

Superconductors without parity symmetry

Daniel Agterberg - University of Wisconsin - Milwaukee

Thanks to Paolo Frigeri, Nobuhiko Hayashi, Manfred Sigrist (ETH-Zurich),
Huiqiu Yuan, Myron Salamon (UIUC), Akihisha Koga (Osaka University) ,
Raminder Kaur, Shantanu Mukherjee, and Zhichao Zheng (UWM)

Lecture 2:

Materials

Spin-Orbit Interaction

Superconducting state: Singlet-triplet mixing

Protected spin-triplet pairing state

Physical Observables- Experiments

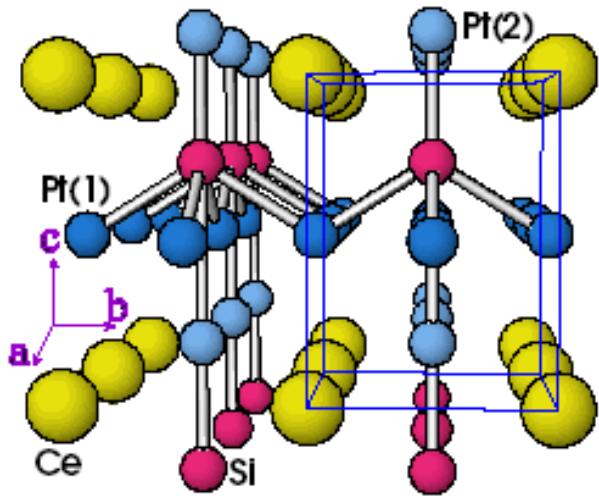
FFLO-like phases

Relevant Materials

- Many broken inversion superconductors:
 $\text{Cd}_2\text{Re}_2\text{O}_7$, UIr , $\text{Mo}_3\text{Al}_2\text{C}$, $\text{La}_5\text{B}_2\text{C}_6$, MoN , Y_2C_3 ,
 La_3S_4 , LaRhSi , NbReSi , Mo_3P , $\text{KO}\text{S}_2\text{O}_6$, $\text{Li}_2\text{Pd}_3\text{B}$, ...
- Superconductivity at the surface of a topological insulator
- Interface superconductors $\text{LaTiO}_3/\text{SrTiO}_3$
- Some of these materials have interesting superconducting properties

CePt_3Si , CeRhSi_3 , CeIrSi_3

- CePt_3Si : Heavy fermion superconductor: E. Bauer *et al* PRL 92 027003.

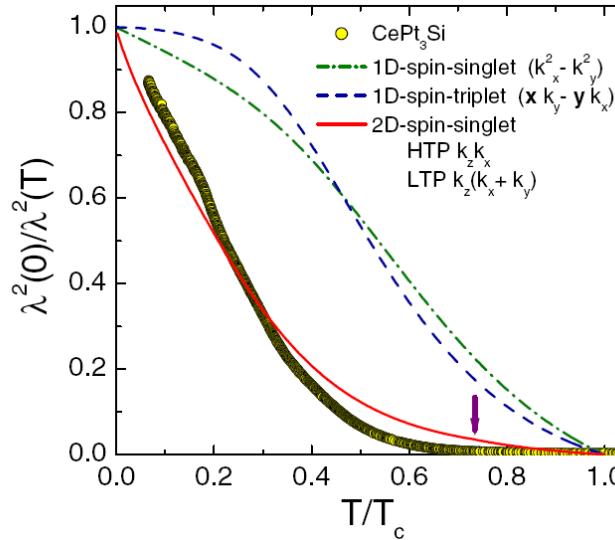


CePt_3Si - P4mm; CePt_3B -type

CeRhSi_3 and CeIrSi_3
also have high H_{c2}

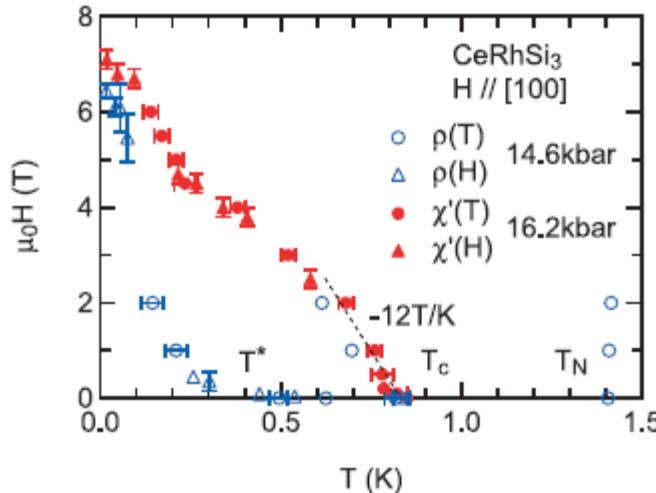
N. Kimura, *et al*, PRL 95, 247004

I. Sugitani, *et al*. JPSJ 75, 043703



Line Nodes in
 CePt_3Si

Bonalde, PRL 2005



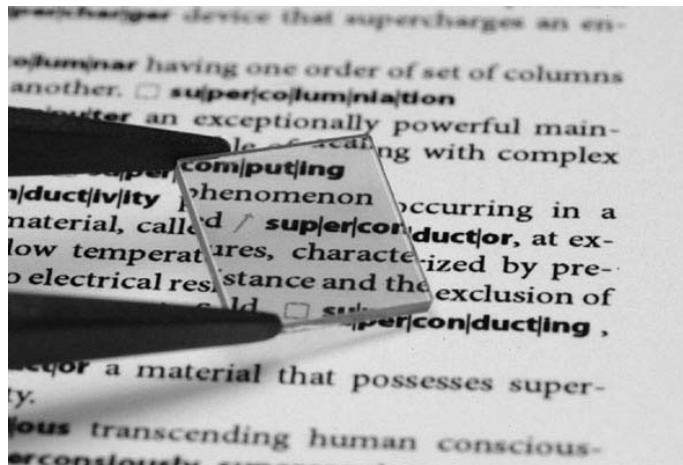
Interface Superconductors

Ohtomo ,Hwang, Nature
427, 423 (2004):

2D electron gas at
 LaAlO_3 and SrTiO_3
interface

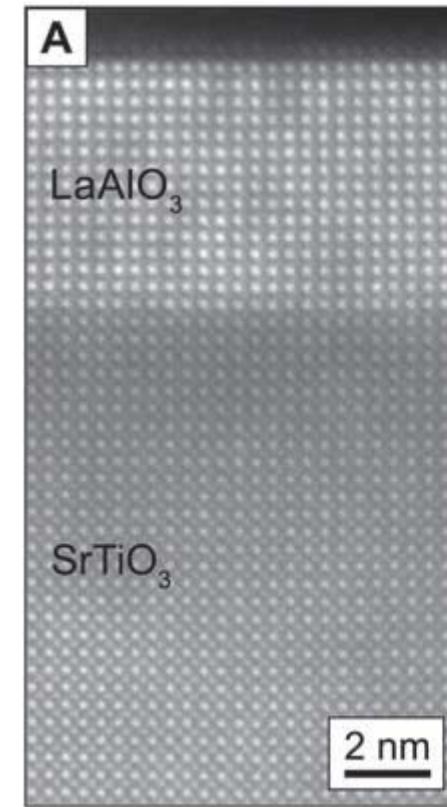
Reyren et al, Science 317,
1196 (2007):

Superconductivity in
the 2D electron gas



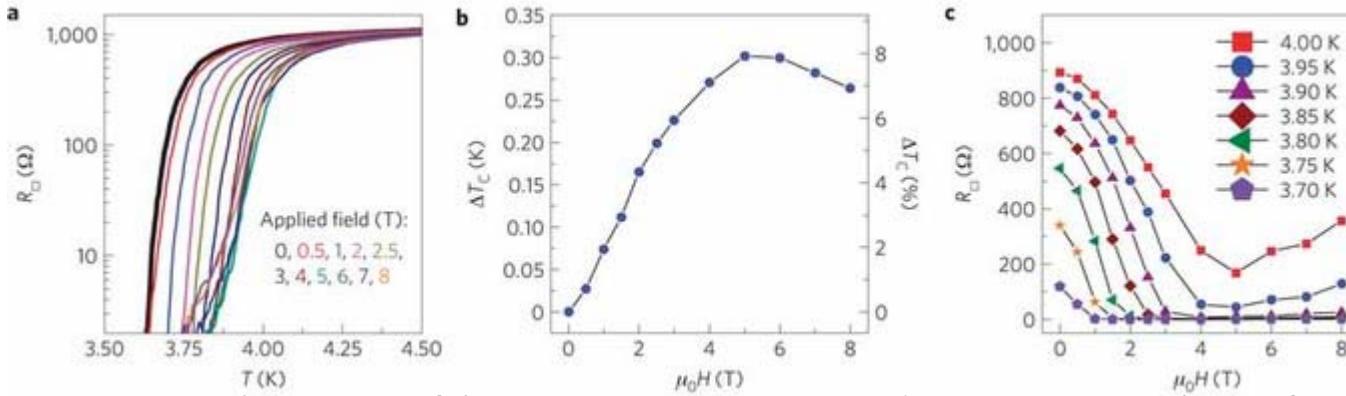
Coexisting superconductivity and ferromagnetism

Dikin et al, Phys. Rev. Lett. (2011); Bert et al,
Nature Phys. (2011); Li et al, Nature Phys (2011)

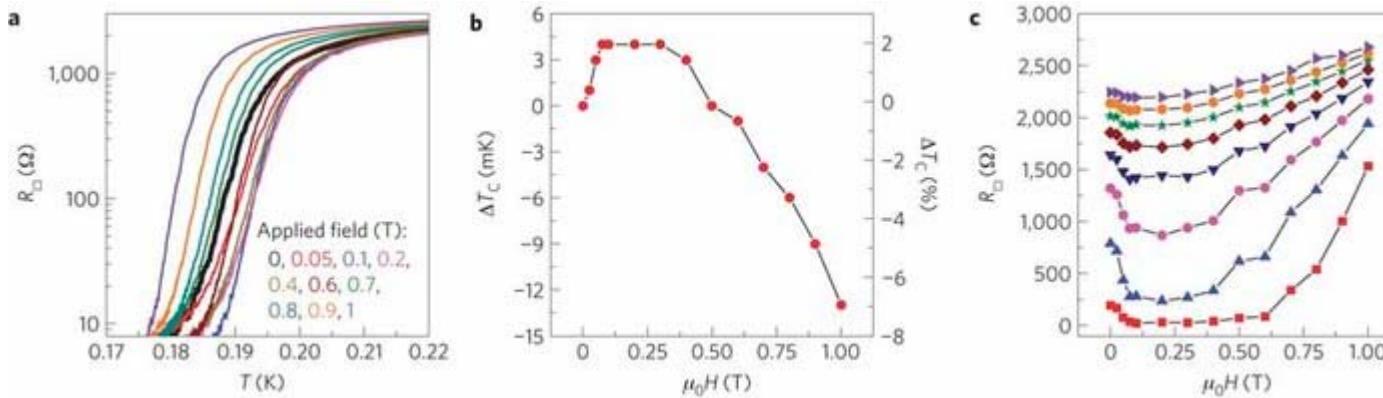


Increase of Tc by Magnetic Field

Gardner et al, Nature Physics 7, 895 (2011)



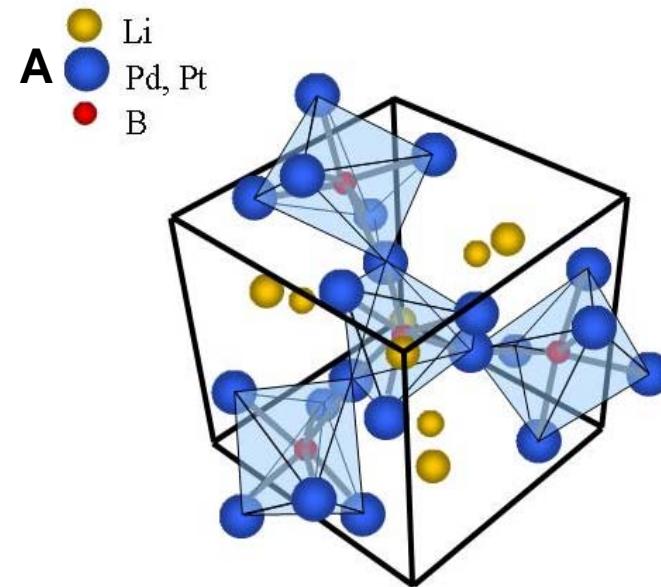
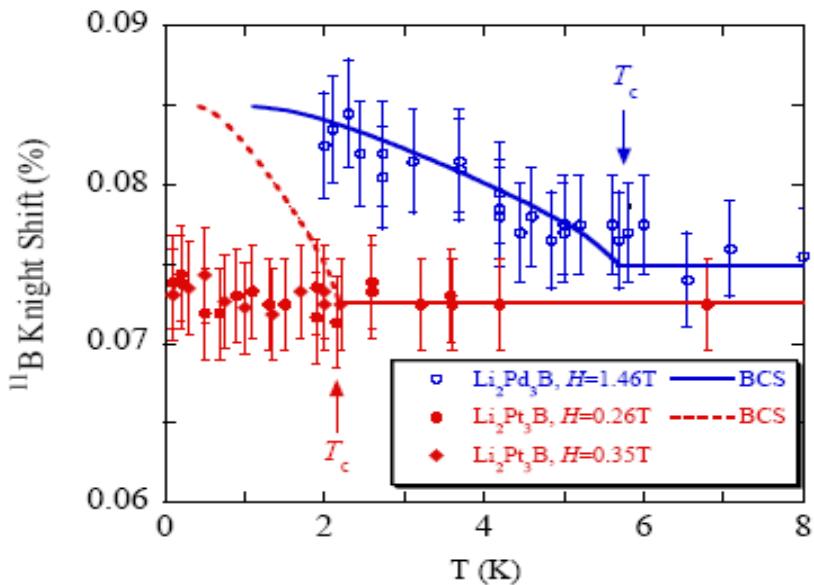
Amorphous Pb film: 21.1 Angstroms (no increased Tc for thicker films)



$\text{LaAlO}_3/\text{SrTiO}_3$ heterostructure

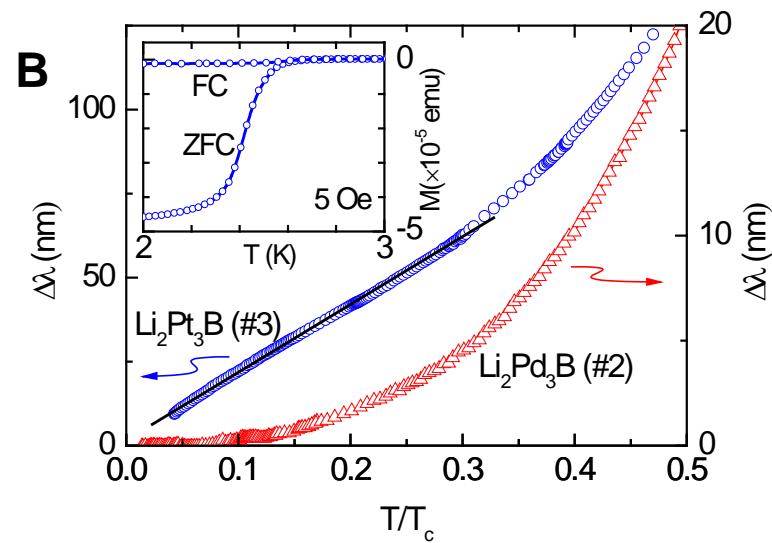
Magnetic fields should decrease Tc.

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



Zheng et al, PRL 98 047002 (2007)

Yuan et al , PRL 97, 017006 (2006)



Spin-Orbit Coupling

$$H_p = \alpha \sum_{k,s,s'} \vec{g}_k \cdot \vec{\sigma}_{s,s'} c_{ks}^t c_{ks'}$$

Time Reversal Symmetry implies $\vec{g}_k = -\vec{g}_{-k}$

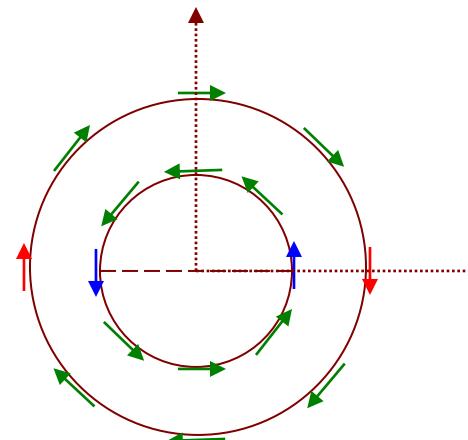
Parity Symmetry implies $\vec{g}_k = \vec{g}_{-k}$

H_p is zero when parity symmetry is also present

$$\epsilon_k = \xi_k \pm \alpha |\vec{g}_k| \quad \text{With spins polarized along } \pm \vec{g}_k$$

Example: 2D Rashba

$$\vec{g}_k = \hat{x}k_y - \hat{y}k_x$$



Spin-Orbit Coupling: Example

Consider Pt-As honeycomb lattice (SrPtAs)

Place d_{xz} , d_{yz} orbitals Fe sites
 p_z orbitals on As sites

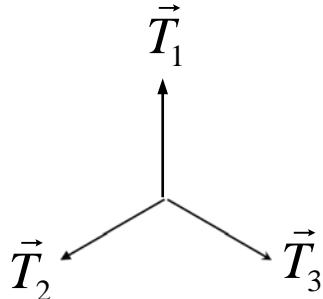
Goal is to find an effective Pt d-hopping Hamiltonian

Let $|+\rangle = |xz + iyz\rangle$
 $|-\rangle = |xz - iyz\rangle$

Lattice has no inversion symmetry. Include large spin-orbit on Fe sites and only hopping between Fe ands As

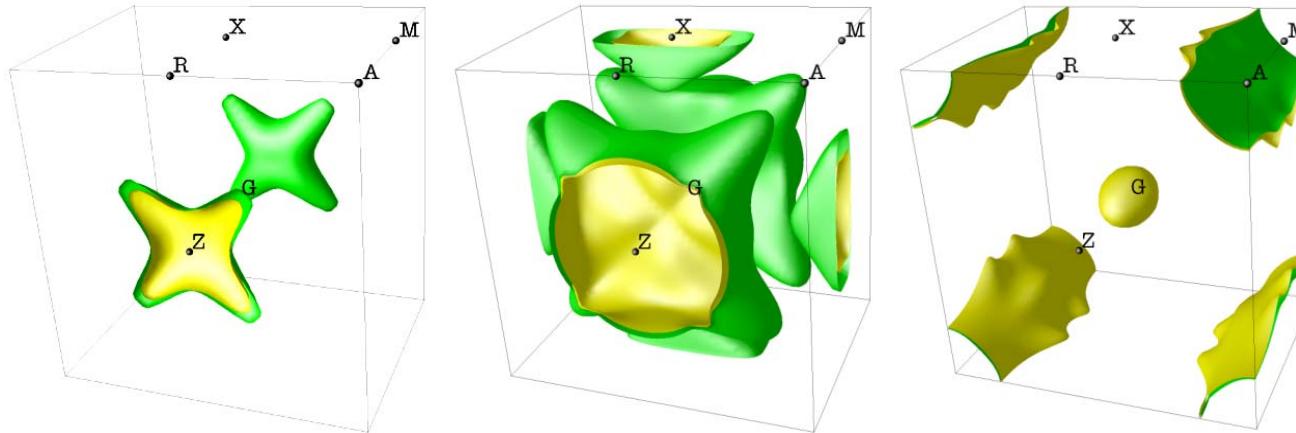
$$\vec{L} \cdot \vec{S} = L_z S_z + L_+ \cancel{\times} L_- S_+$$

$|+, \uparrow\rangle, |-, \downarrow\rangle$
 $|-, \downarrow\rangle, |+, \uparrow\rangle$



$$\vec{g}_k = \alpha \hat{z} [\sin(\vec{k} \cdot \vec{T}_1) + \sin(\vec{k} \cdot \vec{T}_2) + \sin(\vec{k} \cdot \vec{T}_3)]$$

Band splitting: CePt₃Si



Split Fermi surface of
CePt₃Si

A.Kozhevnikov, V. Anisimov

LaAlO₃ SrTiO₃: spin gap is 10 meV and Fermi Energy is 40 meV

Often spin-orbit is a large energy scale with respect to the superconducting gap.

Superconductivity

Symmetry and Cooper pairing

Anderson(1984): degenerate electron states in a $P_{\text{tot}}=0$ Cooper Pair;
Which partners are available by symmetry ?

Spin singlet Pairing:

Time reversal sym. T necessary:

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

Spin triplet Pairing:

Time reversal sym. T and parity sym. I necessary:

$$|\vec{k}, \uparrow\rangle \rightarrow \begin{cases} |-\vec{k}, \downarrow\rangle = T|\vec{k}, \uparrow\rangle \\ |-\vec{k}, \uparrow\rangle = I|\vec{k}, \uparrow\rangle \\ |\vec{k}, \downarrow\rangle = TI|\vec{k}, \uparrow\rangle \end{cases}$$

Superconductivity

$$H = \sum_{k,s} \xi_k c_{ks}^t c_{ks} + \frac{1}{2} \sum_{k,k',s,s'} V(k, k') c_{ks}^t c_{-ks'}^t c_{-k's'} c_{k's}$$

Broken parity appears through:

$$H_p = \alpha \sum_{k,s,s'} \vec{g}_k \cdot \vec{\sigma}_{s,s'} c_{ks}^t c_{ks'} \quad \vec{g}_k = -\vec{g}_{-k}$$

Linear Gap Equation

$$\Delta_{s,s'}(k) = -\frac{1}{\beta} \sum_{k',s2,s1,n} V(k,k') G_{s,s1}^0(k',\omega_n) \Delta_{s1,s2}(k') G_{s',s2}^0(-k,-\omega_n)$$

$$G^0(k, \omega_n) = G_+(k, \omega_n) \sigma_0 + (\hat{g}(k) \cdot \vec{\sigma}) G_-(k, \omega_n)$$

$$G_{\pm}(k, \omega_n) = \frac{1}{2} \left(\frac{1}{i\omega_n - \xi(k) - \alpha |g(k)|} \pm \frac{1}{i\omega_n - \xi(k) + \alpha |g(k)|} \right)$$

$$\Delta(k) = \psi(k) i\sigma_y + \vec{d}(k) \cdot \vec{\sigma} i\sigma_y$$

For spin singlet component find:

$$\psi(k) = -k_B T \sum_{n,k'} V(k, k') \{ [G_+ G_+ + G_- G_-] \psi(k) + [G_+ G_- + G_- G_+] \hat{g}(k') \cdot \vec{d}(k') \}$$

Where: $G_i G_j = G_i(k, \omega_n) G_j(-k, -\omega_n)$ Use: $\sum_k f(k) \approx N(0) \int_{-\varepsilon c}^{\varepsilon c} d\xi < f(k) >_{F.S.}$

Has singlet-triplet mixing - for small spin-orbit triplet part is small - for now we will ignore this ($\Delta \ll \alpha \ll \varepsilon c$)

Results on Stability

$$\ln \frac{T_c}{T_{cs}} = O\left(\frac{\alpha^2}{\epsilon_F^2}\right) \quad \text{spin-singlet}$$

$$\ln \frac{T_c}{T_{ct}} = 2 \left\langle \left[|\vec{d}_k|^2 - |\hat{g}_k \cdot \vec{d}_k|^2 \right] f(\rho_k) \right\rangle_k + O\left(\frac{\alpha^2}{\epsilon_F^2}\right) \quad \text{spin-triplet}$$

$$\rho_k = \frac{\alpha |\vec{g}(k)|}{\pi k_B T_c}$$

$$f(\rho) = \sum_n \left(\frac{1}{n + \frac{1}{2} + i\rho} - \frac{1}{n + \frac{1}{2}} \right)$$

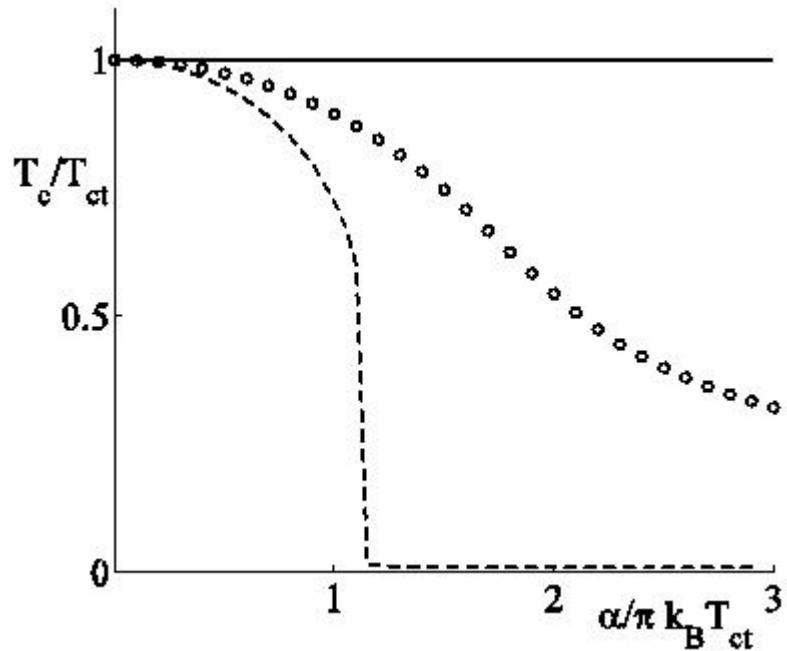
$f(\rho)$ leads to a strong suppression of T_c

T_c for spin-triplet is not suppressed only for a *single protected d* vector (with g and d parallel).

Rashba Case

$$\vec{g}_k = \hat{y}k_x - \hat{x}k_y$$

$$\ln \frac{T_c}{T_{ct}} = 2 \left\langle \left[|\vec{d}_k|^2 - |\hat{g}_k \cdot \vec{d}_k|^2 \right] f(\rho_k) \right\rangle_k + O\left(\frac{\alpha^2}{\epsilon_F^2}\right)$$



$$\vec{d}_k = \hat{y}k_x - \hat{x}k_y$$

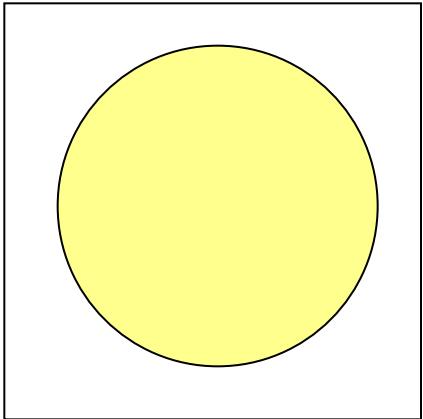
$$\vec{d}_k = \hat{y}k_x + \hat{x}k_y$$

$$\vec{d}_k = \hat{x}k_x + \hat{y}k_y + \hat{z}k_z$$

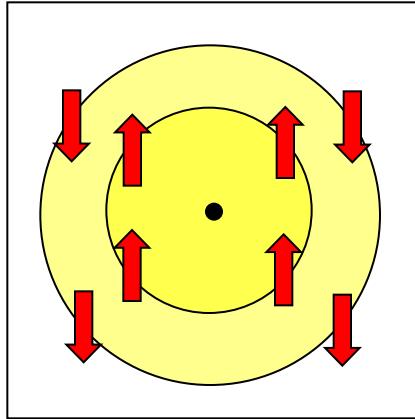
Often, only the protected triplet state (with $d||g$) can survive

Pauli Paramagnetism

Singlet superconductors with parity symmetry: Pauli Field

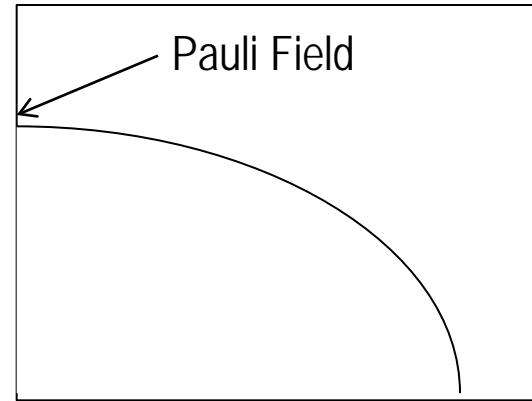


No Zeeman



With Zeeman

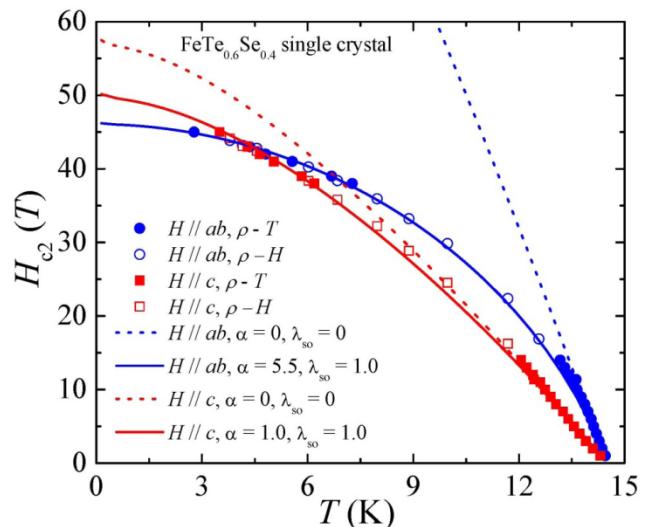
B



T_c

$$\xi_{\pm}(k) = \varepsilon(k) \pm |\mu_B \vec{B}|$$

Spin Singlet Superconductivity suppressed when $\mu B \sim \Delta$



Khim et al (2010)

Broken parity symmetry case

$$H = \sum_{k,s} \xi_k c_{ks}^t c_{ks} + \frac{1}{2} \sum_{k,k',s,s'} V(k, k') c_{ks}^t c_{-ks'}^t c_{-k's'} c_{k's}$$

$$H_{\text{spin}} = \sum_{k,s,s'} (\mu_B \vec{h} + \vec{g}_k) \cdot \vec{\sigma}_{s,s'} c_{ks}^t c_{ks'}$$

Calculate $T_c(h)$:

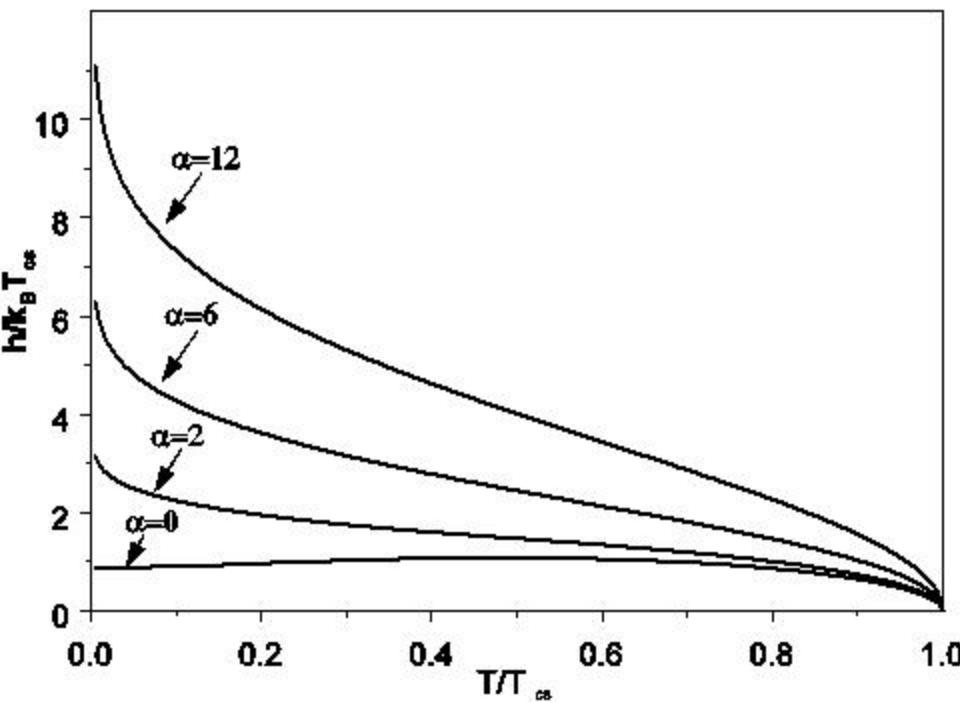
Key result: when $\vec{g} \cdot \vec{h} = 0$ then h diverges at low T :

$$(\mu_B h)^2 \ln \frac{\mu_B h}{\pi k_B T_{cs}} = -\alpha^2 \ln \frac{T_c}{T_{cs}}$$

Will consider $\vec{g} \cdot \vec{h} \neq 0$ later

Suppression of Pauli field: Rashba

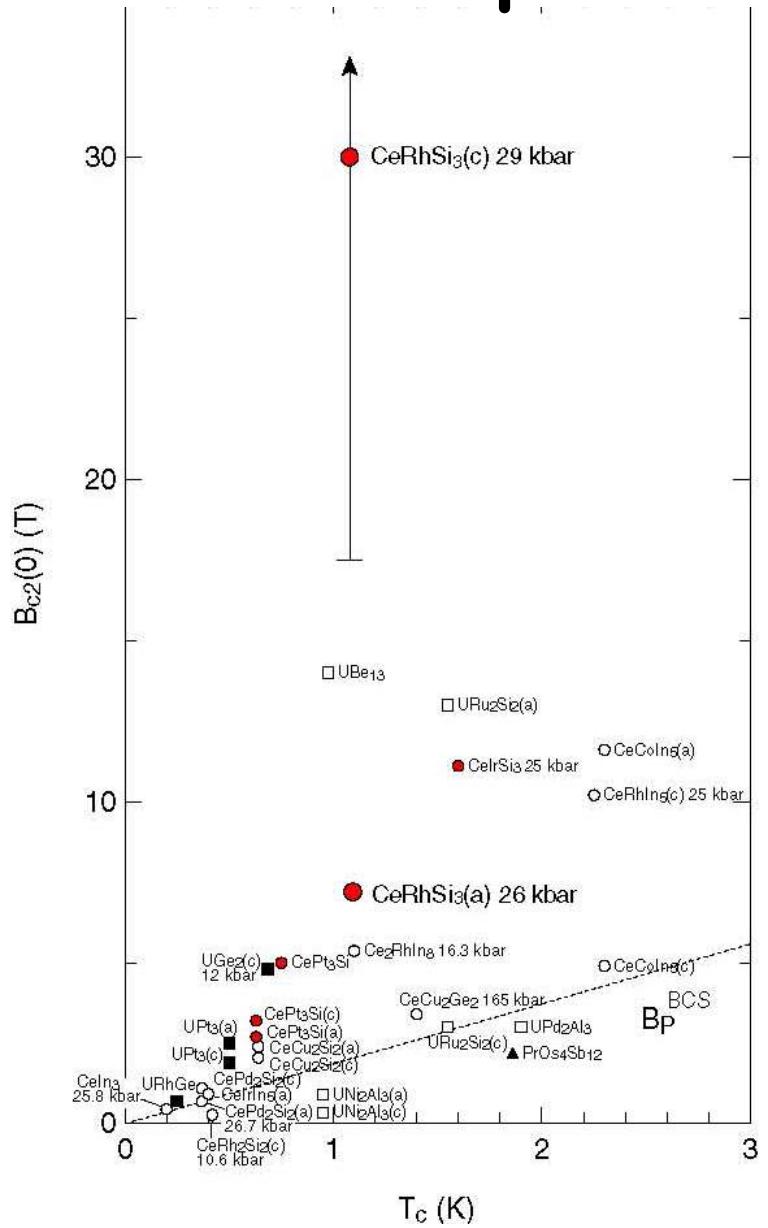
- Pauli field for spin-singlet case is strongly suppressed (also found by Bulaevski):



for $\vec{g} \cdot \vec{h} = 0$

Large $H_c2(0)$ in CePt_3Si can be due to spin-triplet pairing or spin-singlet pairing with suppressed Pauli field.

Experimental Results



Kimura et al, PRL (2007)

Red dots are non-centrosymmetric materials with a Rashba spin-orbit.

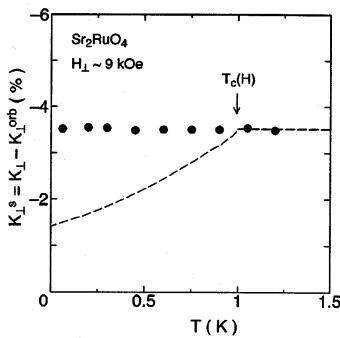
They all surpass the Pauli field.

Critical field determined by vortex physics

Spin Susceptibility

Example Spin-Triplet: Sr_2RuO_4

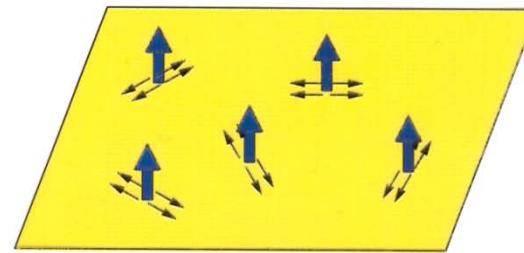
The spin-susceptibility is unchanged when $\mathbf{H} \cdot \mathbf{d}=0$



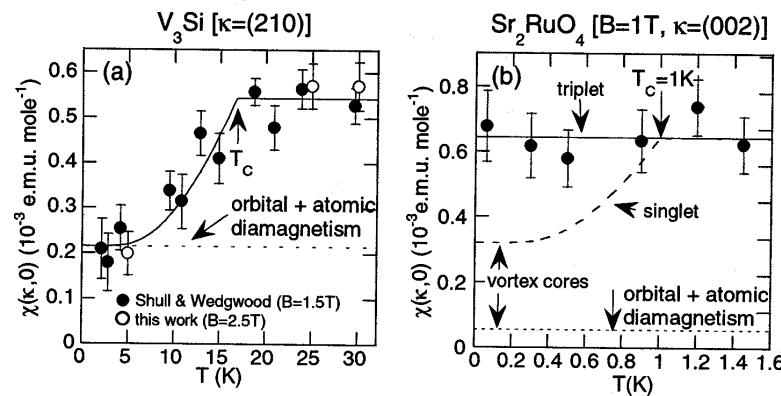
K. Ishida *et al.*, Nature 396, 658 (1998).

Spin triplet: Sr_2RuO_4

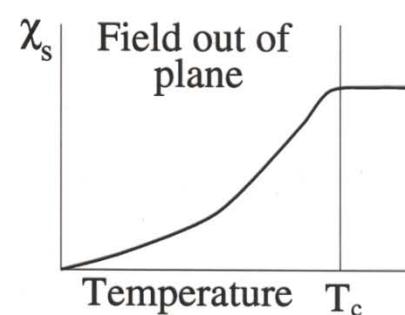
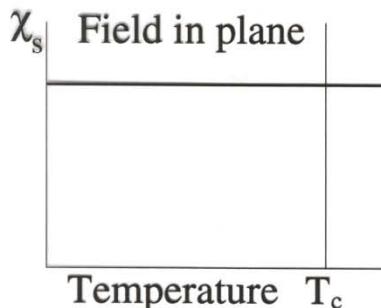
$$\vec{d}(k) = \hat{z}(k_x + ik_y)$$



- Example \vec{d} : Cooper pair spins confined to the plane
- Cooper pairs can respond to a field in plane - but not to one out of plane



J.A.Duffy *et al.*, PRL 85, 5412 (2000).



Spin Susceptibility

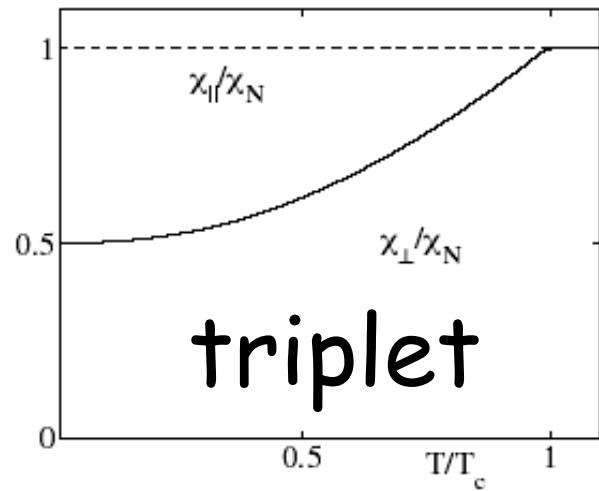
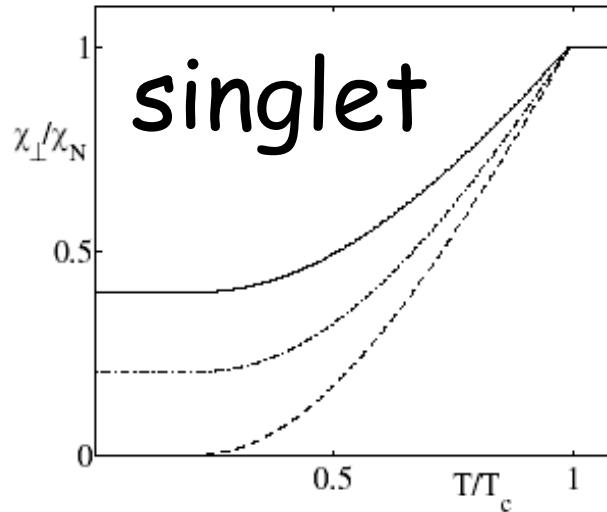
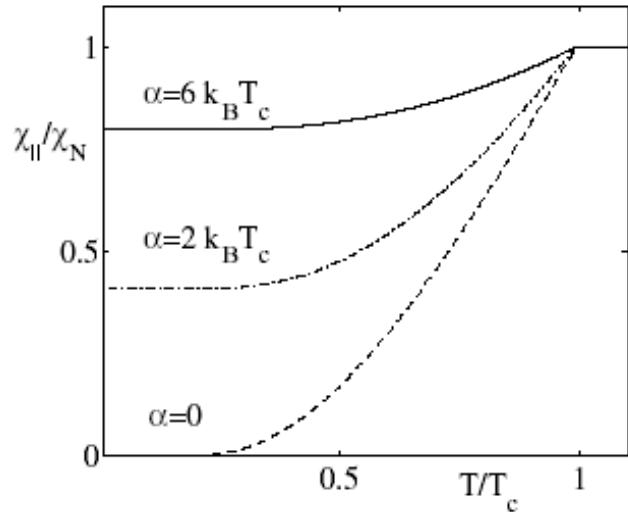
$$\chi_{ij} = -\mu_B^2 k_B T \sum_{k, \omega_n} \text{Tr} \left(\sigma_i G(k, \omega_n) \sigma_j G(k, \omega_n) - \sigma_i F(k, \omega_n) \sigma_j^T F^t(k, \omega_n) \right)$$

Find spin-triplet susceptibility of protected state is independent of spin-orbit (giving the same result as parity symmetric triplet SC)

Find spin-singlet susceptibility becomes the same as the above spin-triplet protected state when $\alpha \gg \Delta$

Gor'kov and Rashba (Rashba spin-orbit) PRL 87, 037004 (2001)
See also Yip PRB 65, 144508 (2002)

Spin Susceptibility

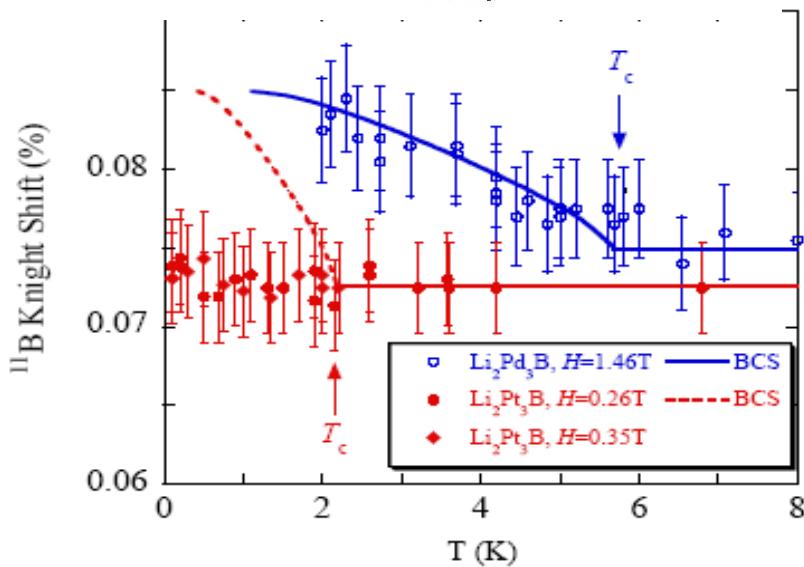
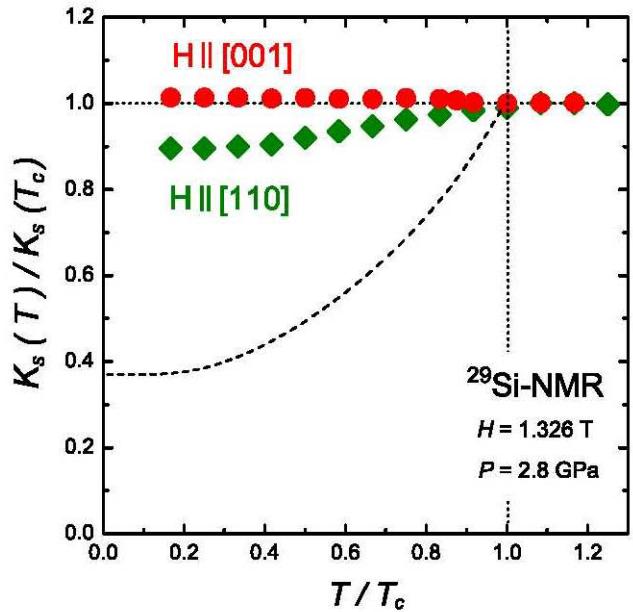


Note $\alpha \gg \Delta$ for CePt_3Si

Singlet approaches triplet in large α limit. The usual Knight shift measurement is not useful

Expect large anisotropy in magnetic response of superconductor.

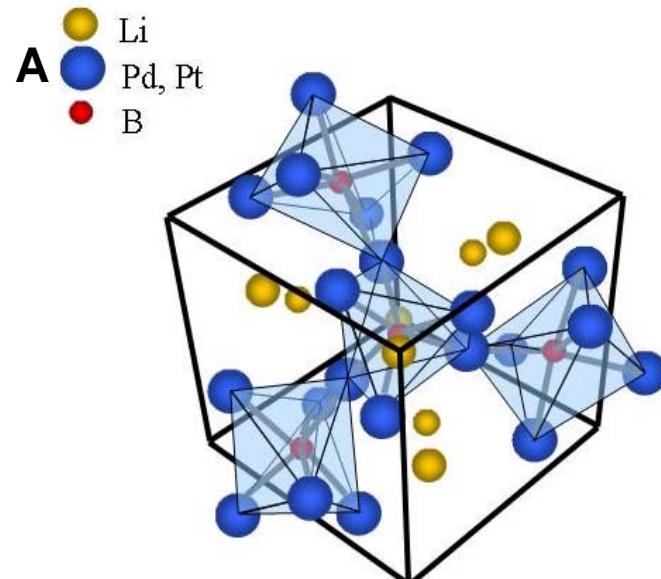
Experimental Results



CeIrSi₃: Rashba

Mukuda *et al*/PRL 2010

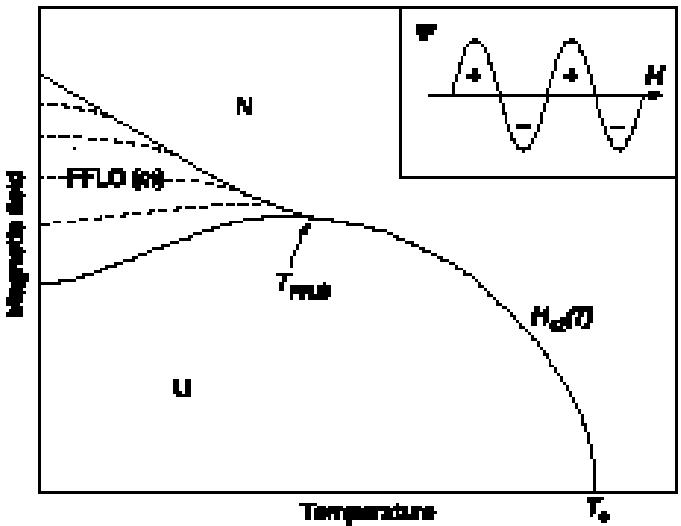
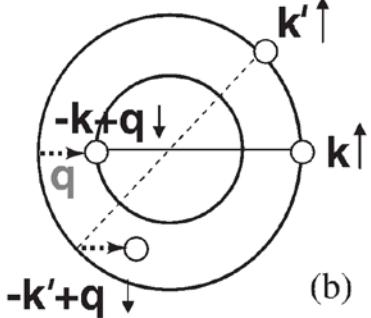
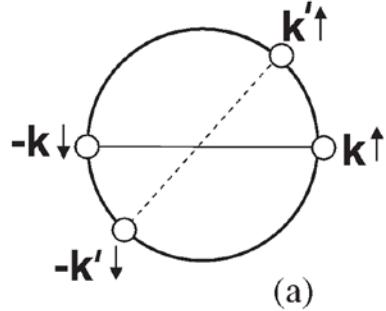
Li₂Pt₃B and Li₂Pd₃B: cubic



Zheng et al, PRL (2007)

FFLO-like phases

Singlet pairing in a Zeeman field: FFLO



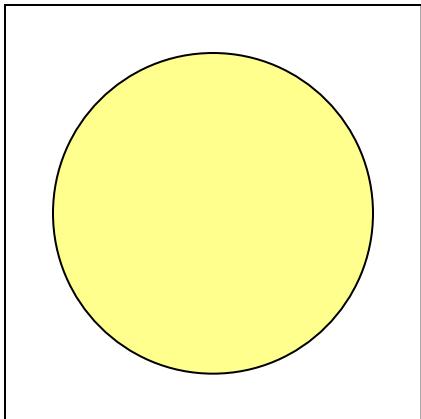
Key Point of FF and LO: Pairing between fermions with different Fermi surfaces leads to "finite momentum" pairing states (FFLO).

$$\Delta(\vec{r}) = \Delta_0 e^{i\vec{q} \cdot \vec{r}} \quad (\text{FF})$$

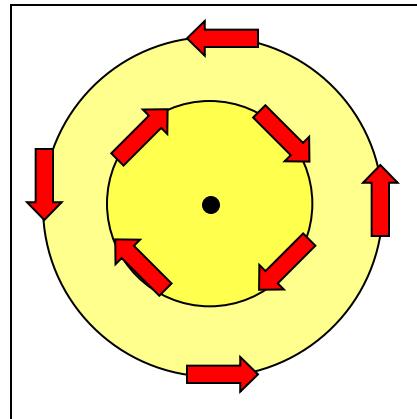
$$\Delta(\vec{r}) = \Delta_0 (e^{i\vec{q} \cdot \vec{r}} + e^{-i\vec{q} \cdot \vec{r}})/2 \quad (\text{LO})$$

Destroyed By Disorder

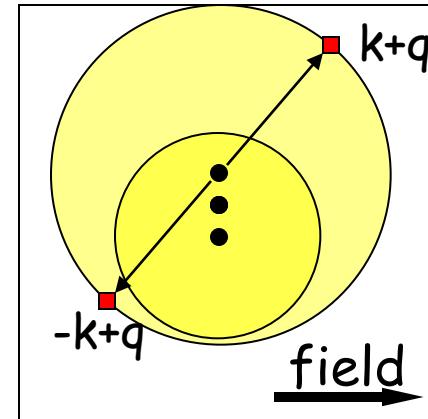
Parity Broken Case



No ASOC



With ASOC



With ASOC and
Zeeman Field

$$\xi_{\pm}(k) = \varepsilon(k) \pm |\alpha \vec{g}(k) + \mu_B \vec{B}|$$

$$\xi_{\pm}(k) \approx \varepsilon(k) \pm \alpha \pm \mu_B \vec{B} \cdot \hat{g}(k)$$

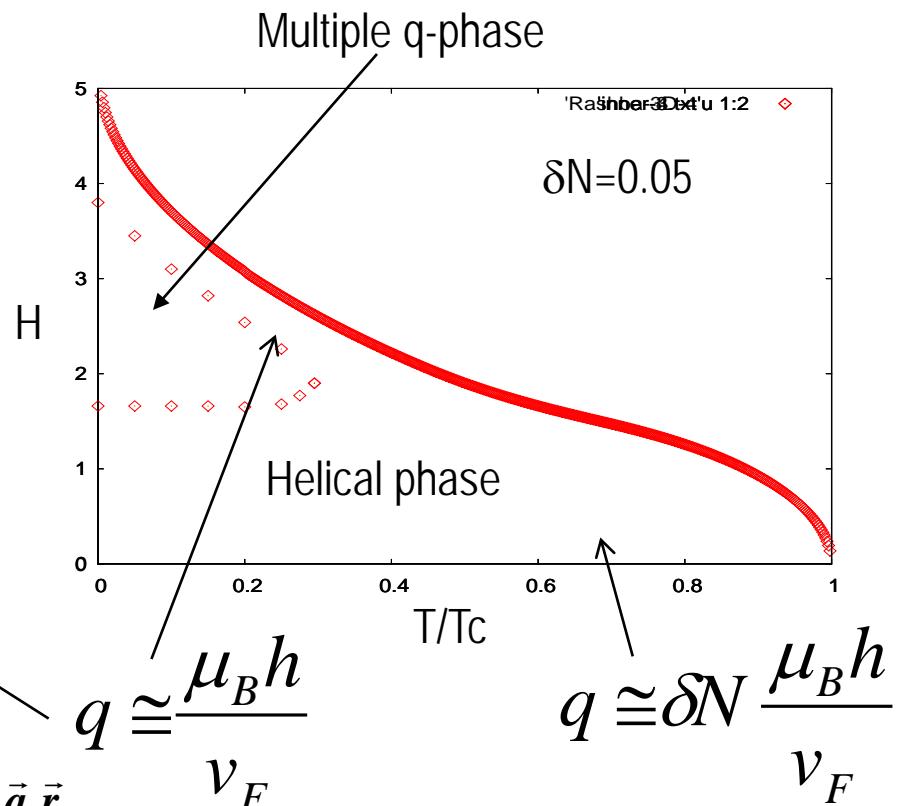
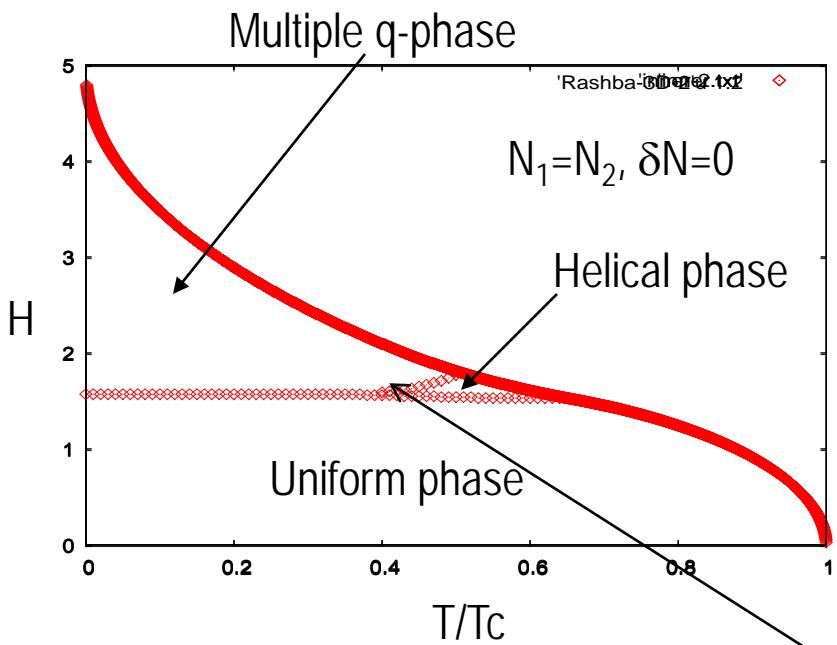
$$\mu_B \vec{B} \cdot \hat{g}(k) = \mu_B B_x k_y / k_F$$

$$\Delta(\vec{r}) = \Delta_0 e^{i 2 \vec{q} \cdot \vec{r}}$$

Can pair every state on one Fermi surface.
The two bands prefer opposite q vectors.

Phase Diagram

$$\delta N = \frac{N_1 - N_2}{N_1 + N_2}$$



Helical phase: $\psi(\vec{r}) = \psi_0 e^{i2\vec{q} \cdot \vec{r}}$

$$q \approx \frac{\mu_B h}{v_F}$$

$$q \approx \delta N \frac{\mu_B h}{v_F}$$

Multiple-q phase: $\psi(\vec{r}) = \psi_1 e^{i2qr} + \psi_2 e^{-2iqr}$

Two different types of q appear - what is the origin?

Ginzburg Landau FFLO/Helical Theories

$$F = \int [\alpha(T, h) |\psi|^2 + \beta(h) |\psi|^4 + \kappa(h) |\vec{\nabla} \psi|^2] d^3 r$$

At FFLO transition: $\kappa(h) = \beta(h) = 0$
 $\Rightarrow \psi = \psi_0 \cos(\vec{q} \cdot \vec{r})$

In broken parity superconductors - new terms appear in the GL theory (Lifschitz invariants)

$$\varepsilon \hat{z} \cdot \vec{B} \times [\psi(i\vec{\nabla} \psi)^* + \psi^*(i\vec{\nabla} \psi)] = \varepsilon \hat{z} \cdot \vec{B} \times \vec{j}_{s,0}$$

Induces a helical solution in a uniform magnetic field

$$\Rightarrow \psi = \psi_0 e^{i\vec{q} \cdot \vec{r}} \text{ with } \vec{q} = -\varepsilon \hat{z} \times \vec{B} / \kappa$$

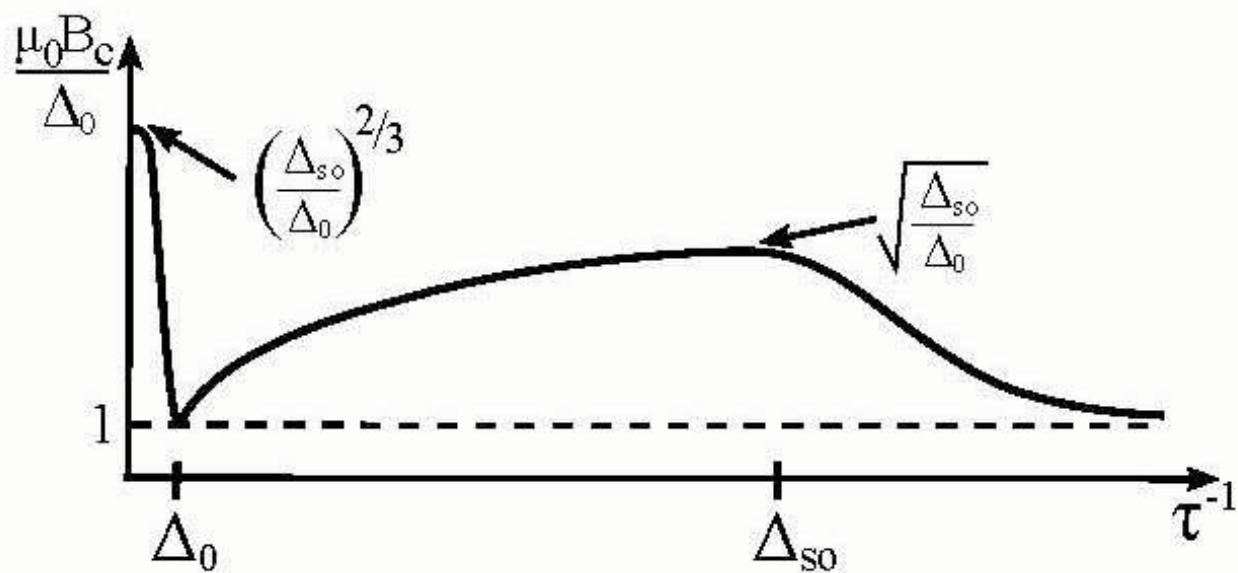
Lifschitz invariant origin suggests helical phase will exist even with impurities. Helical phase has no supercurrent.

Results for 2D Rashba

Barzykin and Gorkov, PRL (2002); DFA, Physica C (2003);
Kaur, DFA, Sigrist PRL (2004); DFA and Kaur PRB (2007);
Dimitrova and Feigel'man , PRB (2007); Samokhin, PRB (2008);
Mineev and Samokhin (2008).

Michaeli, Potter, Lee (2012)

(LaAlO₃/SrTiO₃ interfaces)



Survives to high Fields in disordered 2D Rashba

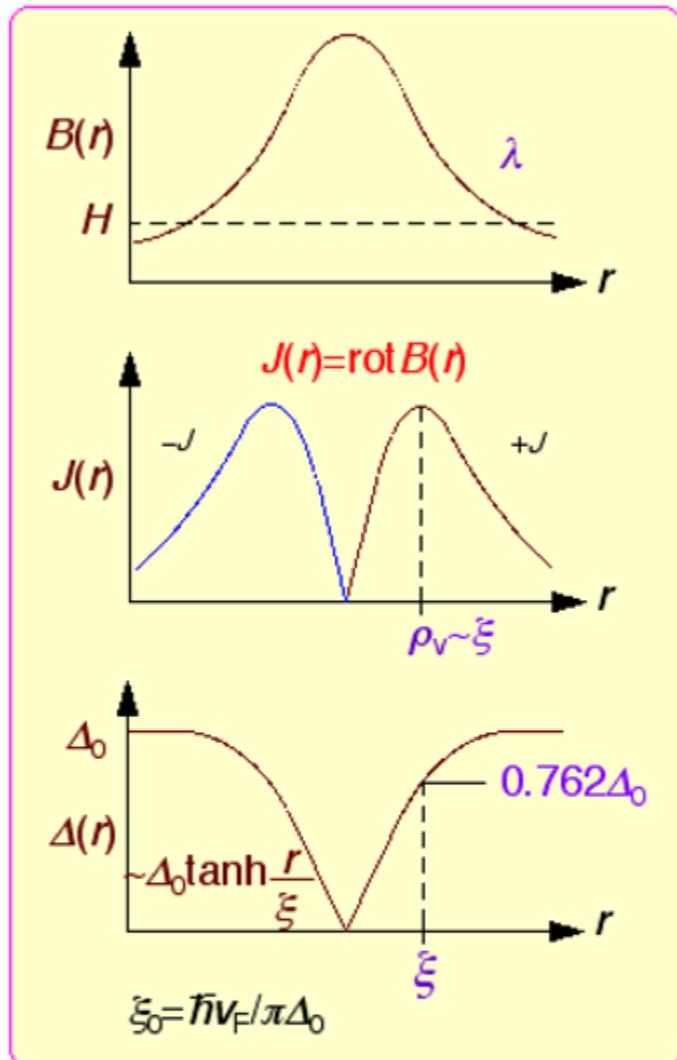
Physics Related to Helical Phase

$$\varepsilon \hat{n} \cdot \vec{B} \times [\psi(\vec{D}\psi)^* + \psi^*(\vec{D}\psi)] = \varepsilon \hat{n} \cdot \vec{B} \times \vec{j}_{s,0}$$

- Edelstein (2D, 1995): in-plane supercurrent will induce a Zeeman field
- Yip (2D, 2002): in-plane Zeeman field will induce a supercurrent. Dimitrova and Feigel'man (2007).
- In $\text{Li}_2\text{Pt}_3\text{B}$ $\varepsilon \vec{B} \cdot \vec{j}_{s,0}$ is allowed by symmetry.
- Levitov, Nazarov, Eliashberg (3D, 1985) magnetic induction jump in Meissner layer at surface and Magnetic field rotates and decays in the superconductor.
- $\text{Li}_2\text{Pt}_3\text{B}$, the helical q-vector will be parallel to the applied magnetic field.

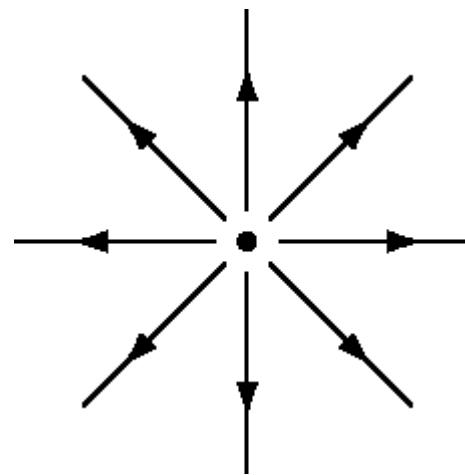
Vortex for c-axis field

$$\varepsilon \hat{n} \cdot \vec{B} \times [\psi(\vec{D}\psi)^* + \psi^*(\vec{D}\psi)] = \varepsilon \hat{n} \cdot \vec{B} \times \vec{j}_{s,0}$$



$$\vec{D} = i\vec{\nabla} - 2e\vec{A}$$

The vortex will develop a *transverse magnetization* that is radial to the applied field.



Fractional Vortices in FFLO-like Phase

Theory of ψ_{Qx} and ψ_{-Qx}

FFLO-like phase:

$$\psi = \psi_{Qx} e^{iQx} + \psi_{-Qx} e^{-iQx}$$

$$f = \alpha_1 |\psi_{Qx}|^2 + \alpha_2 |\psi_{-Qx}|^2 + \beta_1 (|\psi_{Qx}|^2 + |\psi_{-Qx}|^2)^2$$

$$+ \beta_2 |\psi_{Qx}|^2 |\psi_{-Qx}|^2 + \frac{1}{2m} (|\nabla \psi_{Qx}|^2 + |\nabla \psi_{-Qx}|^2)$$

$U(1) \times U(1)$ symmetry!

General feature:

$$(\psi_{Qx})^n (\psi_{Qx}^*)^m (\psi_{-Qx})^p (\psi_{-Qx}^*)^k$$

$$\mathbf{n - m + p - k = 0} \quad \text{Gauge invariance}$$

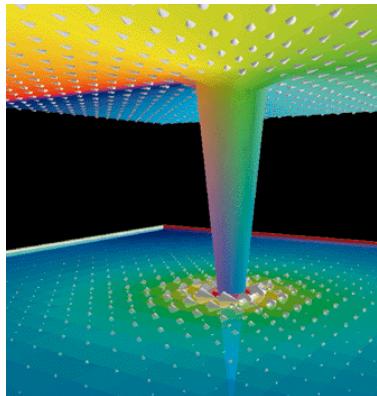
$$\mathbf{n = m}$$

$$\mathbf{n - m - p + k = 0} \quad \text{Translational invariance}$$

$$\mathbf{p = k}$$

FFLO “Vortices”

$$\psi_Q(\mathbf{r}, \phi) = |\psi_1(\mathbf{r})| e^{in\phi} \quad \psi_{-Q}(\mathbf{r}, \phi) = |\psi_2(\mathbf{r})| e^{im\phi}$$



(n,m) vortices. Consider (1,0) vortex in a phase where the magnitudes of the components far from the vortex core are $(|\psi_1|^2, |\psi_2|^2)$

$$\vec{j} = i\hbar m [\psi_1 (\nabla \psi_1)^* - \psi_1^* (\nabla \psi_1)] - \frac{2me}{c} (|\psi_1|^2 + |\psi_2|^2) \vec{A}$$

then

$$\oint A \cdot dl = \frac{|\psi_1|^2}{|\psi_1|^2 + |\psi_2|^2} \Phi_0$$

(1,1) vortex is usual Abrikosov vortex with flux Φ_0

Conclusions

- d_k must be parallel to g_k for spin-triplet superconductivity
- Paramagnetism is strongly suppressed in spin-singlet superconductors (critical fields are increased)
- Spin susceptibility is the same for both singlet and triplet states when spin-orbit is large.
- In Rashba materials, microscopic arguments imply FFLO/helical phases.
- Broken parity materials have new Lifshitz invariants in the free energy with an associated anomalous magnetization.
- FFLO-like phase will have fractional vortices.