Is Sr2RuO4 a triplet superconducor?

---analysis of specific heat under fields---

Kazu. Machida

Okayama Univ

collaborators

M. Ichioka, T. Mizushima,
H. Adachi, N. Nakai, Y. Tsutsumi

Outline

- Phenomena related to Pauli paramagnetism in various superconductors:

  1) Sr_2RuO_4 (214)
  2) $CeCoIn_5$ (115)
  3) $TmNi_2B_2C$ (boro-carbide)
  4) URu_2Si_2 (122)
  5) UPd_2Al_3 (123)

  cf imbalanced Fermi superfluids
  FFLO state

- Theoretical framework;

  quasi-classical Eilenberger

Is Sr2RuO4 a triplet superconductor?

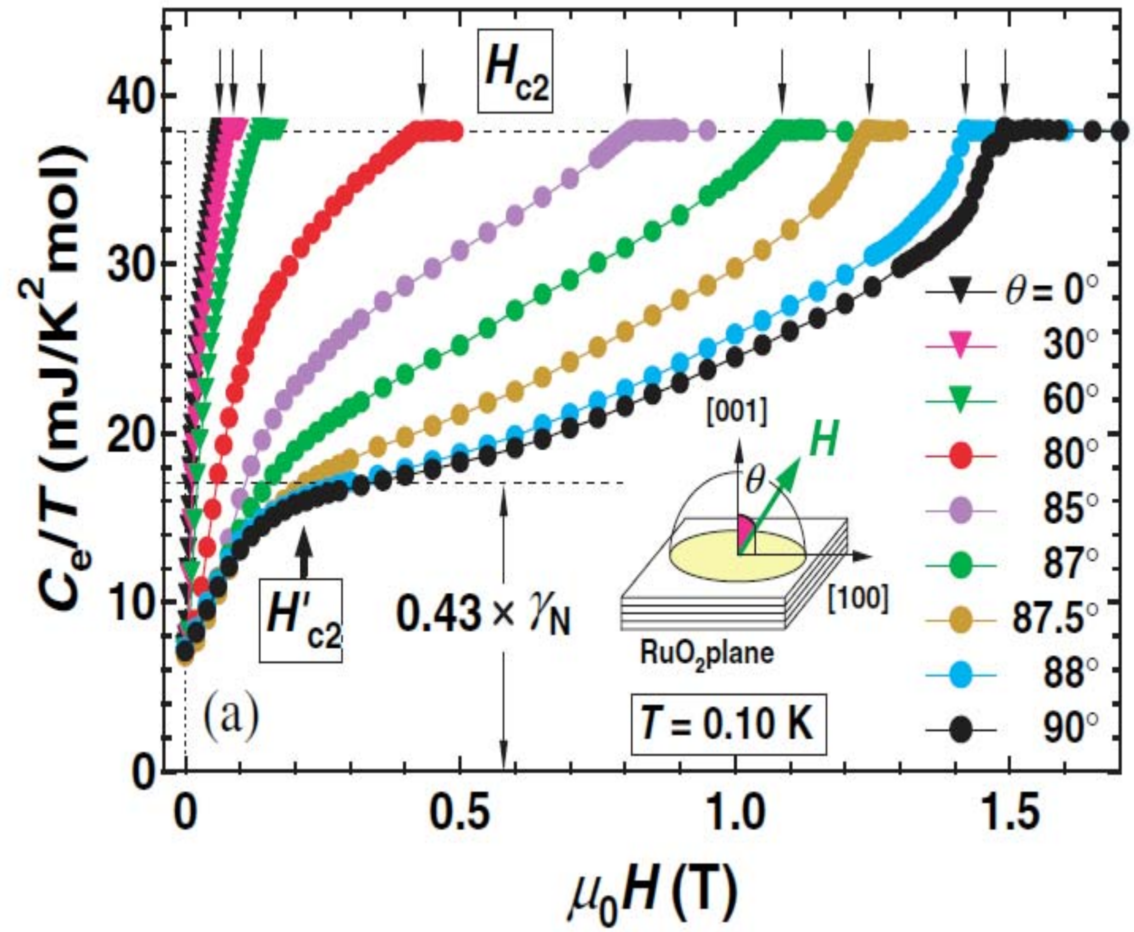
Supporting evidence for triplet pairing

Knight shift (KS) experiments--->
no change for both c-axis and ab-plane

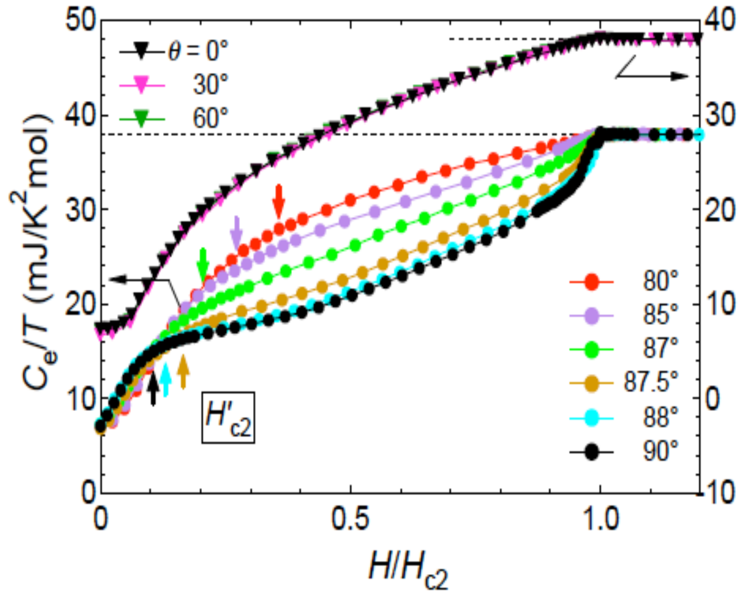
cf
There must be a field direction which shows change of KS when applied parallel to d-vector.

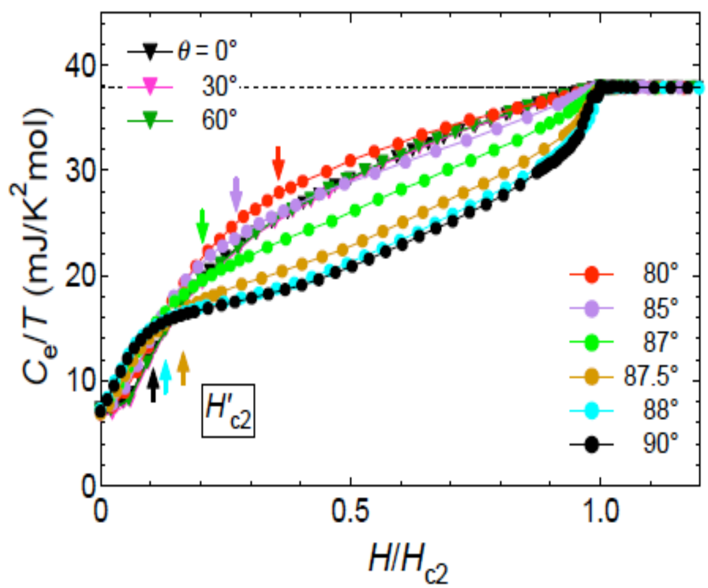
How to understand anomalous $\gamma(H)$ behaviors for H//ab; specific heat---> bulk property

Sr_2RuO_4



K. Deguchi, et al, JPSJ 75 (2004) 1313





K. Deguchi 2005/3/11

Sr_2RuO_4

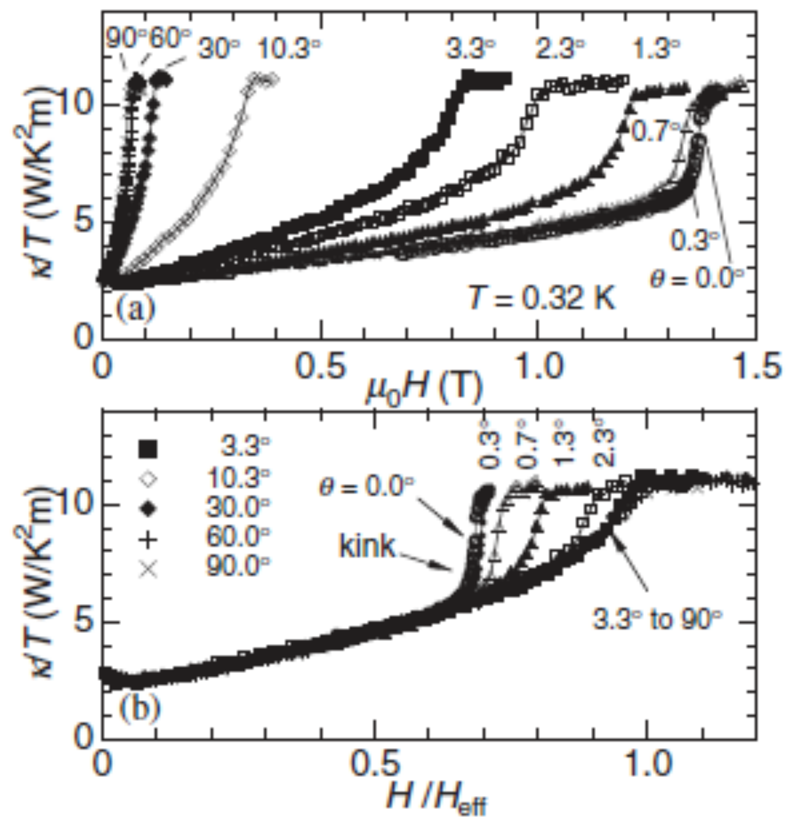
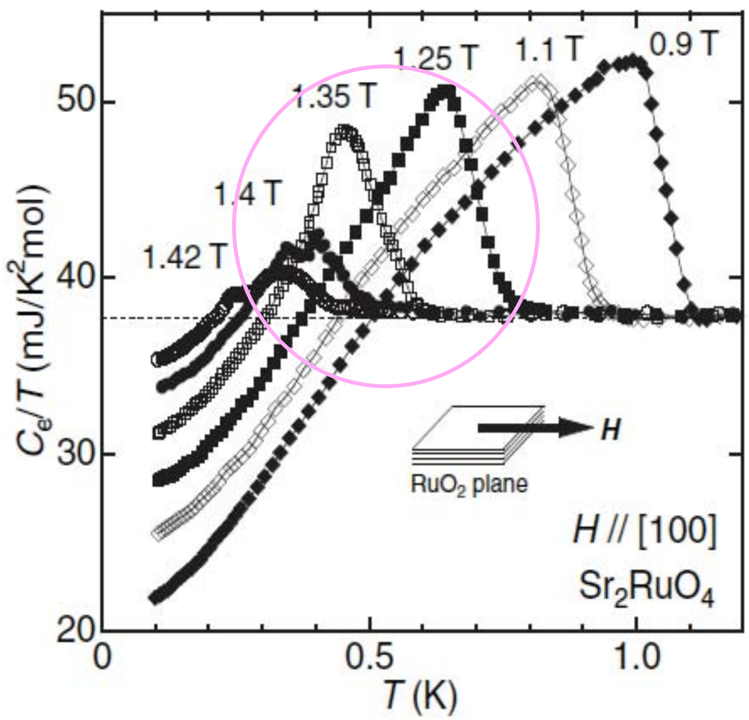
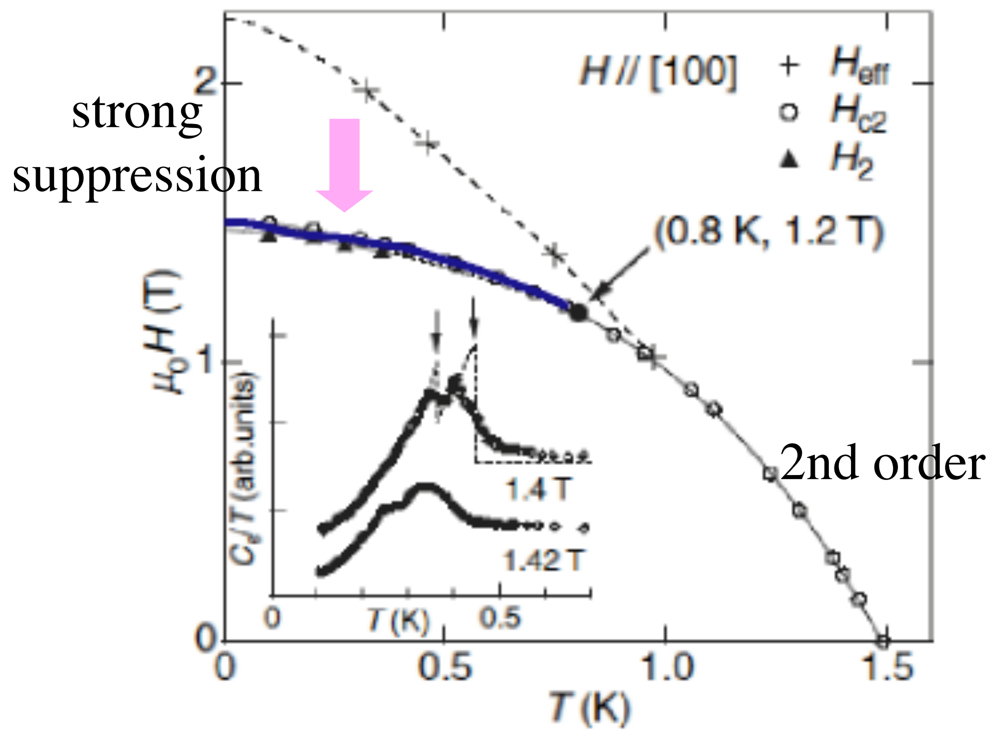


Fig. 4. (a) Transformation of the field dependence of κ/T at 0.32 K on each field angle θ. (b) The same dependence normalized by H_{eff}, treated as a fitting parameter.

Sr_2RuO_4

triplet pairing?

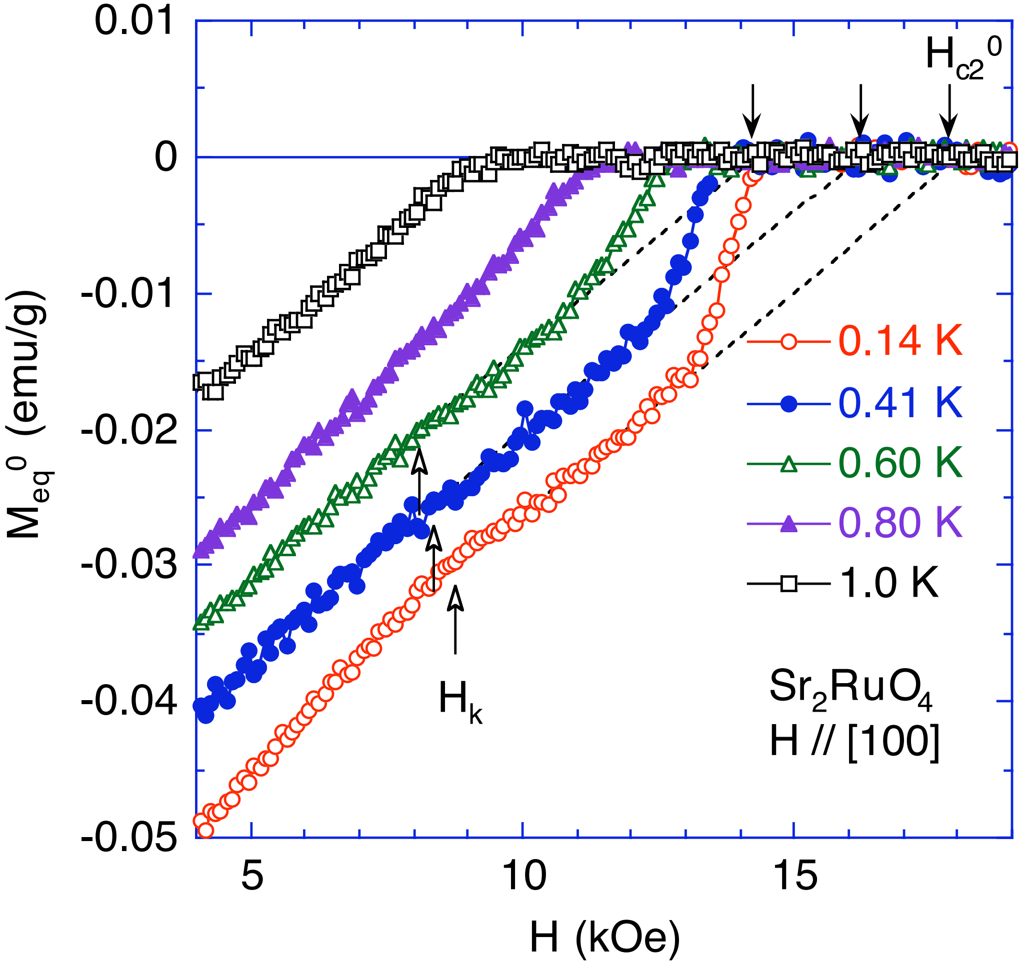




K. Deguchi, et al, JPSJ 71 (02)2839.

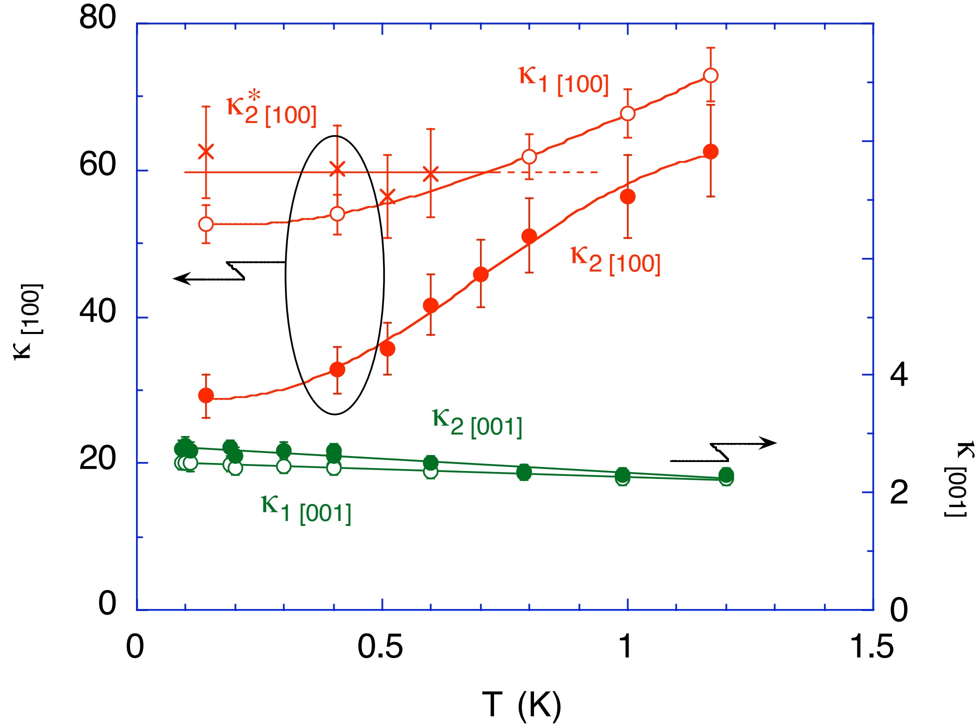
Sr_2RuO_4

Tenya et al



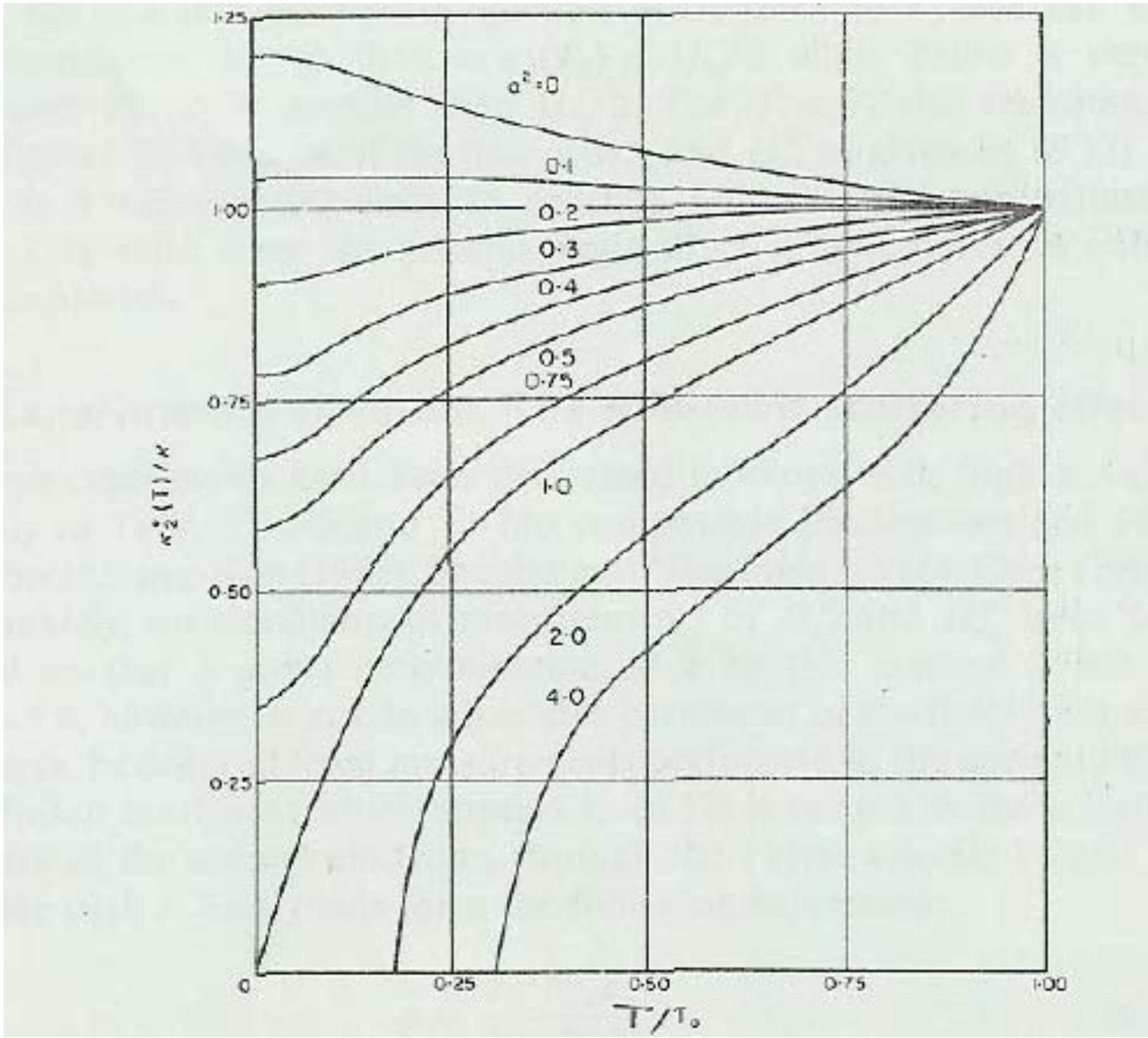
Sr2RuO4

Tenya et al

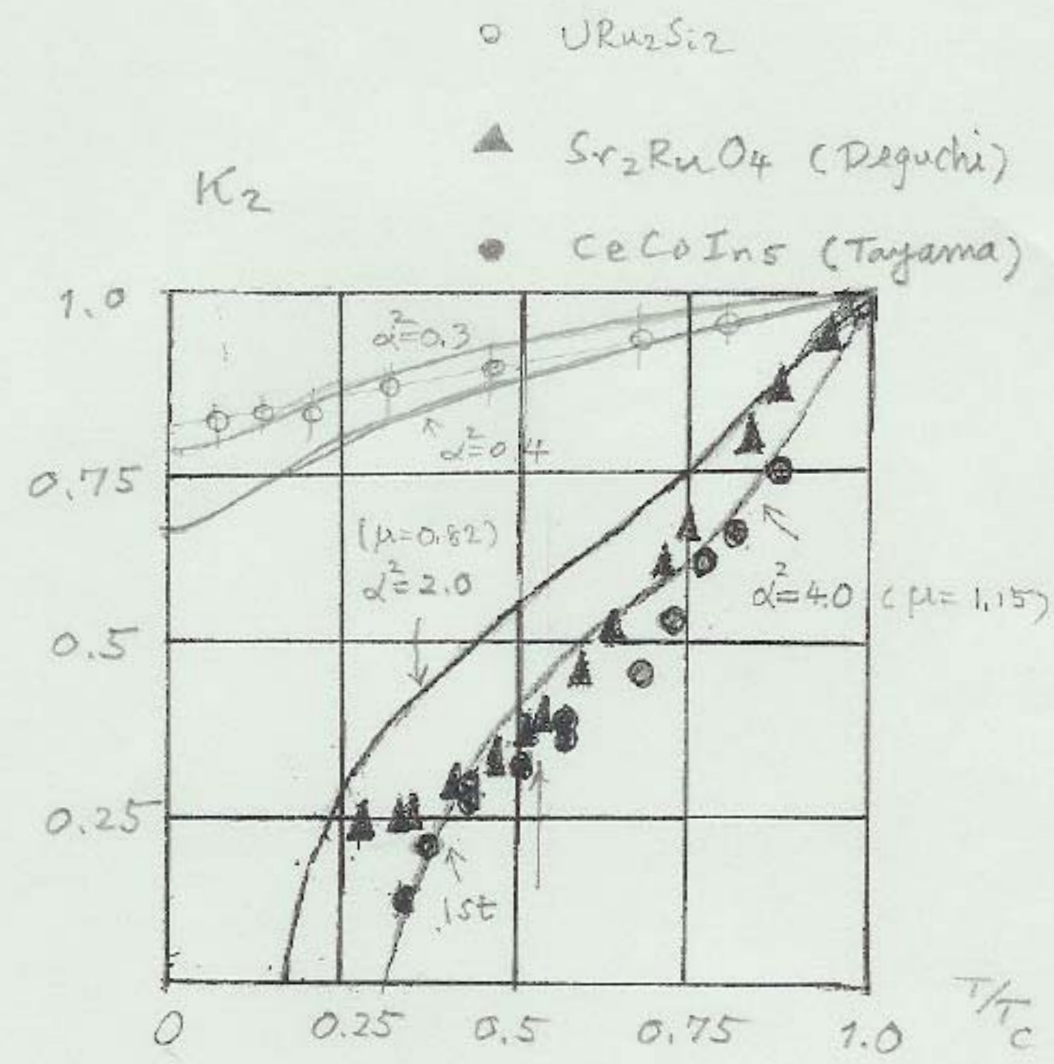


indicating that Pauli effect is important.

κ_2



1·25
1·00
0·75
0·50
0·25
0
0·25
0·50
0·75
1·00
T/T₀
a² = 0
0·1
0·2
0·3
0·4
0·5
0·75
1·0
2·0
4·0



○ URu2Si2
▲ Sr2RuO4 (Deguchi)
● CeCoIn5 (Tayama)
K2
1.0
0.75
0.5
0.25
0
0.25
0.5
0.75
1.0
T/Tc
α²=0.3
α²=0.4
(μ=0.82)
α²=2.0
α²=4.0 (μ=1.15)
1st

Gor'kov equation (Green's function)

$$\sum_{\mathbf{r}''}\left\{ \mathrm{i}\omega_n - \begin{pmatrix} K & \Delta \\ \Delta^\dagger & -K^* \end{pmatrix} \right\}_{\mathbf{r},\mathbf{r}''} \begin{pmatrix} \overset{G}{G_{11}(\omega_n,\mathbf{r}'',\mathbf{r}')} & \overset{F}{G_{12}(\omega_n,\mathbf{r}'',\mathbf{r}')} \\ \underset{F^\dagger}{G_{21}(\omega_n,\mathbf{r}'',\mathbf{r}')} & \underset{\bar{G}}{G_{22}(\omega_n,\mathbf{r}'',\mathbf{r}')} \end{pmatrix} = \hbar\delta(\mathbf{r}'-\mathbf{r})$$

Hamiltonian

$K = -\frac{\hbar^2}{2m}\nabla^2 - \mu,$

Δ : pair potential

$$G_{11}(\omega_n,\mathbf{r},\mathbf{r}') = \sum_\alpha \frac{u_\alpha(\mathbf{r})u^*_\alpha(\mathbf{r}')}{\mathrm{i}\omega_n - E_\alpha}, \qquad G_{12}(\omega_n,\mathbf{r},\mathbf{r}') = \sum_\alpha \frac{u_\alpha(\mathbf{r})v^*_\alpha(\mathbf{r}')}{\mathrm{i}\omega_n - E_\alpha}$$

$$G_{21}(\omega_n,\mathbf{r},\mathbf{r}') = \sum_\alpha \frac{v_\alpha(\mathbf{r})u^*_\alpha(\mathbf{r}')}{\mathrm{i}\omega_n - E_\alpha}, \qquad G_{22}(\omega_n,\mathbf{r},\mathbf{r}') = \sum_\alpha \frac{v_\alpha(\mathbf{r})v^*_\alpha(\mathbf{r}')}{\mathrm{i}\omega_n - E_\alpha}$$

Bogoliubov-de Gennes Equation (eigen-value equation)

Superconductivity-version of Schrodinger eq.

$$\sum_{\mathbf{r}'}\begin{pmatrix} K & \Delta \\ \Delta^\dagger & -K^* \end{pmatrix}_{\mathbf{r},\mathbf{r}'}\begin{pmatrix} u_\alpha(\mathbf{r}') \\ v_\alpha(\mathbf{r}') \end{pmatrix} = E_\alpha \begin{pmatrix} u_\alpha(\mathbf{r}) \\ v_\alpha(\mathbf{r}) \end{pmatrix}$$

E_α : eigen-energy

u_α v_α : wave functions

(α: label of eigen-state)

Quasi-classical approximation

$\xi >> 1/k_F$

$$g(\omega_n,\mathbf{r},\mathbf{k}_F) = \frac{1}{\mathrm{i}\pi}\int d\epsilon G(\omega_n,\mathbf{r},\mathbf{k})$$

$$f(\omega_n,\mathbf{r},\mathbf{k}_F) = \frac{1}{\pi}\int d\epsilon F(\omega_n,\mathbf{r},\mathbf{k})$$

$$f^\dagger(\omega_n,\mathbf{r},\mathbf{k}_F) = \frac{1}{\pi}\int d\epsilon F^\dagger(\omega_n,\mathbf{r},\mathbf{k})$$

$\mathbf{r}$: center of mass coordinate

$\mathbf{k} = (\epsilon, \mathbf{k}_F)$: relative momentum

$\epsilon = \frac{\hbar^2}{2m}k^2 - \mu$: perpendicular to the Fermi surface

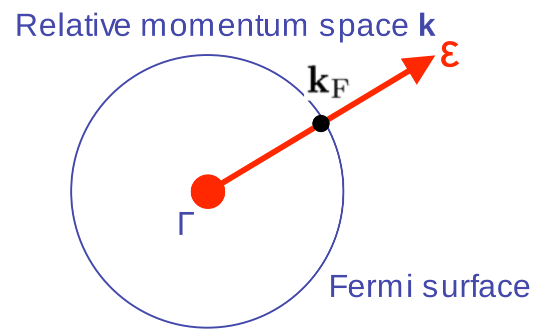
$\mathbf{k}_F$: on the Fermi surface

Eilenberger equation (quasi-classical Green's function)

$$\left\{\omega_n + \frac{\mathrm{i}}{2}\mathbf{v}(\mathbf{k}_F)\cdot\left(\frac{\nabla}{\mathrm{i}} + \frac{2\pi}{\phi_0}\mathbf{A}(\mathbf{r})\right)\right\} f(\mathrm{i}\omega_n,\mathbf{k}_F,\mathbf{r}) = \Delta(\mathbf{k}_F,\mathbf{r})g(\mathrm{i}\omega_n,\mathbf{k}_F,\mathbf{r}),$$

$$\left\{\omega_n - \frac{\mathrm{i}}{2}\mathbf{v}(\mathbf{k}_F)\cdot\left(\frac{\nabla}{\mathrm{i}} - \frac{2\pi}{\phi_0}\mathbf{A}(\mathbf{r})\right)\right\} f^\dagger(\mathrm{i}\omega_n,\mathbf{k}_F,\mathbf{r}) = \Delta^*(\mathbf{k}_F,\mathbf{r})g(\mathrm{i}\omega_n,\mathbf{k}_F,\mathbf{r}),$$

$$g(\mathrm{i}\omega_n,\mathbf{k}_F,\mathbf{r}) = [1 - f(\mathrm{i}\omega_n,\mathbf{k}_F,\mathbf{r})f^\dagger(\mathrm{i}\omega_n,\mathbf{k}_F,\mathbf{r})]^{1/2}$$



Quasiclassical Eilenberger theory

Zeeman effect

Free energy with paramagnetic effect

$$F = \int d\mathbf{r} \left\{ \frac{|B(\mathbf{r})|^2}{8\pi} - \frac{\chi_n}{2}|B(\mathbf{r})|^2 + \frac{\langle|\Delta(\mathbf{r})|^2\rangle_{\mathbf{k}}}{V_{\text{pairing}}} - \pi T \sum_{|l|<l_{\text{cut}}} N_0 \langle I(\mathbf{r},\mathbf{k},\omega_l + \mathrm{i}\mu_{\mathrm{B}} B)\rangle_{\mathbf{k}} \right\}$$

$$= \int d\mathbf{r} \left\{ \frac{|B(\mathbf{r})|^2}{8\pi} - \frac{\chi_n}{2}|B(\mathbf{r})|^2 + \langle|\Delta(\mathbf{r})|^2\rangle_{\mathbf{k}} N_0 \ln\frac{T}{T_{\mathrm{c}}} + \pi T N_0 \sum_{|l|<l_{\text{cut}}} \left[\frac{|\Delta(\mathbf{r})|^2}{|\omega_l|} - \langle I(\mathbf{r},\mathbf{k},\omega_l + \mathrm{i}\mu_{\mathrm{B}} B)\rangle_{\mathbf{k}} \right] \right\}$$

$$\begin{aligned} I(\mathbf{r},\mathbf{k},\omega_l + \mathrm{i}\mu_{\mathrm{B}} B) &= \Delta(\mathbf{r},\mathbf{k}) f^\dagger + \Delta^*(\mathbf{r},\mathbf{k}) f \\ &\quad + (g - \operatorname{sign}(\omega_l)) \left\{ \frac{1}{f}\left(\omega_l + \mathrm{i}\mu_{\mathrm{B}} B + \frac{\hbar}{2}\mathbf{v}_{\mathrm{F}}\cdot\mathbf{\Pi}\right) f + \frac{1}{f^\dagger}\left(\omega_l + \mathrm{i}\mu_{\mathrm{B}} B - \frac{\hbar}{2}\mathbf{v}_{\mathrm{F}}\cdot\mathbf{\Pi}^*\right) f^\dagger \right\} \\ &= \Delta f^\dagger + \Delta^* f + 2(\omega_l + \mathrm{i}\mu_{\mathrm{B}} B)(g - \operatorname{sign}(\omega_l)) - \hbar \frac{f^\dagger(\mathbf{v}_{\mathrm{F}}\cdot\mathbf{\Pi} f) - f(\mathbf{v}_{\mathrm{F}}\cdot\mathbf{\Pi}^* f^\dagger)}{2(g + \operatorname{sign}(\omega_l))} \end{aligned}$$

$\chi_n = 2\mu_{\mathrm{B}}^2 N_0$ Normal state susceptibility

$$\mathbf{\Pi} = \vec{\nabla} - \mathrm{i}\frac{2\pi}{\phi_0}\mathbf{A}(\mathbf{r}) \qquad (\ e = |e|\ )$$

$$\mathbf{B}(\mathbf{r}) = \bar{\mathbf{B}} + \mathbf{b}(\mathbf{r})$$
$$\mathbf{A}(\mathbf{r}) = \tfrac{1}{2}\bar{\mathbf{B}} \times \mathbf{r} + \mathbf{a}(\mathbf{r})$$

$\bar{\mathbf{B}}$ Average flux density

$\mathbf{b}(\mathbf{r}) = \vec{\nabla} \times \mathbf{a}(\mathbf{r})$

Internal field distribution

Self-consistent equation

Pairing potential

$$\frac{\Delta(\mathbf{r})}{\pi k_B T_c}\left(\ln\frac{T}{T_c}+2\frac{T}{T_c}\sum_{0\le l\le l_{cut}}\frac{\pi k_B T_c}{\omega_l}\right)=\frac{T}{T_c}\sum_{|l|\le l_{cut}}\langle\phi^*(\mathbf{k})f(\omega_l+i\tilde{\mu}B,\mathbf{k},\mathbf{r})\rangle_{\mathbf{k}}$$

$$=\frac{T}{T_c}\sum_{0\le l\le l_{cut}}\left\langle\phi^*(\mathbf{k})\left\{f(\omega_l+i\tilde{\mu}B,\mathbf{k},\mathbf{r})+f^{\dagger *}(\omega_l^*+i\tilde{\mu}B,\mathbf{k},\mathbf{r})\right\}\right\rangle_{\mathbf{k}}$$

paramagnetic parameter

Vector potential

$$R_0\vec{\nabla}\times\left(R_0\vec{\nabla}\times\frac{\mathbf{A}(\mathbf{r})}{A_0}\right)=R_0\vec{\nabla}\times\frac{4\pi\mathbf{M}_{para}(\mathbf{r})}{B_0}+\frac{2}{\tilde{\kappa}^2}\frac{T}{T_c}\sum_{0\le l}\left\langle\frac{\mathbf{v}_F}{v_{F0}}\mathrm{Im}\left\{g(\omega_l+i\tilde{\mu}B,\mathbf{k},\mathbf{r})\right\}\right\rangle_{\mathbf{k}}$$

B(r)/B_0
Total internal field

Paramagnetic contribution

Diamagnetic (super-current) contribution

Paramagnetic magnetization

$$\frac{4\pi M_{para}(\mathbf{r})}{B_0}=\frac{4\pi M_0}{B_0}\left(\frac{B(\mathbf{r})}{\bar{B}}-\frac{2}{\tilde{\mu}\bar{B}/B_0}\frac{T}{T_c}\sum_{0\le l}\langle\mathrm{Im}\left\{g(\omega_l+i\tilde{\mu}B,\mathbf{k},\mathbf{r})\right\}\rangle_{\mathbf{k}}\right)$$

$$\frac{4\pi M_0}{B_0}=\frac{\tilde{\mu}^2}{\tilde{\kappa}^2}\frac{\bar{B}}{B_0}$$

Normal state magnetization

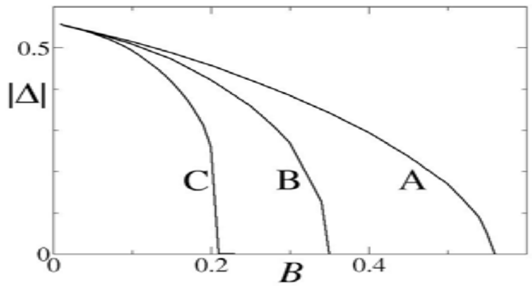
Results of calculation

Magnetic field dependence

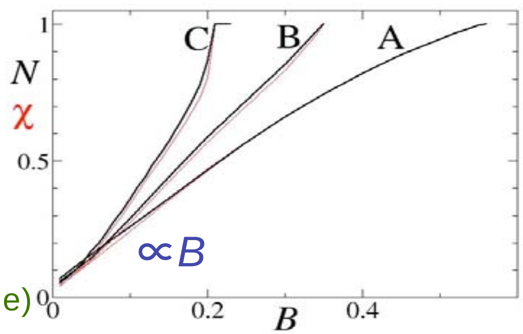
T = 0.1 Tc

s-wave paring

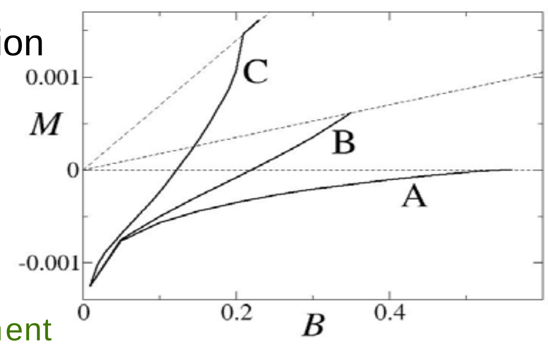
Amplitude of
pair potential
(spatial average)



DOS at E=0
(~Low temp.
specific heat)
≒ Paramagnetic
susceptibility
(if GL parameter is large)



Total magnetization
(Paramagnetic
＋Diamegnetic)



Dotted lines：
Paramagnetic moment
in the normal state

Paramagnetic effect

A: very small $\tilde{\mu} = 0.02$

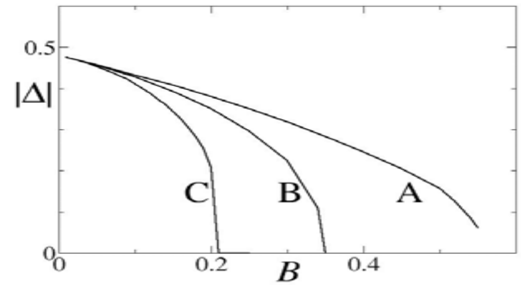
B: $\tilde{\mu} = 0.85$

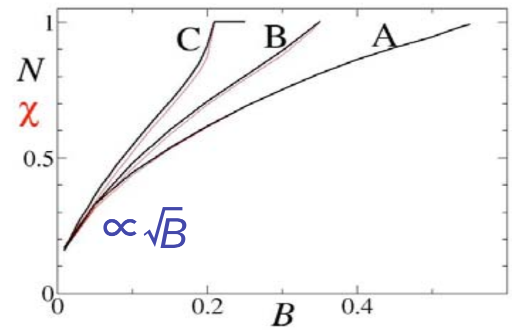
C：Large $\tilde{\mu} = 1.7$

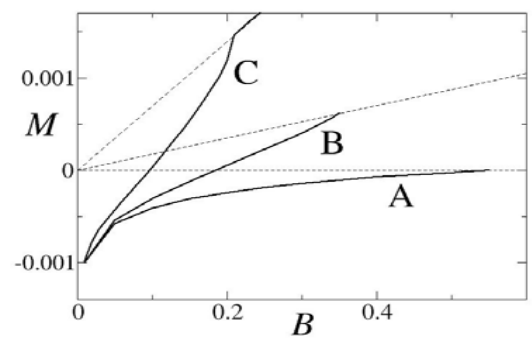
Suppression of
superconductivity
at high field

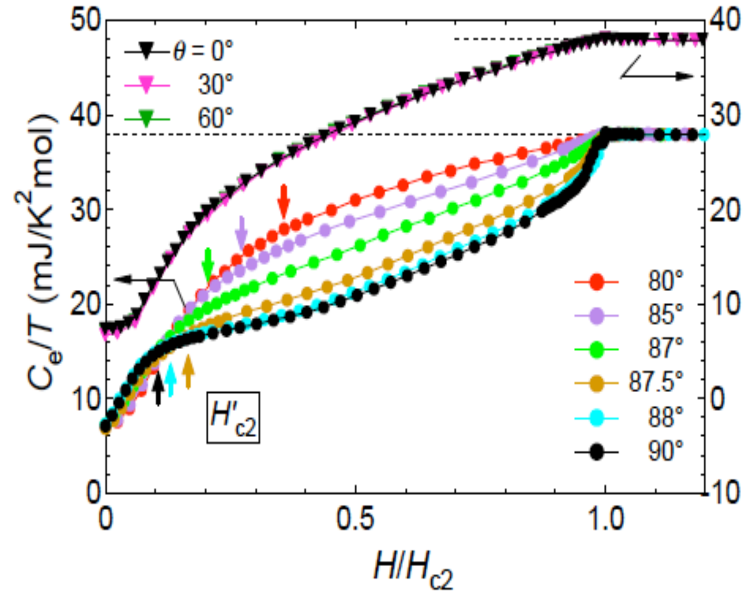
(Similar effect both
for s-wave and
d-wave pairing)

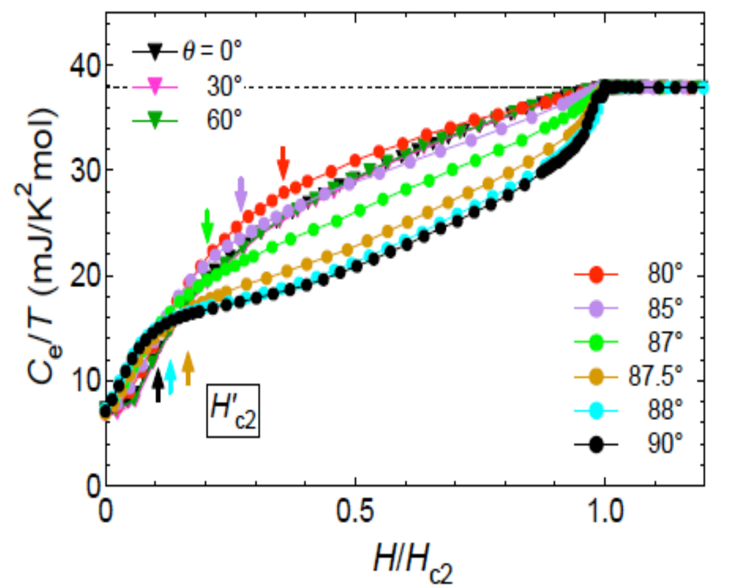
d-wave pairing











K. Deguchi 2005/3/11

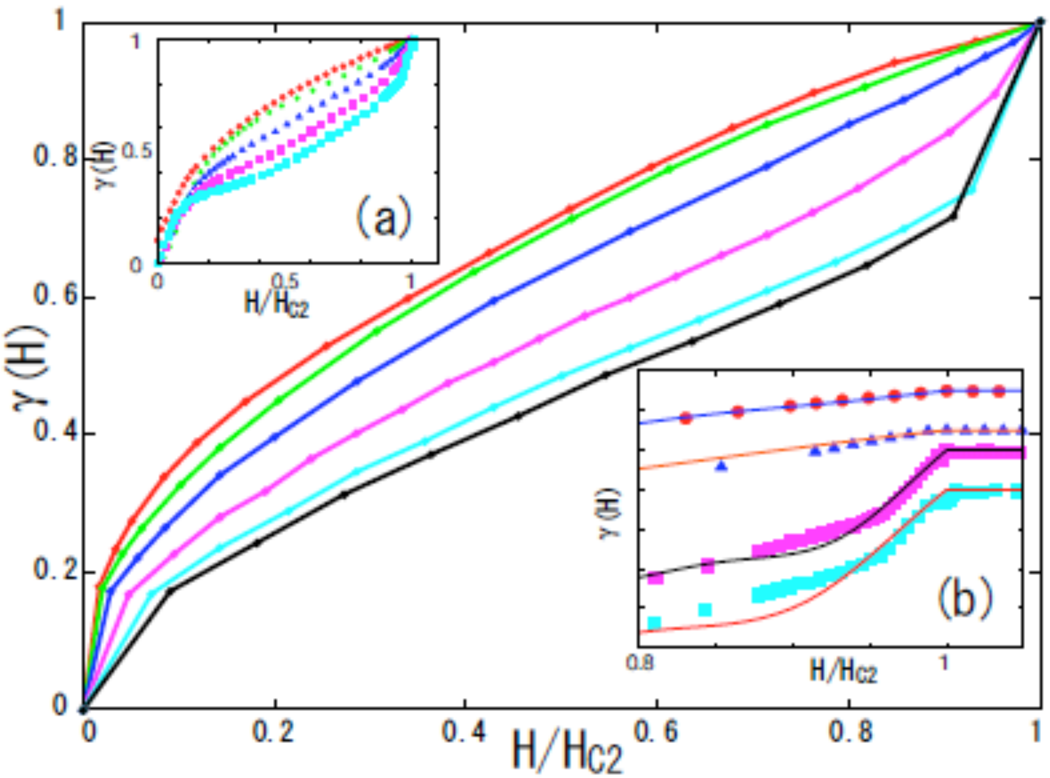


FIG. 3: (color online) Zero-energy DOS $\gamma(H)$ at $T = 0.1T_c$ for $\tilde{\mu} = 0.02$, 0.41, 0.86, 1.71, 2.57 and 3.41 from top to bottom. Inset (a) shows the experimental data [16] for θ=0°, 2.5°, 3.0°, 5.0° and 90° from bottom to top. Inset (b) is the fitting of the data θ=0° by $\tilde{\mu}$=3.41, 0.5° ($\tilde{\mu}$=2.36), 5° ($\tilde{\mu}$=0.33) and 90° ($\tilde{\mu}$=0.03) from bottom to top, which are shifted upwards.

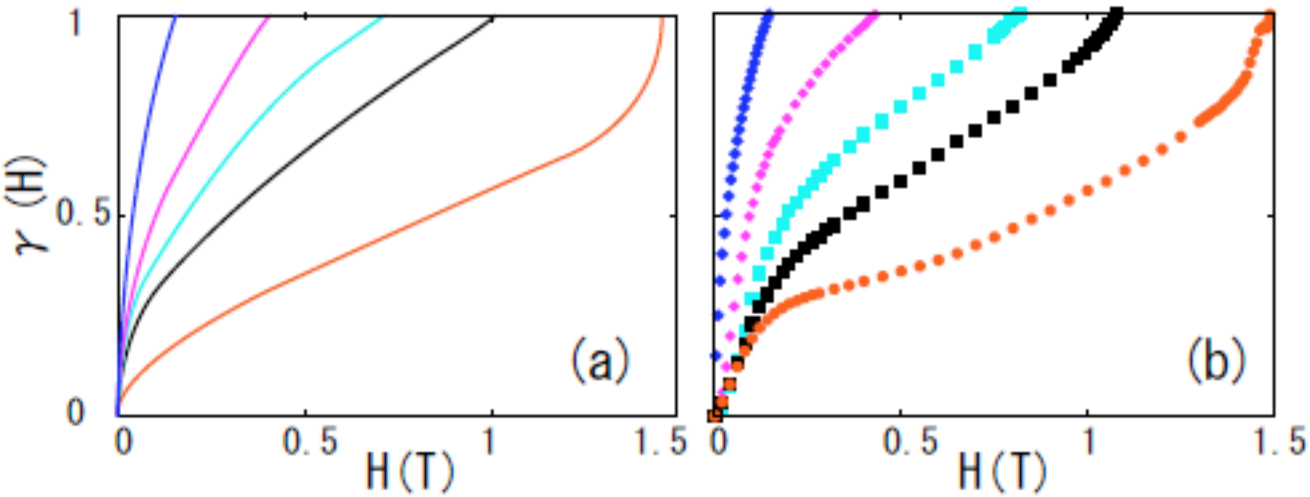


FIG. 4: (color online) (a) $\gamma(H)$ for $\tilde{\mu} = 3.41$, 0.60, 0.36, 0.18 and 0.06 from bottom to top. (b) Corresponding data [16] for θ=0°, 3°, 5°, 10° and 30°.

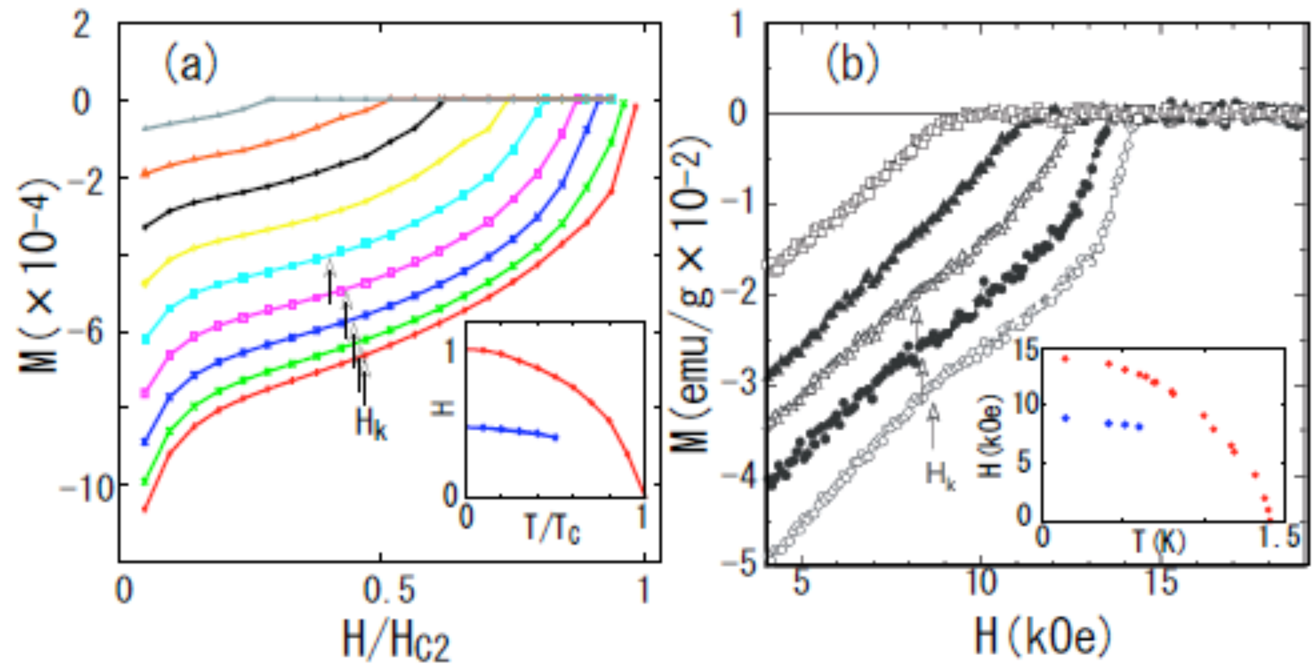


FIG. 5: (color online) (a) Calculated magnetization curves for various $T/T_c = 0.1, 0.2, 0.3 \cdots, 0.9$ from bottom to top for $\tilde{\mu} = 1.71$. Inset shows H_{c2} and the inflection point H_K. (b) Corresponding data [17] for T/T_c=0.1, 0.28, 0.40 and 0.56 from bottom to top for $H \parallel ab$. Inset shows H_{c2} and "kink" field H_K in their terminology [17]. Magnetization of the normal paramagnetic moment is substracted.

Heavy Fermion superconductors

URu_2Si_2, Sr_2RuO_4, $CeCoIn_5$

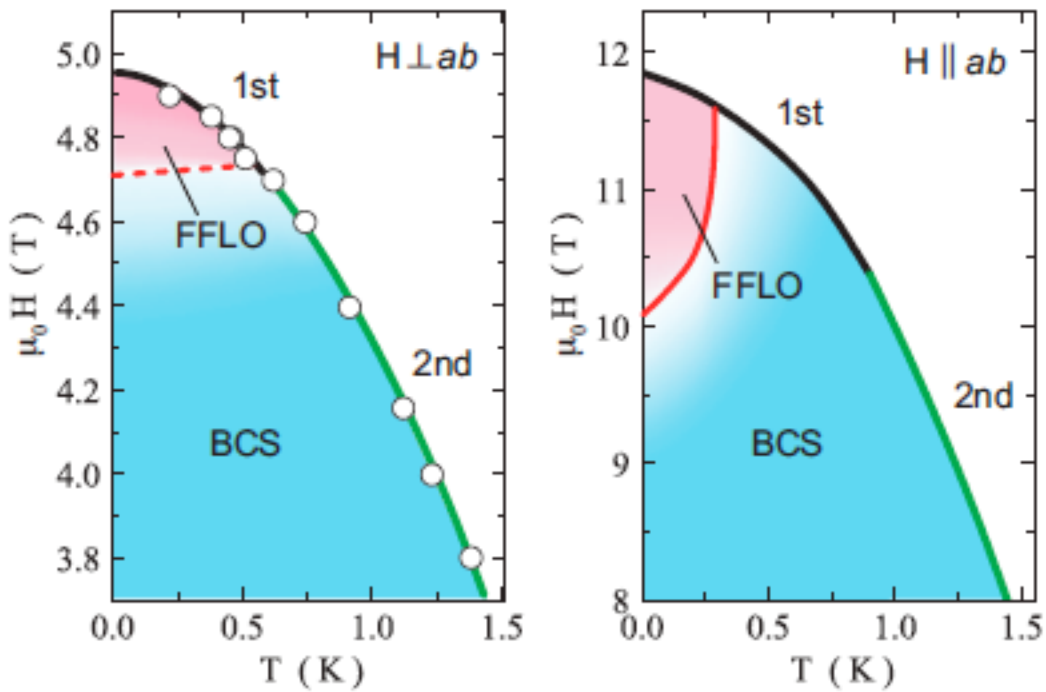
Pauli paramagnetic effect on vortex lattice

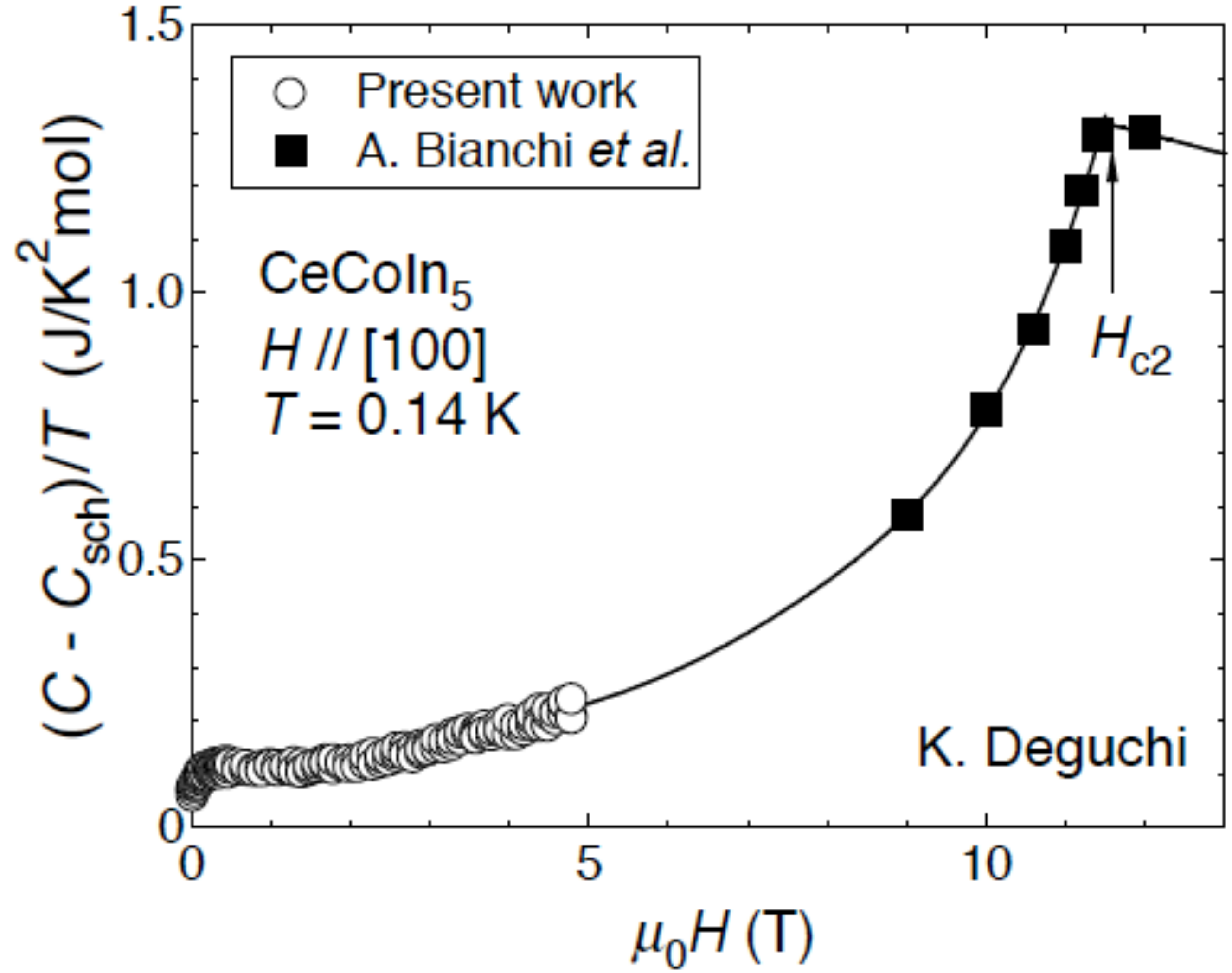
Zeeman effect -----> up spin and down spin population imbalance

-------> Fulde-Ferrell-Larkin-Ovchinikov (FFLO)

Phase diagram in H vs T

$CeCoIn_5$





Present work
A. Bianchi et al.
CeCoIn5
H // [100]
T = 0.14 K
Hc2
K. Deguchi
(C - Csch)/T (J/K2mol)
μ0H (T)
0
0.5
1.0
1.5
0
5
10

URu_2Si_2 another Pauli-limited superconductor

H// c

H// a

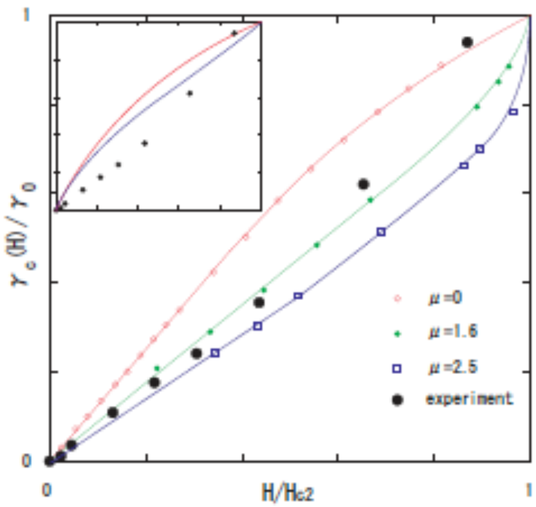


FIG. 5: (Color online) The same as in Fig. 3, but for $H \parallel c$ and $\mu = 0, 1.6, 2.5$. In inset $\mu = 0$ (upper) and $\mu = 1.3$ (lower).

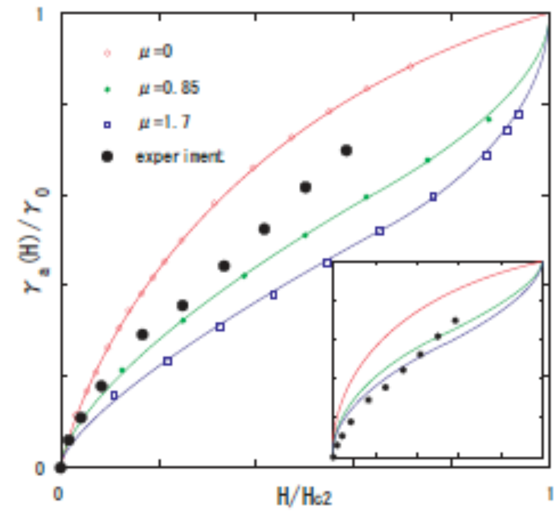
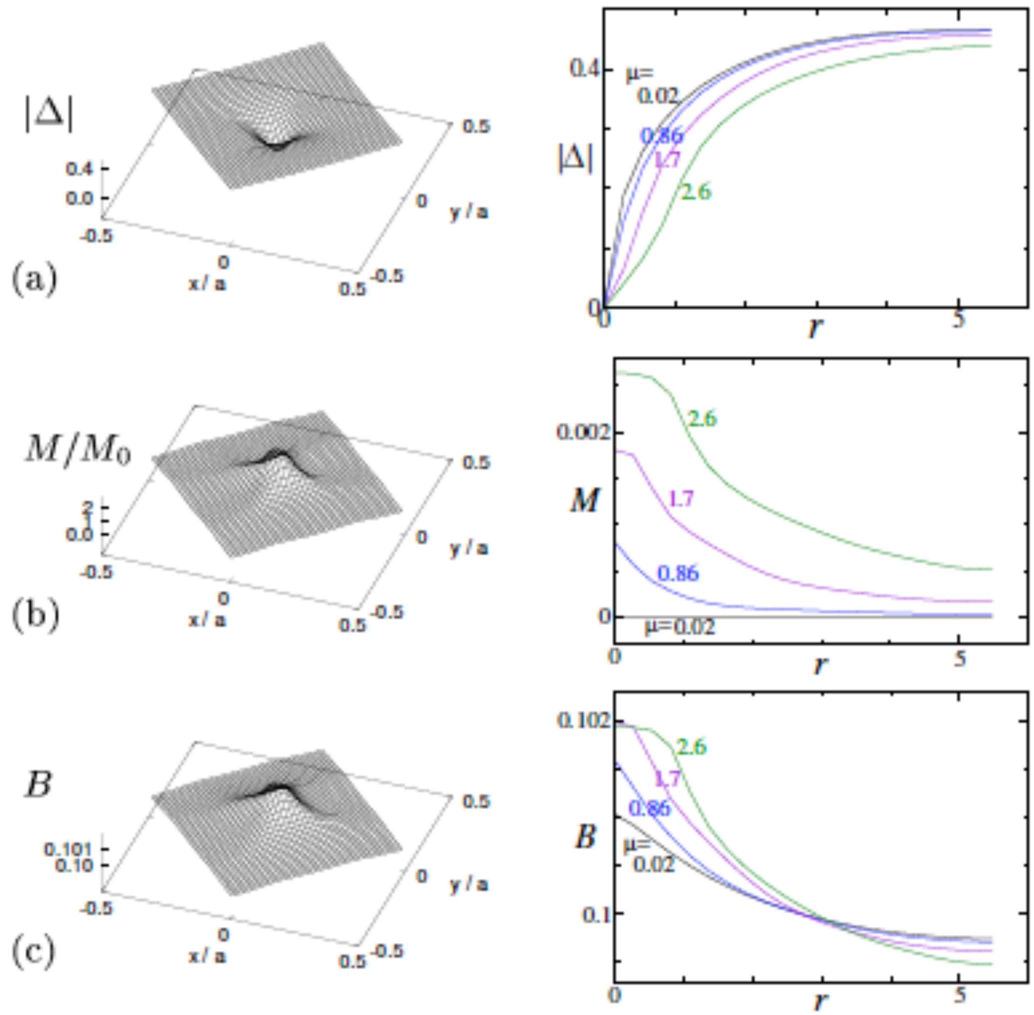


FIG. 4: (Color online) H-dependence of $\gamma(H)$ for $H \parallel a$ when $\phi(\mathbf{k}) = \sin\theta$ and $\mu = 0, 0.85, 1.7$. Solid circles are experimental data in Fig. 2. Inset shows $\gamma(H)$ for the quadratic point node case $\phi(\mathbf{k}) = \sin^2\theta$. $\mu = 0, 0.6, 1.0$ from top to bottom.

point nodes at two poles on Fermi sphere,
but we need paramagnetic effect with rather large μ value

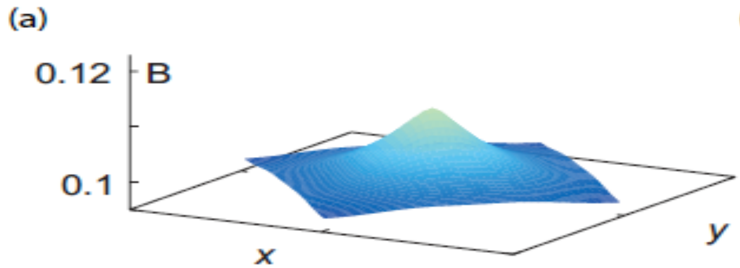


|Δ|
0.4
0.0
-0.5
0
x / a
0.5
-0.5
0
y / a
0.5
(a)
μ=
0.02
0.86
1.7
2.6
0
5
r
M/M0
2
1
0.0
(b)
0.002
M
(c)
B
0.101
0.10
0.102
0.1

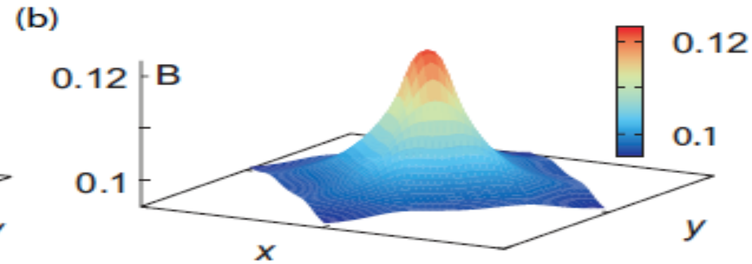
vortex core structures

ordinary Abrikosov vortex

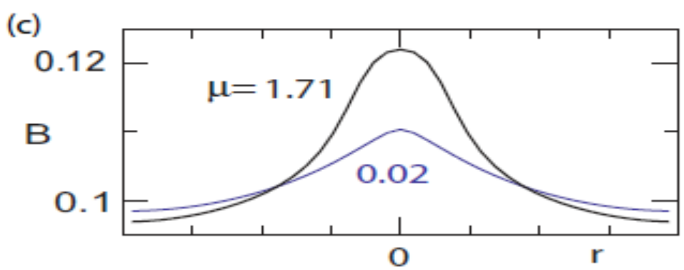
paramagnetic vortex case



small μ-case



large μ-case



enhanced paramagnetic moment accumulated at core

majority spin component accommodated exclusively at core because of π-phase shift physics

$CeCoIn_5$ prime candidate for FFLO

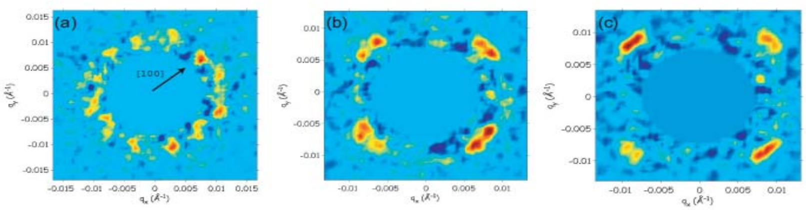
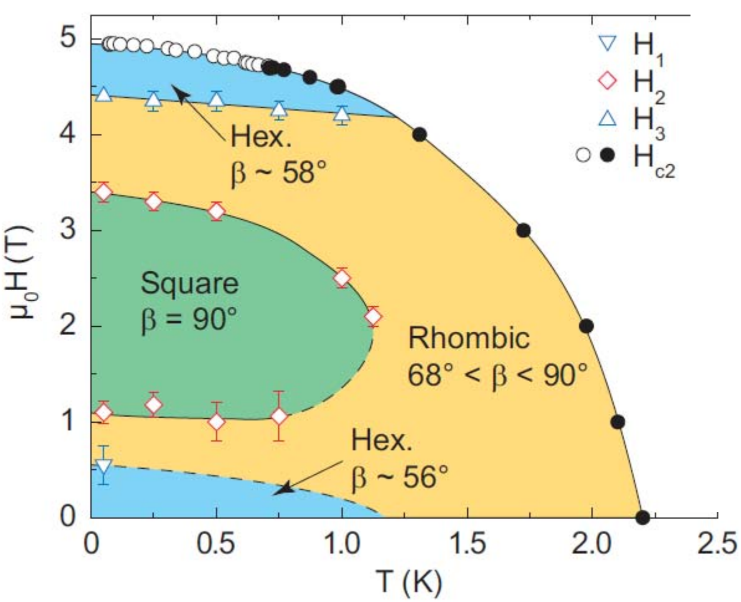
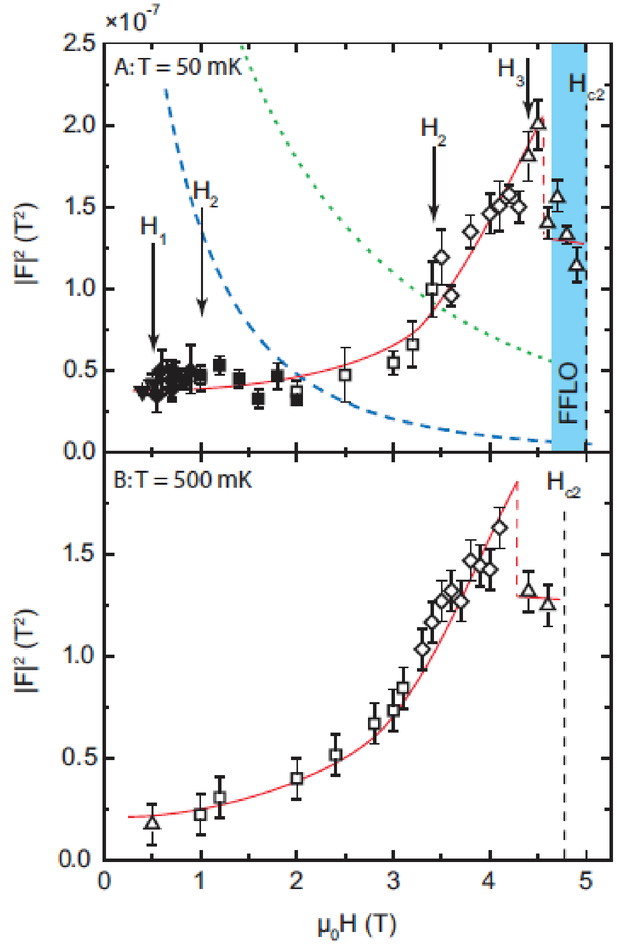


FIG. 1: (Color) FLL diffraction patterns for $CeCoIn_5$ with applied fields 0.5 T (a), 0.55 T (b) and 0.75 T (c), after subtraction of background measurement. The data is smoothed and the center of the image is masked off. The crystalline a axis is vertical.





Eskildsen et al
Science in press

Comparison between quasi-classical theory and exp.

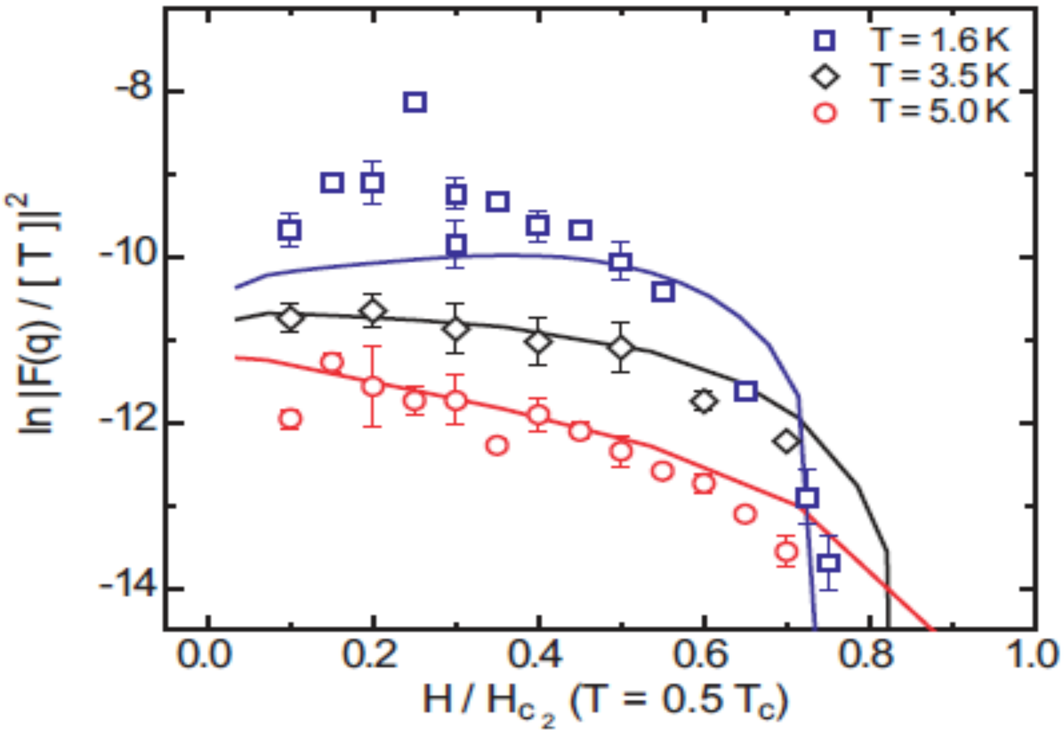


FIG. 3: (Color online) Comparison of measured and calculated VL form factors in $TmNi_2B_2C$ at $T = 1.6$, 3.5, and 5.5 K. The curves were calculated using the model described in the text, for $T = 0.16T_c$ and $\mu = 1.71$ (A), $T = 0.35T_c$ and $\mu = 1.28$ (B), and $T = 0.50T_c$ and $\mu = 0.86$ (C).

Conclusion and perspectives

rich vortex physics associated with Pauli paramagnetic effects
described microscopically by quasi-classical Eilenberger framework

TmNi2B2C
Pauli effect arised from sf exchange int.
between 4f-localized moment and s-electrons

URu2Si2
unconventional pairing with point nodes
substaintial Pauli effect
-->possible first order at Hc2

CeCoIn5
Pauli paramagnetic effect is important
for high field phase in both H-directions,
but several mysteries remain associated
with non-Fermi liquid phenomena.

Sr2RuO4
It seems that Pauli effect may be important,
in particular in understanding of the in-plane
properties; C/T etc
It comes from either

(A) The pairing symmetry is singlet,
(B) or triplet where d-vector locked in plane.

References

1)

PRL 99, 167001 (2007) PHYSICAL REVIEW LETTERS week ending 19 OCTOBER 2007

Pauli Paramagnetic Effects on Vortices in Superconducting $TmNi_2B_2C$

L. DeBeer-Schmitt,[1] M. R. Eskildsen,[1,*] M. Ichioka,[2] K. Machida,[2] N. Jenkins,[3] C. D. Dewhurst,[4] A. B. Abrahamsen,[5] S. L. Bud'ko,[6] and P. C. Canfield[6]
[1]*Department of Physics, University of Notre Dame, Notre Dame, Indiana 46556, USA*
[2]*Department of Physics, Okayama University, Okayama 700-8530, Japan*
[3]*DPMC, University of Geneva, 24 Quai Ernest-Ansermet, CH-1211 Genève 4, Switzerland*
[4]*Institut Laue-Langevin, 6 Rue Jules Horowitz, F-38042 Grenoble, France*
[5]*Materials Research Department, Risø National Laboratory, DK-4000 Roskilde, Denmark*
[6]*Ames Laboratory and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA*
(Received 4 April 2007; published 16 October 2007)

2)

Field-angle-dependent specific heat measurements and gap determination of a heavy fermion superconductor URu_2Si_2

K. Yano,[1] T. Sakakibara,[1] T. Tayama,[1] M. Yokoyama,[2] H. Amitsuka,[3] Y. Homma,[4] P. Miranović,[5] M. Ichioka,[6] Y. Tsutsumi,[6] and K. Machida[6]
[1] *Institute for Solid State Physics, University of Tokyo, Kashiwa, Chiba 270-8581, Japan*
[2] *Faculty of Science, Ibaraki University, Mito 310-8512, Japan*
[3] *Graduate School of Science, Hokkaido University, Sapporo 060-0810, Japan*
[4] *IMR Tohoku University, Oarai 311-1313, Japan*
[5] *Department of Physics, University of Montenegro, Podgorica 81000, Montenegro*
[6] *Department of Physics, Okayama University, Okayama 700-8530, Japan*
(Dated: November 14, 2007)

PRL in press

3)

Is Sr_2RuO_4 a triplet superconductor?

K. Machida and M. Ichioka
Department of Physics, Okayama University, Okayama 700-8530, Japan

arXiv: 0706.1426