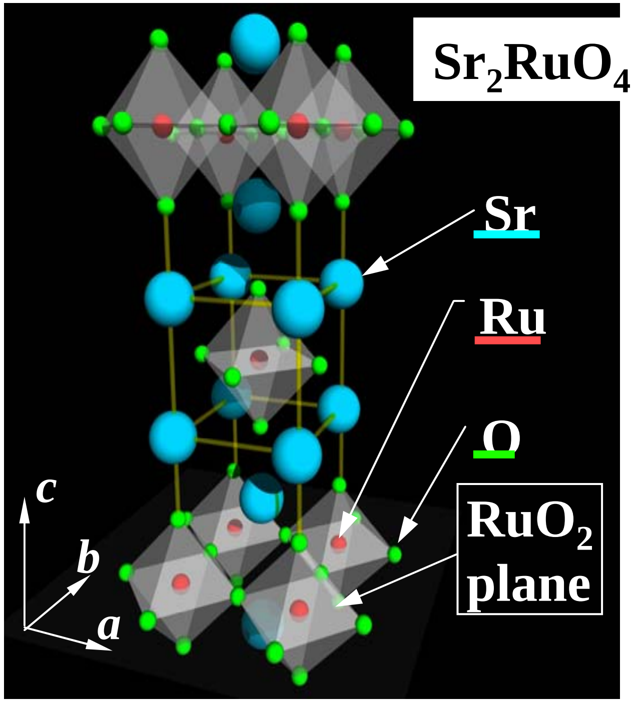
Knight Shift Measurements on Superconducting Sr_2RuO_4



Layered Perovskite structure

Maeno *et al*. Nature 372, 532 ('94)

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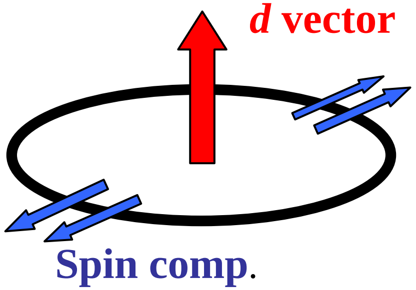
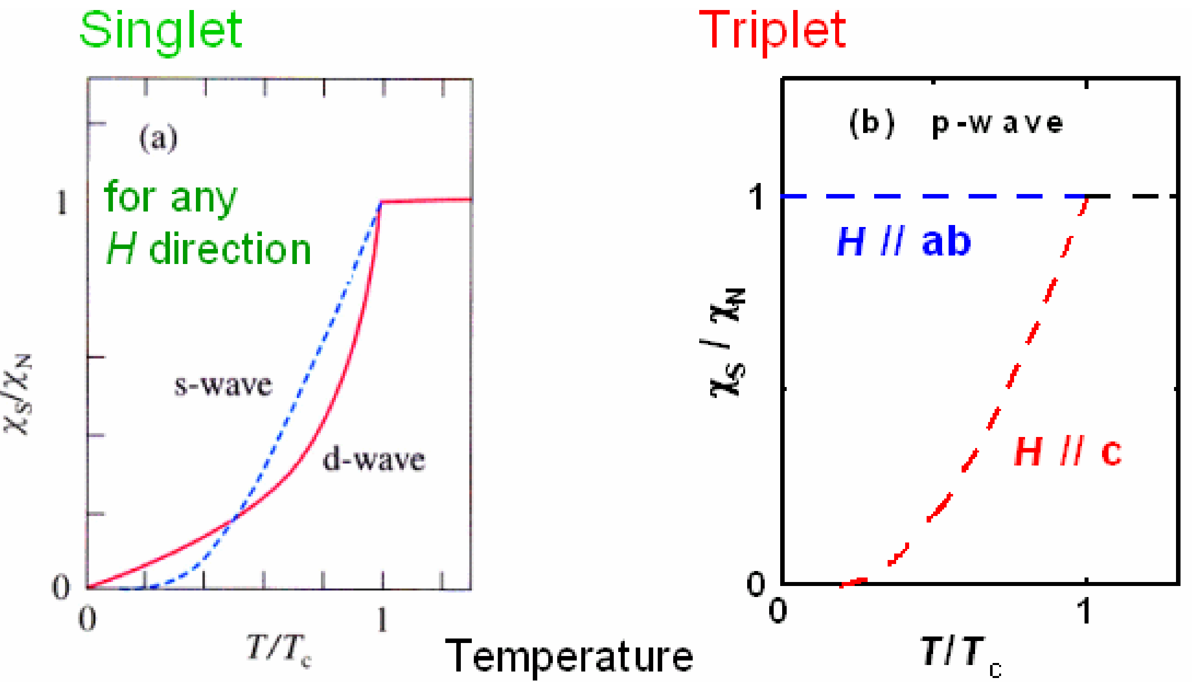
**Tulane Univ.* (USA)

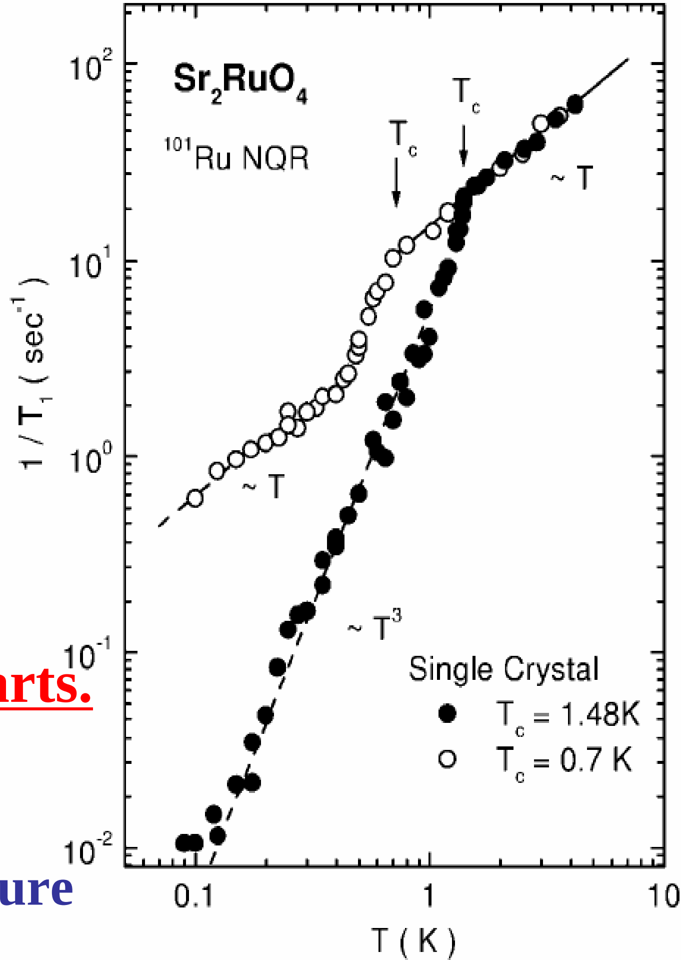
Superconducting wave function

$$\Psi(r_1, \sigma_1 : r_2, \sigma_2) = \chi(\sigma_1, \sigma_2)\ \psi(r_1, r_2)$$

Spin part **Orbital part**







NMR gives important information about both parts.

Knight shift measurements : Spin susceptibility

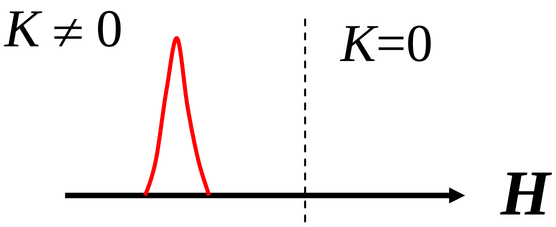
Nuclear spin-lattice relaxation rate $1/T_1$: Gap structure

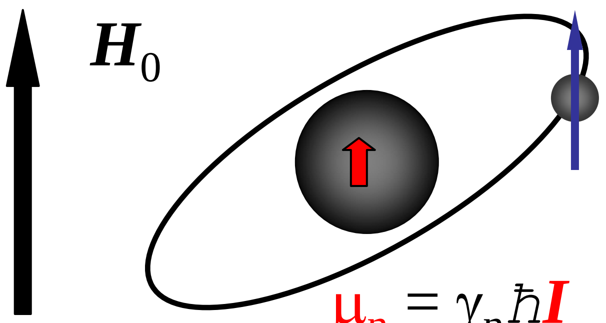
Knight-Shift Measurement

(Hyperfine Interaction)

Interaction between nuclear spins and electronic spins

Nuclear spins ($\boldsymbol{I}$) are coupled with electronic spins ($\boldsymbol{S}$) in the external magnetic field ($\boldsymbol{H}_0$).





$\mu_e = \gamma_e \hbar \boldsymbol{S}$

$\mu_n = \gamma_n \hbar \boldsymbol{I}$

Hamiltonian of the nuclear spins

$$\mathrm{H_Z} = -\gamma_n \hbar\, \boldsymbol{I}\, \boldsymbol{H}_0 + \mathbf{A}\, \boldsymbol{I}\, \boldsymbol{S} = -\gamma_n \hbar\, \boldsymbol{I}\, \boldsymbol{H}_{\mathbf{Loc}}$$

A: Hyperfine coupling constant

$$\boldsymbol{H}_{\mathbf{Loc}} = \boldsymbol{H}_0 - \frac{\mathbf{A}}{\gamma_n \hbar} \boldsymbol{S} = \boldsymbol{H}_0 - \frac{\mathbf{A}}{\gamma_n \hbar} \{ \underbrace{\langle \boldsymbol{S} \rangle}_{\textbf{av. static}} + \underbrace{\delta \boldsymbol{S}}_{\textbf{dynamics}} \}$$

Shift of the spectrum (Static properties)

$$\boxed{\boldsymbol{K} = \frac{\boldsymbol{H}_0 - \langle \boldsymbol{H}_{\mathrm{Loc}} \rangle}{\boldsymbol{H}_0} = \frac{\mathrm{A}}{\gamma_n \hbar} \cdot \frac{\langle \boldsymbol{S} \rangle}{\boldsymbol{H}_0} = \frac{\mathrm{A}}{N_A \gamma_e \gamma_n \hbar^2} \chi}$$

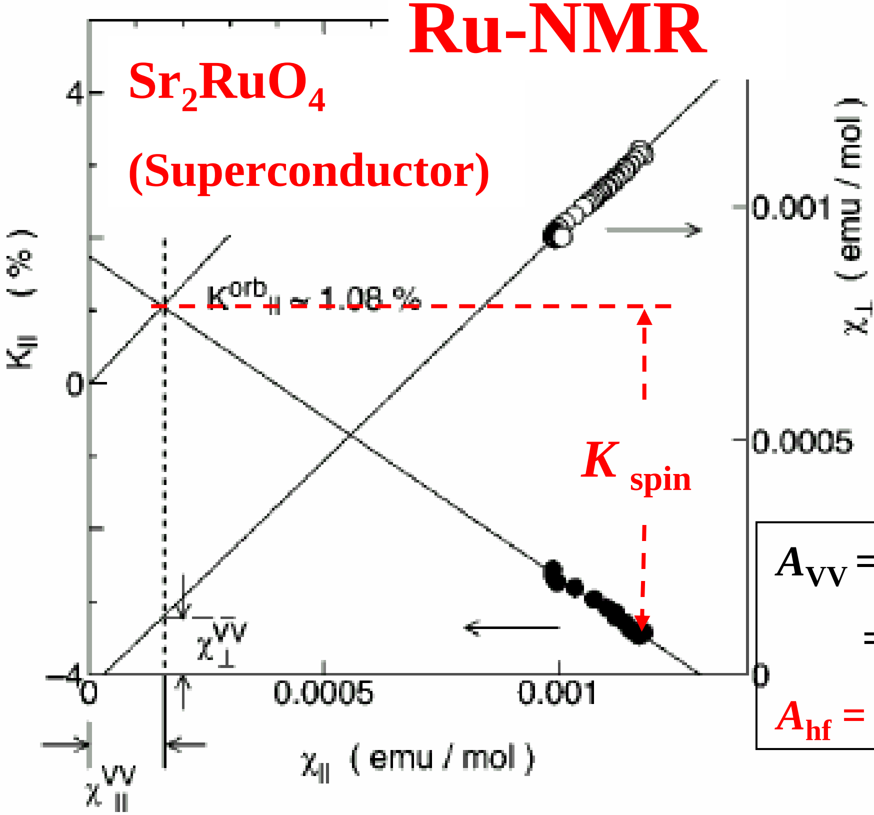
$$\left(\chi = \frac{\boldsymbol{M}}{\boldsymbol{H}_0} = \frac{N_A \gamma_e \hbar \langle \boldsymbol{S} \rangle}{\boldsymbol{H}_0} \right)$$

Example of *K*- χ plot

Ru-NMR

Sr$_2$RuO$_4$

(Superconductor)



***K* spin**

$A_{VV} = 2\mu_B\langle r^{-3}\rangle$

$= 384 \text{kOe}/\mu_B$

$A_{hf} = -250$ kOe/μB

FIG. 2. Plot of $^{99}K_{\parallel}$ (Ref. 18) against $\chi_{\parallel}$ (left scale). The relation between $\chi_{\perp}$ and $\chi_{\parallel}$ are also plotted (right scale).

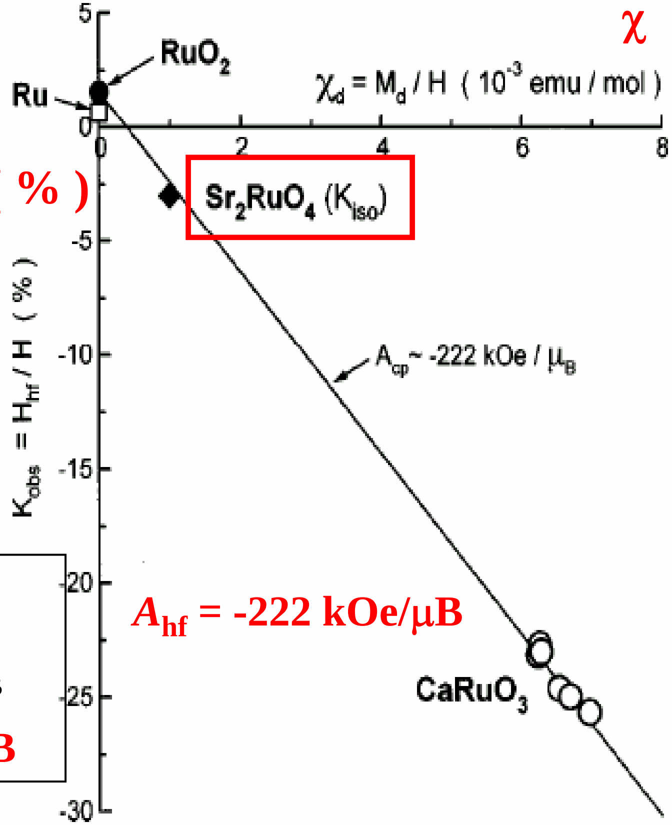
$$K_{\text{spin}} = \frac{A_{\text{hf}}}{\mu_B N_A}\chi_{\text{spin}} \quad \sim -4.5\ \%$$

$$K_{\text{orb}} = \frac{A_{VV}}{\mu_B N_A}\chi_{VV} \quad \sim 1\ \%$$

CaRuO$_3$ (Nearly Ferro. Metal)

χ

***K* (%)**

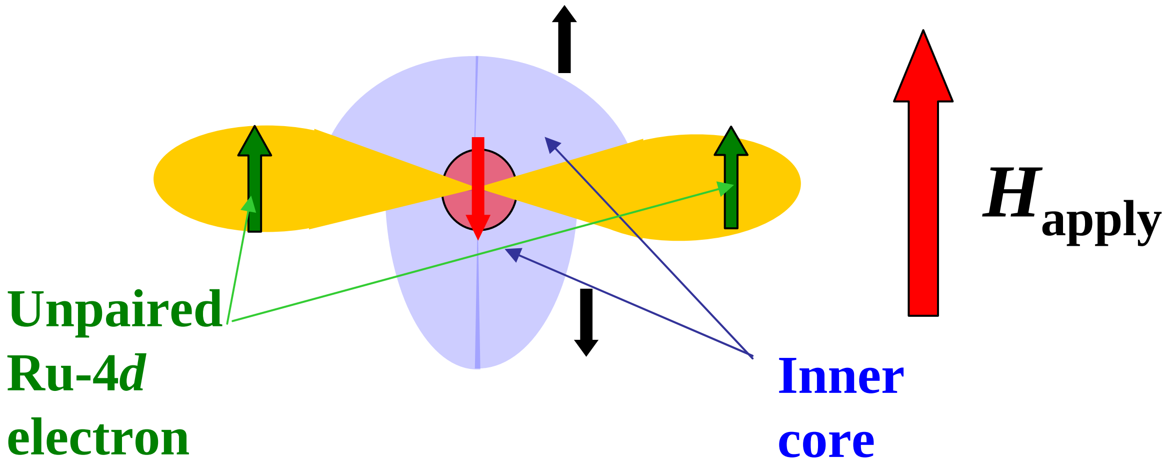


$A_{hf} = -222$ kOe/μB

FIG. 5. Knight shift vs susceptibility $[M_d(H)/H]$ with an implicit parameter of the external field H. The hyperfine coupling constant due to the inner core polarization $A_{cp} \approx -222 \pm 50$ kOe/μ_B is estimated from a slope of linear line when $K_{5s} + K_{orb}$ is assumed to be the same value as $K_{obs} = +1.59\%$ in RuO$_2$. This value is close to $A_{hf} \sim -300 \pm 60$ kOe/μ_B in the FM state of SrRuO$_3$. Note that the Knight shift for Sr$_2$RuO$_4$ lies on the same line of K_{obs} vs χ_{obs} plot as that for CaRuO$_3$.

Core polarization effect

Inner Core Polarization Effect by Unpaired *d* electrons



$$H_{\text{nul.}} \qquad \sum_i \left\{ |\psi_i(0)|_\uparrow^2 - |\psi_i(0)|_\downarrow^2 \right\}$$

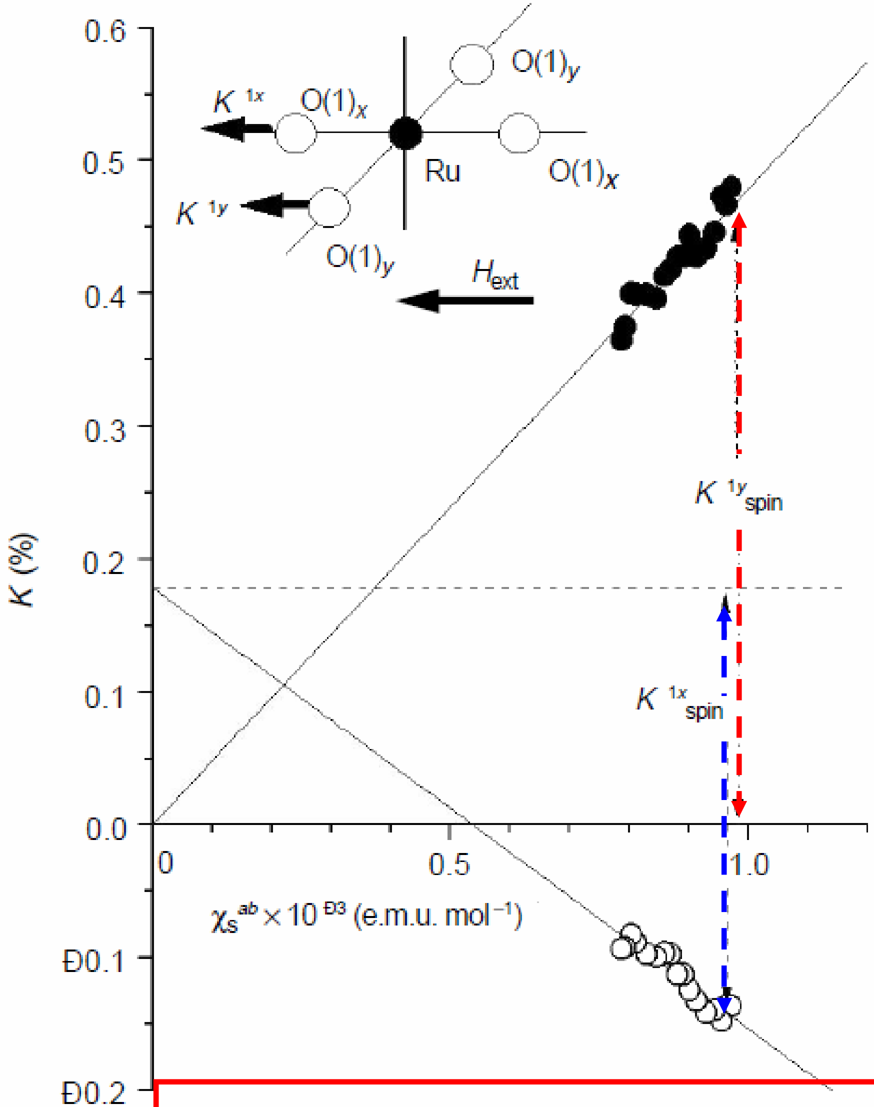
Negative isotropic field is induced

$$K_{\text{CP}} = \frac{8\pi}{3} \chi_{\text{d}} \sum_i \left\{ |\psi_i(0)|_\uparrow^2 - |\psi_i(0)|_\downarrow^2 \right\}$$

	A_{hf}
Sr_2RuO_4 (SC.)	~ -250 kOe/μ_B
c.f. $SrRuO_3$ (Ferro.)	H_{int} / M_0 ~ -300 kOe/μ_B
$CaRuO_3$ (NearlyFerro.)	~ -222 kOe/μ_B

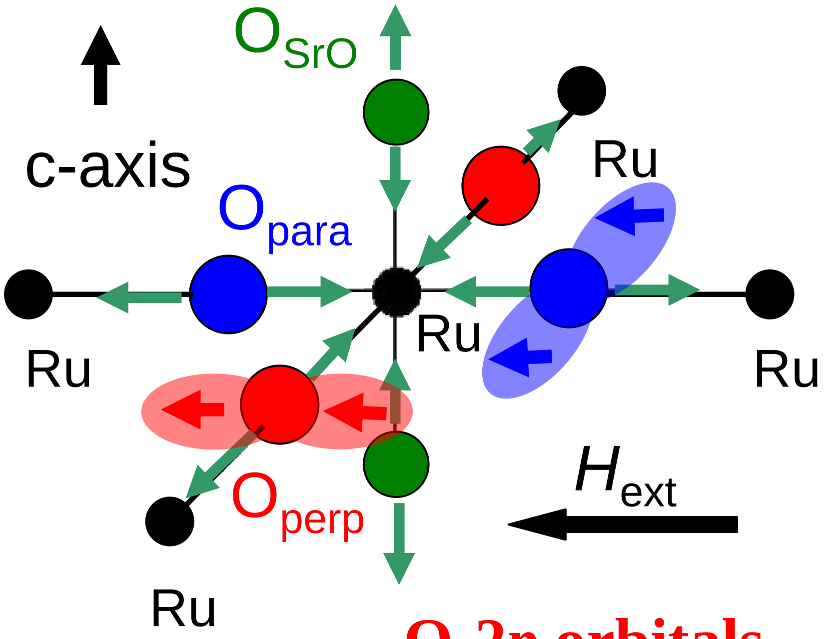
Ru-4*d* state is in the Fermi level in these Ruthenates

Knight-Shift Measurement at O site 17O-NMR

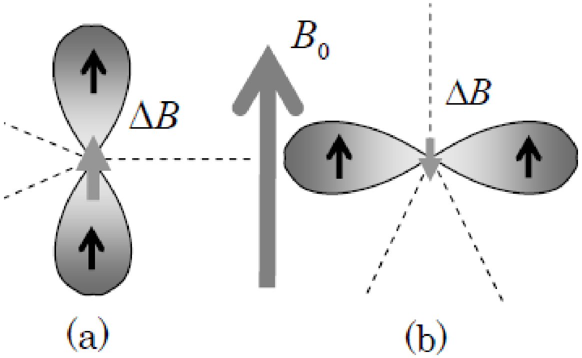


K_{spin}^{x} ~ -0.3 %

K_{spin}^{y} ~ 0.5 %



O-2*p* orbitals



O-2p orbitals hybridized with Ru-4*d*xy orbitals are important.

^{17}O Knight Shift measurement

K. Ishida *et al.*Nature 395, 658 (98)

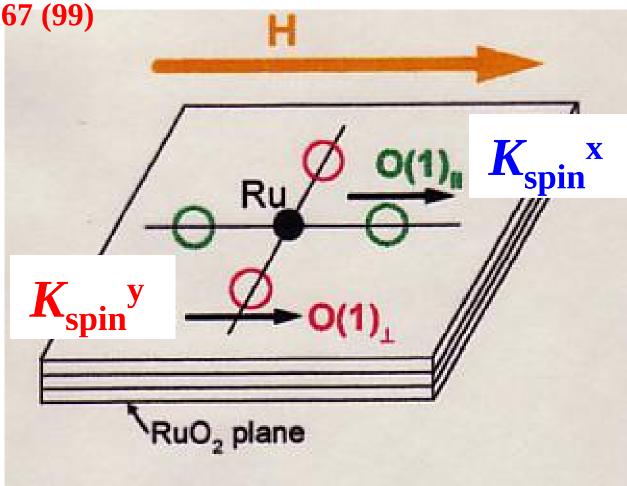
Mukuda *et al.* J. Low Temp. Phys. 117, 1567 (99)

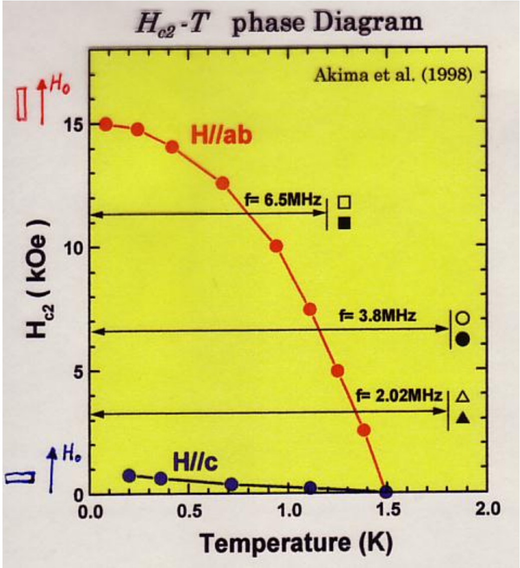
Spin part in *K*

$K_{spin}^{x} = -0.3\ \%$

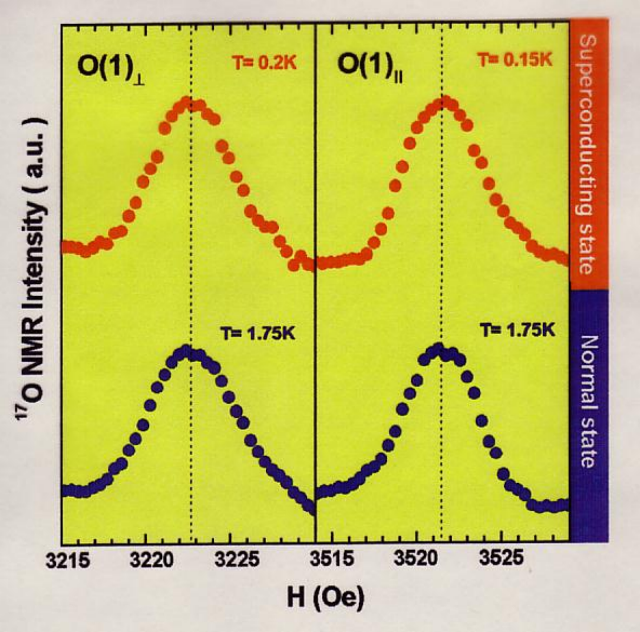
$K_{spin}^{y} = 0.5\ \%$

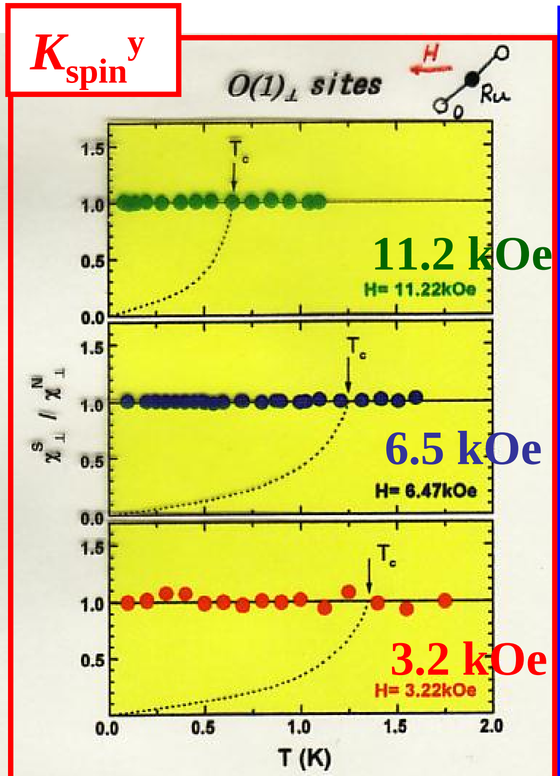
H // ab ~ 3.5 kOe

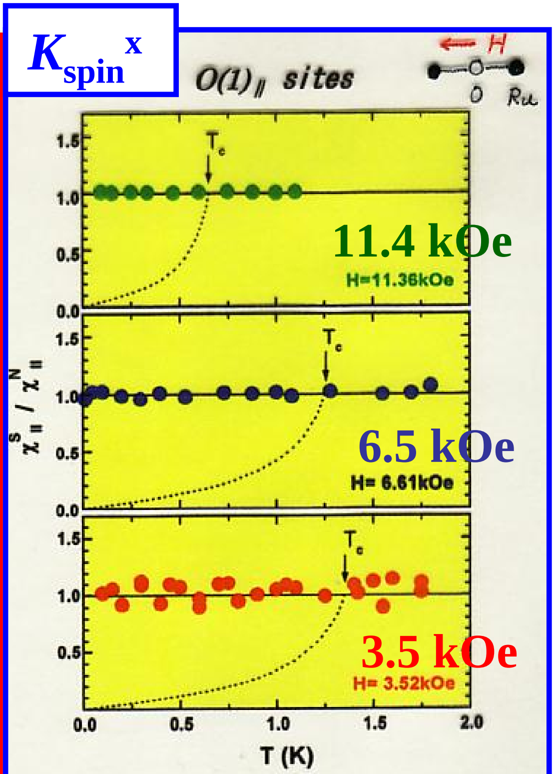




FWHM ~ 5Oe

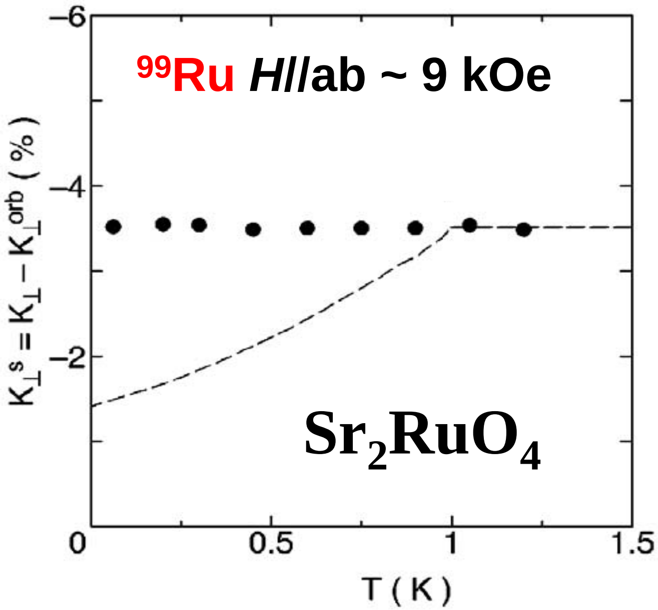


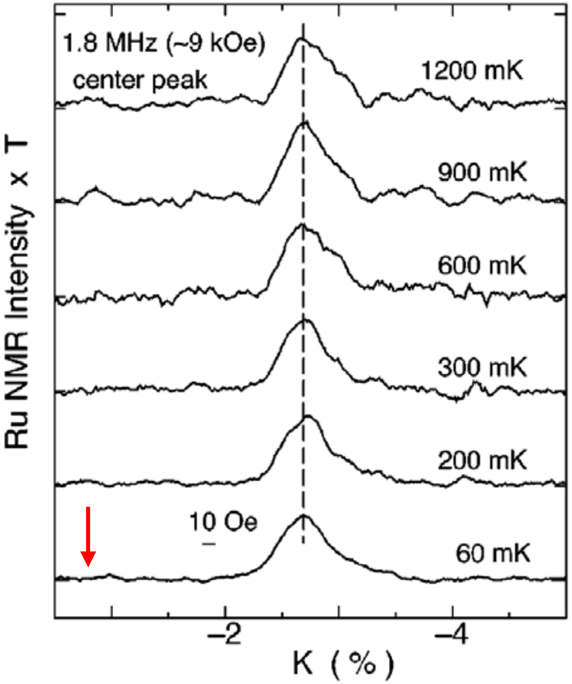




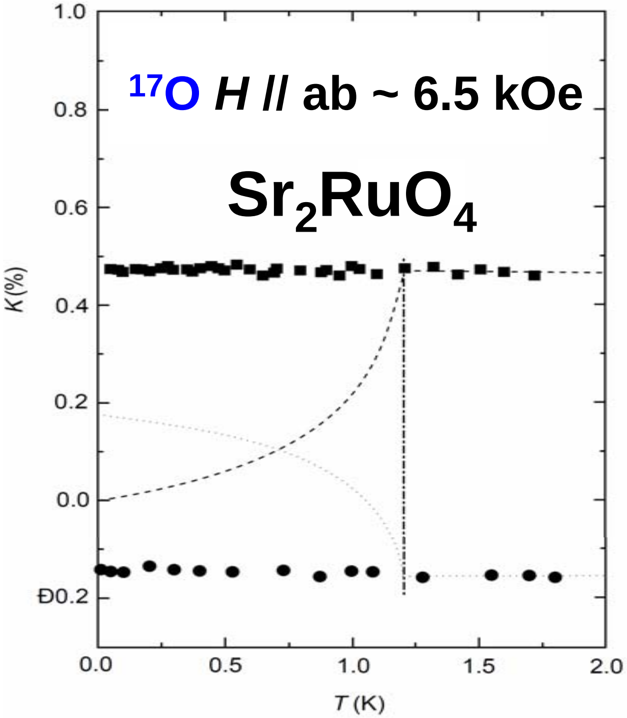
Ru, ^{17}O Knight-shift measurements

H* > 3 kOe // *ab





K.Ishida H. Mukuda, Y. Kitaoka *et al.*
Phys. Rev. B 63 (2001) 060507(R).



K.Ishida H. Mukuda Y. Kitaoka *et al.* Nature. 396 (1998) 658.

Knight-shift is unchanged in the SC state

Spin-triplet superconductivity

KS behavior in the SC state

T-dep. *KS* in Sr_2RuO_4

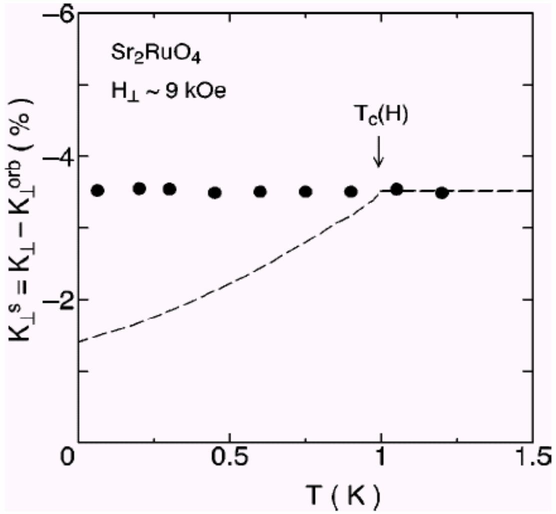
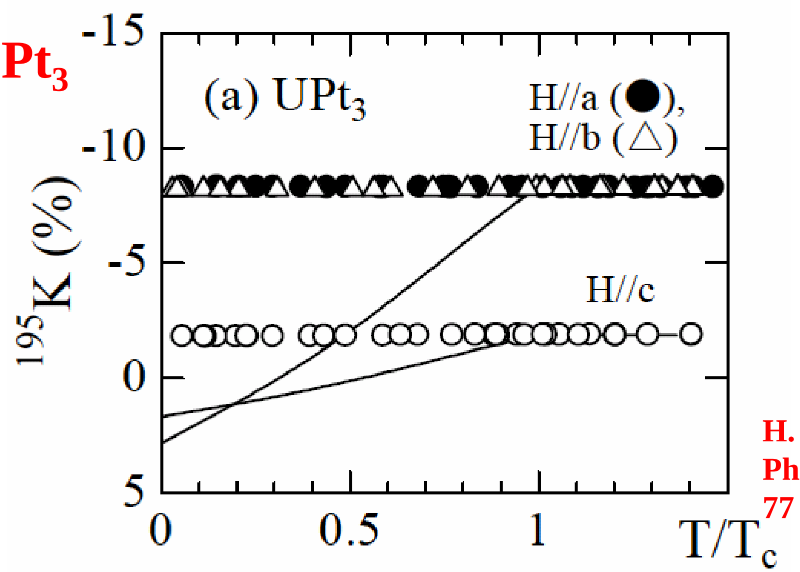


FIG. 6. Temperature dependence of $^{99}K_\perp^s$. The dotted curve is the calculation based on the spin-singlet *d*-wave ($d_{x^2-y^2}$) model with a line node (see text).

K.Ishida *et al.* Phys. Rev. B 63, 060507(R)

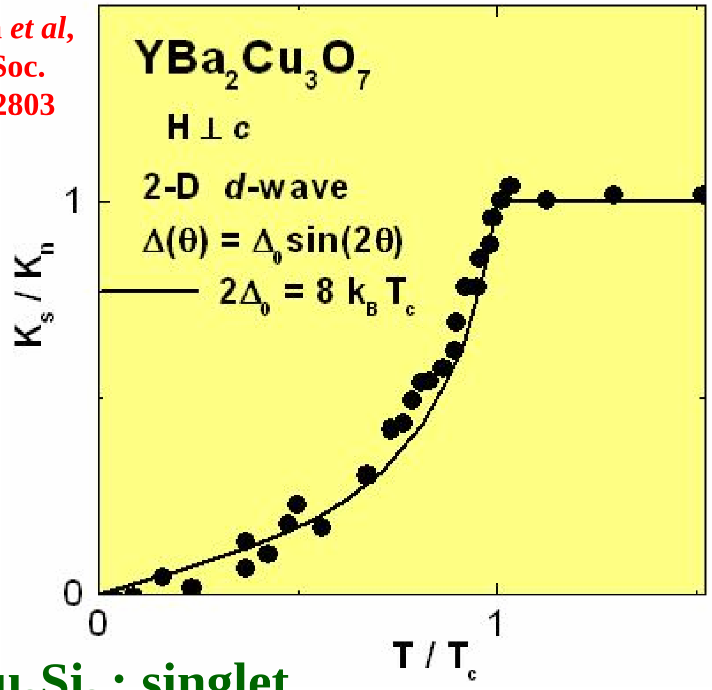
UPt_3



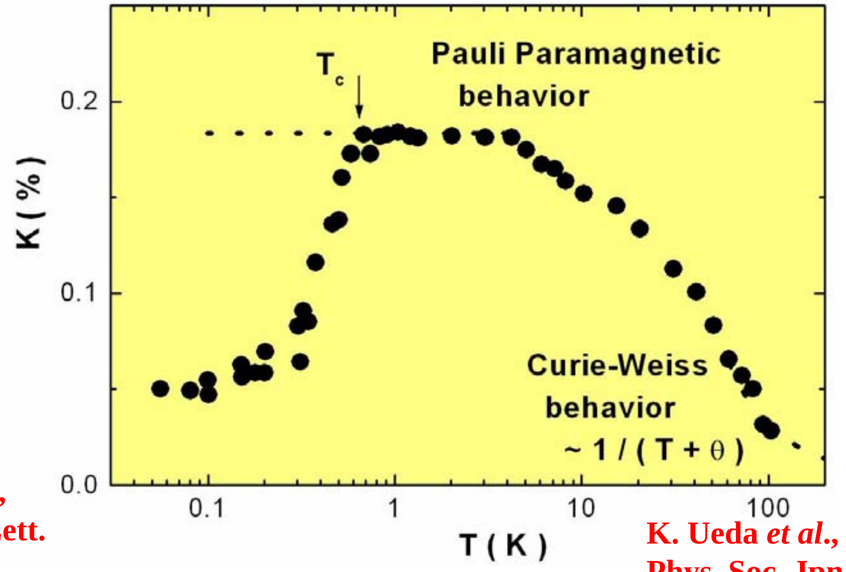
H. Tou *et al.*, Phys. Rev. Lett. 77 1374 (96)

High-T_c : singlet

K. Ishida *et al*, J. Phys. Soc. Jpn. 63, 2803 (93)



$CeCu_2Si_2$: singlet



K. Ueda *et al.*, J. Phys. Soc. Jpn 56, 867 (87)

Other example (Spin-singlet Superconductor)

$PuCoIn_5$ (T_c ~ 20 K)

N. Curro *et al.* Nature 434, 622 (05)

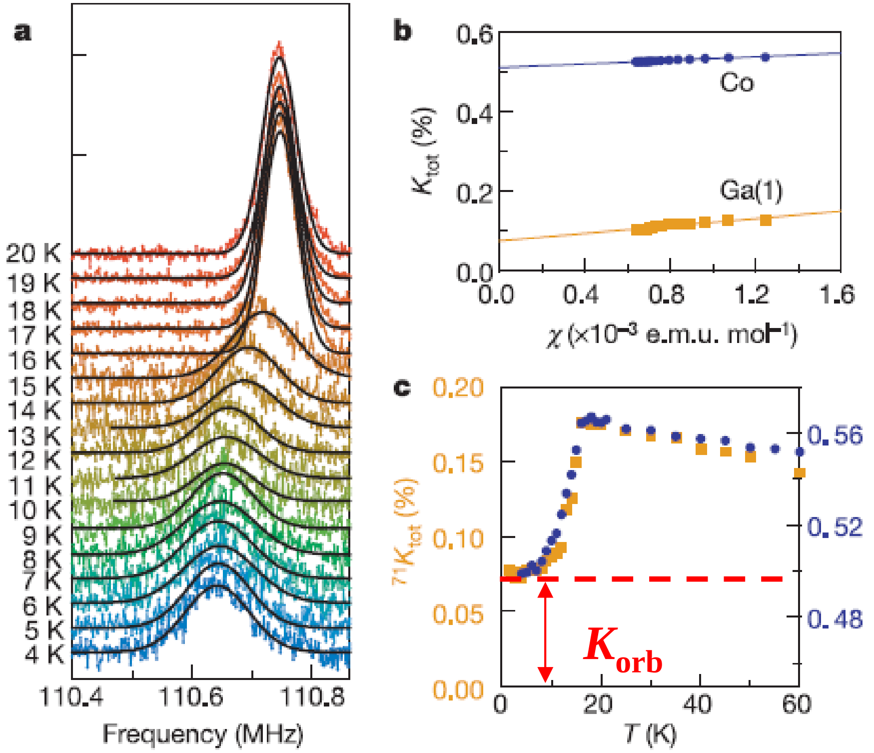
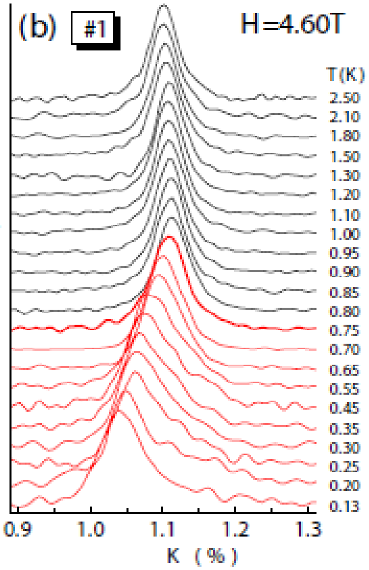


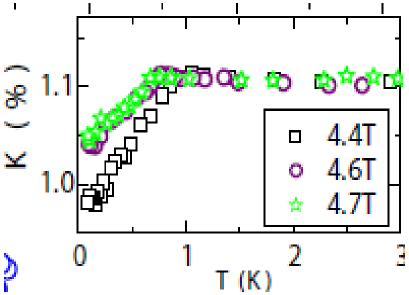
Figure 1 Knight shift measurements in $PuCoGa_5$. **a**, NMR spectra of ^{71}Ga in 8 T at a series of temperatures through T_c. The spectra have been offset vertically for clarity. Solid lines are gaussian fits. **b**, The normal-state magnetic shift K_{tot} of the ^{59}Co and $^{71}Ga(1)$ versus bulk susceptibility χ. The intercepts and hyperfine constants are given by $^{59}K_{orb} = 0.53\%$, $^{71}K_{orb} = 0.088\%$, and $^{59}A = 1.5\,kOe\,\mu_B^{-1}$, $^{71}A = 4.1\,kOe\,\mu_B^{-1}$. Solid lines are fits to the low-temperature data. **c**, The total magnetic shift K_{tot} of the ^{59}Co and $^{71}Ga(1)$ versus temperature.

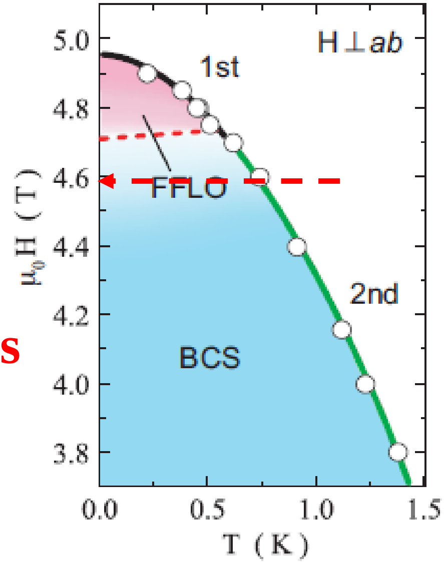
$CeCoIn_5$ (T_c ~ 2.3 K)

Kumagai *et al.*

PRL 97, 267204 (06)



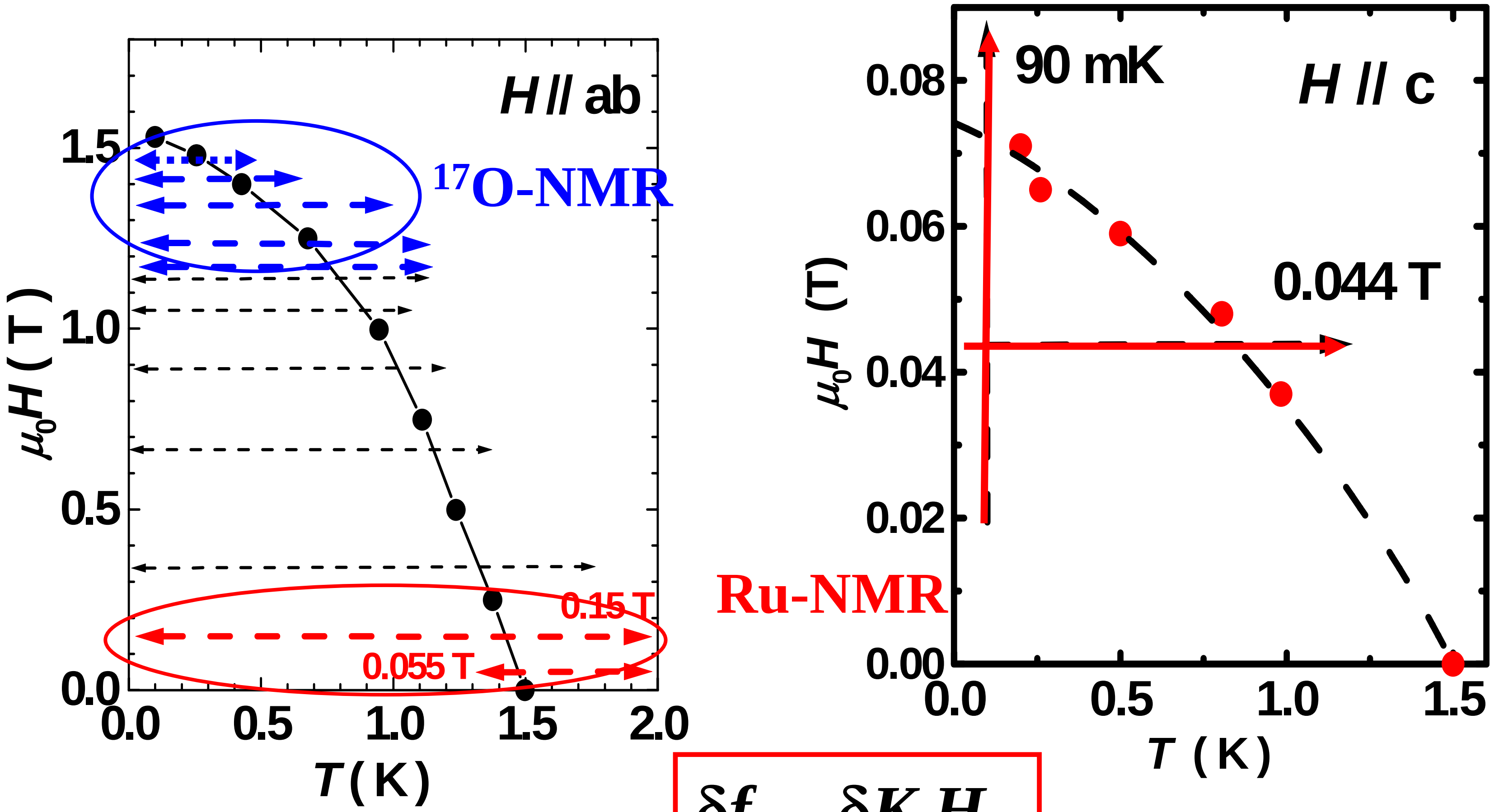




K.S. decreases even near H_{c2}

Summary of the Knight-Shift Measurements so far

Applied fields were controlled with an accuracy less than 0.5 degree.

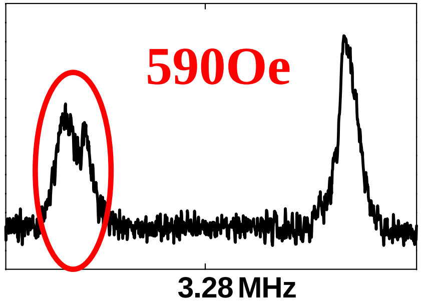


$$\boxed{\delta f \qquad \delta K\, H}$$

Knight shift is unchanged in the field of $\mu_0 H_{ab} > 0.055$ T, $\mu_0 H_c > 0.02$ T.

T dependence of ^{101}K at H = 440 Oe

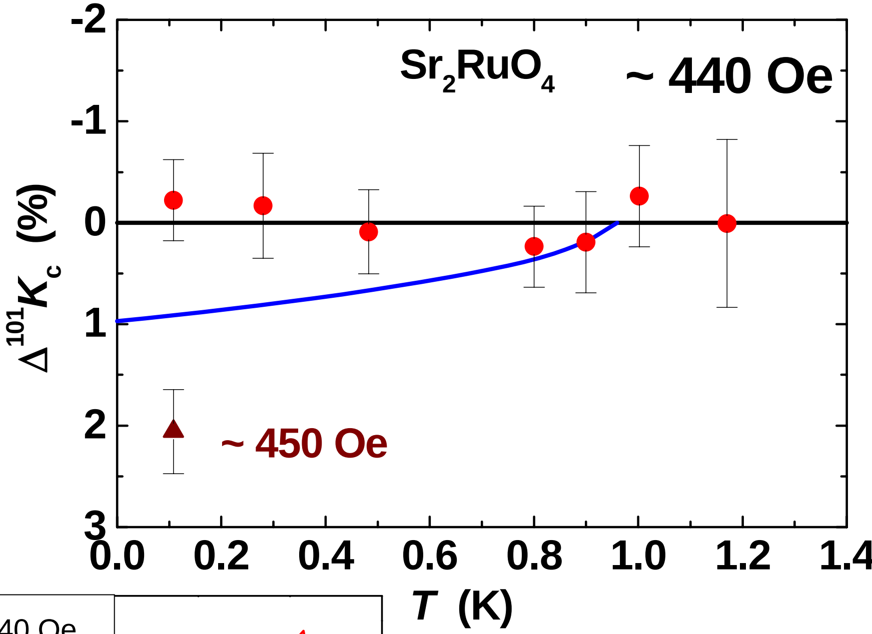
H // c

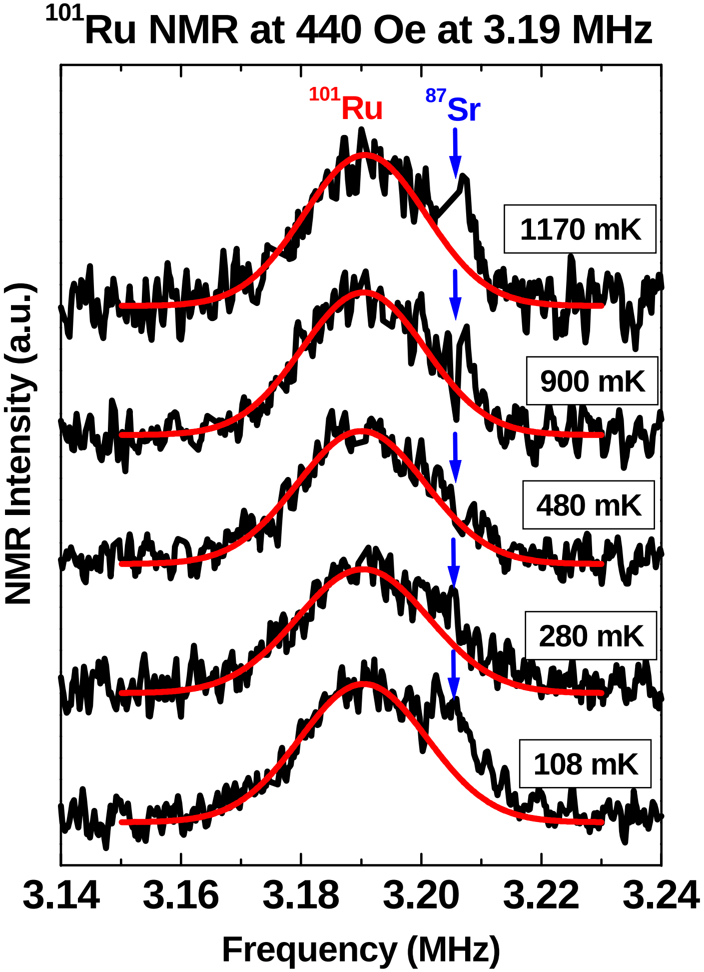


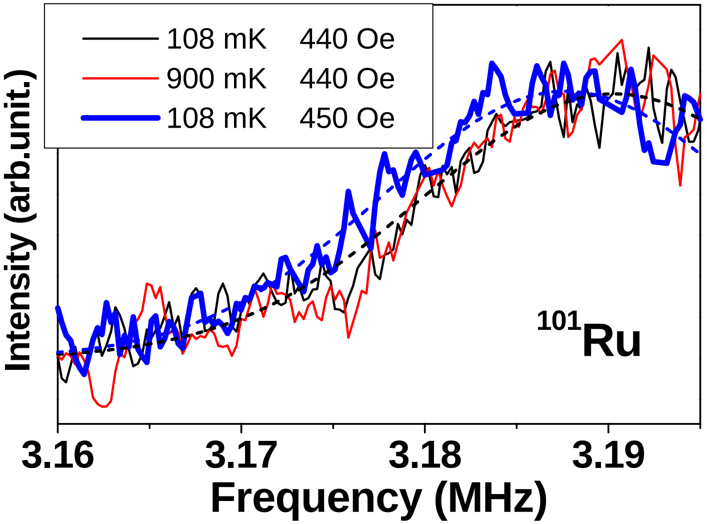
Ru-NMR

H//c

κ ~ 2.3







$\delta K \sim 1\%$

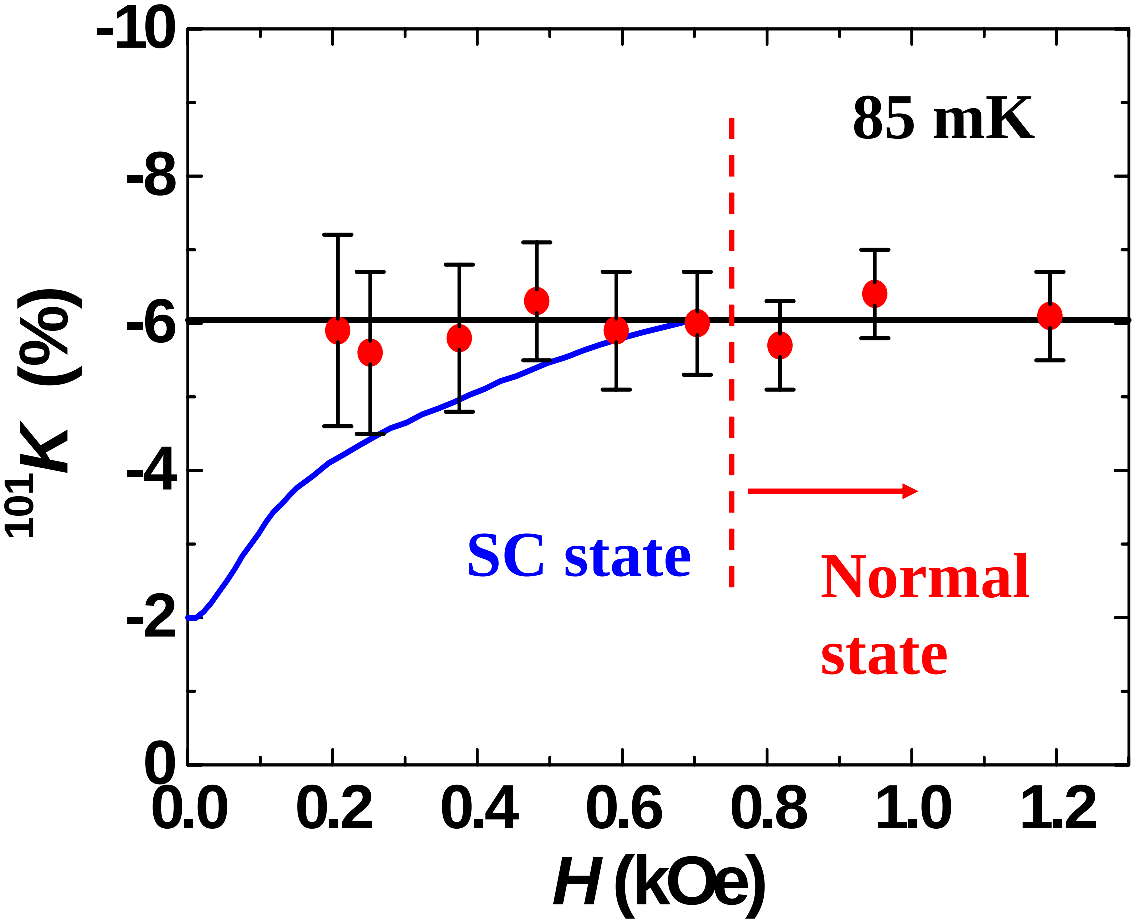
$\delta H = 4.4$ Oe

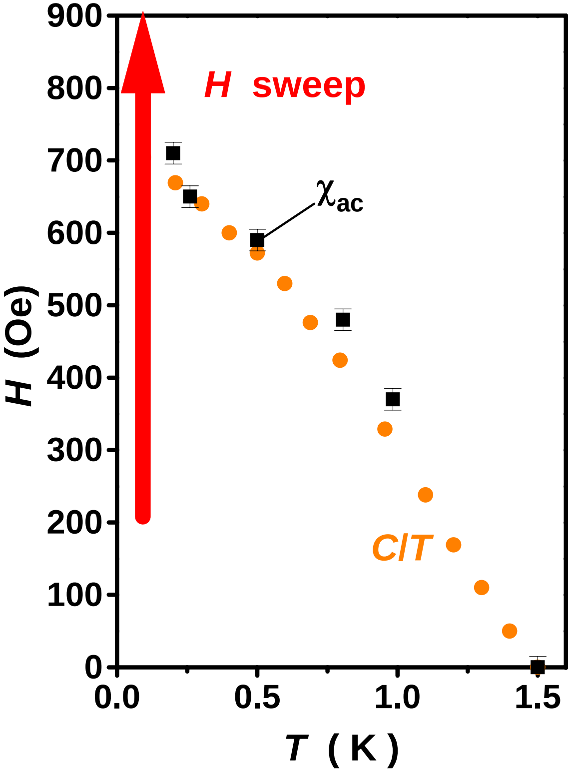
$\delta f = \gamma \times \delta H$

~ 1 kHz

Within the experimental accuracy,
^{101}K is invariant with *T*.

H dependence of the Ru Knight Shift at Low *T*

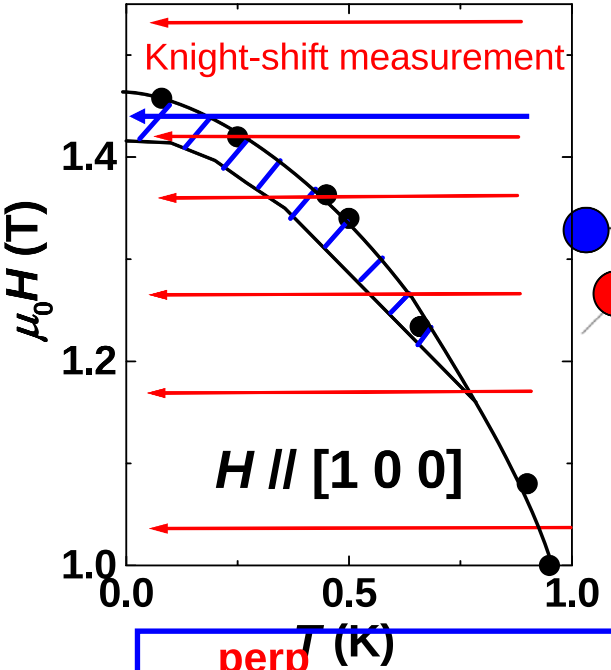


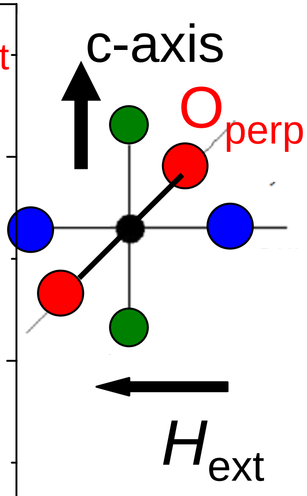


Within the experimental accuracy,

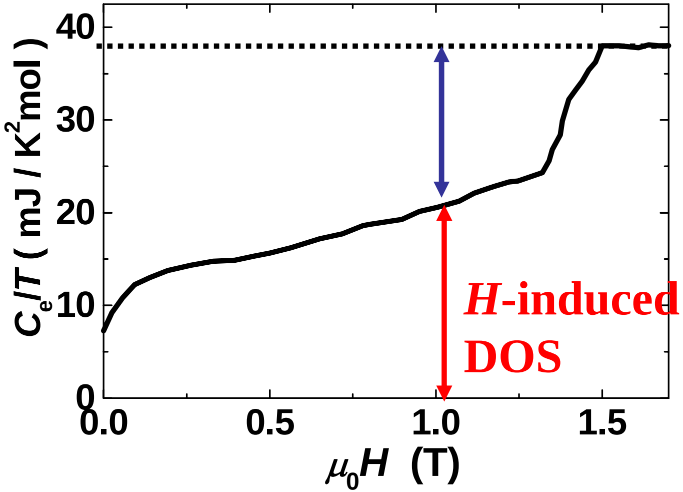
$^{101}K_S$ (~ – 2%) **is unchanged across** T_c.

^{17}O NMR at ``D” phase

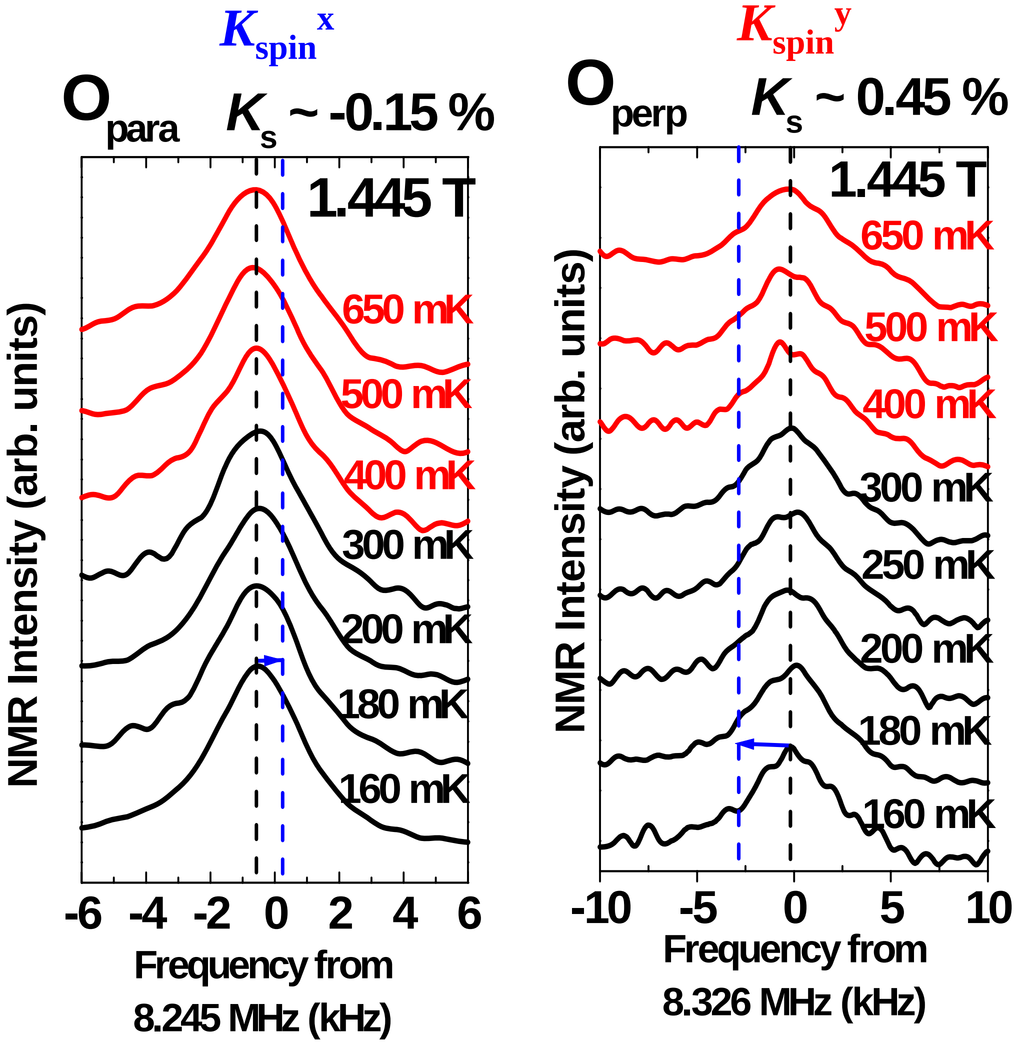




K_{spin}^{perp} ~ 0.47 %



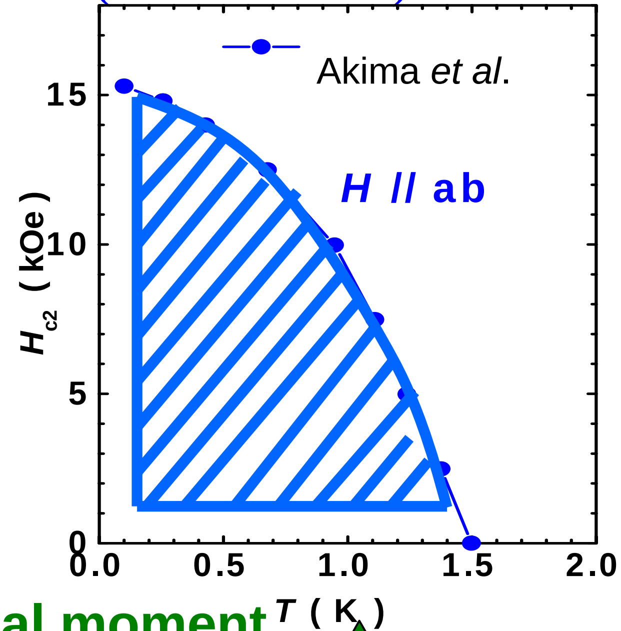
^{17}O NMR



Summary

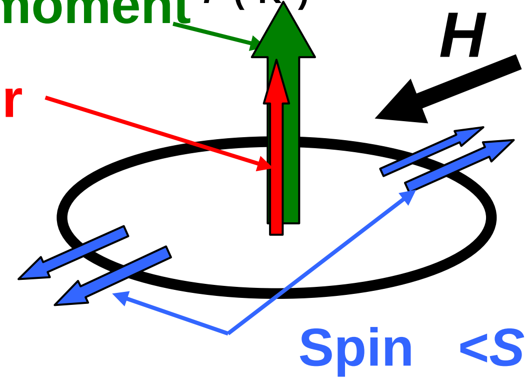
KS was measured in the wider-field range shown below, but the decrease of KS was not observed in the range.

H // ab (***H*** > 550 Oe)



Orbital moment

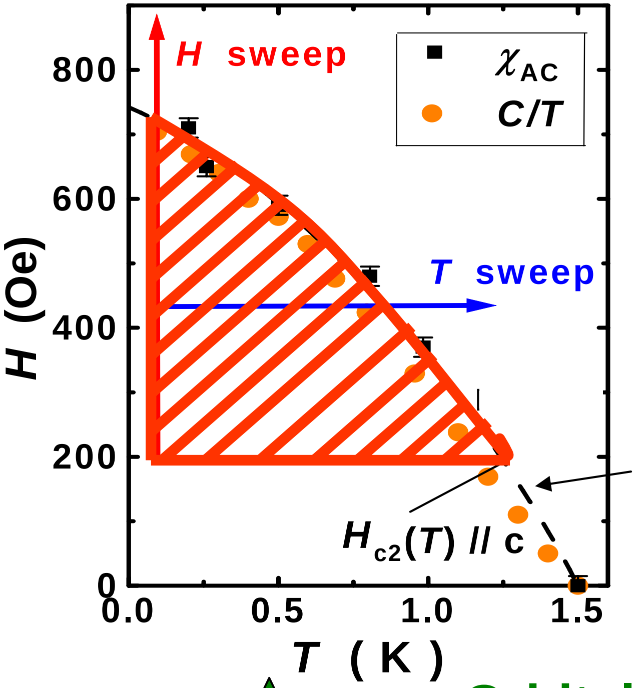
d **-vector**



Spin $\langle S_z \rangle = 0$

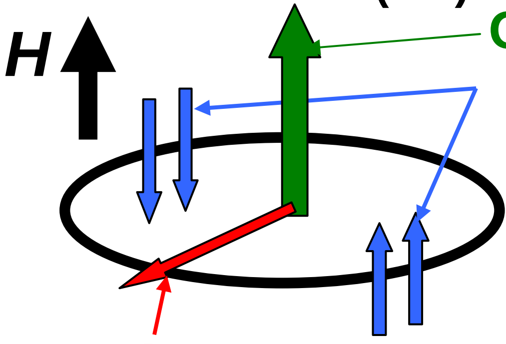
$$d = z\Delta_0(\sin k_x + i \sin k_y) \quad \textbf{(A state)}$$

H **// c (** ***H*** **> 200 Oe)**



Due to Meissner effect, precise measurement of KS was impossible

Orbital moment



Spin

[parallel to the c-axis]

***d*-vector** [in ab (RuO_2) plane]

The effect of the spin-orbit interaction at Ru-4*d* orbitals ($\lambda l \cdot s$)

Y. Yanase and M. Ogata JPSJ 72, 673 (2003).

Ikeda &
Nomura

The symmetry breaking interaction in the ***d***-vector space is **in the second order with respect to λ.**

$$F_{d\perp c} - F_{d//c} \sim UJ_{\mathrm{H}}\lambda^2/W^3$$

Anisotropic energy is reduced to ~ 10^{-4}.

$\Delta T_c \sim 0.01\, T_c$

$H_{\mathrm{flip}} \sim 1$ kOe

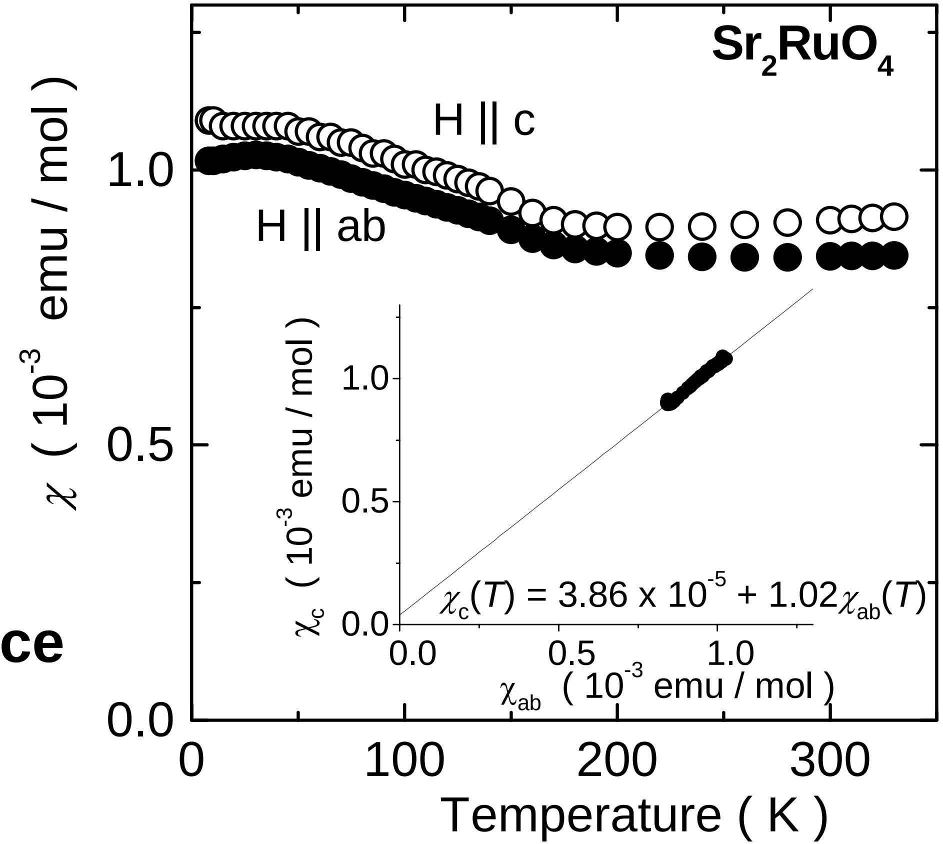
This is the order estimation.

DC susceptibility

The normal state DC susceptibility is almost isotropic.

$\chi_c/\chi_{ab} \sim 1.02$

The anisotropy in the spin space seems to be small.



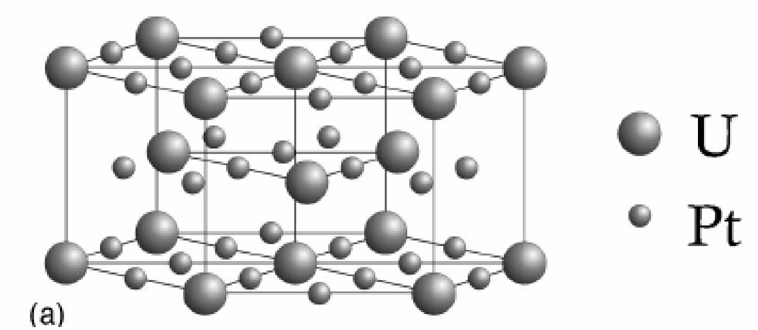
UPt_3 : Spin-triplet Multi-phase superconductor

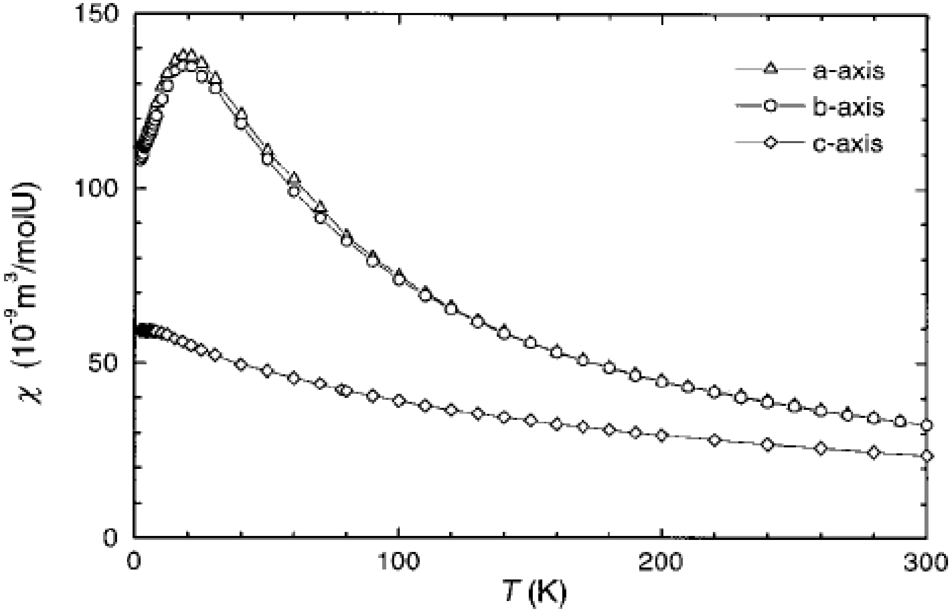
*T*c1 ~ 0.58 K,

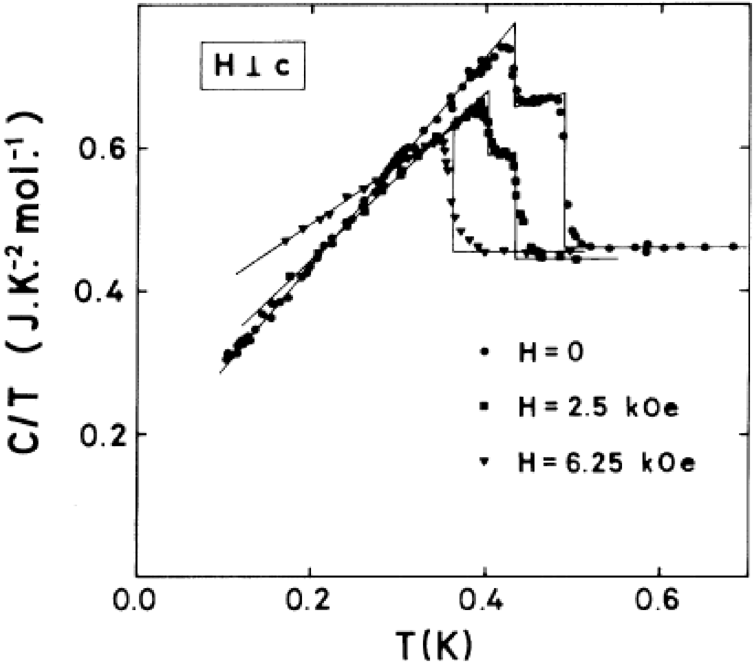
*T*c2 ~ 0.53 K

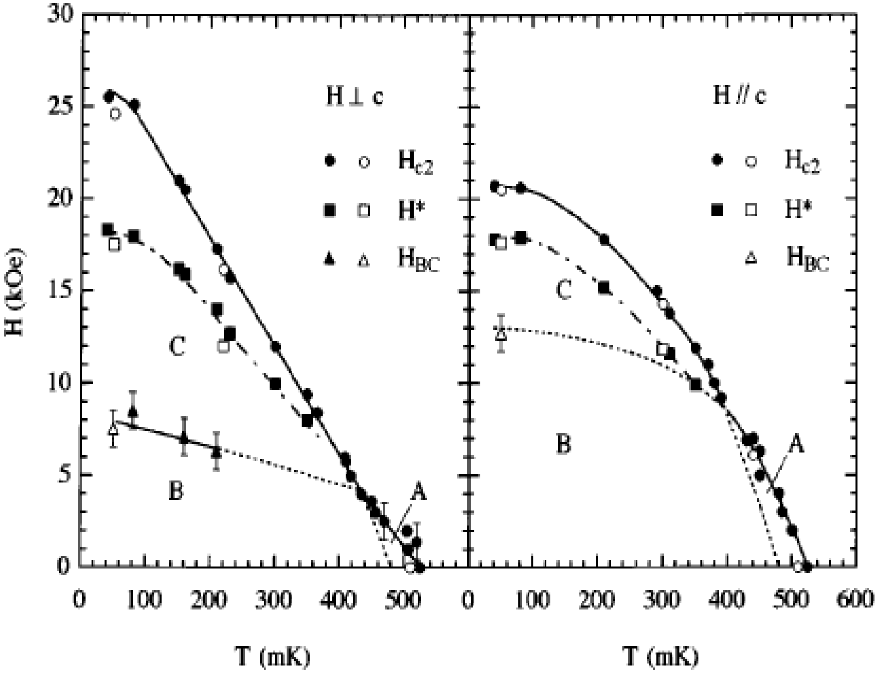
Magnetic anomaly

T_M ~ 5 K



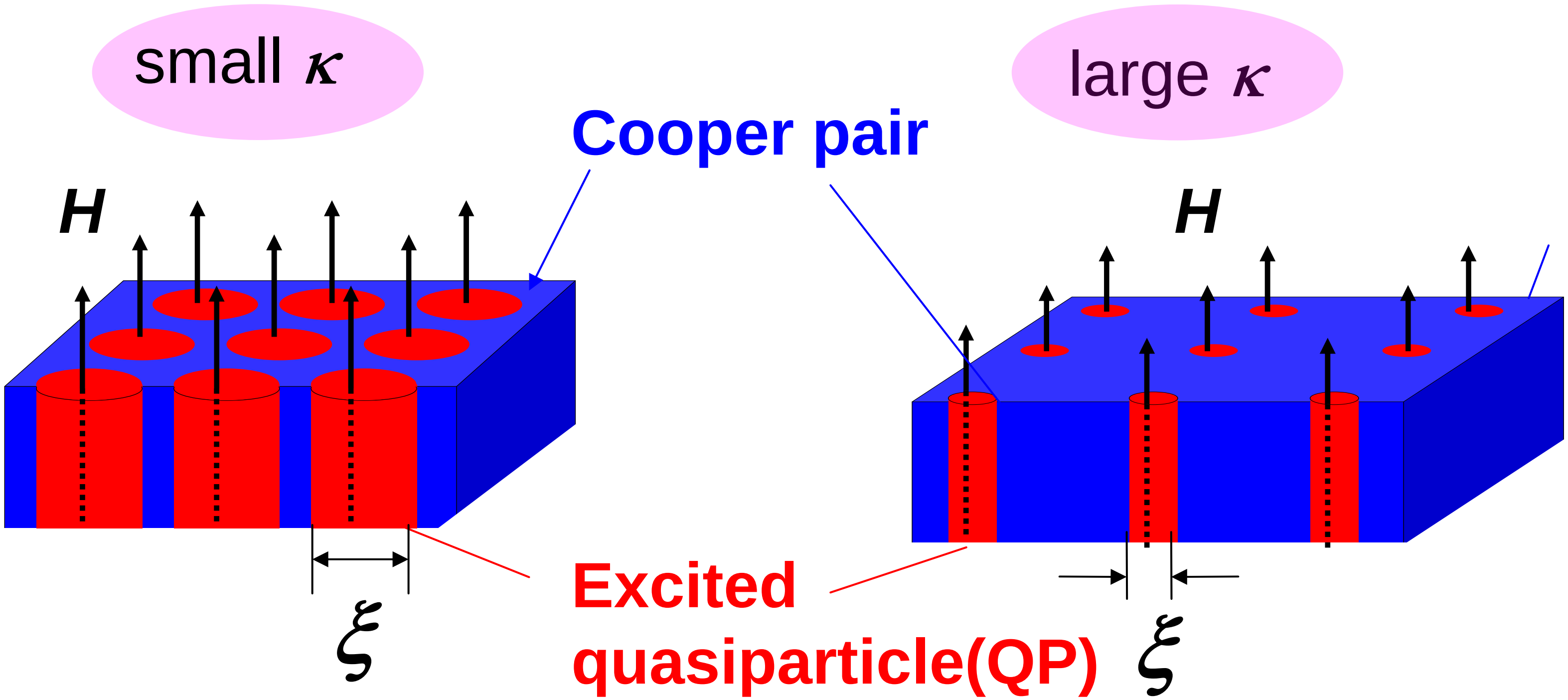






Ginzburg Landau Parameter κ

$\kappa \sim 2.7$ in $H \parallel c$ (Sr_2RuO_4)



small κ

large κ

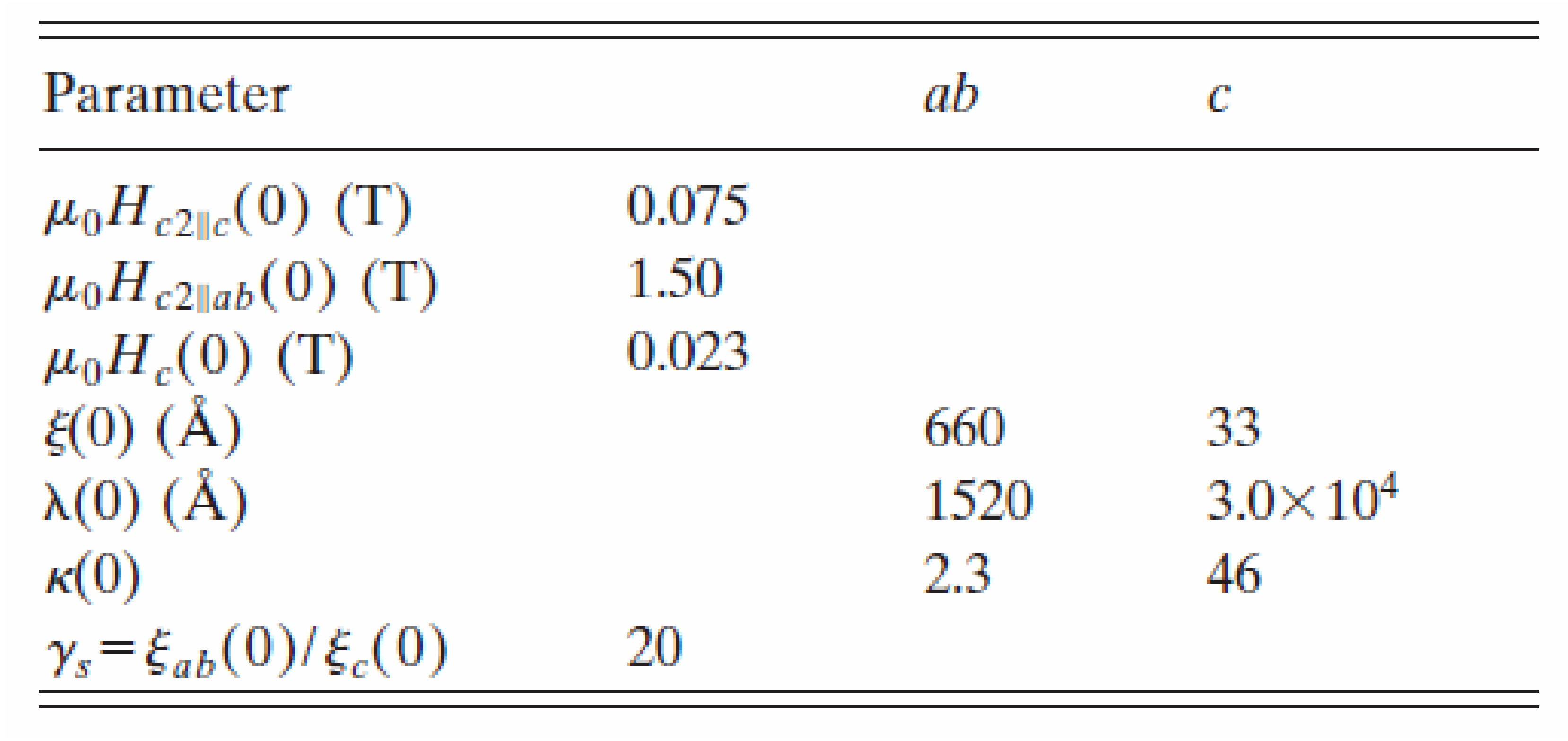
Cooper pair

Excited quasiparticle(QP)

Estimation the ratio of the spin susceptibility from the excited QP is needed.

Specific heat data (Deguchi *et al*.,) is used for estimating the QP’s contribution.

Superconducting Parameter in Sr_2RuO_4



Parameter		*ab*	*c*
$\mu_0 H_{c2\parallel c}(0)$ (T)	0.075		
$\mu_0 H_{c2\parallel ab}(0)$ (T)	1.50		
$\mu_0 H_c(0)$ (T)	0.023		
$\xi(0)$ (Å)		660	33
$\lambda(0)$ (Å)		1520	3.0×10^4
$\kappa(0)$		2.3	46
$\gamma_s = \xi_{ab}(0)/\xi_c(0)$	20		