A brief Introduction of Fe-based SC

Yunkyu Bang (Chonnam National Univ., Kwangju, Korea)

Lecture 1: Introduction

1. Overview

2. What is sign-changing s-wave gap : +/-s-wave gap

Lecture 2: Superconducting properties of +/-s-wave gap

- 1. Impurity effects on the +/-s-wave gap
- 2. NMR : Knight shift and T1 relaxation rate
- 3. Penetration depth versus T
- 4. Volovik effect general principle
- 5. Volovik effect on +/-s-wave gap thermal conductivity

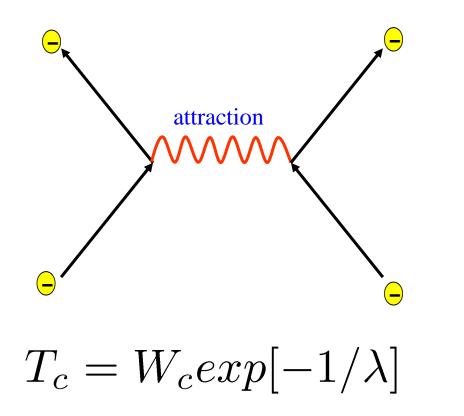
Lecture 3: Specific heat jump and Condensation E vs. Tc

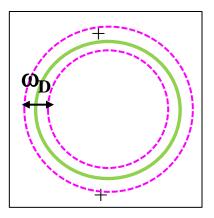
- 1. Specific heat jump vs. Tc : BNC scaling
- 2. Condensation E in BCS superconductor
- 3. Condensation E in multi-band superconductor
- 4. Pairing mechanism

Lecture 4: FeSe system (Tc~100K)

- 1. Possible phonon contribution
- 2. Renormalization of pairing cutoff in incipient band
- superconductors
- 3. Outlook.

BCS theory: Only one proven Theory of Superconductivity





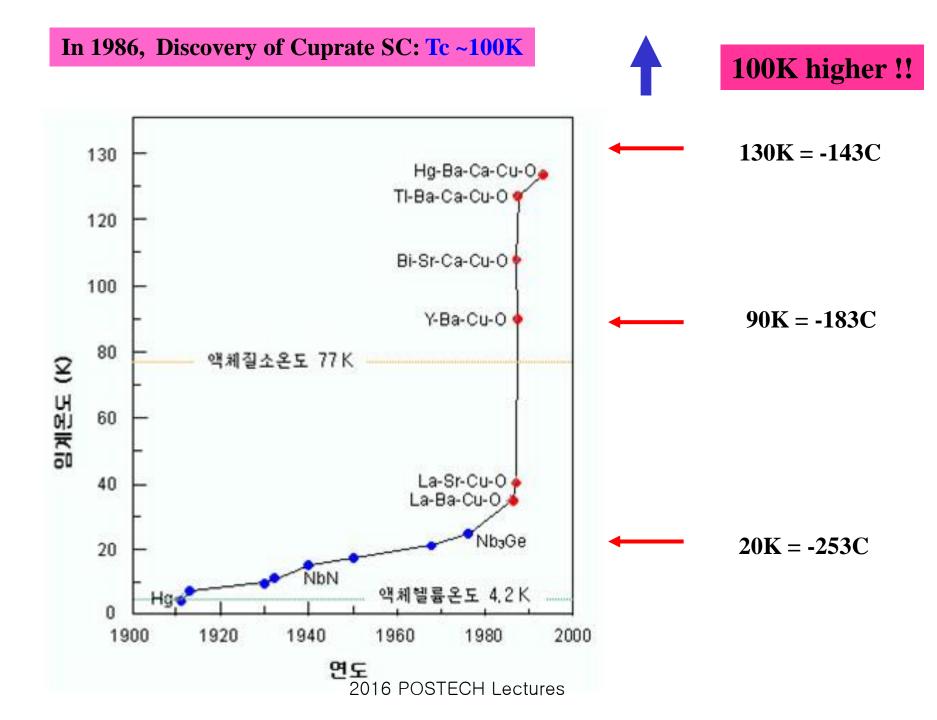


 W_c : energy scale of coupling boson λ : coupling constant

A stronger glue can increase T_c :

But it causes the material unstable (*general stability problem*) : too much strong phonon attraction will cause a lattice collapse.

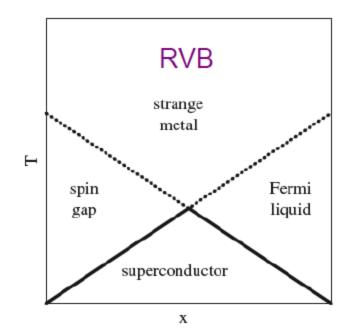
 \rightarrow Maybe T_c^{max} < 30K (Anderson & Cohen) 2016 POSTECH Lectures

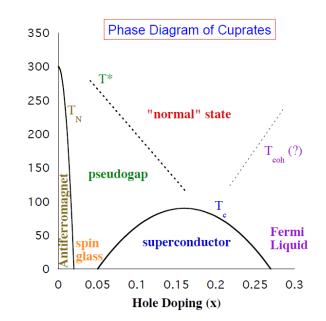


Anderson declared: (In 1987 Science vol. 235 and subsequent papers) "This is Un-conventional SC": non-BCS, non-Fermi liquid

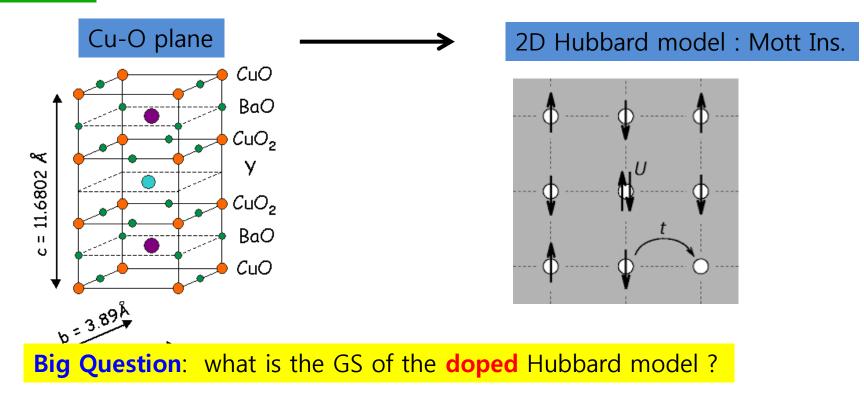
1. Cuprate-SC \rightarrow (RVB + doped holes) condensation

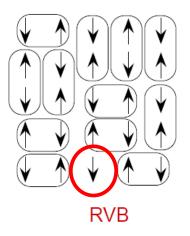
- 2. Cuprate-normal state \rightarrow new quantum liquid (no q.p.)
- 3. high-Tc is a natural manifestation of this new quantum liquid





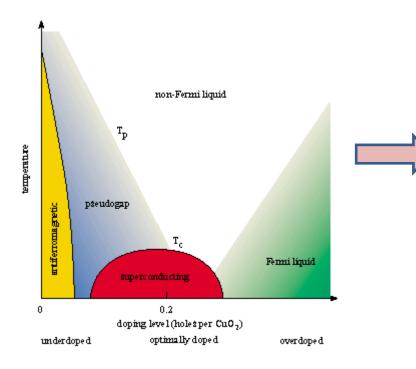
Mott Physics

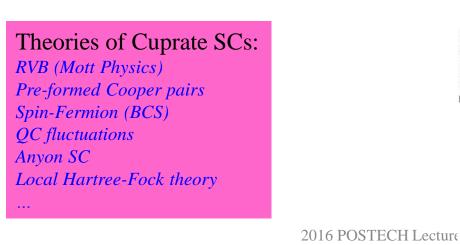


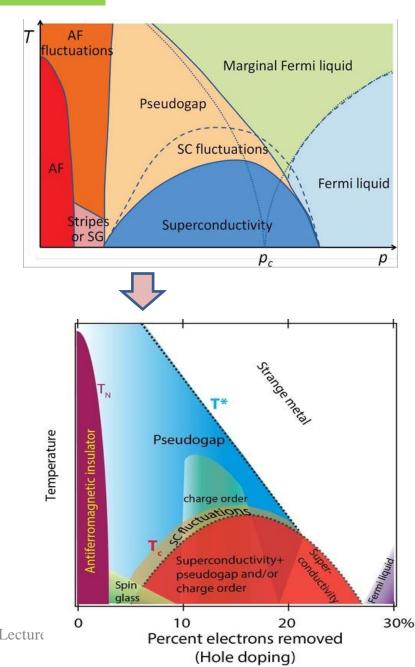


Electron q.p. = spinon + holon (spin-charge separation, Doped Spin liquid, etc., etc)

Last 30 years = history of frustration – still on going



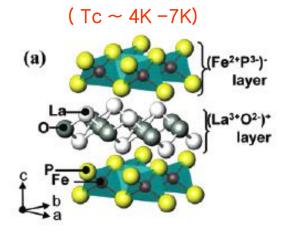


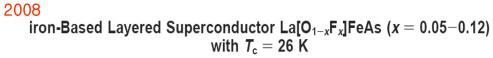


Discovery of Fe-based Superconductor (2006,2008)

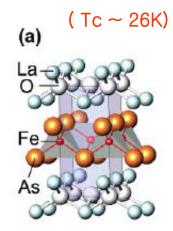
Iron-Based Layered Superconductor: LaOFeP

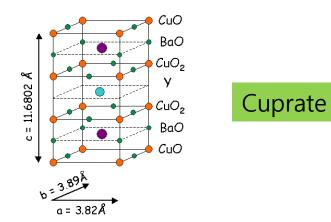
Yoichi Kamihara,[†] Hidenori Hiramatsu,[†] Masahiro Hirano,^{†,‡} Ryuto Kawamura,[§] Hiroshi Ya Toshio Kamiya,^{†,§} and Hideo Hosono^{*,†,‡}



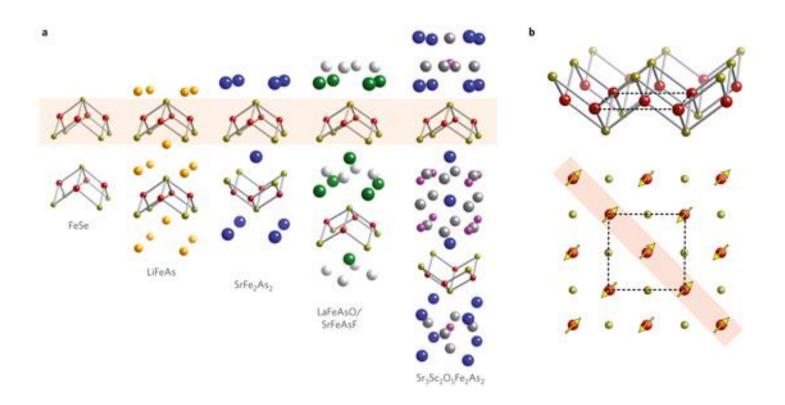


Yoichi Kamihara,*,† Takumi Watanabe,‡ Masahiro Hirano,†,§ and Hideo Hosono†,‡,§



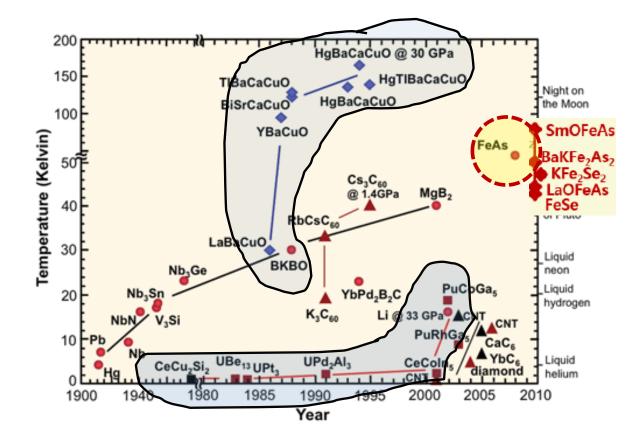


oxypnictide	Т _с (К)	non-oxypnictide	Т _с (К)
LaO _{0.89} F _{0.11} FeAs	26 ^[8]	$Ba_{0.6}K_{0.4}Fe_2As_2$	38 ^[9]
LaO _{0.9} F _{0.2} FeAs	28.5 ^[10]	Ca _{0.6} Na _{0.4} Fe ₂ As ₂	26 ^[11]
CeFeAsO _{0.84} F _{0.16}	41 ^[8]	CaFe _{0.9} Co _{0.1} AsF	22 ^[12]
SmFeAsO _{0.9} F _{0.1}	43 ^[8]	Sr _{0.5} Sm _{0.5} FeAsF	56 ^[13]
La _{0.5} Y _{0.5} FeAsO _{0.6}	43.1 ^[14]	LiFeAs	<18 ^{[15][16]}
NdFeAsO _{0.89} F _{0.11}	52 ^[8]	NaFeAs	9-25 ^{[17][18]}
PrFeAsO _{0.89} F _{0.11}	52 ^[19]	FeSe*	<27 ^{[20][21]}
GdFeAsO _{0.85}	53.5 ^[22]	BaFe _{1.8} Co _{0.2} As ₂ +	25.3 ^[23]
SmFeAsO _{~0.85}	55 ^[24]		



Crystallographic and magnetic structures of the iron-based superconductors.

Three main groups of Un-conventional Superconductors



Key Unconventional Superconductors:

- High-Tc cuprate SC
 Heavy Fermion SC
- 3. Iron-based SC

What do we mean by "Unconventional-SC" ? → Probably, non-BCS SC

When did it start ? \rightarrow because of high-T_c cuprates (1986 Bednorz & Meuller) Why did it start ? \rightarrow because of PW Anderson, partly Ideas of **truly non-BCS** superconductors: e.g.

RVB SC : based on spin-charge separation
 Anyon SC : based on new q.p. (neither fermion nor boson)

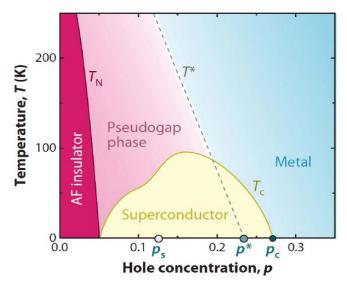
Interesting ideas but didn't pass exp. tests. \rightarrow at least, the cuprate and all other SC seems to consist of Cooper pairs. (*Josephson tunneling* + many other conventional SC properties)

But still many people wish to find a novel (non-BCS) theory.

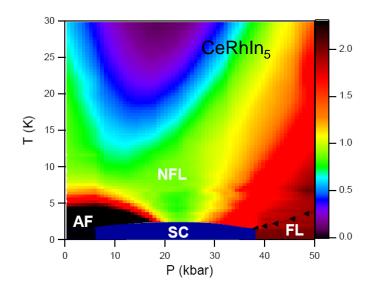
 \rightarrow But, besides RVB, Anyon theories, what non-BCS theory ?

Common Phase diagram of unconventional SCs

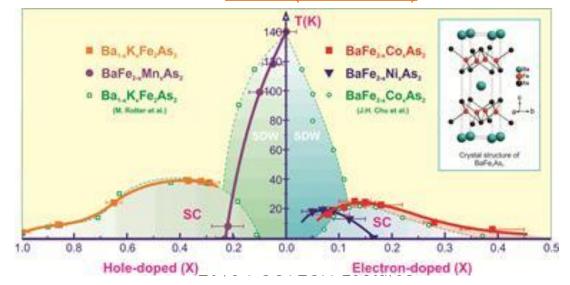




heavy fermion

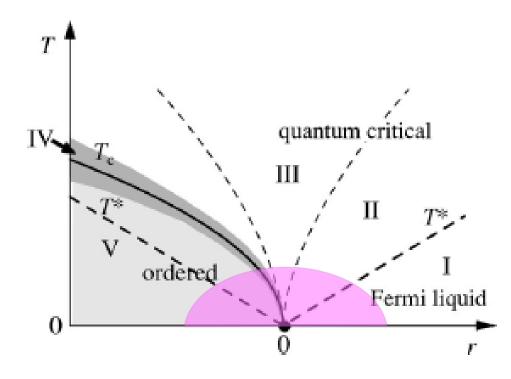


Fe-122(BaFe2 As2)



Common Belief of paradigm:

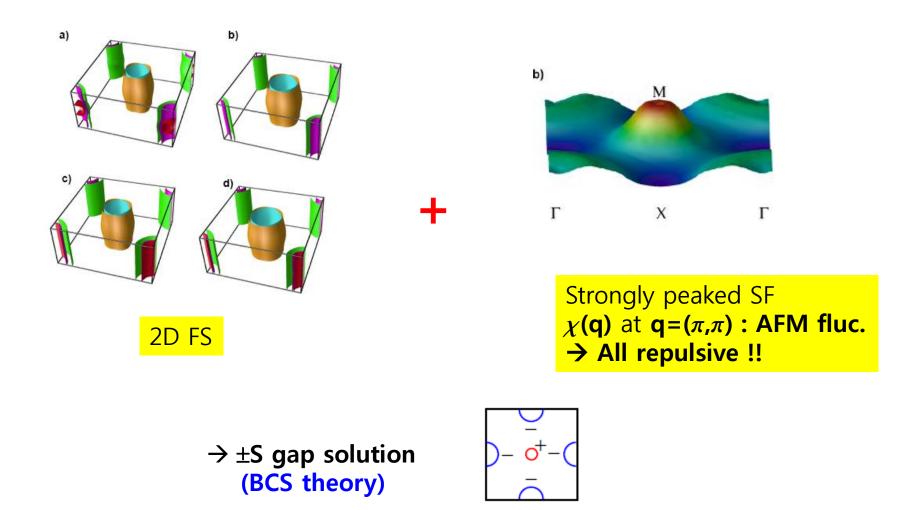
Strong correlation → QCP (?)
 → no q.p → Non-Fermi Liquid normal state
 → Un-conventional SC (perhaps high-T_c)
 → Un-conventional pairing mechanism (non-BCS type ?)

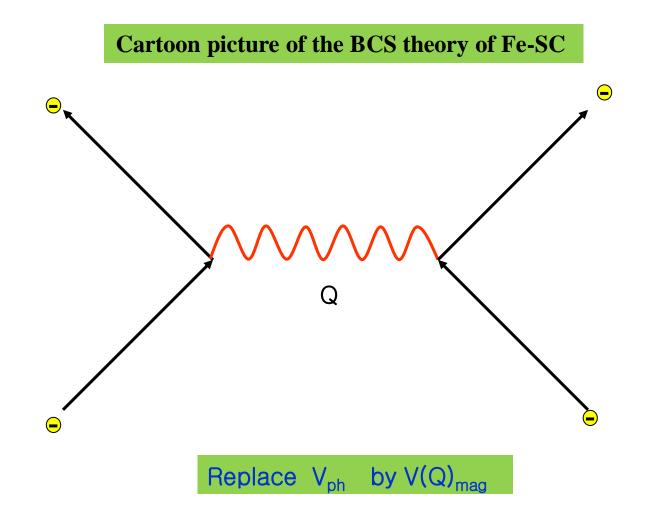


BCS theory of Fe-based Superconductor: **Sign-changing S-wave state** or **±S-wave**

How much can we understand Fe-based SC with BCS theory ?

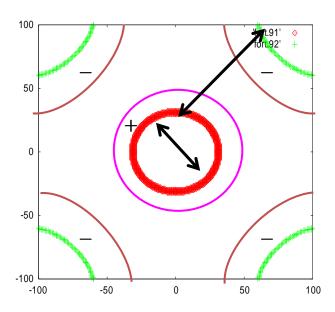
Early theories (2008) just after the discovery of La(OF)FeAs (26K) *Mazin et al, PRL 101, 057003; Kuroki et al., 101, 087004 (later many more)*





Sign-changing S-wave solutions = multi-bands + AFM fluctuations

 \pm S-wave



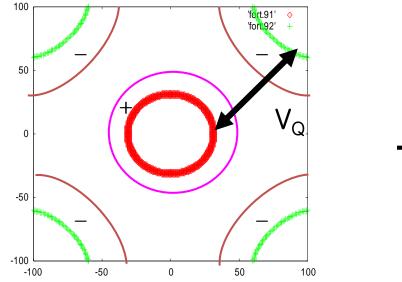


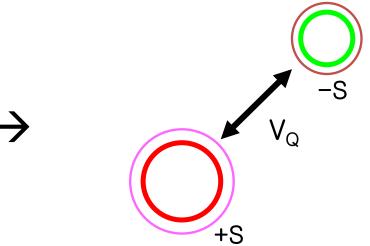
Two band BCS gap Equation

$$\begin{aligned} \Delta_{h}(k) &= (5) \\ &- \sum_{k'} [V_{hh}(k,k')\Delta_{h}(k')\chi_{h}(k') + V_{he}(k,k')\Delta_{e}(k')\chi_{e}(k')], \\ \Delta_{e}(k) &= \\ &- \sum_{k'} [V_{eh}(k,k')\Delta_{h}(k')\chi_{h}(k') + V_{ee}(k,k')\Delta_{e}(k')\chi_{e}(k')]. \end{aligned}$$
(6)

Sign-changing S-wave solutions for multi-bands + AFM interaction

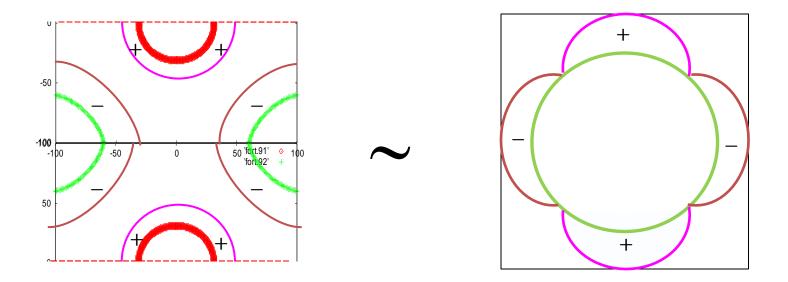
 \pm S-wave pairing





Two band Model

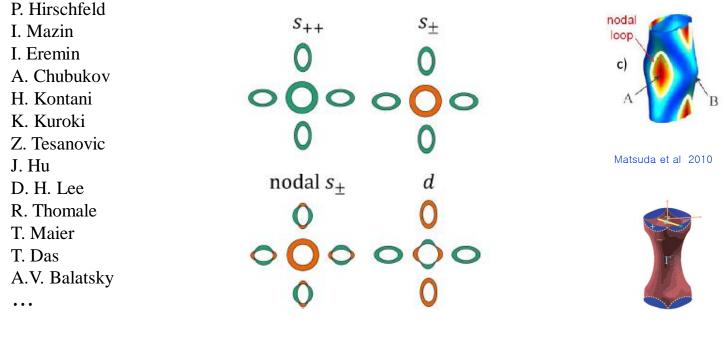
\pm s-wave = d-wave



Universal Pairing Mechanism of AFM spin fluctuation V(Q)

All BCS theory

More realistic calculations with orbital d.o.f., 3D $V_{spin}(q)$, FS shapes, etc found that $\pm s$ -gap is a dominant solution. But with some parameters, other solutions are possible: accidental nodes, horizontal node, d-wave, s++, etc.



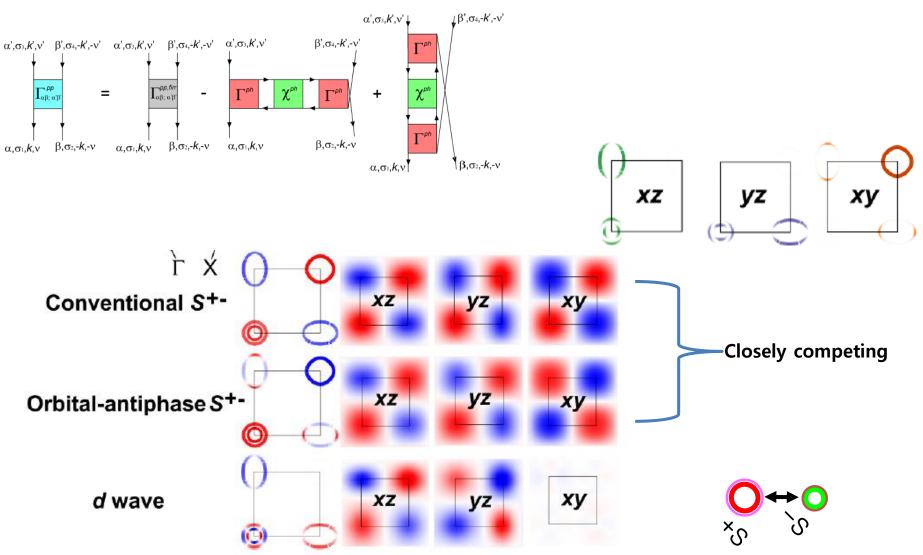
Kuroki et al JPSJ 2010

P. J. Hirschfeld, M. M. Korshunov, I. I. Mazin, Rep. Prog. Phys. 74, 124508 (2011)

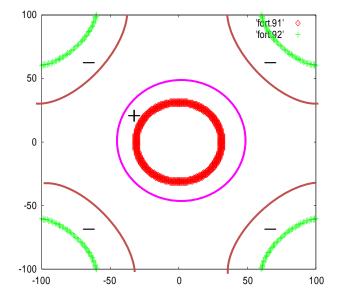
an orbital-antiphase pairing symmetry in iron-based superconductors

More variation

Z. P. Yin,* K. Haule, and G. Kotliar



Standard Paradigm of Pnictide SC



Q: Is it consistent with experiments ?

A: Almost Yes.

Experimental situation of Fe-based SC

1. Most of Experiments (90 % or more) (*ARPES, Raman, Penetration depth, Specific heat, Thermal Conductivity, NMR, etc*) are all consistent with the \pm s-wave gap.

2. Problem is : it is too boring BCS (also s-wave) SC.

Part II:

Superconducting properties of ±s-wave gap

Probing **Pairing Mechanism** is **Religion**, but

Probing **Pairing symmetry** is **Science** $!! \rightarrow$ low energy DOS N(ω , T, H)

$$\setminus \sim e^{-T/\Delta}$$

Activated laws

Many probes for $N(\omega, T, H)$:

•C(T,H)/T
•Thermal conductance κ(T, H)
•Penetration depth λ(T)
•NMR 1/T₁(T,H)
•Tunneling
•Etc.

$$\sim T^{\alpha}$$

Power laws

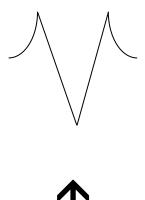
Hallmarks of **D-wave SC (Cuprates)**

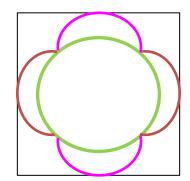
NMR $1/T_1 \sim T^3$

Pene. Depth $\lambda(T) \sim T$ Superfluidity density $\Delta \rho(T) \sim T$

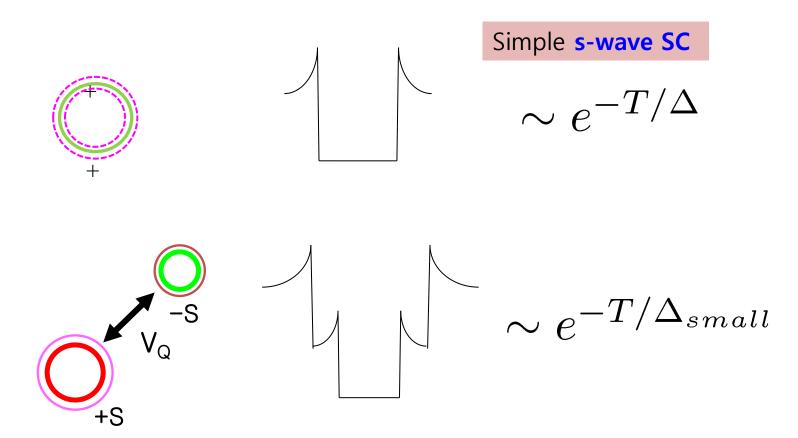
Thermal conduc. $\kappa(H) \sim H^{1/2}$

+ various power laws T^{α}

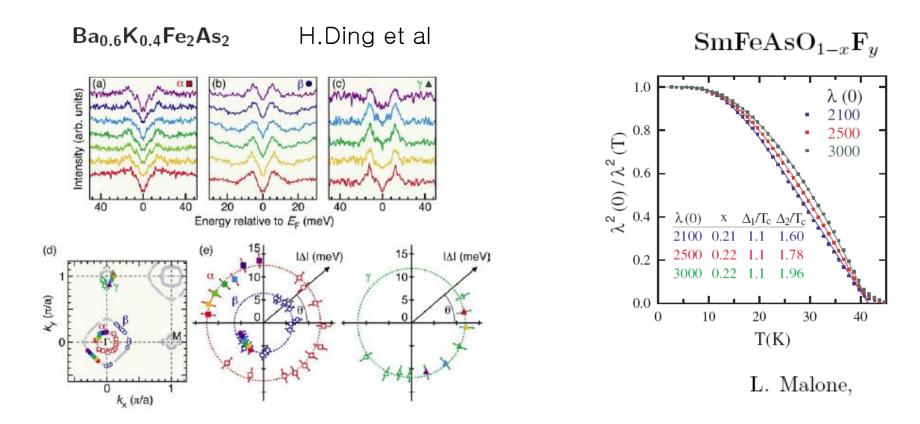




SC properties of $\pm s$ gap (Fe-SC) : exponential behaviors



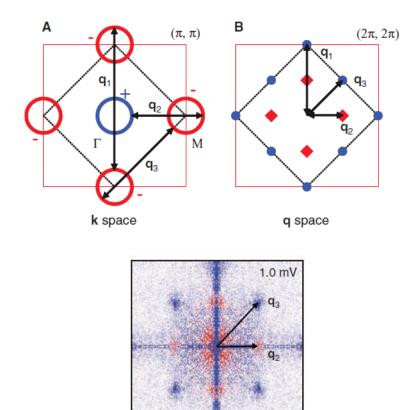
Direct Evidences of isotropic S-wave gaps



Evidence for isotropic full gaps

Unconventional *s*-Wave Superconductivity in Fe(Se,Te)

T. Hanaguri,^{1,2}* S. Niitaka,^{1,2} K. Kuroki,^{2,3} H. Takagi^{1,2,4}



q₂ point signal enhances or decreaces with B fields

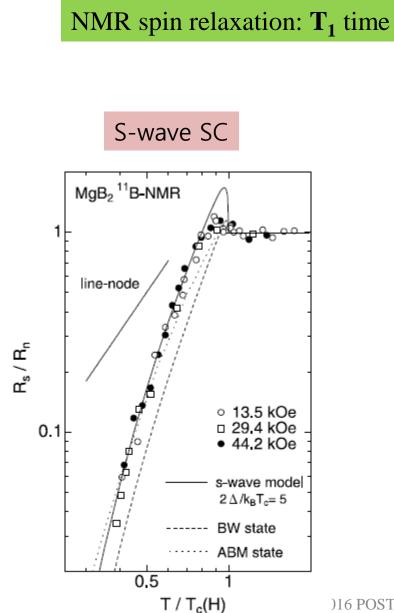
Fig. 4. Magnetic field—induced change in QPI intensities indicates the s_{\pm} -wave symmetry. Differ-

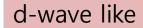
Dec.

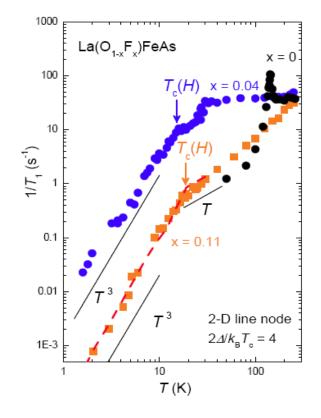
10 T

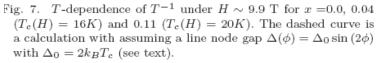
Inc.

(1) First challenge for full s-wave gap





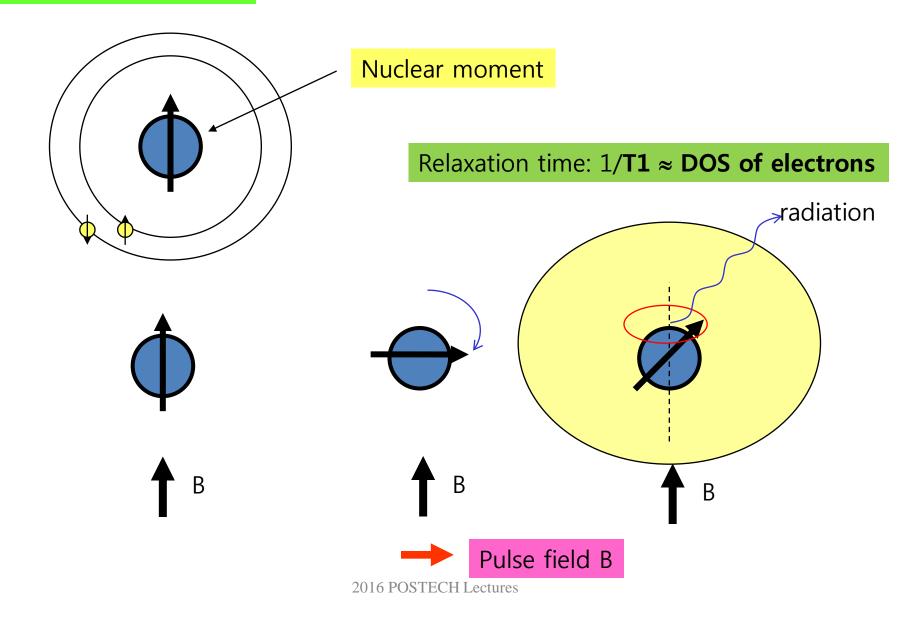




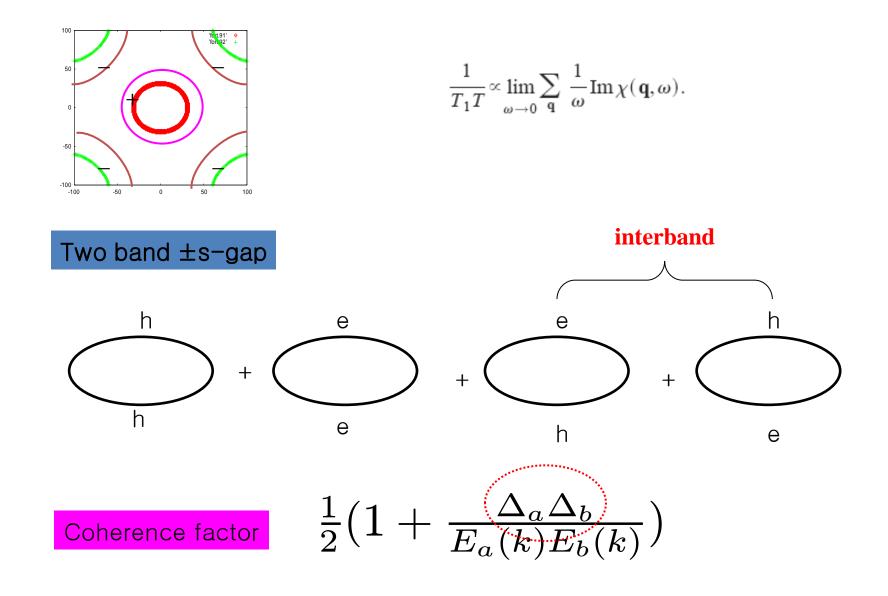
)16 POSTECH Lectures

Evidence for nodal gap

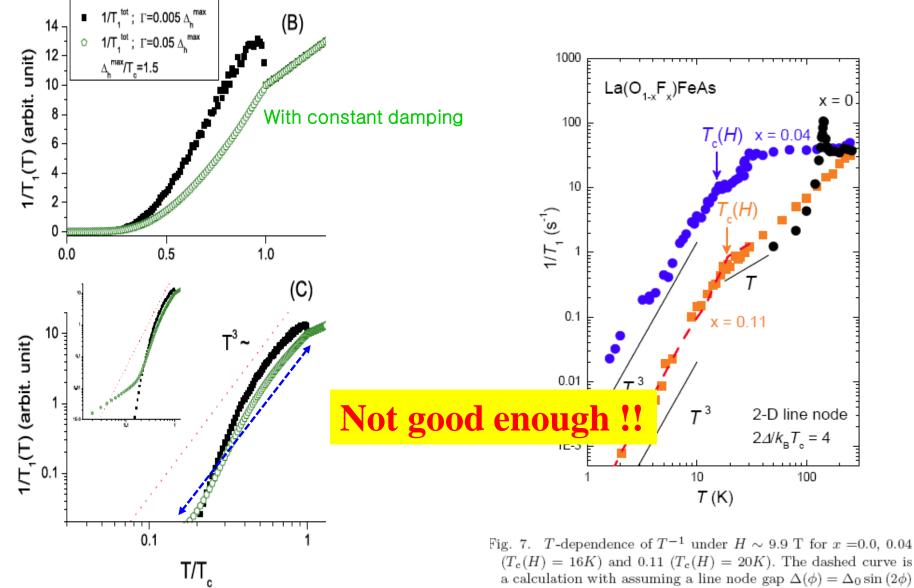
NMR cartoon picture



Spin-lattice relaxation rate 1/T₁



 $\pm \Delta$ interband term gives (-)suppression \rightarrow No Hebel-Slichter peak

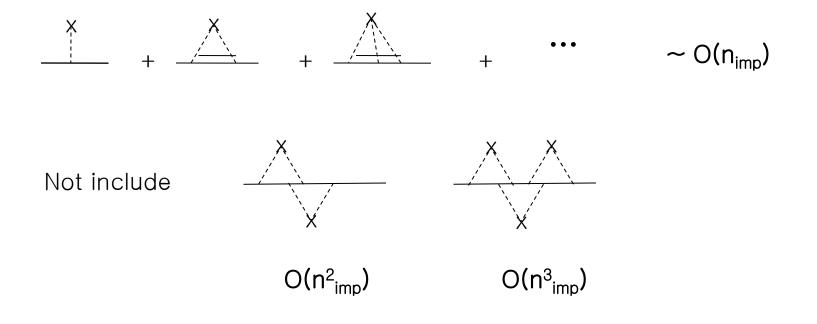


a calculation with assuming a line node gap $\Delta(\phi) = \Delta_0 \sin(2\phi)$ with $\Delta_0 = 2k_BT_c$ (see text).

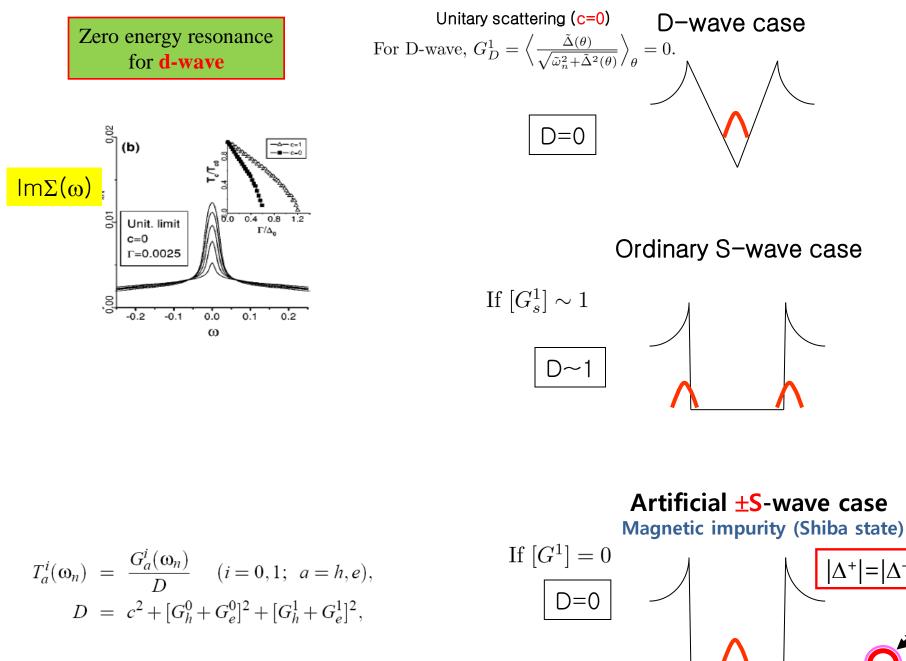
Impurity effect

T-matrix approximation for imp. scattering

(summation of a infinite series of single impurity scattering) x (imp. concentration n_{imp})



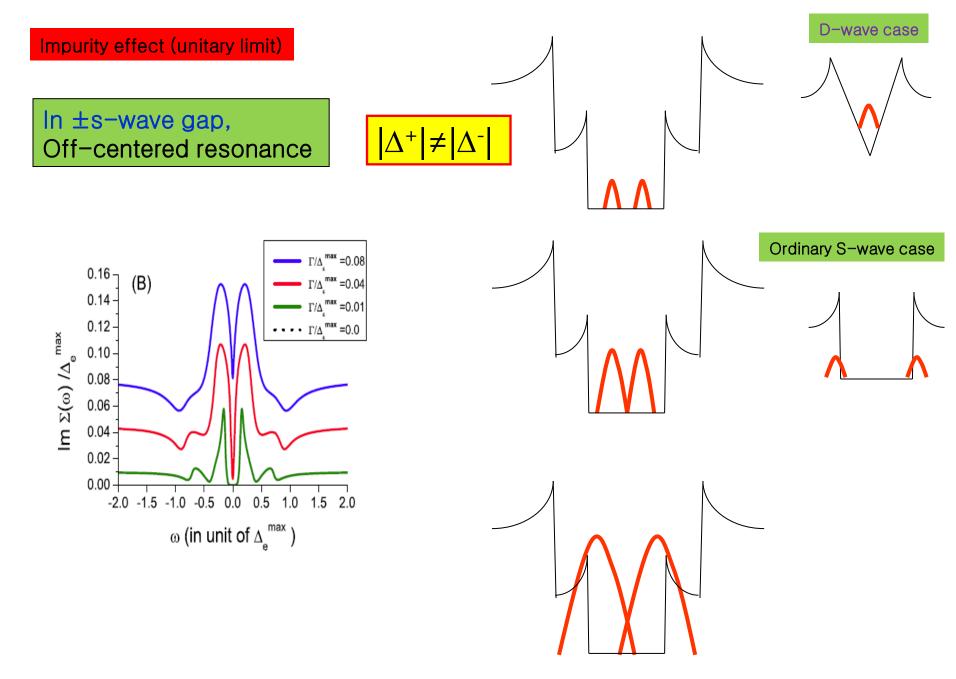
- 1. Low concentration expansion.
- 2. Interaction strength can be strong or weak.

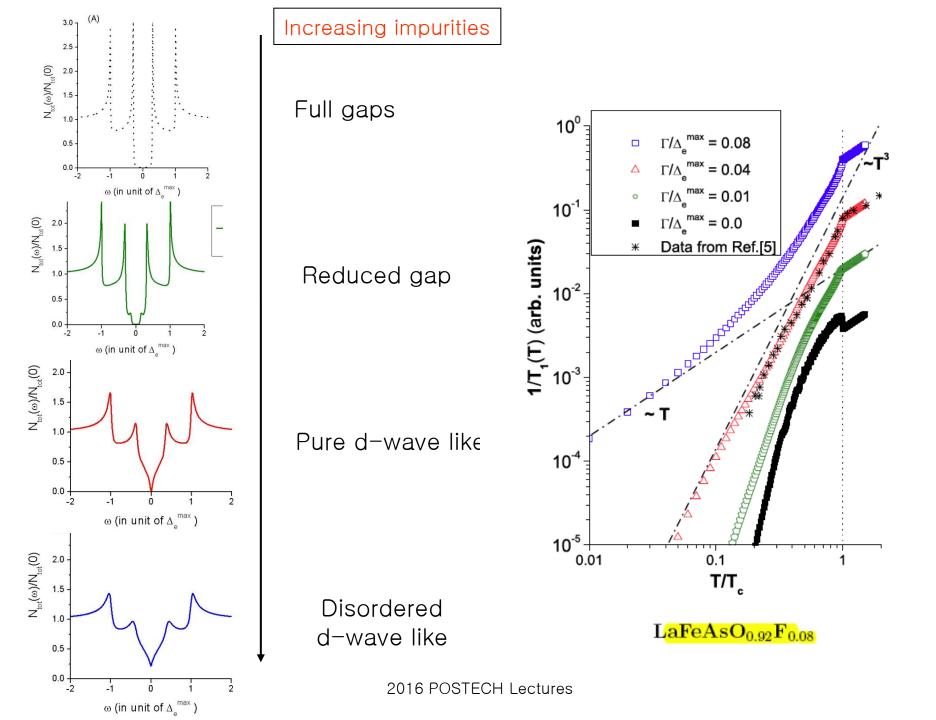


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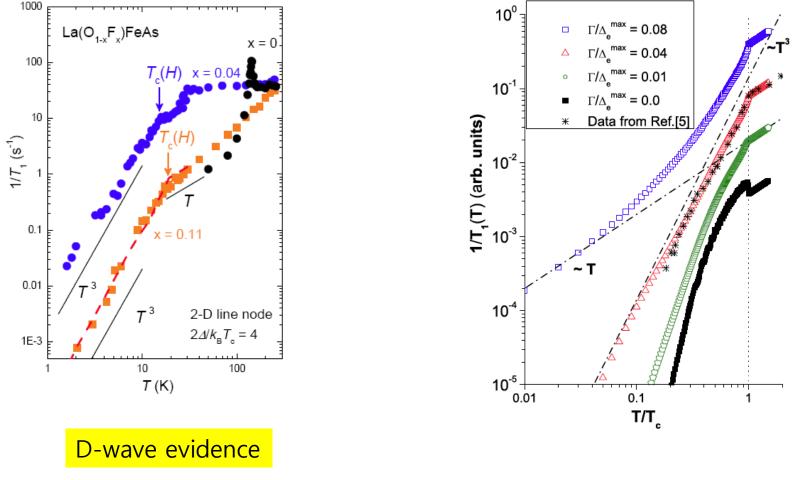
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(2) Spin-lattice relaxation rate $1/T_1 \rightarrow T^3 \rightarrow \text{lines of node (D-wave)}$

Y.Bang, PRB 79, 054529 (2009)



More consistent with $\pm S$ -wave

Y. Nakai et al, PRB 79, 212506 (2009)

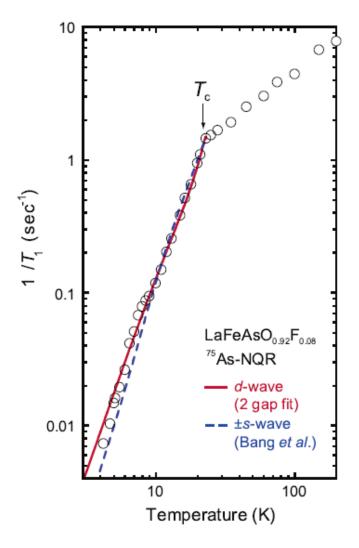
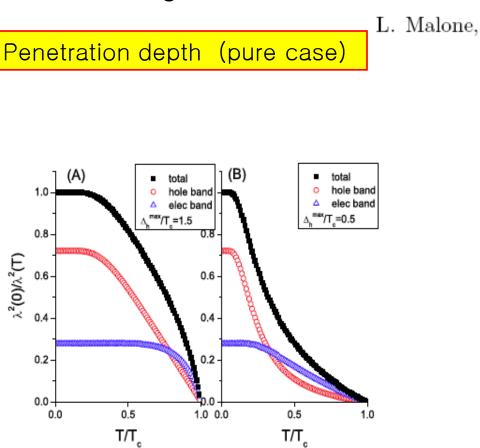


FIG. 3: (color online) The temperature dependence of $^{75}(1/T_1)$ in LaFeAsO_{0.92}F_{0.08} measured at zero magnetic field. The solid curve is a two gap fit assuming a *d*-wave symmetry with parameters, $\Delta_1(0) = 4.2k_{\rm B}T_{\rm c}$, $\Delta_2(0) = 1.6k_{\rm B}T_{\rm c}$, and $\alpha = 0.6$ (see text). The dotted curve is a simulation assuming two *s*-wave gaps that change signs with parameters, $\Delta_1(0) = 3.75k_{\rm B}T_{\rm c}$, $\Delta_2(0) = 1.5k_{\rm B}T_{\rm c}$, and $\alpha = 0.38$ referred from literature.^{30,31}2The BOETERIOV circle at the state of the st

Penetration depth $\lambda(T)$

2nd challenge



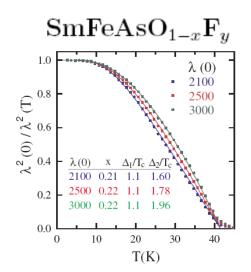
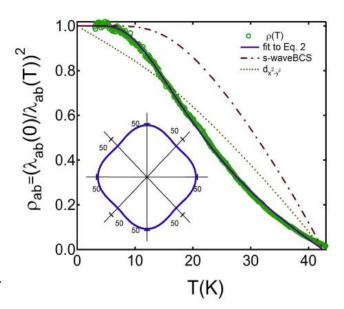


FIG. 2: (color online). Calculated normalized superfluid density $[\lambda^2(0)/\lambda^2(T)]$ versus temperature for sample #1, using different assumed values for the zero temperature penetration depth $\lambda(0)$. The solid lines are fits to the two gap model described in the text, and the inset table shows the fit parameters.



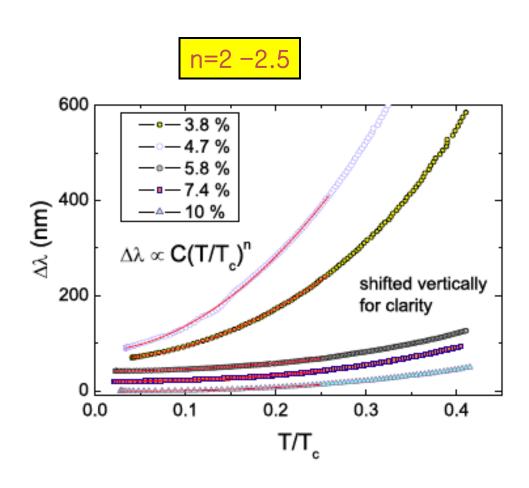


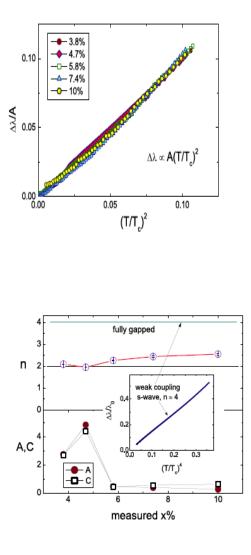
C. Martin, R. T. C P. C. Canfield,

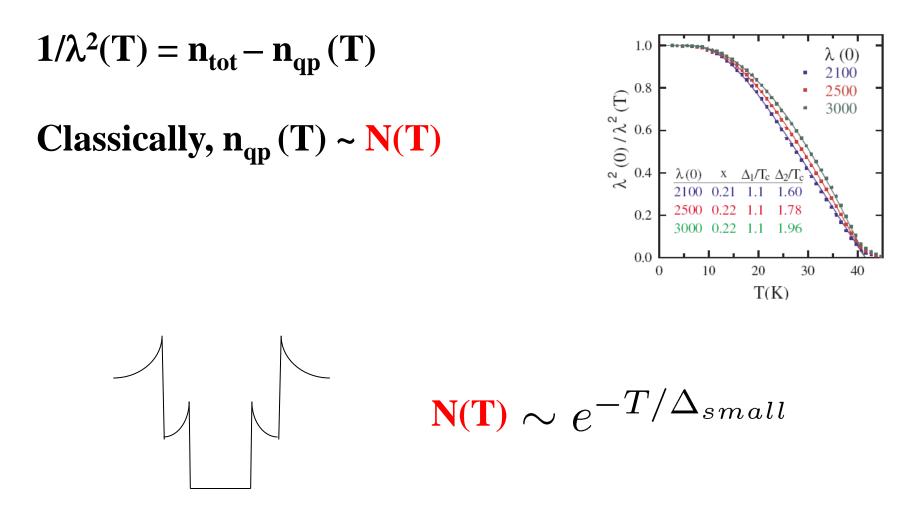
2016 POSTECH Lectu

Prozorov et al

 $Ba(Fe_{1-x}Co_x)_2As_2$

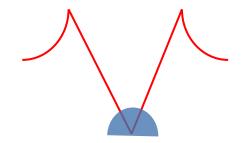




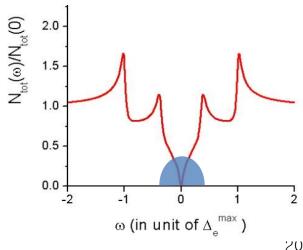


This is not exactly true with impurities.

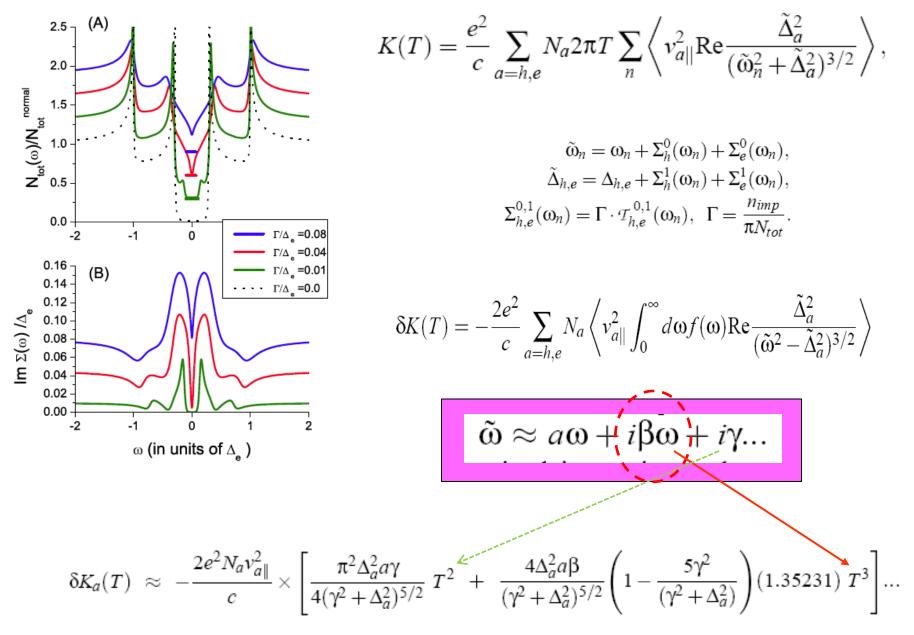
D-wave gap : kinematically driven V-shape DOS



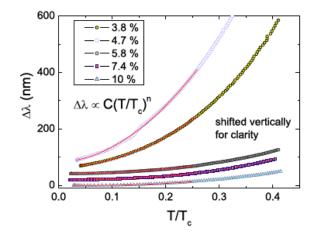
±S-wave gap : dynamically driven V-shape DOS



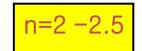
$$\delta\lambda_{const}(T) \sim T^2$$



Penetration depth $\delta\lambda(T)$

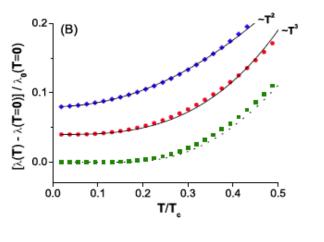


 $Ba(Fe_{1-x}Co_x)_2As_2$

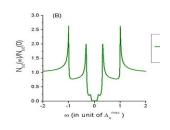


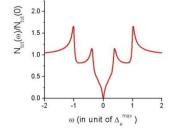
Prozorov et al, PRB 79, 100506 (2009)

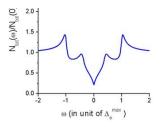
Exponentially flat \rightarrow T³ \rightarrow T²



Bang, EPL 86, 47001 (2009)







Some challenge for nodal gap ? LaFePO, $BaFe_2(As_{0.67}P_{0.33})_2$, KFe_2As_2

Some evidence for nodal gap: $\lambda(T) \sim T$

PRL 102, 147001 (2009) PH Y	PRI	L 102	147001	(2009)	PHYS
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SICAL REVIEW LETTERS

Evidence for a Nodal-Line Superconducting State in LaFePO

J. D. Fletcher,¹ A. Serafin,¹ L. Malone,¹ J. G. Analytis,² J.-H. Chu,² A. S. Erickson,² I. R. Fisher,² and A. Carrington¹ ¹H. H. Wills Physics Laboratory, University of Bristol, Tyndall Avenue, BS8 1TL, United Kingdom ²Geballe Laboratory for Advanced Materials and Department of Applied Physics, Stanford University, Stanford, California 94305-4045, USA



PRL 103, 127003 (2009)

week ending

10 APRIL 2009

Evidence for a Nodal Energy Gap in the Iron-Pnictide Superconductor LaFePO from Penetration Depth Measurements by Scanning SQUID Susceptometry

Clifford W. Hicks,¹ Thomas M. Lippman,¹ Martin E. Huber,² James G. Analytis,¹ Jiun-Haw Chu,¹ Ann S. Erickson,¹ Ian R. Fisher,¹ and Kathryn A. Moler¹ ¹Geballe Laboratory for Advanced Materials, Stanford University, Stanford, California, 94305, USA

and Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, 2575 Sand Hill Road, Menlo Park, California 94025, USA

²Departments of Physics and Electrical Engineering, University of Colorado Denver, Denver, Colorado, 80217, USA

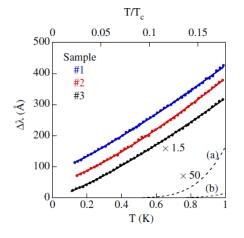


FIG. 2 (color online). Temperature dependence of the in-plane penetration depth $\Delta \lambda_a$ in three single crystals of LaFePO. Data for sample 3 has been multiplied by 1.5. The curves are offset for clarity. Solid lines are power-law fits giving an exponent of 1.2 ± 0.1 . The dashed lines are the behavior expected for a fully gapped Fermi surface (a) with parameter relevant to Sm-1111 [5] and (b) the conventional isotropic BCS case. Both curves have been multiplied by 50 for clarity.

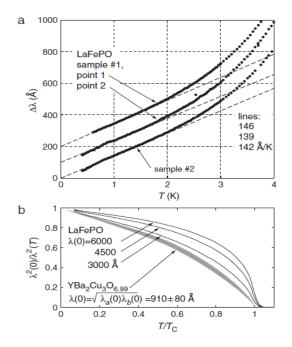
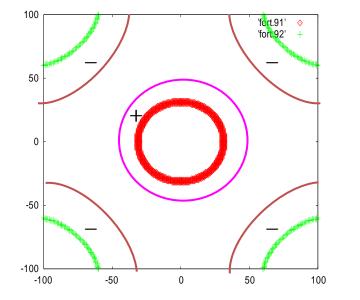
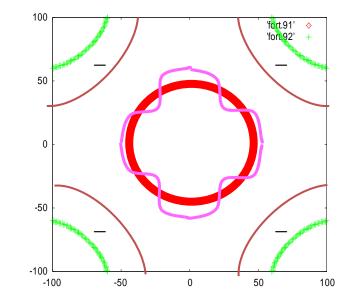


FIG. 3. Top: $\Delta\lambda$ of two LaFePO specimens, at the points indicated in Fig. 4. The lines were fit over 0.7 < T < 1.6 K. Bottom: black lines are possible superfluid densities for LaFePO sample #1, point 2, with different $\lambda(0)$. Shaded area: superfluid density of YBa₂Cu₃O_{6.99} [1/($\lambda_a\lambda_b$)], from [30,31]; the width of the shaded area reflects uncertainty in $\lambda(0)$.

Continuous evolution from $\pm S$ gap \rightarrow Nodal gap which is the same Mechanism.





±S

g+S: nodal gap (A1g) Another challenge for nodal gap

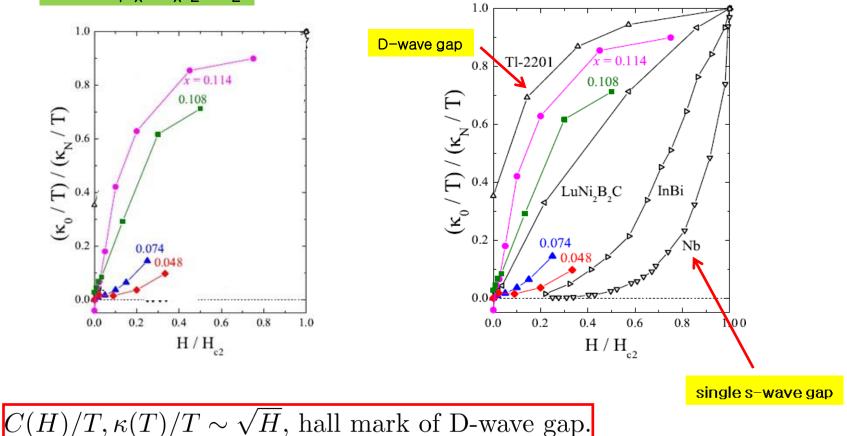
Volovik Effect : thermal conductivity κ(H)

Volovik Effect

C(T,H)/T and $\kappa(T,H)$: probe N(0,H) in mixed state with mag. field H

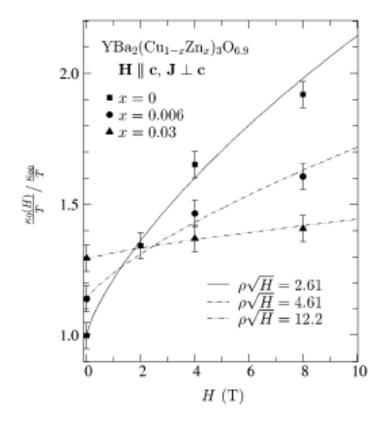
 $Ba(Fe_{1-x}Co_x)_2As_2$

M. Tanatar et al, PRL, 104, 067002 (2010)



D-wave : nodal gap $\rightarrow \kappa(H) \sim \sqrt{H}$

Volovik effect



L. Taillefer et al

But, strong field dependence is not unique with d-wave gap. Some S-wave also show strong field dependence.

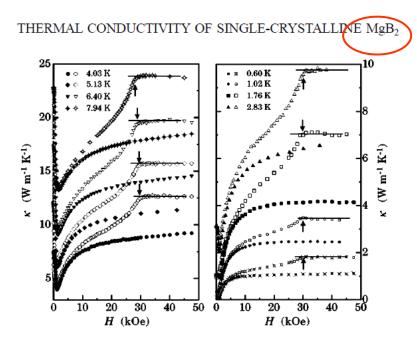
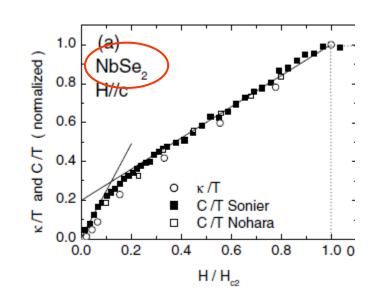


FIG. 4. Thermal conductivity in the basal plane of MgB₂ vs H at several fixed temperatures. The arrows denote the upper critical field H_{c2} for $H \| c$. The solid and open symbols correspond to the field direction perpendicular and parallel to the c axis, respectively.



$$egin{aligned} C\left(T\,,\,H\,
ight)/T &\propto & \int\,d\,\omega\,(-\,rac{\partial\,f}{\partial\,\omega})N\left(\omega\,,\,H\,
ight) \ &\kappa\left(T\,,\,H\,
ight) &\propto & \int\,d\,\omega\,(-\,rac{\partial\,f}{\partial\,\omega})S\left(\omega\,,\,H\,
ight) \end{aligned}$$

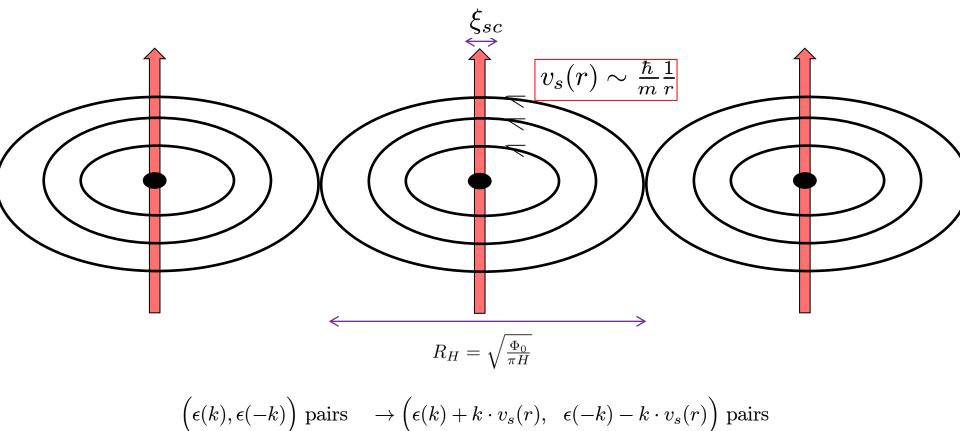
$$N(\omega, H) = \sum_{n} \delta(\omega - E_n(H))$$

$$S(\omega, H) = \sum_{n,m} v_x^2 \delta(\omega - E_n(H)) \delta(E_n - E_m)$$

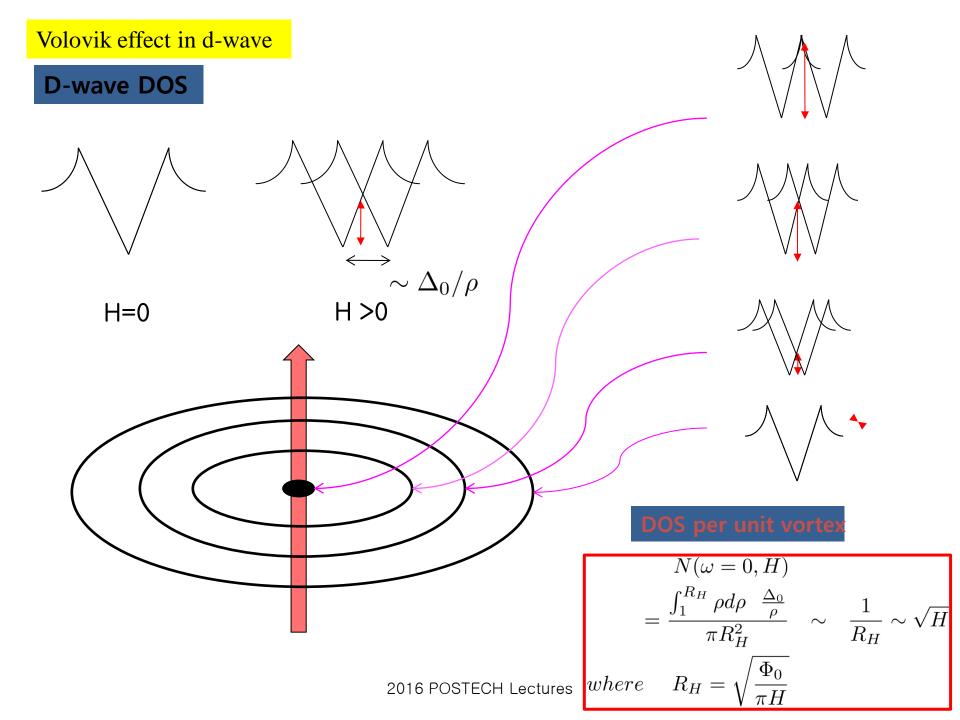
Volovik effect :

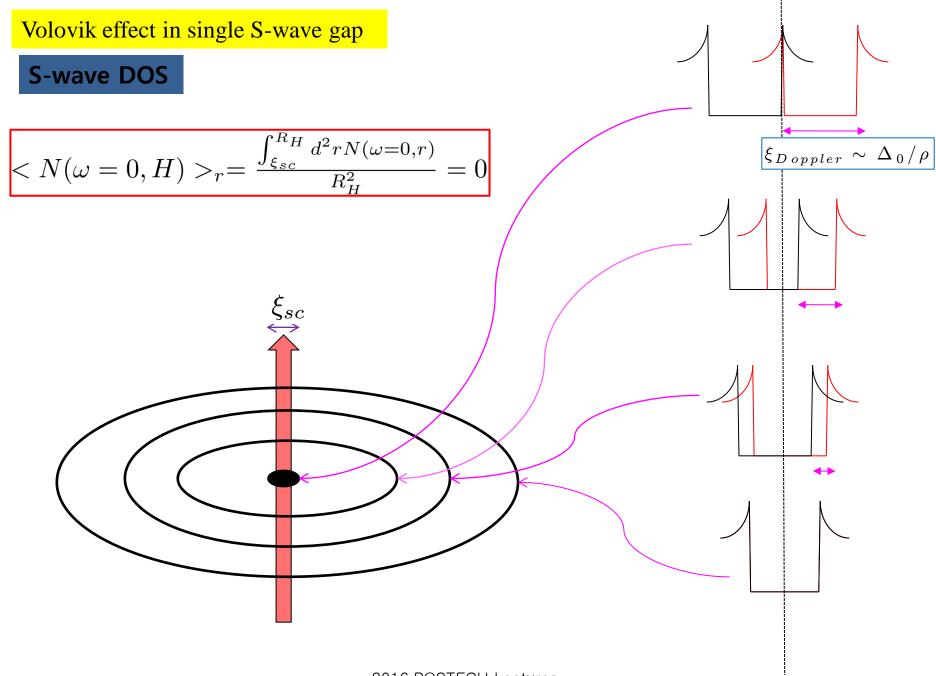
Fully Q.M treatment (Tesanovic et al, Mishra et al.)

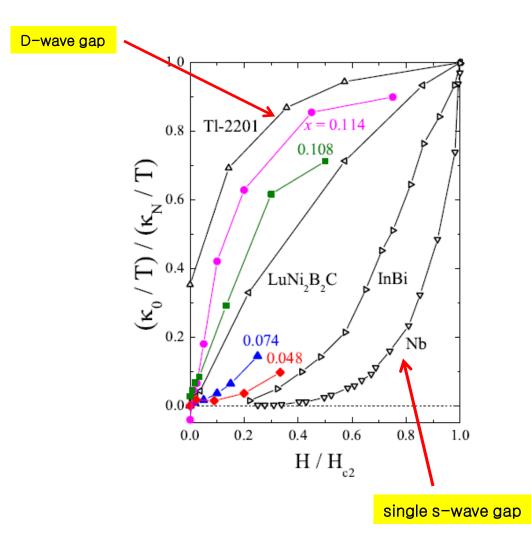
semiclassical approximation valid for $H_{c1} < H << H_{c2}$. Replace $\mathbf{A}(\mathbf{r})$ by $v_s(\mathbf{r})$ and have Doppler shift of q.p. energy ξ_k .



Pair breaking due to Doppler shift of q.p. energy

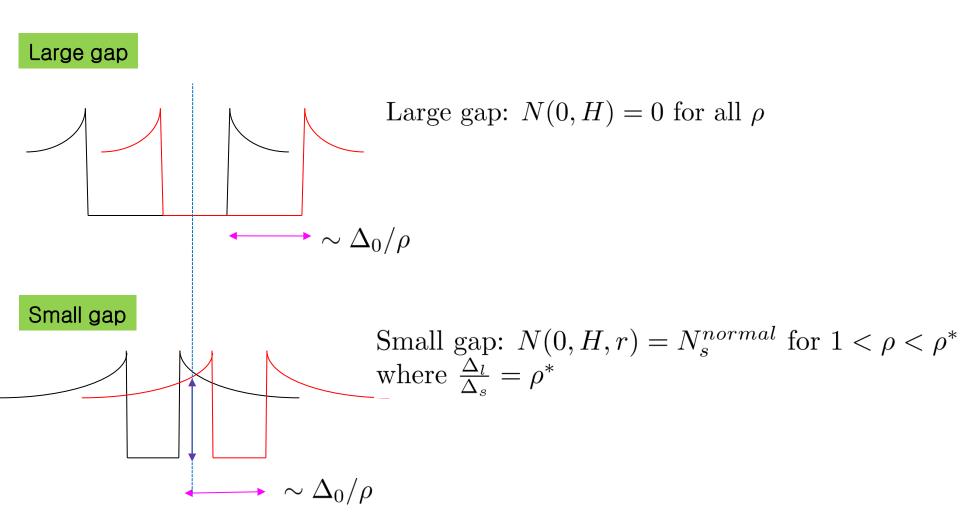




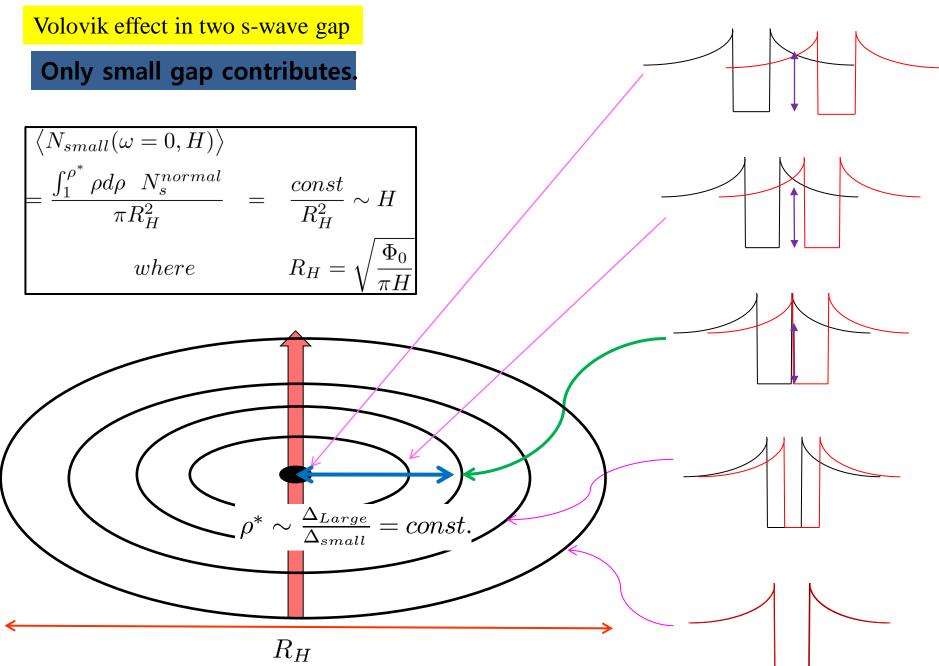








Small Gap OP doesn't collapse because Δ_{large} and Δ_{small} are coupled each other.



²⁰¹⁶ POSTECH Lectures

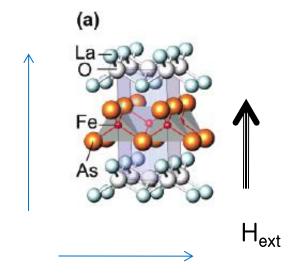
$$C(T,H) = \int d\omega < N(\omega,H) > \frac{\omega^2}{T^2} sech^2(\frac{\omega}{2T})$$

$$\kappa(T, H, r) \sim \frac{1}{T^2} \int_0^\infty d\omega \omega^2 \operatorname{sech}^2(\frac{\omega}{2T}) K_i(\omega, T, H, r)$$

where,
$$K_i(\omega, T, H, r) = \frac{1}{Im\sqrt{\tilde{z}^2 - \tilde{\Delta}_i^2}} \times \left(1 + \frac{\tilde{z}^2 - \tilde{\Delta}_i^2}{|\tilde{z}^2 - \tilde{\Delta}_i^2|}\right)$$

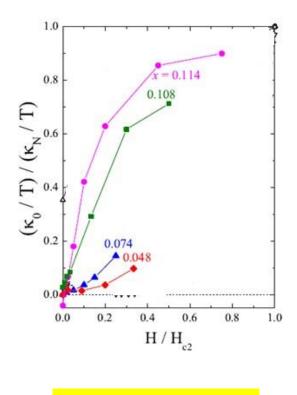
and $\tilde{z} = \tilde{\omega} + \mathbf{v}_s(\mathbf{r}) \cdot \mathbf{k}_{\mathbf{F}}$

$$\begin{split} \kappa_{\parallel}(T,H) &= \int dr^2 \kappa(T,H,r)/\pi R_H^2 \\ \kappa_{\perp}^{-1}(T,H) &= \int dr^2 \kappa^{-1}(T,H,r)/\pi R_H^2 \end{split}$$



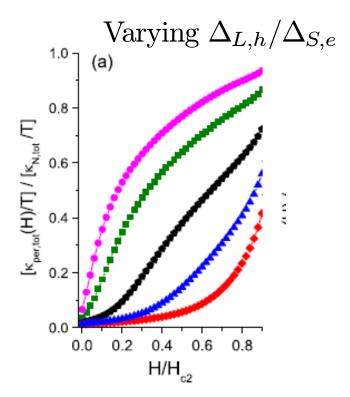
Thermal conductivity $\kappa(\mathbf{H})$: probe $N(0,\mathbf{H})$ in mixed state with mag. field \mathbf{H}

 $Ba(Fe_{1-x}Co_x)_2As_2$



D-wave evidence

M. Tanatar et al, PRL, 104, 067002 (2010)



Absolute evidence for ±S-wave

Y Bang, PRL,, 104, 217001 (2010)

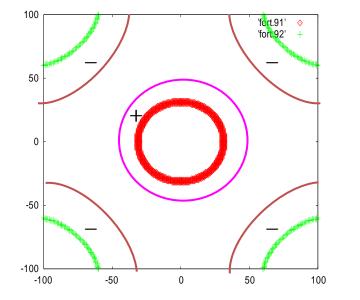
1. We have no consensus yet for a microscopic theory of IBS.

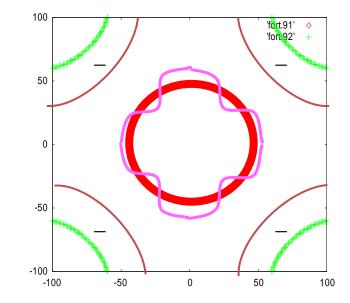
2. But, the **±s-wave gap** symmetry conforms with most of Experiments (90 % or mo (*ARPES, Raman, Penetration depth, Specific heat, Thermal Conductivity, NMR, etc*)

3. Problem is : it is too boring BCS (also s-wave) SC.

4. Some people likes to find, at least, some nodes.

Continuous evolution from \pm S gap \rightarrow Nodal gap which is the same Mechanism.





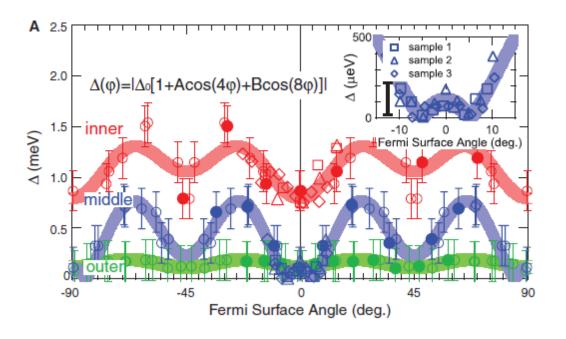
±S

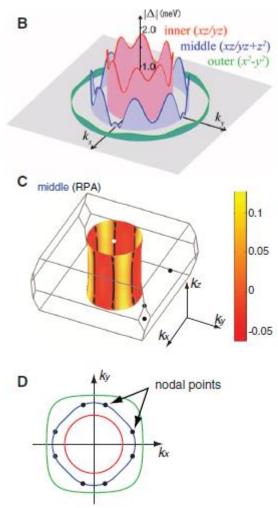
g+S: nodal gap (A1g)



Octet-Line Node Structure of Superconducting Order Parameter in KFe2As2 K. Okazaki *et al.*

Science 337, 1314 (2012);





We are obsessed with Un-conventional Superconductivity in the past 30 yrs. Many people have different meaning with it. We need to clarify our questions and wishes more clearly.

- 1. Normal state properties show abundant NFL, QC behaviors, and Mott physics.
- 2. But, all SC properties are very conventional with Cooper pairs.
- 3. Do we think a Non-BCS theory is only option for explaining high Tc?
- 4. Do we have any idea of non-BCS SC theory ?