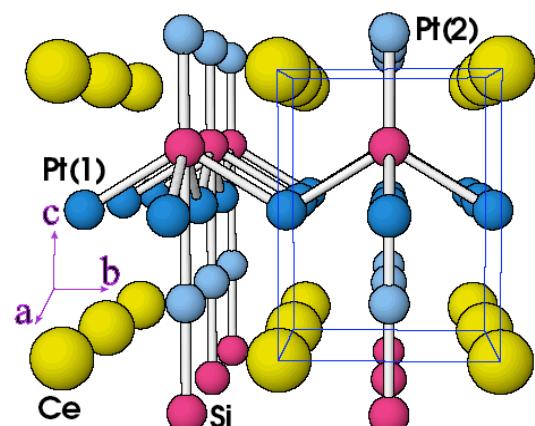


Spin-orbit coupling and superconductivity in materials without inversion symmetry

Sendai, June 29, 2006

Manfred Sigrist, ETH Zürich



- ◆ Parity as a key symmetry
for superconductivity
role of antisymmetric spin-orbit coupling
- ◆ Physical properties
discussion of experimental results

Collaborators:

Theory

- ETH Zurich:* P.A. Frigeri, N. Hayashi, K. Wakabayashi, I. Milat, Y. Yanase
Uni Wisconsin: D.F. Agterberg, R.P. Kaur
Osaka Uni: A. Koga

Experiment

- TU Wien:* E. Bauer and his team
Uni Illinois: H-Q. Yuan, ...
Kyoto Uni: T. Shibauchi, Y. Matsuda, ...
IBM Watson Lab: L. Kruzin-Elbaum

Funding:

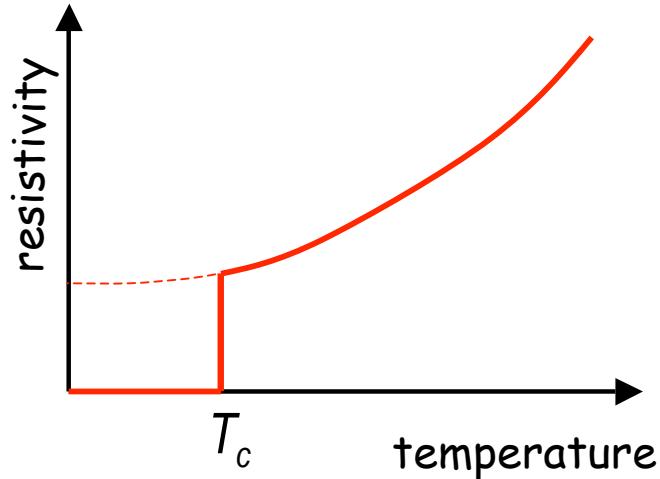


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SCHWEIZERISCHER NATIONALFONDS
FONDO NAZIONALE SVIZZERO
SWISS NATIONAL SCIENCE FOUNDATION

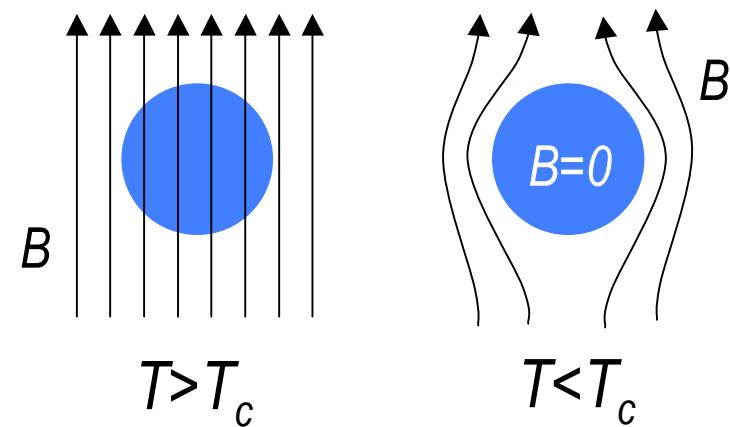


Superconductivity

Electrical resistance (1911)



Field expulsion (1933)
Meissner-Ochsenfeld effect



Superconductivity as a thermodynamic phase

London theory (1935)

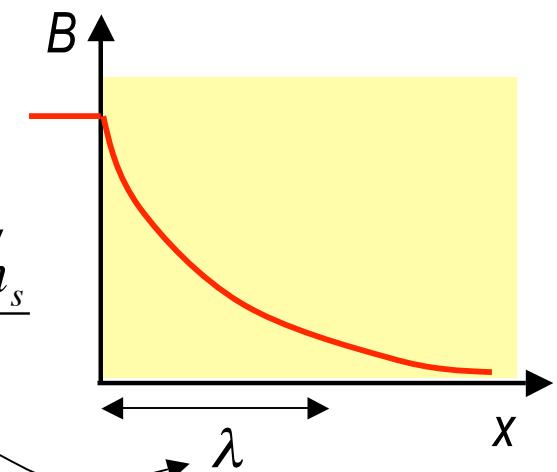
$$\left. \begin{aligned} \nabla \times \lambda^2 \vec{j} &= -\vec{B} \\ \nabla \times \vec{B} &= \frac{4\pi}{c} \vec{j} \end{aligned} \right\}$$

density of superconducting electrons

$$\nabla^2 \vec{B} = \lambda^{-2} \vec{B}$$

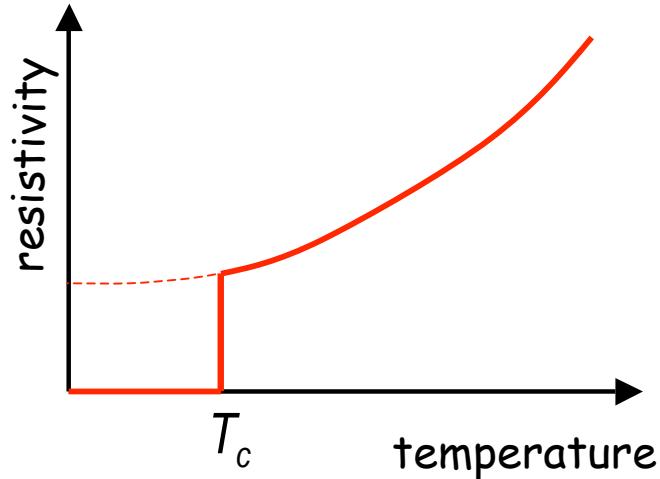
$$\lambda^{-2} = \frac{4\pi e^2 n_s}{mc^2}$$

London penetration depth

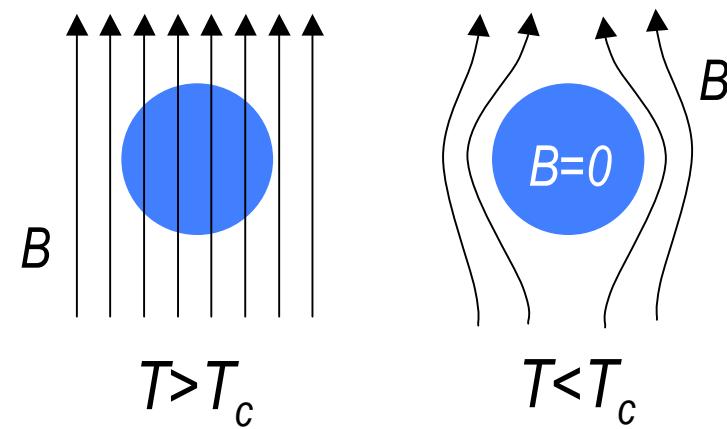


Superconductivity

Electrical resistance (1911)



Field expulsion (1933)
Meissner-Ochsenfeld effect



Superconductivity as a thermodynamic phase

Order parameter: $\Psi(\vec{r}) = |\Psi(\vec{r})| e^{i\varphi(\vec{r})}$ condensate with a broken $U(1)$ -gauge symmetry

$$F[\Psi, \vec{A}] = \int d^3r \left[a(T) |\Psi|^2 + b |\Psi|^4 + K |\vec{D}\Psi|^2 + \frac{1}{8\pi} (\vec{\nabla} \times \vec{A})^2 \right]$$

Ginzburg-Landau theory (1950)

minimal coupling $\vec{D} = \vec{\nabla} + i \frac{2e}{\hbar c} \vec{A}$

Mikroscopic viewpoint of superconductivity

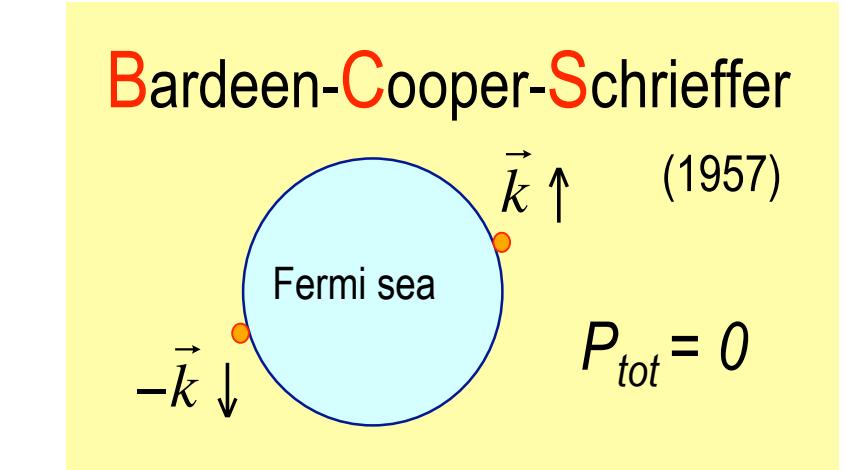
Order parameter $\Psi(\vec{r}) = |\Psi(\vec{r})| e^{i\varphi(\vec{r})}$ complex condensate wave function

Coherent state of electron pairs (Cooper pairs)

$$|\psi\rangle = \prod_{\vec{k}} \left\{ u_{\vec{k}} + v_{\vec{k}} c_{\vec{k}\uparrow}^\dagger c_{-\vec{k}\downarrow}^\dagger \right\} |0\rangle$$

not a state of fixed particle number

$$c_{-\vec{k}\downarrow} c_{\vec{k}\uparrow} |\psi\rangle = u_{\vec{k}} v_{\vec{k}} |\psi\rangle$$



fixed phase

violation of $U(1)$ -gauge symmetry

$$\begin{aligned} c_{\vec{k}} &\rightarrow e^{i\alpha} c_{\vec{k}} \\ \Rightarrow \Psi_{\vec{k}} &\rightarrow e^{2i\alpha} \Psi_{\vec{k}} \end{aligned}$$

condensate wavefunction

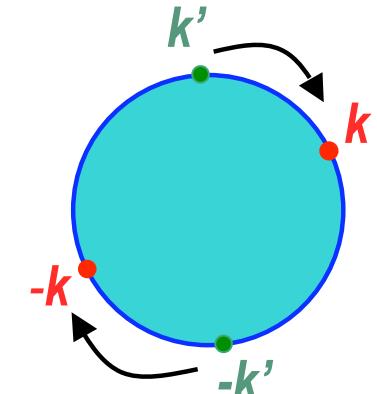
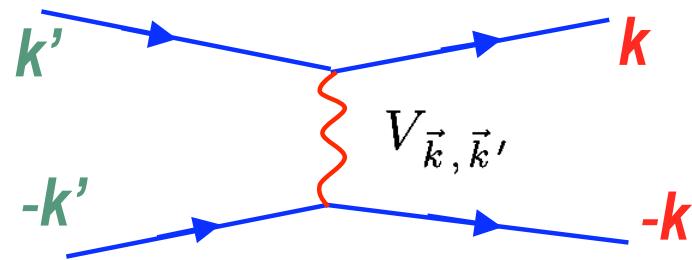
$$\Psi_{\vec{k}} = \langle \psi | c_{-\vec{k}\downarrow} c_{\vec{k}\uparrow} | \psi \rangle = u_{\vec{k}} v_{\vec{k}}$$

" $U(1)$ - Higgs field"

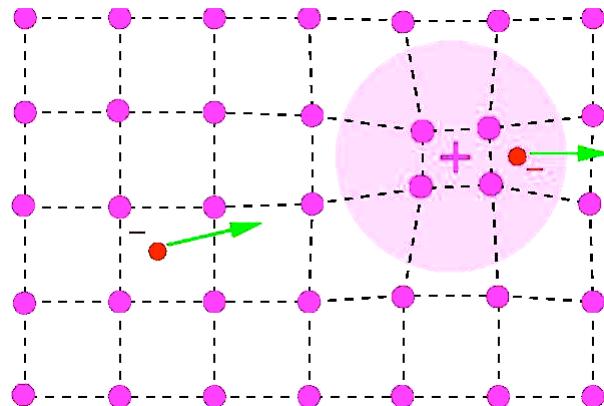
Pairing interaction

Cooper pair formation (bound state of 2 electrons) needs attractive interaction

$$\mathcal{H}_{pair} = \frac{1}{2\Omega} \sum_{\vec{k}, \vec{k}'} \sum_{s, s'} V_{\vec{k}, \vec{k}'} c_{\vec{k}, s}^\dagger c_{-\vec{k}, s'}^\dagger c_{-\vec{k}', s'} c_{\vec{k}', s}$$



electron phonon interaction:



attractive interaction



scattering between electron states
with degenerate energy

$$\varepsilon_{\vec{k}} = \varepsilon_{-\vec{k}}$$

Alternative mechanism for Cooper pairing

Pairing from purely repulsive interactions: Kohn & Luttinger (1965)

screened Coulomb potential in metal has long-ranged oscillatory tail (sharp Fermi edge)

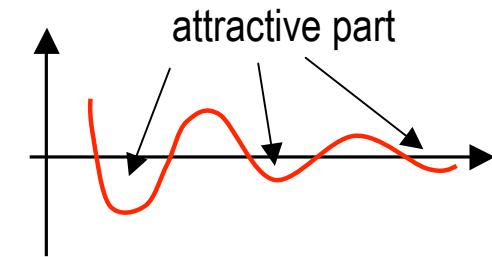
Friedel oscillations:

$$V(r) \propto r^{-3} \cos(2k_F r)$$

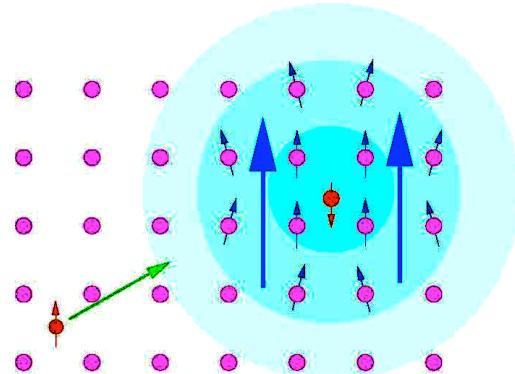
pairing in high-angular momentum channel $l > 0$

$$T_c/T_F \sim \exp\{-(2l)^4\}$$

very low !



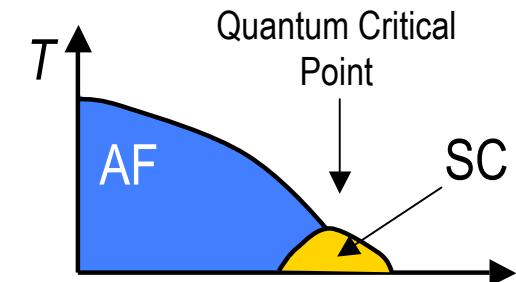
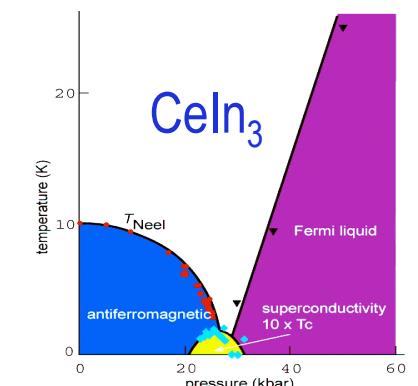
Pairing by magnetic fluctuations: Berk & Schrieffer (1966)



easily spin polarizable medium

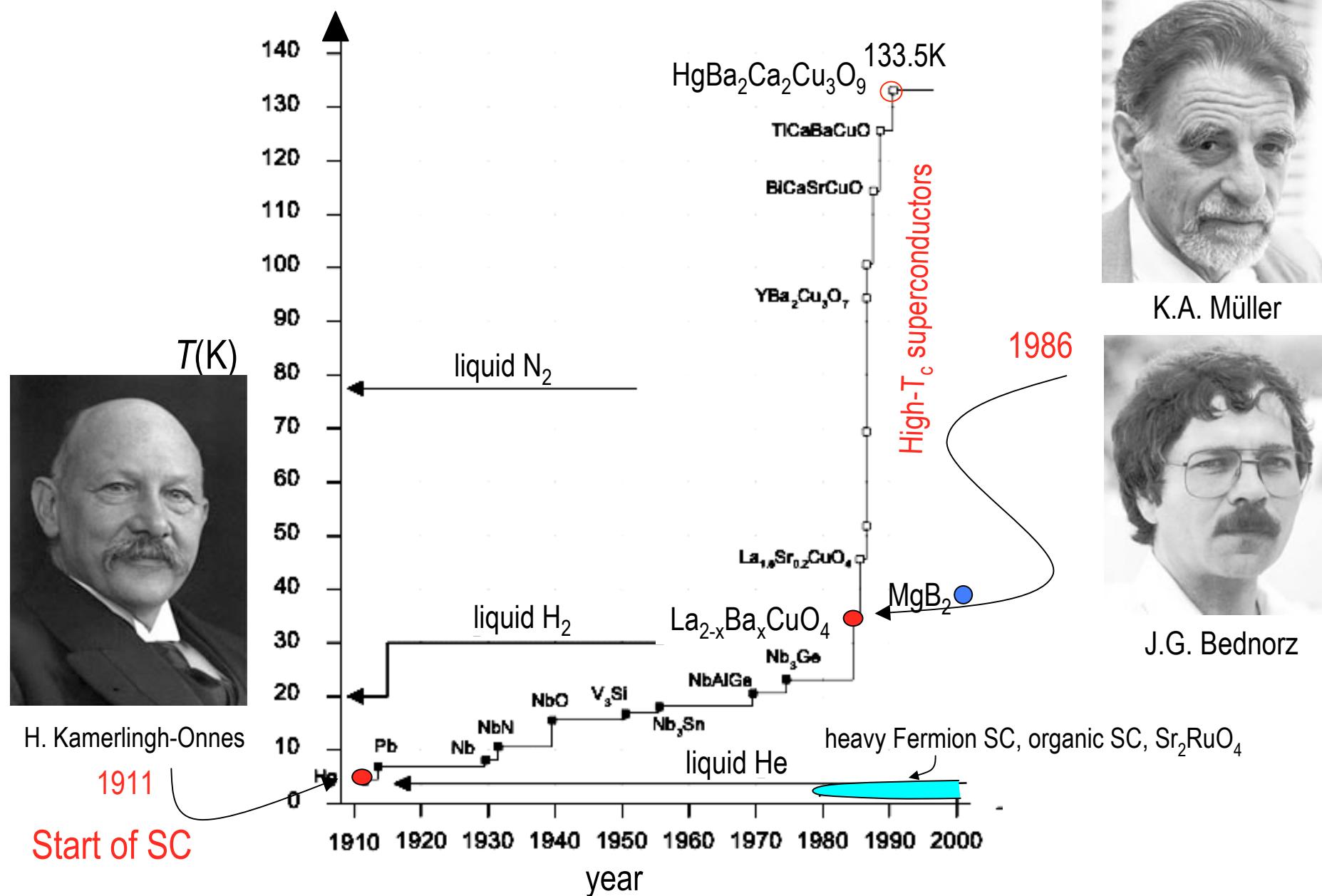
longer ranged interaction

T_c reasonable for higher angular momentum pairing



Novel Superconductors

Unexpected breakthroughs

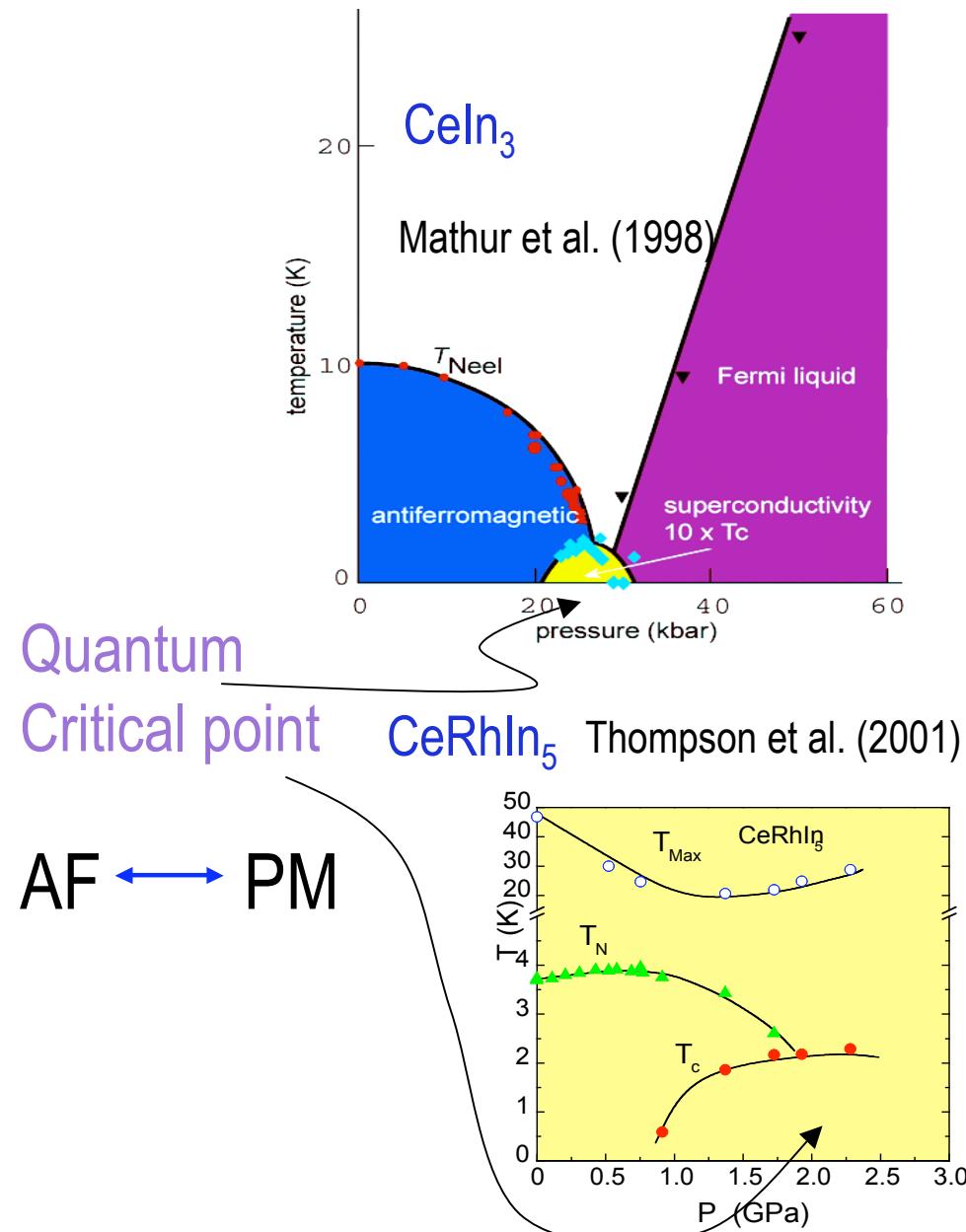
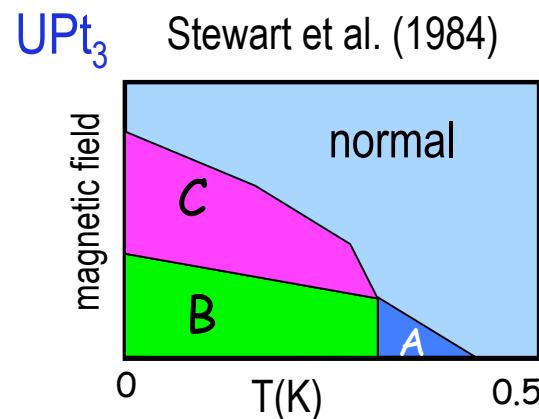
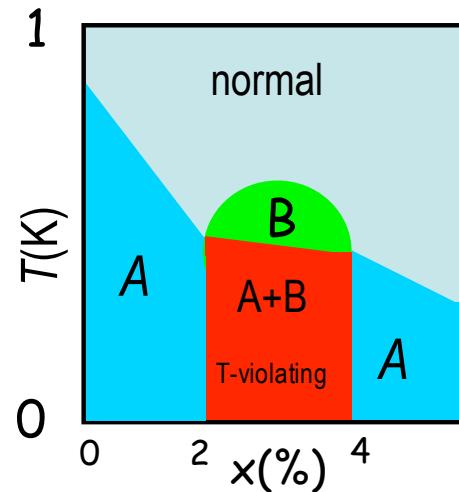


The novel superconductors

Heavy Fermion superconductors:

CeCu_2Si_2 Steglich et al. (1979)

$\text{U}_{1-x}\text{Th}_x\text{Be}_{13}$ Ott et al. (1983)



The novel superconductors

High-temperature superconductors

Layered perovskite cooper-oxides

Müller & Bednorz (1986)



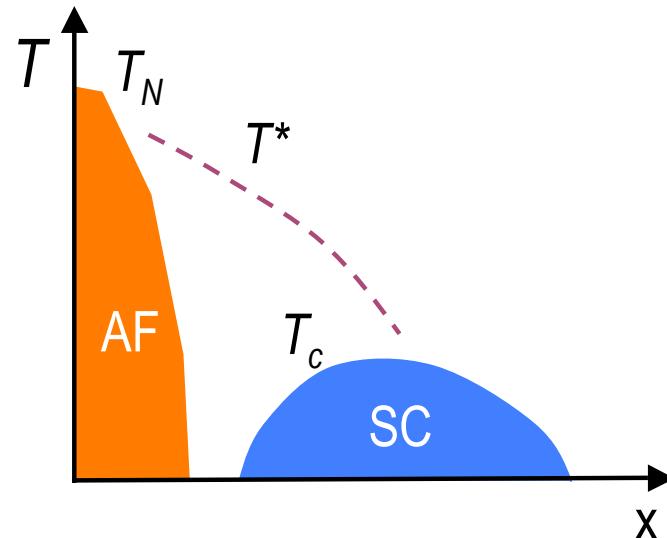
$T_c = 45\text{K}$



$T_c = 92\text{K}$



$T_c = 133.5\text{K}$



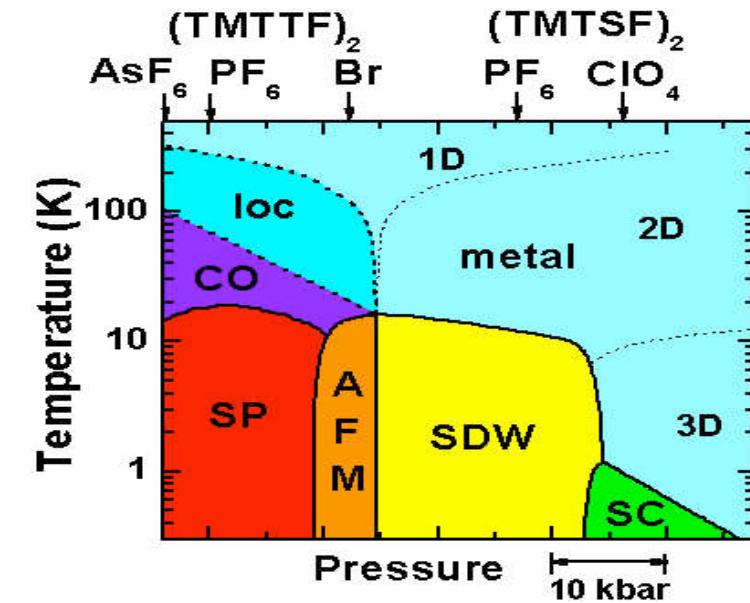
Organic superconductors

Jerome, Bechtgard et al (1980)

$(\text{TMTSF})_2\text{M}$ ($\text{M}=\text{PF}_6^-$, SbF_6^- , ReO_4^- , ...) $T_c \sim 1\text{K}$

$(\text{BEDT-TTF})_2\text{M}$

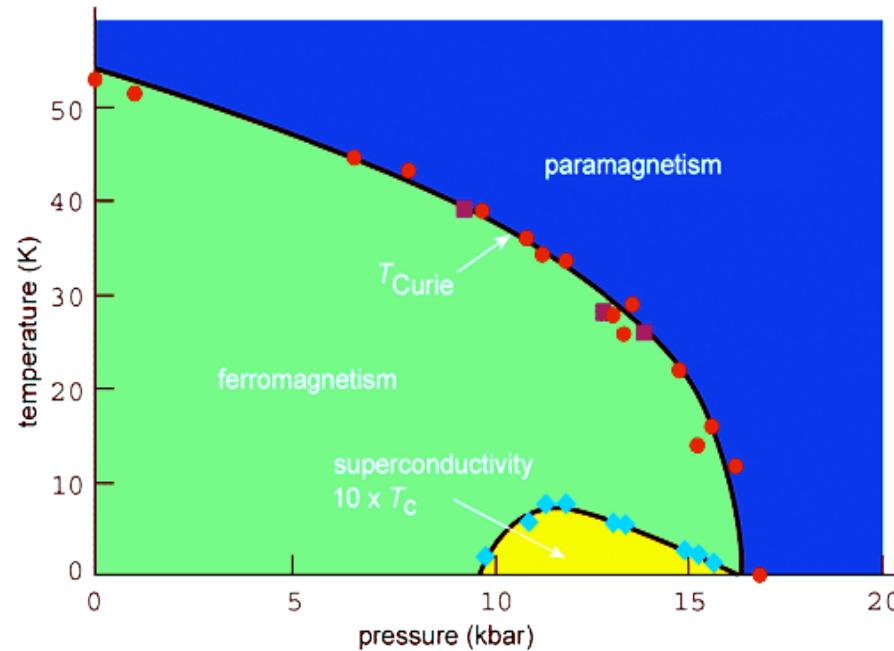
$T_c \sim 10\text{K}$



The novel superconductors

Ferromagnetic superconductors:

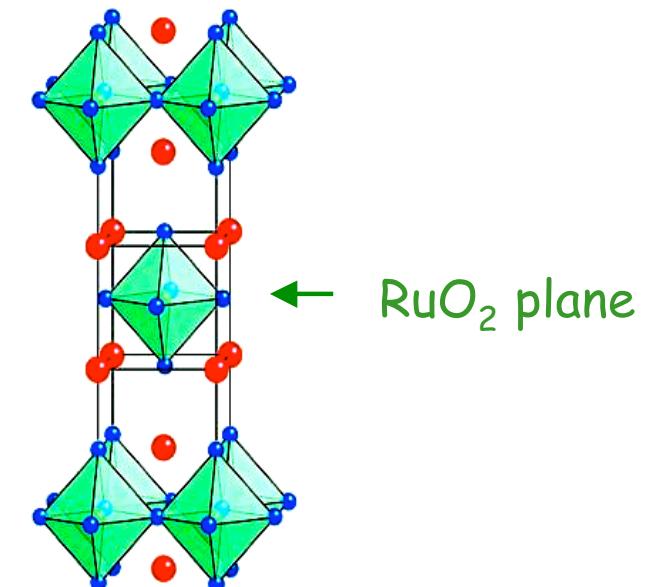
UGe_2 Saxena et a. (2000)



ZrZn_2 Pfleiderer et al. (2001)

Superconductivity within
the ferromagnetic phase

Sr_2RuO_4



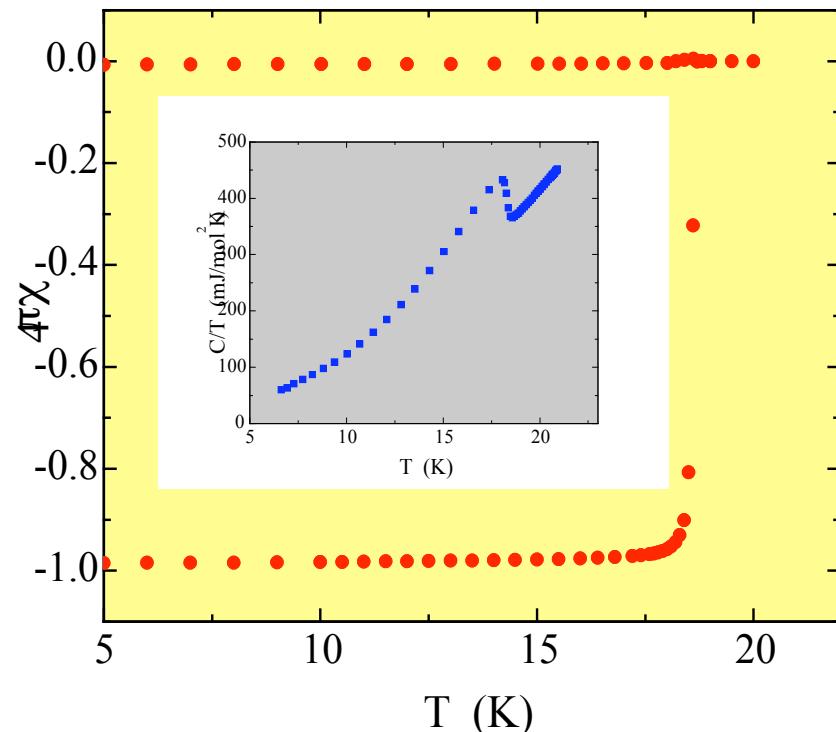
some similarities with
high- T_c superconductors,

but $T_c = 1.5 \text{ K}$

spin-triplet superconductor

The novel superconductors

Plutonium compounds

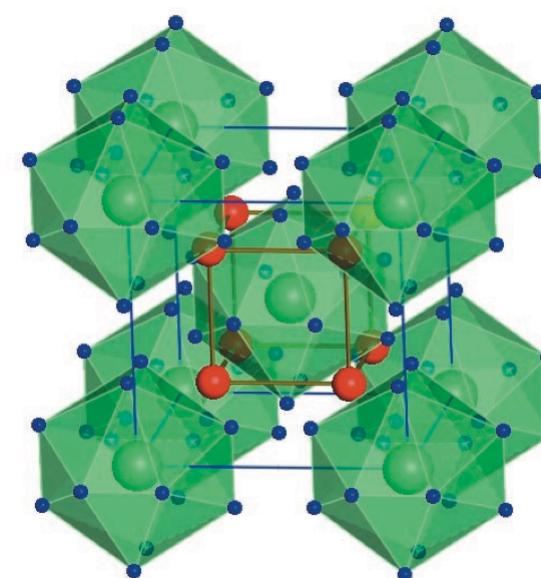


PuCoGa_5

$T_c = 18 \text{ K}$

Thompson et al. (Los Alamos)

Skutterudite



$\text{PrOs}_4\text{Sb}_{12}$ $T_c = 1.8 \text{ K}$

Bauer et al. PRB 65, R100506 (2002)

Multiple phases

Cooper pairing
and
Symmetry

Alternative ways to Cooper pairing

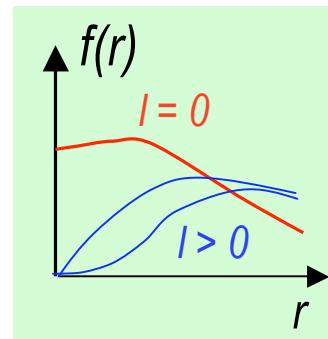
Coulomb and electron-phonon interaction very short-ranged (λ_{TF}) “*contact interaction*”

Bound Cooper pair wavefunction:

$$\psi(\vec{r}, s; \vec{r}', s') = f(|\vec{r} - \vec{r}'|) \chi(s, s')$$

with $f(r \rightarrow 0) \neq 0$

relative angular momentum $I=0$
important for “contact interaction”



How to avoid Coulomb repulsion?

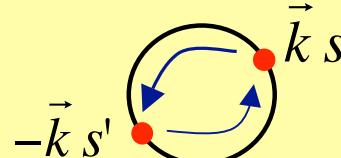
higher-angular momentum pairing

$$I > 0 \quad \rightarrow \quad f(r \rightarrow 0) \propto r^l$$

“contact interaction” not effective

Symmetry of pairs of identical electrons: $\Psi_{ss'}(\vec{k}) = \langle \hat{c}_{\vec{k}s} \hat{c}_{-\vec{k}s'} \rangle = \underbrace{\Phi(\vec{k})}_{\text{orbital}} \underbrace{\chi(s, s')}_{\text{spin}}$

wave function totally antisymmetric
under particle exchange



$$\vec{k} \rightarrow -\vec{k} \quad s \leftrightarrow s'$$

even parity: $I = 0, 2, 4, \dots$, $S=0$ singlet
even odd

odd parity: $I = 1, 3, 5, \dots$, $S=1$ triplet
odd even

Requirements for the formation of Cooper pairs

Anderson's Theorems (1959, 1984)

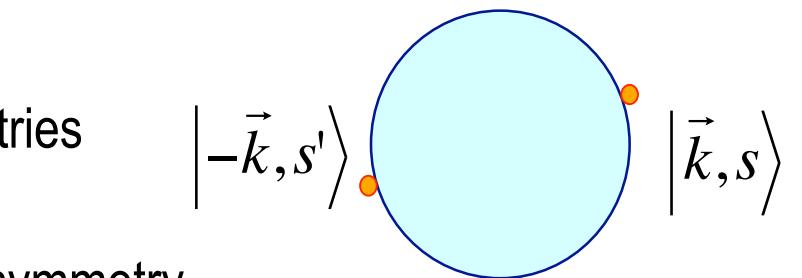
Cooper pair formation with $P=0$ relies on symmetries which guarantee **degenerate partner electrons**

- Spin singlet pairing: time reversal symmetry

$$|\vec{k} \uparrow\rangle$$

$$T|\vec{k} \uparrow\rangle = |\vec{-k} \downarrow\rangle$$

time reversal



harmful:
magnetic impurities
ferromagnetism
paramagnetic limiting

- Spin triplet pairing: time reversal & inversion symmetry

$$|\vec{k} \uparrow\rangle$$

$$I|\vec{k} \uparrow\rangle = |\vec{-k} \uparrow\rangle$$

inversion

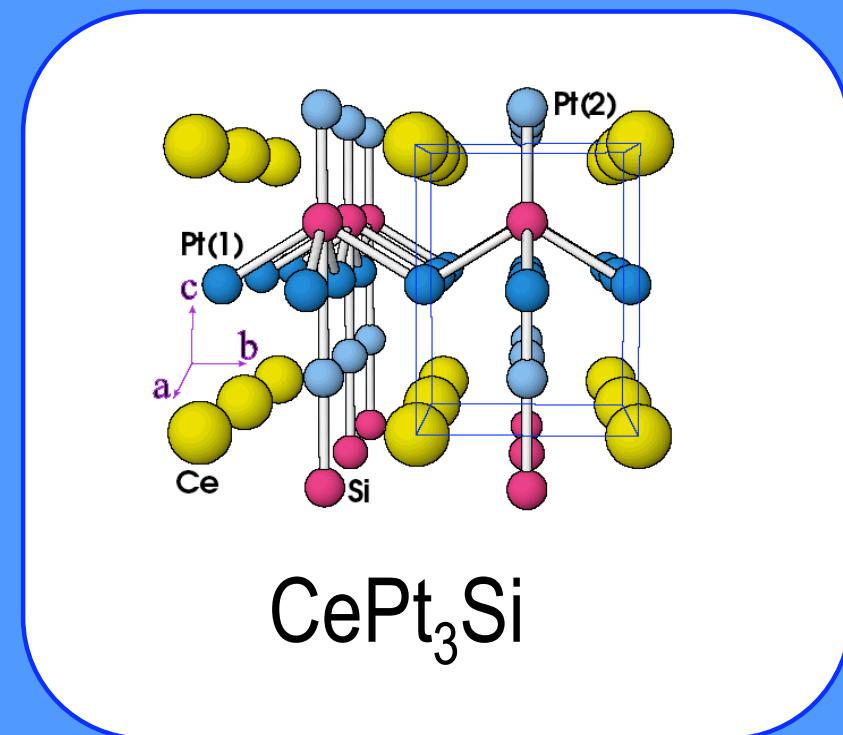
$$T|\vec{k} \uparrow\rangle = |\vec{-k} \downarrow\rangle$$

$$IT|\vec{k} \uparrow\rangle = |\vec{k} \downarrow\rangle$$

harmful: crystal structure without inversion center

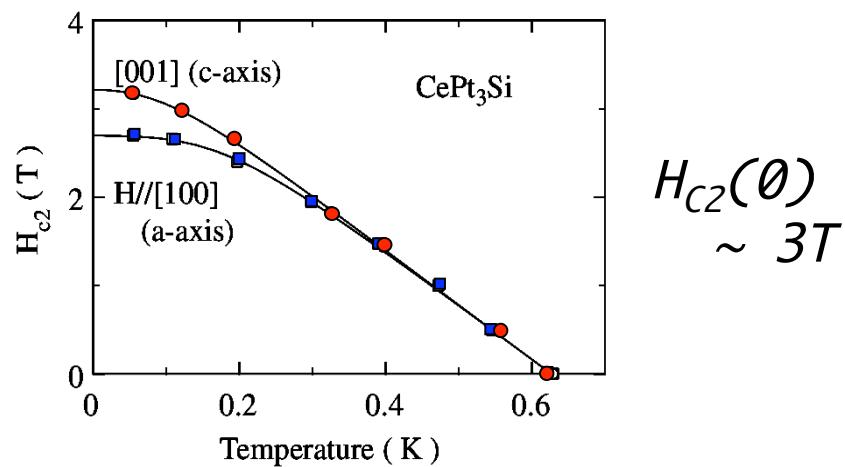
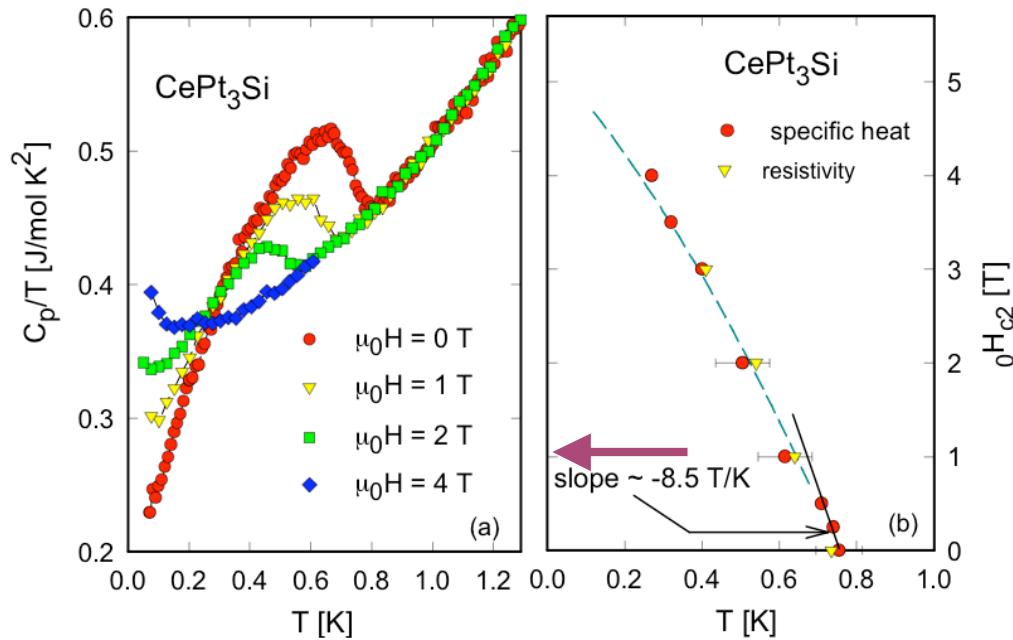
The essential symmetries

Non-centrosymmetric superconductors



CePt₃Si Heavy Fermion superconductor: $T_c = 0.75$ K

E. Bauer et al. PRL 92, 027003 (2004)



$$\gamma \approx 350 \frac{mJ}{molK^2}$$

$$H_{c2}(T=0) \rightarrow 5T$$

paramagnetic limiting

$$H_p \approx \frac{\Delta_0}{\sqrt{2}\mu_B} \approx \frac{k_B T_C}{\mu_B} \approx 1T$$

No paramagnetic limiting

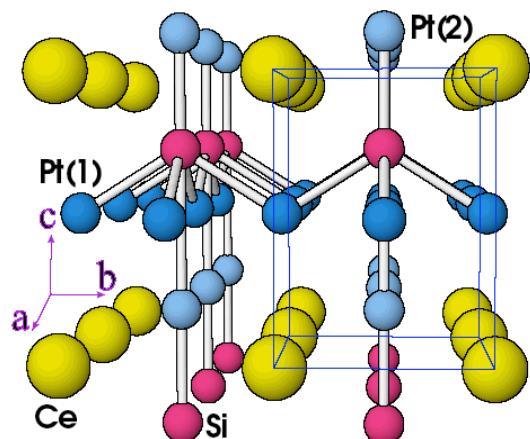


spin triplet pairing ?

T. Yasuda et al., JPSJ 73, 1657 (2004)

Symmetry of superconducting phase

CePt₃Si



Crystal space group

P4mm tetragonal

generating
point group

C_{4v}

(mirror plane z → -z missing)



No inversion center:

spin triplet pairing?

Anderson's second theorem

Basic Model of a system without inversion center

Lack of inversion symmetry

$$\mathcal{H} = \underbrace{\sum_{\vec{k}, s} (\epsilon_{\vec{k}} - \mu) c_{\vec{k}s}^\dagger c_{\vec{k}s}}_{\text{Electron band}} + \alpha \underbrace{\sum_{\vec{k}, s, s'} \vec{\lambda}_{\vec{k}} \cdot \{c_{\vec{k}s}^\dagger \vec{\sigma}_{ss'} c_{\vec{k}s'}\}}_{\text{Spin-orbit coupling}}$$

Symmetry conditions

- time reversal symmetry: $\epsilon_{\vec{k}} = \epsilon_{-\vec{k}}$ and $\vec{\lambda}_{\vec{k}} = -\vec{\lambda}_{-\vec{k}}$

$$\vec{k} \rightarrow -\vec{k}, \vec{S} \rightarrow -\vec{S}$$

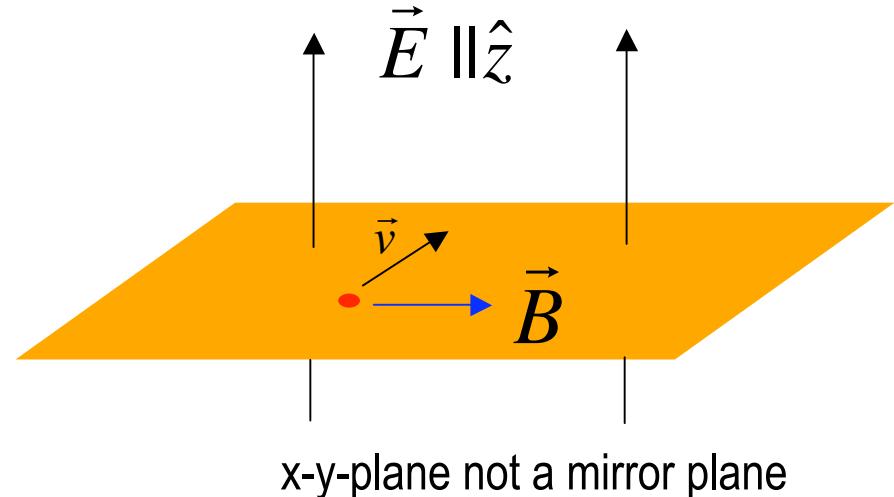
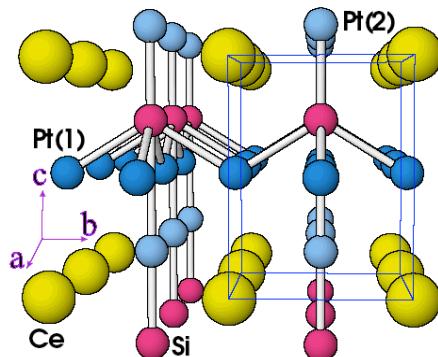
- inversion symmetry: $\epsilon_{\vec{k}} = \epsilon_{-\vec{k}}$ and $\vec{\lambda}_{\vec{k}} = \vec{\lambda}_{-\vec{k}}$

$$\vec{k} \rightarrow -\vec{k}, \vec{S} \rightarrow \vec{S}$$

$\vec{\lambda}_{\vec{k}} \neq 0 \quad \rightarrow \quad$ time reversal and/or inversion symmetry absent

Lack of inversion symmetry

Dresselhaus 1955; Rashba 1960



x-y-plane not a mirror plane

Special relativity: $\vec{B} \approx -\frac{\vec{v}}{c} \times \vec{E}$

Zeeman coupling: $\vec{B} \cdot \vec{S} \propto (\vec{v} \times \hat{z}) \cdot \vec{S} \propto \vec{\lambda} \cdot \vec{S} \rightarrow \vec{\lambda}_{\vec{k}} \propto \begin{pmatrix} k_y \\ -k_x \\ 0 \end{pmatrix}$

$$\vec{\lambda}_{\vec{k}} = -\vec{\lambda}_{-\vec{k}}$$

time reversal symmetry conserved

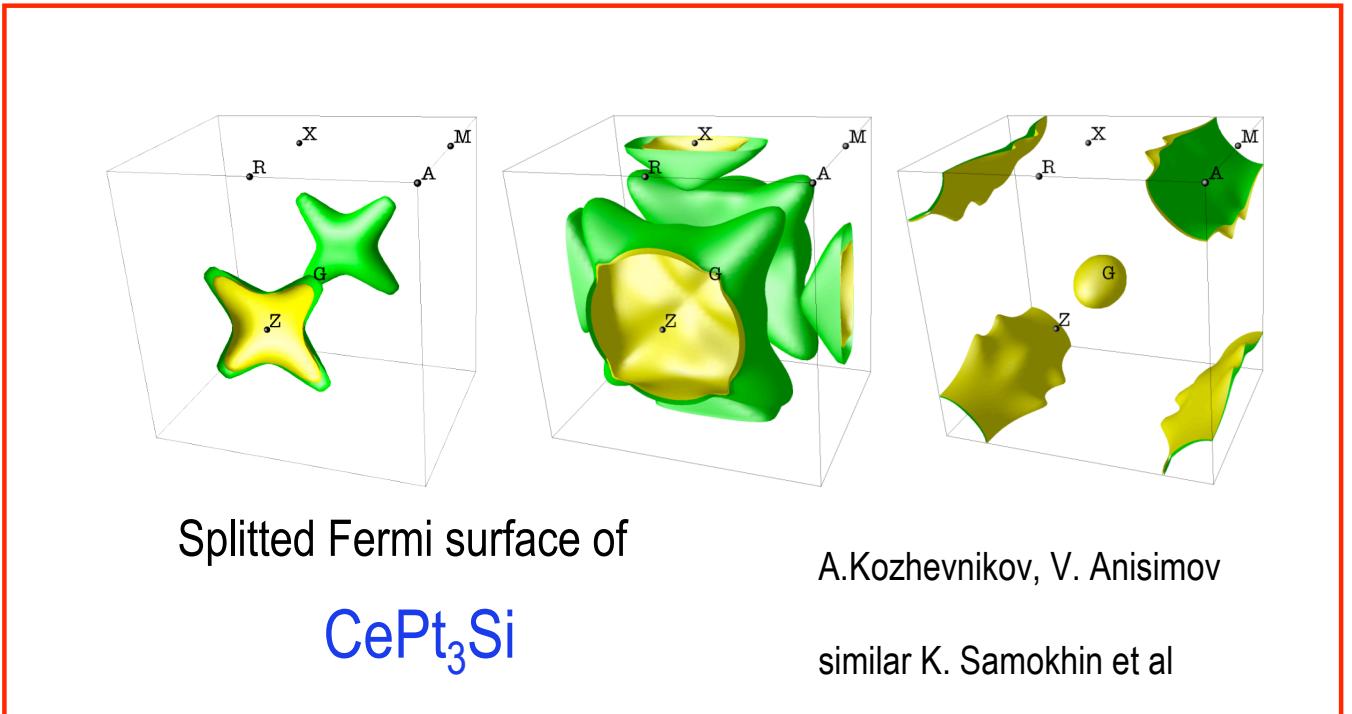
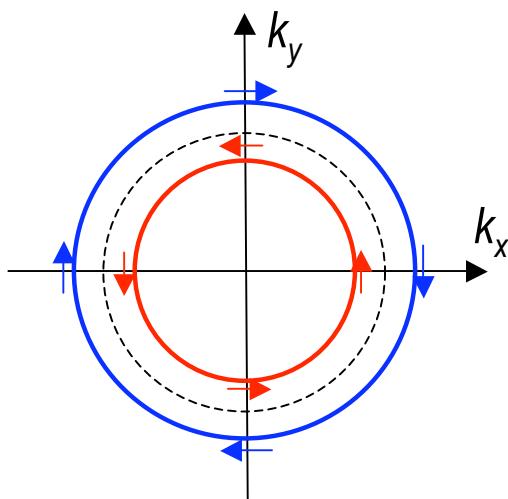
Band splitting

$$\mathcal{H} = \sum_{\vec{k}, s} (\epsilon_{\vec{k}} - \mu) c_{\vec{k}s}^\dagger c_{\vec{k}s} + \alpha \sum_{\vec{k}, s, s'} \vec{\lambda}_{\vec{k}} \cdot \{ c_{\vec{k}s}^\dagger \vec{\sigma}_{ss'} c_{\vec{k}s'} \}$$

*k-dependent spin splitting
(Zeeman)*

Energy spectrum:

$$E_{\vec{k}\pm} = \epsilon_{\vec{k}} - \mu \pm \alpha |\lambda_{\vec{k}}|$$



Superconductivity

Hamiltonian: $\hat{H} = \sum_{\vec{k}, s, s'} [\xi_{\vec{k}} \sigma^0 + \alpha \vec{\lambda}_k \cdot \vec{\sigma}]_{s, s'} \hat{c}_{\vec{k}, s}^\dagger \hat{c}_{\vec{k}, s'} + \frac{1}{2} \sum_{\vec{k}, \vec{k}', s, s'} V_{\vec{k}, \vec{k}'} \hat{c}_{\vec{k}, s}^\dagger \hat{c}_{-\vec{k}, s'}^\dagger \hat{c}_{-\vec{k}', s'} \hat{c}_{\vec{k}', s}$

Mean field:

$$\Psi_{\vec{k}, ss'} = \langle c_{-\vec{k}s'} c_{\vec{k}s} \rangle$$

spin singlet, even parity

$$\Psi_{\vec{k}, ss'} = \begin{pmatrix} 0 & \psi(\vec{k}) \\ -\psi(\vec{k}) & 0 \end{pmatrix}$$

1 configuration $\frac{\psi(\vec{k})}{\sqrt{2}} (| \uparrow\downarrow \rangle - | \downarrow\uparrow \rangle)$

$$\psi(-\vec{k}) = \psi(\vec{k})$$

spin triplet, odd parity

$$\Psi_{\vec{k}, ss'} = \begin{pmatrix} -d_x + id_y & d_z \\ d_z & d_x + id_y \end{pmatrix}$$

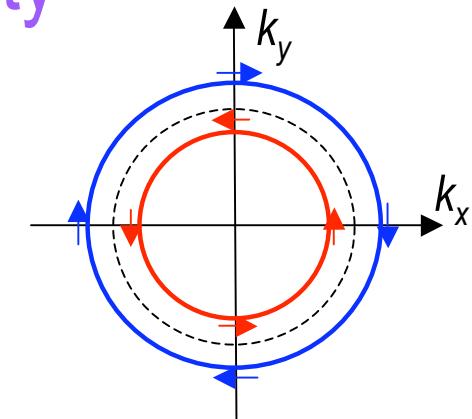
3 configurations $\left\{ \begin{array}{l} (-d_x(\vec{k}) + id_y(\vec{k})) | \uparrow\uparrow \rangle \\ \frac{d_z(\vec{k})}{\sqrt{2}} (| \uparrow\downarrow \rangle + | \downarrow\uparrow \rangle) \\ (d_x(\vec{k}) + id_y(\vec{k})) | \downarrow\downarrow \rangle \end{array} \right.$

$$\vec{d}(-\vec{k}) = -\vec{d}(\vec{k})$$

Spin-orbit coupling and superconductivity

spin-orbit coupling as a perturbation

spin singlet pairing: minor effect



spin triplet pairing: almost all pairing states severely suppressed

weakly affected pairing states:

$$\vec{\lambda}_{\vec{k}} \parallel \vec{d}(\vec{k})$$

$$\text{CePt}_3\text{Si: } \vec{d}(\vec{k}) \propto \begin{pmatrix} k_y \\ -k_x \\ o \end{pmatrix}$$

The Superconducting Phase

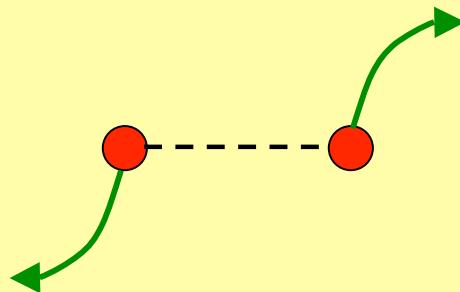
and

the Magnetic Field

Upper critical field

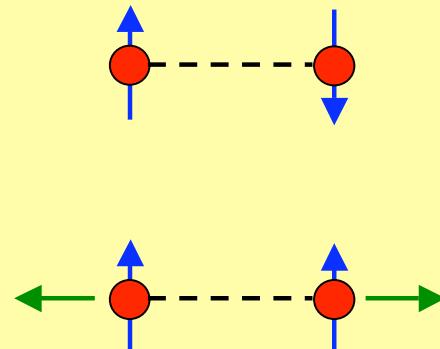
How to destroy Cooper pairs by a magnetic field?

Orbital depairing:



Lorentz force
on moving
charged particles

Spin depairing:

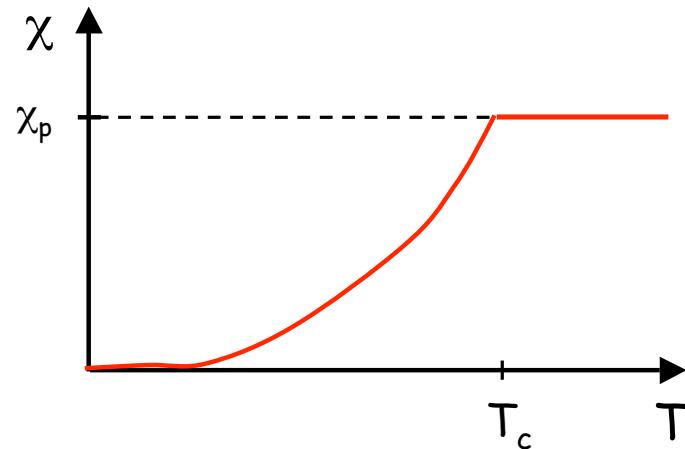


Zeeman coupling
spin polarization

Spin anisotropy

- spin singlet pairing \rightarrow Yosida behavior of spin susceptibility

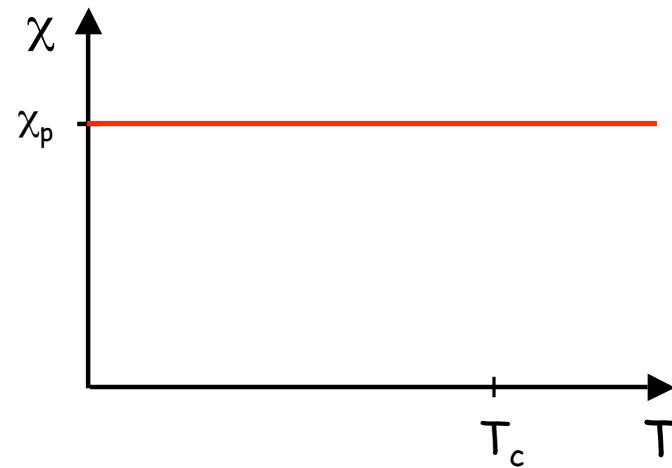
pair breaking
by spin polarization



- spin triplet pairing

no pair breaking
for equal spin pairing

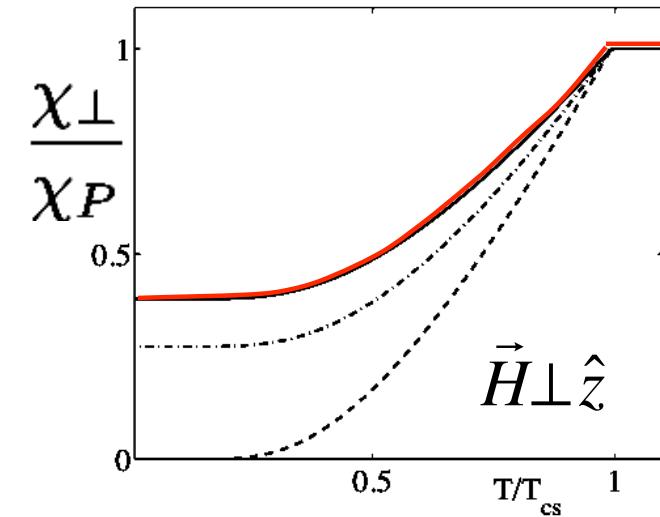
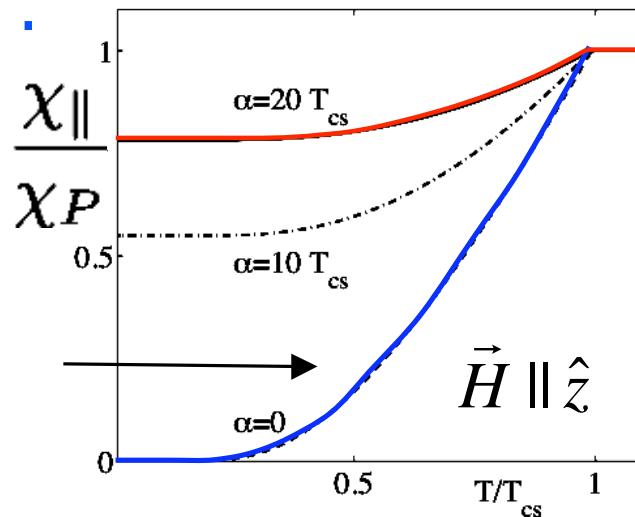
$$\chi = \text{const. for } \vec{d}(\vec{k}) \cdot \vec{H} = 0$$



Modified spin susceptibility

"Spin singlet":

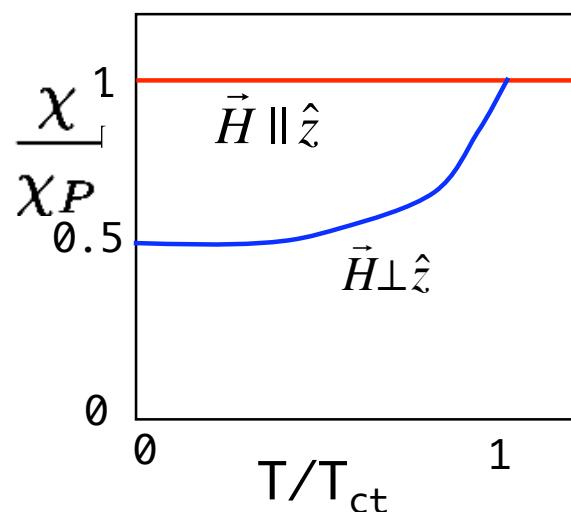
Yosida behavior



"Spin triplet":

$$\vec{\lambda}_k \parallel \vec{d}(k)$$

independent of α



singlet and triplet
become similar

Paramagnetic limiting

destruction of superconductivity due to Zeeman splitting of electron spins

Comparison of

$$E_{cond} = \frac{1}{2}N(0)|\Delta(0)|^2 = \frac{H_c(0)^2}{8\pi} \quad \longleftrightarrow \quad E_{para} = \frac{1}{2}\{\chi_P - \chi(0)\}H^2$$

quasiparticle gap

Pauli susceptibility

$$H_p = \frac{|\Delta(0)|/\mu_B\sqrt{2}}{\sqrt{1 - \chi(0)/\chi_P}}$$

paramagnetic limiting field

Paramagnetic limiting

destruction of superconductivity due to Zeeman splitting of spin

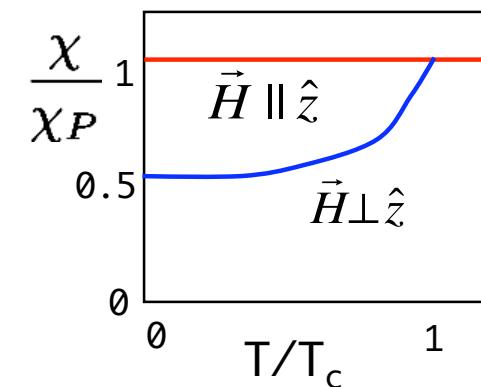
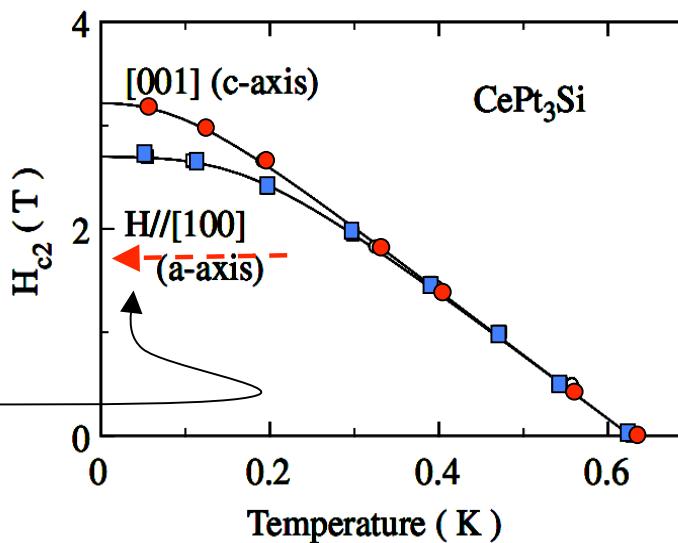
$$H_p = \frac{|\Delta(0)|/\mu_B\sqrt{2}}{\sqrt{1 - \chi(0)/\chi_P}}$$

Susceptibility:	$H \parallel c\text{-axis}$	weak limiting
	$H \parallel ab\text{-axis}$	intermediate limiting

Experiment:

T. Yasuda et al.
JPSJ 73, 1657 (2004)

expected
in-plane H_p

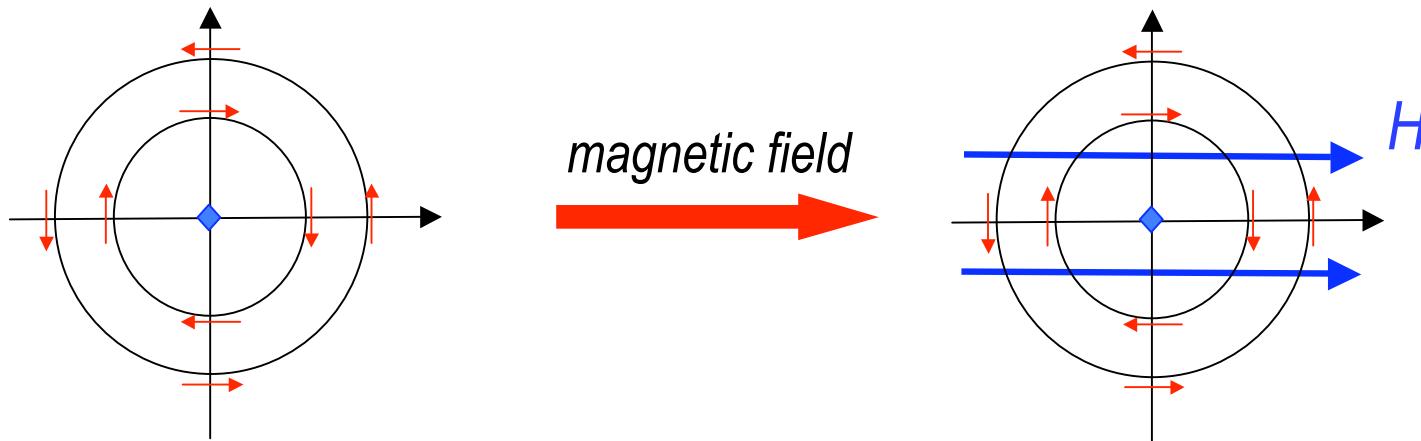


upper critical fields
almost identical for
both field directions

Helical Phase

Helical phase in a magnetic field

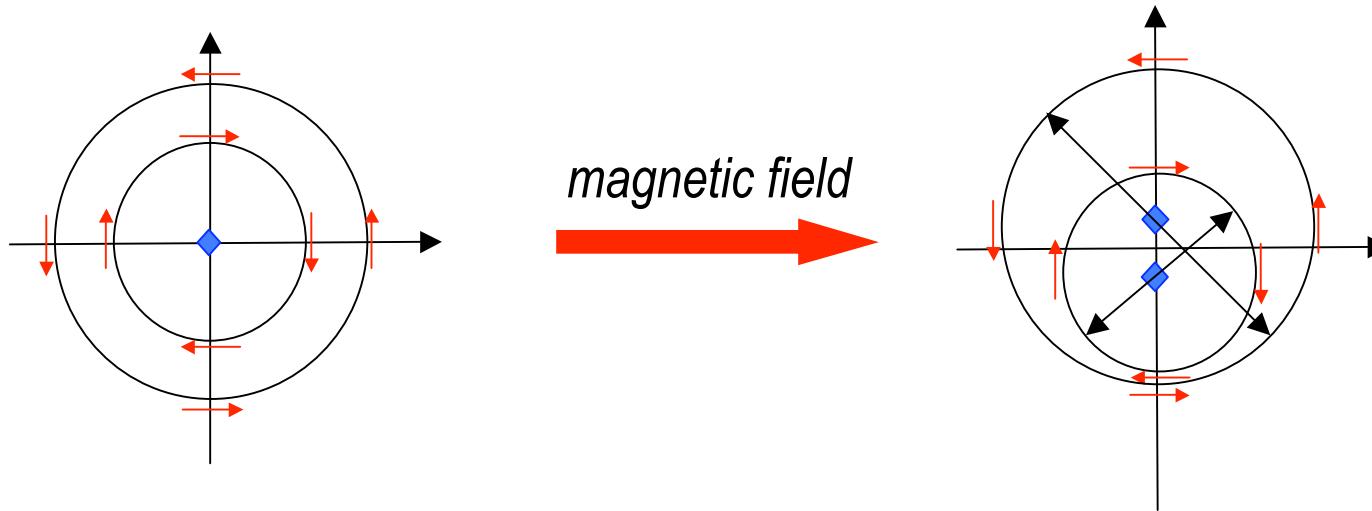
effect of magnetic field on the Fermi surfaces



$$\mathcal{H} = \mathcal{H}_{band} + \sum_{\vec{k}, s, s'} (\vec{\lambda}_{\vec{k}} - \mu_B \vec{H}) \cdot \{ c_{\vec{k}s}^\dagger \vec{\sigma}_{ss'} c_{\vec{k}s'} \}$$

Helical phase in a magnetic field

effect of magnetic field

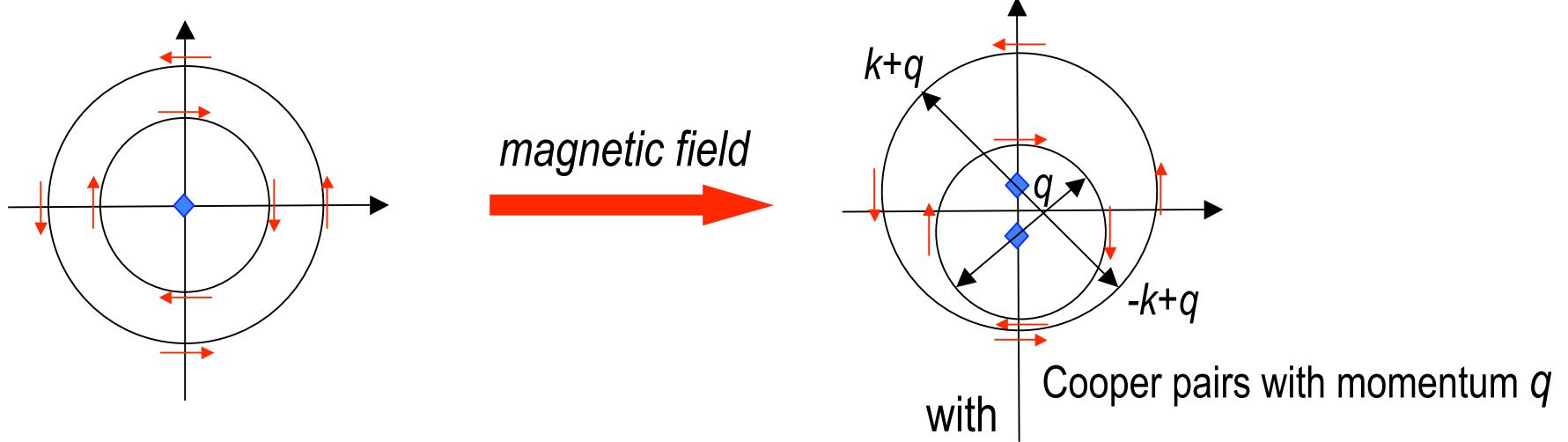


$$\mathcal{H} = \mathcal{H}_{band} + \sum_{\vec{k}, s, s'} (\vec{\lambda}_{\vec{k}} - \mu_B \vec{H}) \cdot \{ c_{\vec{k}s}^\dagger \vec{\sigma}_{ss'} c_{\vec{k}s'} \}$$

Fermi surface shifts by $\pm q \propto B$

Helical phase in a magnetic field

effect of magnetic field



Ginzburg-Landau expansion for single-component order parameter:

$$F = a|\psi|^2 + b|\psi|^4 + K|\vec{D}\psi|^2 + \underbrace{\epsilon \vec{H} \cdot \hat{z} \times \left\{ \psi(\vec{D}\psi)^* + \psi^*(\vec{D}\psi) \right\}}_{\text{new term}} + \frac{\vec{H}^2}{8\pi}$$

$$\vec{D} = \frac{\hbar}{i} \vec{\nabla} + \frac{e}{c} \vec{A}$$

new term possible Mineev & Samokhin (1994)

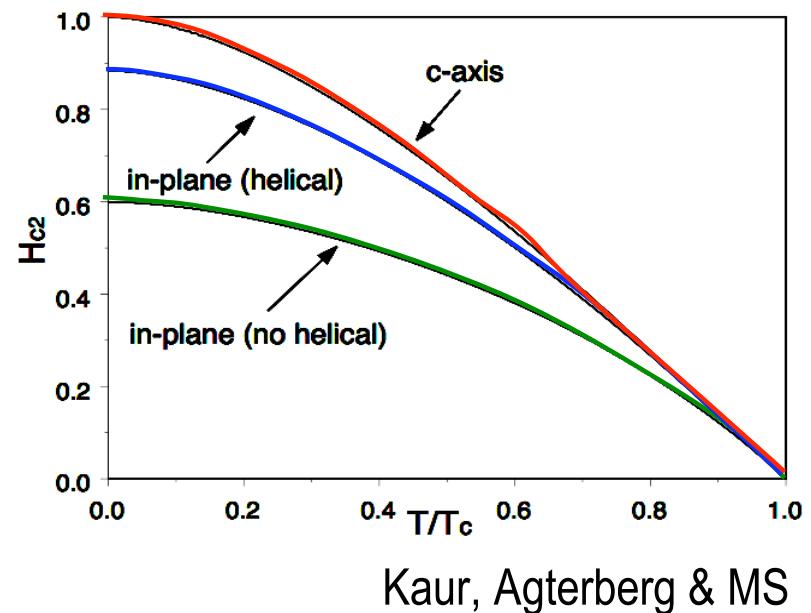
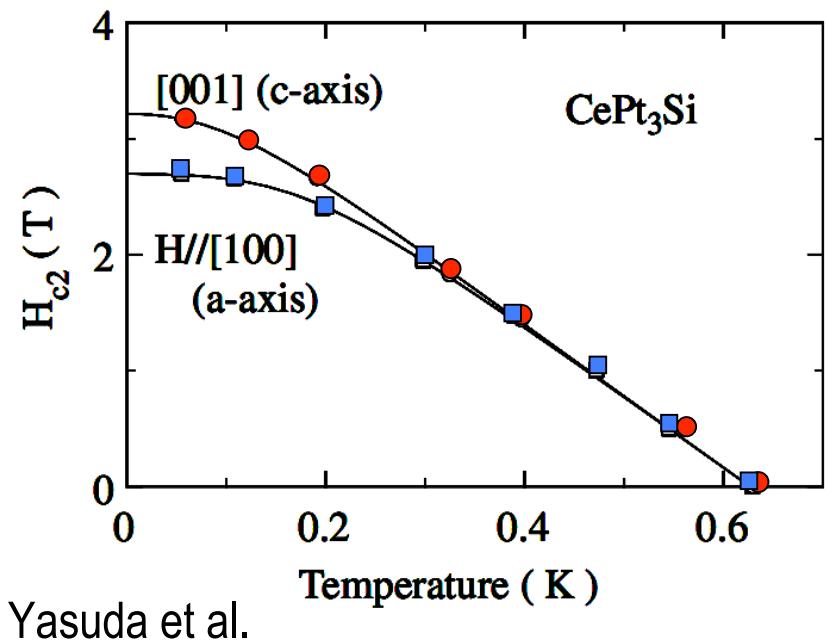
$$\epsilon \vec{H} \cdot \hat{z} \times \vec{J}_s$$

Helical state:

$$\psi(\vec{r}) = f(\vec{r}) e^{i\vec{q} \cdot \vec{r}} \quad \vec{q} = \frac{\epsilon}{K} \hat{z} \times \vec{H}$$

Helical phase and upper critical field

Additional structure in the order parameter possible in non-centrosym. systems



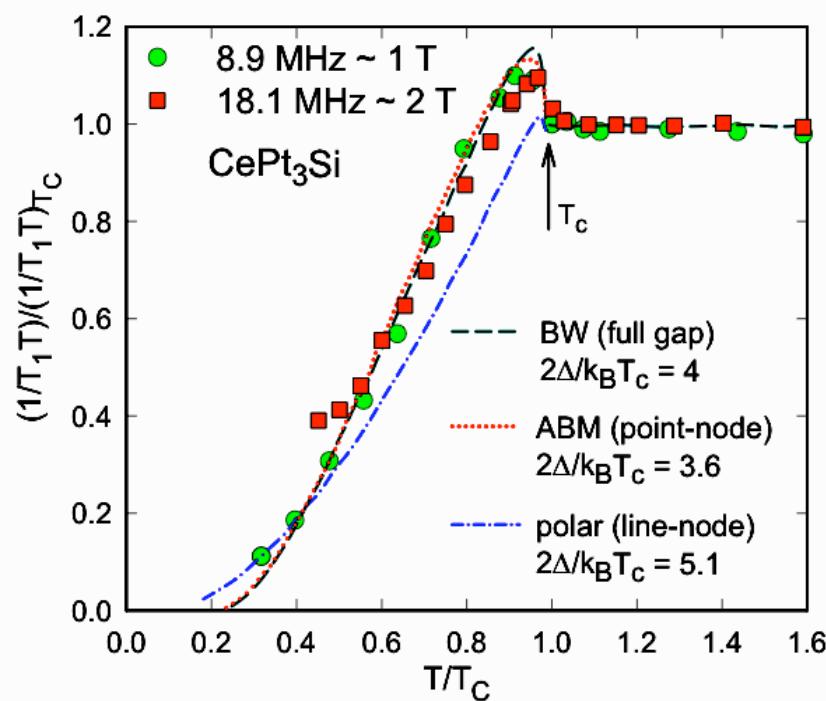
Enhanced H_{c2} : $T_c(H) = T_c(0) - \frac{\pi H}{\Phi_0 K a'} - \gamma \delta \hat{\chi} \vec{H}^2 + \frac{\epsilon^2 (\hat{z} \times \vec{H})^2}{4 K a'}$

orbital	paramagnetic	<i>helical</i>
		depairing

Indications of the
pairing symmetry

Quasiparticle gap structure

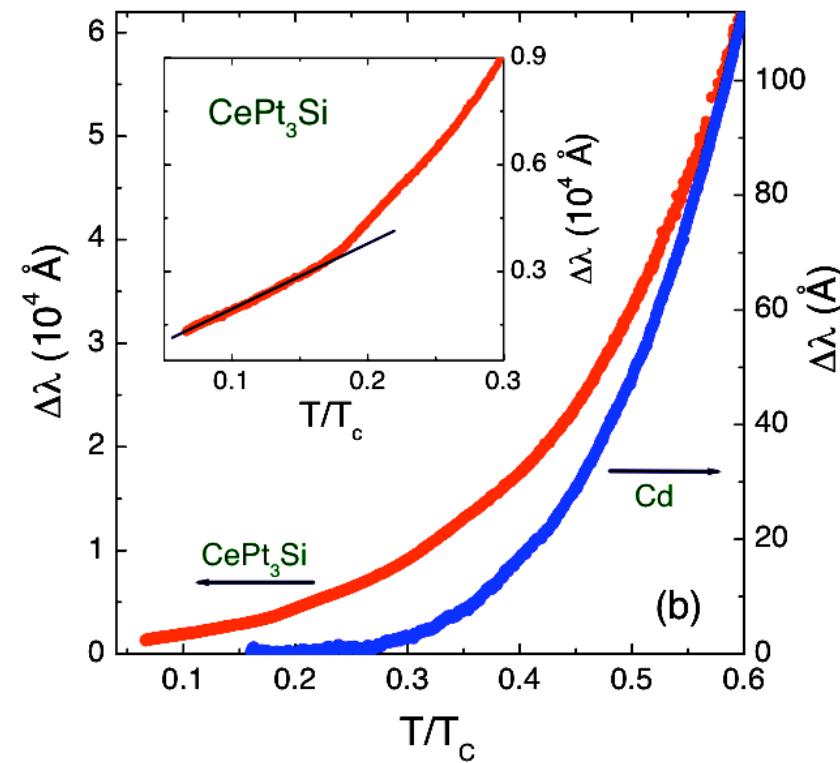
NMR- $1/T_1$



Hebel-Slichter peak
powerlaw T^3 for $T \rightarrow 0$

Bauer et al.

London penetration depth



powerlaw $\Delta\lambda \propto T$ for $T \rightarrow 0$

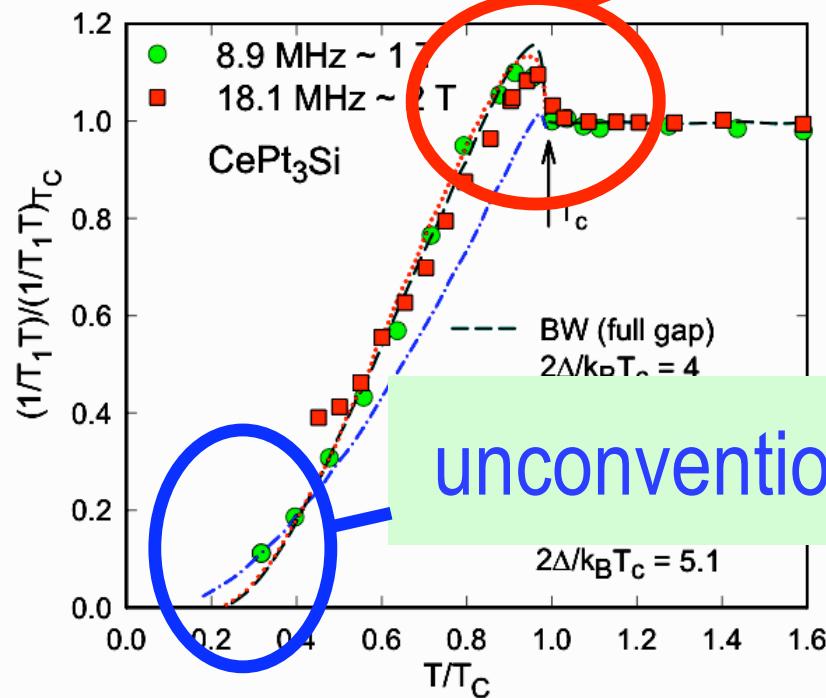
Bonalde et al.

Quasiparticle gap structure

NMR- $1/T_1$

conventional

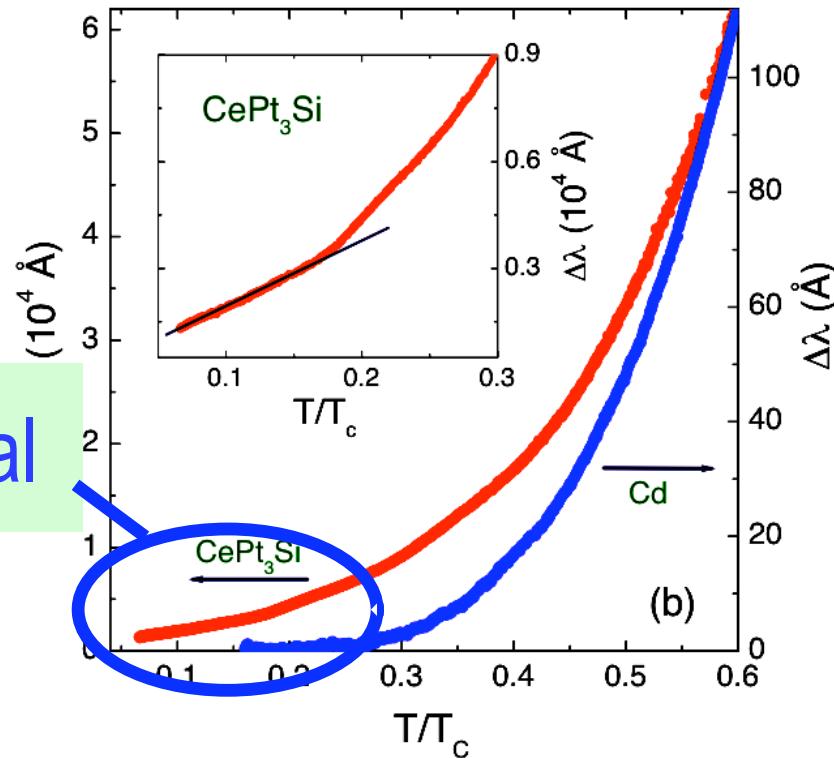
n penetration depth



unconventional

Hebel-Slichter peak
powerlaw T^3 for $T \rightarrow 0$

Bauer et al.



powerlaw $\Delta\lambda \propto T$ for $T \rightarrow 0$

Bonalde et al.

Quasiparticle gap structure

Parity mixing

"even + odd-parity"

inversion symmetry

even-parity state

$$\Delta_{\vec{k},ss'} =$$

$$\psi(\vec{k}) i \sigma^y_{ss'}$$

no inversion symmetry

$$\Delta_{\vec{k},ss'} =$$

$$\psi(\vec{k}) \left\{ (\sigma^0 + \gamma \vec{\lambda}_{\vec{k}} \cdot \vec{\sigma}) i \sigma^y \right\}_{ss'}$$

gaps on two split Fermi surfaces

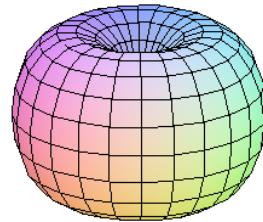
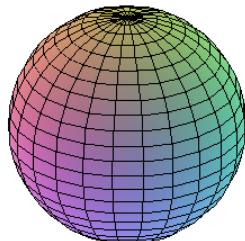
$$|\Delta_{\vec{k}\pm}| = |\psi(\vec{k})| \left| 1 \pm \gamma |\vec{\lambda}_{\vec{k}}| \right|$$

Quasiparticle gap structure

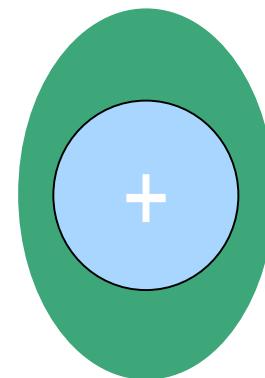
Parity mixing s - + p -wave

$$|\Delta_{\vec{k}\pm}| = |\psi(\vec{k})| \left| 1 \pm \gamma |\vec{\lambda}_{\vec{k}}| \right|$$

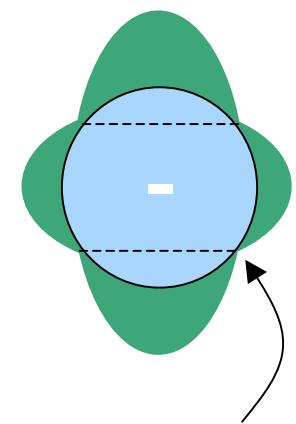
$$\psi = \Delta_s \quad \vec{\lambda}_{\vec{k}} = \hat{x}k_y - \hat{y}k_x$$



2 Fermi surfaces: + and -



full gap



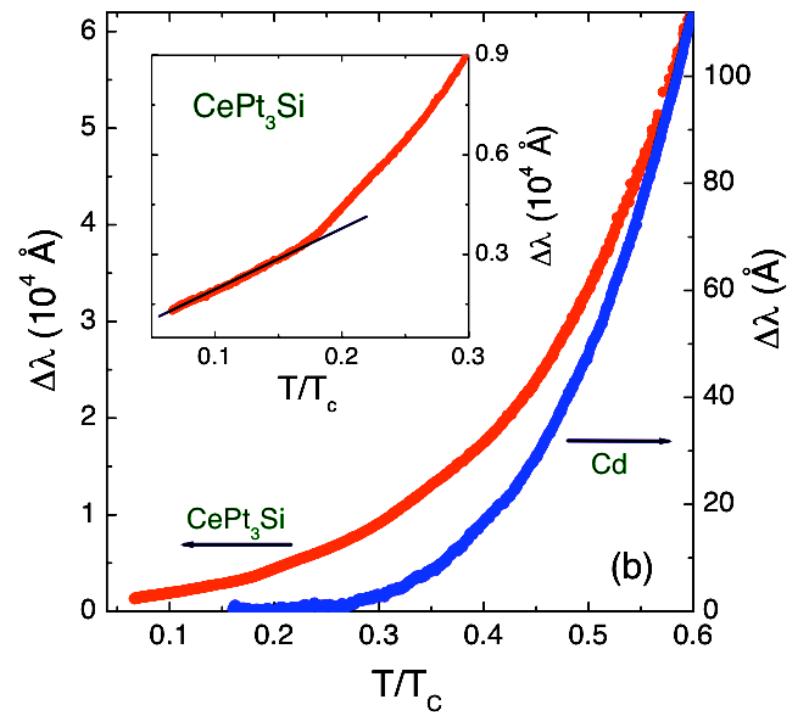
line nodes

Anisotropic gaps:

- different on the two Fermi surfaces
- no spin degeneracy ("spinless Fermions")
- accidental line nodes possible!

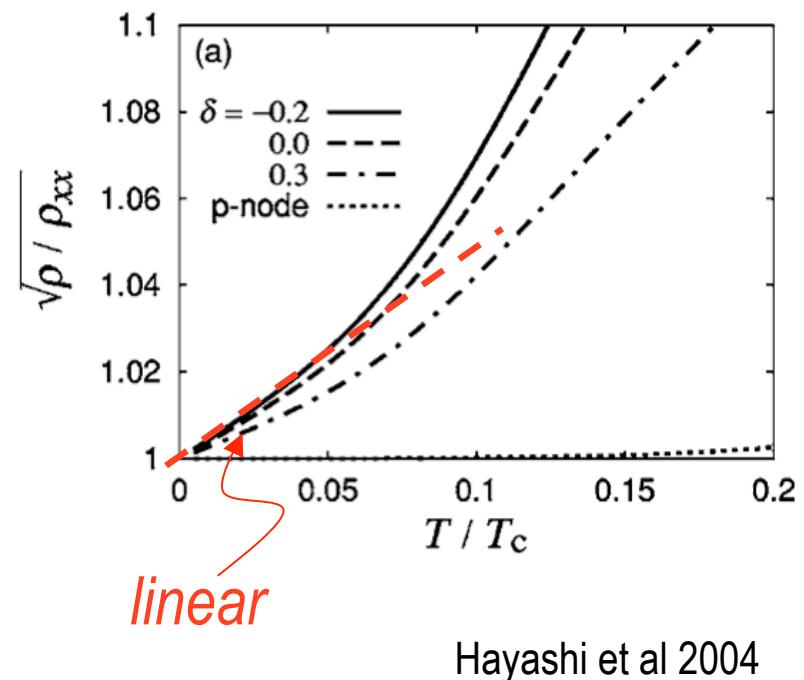
London penetration depth and superfluid density

T -linear behavior for $T \rightarrow 0$



Bonalde et al 2004

mixed parity state with nodes



Hayashi et al 2004

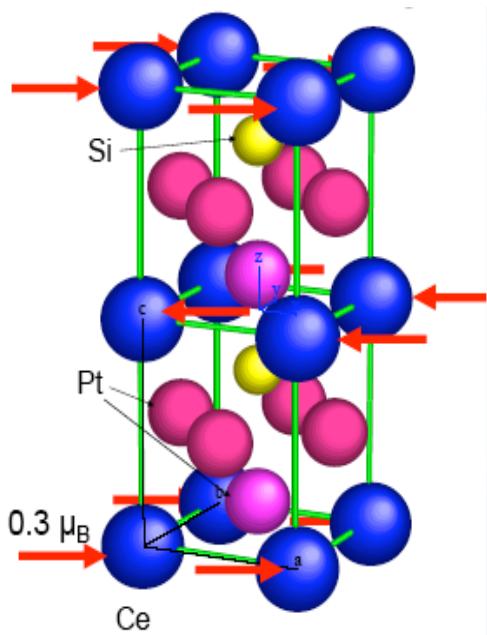
effect of accidental nodes !?

Complication for CePt₃Si

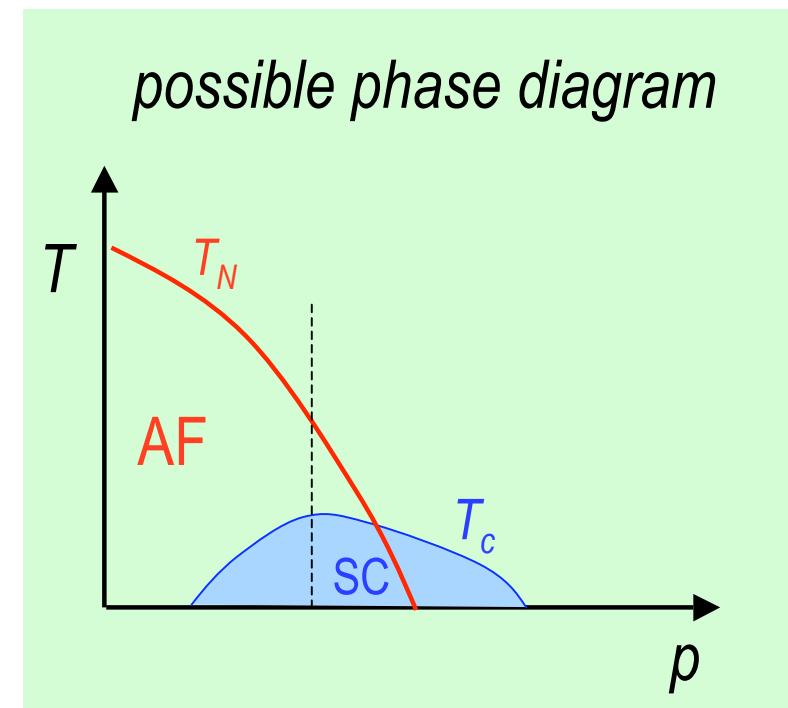
heavy Fermion compound: localized 4f-moments of Ce

◆ *superconductivity:* $T_c = 0.75 \text{ K}$

◆ *antiferromagnetism:* $T_N = 2.2 \text{ K}$



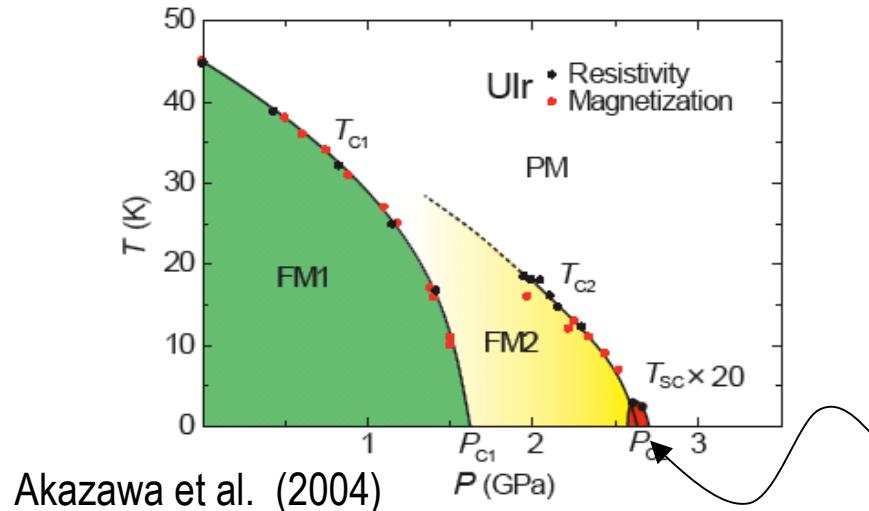
N. Metoki et al. (2004)



Other recently discovered
non-centrosymmetric
superconductors

Ulr

Ferromagnetic quantum phase transition



Akazawa et al. (2004)

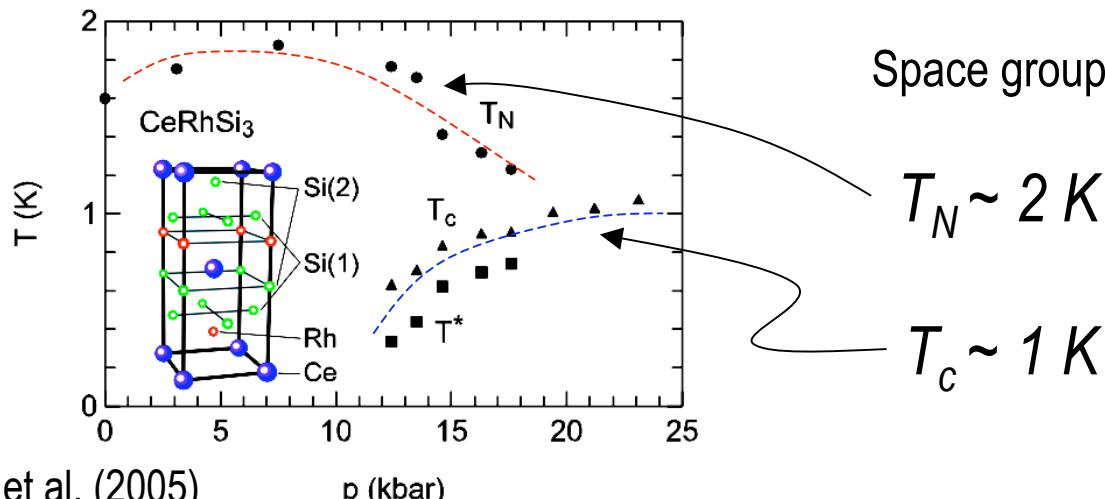
Space group: **P2₁** monoclinic

Coexistence of
Superconductivity and Ferromagnetism ! ?

superconductivity $T_c = 0.15$ K

CeRhSi₃

Antiferromagnetic quantum phase transition



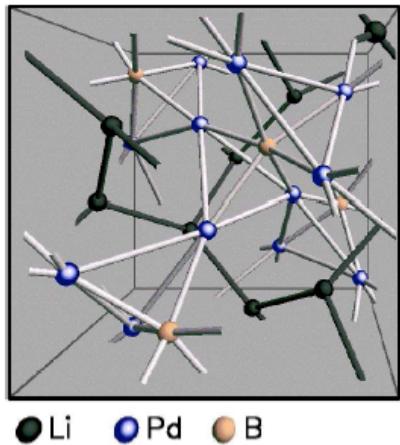
Kimura et al. (2005)

Space group: **I4mm** tetragonal

$T_N \sim 2$ K

$T_c \sim 1$ K

$\text{Li}_2\text{Pd}_3\text{B}$, $\text{Li}_2\text{Pt}_3\text{B}$

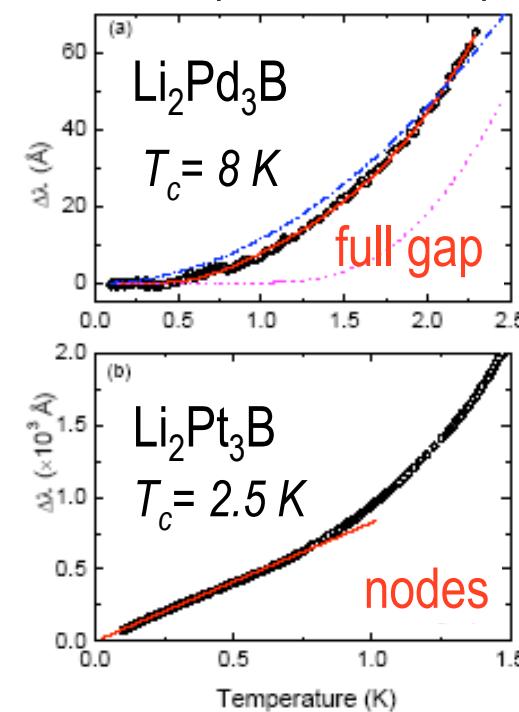


Togano et al. (2004)

Space group:
 $\text{P}4_3\text{3}2$ cubic

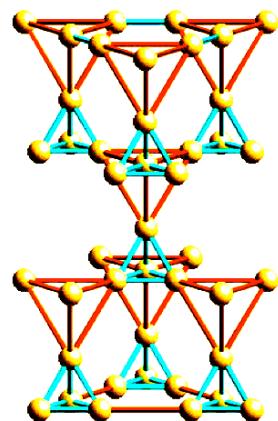
alloy interpolation:
 $\text{Li}_2(\text{Pd}_x\text{Pt}_{1-x})_3\text{B}$
varying spin-orbit coupling

London penetration depth



Yuan et al.
(2005)

$\text{KO}_{\text{S}_2}\text{O}_6$

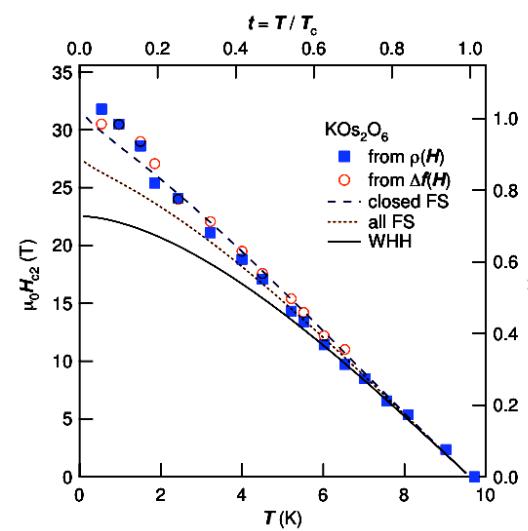


distorted pyrochlore
lattice

Space group: $\bar{\text{F}}4\text{3m}$
tetrahedral

Yonezawa et al. (2004)

H_{c2}



$T_c = 9.6\text{ K}$

Shibauchi et al.
(2006)

Conclusions

Symmetry of Cooper pairs:

inversion symmetry

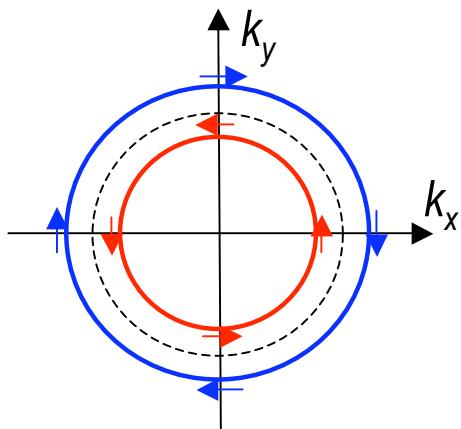
even-parity	spin-singlet
odd-parity	spin-triplet

no inversion symmetry

mixed-parity	mixed-spin
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no inversion symmetry → **antisymmetric spin-orbit coupling**

strong Fermi surface effect:



- paramagnetic effect
- gap structure
- helical phase in high magnetic fields
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