



<http://www.topological-qp.jp/english/index.html>

# Theory of superconducting topological insulator

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ISSP June 13 (2013)

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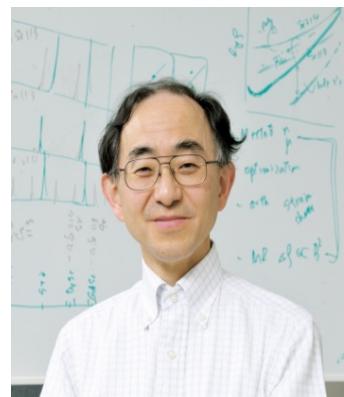


T. Hashimoto (Nagoya)



# Main collaborators

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Y. Ando (Osaka)



S. Nakosai (Univ. Tokyo)



K. Segawa (Osaka)



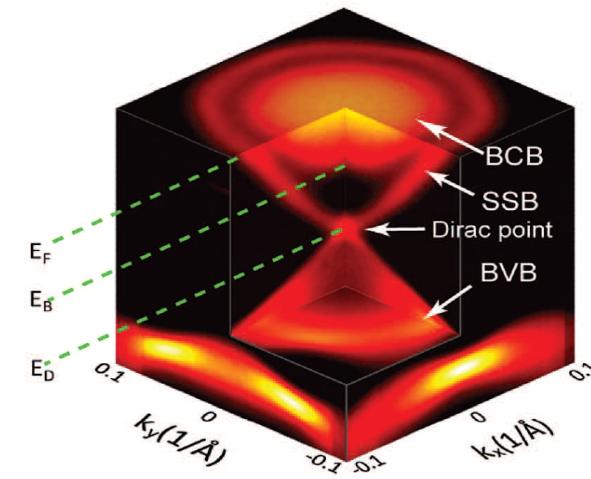
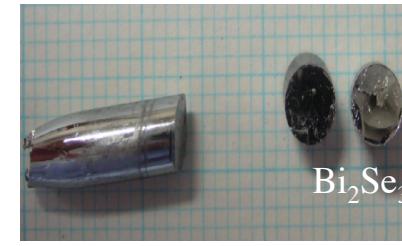
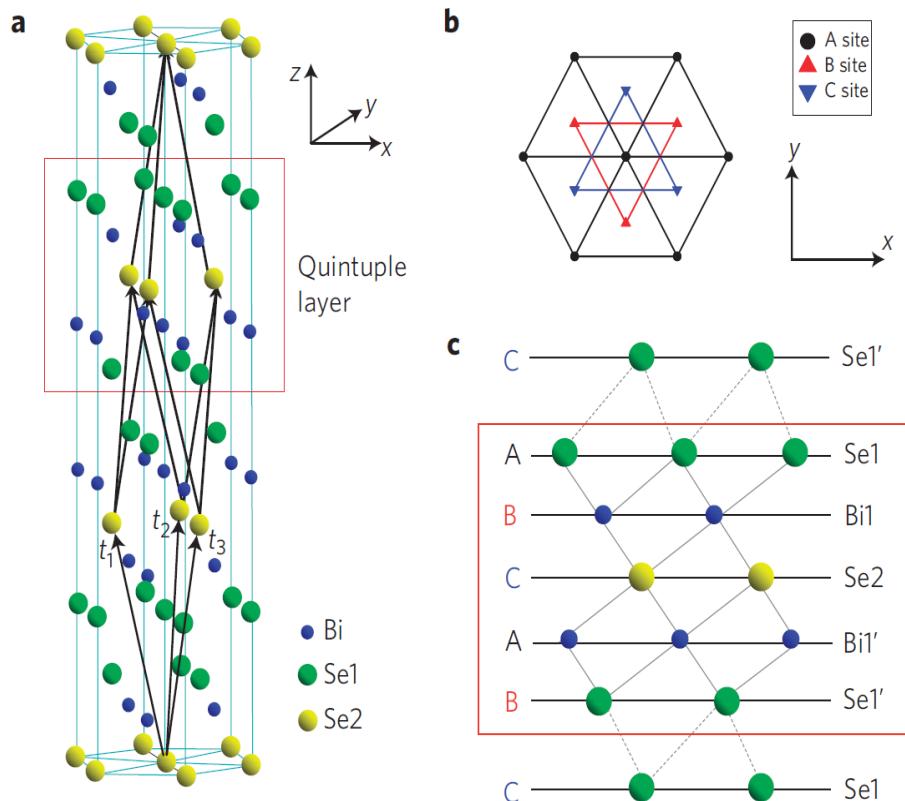
# Contents of our talk

- (1)What is superconducting topological insulator
- (2)Andreev bound state and quasi particle tunneling
- (3)Josephson current
- (4)Spin susceptibility
- (5)Relevant Rashba superconductor system

# Topological insulator $\text{Bi}_2\text{Se}_3$

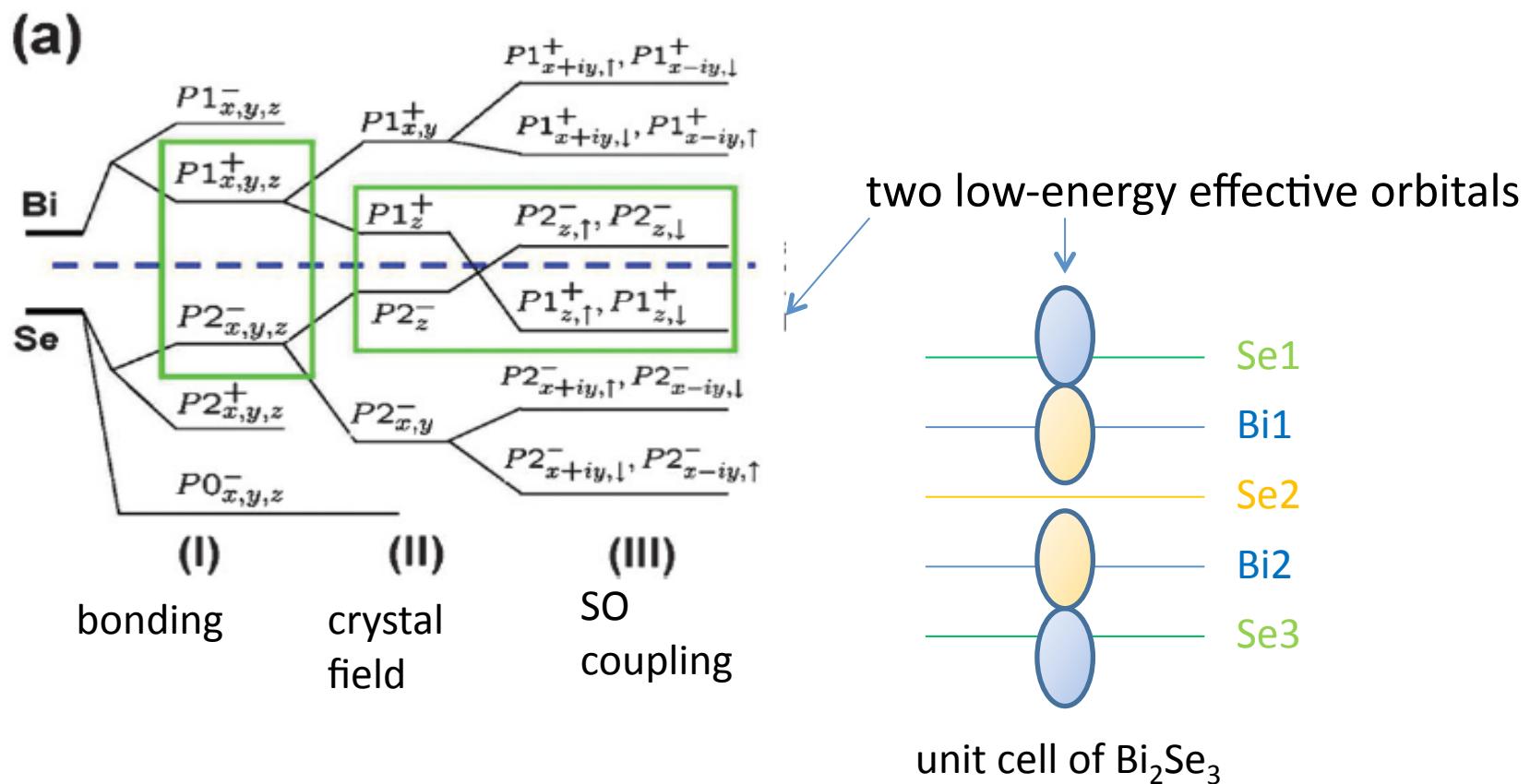
- Nonzero topological number  $Z_2$
- Helical Dirac Cone as a surface state
- Strong spin-orbit coupling

## Crystal structure $\text{Bi}_2\text{Se}_3$



Electronic band structure of  $\text{Bi}_2\text{Se}_3$  measured by ARPES  
Y. L. Chen *et al.* Science 329, 659 (2010)

# Electronic states of $\text{Bi}_2\text{Se}_3$



energy levels of the atomic orbitals  
in  $\text{Bi}_2\text{Se}_3$

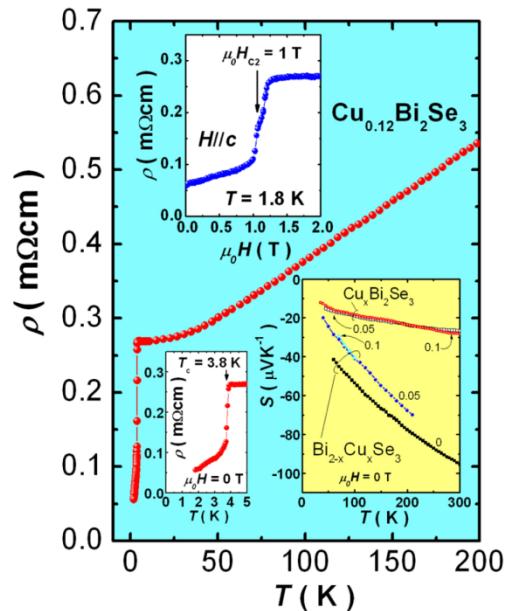
Zhang et al, Nature 09

# Superconducting topological insulator

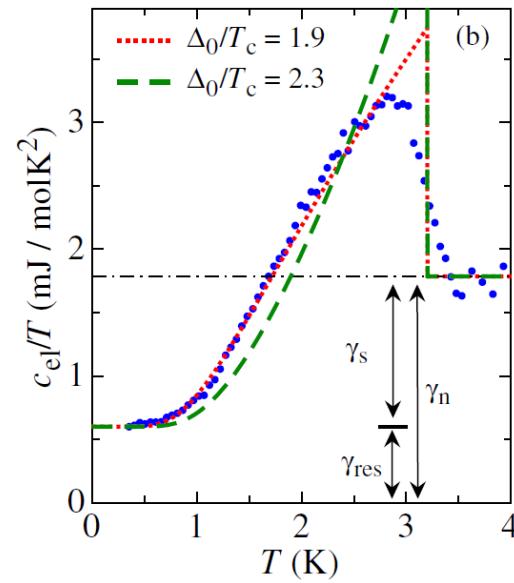
## $\text{Cu}_x\text{Bi}_2\text{Se}_3$

Cu doped topological insulator

### Resistivity



### Specific heat



Y.S.Hor *et al.*, PRL 104, 057001 (2010)

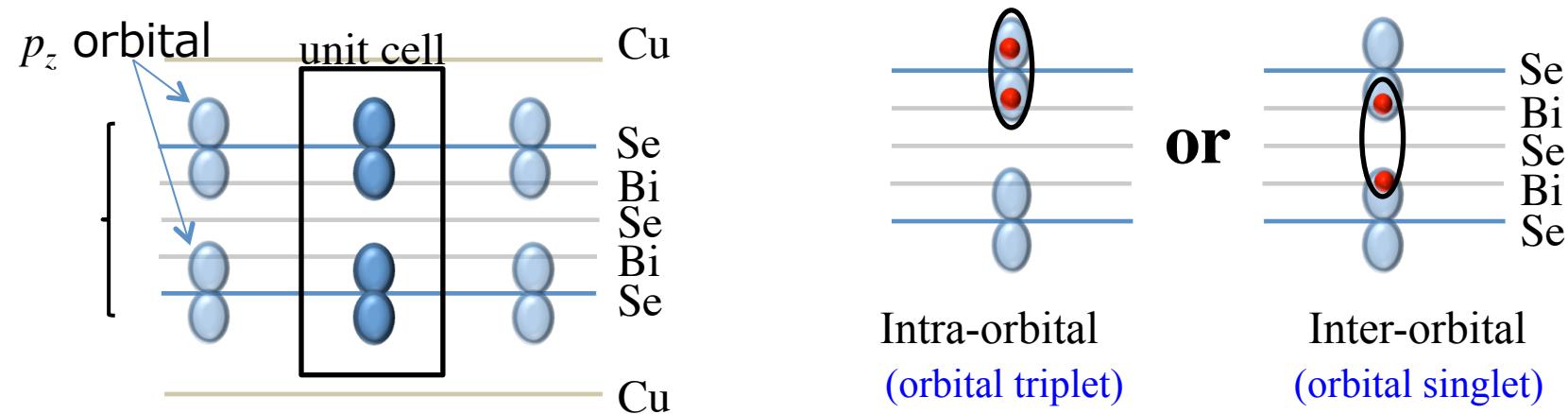
M. Kriener *et al.*, PRL 106, 127001 (2011)

$T_c = 3.8$ K

# Candidate of pair potentials

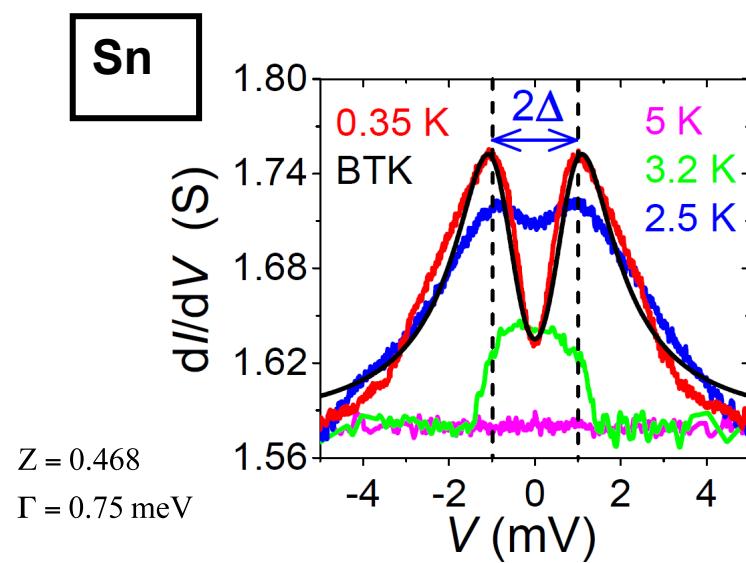
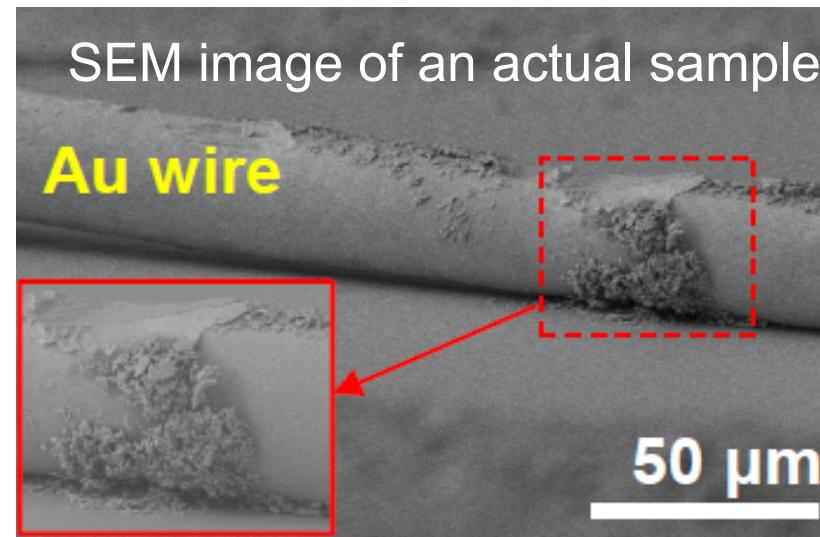
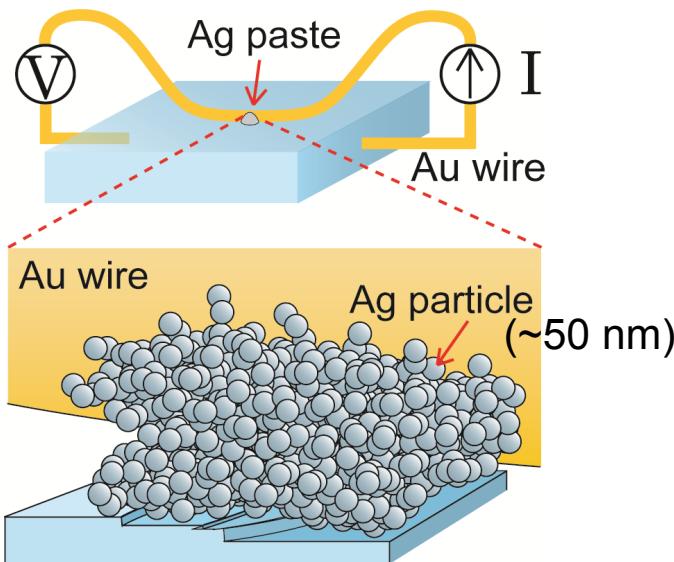
Liang Fu, Erez Berg, PRL,105, 097001 (2010)

	Energy gap	irreducible representation	spin	Orbital	Inversion symmetry
$\Delta_1$	full gap	$A_{1g}$	singlet	intra	even
$\Delta_2$	full gap	$A_{1u}$	triplet	inter	odd
$\Delta_3$	point node	$A_{2u}$	singlet	intra	odd
$\Delta_4$	point node	$E_u$	triplet	inter	odd

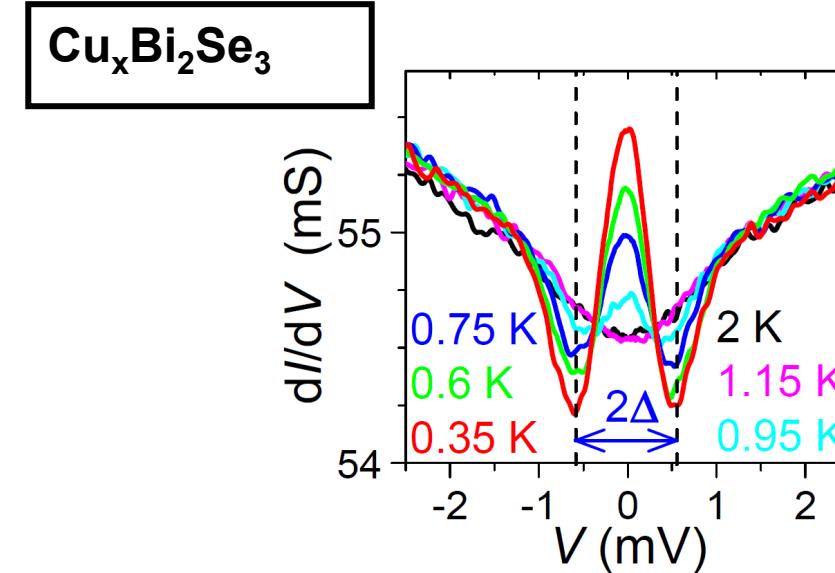


$\text{Cu}_x\text{Bi}_2\text{Se}_3$  Effective orbital  $p_z$  orbital      **(No momentum dependence)**

# Tunneling spectroscopy



Ando's group (Osaka)

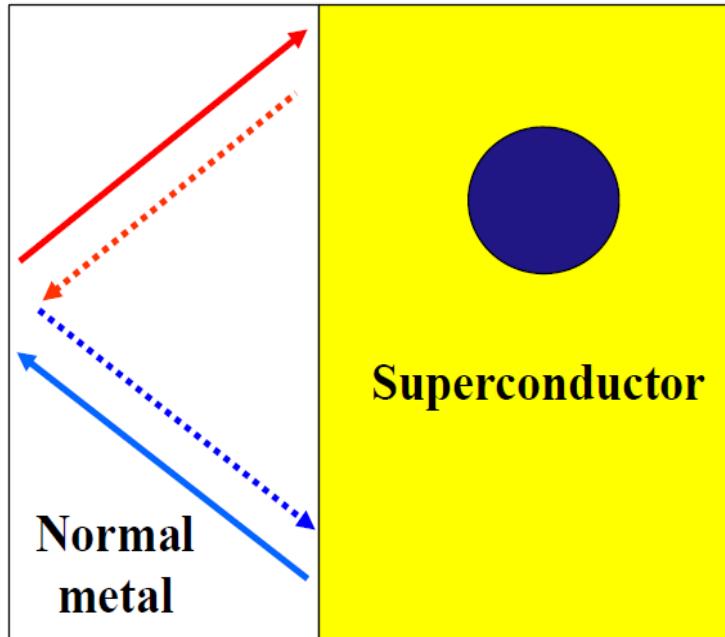


S. Sasaki et al PRL 107 217001 (2011)

# Contents of our talk

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- (5) Relevant Rashba superconductor system

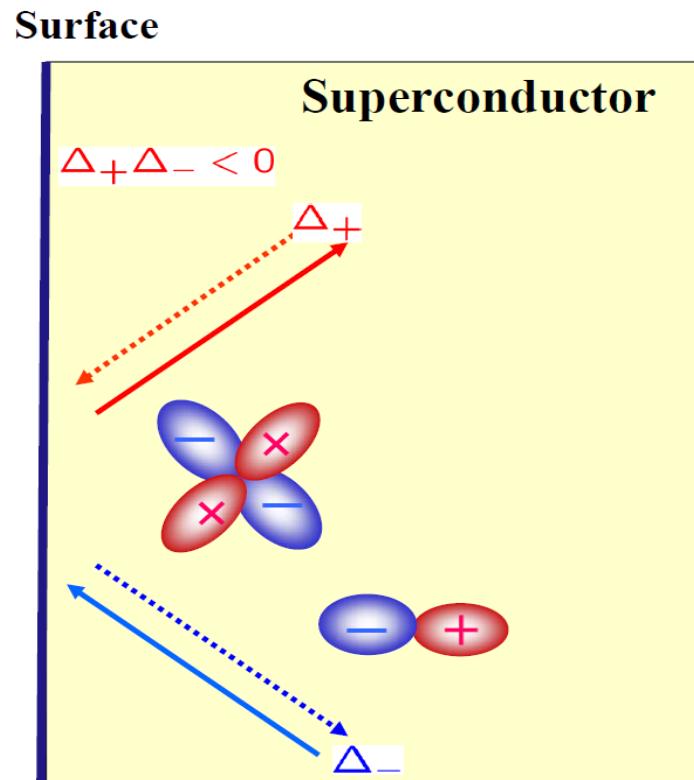
# Andreev bound state (non-topological and topological)



Andreev bound state with non zero energy (de Gennes, Saint James)

Not edge state

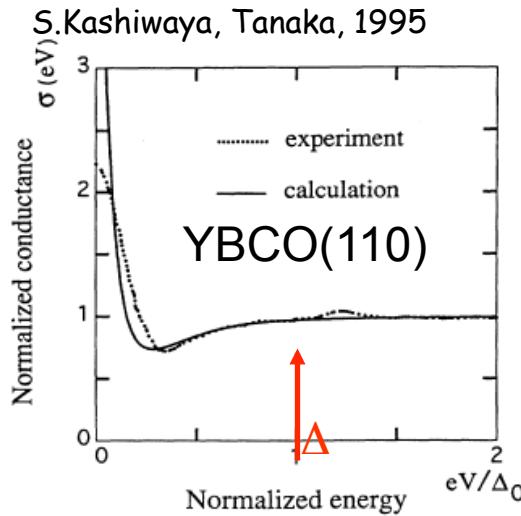
Non topological



Mid gap (zero energy) Andreev bound state  
Surface Andreev bound state  
**Edge state Topological**

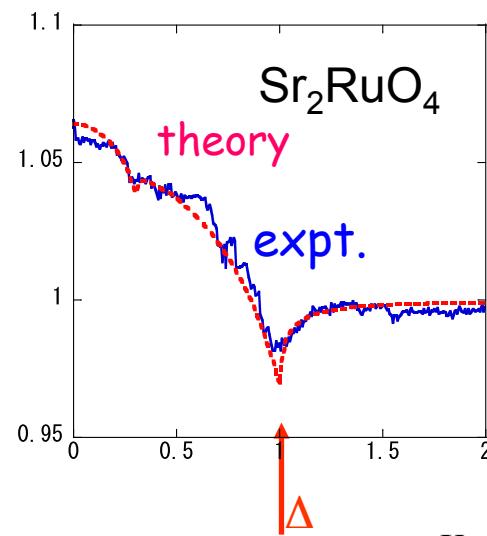
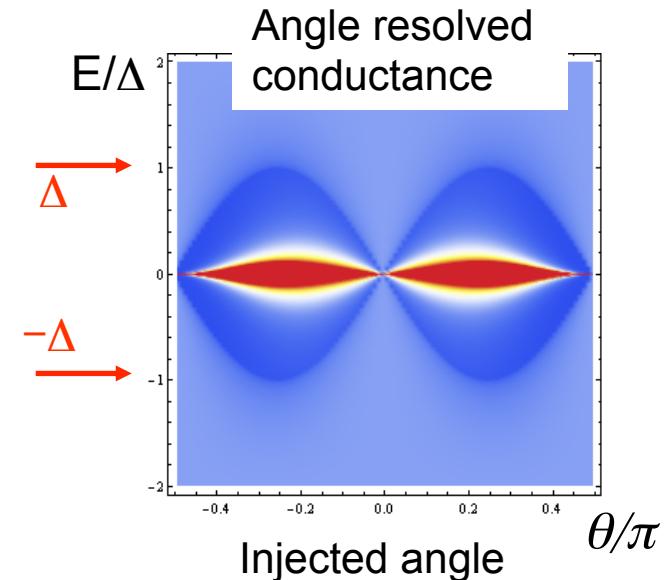
L. Buchholtz & G. Zwicknagl (81); J. Hara & K. Nagai : Prog. Theor. Phys. 74 (86)  
C.R. Hu : (94) Tanaka Kashiwaya (95), .....

# Tunneling spectrum in two-dimensional topological superconductors



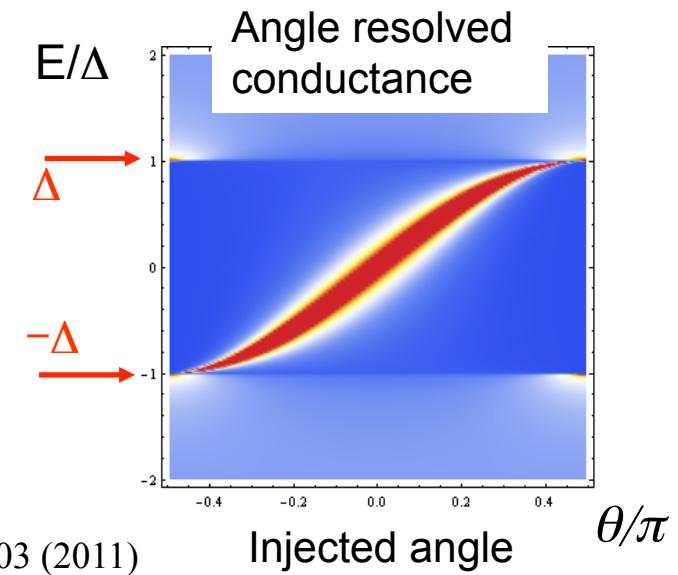
$d_{x^2-y^2}$ -wave  
nodal gap

zero energy flat band  
of surface ABS



chiral  $p$ -wave  
full gap  
chiral edge state (ABS)

broad zero-bias peak  
due to linear dispersion

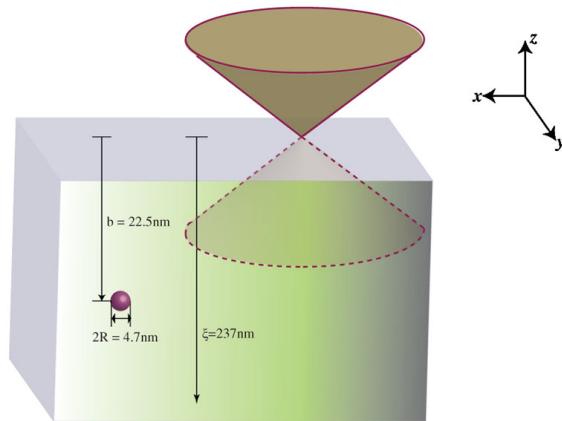


Kashiwaya *et al*, Phys. Rev. Lett. **107**, 077003 (2011)

# Andreev bound state (topological edge state) and topological invariant

Andreev bound state	Topological invariant	Time reversal symmetry	Materials	Theory of tunneling	Insulator (semi-metal)
Flat	1d winding Number $Z$ for fixed $k_y$ AIII (BDI) class	○	Cuprate $p_x$ -wave	PRL (1995) JPSJ(1998)	Graphene (zigzag edge)
Chiral	2d winding Number $Z$ D class	✗	$Sr_2RuO_4$ $^3He A$	PRB (1997)	QHS QAHS
Helical	$Z_2$ DIII class	○	$s+p$ -wave (NCS)	PRB (2007)	QSHS (2D Topological insulator)
Cone	3d winding Number $Z$ DIII class	○	$^3He B$	PRB (2003)	Topological insulator

# ABS in B-phase of superfluid $^3\text{He}$

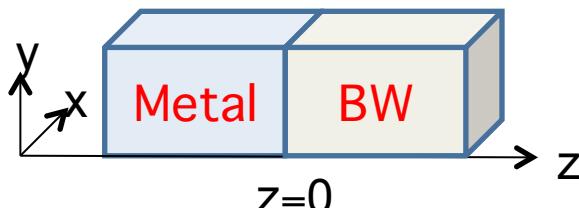


Cone type ABS

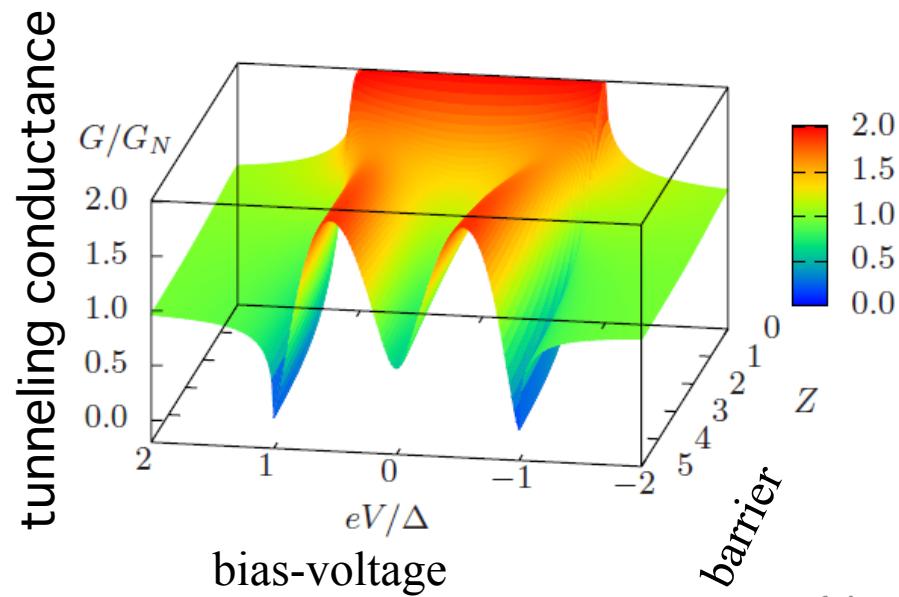
Salomaa Volovik (1988)  
Schnyder (2008)  
Roy (2008) Nagai (2009)  
Qi (2009)  
Kitaev(2009)  
Chung, S.C. Zhang (2009)  
Volovik (2009)

perpendicular injection ZES: Buchholtz and Zwicknagle (1981)

BW state (B-phase in  $^3\text{He}$ )  
full gap superconductor

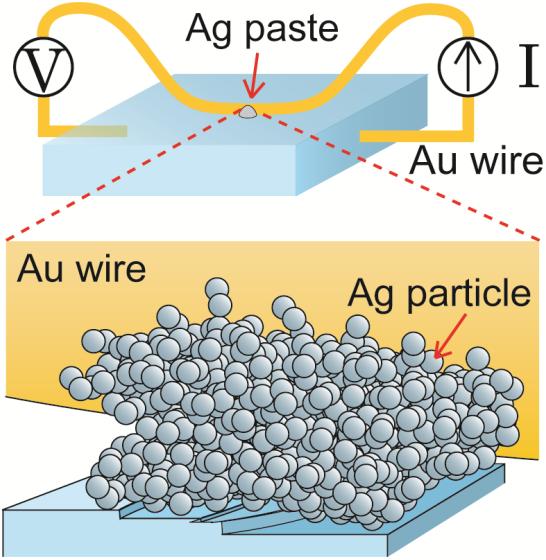


no zero-bias peak  
due to linear dispersion  
of surface ABS

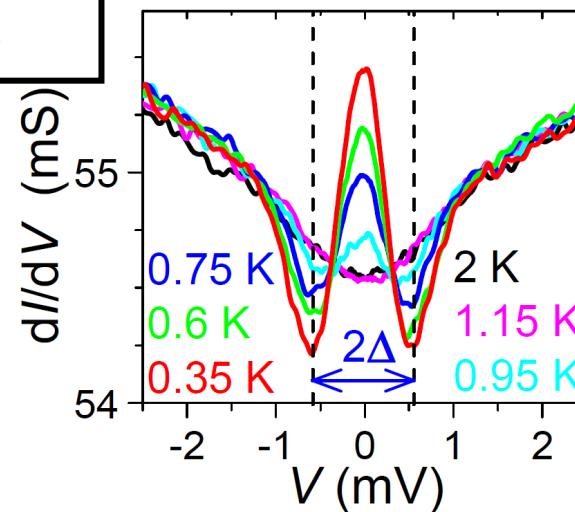


Y. Asano *et al*, PRB '03

# Tunneling experiment



$\mathbf{Cu_xBi_2Se_3}$

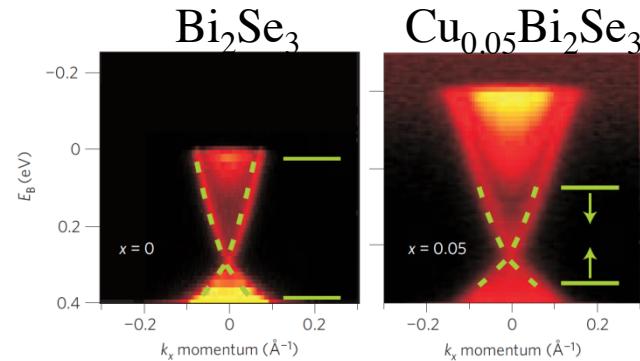
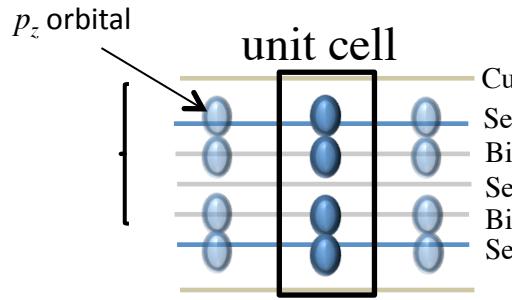


S. Sasaki et al PRL 107 217001 (2011)

If  $\mathbf{Cu_xBi_2Se_3}$  is a 3D topological superconductor with odd-parity, Tunneling spectroscopy can not be explained by pair potential realized in B-phase in  ${}^3\text{He}$ , which is a typical example of 3d full gap superconductor.

# Effective Hamiltonian of Cu<sub>x</sub>Bi<sub>2</sub>Se<sub>3</sub>

ARPES



Model Hamiltonian (Normal state) H.Zhang *et al*, Nature Phys. 5, 438 (2009)

$$H_0(k) = m\sigma_x + v(k_x\sigma_z s_y - k_y\sigma_z s_x) + v_z k_z \sigma_y$$



Model Hamiltonian (superconducting state)

BdG Hamiltonian

$$H(k) = [H_0(k) - \mu]\tau_z + \hat{\Delta}\tau_x$$

$8 \times 8$  matrix

**Pauli matrix**  $\sigma$ : orbital,  $s$  : spin,  $\tau$  : particle hole

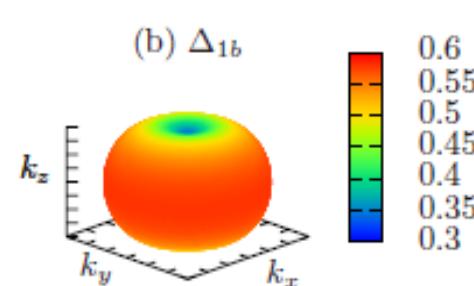
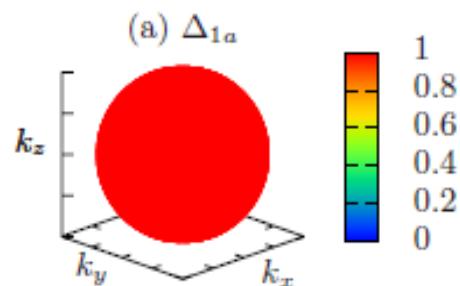
# Possible pairings

		Matrix representation	Parity (spatial inversion)
$\hat{\Delta}_{1a}$	$c_{1\uparrow}c_{1\downarrow} + c_{2\uparrow}c_{2\downarrow}$	$\Delta$	Even
$\hat{\Delta}_{1b}$	$c_{1\uparrow}c_{2\downarrow} - c_{1\downarrow}c_{2\uparrow}$	$\Delta\sigma_x$	Even
$\hat{\Delta}_2$	$c_{1\uparrow}c_{2\downarrow} + c_{1\downarrow}c_{2\uparrow}$	$\Delta\sigma_y s_z$	Odd
$\hat{\Delta}_3$	$c_{1\uparrow}c_{1\downarrow} - c_{2\uparrow}c_{2\downarrow}$	$\Delta\sigma_z$	Odd
$\hat{\Delta}_4$	$c_{1\uparrow}c_{2\uparrow} \mp c_{1\downarrow}c_{2\downarrow}$	$\Delta\sigma_y s_x$ $(\Delta\sigma_y s_y)$	Odd

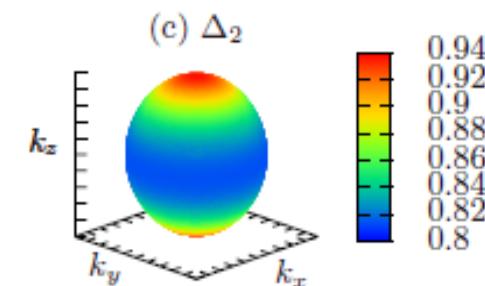
# Energy Gap function

Full Gap

spin-singlet intra-orbital

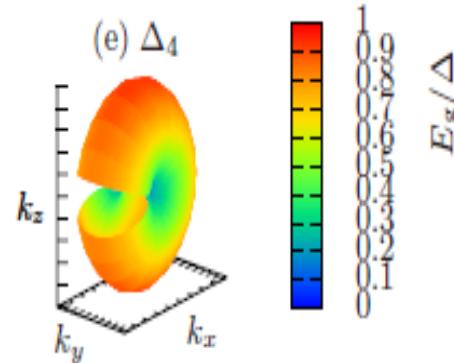
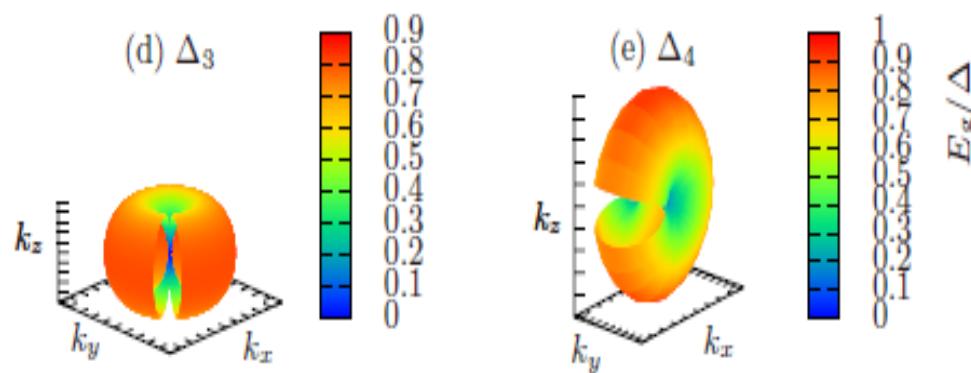


spin-triplet inter-orbital  
spatial inversion odd



Point Node

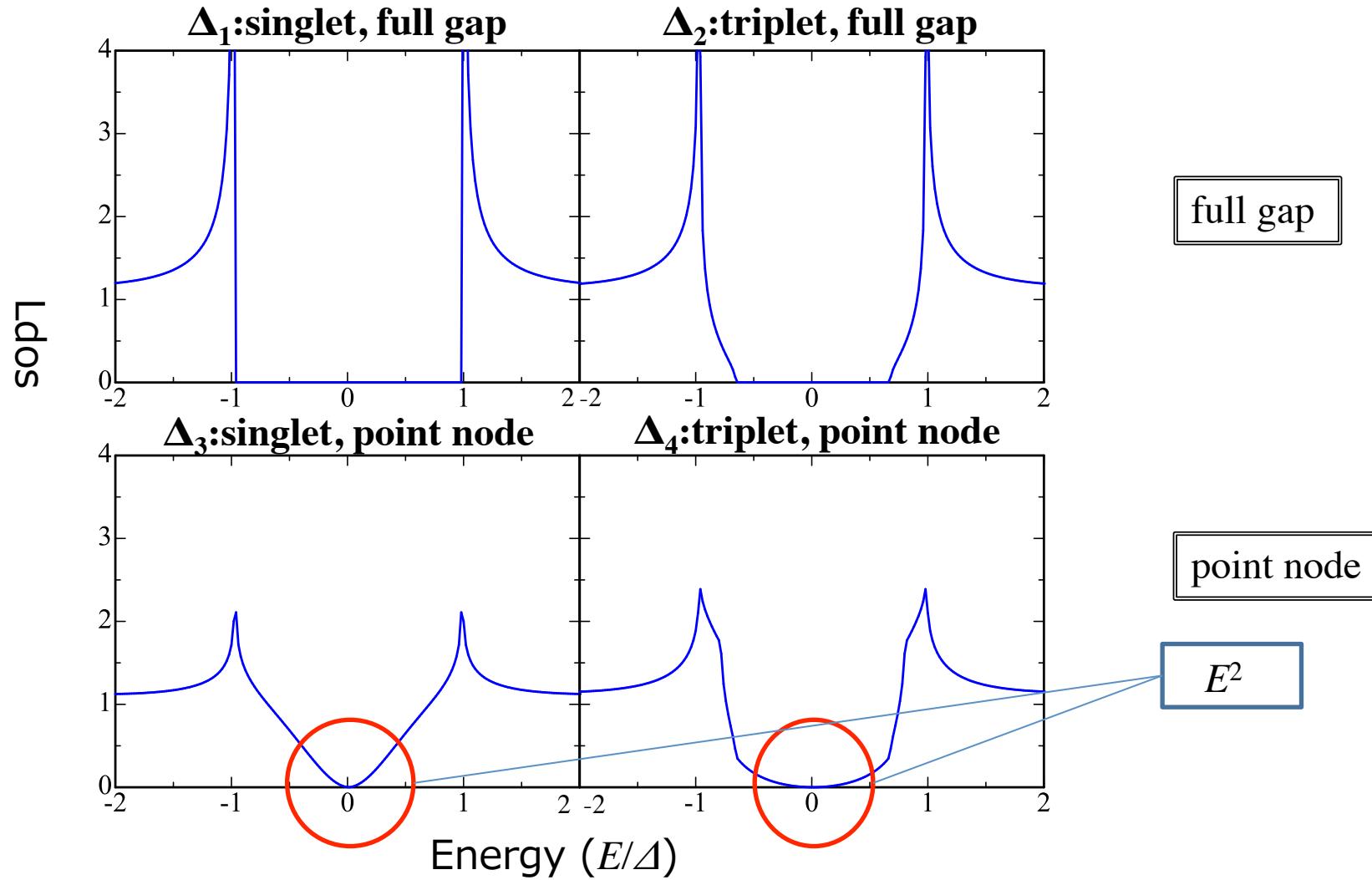
spatial inversion odd



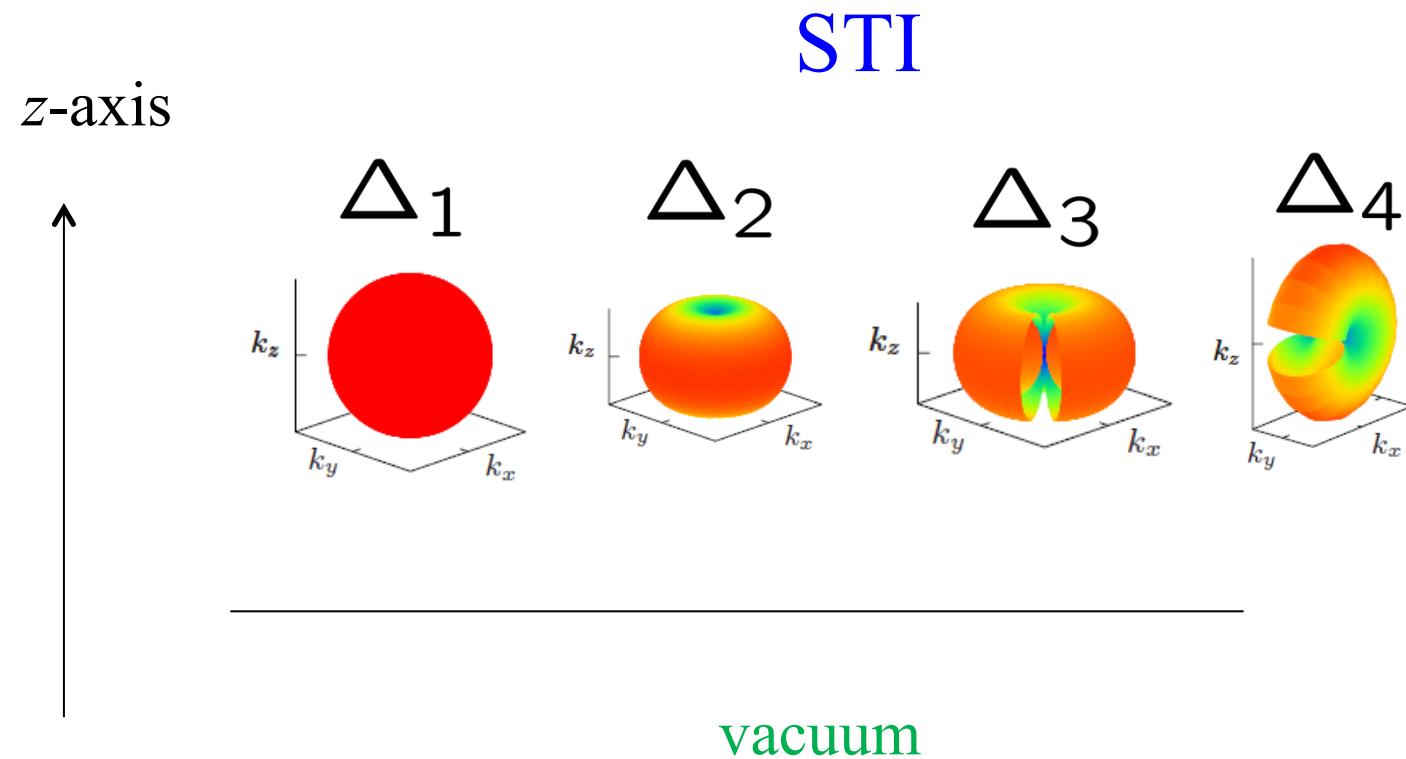
Fu and Berg, Phys. Rev. Lett. 105 097001(2010)

Yamakage et al., PRB Rapid (2011)

# Bulk local density of state



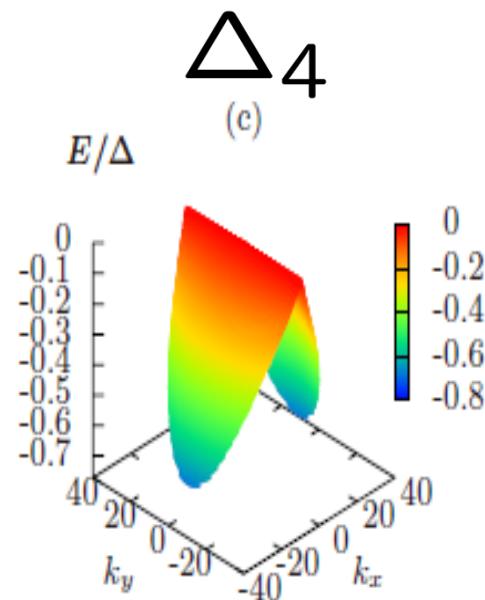
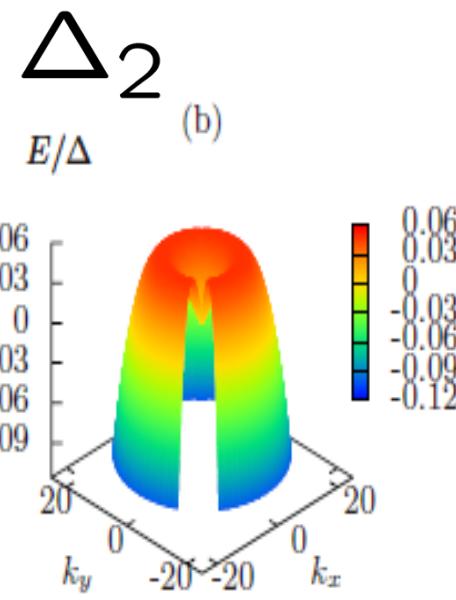
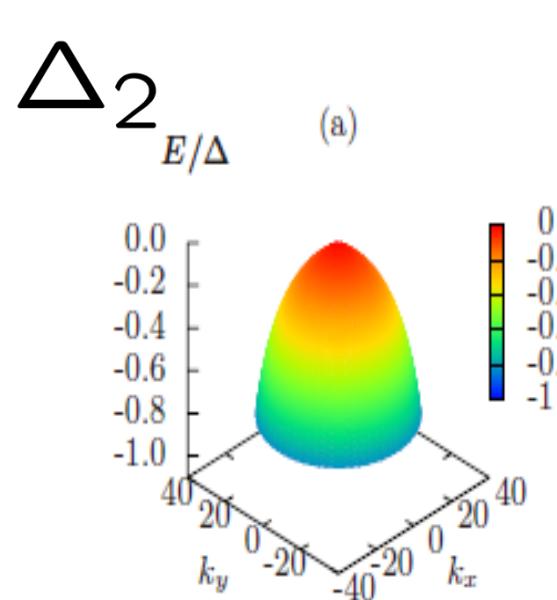
# Surface state generated at $z=0$



STI (Superconducting topological insulator)

# Dispersions of Andreev bound state

## spin-triplet inter-orbital spatial inversion odd-parity



Normal Cone

(Only positive spin helicity  
 $k_x s_y - k_y s_x = +k$  states  
 are shown.)

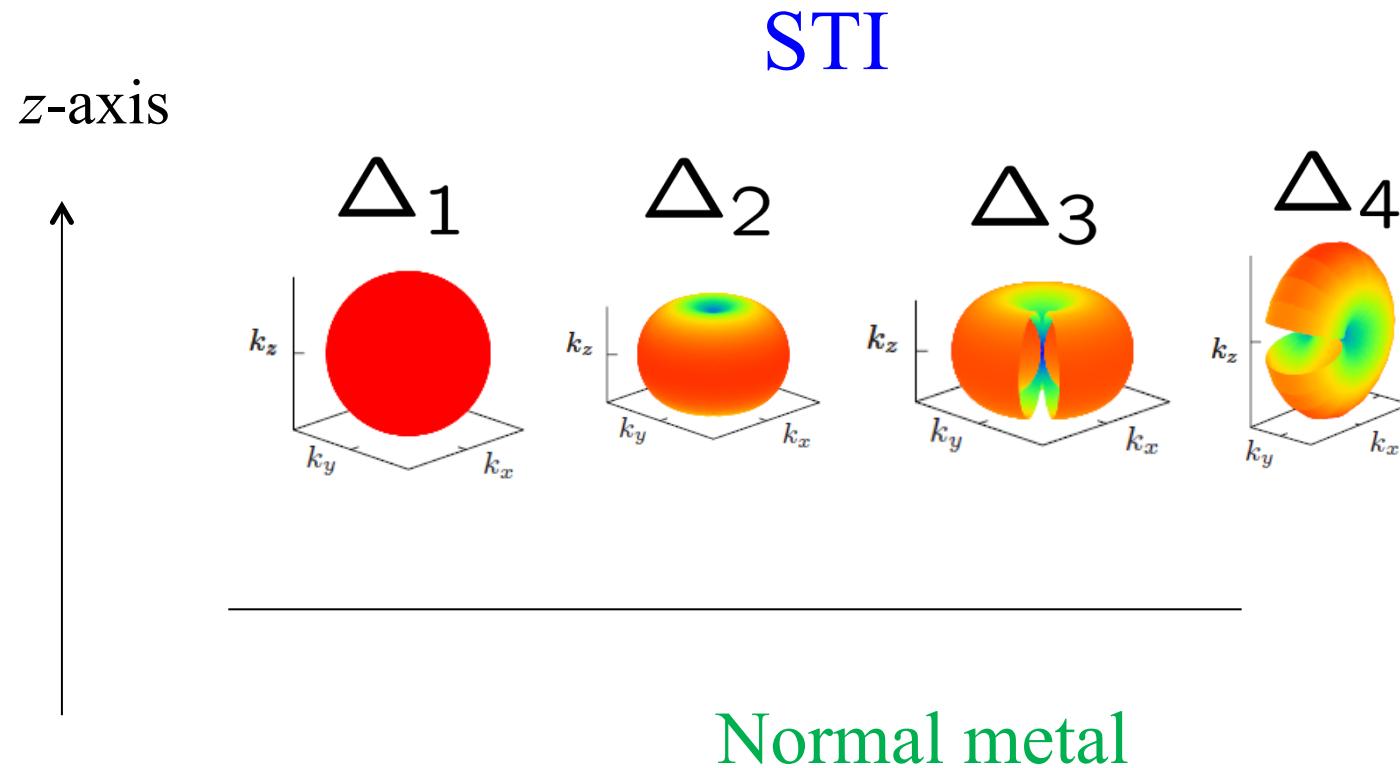
Caldera Cone

(solution of confinement condition  $\psi(z=0)=0$ )

Deformed Cone

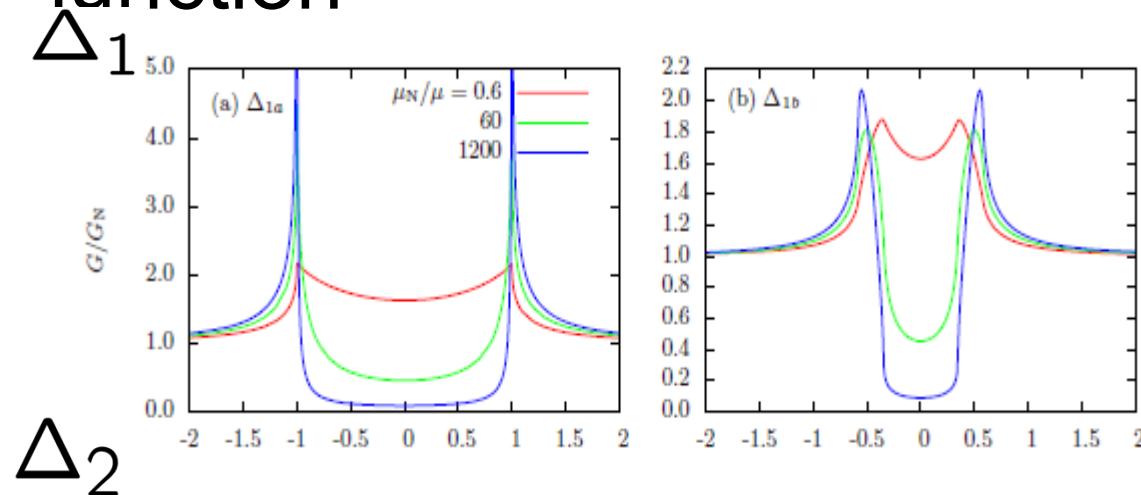
(Only negative energy  
 states are shown.)

# Charge transport in normal metal / STI junctions

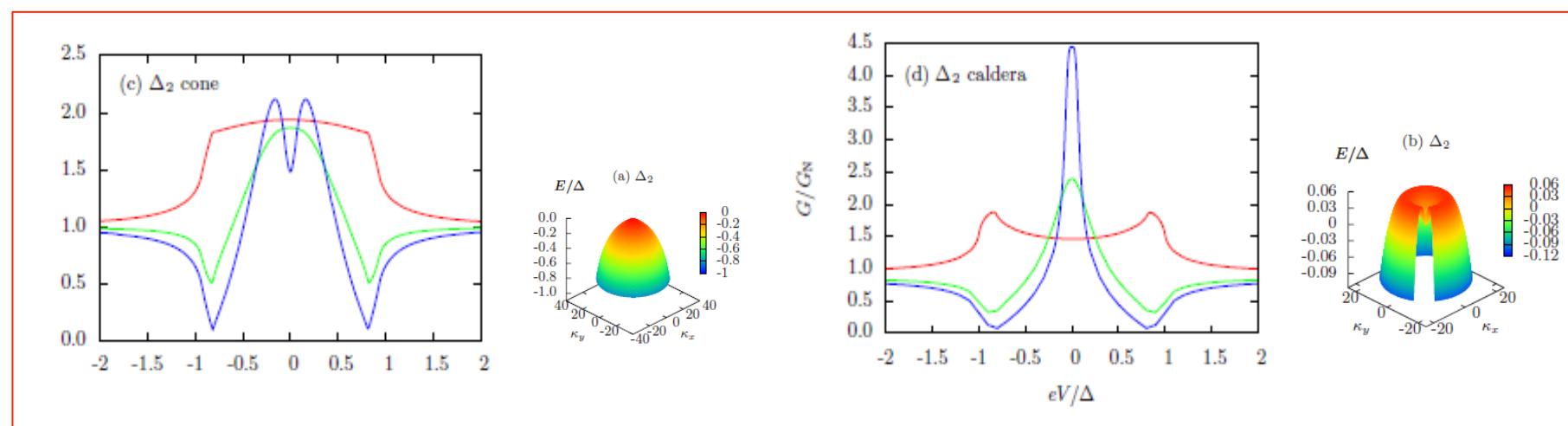


STI (Superconducting topological insulator)

# Tunneling conductance between normal metal / superconducting topological insulator junction



Similar to conventional spin-singlet s-wave superconductor

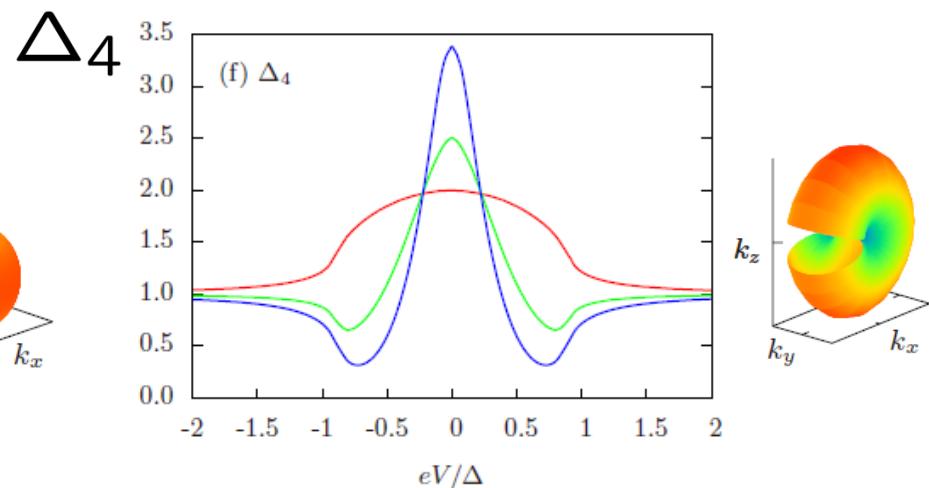
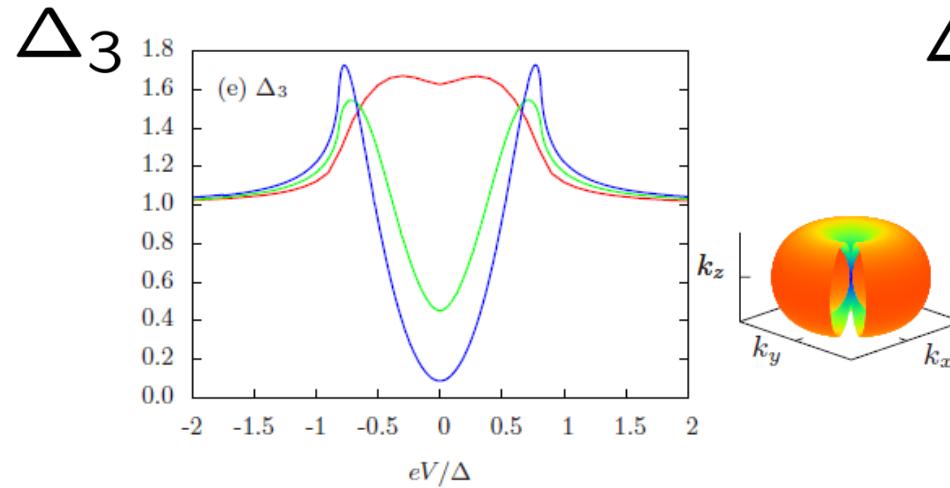


**Zero bias conductance peak is possible even for  $\Delta_2$  case with full gap**

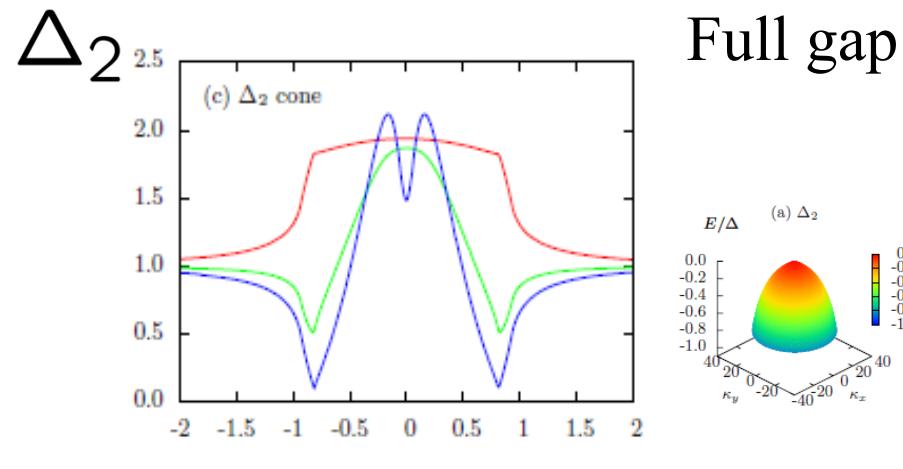
# Conductance between normal metal / STI junction

(Spatial inversion odd-parity)

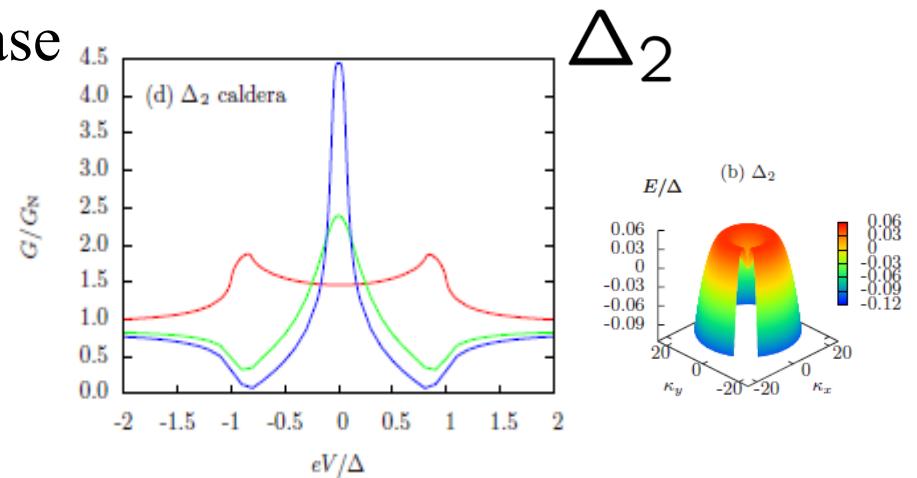
Point node case



Tunneling conductance strongly depends on the direction of nodes.



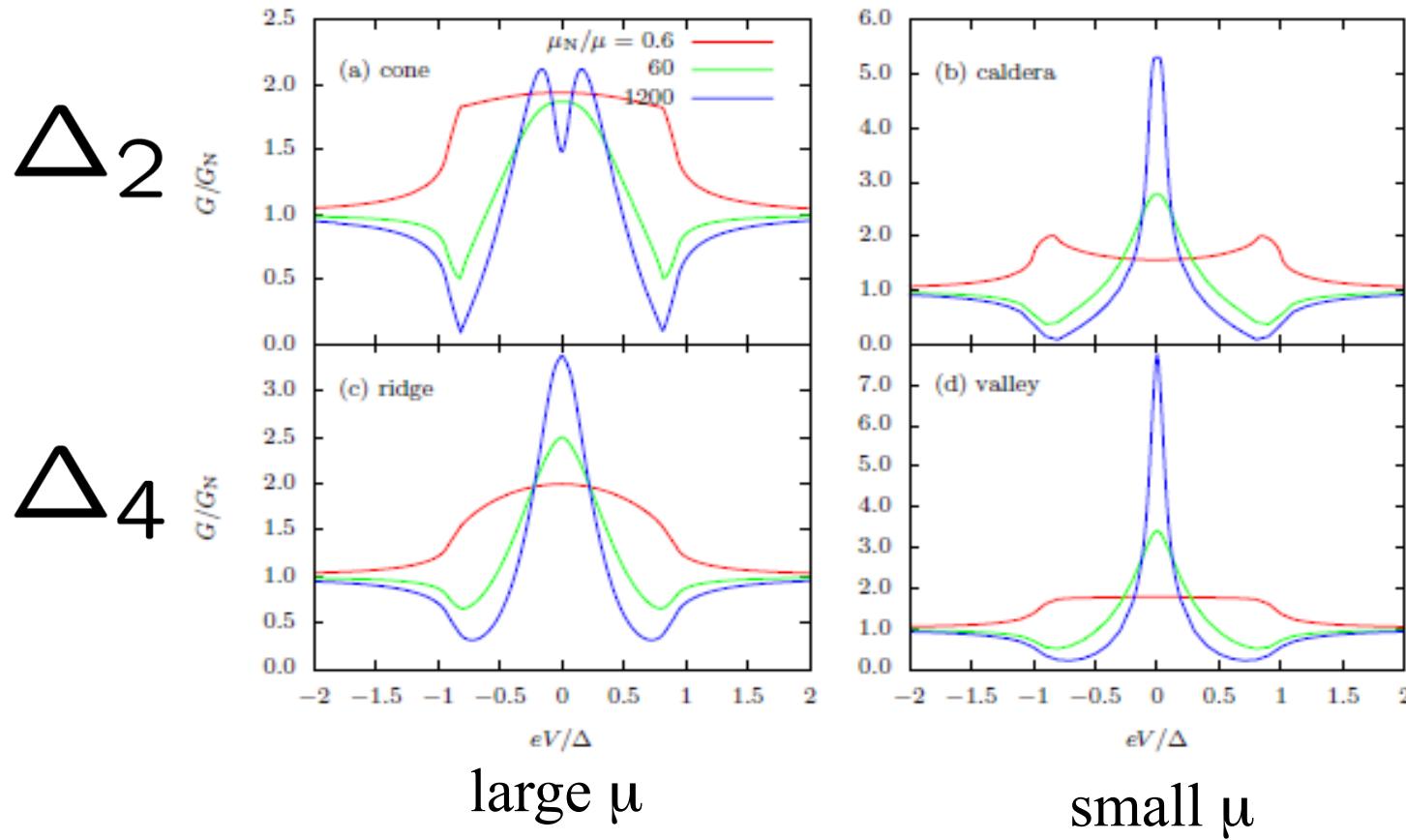
Full gap case



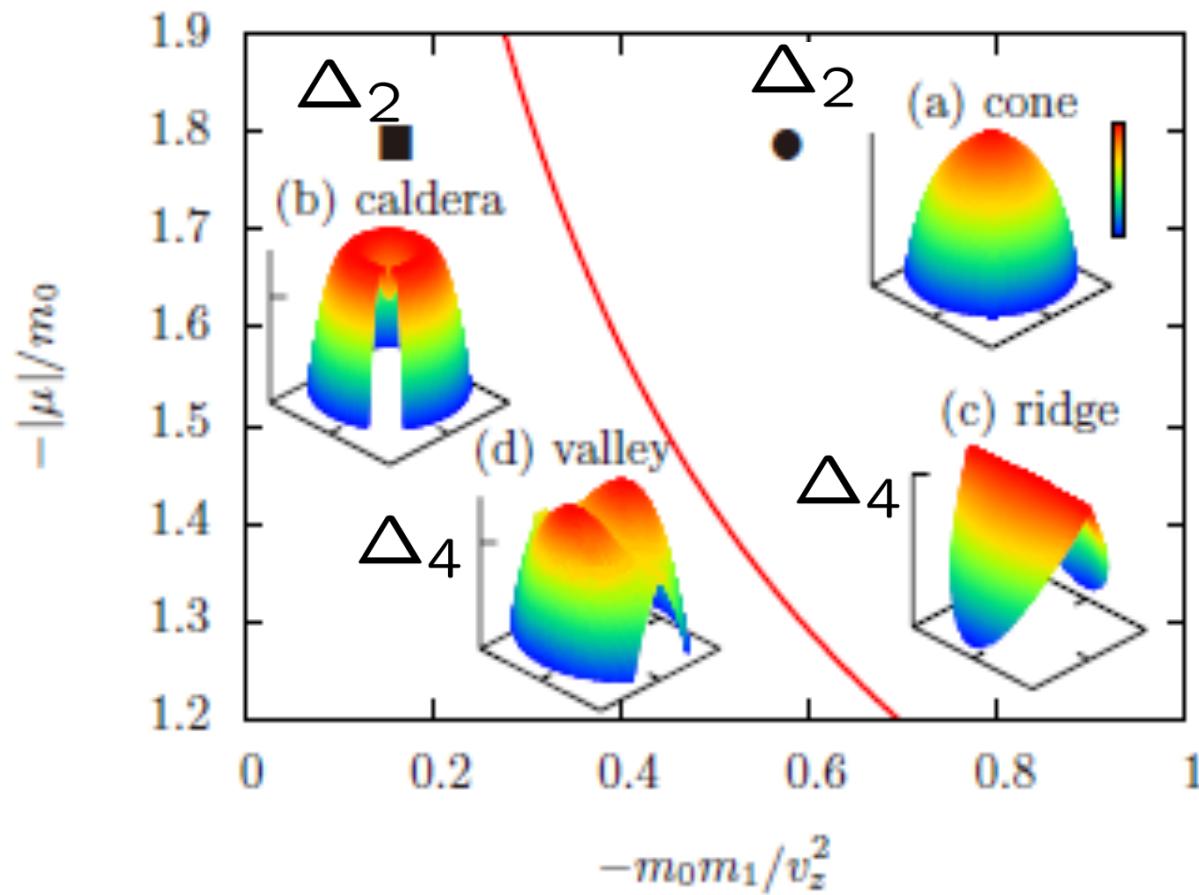
# Tunneling conductance with ABS

Andreev bound state (Majorana Fermion)

**spin-triplet inter-orbital spatial inversion odd-parity**



# Structural transition of the energy dispersion of Andreev bound state

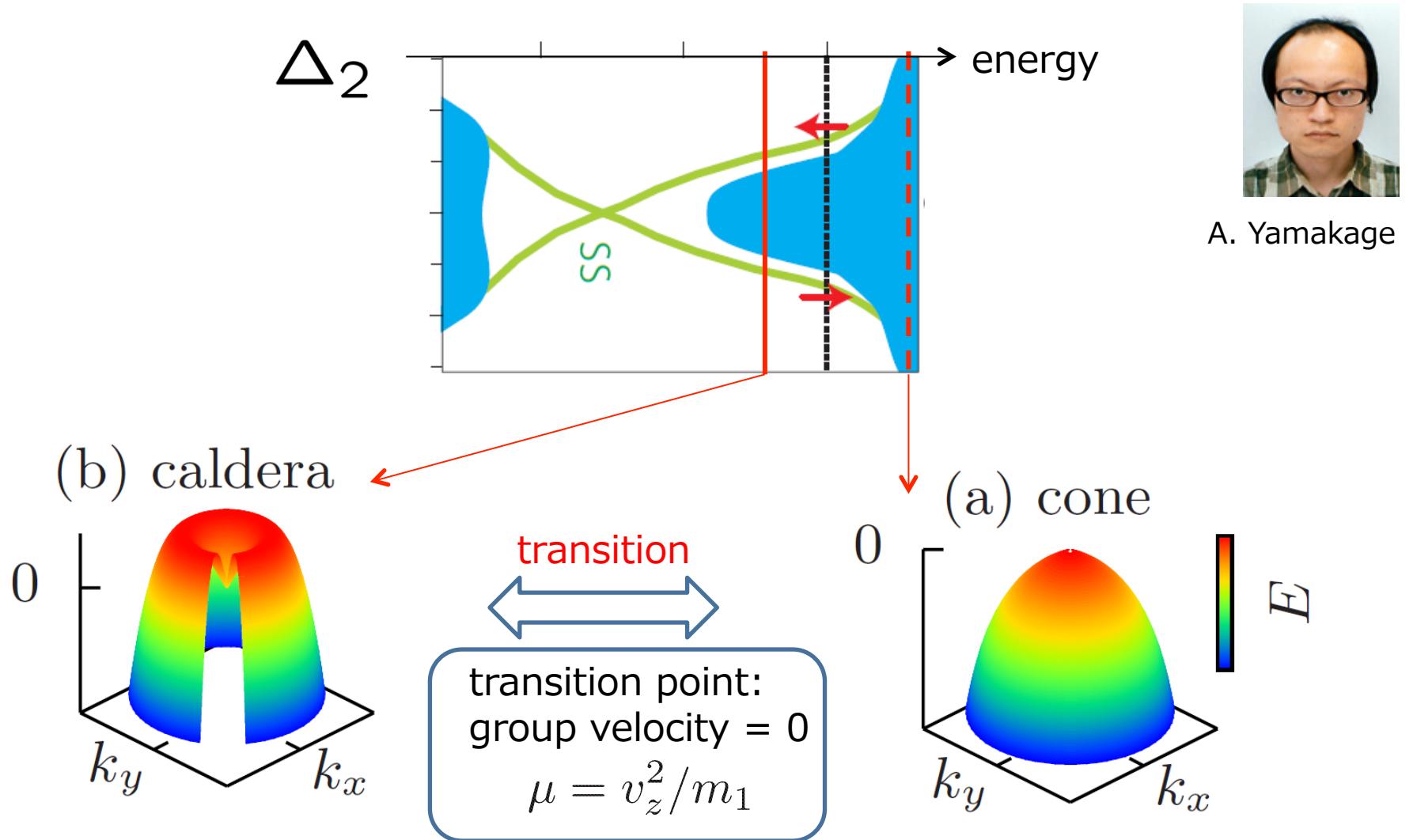


Transition line       $\mu^2 = -m_0 v_z^2 / m_1$



Yamakage

# Structural transition of the dispersion of ABS



L. Hao and T. K. Lee, PRB '11    T. H. Hsieh and L. Fu, PRL '12  
A. Yamakage, K. Yada, M. Sato, and Y. Tanaka, PRB 2012

## Summary (1)

### Theory of tunneling spectroscopy of superconducting topological insulators

1.  $\Delta_2$  and  $\Delta_4$  are consistent with point-contact experiment by Ando's group.
2. Zero-bias conductance peak is possible even in full-gap topological 3d superconductors, differently from the case of BW states.
3. This originates from the structural transition of energy dispersion of ABS.

# Summary of the Topological natures of four pairings

Pair potential	Irreducible representation	spin	orbital	Gap structure	Parity (spatial inversion)	Topological
$\Delta_1 = \Delta$	$A_{1g}$	Singlet	intra	isotropic full gap	even	No
$\Delta_2 = \Delta \sigma_y s_z$	$A_{1u}$	triplet	inter	anisotropic full gap	odd	DIII Z
$\Delta_3 = \Delta \sigma_z$	$A_{2u}$	singlet	intra	Point node ( $z$ -direction)	odd	DIII $Z_2$
$\Delta_4 = \Delta \sigma_y s_x$	$E_u$	triplet	inter	Point node ( $z$ -direction)	odd	DIII $Z_2$

Supplementary materials in  
S. Sasaki et al PRL 107 217001 (2011)

# Current status of tunneling experiments

## **Consistent with Ando's group with ZBCP**

- G. Koren, et al, Phys. Rev. B 84, 224521 (2011).
- T. Kirzhner, et. al, Phys. Rev. B 86, 064517 (2012).
- G. Koren and T. Kirzhner, Phys. Rev. B 86, 144508 (2012).

## **Contradict with Ando's group with full gap (STM)**

- N. Levy, et al, Phys. Rev. Lett. 110 117001 (2013)

Composition and crystal structures of the actual samples have not fully clarified yet.

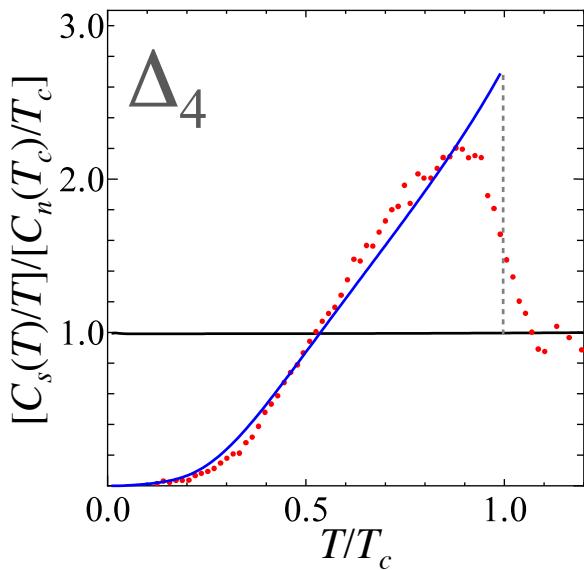
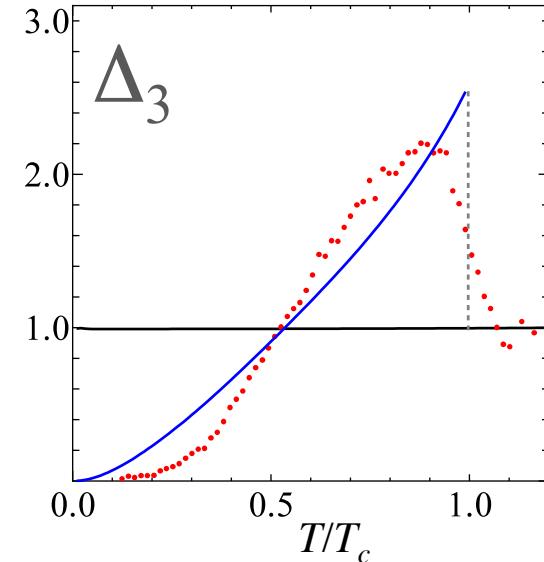
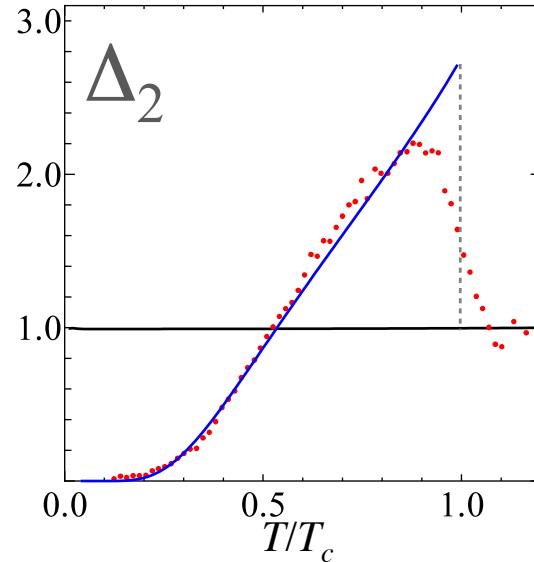
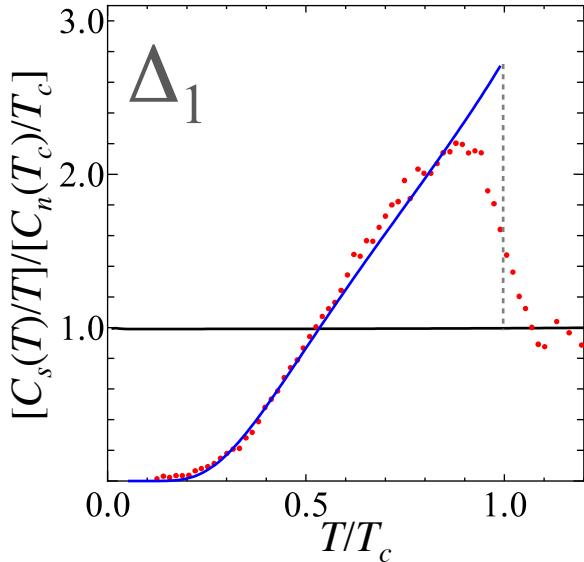


We must need further experimental research.  
Theoretical works in bulk properties become important.

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- (4)Spin susceptibility and specific heat
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# Temperature dependence of specific heat



— calculation

● Experimental results in Ando's group

M. Kriener *et al.*, PRL **106**, 127001 (2011).

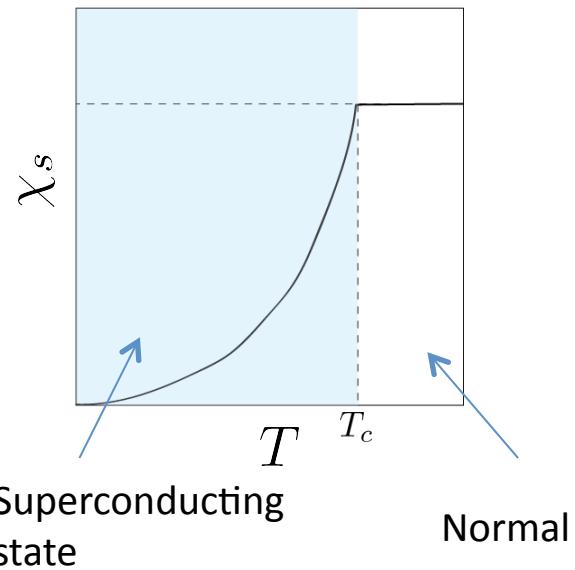
Experimental data can be fitted for  $\Delta_1$ ,  $\Delta_2$ , and  $\Delta_4$  pairings.

$\Delta_3$  is not consistent with experiment.

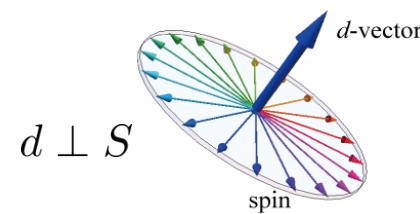
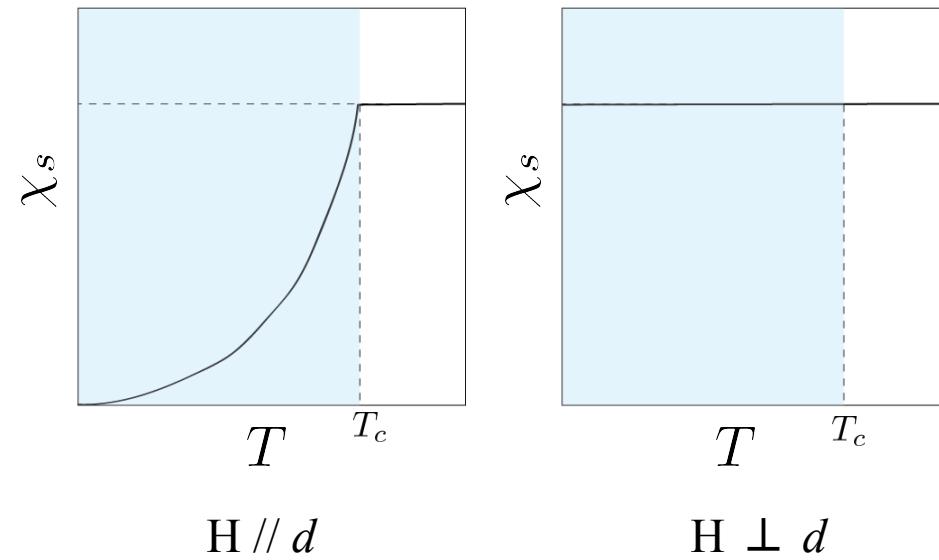
# Temperature dependence of spin-susceptibility

## Standard case

Spin-singlet pairing



Spin-triplet pairing



In the actual  $\text{Cu}_x\text{Bi}_2\text{Se}_3$ , the situation becomes complex due to strong spin-orbit coupling.

# Spin susceptibility of superconducting topological insulator Cu<sub>x</sub>Bi<sub>2</sub>Se<sub>3</sub>

$$\chi_i = -\mu_B^2 \lim_{\mathbf{q} \rightarrow 0} \frac{1}{V} \sum_{\mathbf{k}\alpha\beta\mu} \frac{f(E_\alpha(\mathbf{k})) - f(E_\beta(\mathbf{k} + \mathbf{q}))}{E_\alpha(\mathbf{k}) - E_\beta(\mathbf{k} + \mathbf{q}) + i0} \\ \times \langle \alpha | s_i | \beta \rangle \langle \beta | \frac{g_{i\mu}}{2} s_i \sigma_\mu | \alpha \rangle.$$

We calculate spin susceptibility for four possible pairing states.

With spin-orbit (SO) Coupling

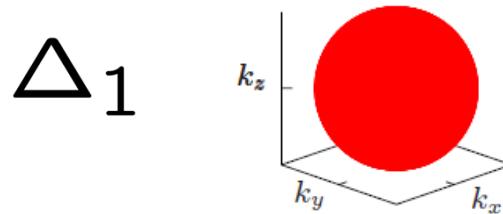
$$H_0(\mathbf{k}) = m\sigma_x + v(k_x\sigma_z s_y - k_y\sigma_z s_x) + v_z k_z \sigma_y$$

Without spin-orbit (SO) coupling

$$H_0(\mathbf{k}) = m\sigma_x + v(k_x\sigma_z s_y - k_y\sigma_z s_x) + v_z k_z \sigma_y$$

Spin orbit coupling term  $\longrightarrow 0$

# Calculated spin-susceptibility (1)

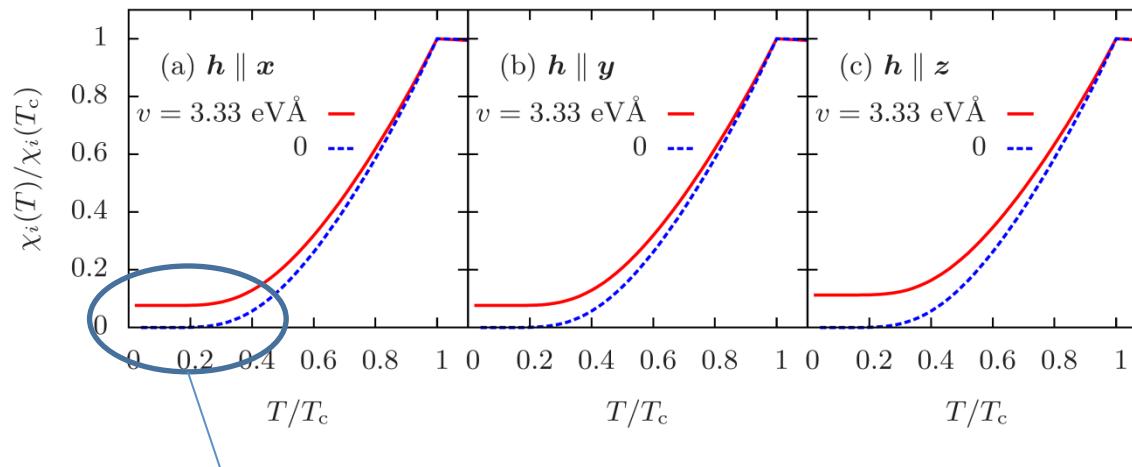


Spin-singlet intra-orbital spatial inversion even

Similar to conventional spin-singlet pairing

— with SO

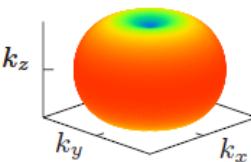
- - - without SO



Due to the Van Vleck susceptibility,  $\chi$  does not become zero even at  $T=0$ .

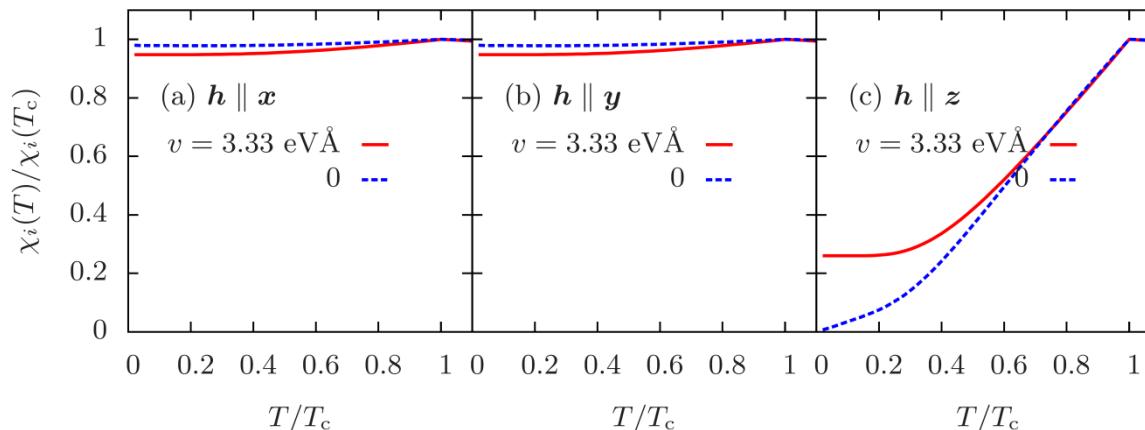
# Calculated spin-susceptibility (2)

$\Delta_2$



— with SO  
- - without SO

Spin-triplet inter-orbital spatial inversion odd



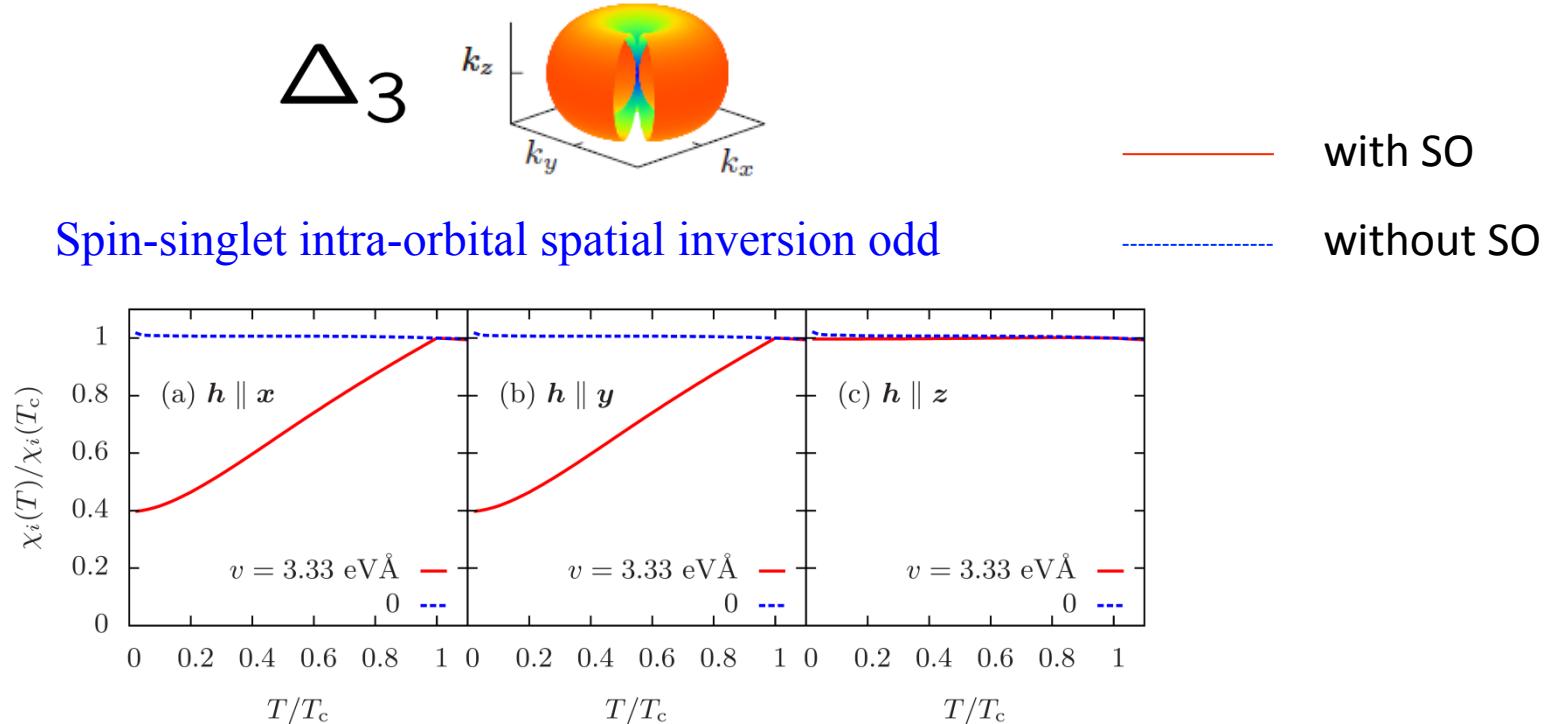
Susceptibility decreases when the magnetic field is along the z-direction.

$$\mathbf{d} = \Delta(0, 0, \sigma_y) \quad (\text{orbital basis})$$



$$\tilde{\mathbf{d}}(\mathbf{k}) = \Delta \left( \frac{v k_x}{m_0}, \frac{v k_y}{m_0}, \frac{v_z k_z}{|m_0|} \tilde{\sigma}_z - \text{sgn}(m_0) \tilde{\sigma}_y \right) \quad \text{band basis}$$

# Calculated spin-susceptibility (3)

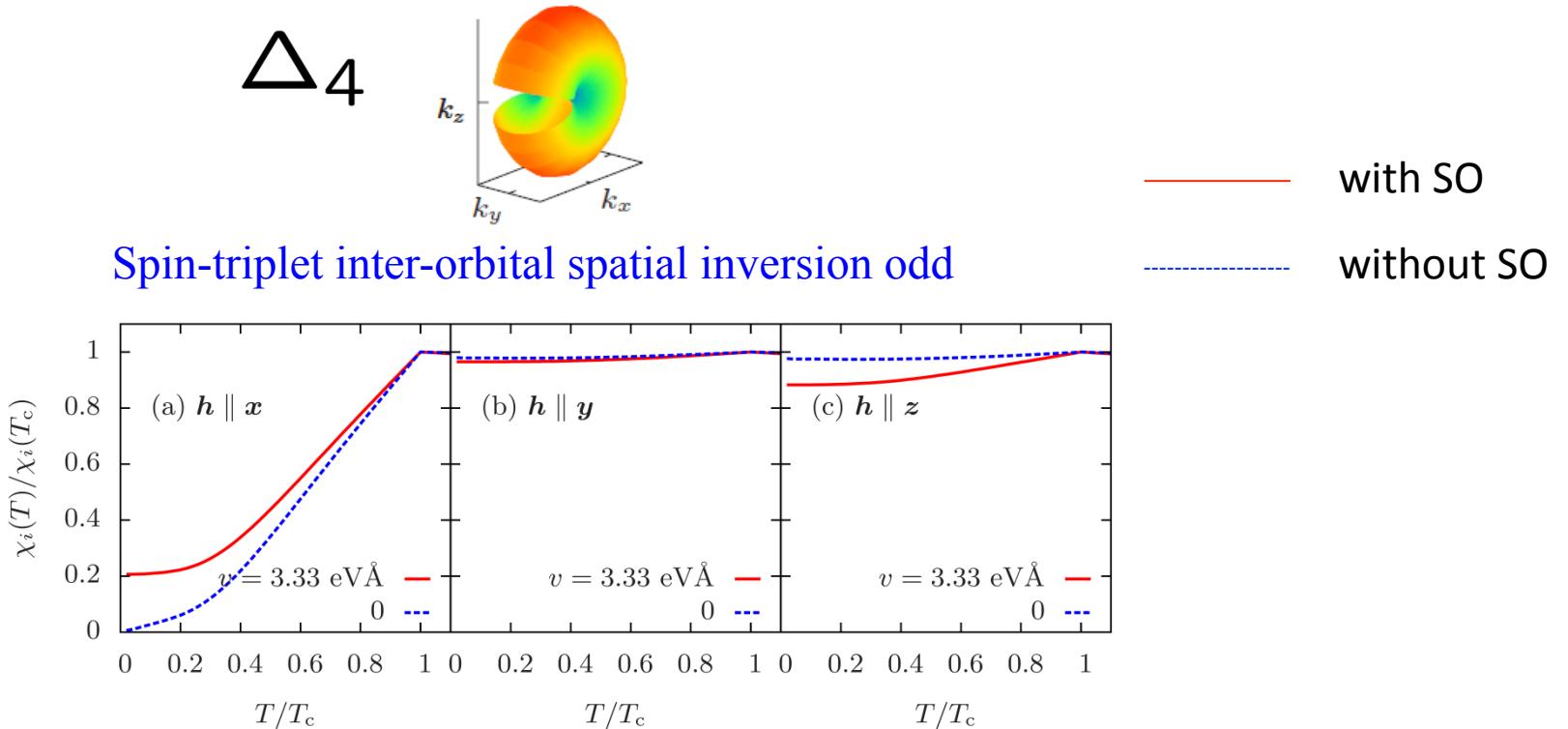


Susceptibility decreases when the magnetic field is along the xy-plane consistent with the direction of d-vector in the band basis.

spin-singlet (orbital basis)

band basis       $\tilde{d}(\mathbf{k}) = \Delta \tilde{\sigma}_z \left( -\frac{vk_y}{|m_0|}, \frac{vk_x}{|m_0|}, 0 \right)$

# Calculated spin-susceptibility (4)



Susceptibility decreases seriously when the magnetic field is along the x-direction.

orbital basis       $\mathbf{d} = \Delta (\sigma_y, 0, 0)$

band basis       $\tilde{\mathbf{d}}(\mathbf{k}) = \Delta \left( \frac{v_z k_z}{|m_0|} \tilde{\sigma}_z - \tilde{\sigma}_y, 0, -\frac{v k_x}{m_0} \right)$



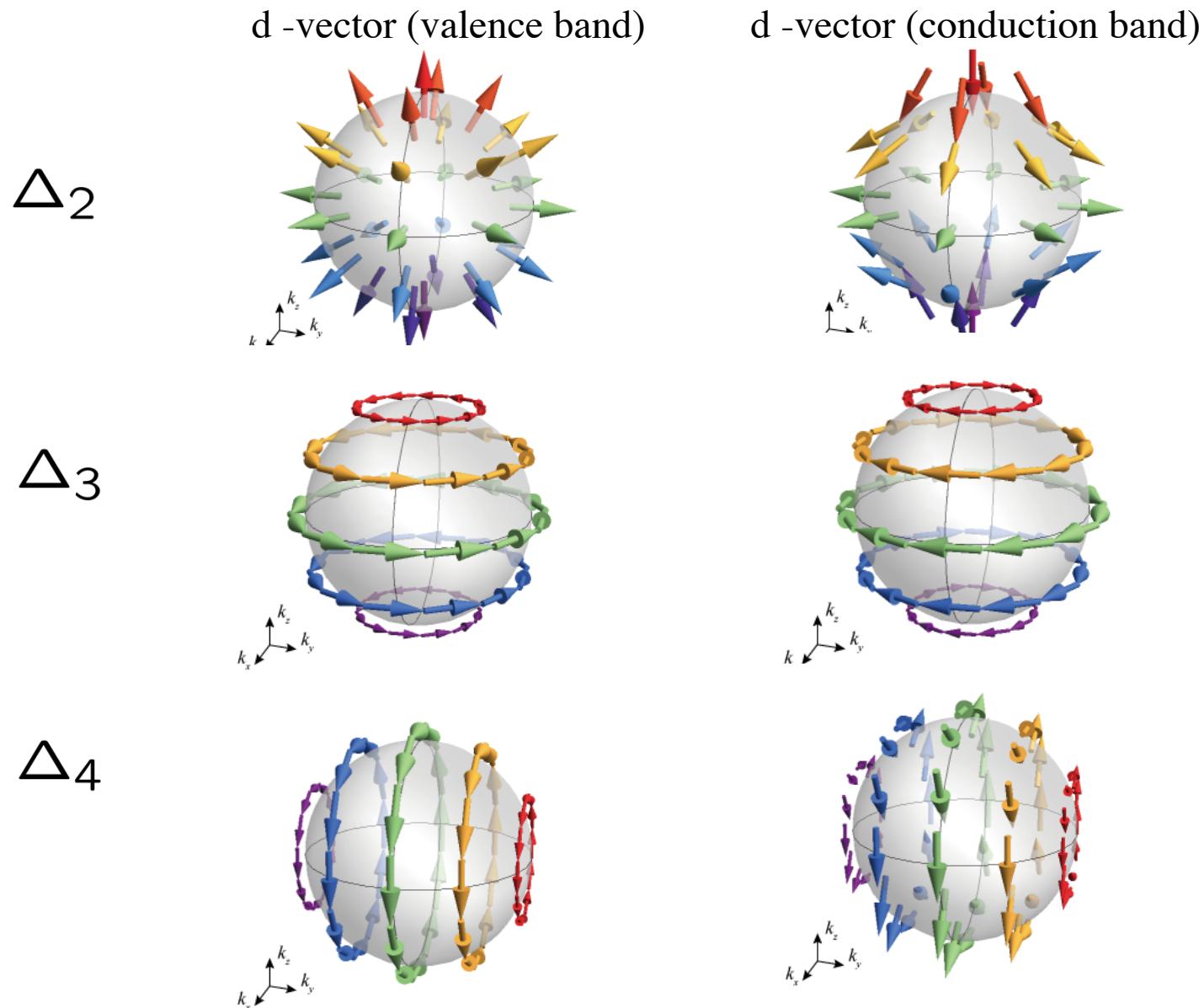
Hashimoto

## Summary (2)

	Rep.	Gap structure	Specific heat	Andreev bound state (xy-plane)	Spin susceptibility		
					$\chi_x$	$\chi_y$	$\chi_z$
$\Delta_1$	$A_{1g}$	Isotropic full gap	Yes	No	↖	↖	↖
$\Delta_2$	$A_{1u}$	Anisotropic full gap	Yes	Yes	—	—	↖
$\Delta_3$	$A_{2u}$	Point nodes at pole	No	No	↖	↖	—
$\Delta_4$	$E_u$	Point nodes on equator	Yes	Yes	↖	—	—

- We find that the temperature dependence of specific heat and the susceptibility are different in each pairing symmetry.
- It is possible to determine pairing symmetry only from bulk quantities.
- We think  $\Delta_2$  and  $\Delta_4$  are most probable candidates consistent with specific heat and point contact experiments by Ando's group.

# Direction of d-vector in the band basis



# Contents of our talk

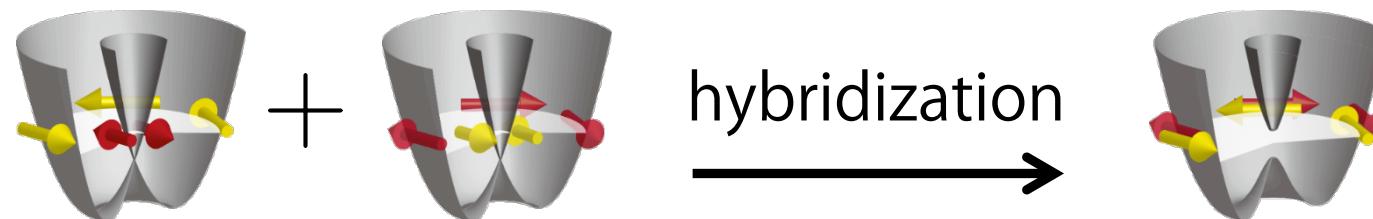
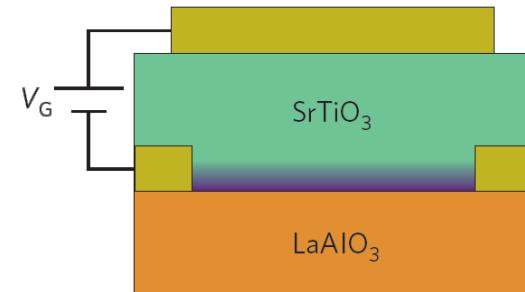
- (1) What is superconducting topological insulator
- (2) Andreev bound state and quasi particle tunneling
- (3) Josephson current
- (4) Spin susceptibility and specific heat
- (5) Relevant Rashba superconductor system

# DIII superconductor from conventional systems

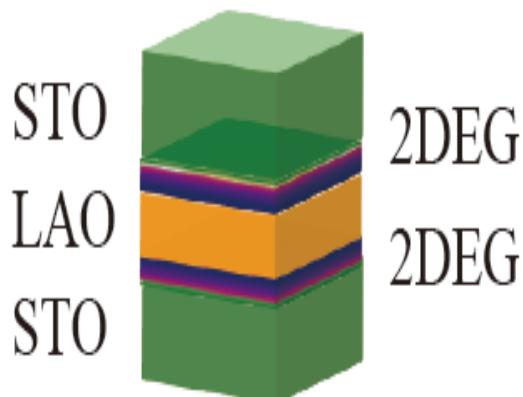
## Using Interface superconductivity

### Interface of transition metal oxides

- 2d electron gas Ohtomo & Hwang Nature 2004
- superconductivity Reyren *et al.* Science 2007
- tunable Rashba SOI Caviglia *et al.* PRL 2010



**One-dimensional Majorana (Helical)**



$$\Delta_1 = -\Delta_2$$

**Intra-layer pairing with different sign**

Nakosai, Tanaka Nagaosa, PRL(2012)

# Model construction

kinetic Hamiltonian

$$\mathcal{H}_0(\mathbf{k}) = \frac{k^2}{2m} - \varepsilon \sigma_x + \alpha (k_x s_y - k_y s_x) \sigma_z$$

hybridize

: transfer

SOI

: Rashba SOI

$s$  : spin     $\sigma$  : layer

electron density-density interaction

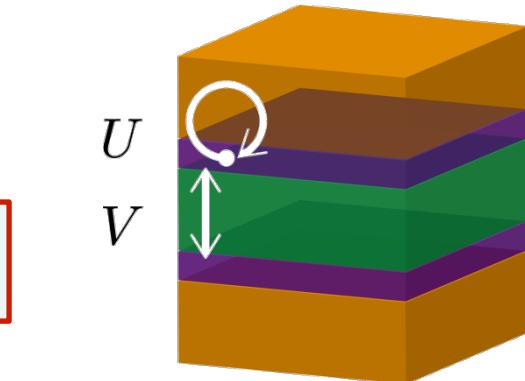
$$\mathcal{H}_{\text{int}}(\mathbf{x}) = -U(n_1^2(\mathbf{x}) + n_2^2(\mathbf{x})) - 2V n_1(\mathbf{x}) n_2(\mathbf{x})$$

intra-layer

inter-layer

Bogoliubov de-Gennes Hamiltonian

$$\mathcal{H}_{\text{BdG}} = \begin{pmatrix} \mathcal{H}_0 - \mu & \Delta \\ \Delta & -\mathcal{H}_0 + \mu \end{pmatrix}$$



cf. Fu and Berg PRL 2010

S. Nakosai , Y . Tanaka and N. Nagaosa PRL(2012)

# Pair potentials

As compared to 3-d superconducting topological insulator  $\text{Cu}_x\text{Bi}_2\text{Se}_3$ , the **orbital index** changes into **layer index**.

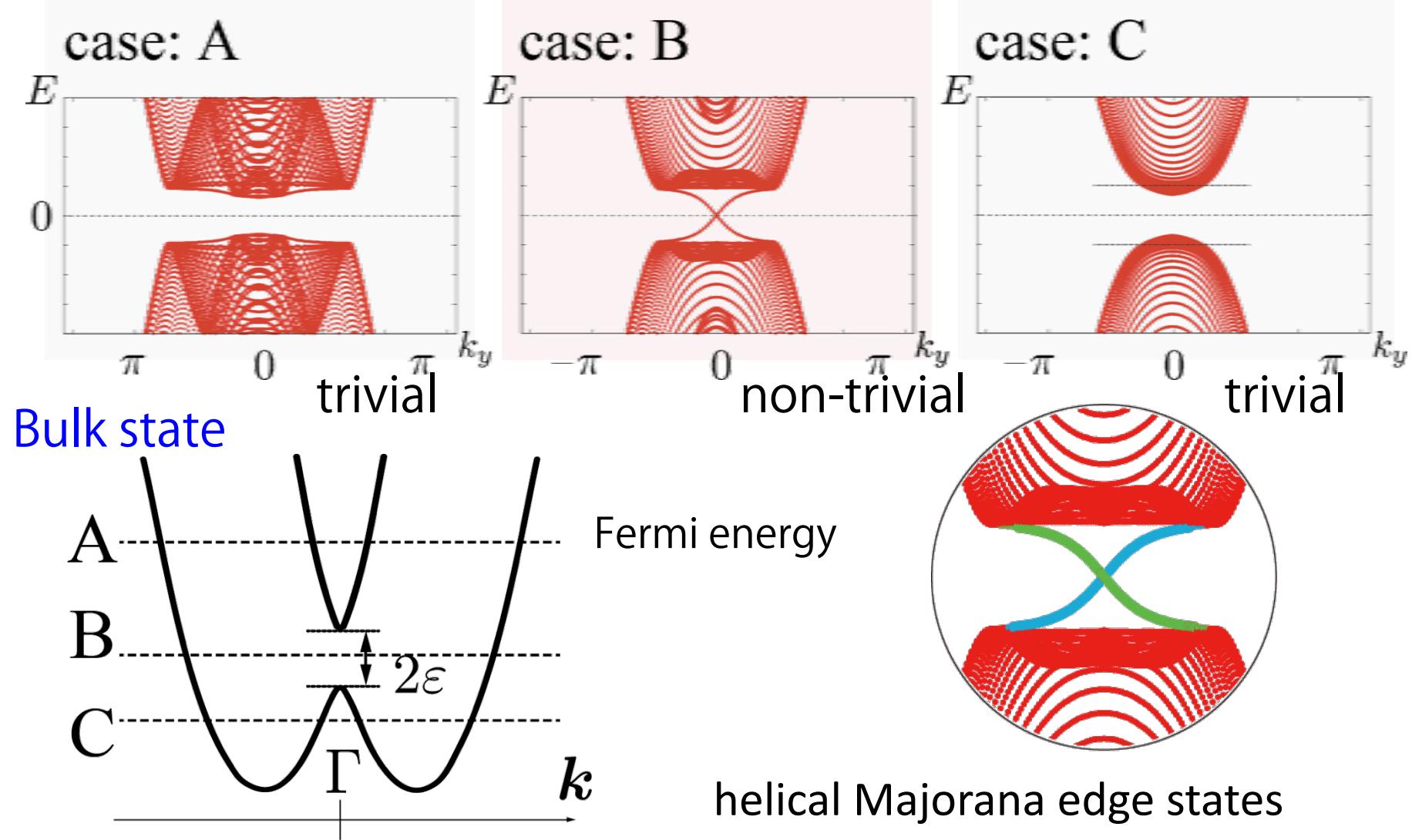
parity under an  
inversion operation

	irreps	matrix	spin	orbital	inversion	gap	topological
$\hat{\Delta}_1$	$A_{1g}$	$I$ $\sigma_x$	singlet	inter	+	full	no
$\hat{\Delta}_2$	$A_{1u}$	$s_z \sigma_y$	triplet	inter	-	full	DIII $Z_2$
$\hat{\Delta}_3$	$A_{2u}$	$\sigma_z$	singlet	intra	-	full	DIII $Z_2$
$\hat{\Delta}_4$	$E_u$	$\begin{pmatrix} s_x \sigma_y \\ s_y \sigma_y \end{pmatrix}$	triplet	inter	-	point node	DIII $Z_2$

Topological superconducting state with  $\Delta_3$  pairing  
 (intra-site inversion symmetry odd) is realized by  
 choosing chemical potential.



S. Nakosai



# Summary (3)

## Topological superconductivity from Rashba system

1. We have proposed a new way to design DIII superconductor in 2D systems.

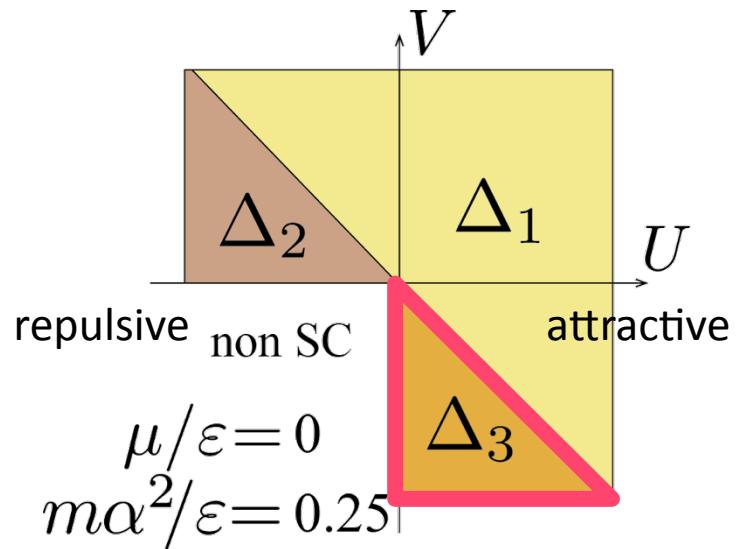
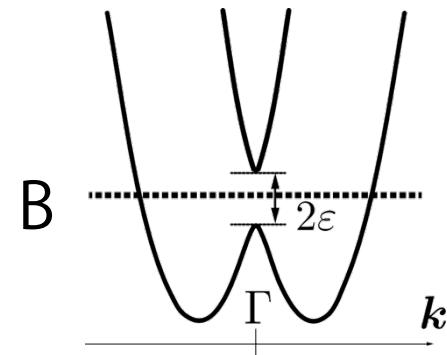
(Bilayer Rashba system realized at the interface of transition metal oxides.)

2. Andreev bound state appears as a helical edge modes without anisotropic pairing.

# Topological SC ?

We set the Fermi energy  
within the hybridization gap.

1. [Fermi level] **OK**



2. [odd parity pairing potential] **OK**

NOTE:

Pairing amplitudes for  $\Delta_2$  and  $\Delta_3$   
are proportional to  $\alpha$ .

SOI-induced SC phases

Unconventional SC phase appears  
in a feasible parameter region.

intra-layer : attractive (phonon mechanism)  
inter-layer : repulsive (Coulomb interaction)