Possible symmetry of the order parameter in noncentrosymmetric superconductor Li_2Pt_3B

Soumya Prasad Mukherjee

In collaboration with: Dr. Tetsuya Takimoto (APCTP)

Asia Pacific Center for Theoretical Physics
Pohang, South Korea

QC11, HongKong

Plan of the talk

- Interesting facts about noncentrosymmetric superconductors
- Motivation to work on the specific compound
- Experimental scenario
- Our model
- Possible symmetry of the gap function
- Conclusion

What we know already

The gap function of a superconductor has the form:

$$\Delta(\vec{k}) = [\Delta_0(\vec{k}) + \vec{\sigma}.\vec{d}(\vec{k})] i\hat{\sigma}_y$$

$$\Delta_0(-\vec{k}) = \Delta_0(\vec{k}) \quad , \quad \vec{d}(-\vec{k}) = -\vec{d}(\vec{k})$$

If the crystal has inversion symmetry,
even parity states have zero spin (d(k)=0) and
odd parity states have unit spin (Δ_0(k)=0)

What happens when the crystal lacks a center of inversion ?

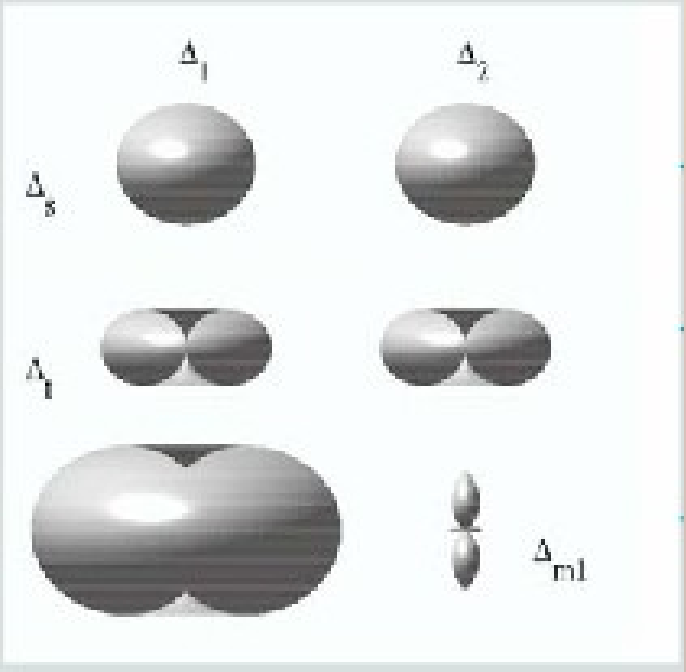
Consequences of missing inversion symmetry

- There appear a anti-symmetric spin-orbit(*ASOC*) coupling (eg. Rashba spin-orbit coupling for which $a\boldsymbol{g}_k.\boldsymbol{S}$ with $\boldsymbol{g}_{-k}=-\boldsymbol{g}_k$)
- This lifts the spin degeneracy of the bands,causing the spin in each sub-band to rotate around the Fermi surface
- The Cooper-pair wave-function may be a mixture of spin-singlet and spin-triplet pairing {Gor'kov and Rashba, PRL 87,037004(2001)}
- The pairing potential must reflect broken parity
- We can treat g(k) as the basis for an odd parity representation
- Triplet d-vector parallel to g-vector stabilize the superconducting state
- A pure triplet potential can exist in each band along with an inter-band term

Each ASOC-split band has its own gap function

$$\Delta_{1,2} = \Psi \pm t|g_k|$$

The relative magnitude of Ψ and t depends on the strength of the ASOC



Ψ dominates - pure singlet

t dominates - pure triplet

Ψ< t – nodes in one gap

Are there any other possibilities?

YES!!! Nodal structure can appear itself from the momentum dependence of the singlet component

Which material might exhibit this?

- $CePt_3Si$ (P4mm) magnetic and heavy fermionic superconductor
- UIr lacks inversion symmetry under pressure, very low T_c
- Li_2Pd_3B and Li_2Pt_3B ($P4_332$) Tc=7.5K and 2.5K respectively, non-magnetic, good to study the effect of inversion symmetry breaking
- LaRhSi and LaIrSi ($P2_13$) T_c=4.3K and 2.3K respectively. Not magnetic.
- Electron gas at the interface of $LaAlO_3/SrTiO_3$ behaving as a two dimensional superconductor with very low T_c

We briefly visit the Pd compound

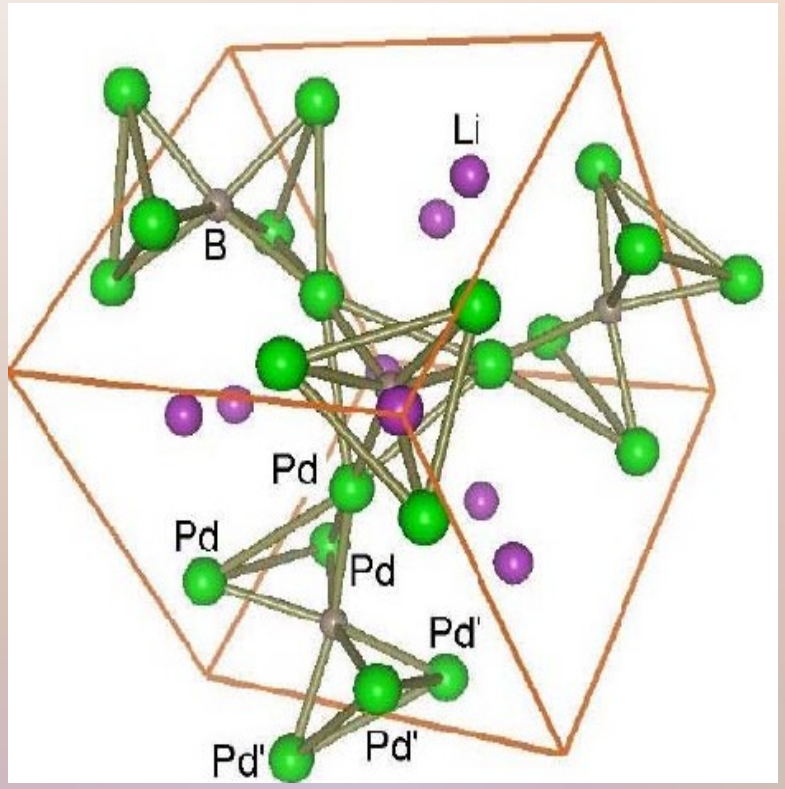
- Effect of ASOC is much less compared to the Pt compound

- In the band structure calculation although the major contribution is still coming from the Pd d-band but the DOS is much smaller and no substantial nesting present

- The order parameter is predominately singlet isotropic s-wave kind with no nodal structure and is confirmed in almost all experiments

We will now see how dramatic the effect of ASOC can be.

Li_2Pd_3B (Pt version is the same)



Space group: cubic $P4_332$

Point group symmetry: O

Contains 4 BPd_6 octahedra

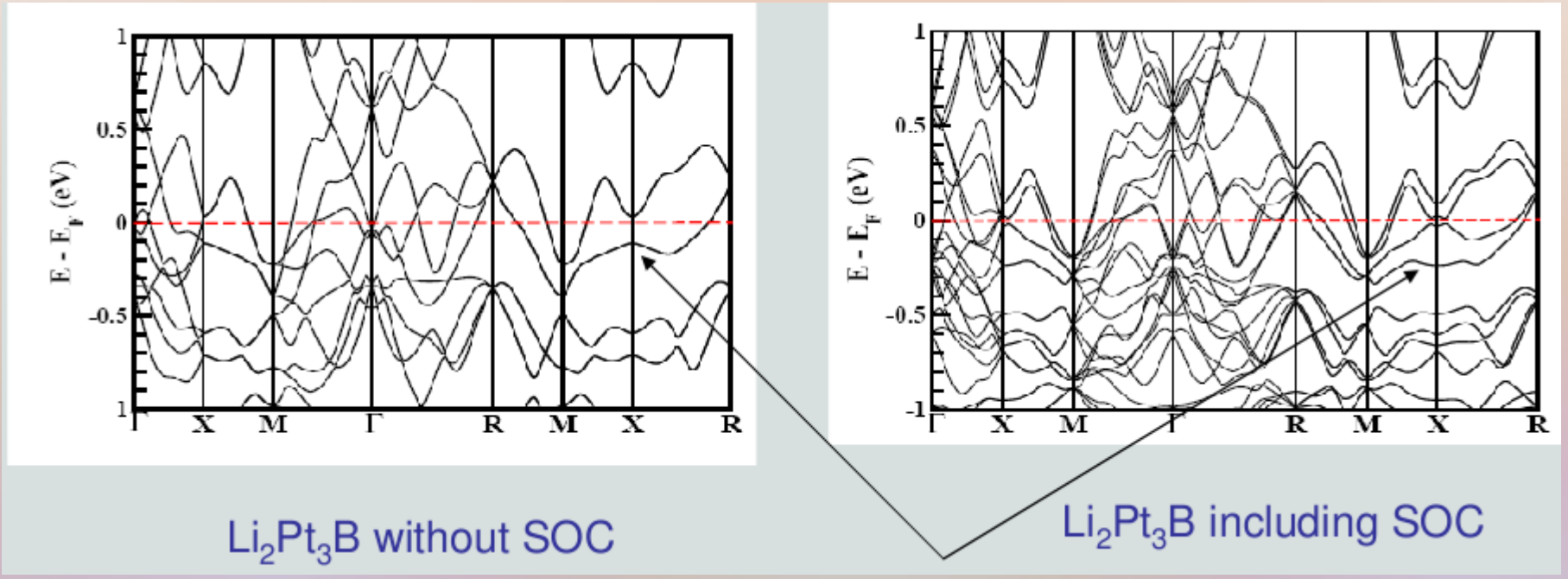
Distinct from perovskite- distorted antiperovskite

Lacks inversion symmetry

[Togano et al. PRL93,247004(2004);Badica et al. JPSJ 74,1014 (2005)]

Effect of ASOC important?

The two compounds only differ in the mass of Pd vs Pt. This induce more ASOC in Pt compound and affects the band structure significantly

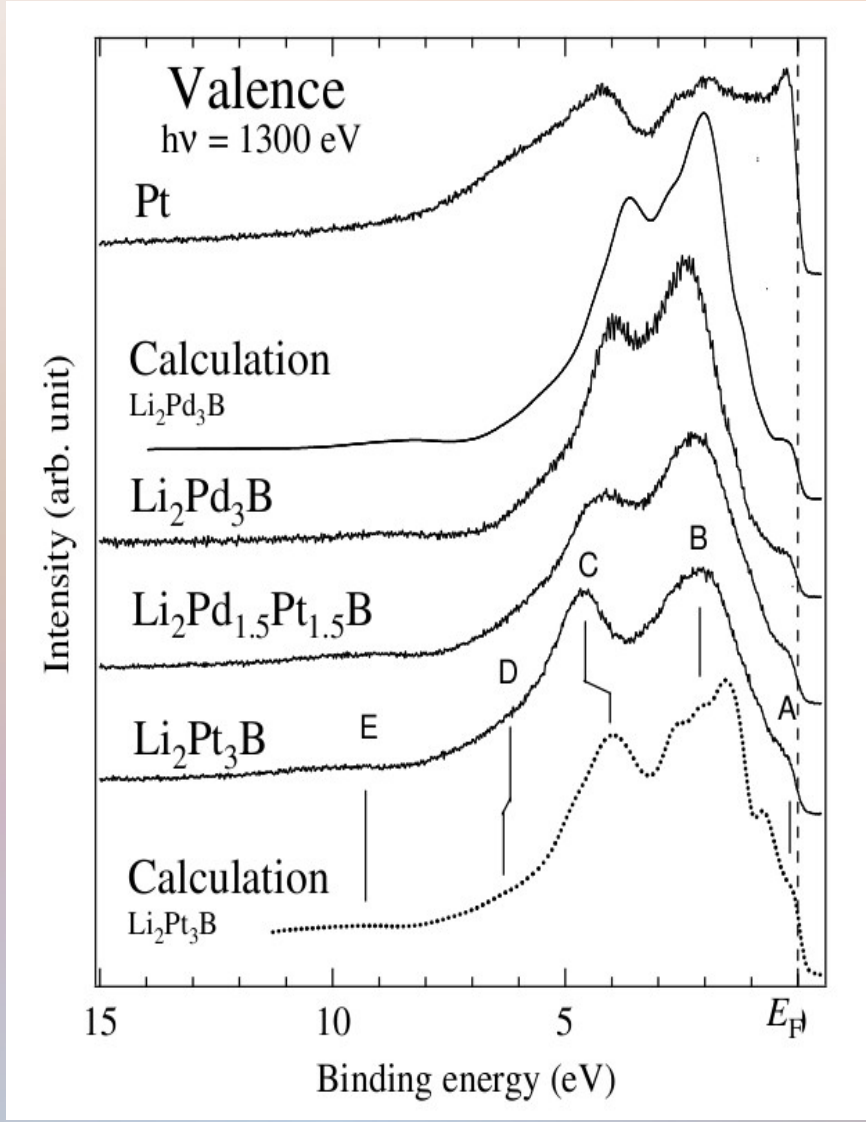


Compare-sizable fraction of the bandwidth

Large nesting between Γ point and R point

[Lee and Pickett PRB 72, 174505(2005)]

X-ray photo-emission spectroscopy data



In complete agreement with band structure calculation

Major contribution to the DOS is from Pt 5d (feature B and C)

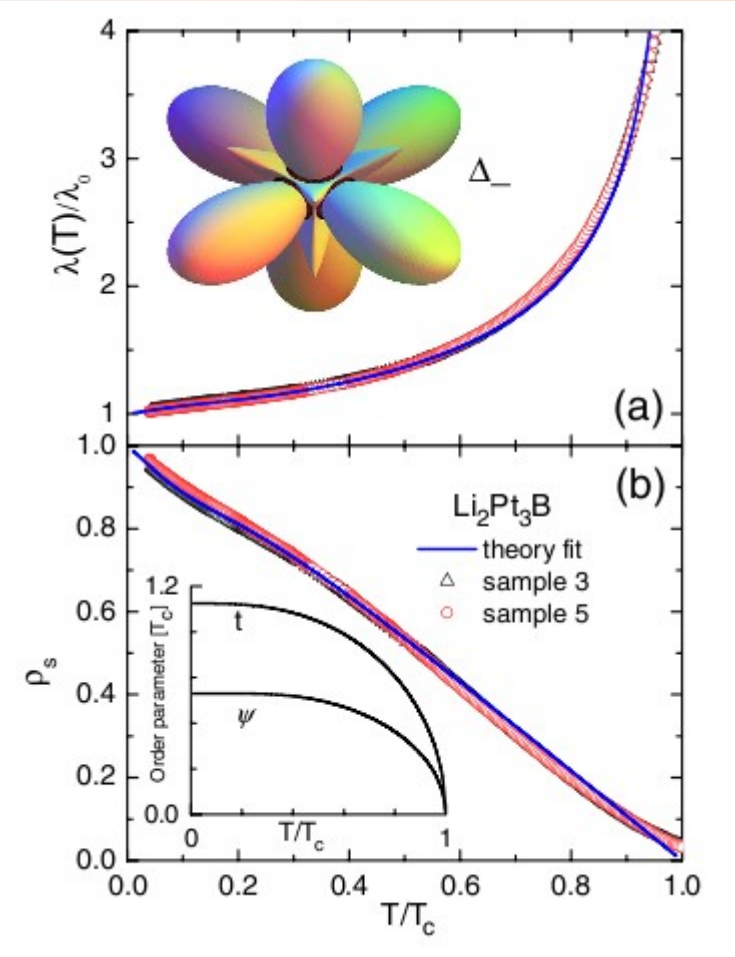
Bandwidth increases with more Pt doping

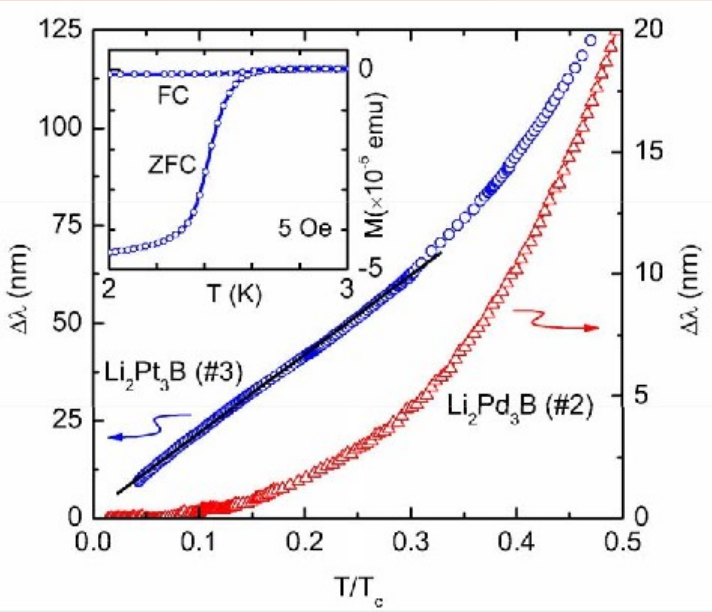
[Yoshida et. al. arXiv 0808.2394]

Larger ASOC in Pt compound responsible for:

- Increased DOS at the Fermi level
- Increase in bandwidth to 7.6 ev (6.7ev in Pd)
- Major contribution from Pt d-bands whose width is 15% wider and extends more strongly to E_f
- More added 'd' character within 1ev of the Fermi surface, hence correlation effects become significant
- Comparable large electron Fermi surface at r point (for Pd it includes no states) and hole pockets at M and R points gives rise to extensive nesting

Measurement on penetration depth λ(T)



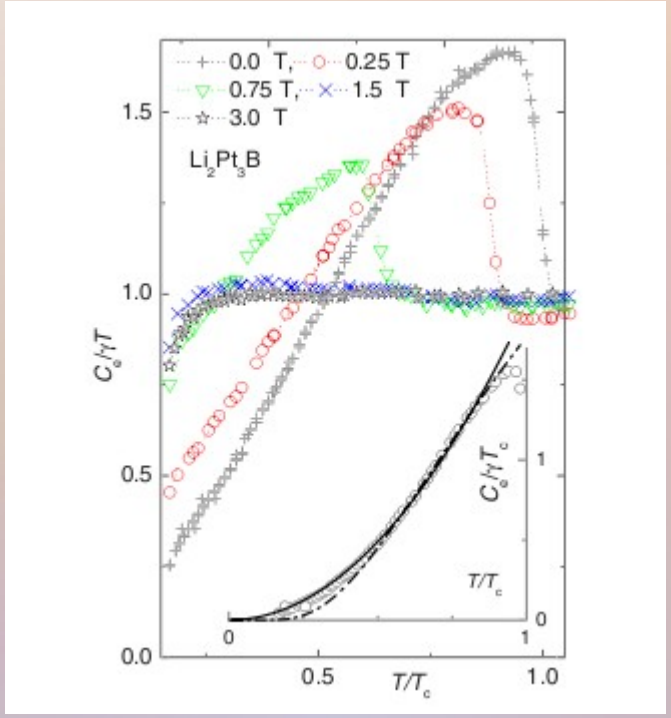


Line node in the energy gap as evidenced by the linear temperature dependence of λ(T)

- Prediction of a larger triplet order parameter with line nodes which fits the experimental data

[Yuan et. al. PRL 97,017006(2006)]

Specific heat measurement and alloy system



T^2 behavior of specific heat below T_c rather than exponential behavior also indicates line nodes in the gap function

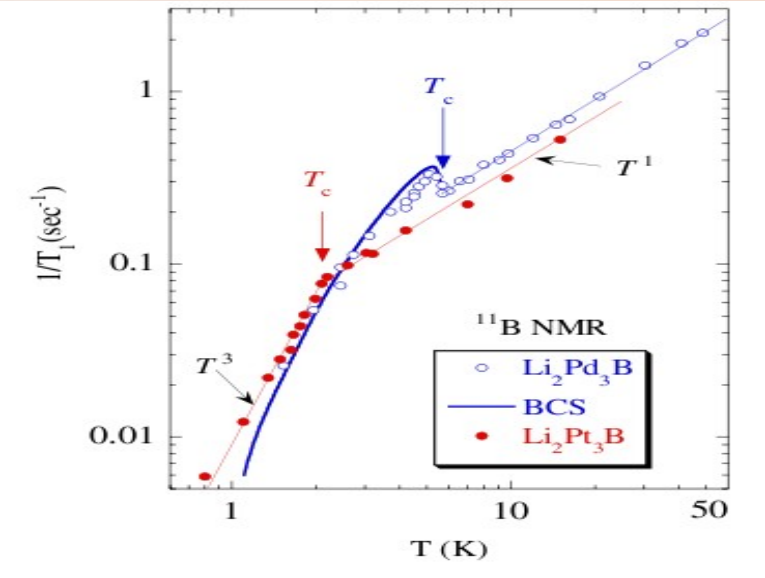
The similar experimental data for the alloy $Li_2Pd_xPt_{3-x}B$ gives similar behavior indicating the robustness of this line node even in a 50% Pd-diluted material

T_c increases linearly with increasing x.

This indicate that there is some parameter which also scales linearly with x

[Takeya et. al. PRB 76, 104506 (2007)]

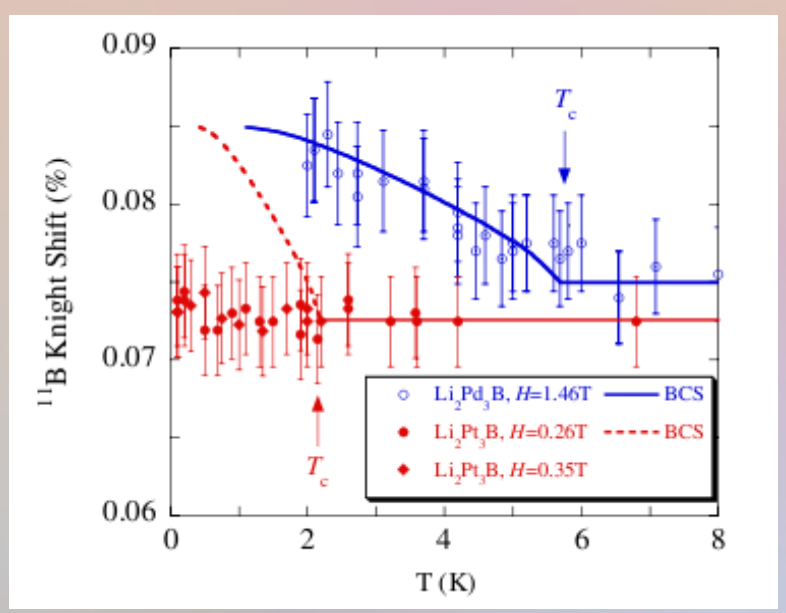
NMR and spin-lattice relaxation rate measurements



No deviation in Knight shift below T_c

Does this exclude singlet OP completely ?

The T^3 behavior of spin-lattice relaxation rate hints for line node in the gap function



[Nishiyama et. al. PRL 98,047002 (2007)]

So what we know now?

- Almost all experiments confirms the existence of line node in the gap function

- This line node is suggested to appear from some triplet gap function , but no conclusive evidence

- Experiment like NMR Knight shift which indicates some triplet pairing have to be taken seriously and one needs to consider the nature of triplet d-vector more seriously

- Appearance of nesting and more d-character near Fermi energy

Model Hamiltonian for the Pt system

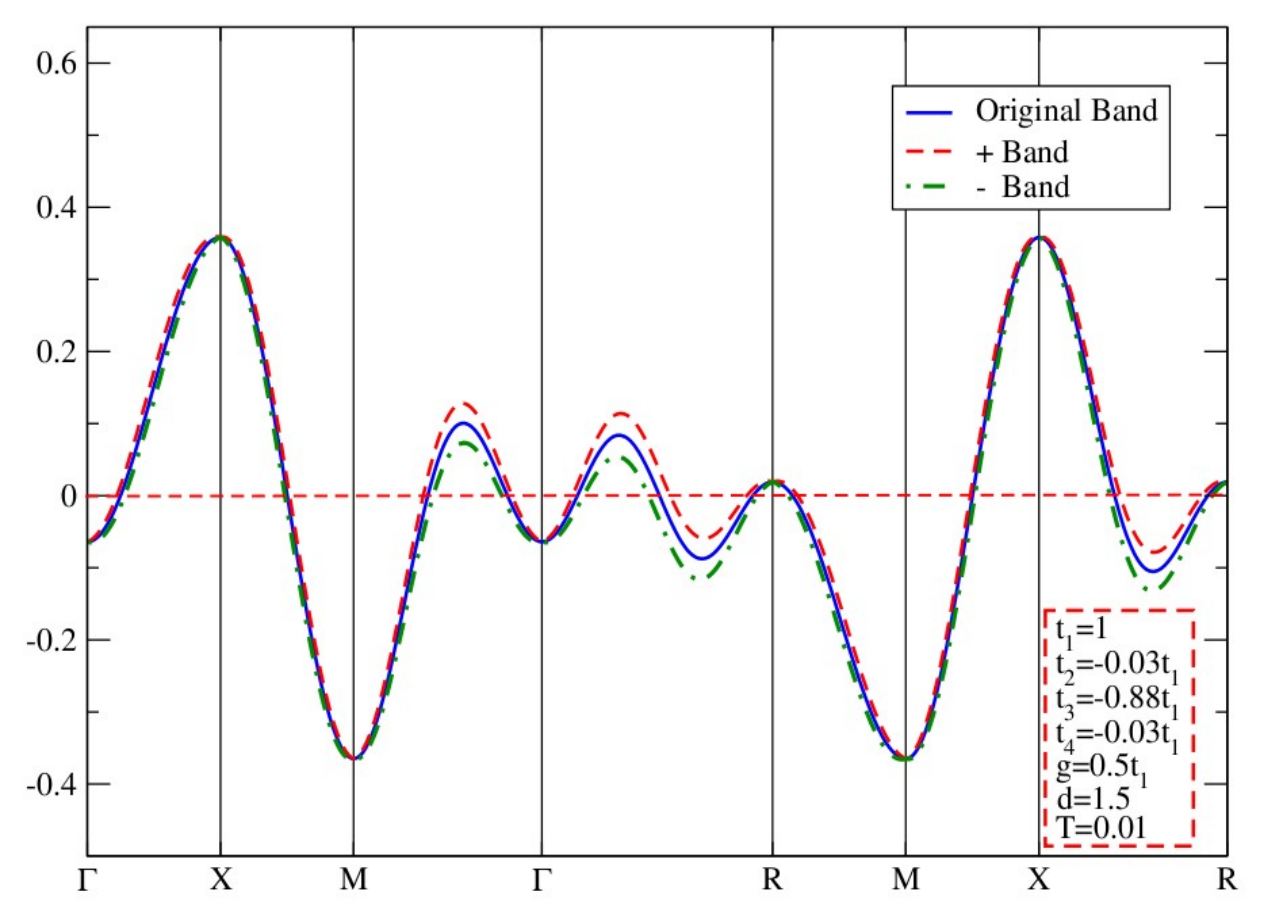
- We introduce an on-site screened interaction U to capture the physics of strong correlation
- The H_0 part of the Hamiltonian describe the usual kinetic term and ASOC term and describe the usual noncentrosymmetric system
- The BZ is simple cubic from the consideration of the space group symmetry of the compound
- The form of ASOC vector g_k is $g_k = g(\mathrm{Sin}(k_x),\mathrm{Sin}(k_y),\mathrm{Sin}(k_z))$ (in accordance with the point group symmetry) which satisfy $g_k = -g_{-k}$
- ε_k is determined from the fitting of the band structure to catch the essential features (particularly the location of the electron and hole Fermi surfaces)

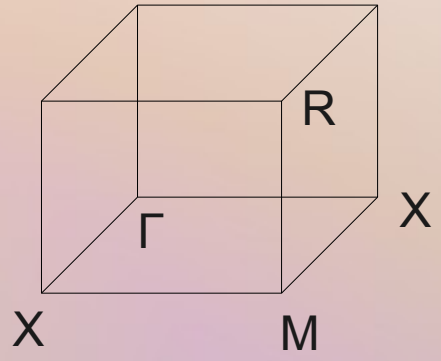
$$H = H_0 + H_1$$

$$H_0 = \sum_{k\sigma\sigma'} [(\varepsilon_k - \mu)\hat{\sigma}_0 + \vec{g}_k . \hat{\sigma}]_{\sigma\sigma'} c^{\dagger}_{k\sigma} c_{k\sigma'},$$

$$H_1 = U \sum_i n_{i\uparrow} n_{i\downarrow}$$

Fitting of the band





This fitting captures most of the essential characteristics obtained from the band structure. It also shows the nesting between electron pocket at Γ point and hole pocket at R point.

Form of matrix gap function

The most general matrix gap function is given as

$$\hat{\Delta}_k = [\Psi(k)\hat{\sigma}_0 + \vec{d}(k).\hat{\sigma}]i\hat{\sigma}_y$$

Here Ψ(k) is the spin-singlet component and d(k) is the d-vector of the triplet component

Only triplet component satisfying $|\vec{d}(k).\vec{g}_k| = |\vec{d}(k)||\vec{g}_k|$ survive the suppression of pairing potential due to lack of inversion symmetry

The spin-triplet component will be given by $\vec{d}(k) = \Phi(k)\vec{g}_k$ where Φ(k) has the same symmetry of the momentum dependence as Ψ(k)

Matrix Green's functions

The normal and anomalous matrix Green's functions is defined as

$$\hat{G}(k,i\omega_n) = G_+(k,i\omega_n)\hat{\sigma}_0 + G_-(k,i\omega_n)\tilde{g}_k.\hat{\sigma},$$
$$\hat{F}(k,i\omega_n) = [F_+(k,i\omega_n)\hat{\sigma}_0 + F_-(k,i\omega_n)\tilde{g}_k.\hat{\sigma}]i\hat{\sigma}_y$$

Where $G_\pm$ and $F_\pm$ are given by

$$G_\pm(k,i\omega_n) = \frac{1}{2}\left(\frac{-i\omega_n-\varepsilon_{k+}}{\omega_n^2+E_{k+}^2} \pm \frac{-i\omega_n-\varepsilon_{k-}}{\omega_n^2+E_{k-}^2}\right),$$
$$F_\pm(k,i\omega_n) = \frac{1}{2}\left(\frac{\Delta_{k+}}{\omega_n^2+E_{k+}^2} \pm \frac{\Delta_{k-}}{\omega_n^2+E_{k-}^2}\right)$$

With $\tilde{g}_k=\frac{\vec{g}_k}{|\vec{g}_k|}$, $\Delta_{k\pm}=\Psi(k)\pm\Phi(k)|\vec{g}_k|$, $E_{k\pm}=\sqrt{\varepsilon_{k\pm}^2+\Delta_{k\pm}^2}$, $\varepsilon_{k\pm}=\varepsilon_k\pm|g_k|-\mu$

Calculation of normal and anomalous spin and charge fluctuations

The dynamical susceptibility is expressed by the following equation

$$\chi_{\alpha\alpha'}(q, i\Omega_n) = \int_0^{\frac{1}{T}} d\tau e^{i\Omega_n \tau} T_\tau \langle [(S_q^\alpha(\tau) - \langle S_q^\alpha \rangle)(S_{-q}^{\alpha'}(0) - \langle S_{-q}^{\alpha'} \rangle)] \rangle$$

Where $\Omega_n = 2n\pi T$ is Bosonic Matsubara frequency. The charge S^c_q and spin S^a_q (a=x,y,z) operators with wave vector q are defined as

$$S_q^c = \frac{1}{2}\sum_{k\sigma} c_{k\sigma}^\dagger c_{k+q\sigma'} \quad , \quad S_q^\alpha = \frac{1}{2}\sum_{k\sigma\sigma'} \sigma_{\sigma\sigma'}^\alpha c_{k\sigma}^\dagger c_{k+q\sigma'}$$

Static charge and spin susceptibility

The matrix element of static spin susceptibility $X^0_{\alpha\beta}(q)$ ($\alpha,\beta=x,y,z$) is given by

$$\chi^0_{\alpha\beta}(q) = \frac{1}{8N_0}\sum_k \sum_{\xi\zeta} \Gamma^{\alpha\beta}_{\xi\zeta}(k;q)\frac{f(\epsilon_{k\zeta})-f(\epsilon_{k+q\xi})}{\epsilon_{k+q\xi}-\epsilon_{k\zeta}}$$

$$\Gamma^{\alpha\beta}_{\xi\zeta}(k;q) = \delta_{\alpha\beta}(1-\xi\zeta\,\tilde{g}_k\cdot\tilde{g}_{k+q}) + \xi\zeta(\tilde{g}_{k\alpha}\tilde{g}_{k+q\beta}+\tilde{g}_{k\beta}\tilde{g}_{k+q\alpha})-\epsilon_{\alpha\beta\gamma}i(\xi\tilde{g}_{k+q\gamma}-\zeta\tilde{g}_{k\gamma})$$

Similarly the charge fluctuation is described by static charge susceptibility $X^0_{cc}(q)$ by the replacement of $\Gamma^{\alpha\beta}_{\xi\zeta}(k;q)$ with

$$\Gamma^{cc}_{\xi\zeta}(k,q) = 1 + \xi\zeta\,\tilde{g}_k\cdot\tilde{g}_{k+q}$$

$[\chi_{xx}(q) + \chi_{yy}(q) + \chi_{zz}(q)]$

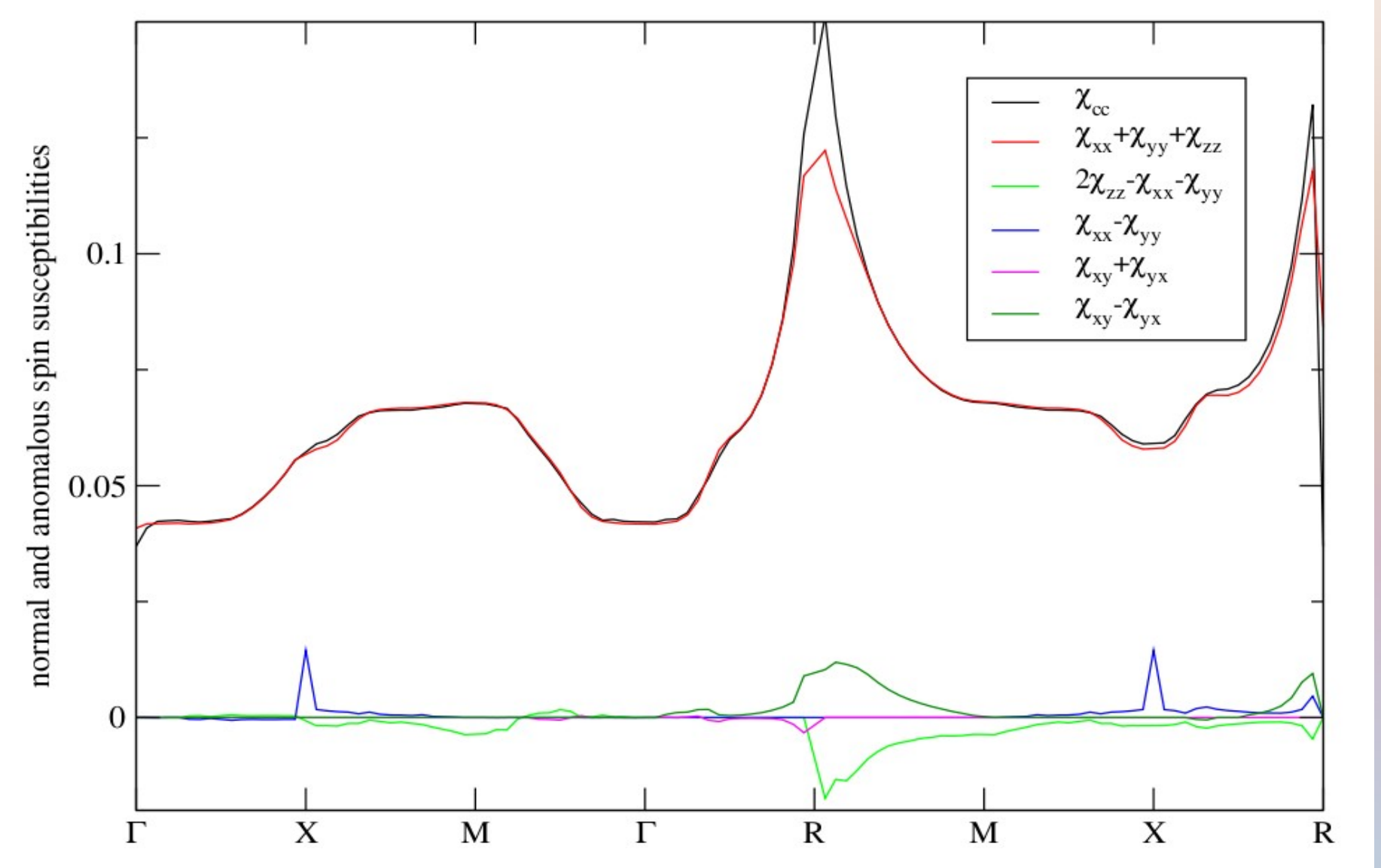
Normal spin fluctuation (exists even in centrosymmetric case)

$(\chi_{xx}(q)-\chi_{yy}(q)),(2\chi_{zz}(q)-\chi_{xx}(q)-\chi_{yy}(q)),$
$(\chi_{\alpha\beta}(q)+\chi_{\beta\alpha}(q)),i(\chi_{\alpha\beta}(q)-\chi_{\beta\alpha}(q)),\alpha\neq\beta$

Symmetric and anti-symmetric anomalous spin fluctuations (non zero only in noncentrosymmetric case)

[T. Takimoto JPSJ 77,113706 (2008)]

Normal and anomalous spin susceptibilities

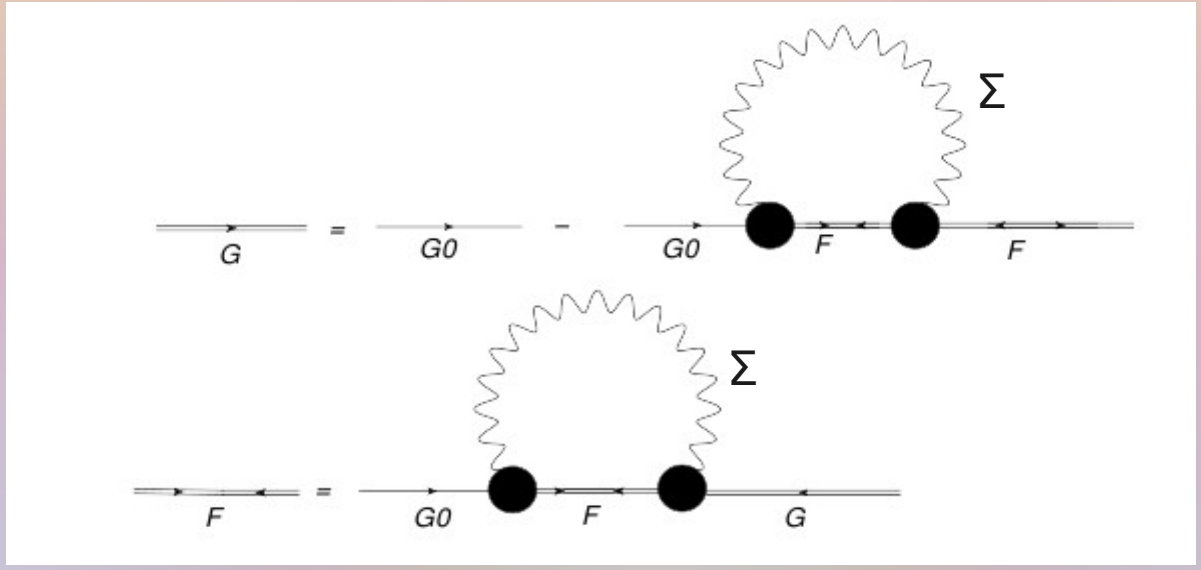


Calculation of superconducting OP

Using second order perturbation theory for pairing potential one can expand the Green's function in the superconducting state and can identify it with the Dyson-Gor'kov equation

$$\hat{G}(k) = \hat{G}_0(k) - \hat{G}_0(k)\hat{\Sigma}_s(k)\hat{F}^{\dagger}(k)$$

Diagrammatically it can be framed as



The self energy gives us the superconducting OP

$$\hat{\Delta}(k) = \hat{\Sigma}_s(k) = \sum_p V(k-p)\hat{F}(p)$$

Superconducting matrix gap equation

The superconducting matrix gap equation takes the form

$$\begin{pmatrix} \Psi(k) \\ d_x(k) \\ d_y(k) \\ d_z(k) \end{pmatrix} = \frac{1}{N_0} \sum_q \begin{pmatrix} V_{ss}(q) & V_{sx}(q) & V_{sy}(q) & V_{sz}(q) \\ V_{xs}(q) & V_{xx}(q) & V_{xy}(q) & V_{xz}(q) \\ V_{ys}(q) & V_{yx}(q) & V_{yy}(q) & V_{yz}(q) \\ V_{zs}(q) & V_{zx}(q) & V_{zy}(q) & V_{zz}(q) \end{pmatrix} \begin{pmatrix} F_s(k-q) \\ F_x(k-q) \\ F_y(k-q) \\ F_z(k-q) \end{pmatrix}$$

With

$$V_{ss}(q) = -U - U^2[\chi_{xx} + \chi_{yy} + \chi_{zz} - \chi_{cc}]$$
$$V_{\alpha\alpha}(q) = U^2[\chi_{cc} + \chi_{\beta\beta} + \chi_{\gamma\gamma} - \chi_{\alpha\alpha}], \ (\alpha \neq \beta \neq \gamma)$$
$$V_{\alpha\beta} = V_{\beta\alpha} = -U^2[\chi_{\alpha\beta} + \chi_{\beta\alpha}]$$
$$V_{s\alpha} = -V_{\alpha s} = iU^2[\chi_{\beta\gamma} - \chi_{\gamma\beta}]$$

Where $F_\alpha(k)$ and $F_s(k)$ are given by the equations

$$F_s(k) = [\Psi(k)\phi_+(k) + \vec{d}(k).\tilde{g}_k\phi_-(k)]/2 \ ,$$
$$F_\alpha(k) = \tilde{g}_{k\alpha}[\Psi(k)\phi_-(k) + \vec{d}(k).\tilde{g}_k\phi_+(k)]/2 \ ,$$
$$\phi_\pm = \frac{1}{2E_{k+}}\tanh\left(\frac{E_{k+}}{2T}\right) \pm \frac{1}{2E_{k-}}\tanh\left(\frac{E_{k-}}{2T}\right)$$

How spin fluctuation contribute to superconductivity?

- For centrosymmetric case V_{ss} gives rise to the singlet OP and $V_{xx} = V_{yy} = V_{zz}$ (since contribution from anomalous spin fluctuation vanishes) contribute to the triplet pairing

- For noncentrosymmetric case the contribution from the symmetric anomalous spin fluctuation affects the triplet pairing only

- The spin-singlet pairing having the same form but changes due to non zero ASOC field g_k

- The mixing interactions $V_{\alpha\beta}$ ($\alpha \neq \beta$) between spin singlet and spin triplet pairs are only affected by the anti-symmetric spin fluctuation

- The anomalous spin fluctuation is significantly lower than the normal spin fluctuation giving rise to weaker spin-triplet OP

Finding Tc

- At $T=T_c$ the matrix gap equation gets converted to the eigenvalue problem

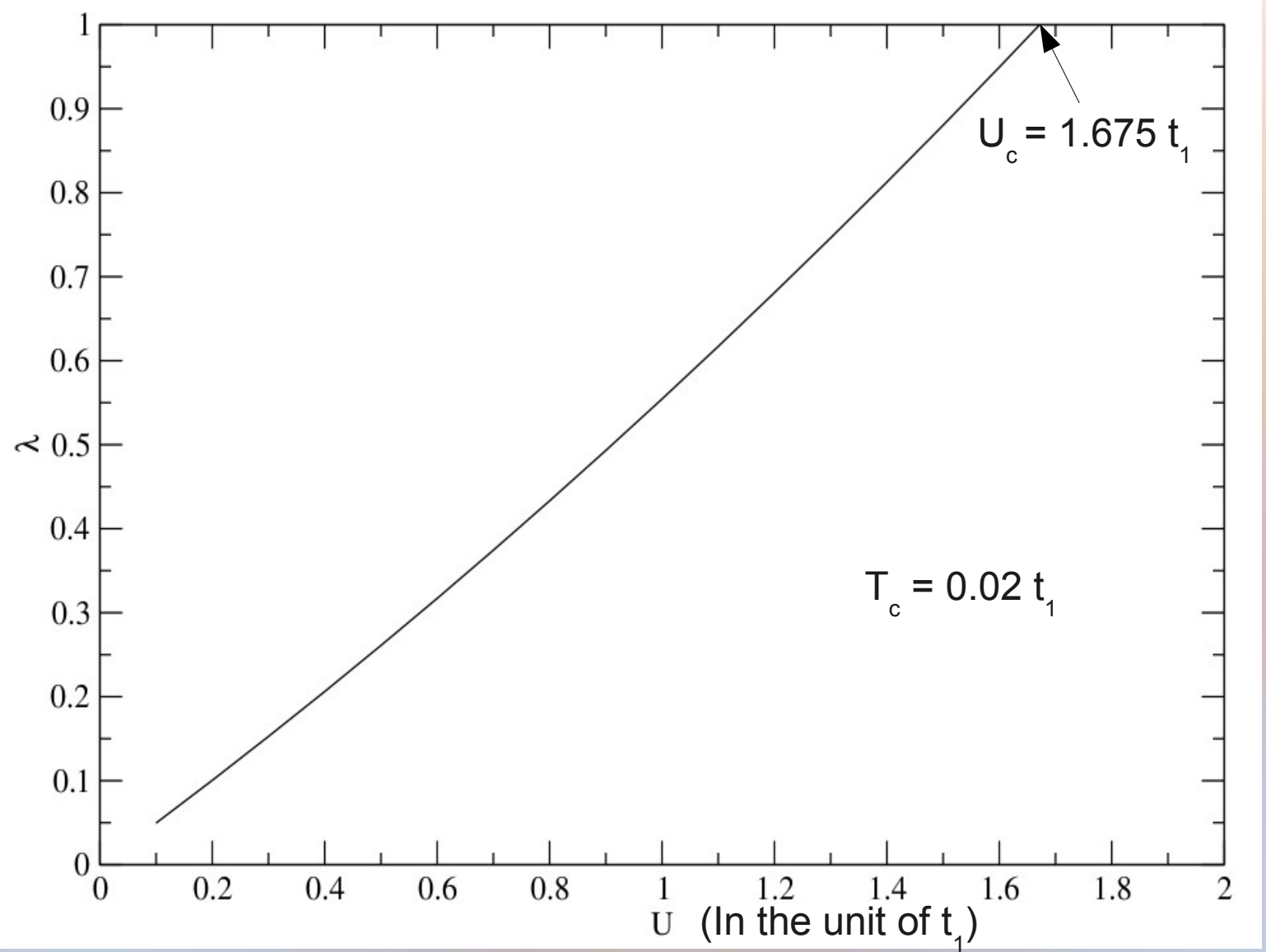
- We fix the T_c at $0.02t_1$ and vary U to see when the maximum eigenvalue is unity, this gives U_c

- The matrix gap equation is solved iteratively at T_c with $U = U_c$

- This process will automatically choose the proper irreducible representation of the Cubic space group

- This gives A_1 representation as the most suitable description for the superconducting state and the momentum dependence of the gap function is obtained

Finding maximum eigenvalue



Nature of the order parameter symmetry

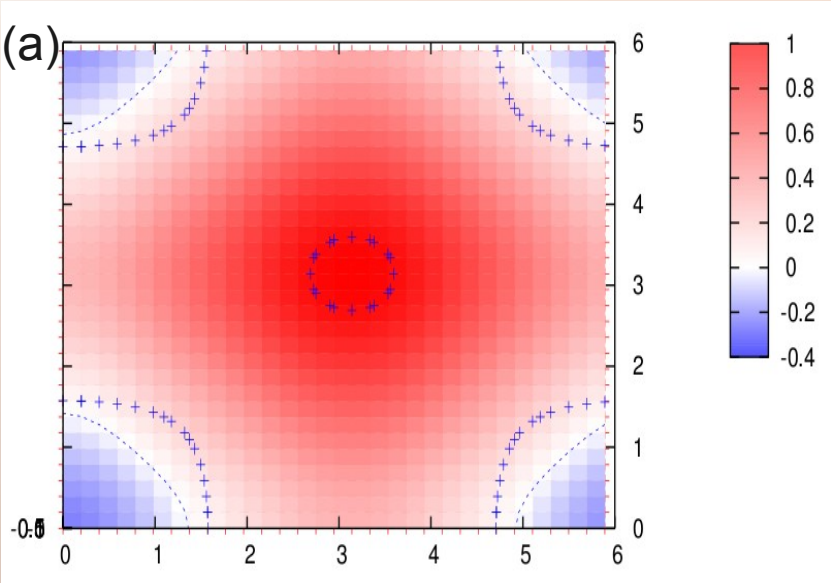
- The OP in the superconducting state is predominantly spin-singlet with very little (perhaps negligible) contribution from the spin-triplet part

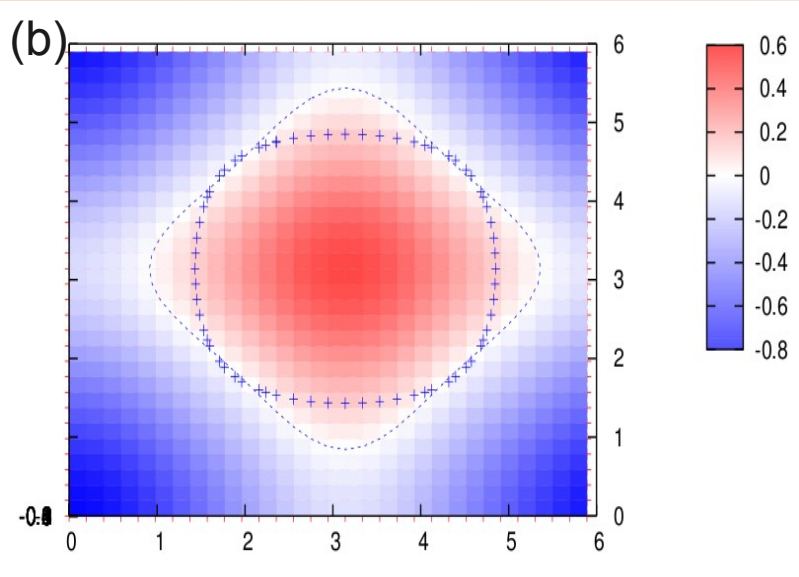
- This largerness of the singlet OP is in the heart of many contradicting experimental behavior

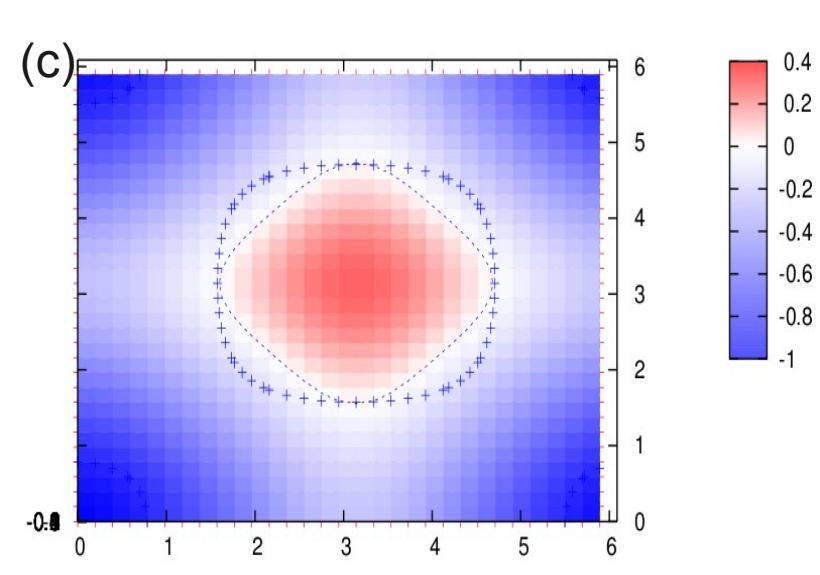
  - The singlet order parameter is of $S_{\pm}$ type and belonging to the A_1 irreducible representation of the underlying cubic space group

  - There appear accidental line nodes in the singlet gap function and this explain many experiments

Contour plot of the singlet order parameter







(a) kz = 0

(b) kz = 0.7 Π

(c) kz = Π

++++++ Fermi surface

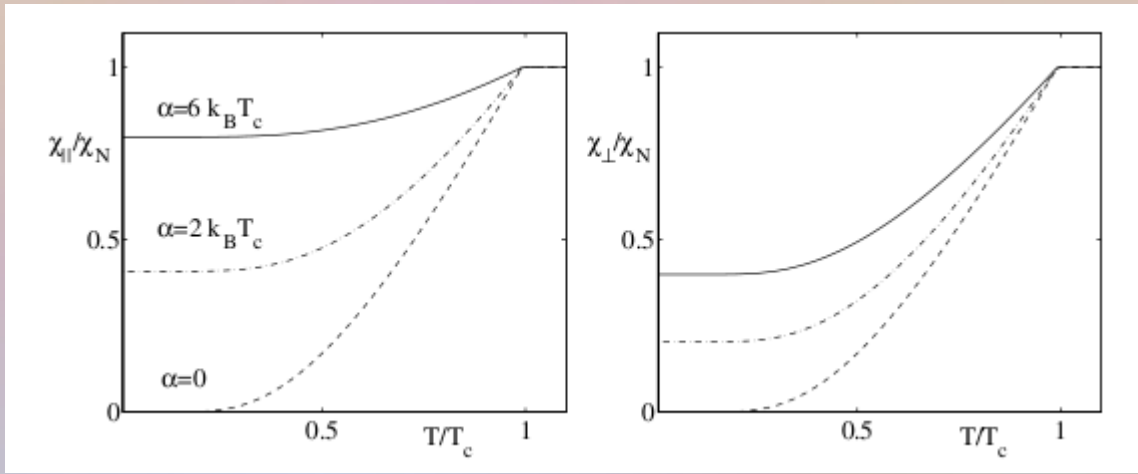
..... Nodal line of singlet OP

Explanation of the Knight Shift data

Frigeri et. al. found the following contribution of the singlet gap function to spin susceptibility

$$\chi_{ii}^{s} = \chi_n \left\{ 1 - k_B T \pi \sum_{\omega_n} \left\langle \frac{1 - \hat{g}_{k,i}^2}{(\omega_n^2 + |\psi(\boldsymbol{k})|^2 + \alpha^2 |\boldsymbol{g}_k|^2)} \frac{|\psi(\boldsymbol{k})|^2}{\sqrt{\omega_n^2 + |\psi(\boldsymbol{k})|^2}} + \hat{g}_{k,i}^2 \frac{|\psi(\boldsymbol{k})|^2}{(\omega_n^2 + |\psi(\boldsymbol{k})|^2)^{3/2}} \right\rangle_k \right\}.$$

Their calculation shows susceptibility (for singlet OP) increases with increasing Rashba spin-orbit coupling α



In our case α~25 T_c

So we expect no substantial deviation of spin susceptibility from the normal state as also found in the experiment

[P A Frigeri et. al. New J Phys 6 115 (2004)]

Work in progress

Conclusion

- The physics of strong Coulomb correlation accompanied with the nesting of the Fermi surface is responsible for contradicting experimental observations in the noncentrosymmetric superconductor Li_2Pt_3B

- The presence of line nodes in the gap function is predicted in every experiments and arise from the Fermi surface topology and is accidental (ie. Not allowed by the symmetry)

- The superconducting OP is of strongly singlet nature ($S_{\pm}$) with negligible triplet pairing in-spite-of the fact that the system has strong ASOC

- The presence of strong ASOC is felt in the Knight shift data below T_c

- More work is underway to verify our claim