Parity and Pairing Symmetry in Iron-Based Superconductors

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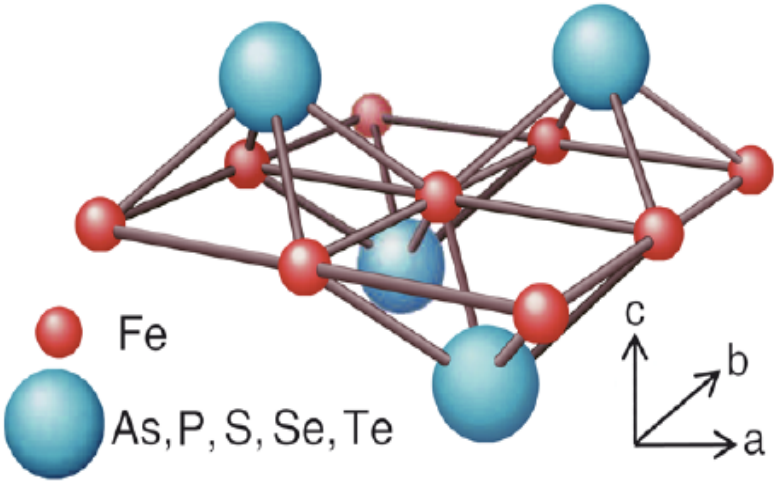
Institute of Physics, CAS



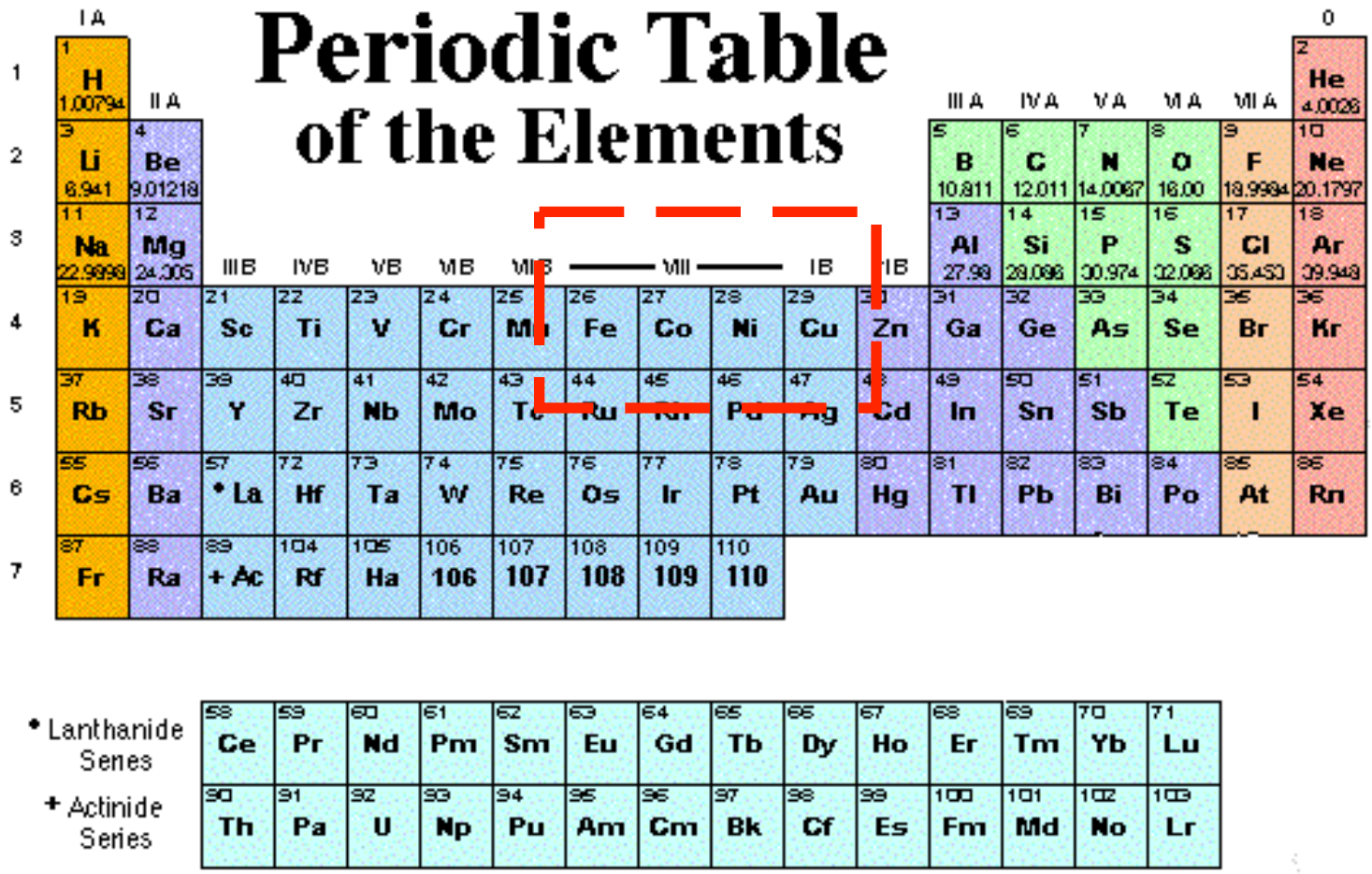
High energy
C.N. Yang & T. D. Lee
Parity unconserved

J.P. Hu, Phys. Rev. X, in Press 1301.6342
N.N. Hao & J.P. Hu, arXiv: 1305.5034
J.P. Hu and N. Hao, Phys. Rev. X, 021009 (2012)

9/3/2013 Long Island, New York

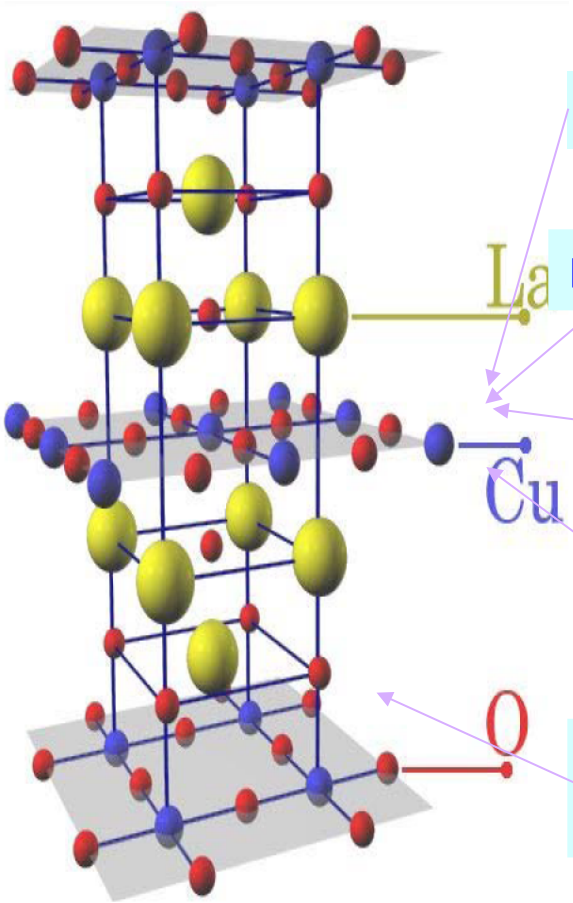
Key Question

- Are the Fe-based superconductors siblings of cuprates?

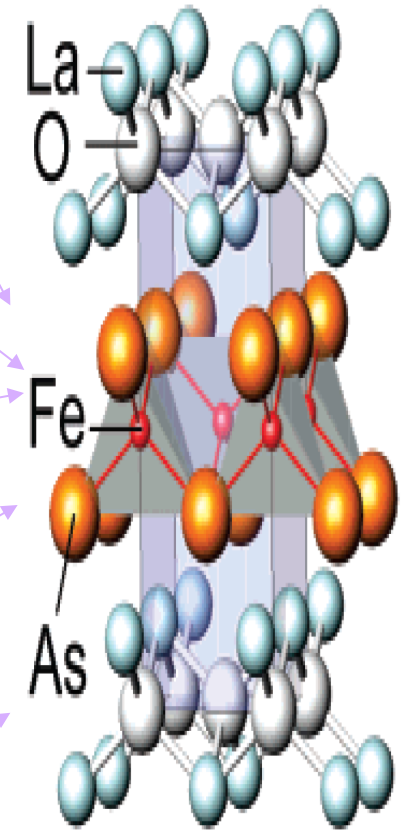


Motivation (I)

- Cuprates ($LaCuO_2$):



- Iron High Tc:



Transition Metal: 3d electron

Layer structure: two dimensions

Magnetic ordered state in parent compounds

Superconductivity induced by doping

Very similar phase diagrams
Very short coherent length

Is the induction method in physics working here?

History Comparison

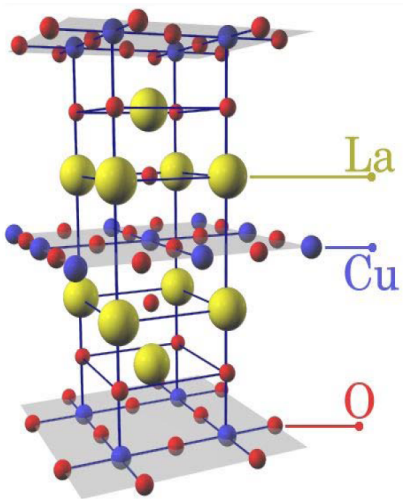
VOLUME 70, NUMBER 10 PHYSICAL REVIEW LETTERS 8 MARCH 1993

Anomalously Large Gap Anisotropy in the *a-b* Plane of $Bi_2Sr_2CaCu_2O_{8+\delta}$

Z.-X. Shen,[(1),(2)] D. S. Dessau,[(1),(2)] B. O. Wells,[(1),(2),(a)] D. M. King,[(2)] W. E. Spicer,[(2)] A. J. Arko,[(3)] D. Marshall,[(2)] L. W. Lombardo,[(1)] A. Kapitulnik,[(1)] P. Dickinson,[(1)] S. Doniach,[(1)] J. DiCarlo,[(1),(2)] A. G. Loeser,[(1),(2)] and C. H. Park[(1),(2)]

[(1)]*Department of Applied Physics, Stanford University, Stanford, California 94305*
[(2)]*Solid State Electronics Laboratory and Stanford Synchrotron Radiation Laboratory, Stanford University, Stanford, California 94305-4055*
[(3)]*Los Alamos National Laboratory, Los Alamos, New Mexico 87545*
(Received 11 November 1992)

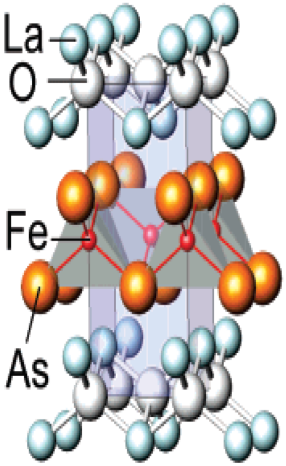
Superconducting gap anisotropy at least an order of magnitude larger than that of the conventional superconductors has been observed in the *a-b* plane of $Bi_2Sr_2CaCu_2O_{8+\delta}$ in angle-resolved photoemission spectroscopy. For samples with T_c of 88 K, the gap size reaches a maximum of approximately 20 meV along the Cu-O bond direction, and a minimum of much smaller or vanishing magnitude 45° away. The experimental data are discussed within the context of various theoretical models. In particular, a detailed comparison with what is expected from a superconductor with a $d_{x^2-y^2}$ order parameter is carried out, yielding a consistent picture.



Discover: 1986

d-wave: 1993

Establish: 2000



Discover: 2008

? –wave: 2013?

Establish: ?

Pairing Symmetry

- black or white
- important to mechanism

Question?

Why is hard to determine the pairing symmetry ?

- Something must be special about the state!

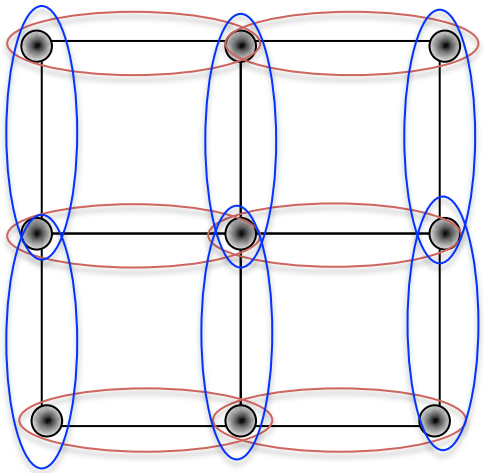
- Why is parity an issue in Iron-Based superconductors?

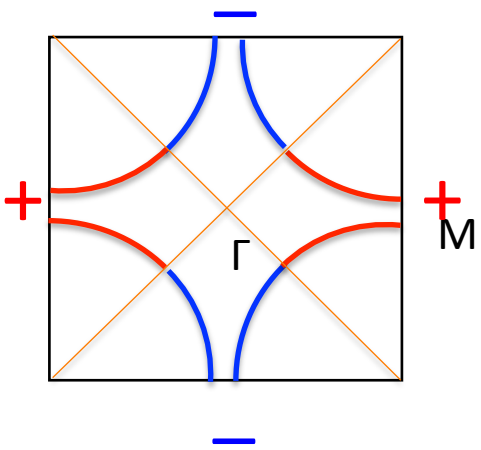
  Even parity vs odd parity spin singlet pairing

- How to test even or odd parity?

- What is possible microscopic mechanism?

d-wave Pairing Symmetry in Curpates





D-wave:

- Group: B1 representation of D_{4h}
- Odd parameter has sign change in both real space and momentum space
- Parity Even: Spin-singlet

Conventional Wisdom from Curpates

Gap Structure:	Sign Change:
• S-wave: Full gap	• In-plane
• D-wave: Gapless Nodes	• Both Reciprocal and real space

Parity and Spin:

- Parity even= Spin singlet, s or d wave
- Parity odd = Spin triplet, p-wave

Parity Operation

$$\Delta(k) = < C_{\uparrow}(k) C_{\downarrow}(-k) > \quad \longleftrightarrow \quad \Delta(-k) = < C_{\uparrow}(-k) C_{\downarrow}(k) >$$

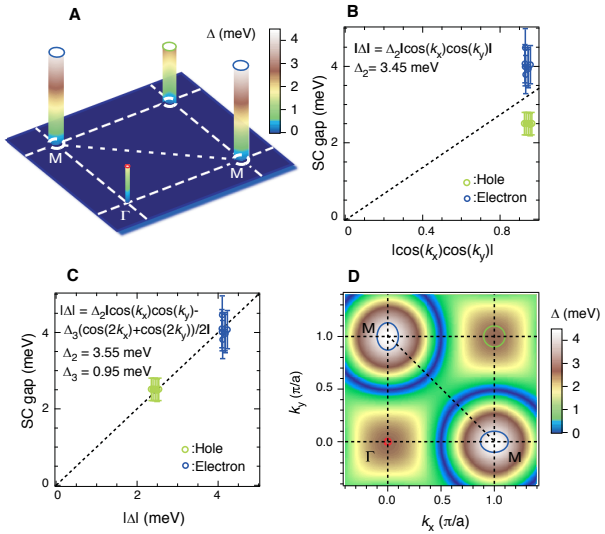
$$\Delta_{even}(k) = < C_{\uparrow}(k) C_{\downarrow}(-k) + C_{\uparrow}(-k) C_{\downarrow}(k) > = < C_{\uparrow}(k) C_{\downarrow}(-k) - C_{\downarrow}(k) C_{\uparrow}(-k) >$$

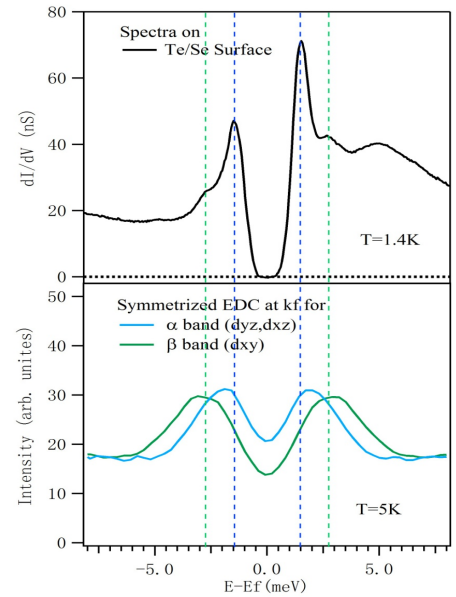
$$\Delta_{odd}(k) = < C_{\uparrow}(k) C_{\downarrow}(-k) - C_{\uparrow}(-k) C_{\downarrow}(k) > = < C_{\uparrow}(k) C_{\downarrow}(-k) + C_{\downarrow}(k) C_{\uparrow}(-k) >$$

Iron-Based Superconductors: Gap structure (I)

$BakFe_2As_2$

H. Ding



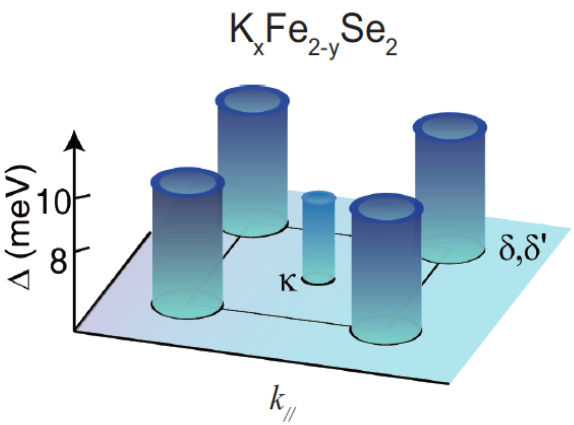


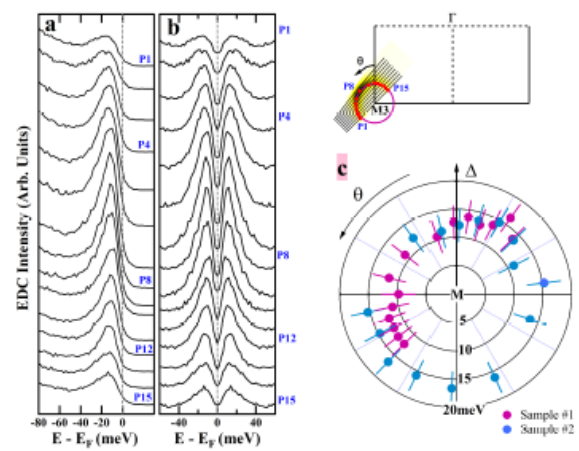
FeSeTe

H.H. Wen
S.H. Pan

KFe_2Se_2

D.L. Feng
H.Ding
X.J. Zhou



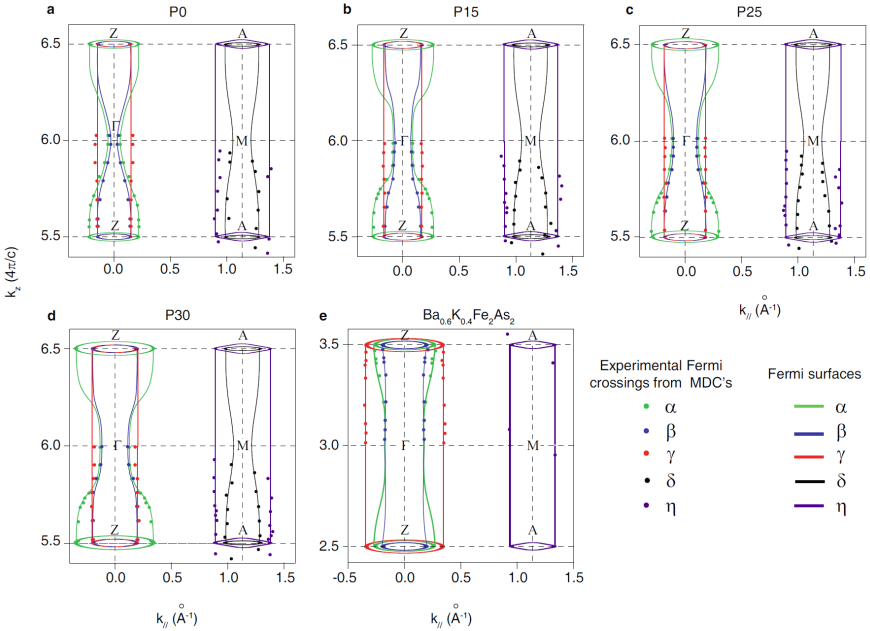


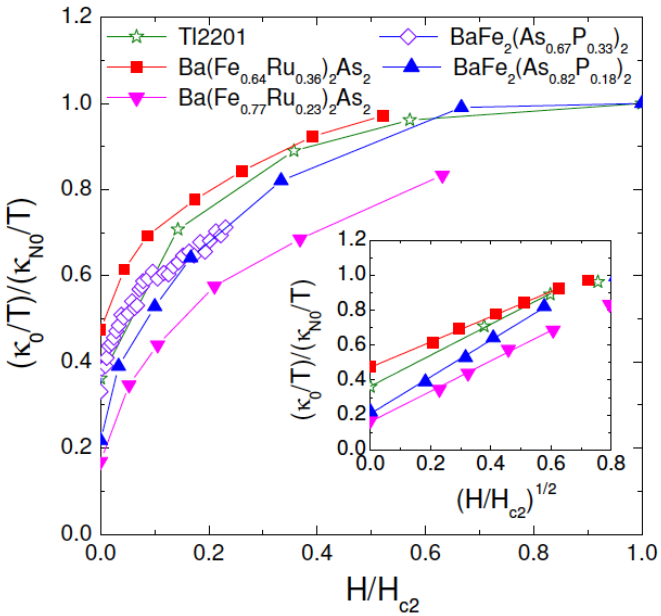
FeSe
Single Layer

X. J. Zhou
X.Q. Kun
D.L. Feng

Full gap structure

Iron-Based Superconductors: Gap structure (II)





$BaFe_2As_{2-x}P_x$

D.L. Feng

S.Y. Li

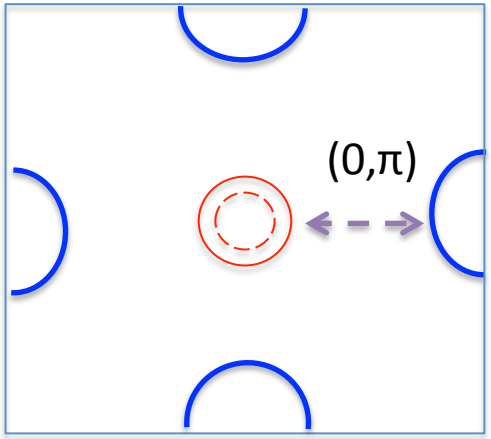
Accidental nodes can be developed in some Fermi surfaces.

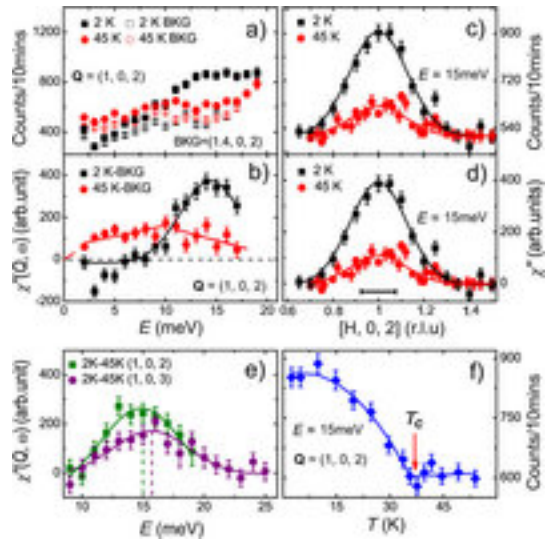
Iron-based superconductors: Sign change evidence (I)

Magnetic Resonance

$BaFe_2As_2$

P.C. Dai
Wei Bao

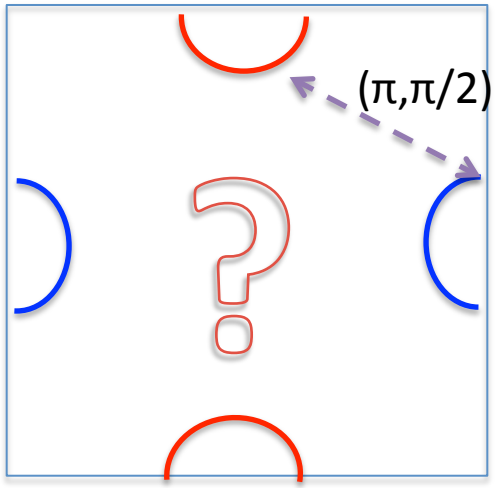


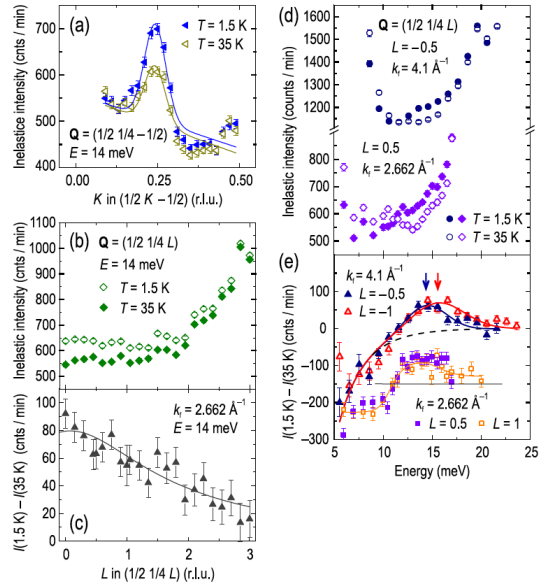


Sign change between Hole and electron Pockets!

KFe_2Se_2

Park et al

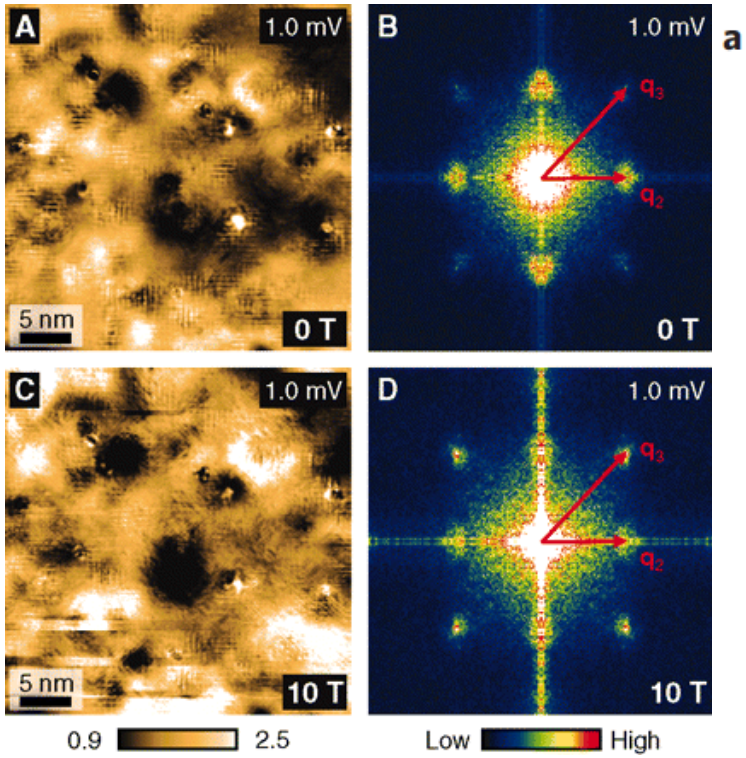


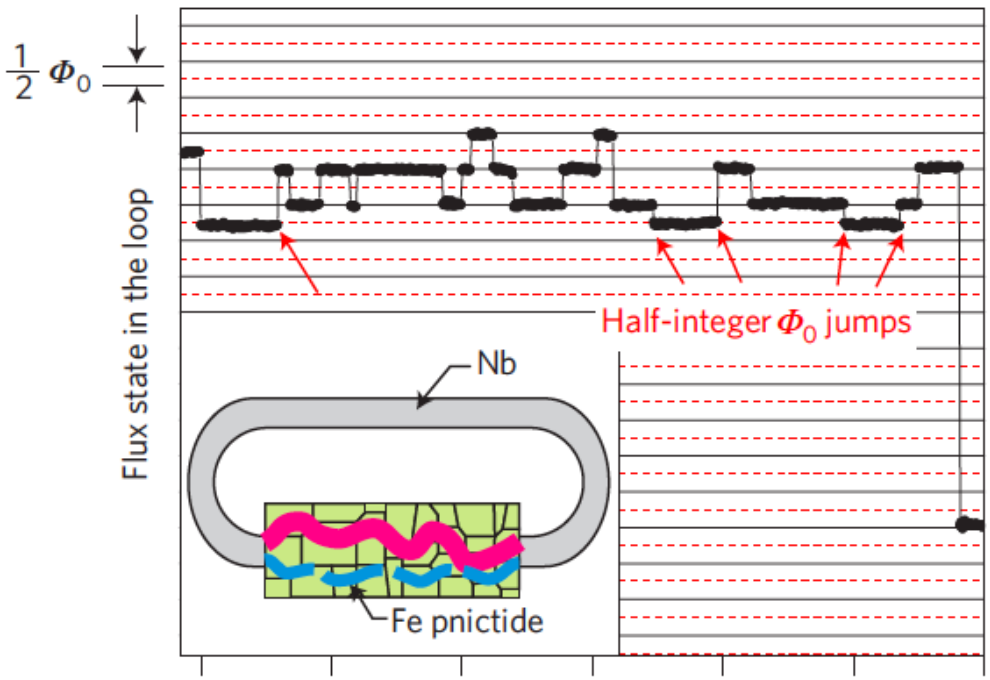


Sign change between electron pockets!

Iron-based superconductors: Sign change evidence (II)

Junction and STM





Sign change between hole and electron pockets!

Real space ?

T. Hanaguri, et al

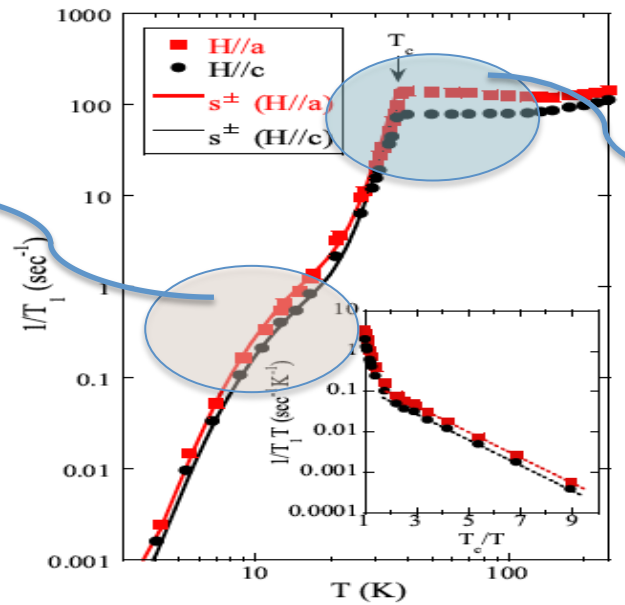
Chen. C. T. et al

Dual Symmetry Characters and Sign Change Principle (III)

NMR

Full gap

S-wave



GQ Zheng, PRB 43 140506

No coherent peak

d-wave

- Sign change is likely symmetry protected!

Summary of Gap Symmetry

- Full gap in most optimally doped materials.
- Accidental nodes ---- but not symmetry protected.
- Sign change----Yes. Is it symmetry protected?
- Dual character of s-wave (gap like conventional s-wave) and d-wave (sign change like cuprates)

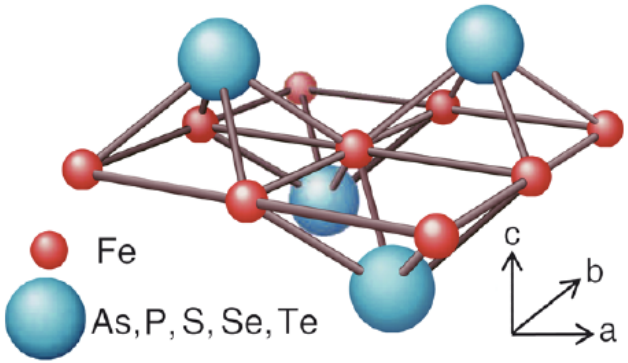
A Chameleon

Uniqueness of Symmetry

- Why is it hard to determine the pairing symmetry in iron-based superconductors?

There must be an uniqueness of the pairing symmetry in iron-based superconductors.

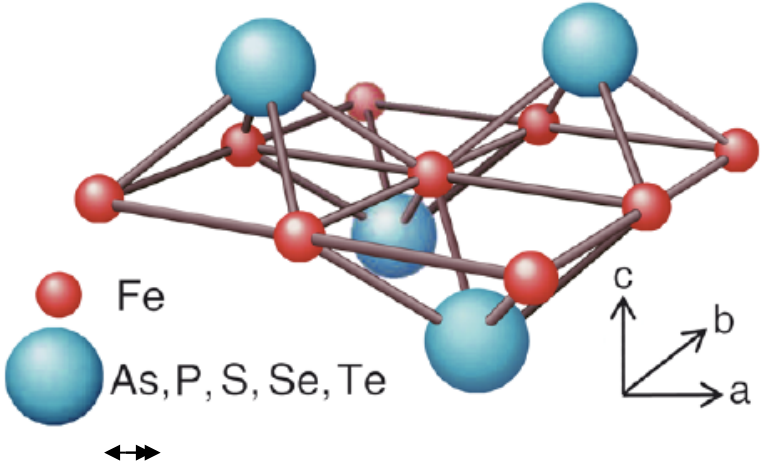
Not multi-orbital!



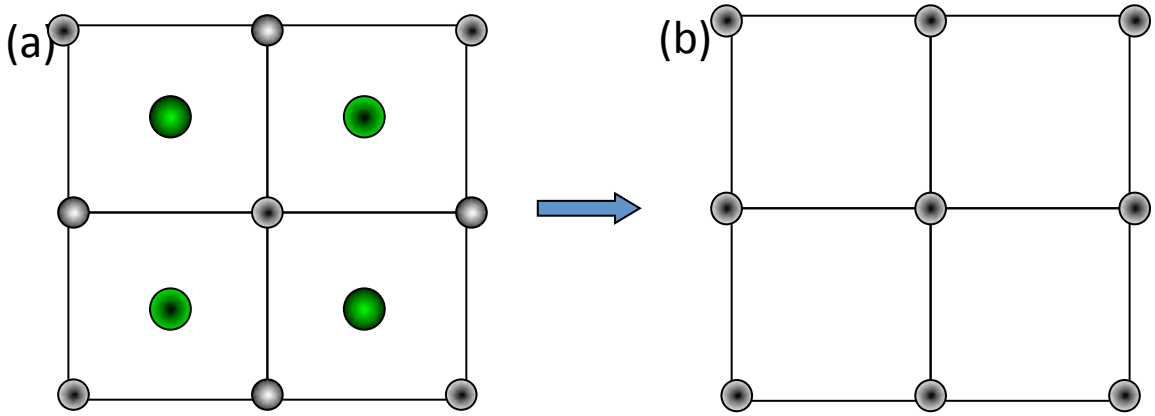
Symmetry Principle

A physical system is characterized by its own symmetry!

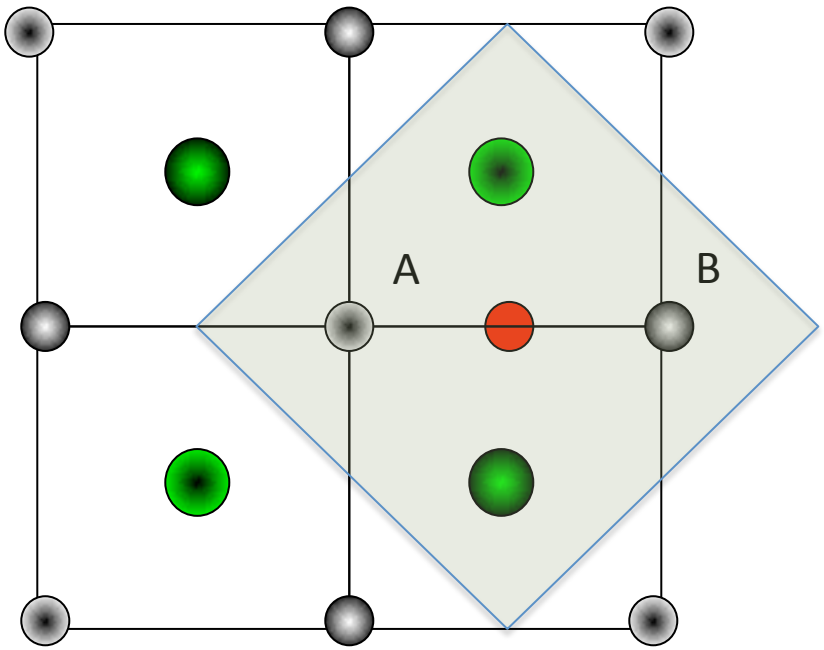
Symmetry Principle May Be Violated

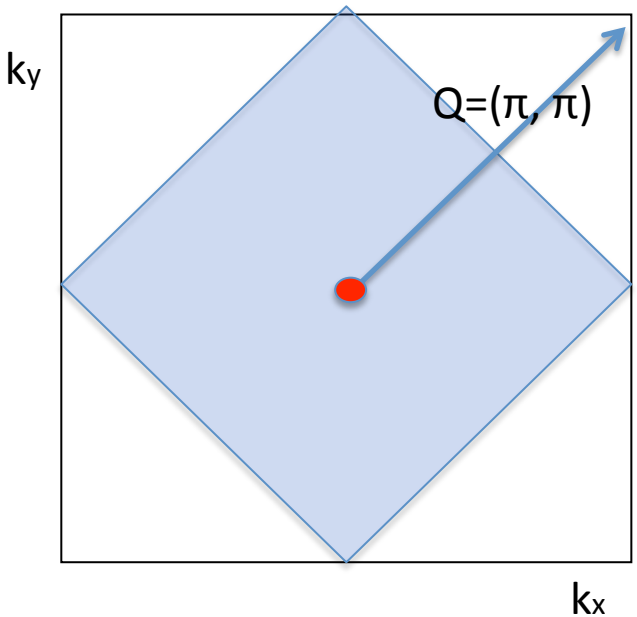


Symmetry changes in effective model!



Symmetry of Single Trilayer Fe-As(Se)





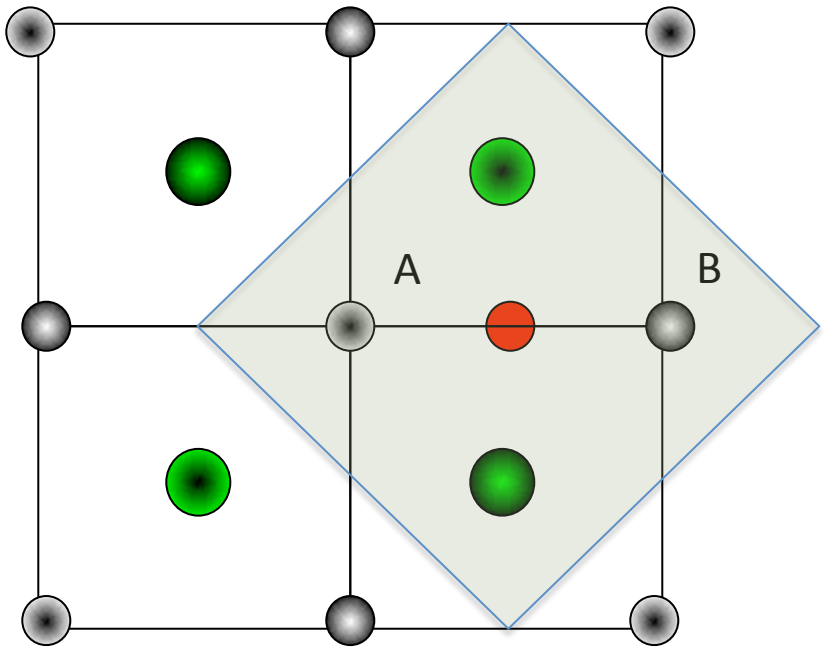
- Point group at Fe: D_{2d}
- Point group at As: C_{4v}

- Total symmetry:

$$(E,I)\otimes D_{2d}^{Fe} = (E,I)\otimes C_{4v}^{As}$$

Non-symmorphic space group!

Parity in Iron-Based Superconductors



$$\Delta_A = < C_{i\uparrow} C_{i\downarrow} >_A$$

Parity Operation

$$\Delta_B = < C_{i\uparrow} C_{i\downarrow} >_B$$

$$\Delta_{even} = < C_{i\uparrow} C_{i\downarrow} >_A + < C_{i\uparrow} C_{i\downarrow} >_B$$

$$\Delta_{odd} = < C_{i\uparrow} C_{i\downarrow} >_A - < C_{i\uparrow} C_{i\downarrow} >_B$$

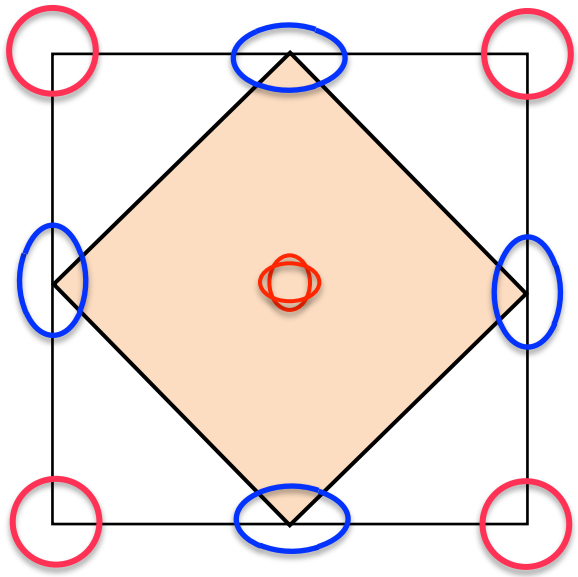
- Spin Singlet
- 1-Fe Unit cell
- Parity even

- Spin Singlet
- 2-Fe Unit cell
- Parity Odd

C. N. Yang, Phys. Rev. Lett., 63, 2144 (1989)

η-pairing

Even Parity in Iron-Based Superconductors– S±

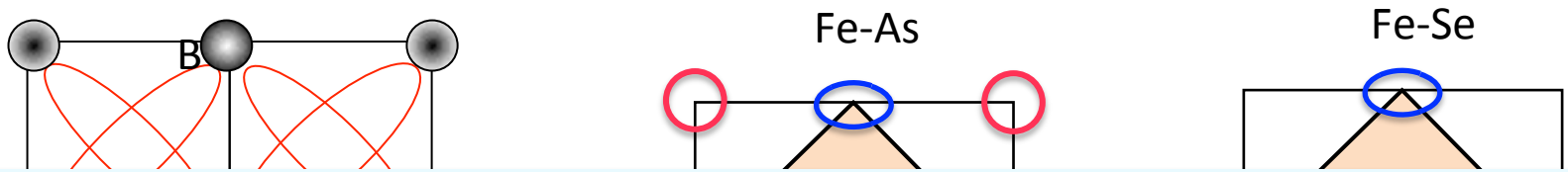


Even parity state:

- Sign change between electron and hole pockets
- The model can be reduced to 1-Fe unit cell

Mazin, Kuroki, Scalapino, Hirschfeld, Chubukov, Dung-Hai Lee, J.P. Hu….

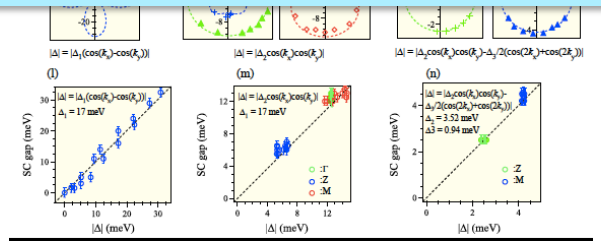
AFM Mechanism in Iron-Based Superconductors– S±



Troublesome for an even parity S± state:

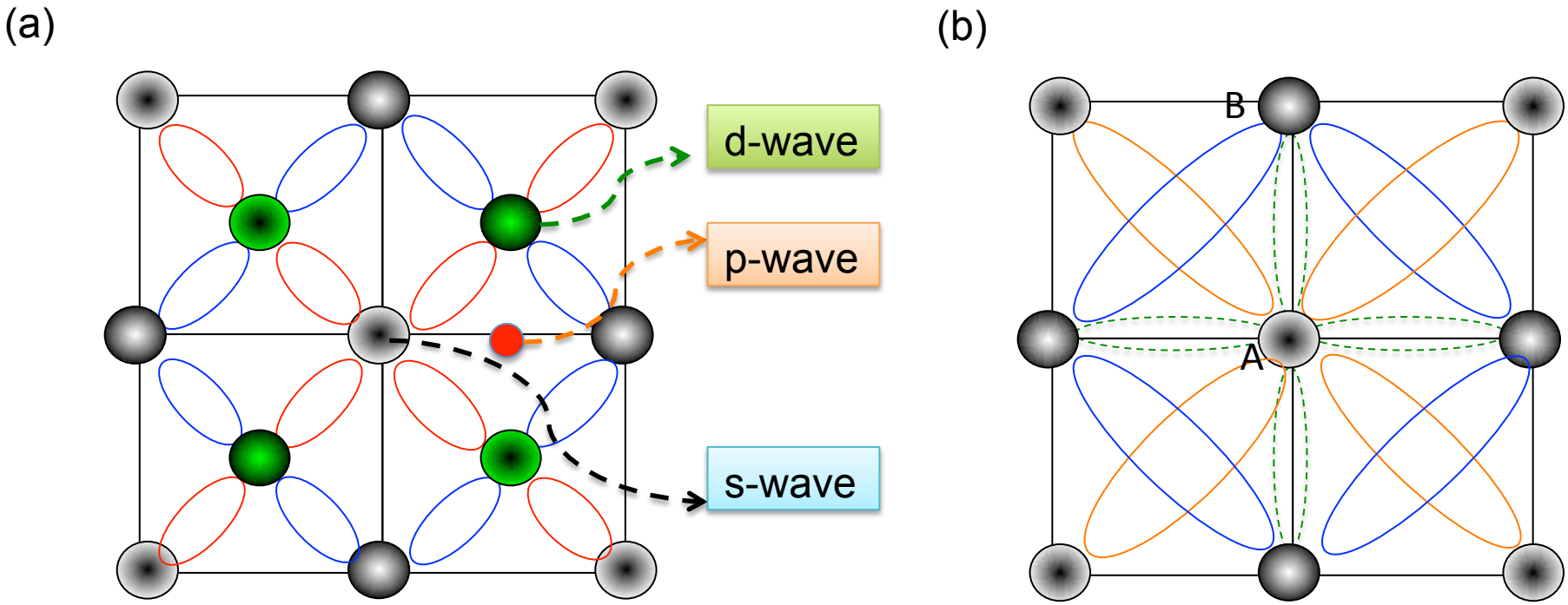
- Sign change is not symmetry protected.
- No Sign change on the Fermi Surfaces of KFe_2Se_2 and single layer FeSe.
- No real space sign change.

K.Seo, et al, PRL 101, 206404 (2008)
C. Fang, et al, PRX, 1,011009 (2011)
J.P. Hu and N. Hao, Phys. Rev. X, 021009 (2012))
J.P. Hu and H. Ding, Scientific Reports 2,381 (2012)



Odd Parity Spin-Singlet!

Odd Parity in Iron-Based Superconductors

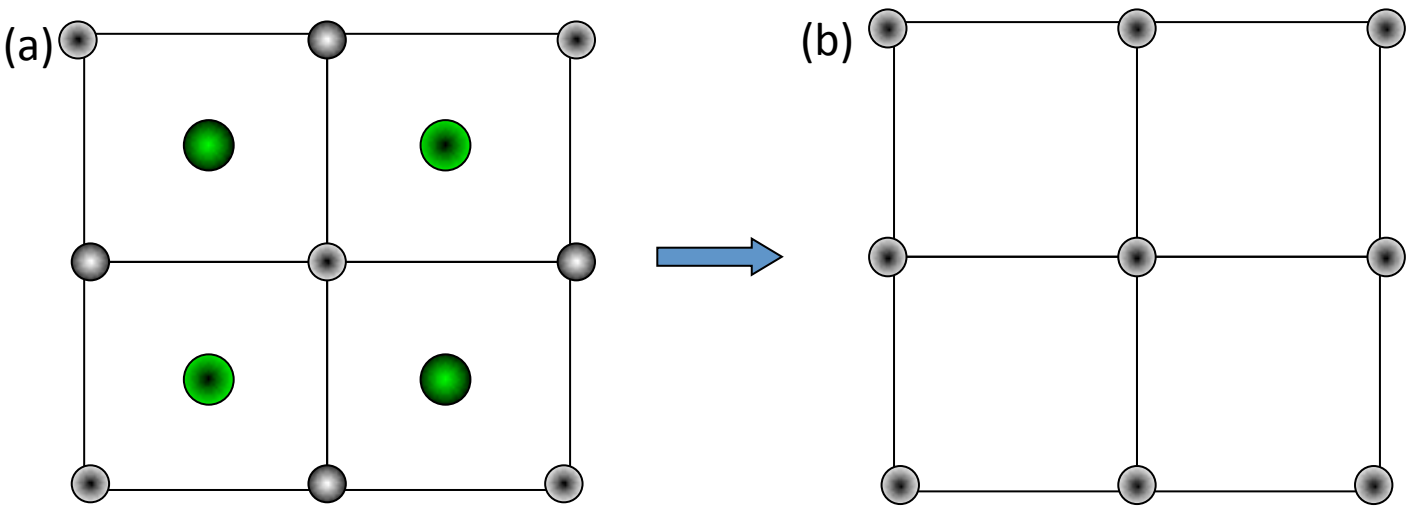


Odd parity state:

- Sign change between top and bottom As(Se) layers
- Sign change between two Iron sublattices
- S-wave at Fe sites = d-wave at As(Se) sites

Like a Chameleon

Effective Model

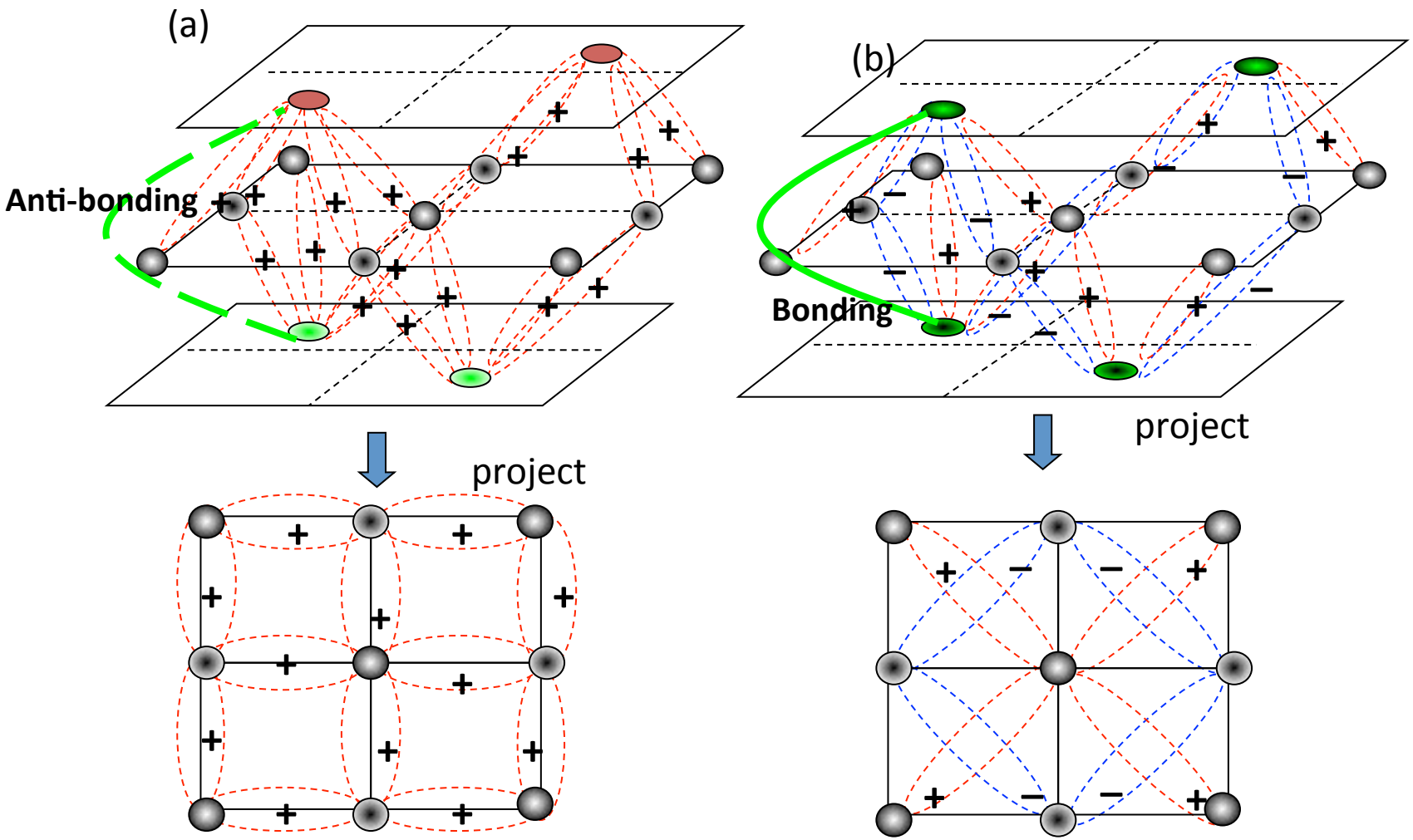


$$H = H_{dp} + \ldots \quad \Rightarrow \quad H_{eff} = H_{dpd} + \ldots$$

We know!!

Kuroki, Hirschfeld….

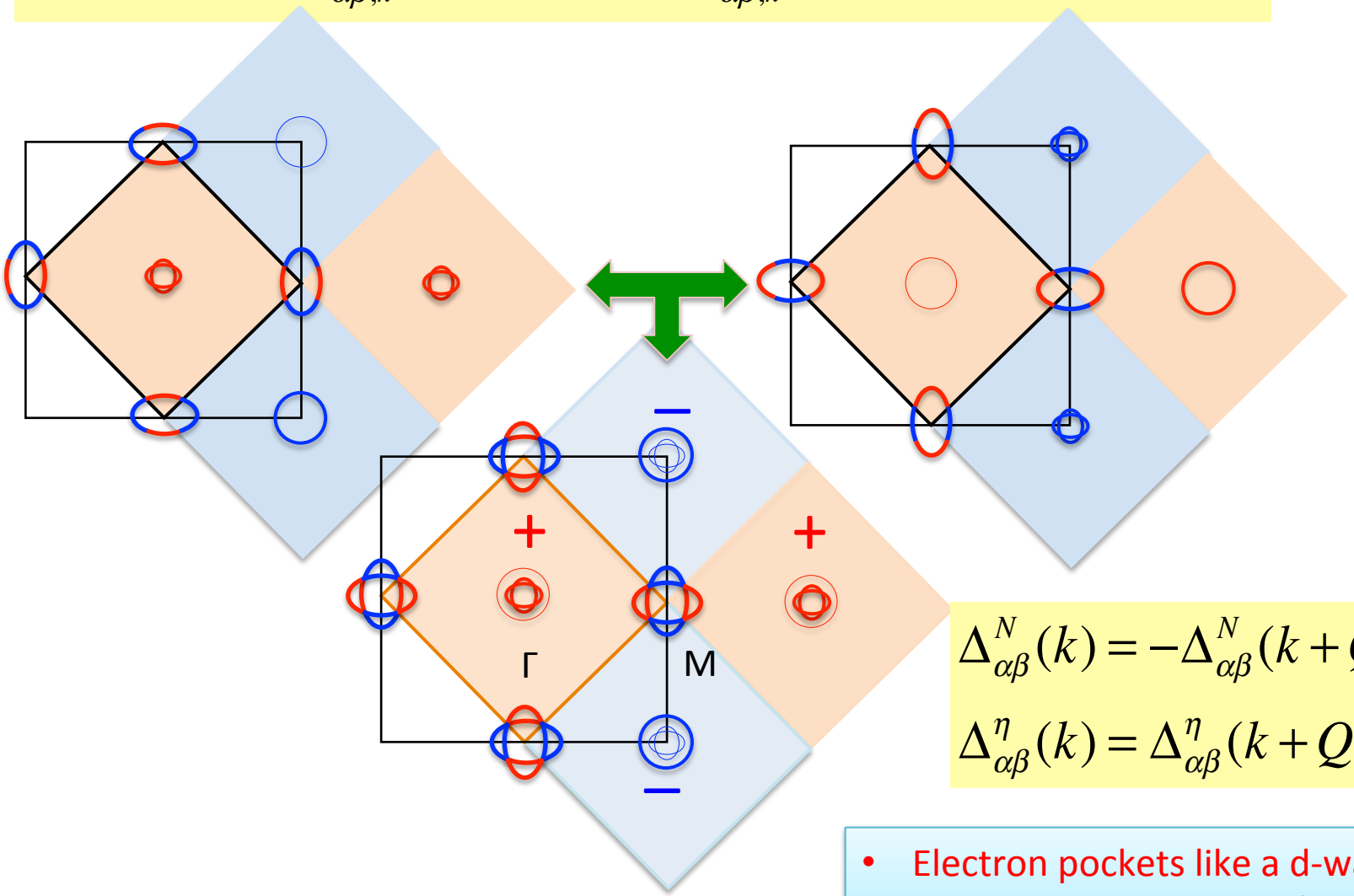
Odd parity s-wave: normal pairing + eta pairing



Inter-sublattice pairing takes different parity from intra-sublattice pairing in an iron effective model!

The Odd Parity State in 1-Fe unite cell

$$H_{BCS} = H_{0,eff} + \sum_{\alpha\beta,k} \Delta^{N}_{\alpha\beta}(k)(k,-k) + \sum_{\alpha\beta,k} \Delta^{\eta}_{\alpha\beta}(k)(k,-k+Q) + h.c.$$



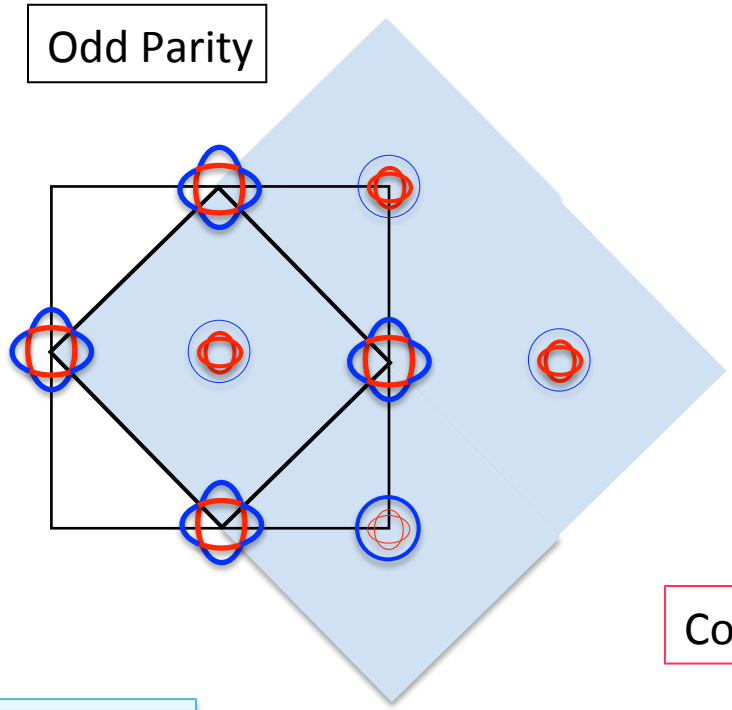
$$\Delta^{N}_{\alpha\beta}(k) = -\Delta^{N}_{\alpha\beta}(k+Q)$$

$$\Delta^{\eta}_{\alpha\beta}(k) = \Delta^{\eta}_{\alpha\beta}(k+Q)$$

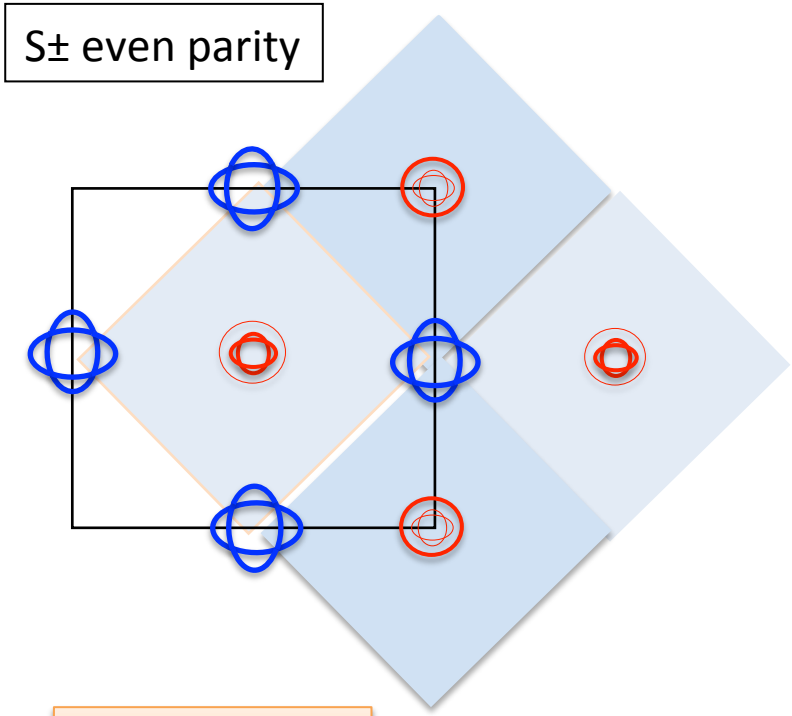
- Electron pockets like a d-wave
- No Symmetry Protected Nodes

The Odd Parity State in 2-Fe unite cell

Odd Parity



S± even parity



Comparison

Odd Parity

- Two Electron pockets
- 2-Fe unit cell
- Sign change between two electron pockets
- Sign change between two hole pockets by dxy and dxz,yz
- Sign change between electron and hole pockets

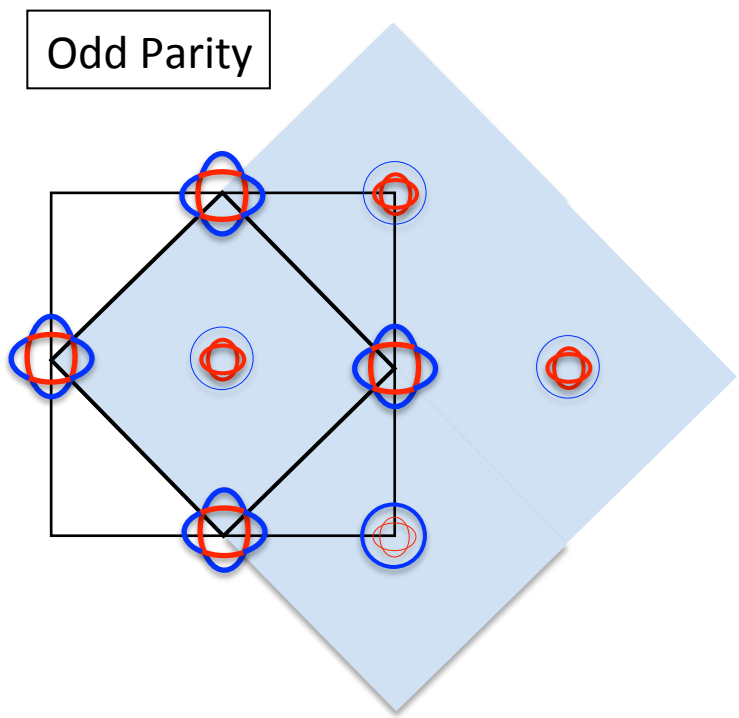
S± even parity

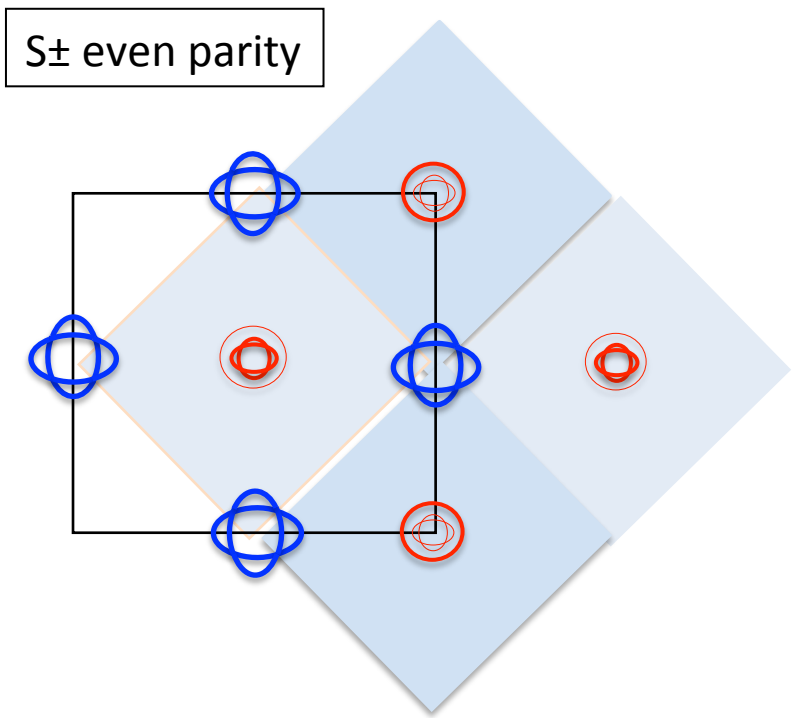
- One Electron pockets
- 1-Fe Unit Cell
- No sign change on electron pockets
- No sign change between hole pockets
- Sign Change between electron and hole pockets

Comparison: Iron-Pnictides

- Iron-Pnictides:

Is there a sign change between two hole pockets?

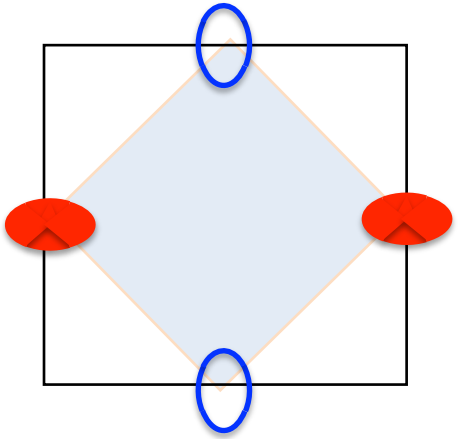




Even parity proposals for 122* FeSe

- Iron-Chalcogenides:

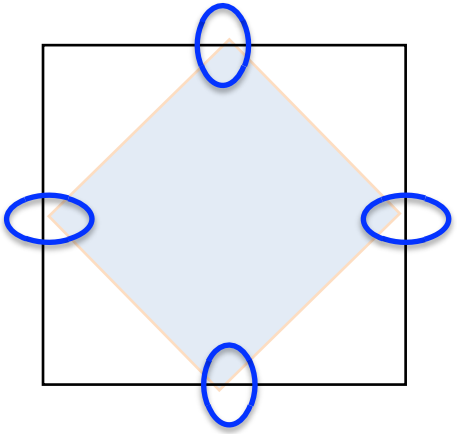
d-wave even parity



Scalapino, Hirshfeld, Lee, Chubukov
....

- Capture sign change between electron pockets
- Inter-sublattice pairing dominates.
- Problem: nodes should appear at Z and C-axis

s-wave even parity

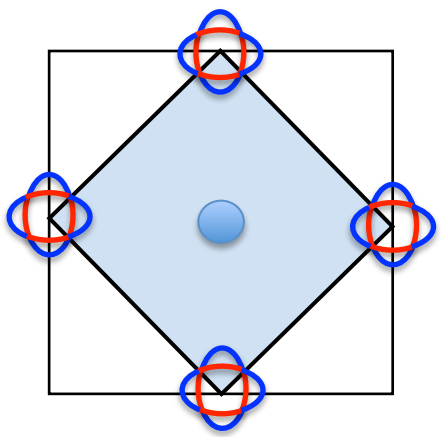


JP Hu, H.Ding, Lee, Si, ...
....

- No Symmetry protected nodes
- Intra-sublattice pairing dominates.
- Problem: no sign change between electron pockets

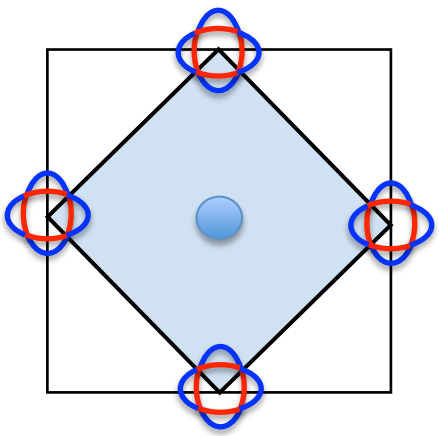
Odd parity proposals for 122* FeSe

- Iron-Chalcogenides:



Maxin: incipient S± (odd)
Chubukov: S (odd) +id (even)

- Intra-sublattice pairing dominates (odd).
- Pure η-pairing (for bonding and anti-bonding)
- Problem:
  - a pure η-pairing generally has nodes.
  - Cannot explain gap structure at Z.



JP Hu: Two S-wave (Even+Odd) in an effective d-orbital models

- Intra-sublattice pairing (odd)
- Inter-sublattice pairing (even)
- No time reversal symmetry breaking
- No general nodes and explain the gap structure at Z.

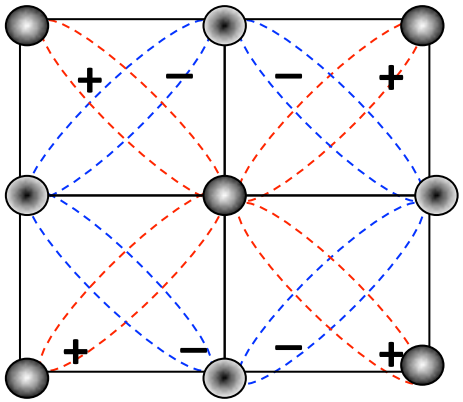
Odd Parity Superconducting State

- Unify iron-pnictides and iron-chalcogenides

  NN pairing is weakened in iron-chalcogenides.
- Explain the SC gap structures:

  From Full gap to accidental nodes
- Answer where is the sign change

  Both momentum and real space
- Explain the dual characters of s-wave and d-wave
- ….

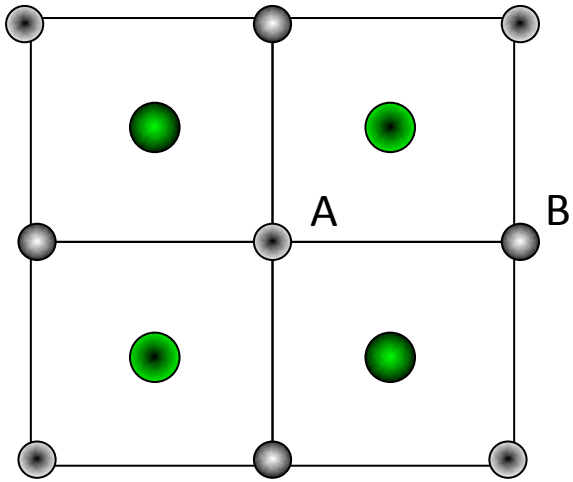


- s-wave like viewed at Fe sites
- d-wave like viewed at As sites

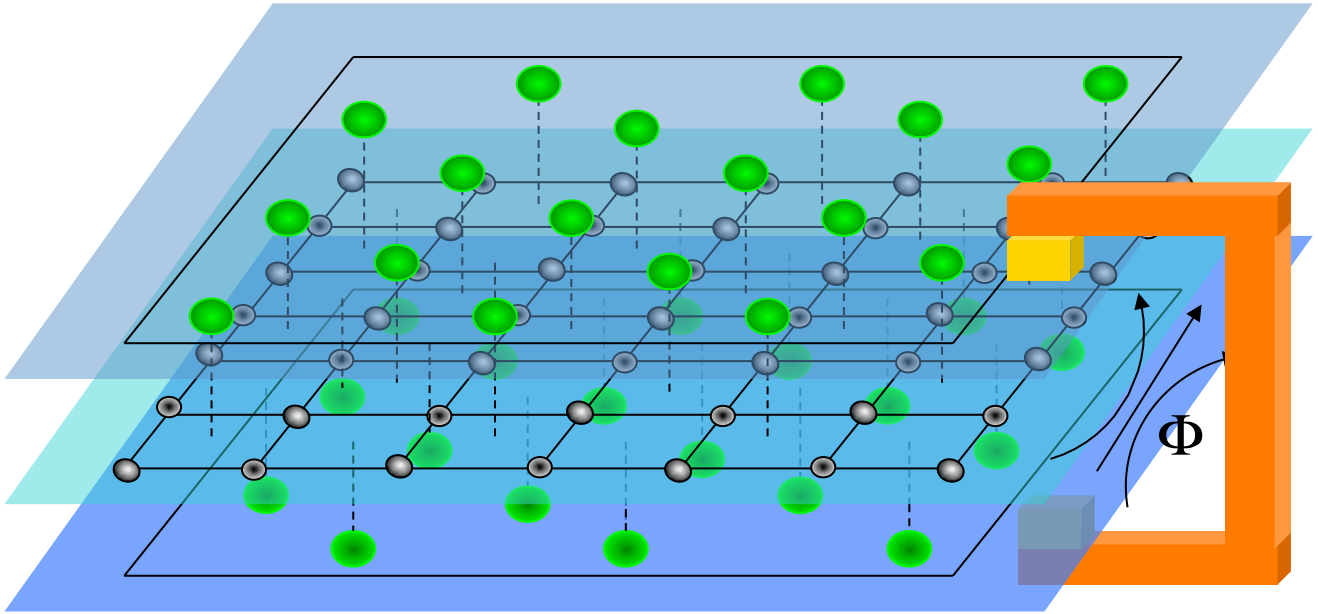
Odd parity spin-singlet s-wave

Smoking gun experiments to distinguish parity!

Signature of Parity Odd Superconductivity



Sign change between top and bottom As(Se) layers !



Signature of Parity Odd Superconductivity in bulk materials

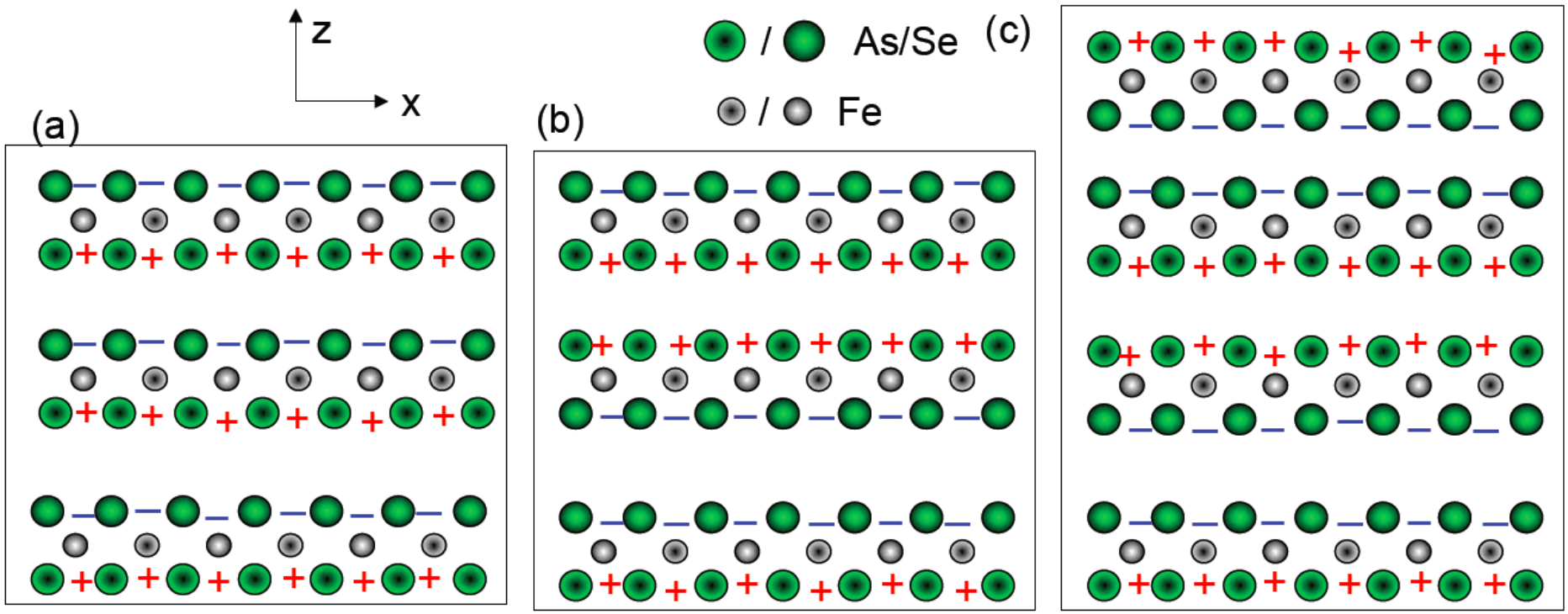
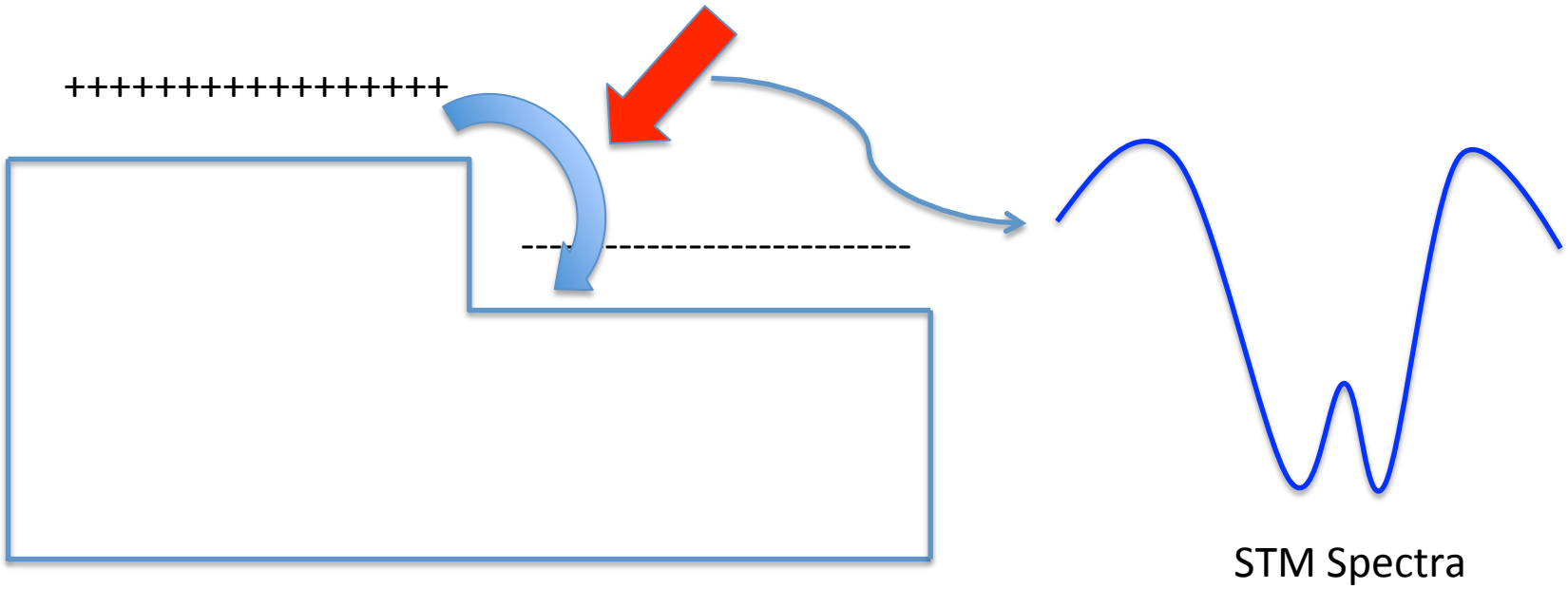


FIG. 4. Sketch of real space sign distribution along c-axis for an η-pairing state in (a) 11-type structure, (b) 122-type structure with odd number of layers and (c) 122-type structure with even number of layers.

Step Edges for Zero Bias Peak



- Andreev Bound States could appear on step edges
- Andreev Bound States can be induced if simultaneously tunneling to bottom and top As(Se) layers

Implication for High Tc Mechanism
- AFM Exchange Coupling

$$H = H_0 + \sum_{<ij>_{NN}} J_{1\alpha} S_{i\alpha} S_{j\alpha} + \sum_{<ij>_{NNN}} J_{2\alpha} S_{i\alpha} S_{j\alpha}$$

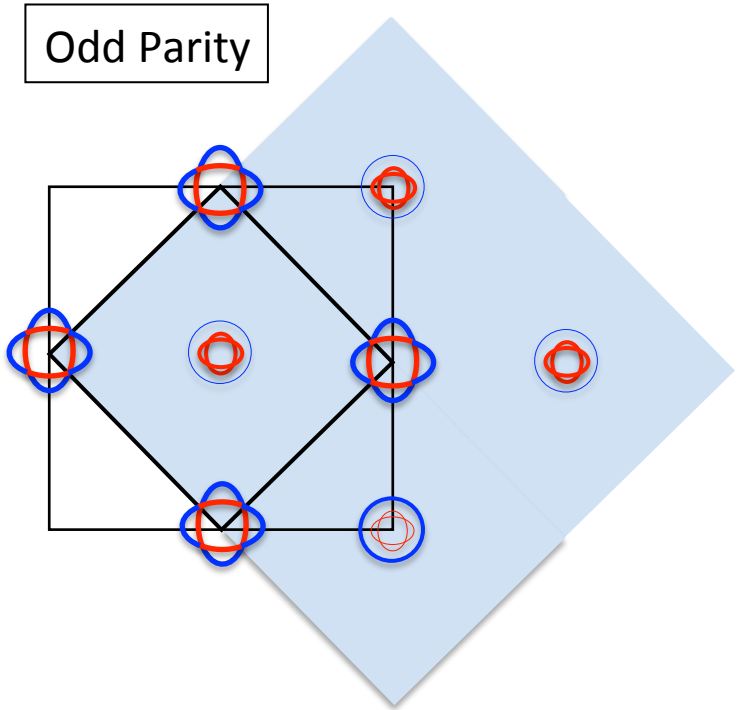
Odd Parity

- J_1, J_2 collaborates
- J_2 is in η-channel, J_1 is in normal-channel

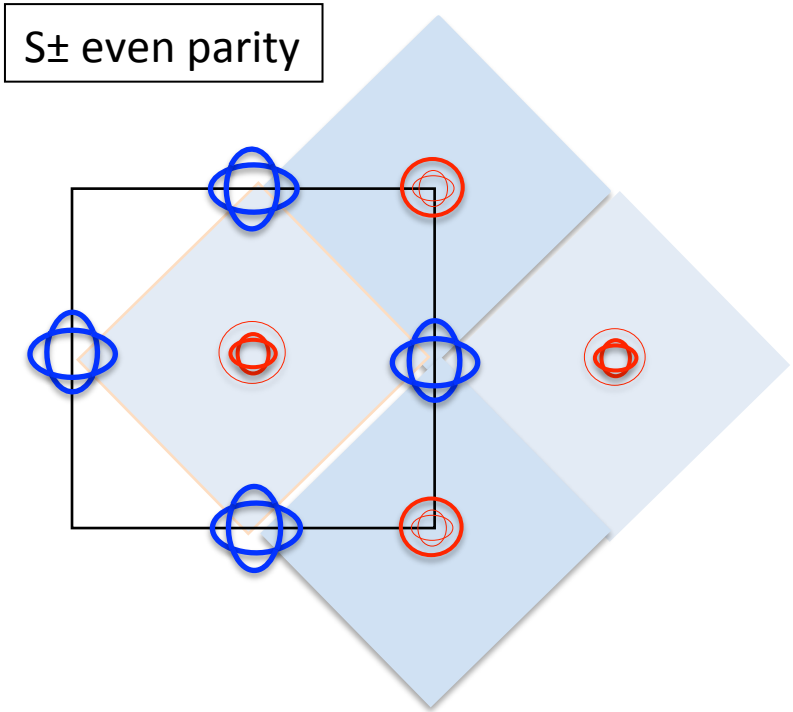
Even Parity

- J_1, J_2 compete with each other
- S± : J_2 dominates

Odd Parity

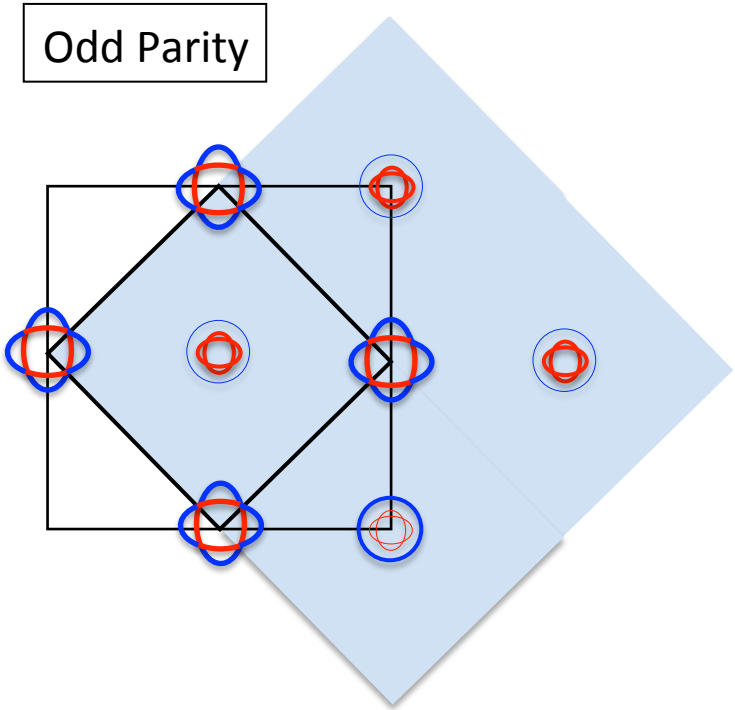


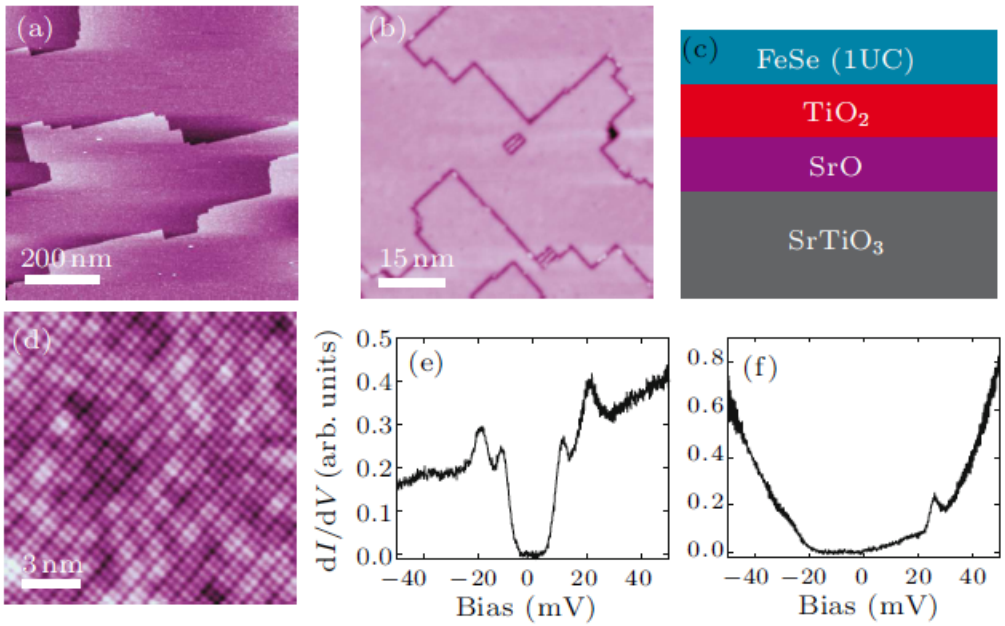
S± even parity



Two Gaps at Electron Pockets: Evidence for odd pairty

Odd Parity

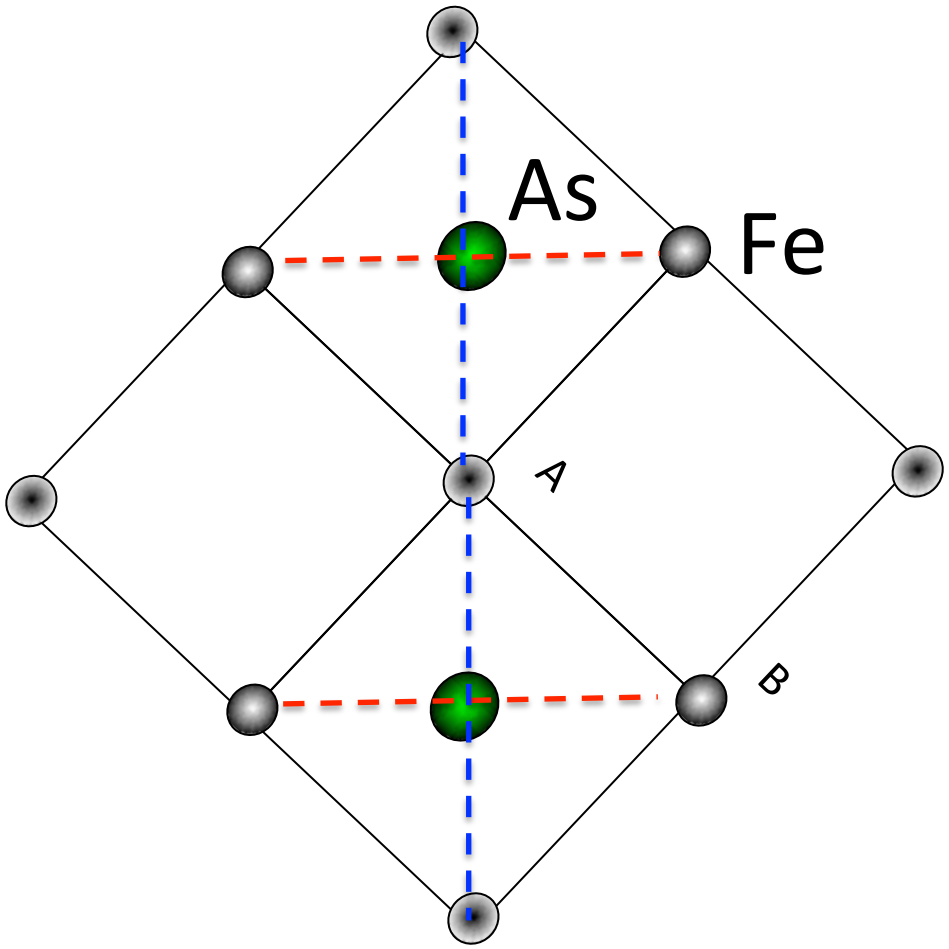


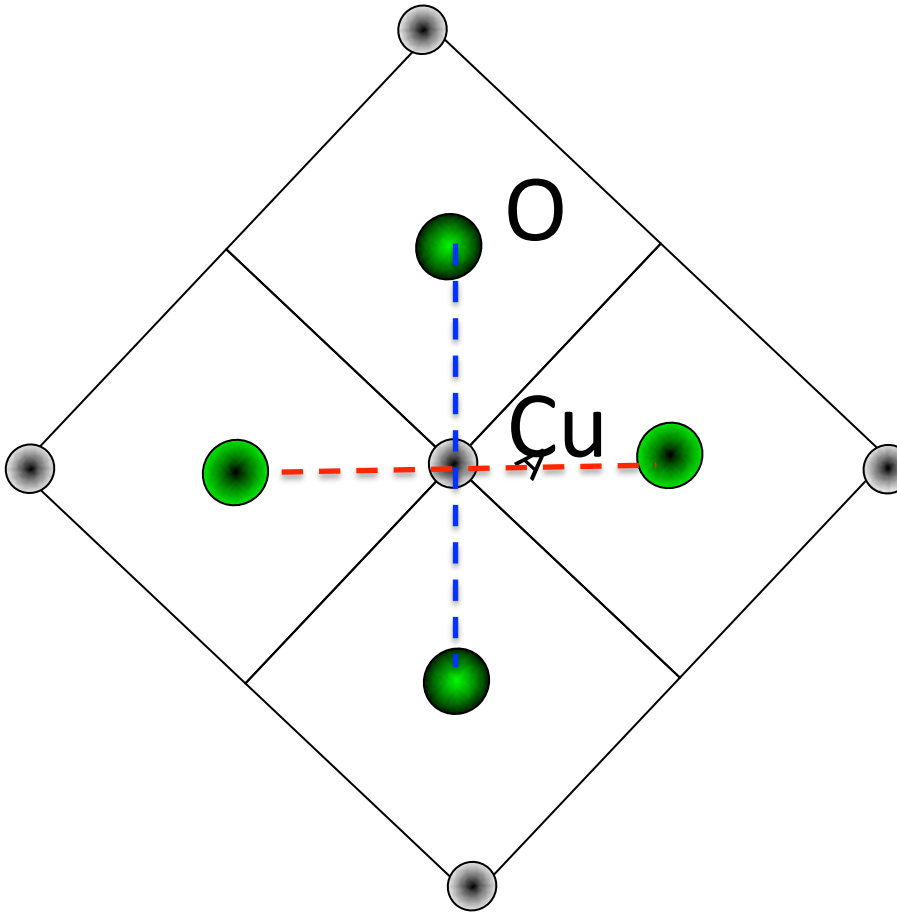


Two Gap features on Single-layer FeSe

Supporting odd parity!

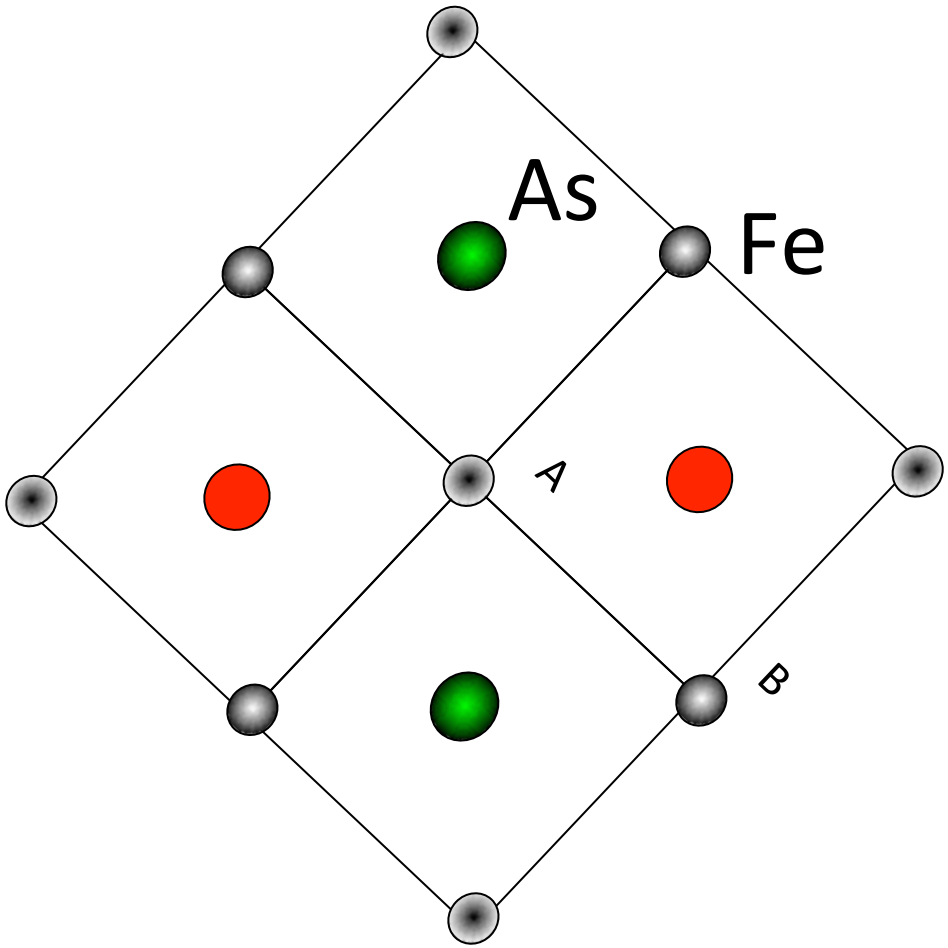
Implication for High Tc Mechanism
- Unify cuprates and iron-based superconductors

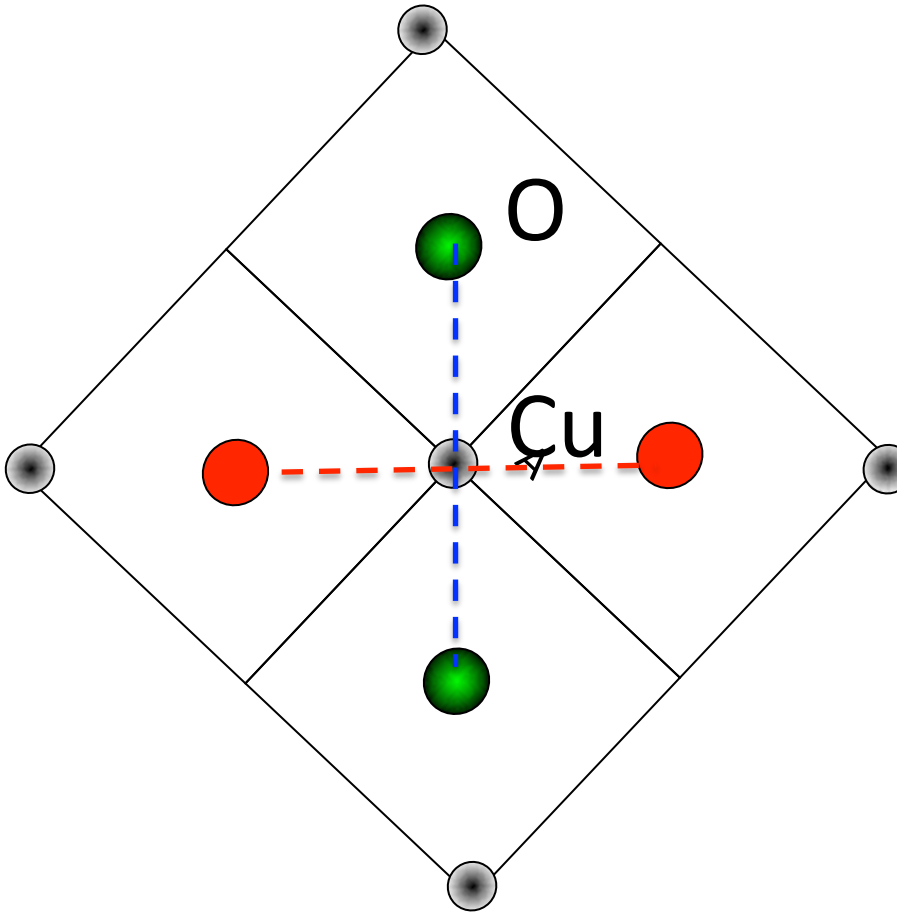




- Local pairing picture comparison between Fe-As and Cu-O

Implication for High Tc Mechanism
- Unify cuprates and iron-based superconductors





- Local pairing picture comparison between Fe-As and Cu-O

Implications to Mechanism From Pairing Symmetry

- AFM fluctuation (even parity) (RPA)

1. S-wave with the existence of hole pockets
2. d-wave for 122*

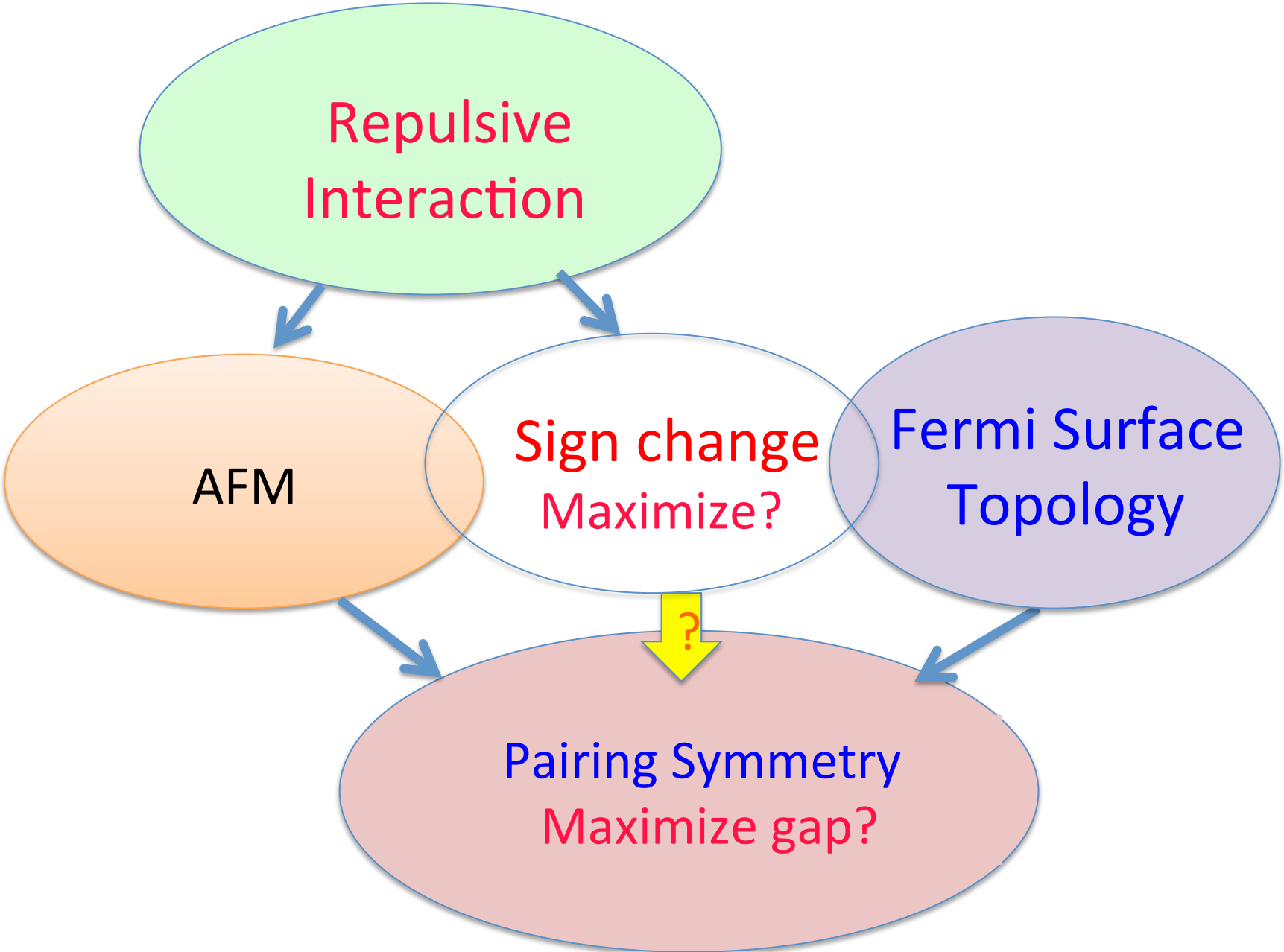
- Local AFM exchange coupling model

S-wave (even) for both all iron-based Scs.

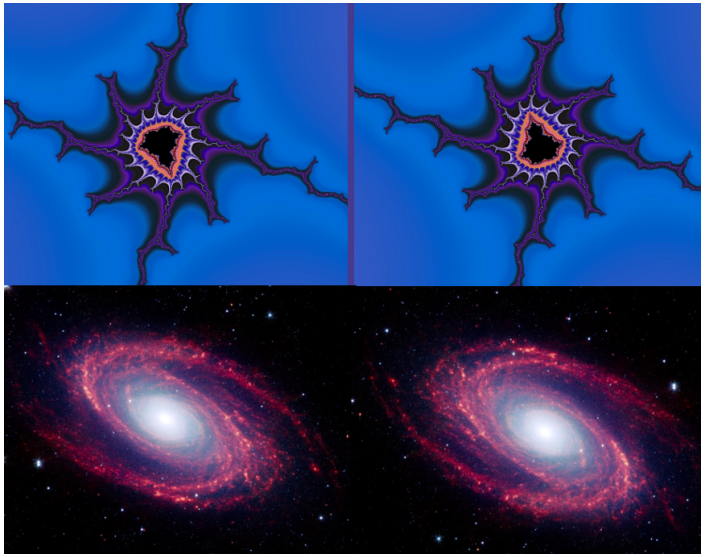
- What if it is odd parity s-wave?

New Principle: maximizing the sign change?

Paradigm For High Tc



Possibilities: wide open!



- Even parity?
- Odd parity(Parity Breaking) ?
- Different symmetry for different families?

Message to Experimentists

Begging for the answer:
even or odd?

- Determining pairing symmetry of iron-based superconductors starts from parity.

Results

- Iron-based superconductor: odd parity spin-singlet pairing (a new quantum state of matter)
- Sign Change is protected by symmetry
- Iron-Pnictides and Iron-Chalcogenides are unified and share same mechanism.
- Establishing Gauge principle
- Suggesting unification of iron-based superconductors and cuprates

New Adventures

Acknowledge

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- Kivelson, Bernevig, T. Xiang, Thomale, Y.P. Wang, X. Dai