{r}} \frac{1}{r^3}\left(\frac{3(\mathbf{r}\cdot\mathbf{m}(\mathbf{r}))\mathbf{r}}{r^2} - \mathbf{m}(\mathbf{r})\right)$$

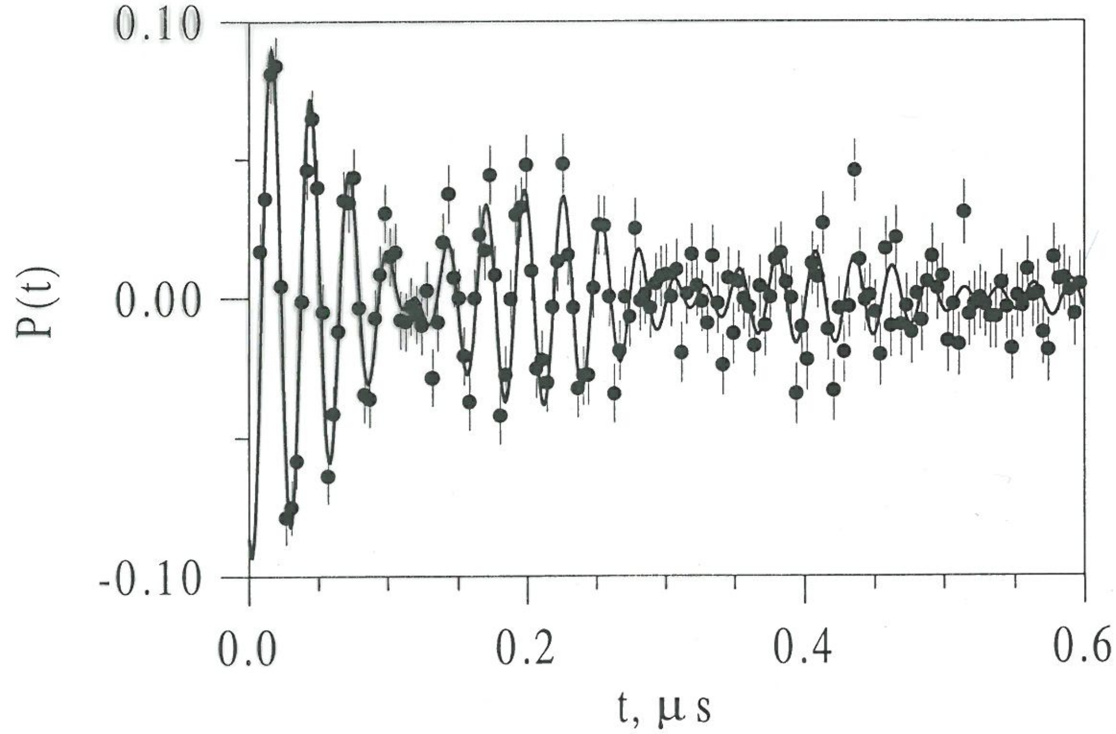


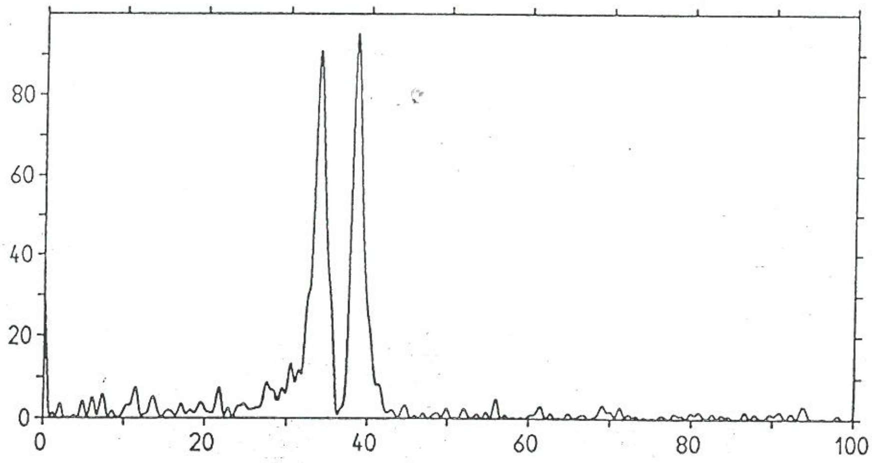


$$\mathbf{B}_c \sim J_{sf}(0)/E_F\, n_s \sum_{\mathbf{r}} F(2k_F r)\, \mathbf{m}(\mathbf{r})$$

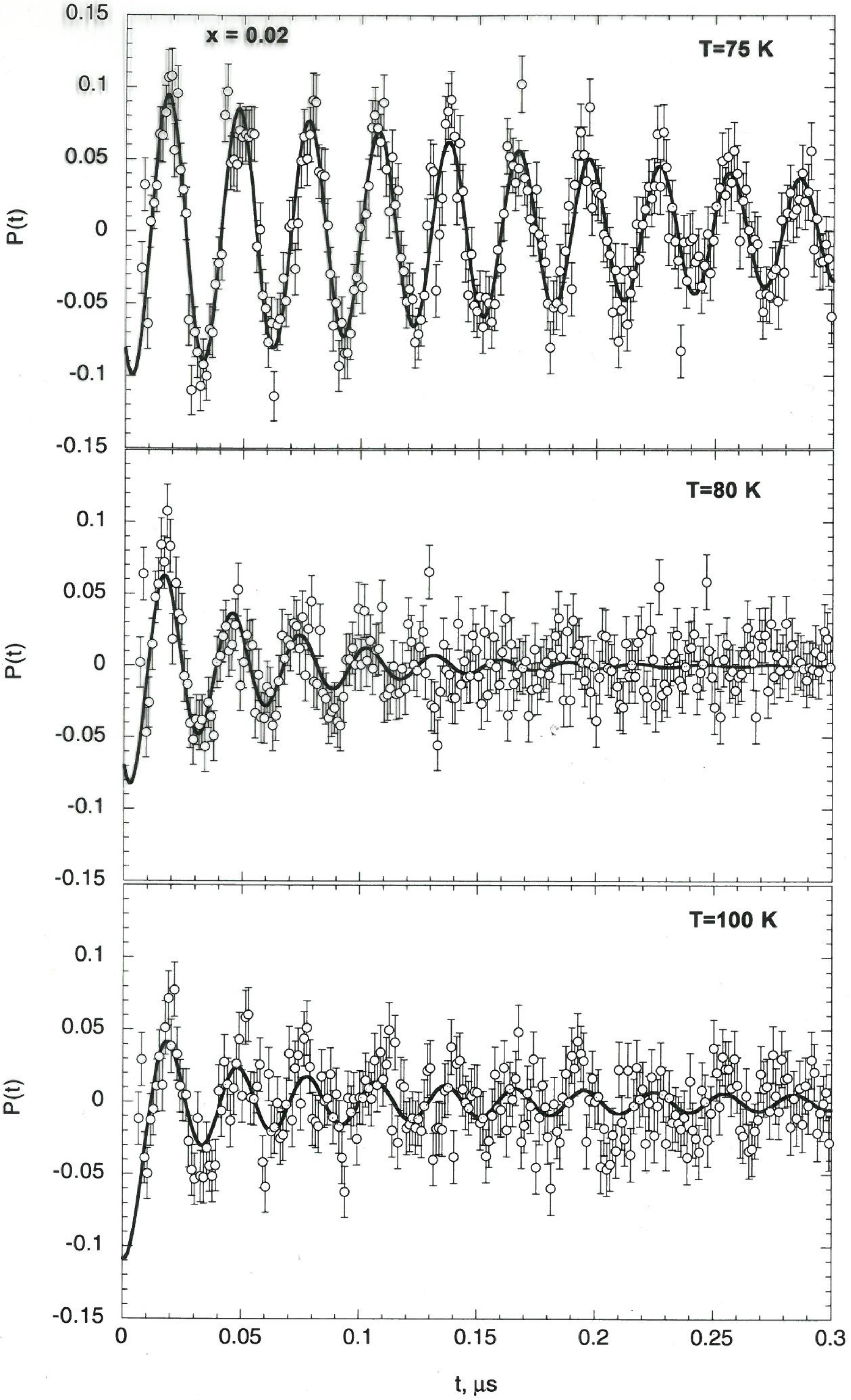
$\mathbf{m}(\mathbf{r})$: local magnetic moments
n_s electron spin density
$J_{sf}(0)$ is the s-f exchange integral

$\boxed{F(x)=(1/x^4)(x \cos x - \sin x)}$ /Rudderman-Kittel/

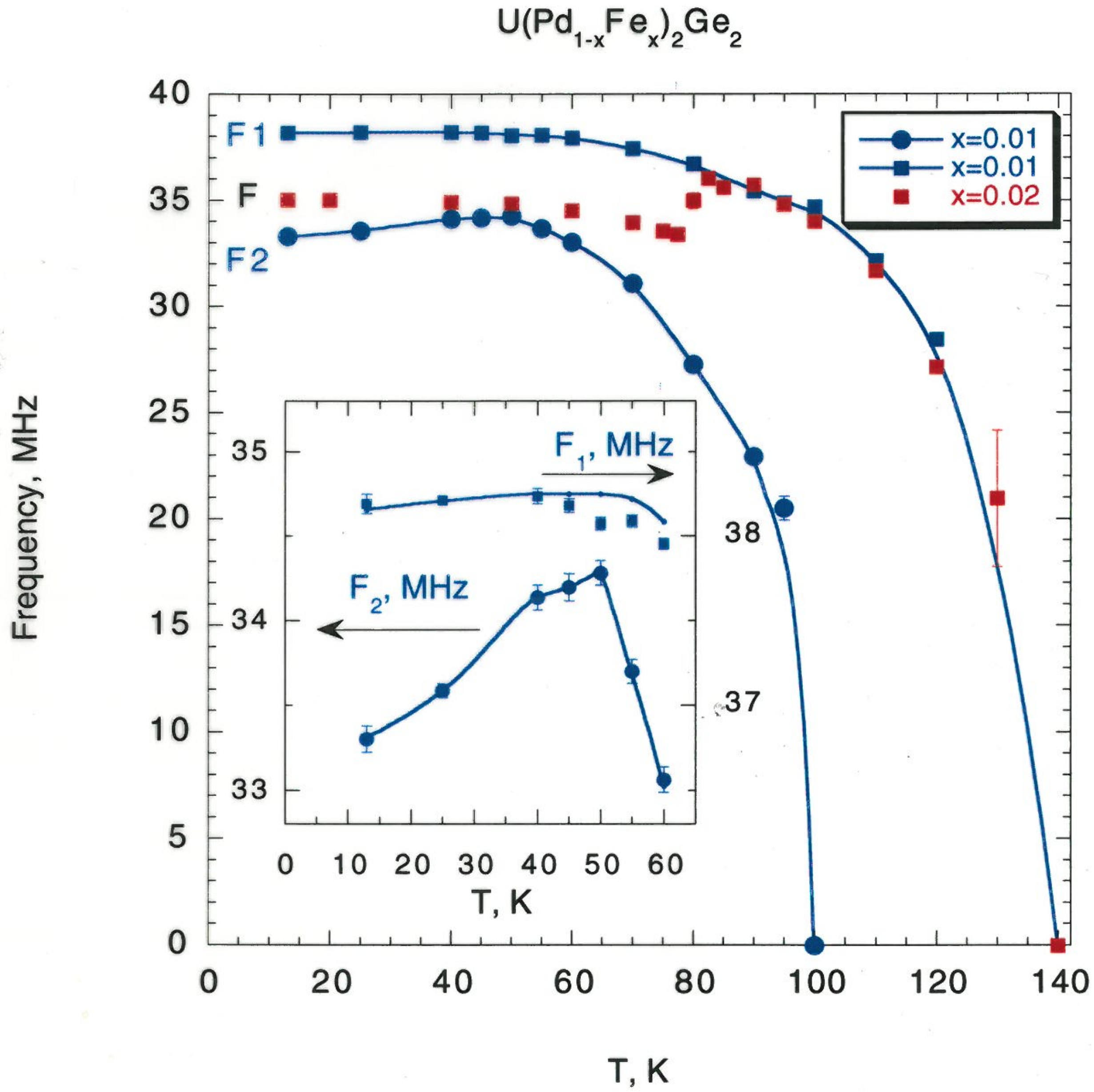




Time dependence of the muon spin polarization in the $U(Pd_{0.99}Fe_{0.01})_2Ge_2$ in zero external field at temperature T=40K and its Fourier transform



x = 0.02
T=75 K
T=80 K
T=100 K
P(t)
0.15
0.1
0.05
0
-0.05
-0.1
-0.15
0
0.05
0.1
0.15
0.2
0.25
0.3
t, μs

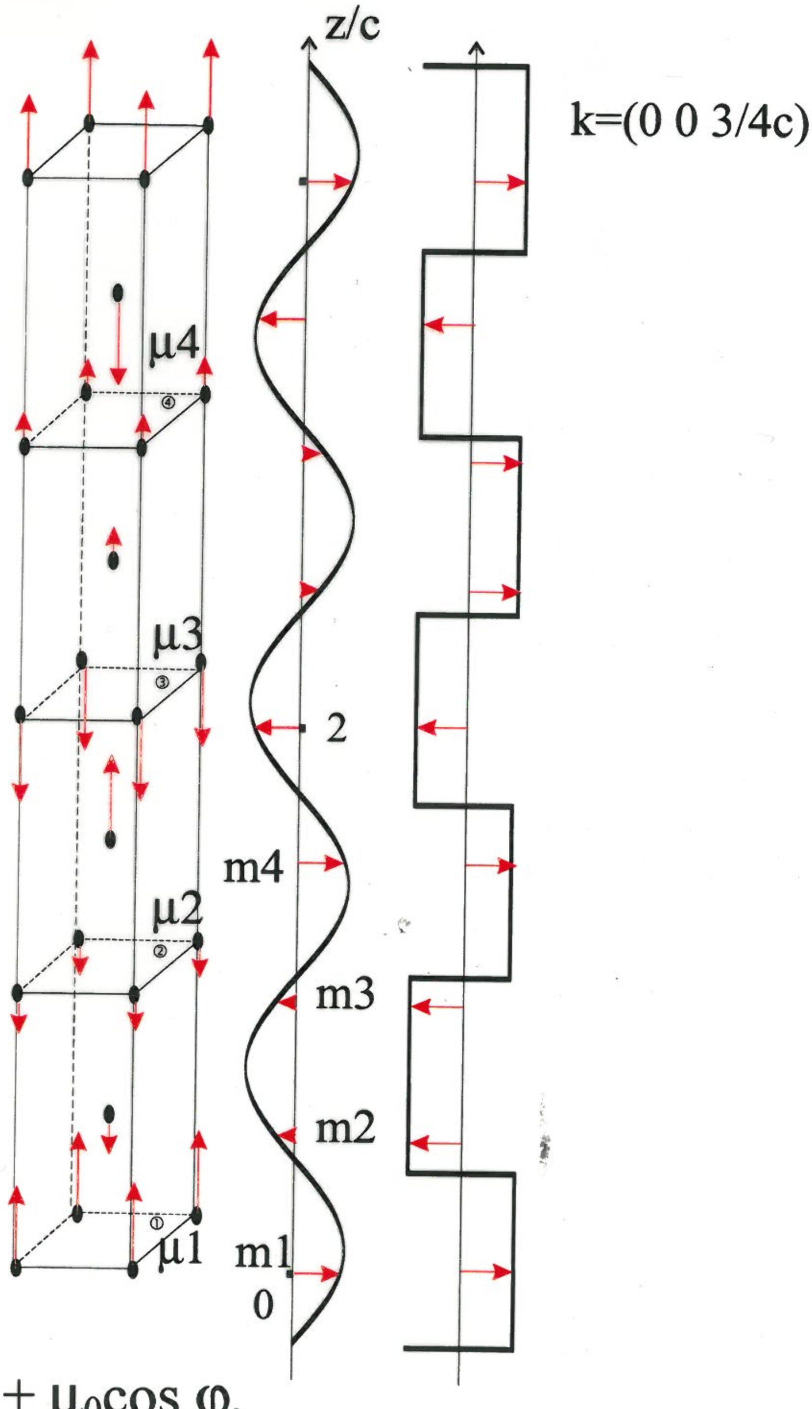


Muon spin precession frequencies F:

$F_1 = \alpha_1 m_1 + \alpha_2 m_2 \qquad F_3 = F_1$

$F_2 = \alpha_1' m_3 + \alpha_2' m_4 \qquad F_4 = F_2$

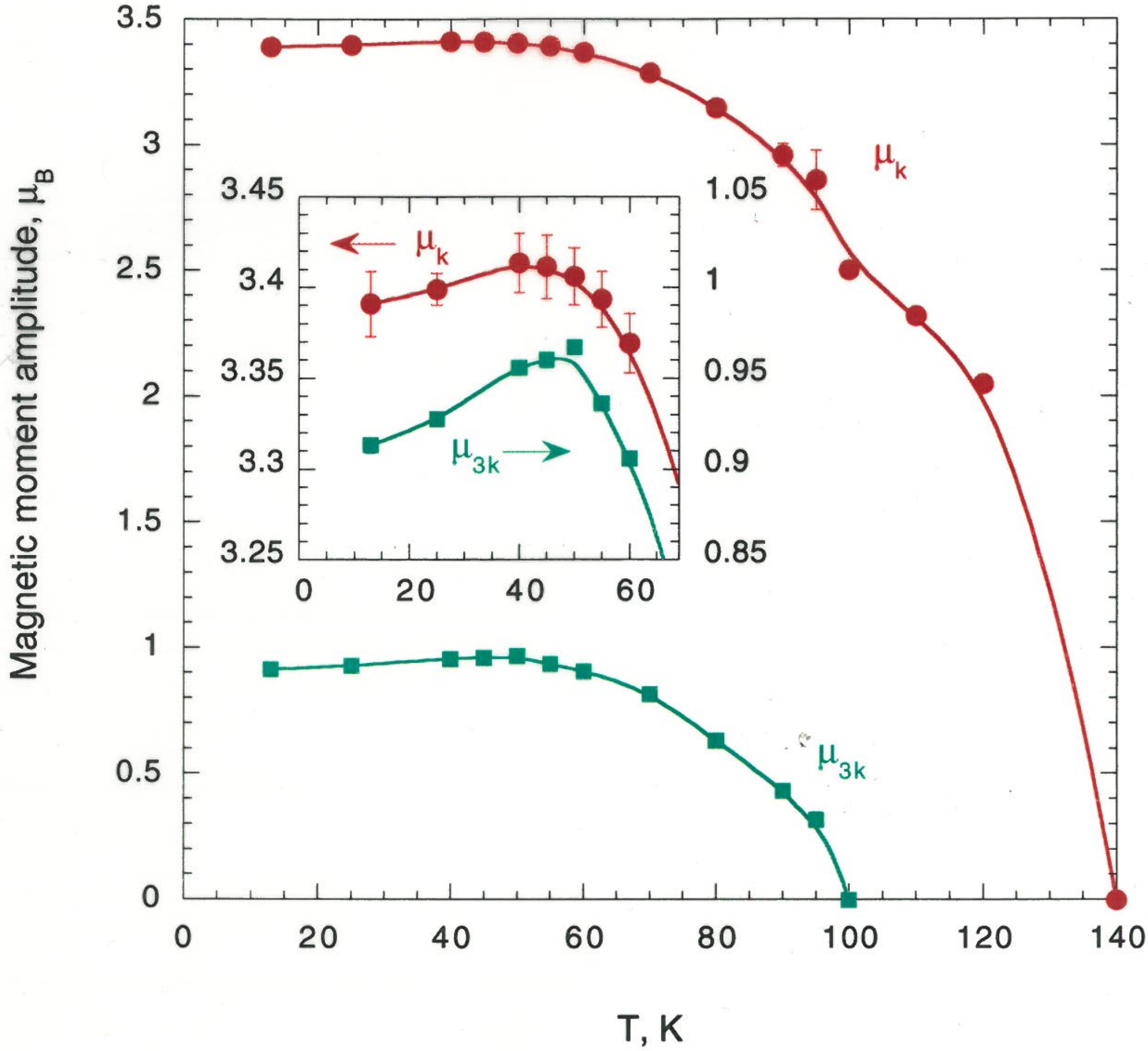
$\alpha_1 \gg \alpha_2,\ \alpha_1' \approx \alpha_1$



$m_1 = m_{\square} + \mu_0 \cos \varphi,$

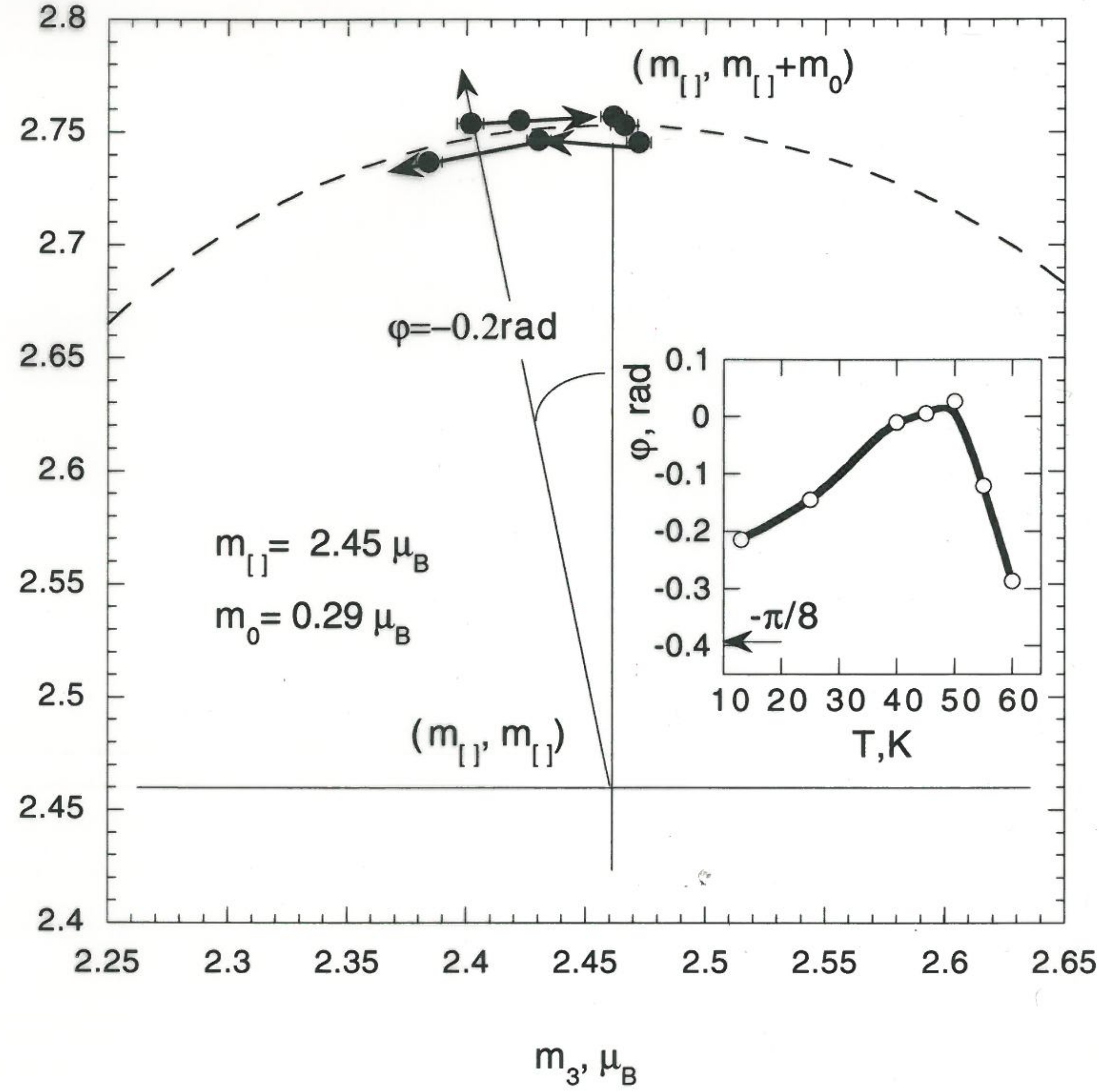
$m_3 = m_{\square} - \mu_0 \sin \varphi,$

μ_0 and $m_{\square}$ are the amplitudes of square and sine modulation.



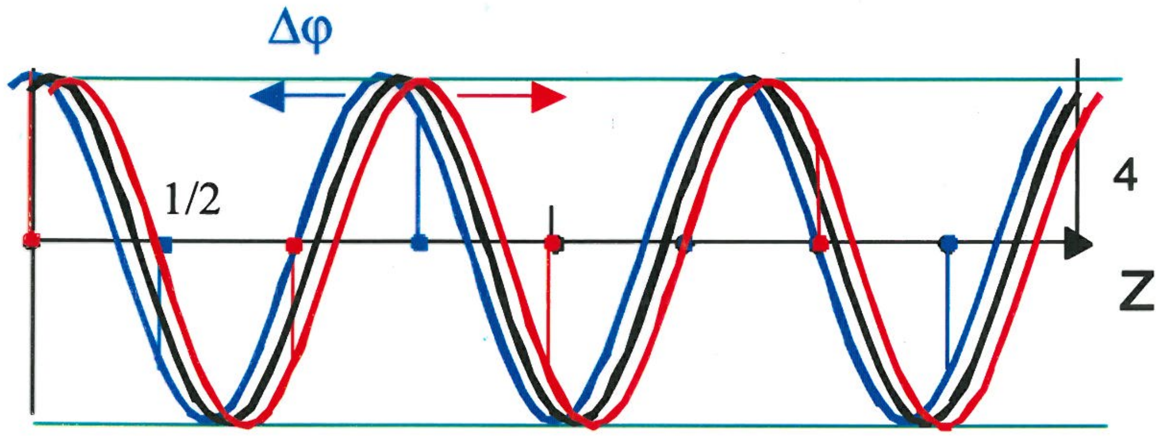
$$\mu_k = \mu_0 + 4/\pi \, m_\square$$

$$\mu_{3k} = 4/3\pi \, m_\square$$



$$m_1(m_3) = m_{\square} + (\mu_0{}^2 - (m_3 - m_{\square})^2)^{1/2}$$

The initial phase shift of modulation.



$$\varphi_1 = \Delta\varphi - \pi/8 \quad (0\ 0\ 0)$$

$$\varphi_2 = -\Delta\varphi - \pi/8 \quad (+1/2\ +1/2\ +1/2)$$

$$\varphi_1 = -\varphi_2 \ -\pi/4$$

Conclusion

In the LSDW phase of $U(Pd_{1-x}Fe_x)_2Ge_2$ (x=0.01) the peculiar temperature behavior of the uranium magnetic moments determined by μSR is connected to the variation of the initial phase φ of the LSDW modulation by $\Delta\varphi \approx 10^\circ$ – a parameter inaccessible in neutron diffraction experiment.

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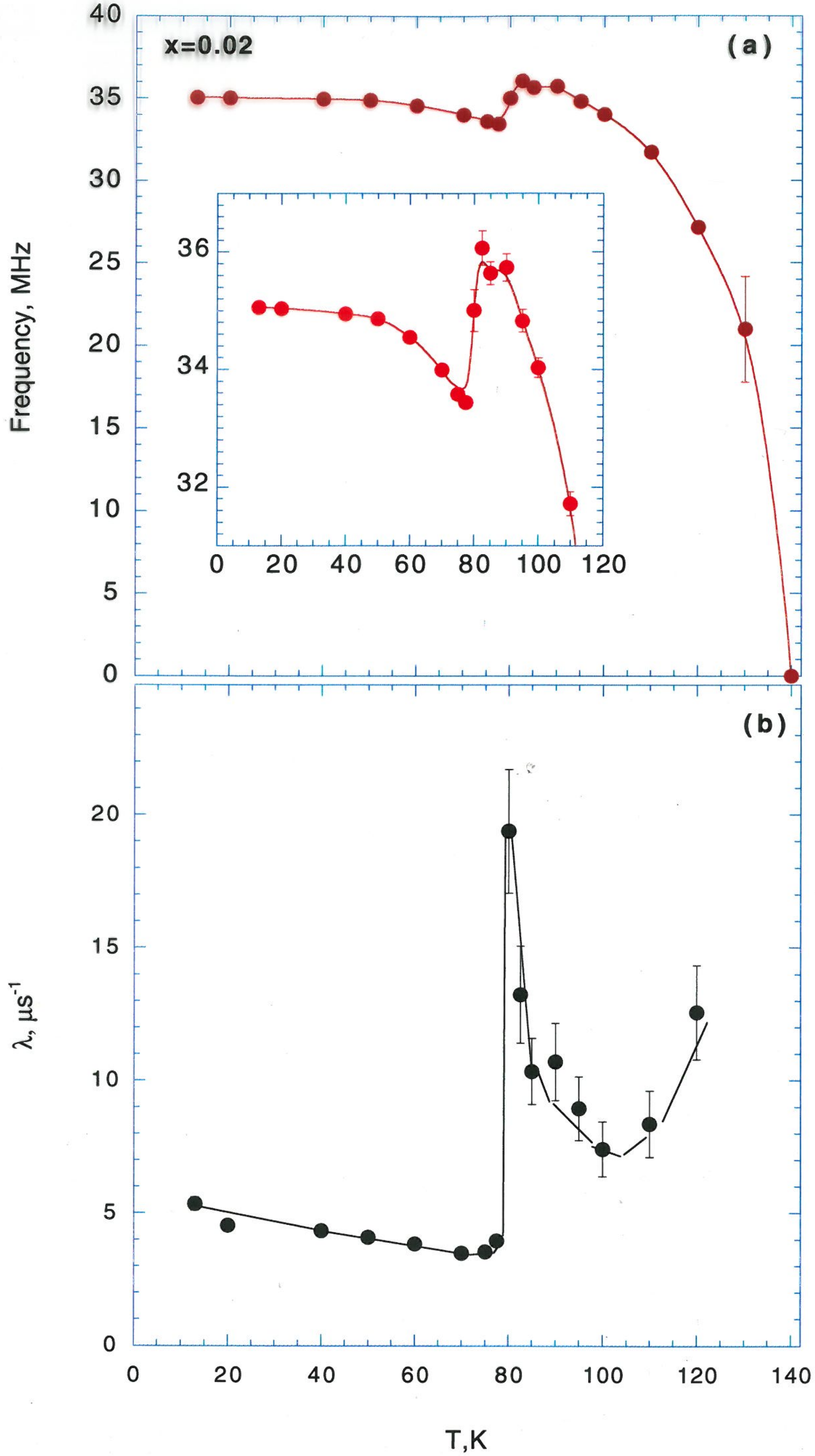
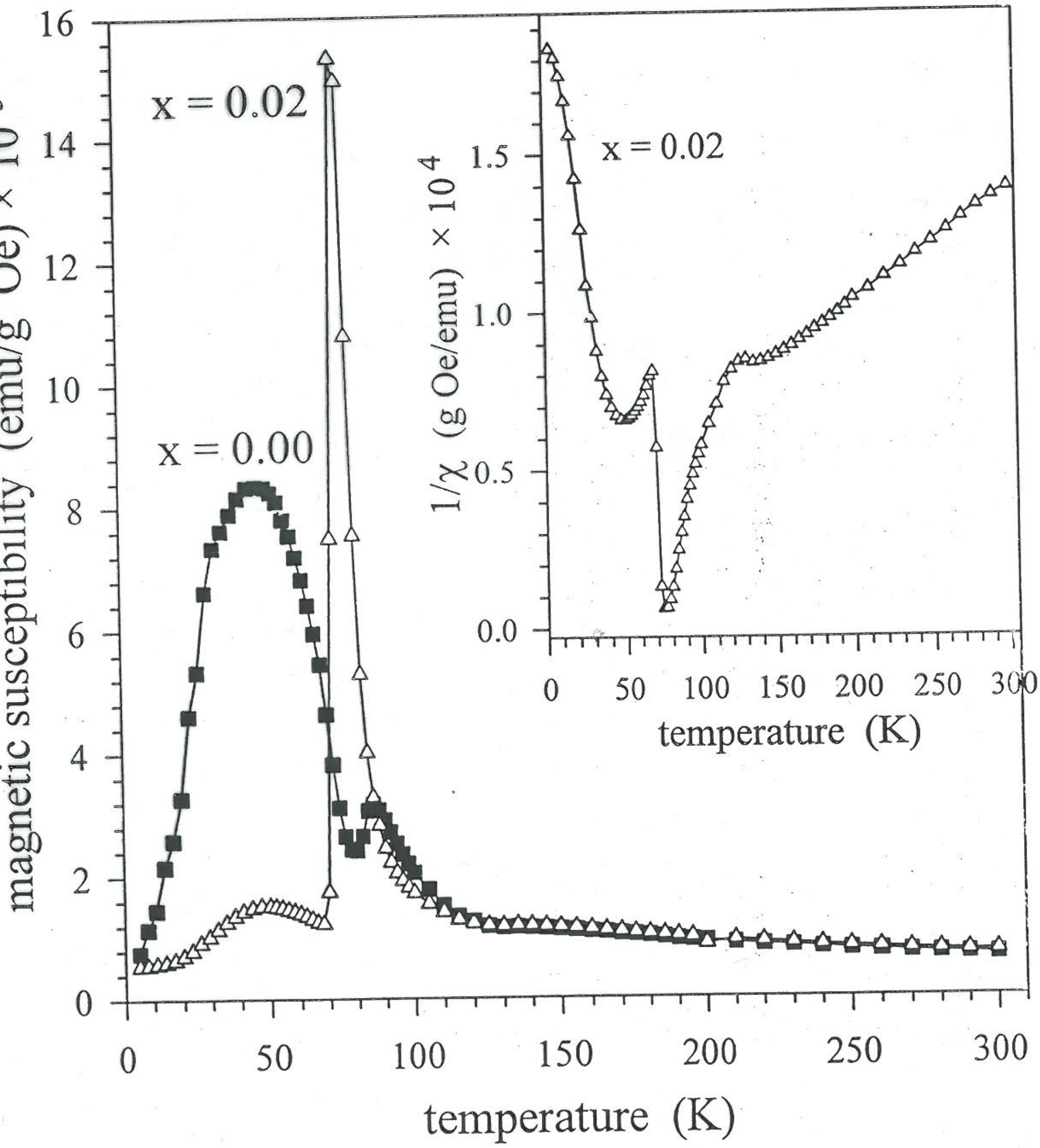
Muon site	B_{dip} /1 μ_B , (G)	μ_U, μ_B
0 1/2 1/8	1016	2.55
0 0 1/2	2113	1.22
1/2 1/2 0	2113	1.22
1/4 1/4 1/4	0	-
0 0 1/4	901	2.87
1/2 1/2 5/16	2067	1.25
1/2 1/4 0	2485	1.04
1/2 0 1/16	2212	1.17
1/8 1/2 3/32	1607	1.61
1/4 1/4 5/32	1099	2.35
1/8 1/8 7/32	884	2.93
Experimental B_μ	2588(3)	

Table 1. The dipole field B_{dip} calculated for possible muon sites in $U(Pd_{0.98}Fe_{0.02})_2Ge_2$ lattice (*I4/mmm*, unit cell parameters a = b = 4.18 Å, c = 10.21 Å) for the simple antiferromagnetic structure with **k** = [0 0 1] for the uranium magnetic moment $\mu_U = 1\ \mu_B$ along the c-axis and the experimentally measured B_μ at T=15 K. The column μ_U shows the uranium magnetic moment expected in dipolar approximation from the experimentally measured B_μ.


x=0.02
(a)
(b)
Frequency, MHz
λ, μs-1
T,K
0
20
40
60
80
100
120
140
0
5
10
15
20
25
30
35
40
32
34
36



magnetic susceptibility (emu/g Oe) × 10^-5
temperature (K)
x = 0.02
x = 0.00
1/χ (g Oe/emu) × 10^4
x = 0.02
temperature (K)