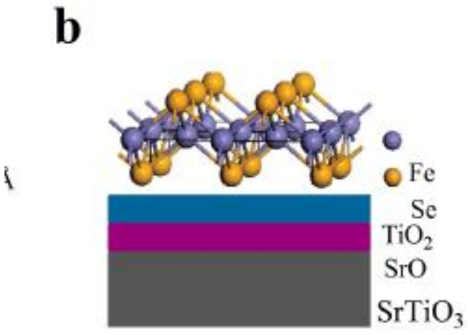
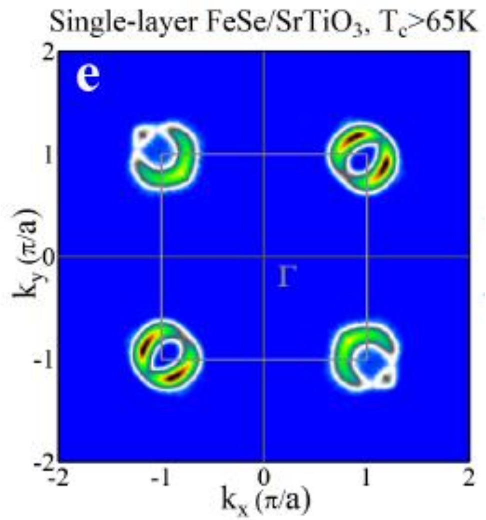
Part IV: one last challenge of IBS

Pairing Mechanism for FeSe systems:

HEDIS (highly electron doped FeSe)

FeSe Problem ?



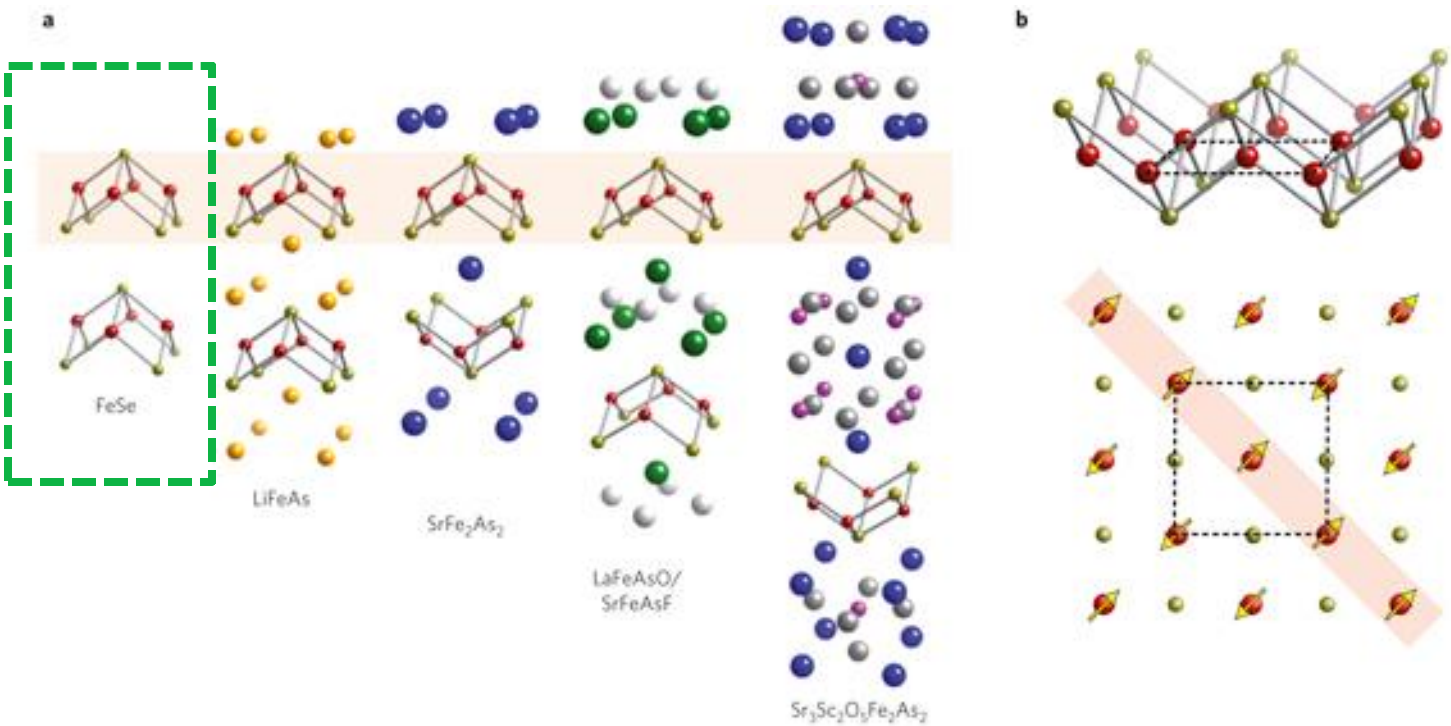


One layer system.
Only Electron pockets.
Tc ~ 100K

Standard Paradigm of IBS:
±S-wave pairing

Nature Physics (2010)
J Paglione R L. Greene

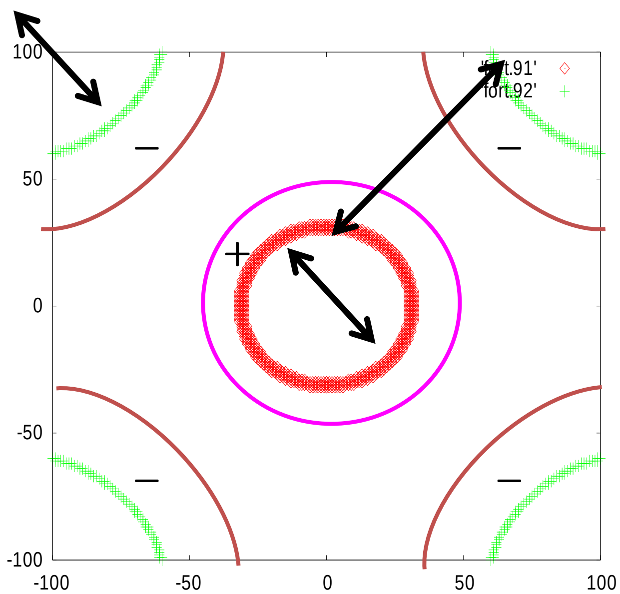
Different family of Fe/Pnctides n Fe/Chacogenides

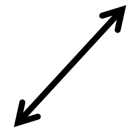


Crystallographic and magnetic structures of the iron-based superconductors.

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

±S-wave





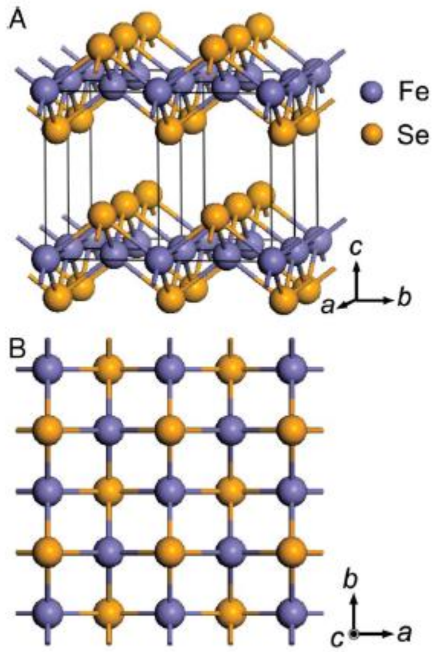
$\mathbf{V_{int}(q)}$: All repulsive interaction

Two band BCS gap Equation

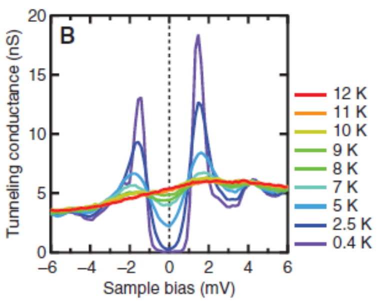
$$\Delta_h(k) = - \sum_{k'} [V_{hh}(k,k')\Delta_h(k')\chi_h(k') + V_{he}(k,k')\Delta_e(k')\chi_e(k')], \quad (5)$$

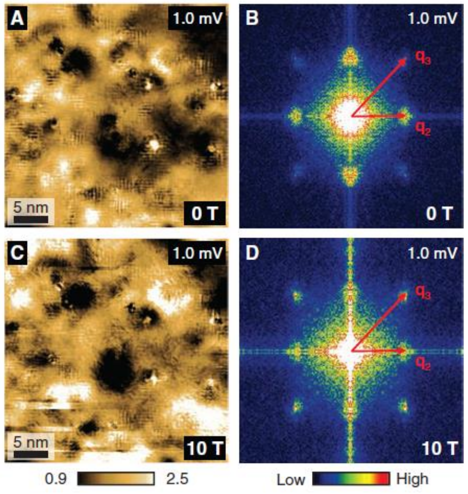
$$\Delta_e(k) = - \sum_{k'} [V_{eh}(k,k')\Delta_h(k')\chi_h(k') + V_{ee}(k,k')\Delta_e(k')\chi_e(k')]. \quad (6)$$

Bulk FeSe crystal: Tc ~8K (PNAS 2008 M.K. Wu et al.)

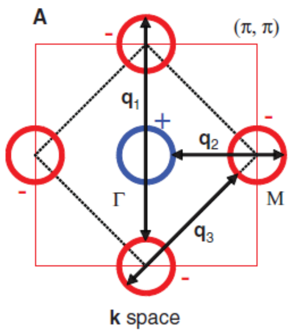


Hanaguri, Science 2010



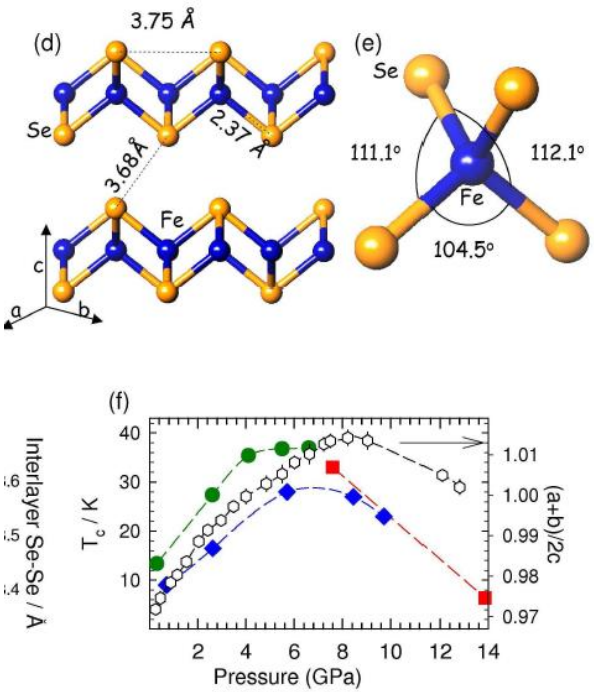


Evidence: the same **±S-wave** gap in **Bulk FeSe**



Tc increases by

1. FeSe pressure → 37K,
2. Alkali element (K,Rb,Cs,Tl)doping → 30-40K,
3. (LiFeOH)FeSe → 40K,
4. some vacancies Fe(SeTe) → 20K,
5. FeSe monolayer → **100K**

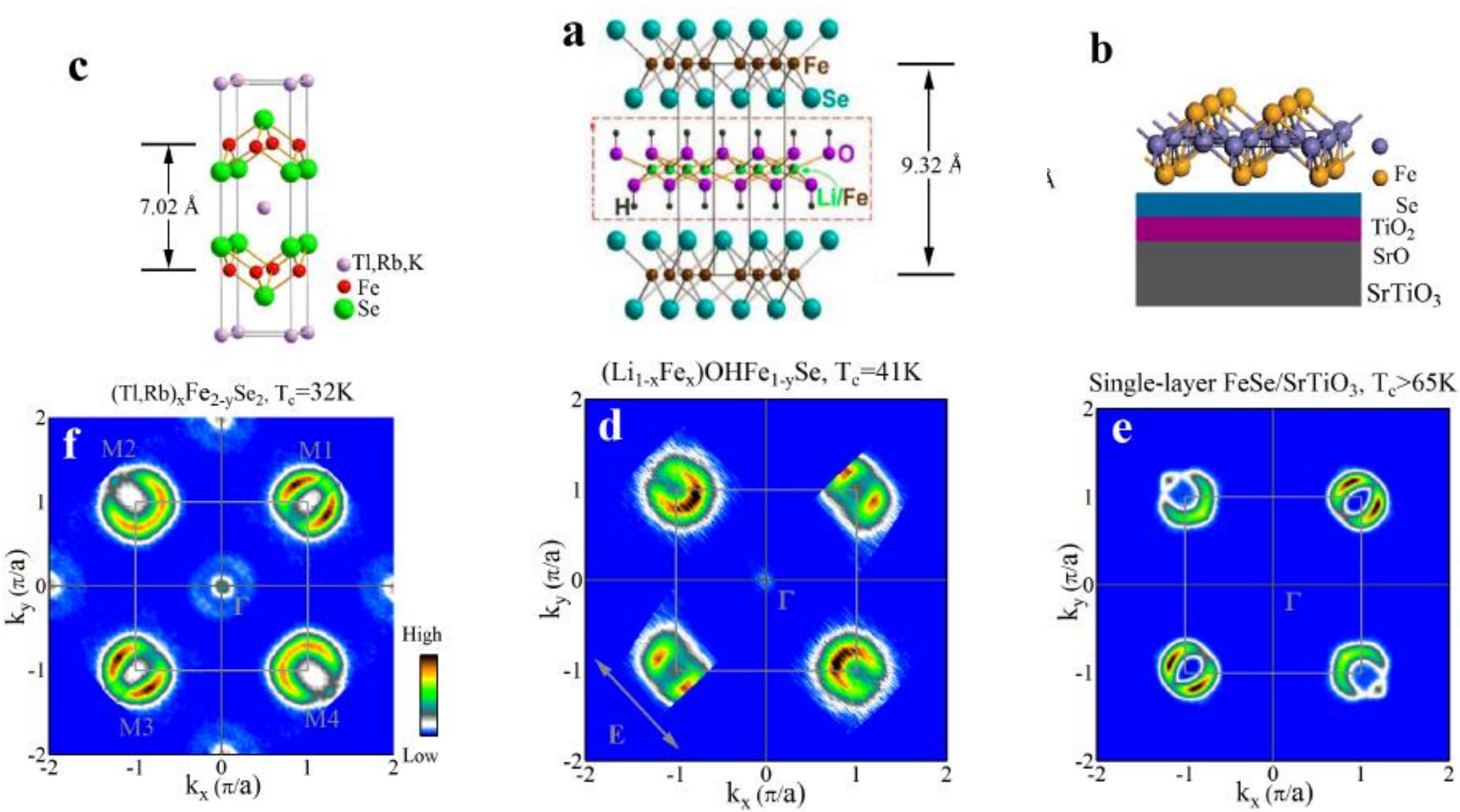


What happens ?

1. Fermi surface change ? → common
2. Magnetic fluc changes (AFM1, AFM2, FM) ?
3. Phonon ?

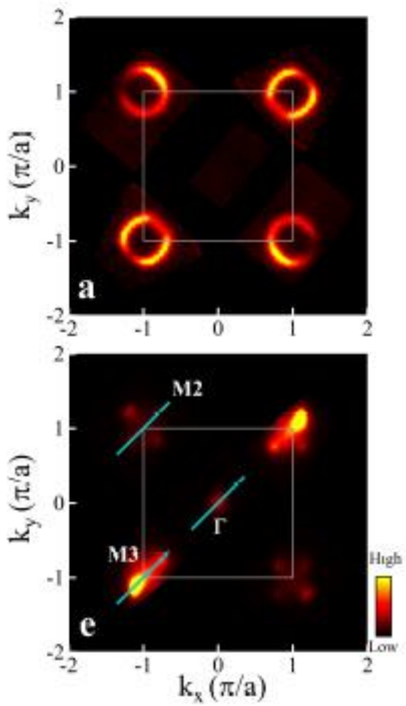
Heavily Electron Doped FeSe systems (X J Zhou et al)

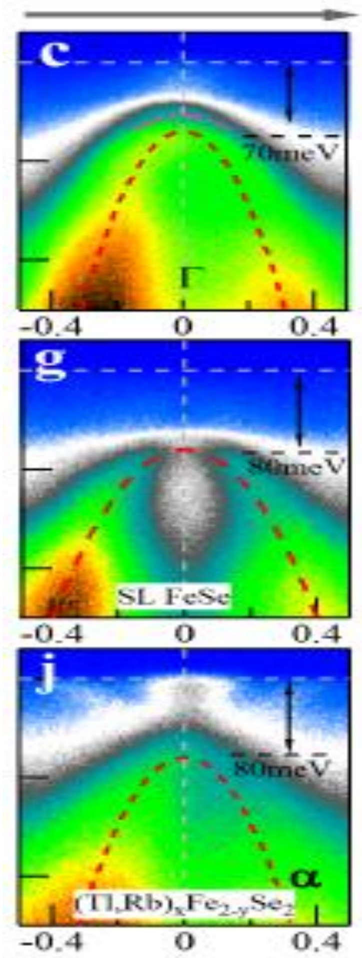
→ Main change: only electron pockets

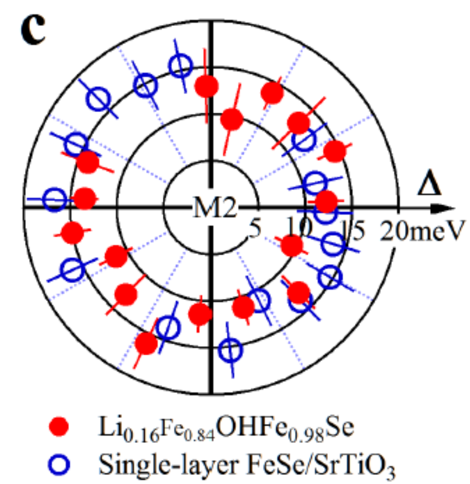


Common features:

1. No Γ band + **S-wave gap** on **M** band.

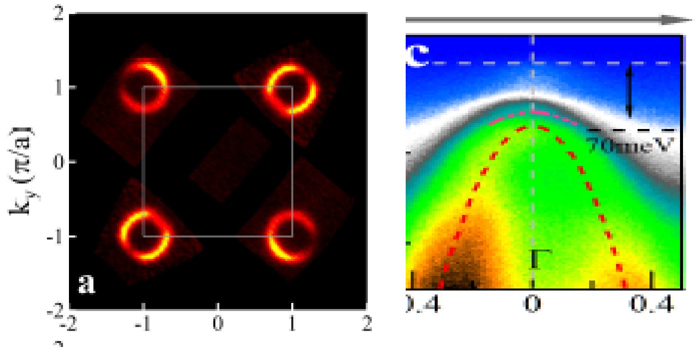


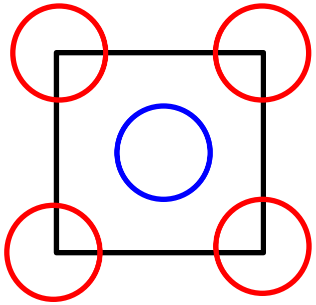




Key Questions:

1. Only Electron Band → how to pair ?
2. T_c (~ 100K) is too high.





Typical bands of Fe-based SC

Answers :

1. **Only Electron Pockets →** (Bang, NJP 2014; arXiv:1605.01509)
2. **T_c (~ 100K) is too high →** (Bang, prb 2008, 2009)

Phonon Boost Effect
for Un-conventional Superconductivity

(Bang, prb 2008, 2009)

Let us separate the questions:

1. HEDIS with only electron pockets typically have $T_{c,max}$ ~ 30-40K
2. FeSe monolayer with Tc ~100K needs **extra boosting mechanism.**

No. 2 is simple:
extra mechanism → small angle phonon + large angle AFM repulsion

$$T_c \simeq 1.14\, \omega_{sf}^{\tilde{\lambda}_{sf}} \cdot \omega_{ph}^{\tilde{\lambda}_{ph}} \;\; e^{-1/\lambda_{tot}}$$

$$\lambda_{tot} = \lambda_{sf} + \lambda_{ph}$$

$$\tilde{\lambda}_{sf} = \lambda_{sf}/\lambda_{tot}, \tilde{\lambda}_{ph} = \lambda_{ph}/\lambda_{tot}$$

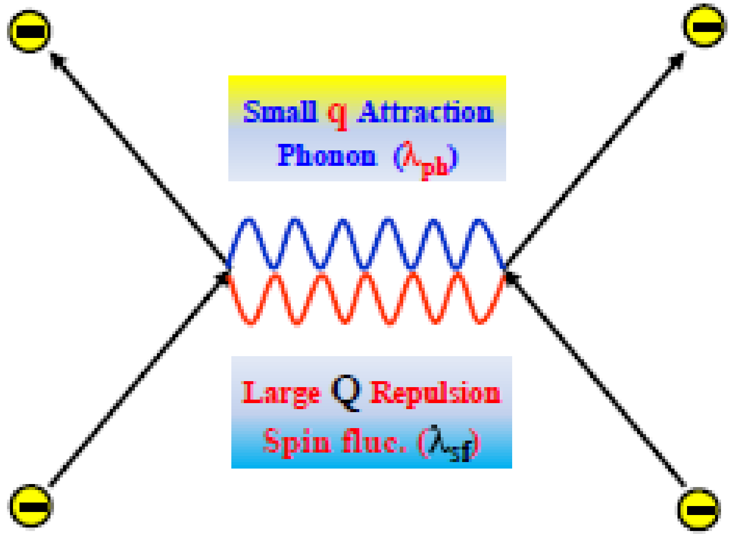
Bang, prb 78, 075116 (2008); prb 79, 092503 (2009)

Effects of phonon interaction on pairing in high-T_c superconductors

Isotope effect and the role of phonons in the iron-based superconductors

$$T_c \simeq 1.14\, \omega_{sf}^{\tilde{\lambda}_{sf}} \cdot \omega_{ph}^{\tilde{\lambda}_{ph}} \;\; e^{-1/\lambda_{tot}}$$

$$\lambda_{tot} = \lambda_{sf} + \lambda_{ph}$$



Both interactions utilize different mom. Spaces !!

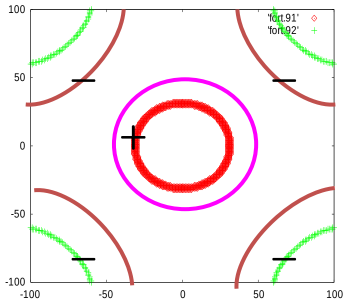
Simple toy model

Bang, PRB 78 (2008), 79(2009)

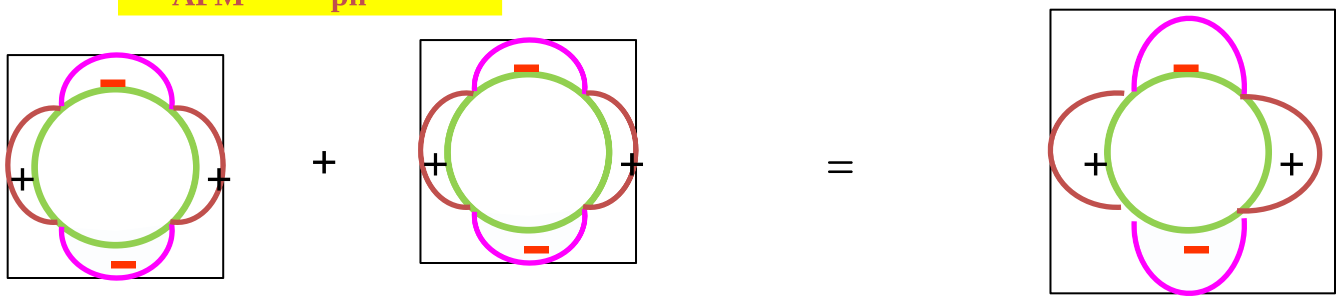
$$H = \sum_{k\sigma} \epsilon(k) c^{\dagger}_{k\sigma} c_{k\sigma} + \sum_{kk'\uparrow\downarrow} V_{\rm AFM}(k,k') c^{\dagger}_{k\uparrow} c^{\dagger}_{-k\downarrow} c_{k'\downarrow} c_{-k'\uparrow},$$

$$\sum_{kk'\uparrow\downarrow} V_{\rm ph}(k,k') c^{\dagger}_{k\uparrow} c^{\dagger}_{-k\downarrow} c_{k'\downarrow} c_{-k'\uparrow},$$

$\pm S_{AFM} + S_{ph}$ wave



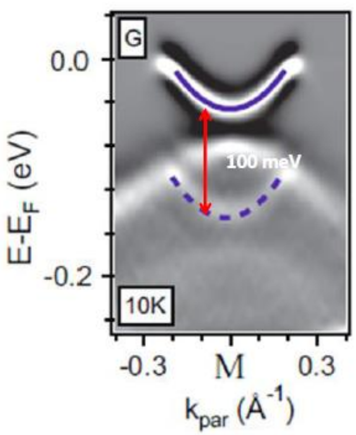
$D_{AFM} + D_{ph}$ wave



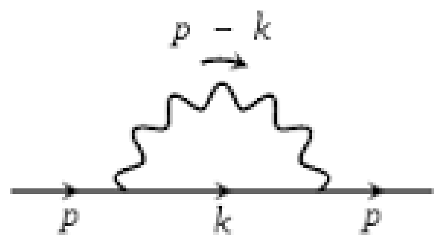
Required condition: **small angle phonon interaction**

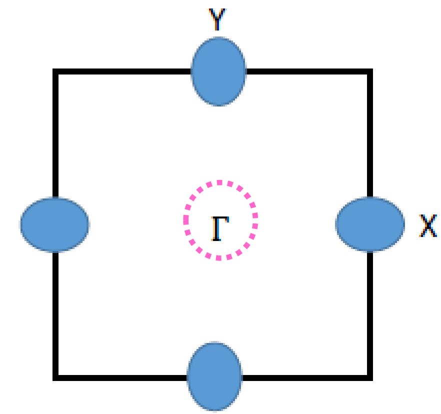
T_c (~ 100K) is too high.

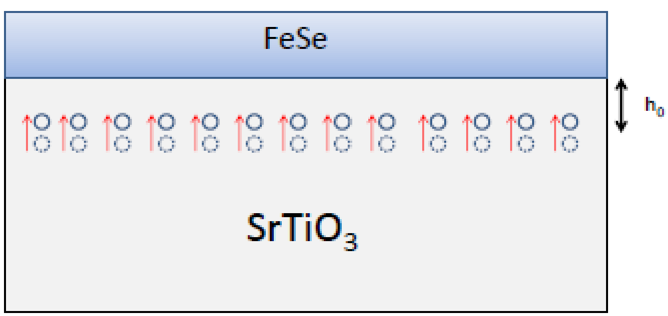
Evidence for small angle phonon + strong coupling



ZX Shen et al 2014

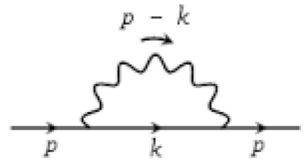




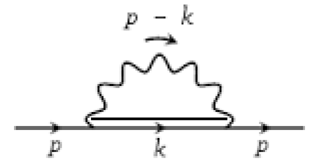


DH Lee 2015, ***small angle phonon scattering***

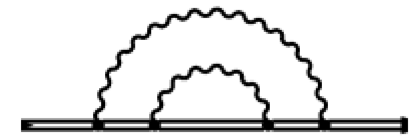
In reality,

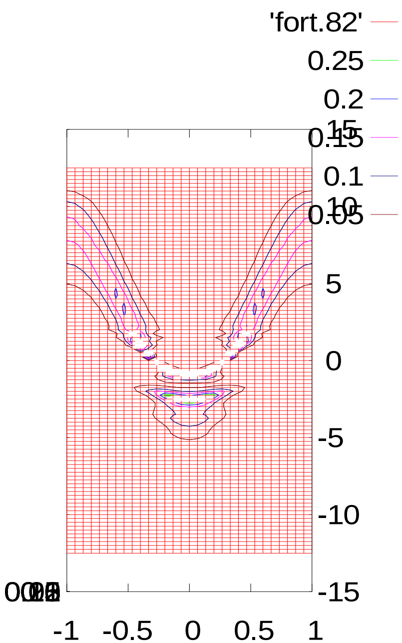


p − k
p
k
p

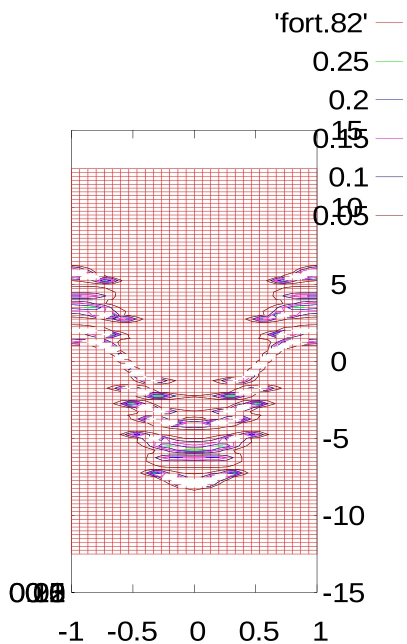


p − k
p
k
p

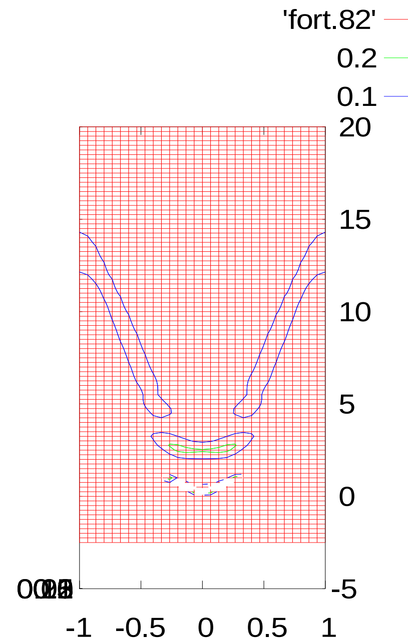




'fort.82'
0.25
0.2
0.15
0.1
0.05



'fort.82'
0.25
0.2
0.15
0.1
0.05



'fort.82'
0.2
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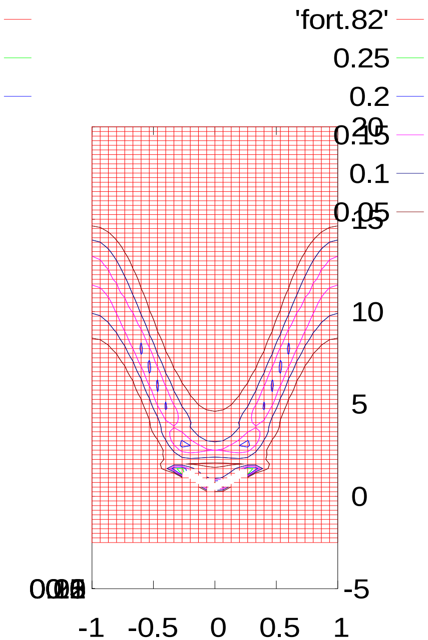

'fort.82'
0.25
0.2
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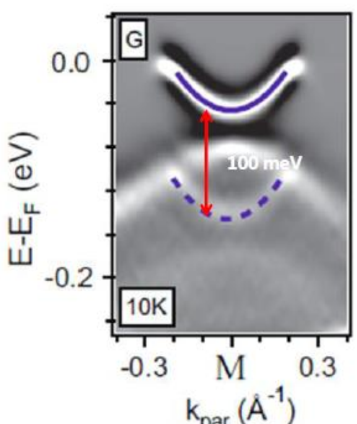
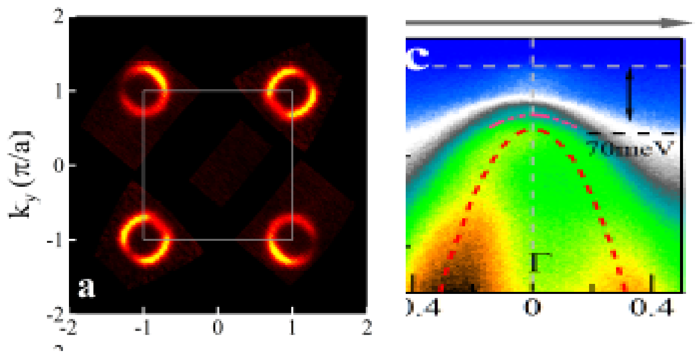
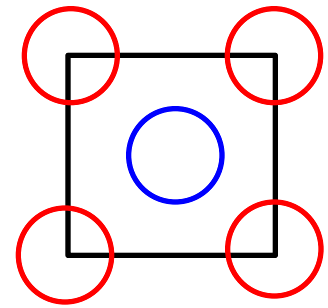


G
100 meV
10K
0.0
-0.2
E-E$_F$ (eV)
-0.3
M
0.3
k$_{par}$ (Å^{-1})

More difficult question:

1. Pairing with only electron pockets : $T_{c,max}$ ~ 30-40K





Typical bands of Fe-based SC

$T_{c,max}$ ~ 30-40K

$T_{c,max}$ ~ 30-50K

Pairing is possible with the same V_{sf} interaction, but **Tc should decrease**.
- *Bang NJP 2014*

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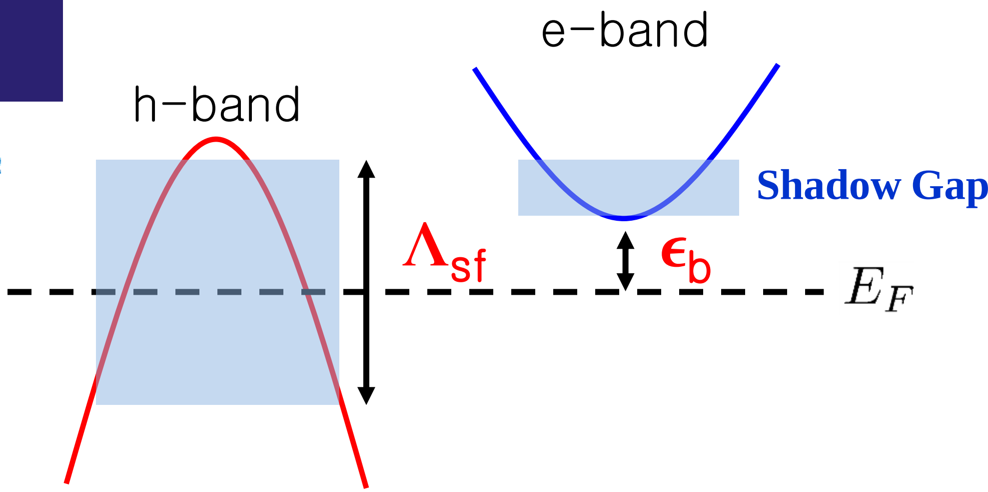
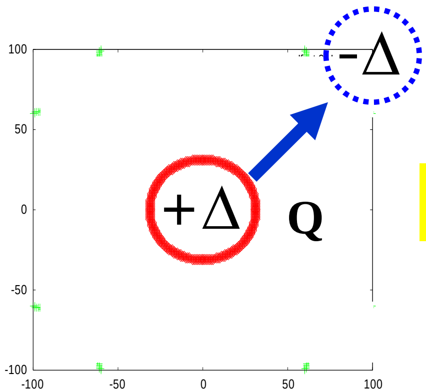
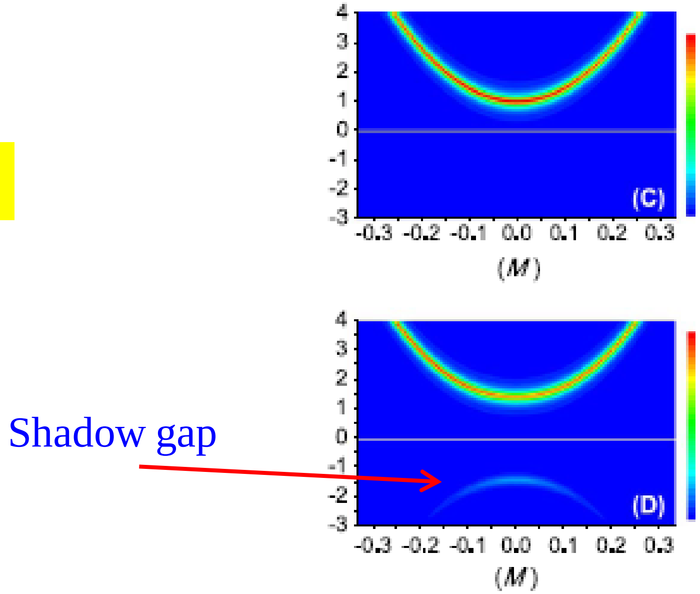
A shadow gap in the over-doped $(Ba_{1-x}K_x)Fe_2As_2$ compound

Yunkyu Bang





Hidden ±S-gap

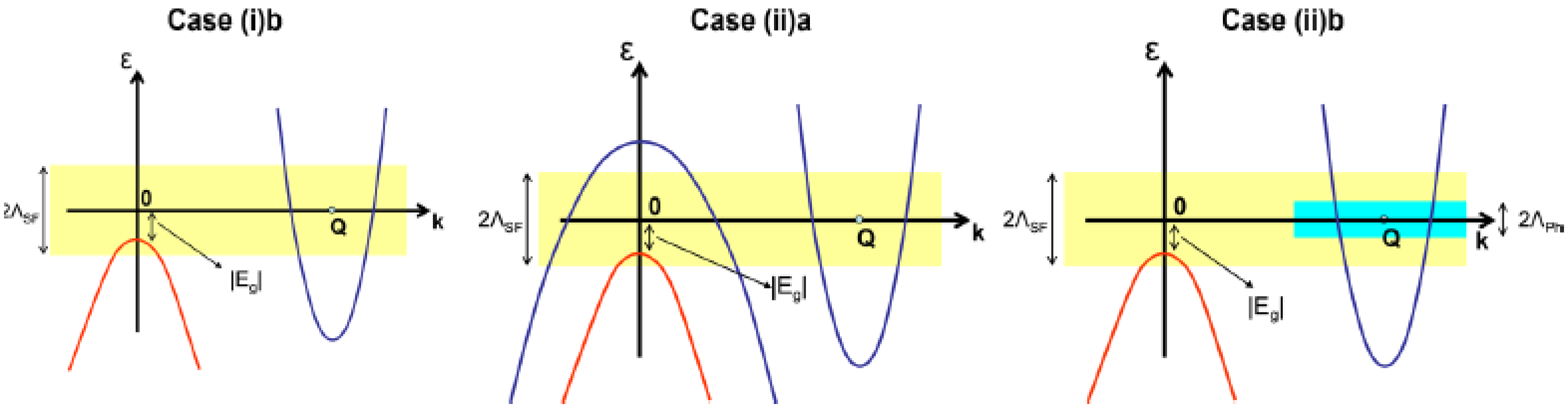


Electron pockets sink down Now !!.

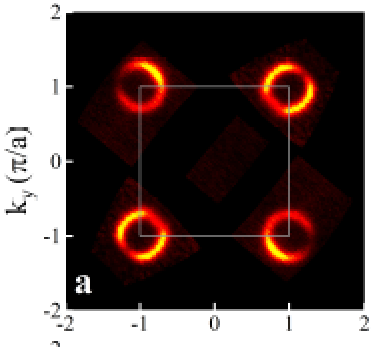
PHYSICAL REVIEW B **92**, 224514 (2015)

Electron pairing in the presence of incipient bands in iron-based superconductors

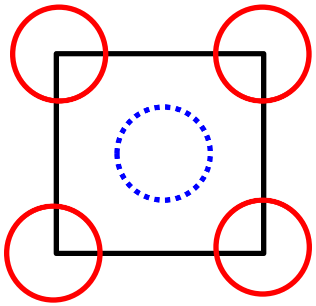
Xiao Chen,[1] S. Maiti,[1,2] A. Linscheid,[1] and P. J. Hirschfeld[1]



So, only Electron Band → No problem



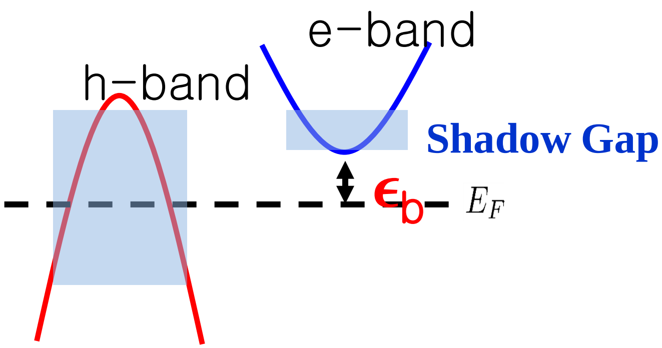
$$\Delta_h(k) = \quad (5)$$
$$- \sum_{k'} [V_{hh}(k,k')\Delta_h(k')\chi_h(k') + V_{he}(k,k')\Delta_e(k')\chi_e(k')],$$
$$\Delta_e(k) =$$
$$- \sum_{k'} [V_{eh}(k,k')\Delta_h(k')\chi_h(k') + V_{ee}(k,k')\Delta_e(k')\chi_e(k')]. \quad (6)$$

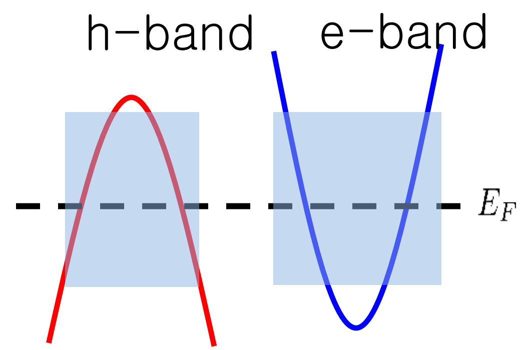


$$\chi_{h,e}(T) = \int_0^{\Lambda_{hi}} \frac{d\xi}{\xi} \tanh\left(\frac{\xi}{2T}\right) \approx \ln\left[\frac{1.14\Lambda_{hi}}{T}\right]$$

$$\chi_e = \int_{\epsilon_b}^{\Lambda_{hi}} \frac{d\xi}{\xi} \tanh\left(\frac{\xi}{2T}\right) \approx \ln\left[\frac{1.14\Lambda_{hi}}{\epsilon_b}\right]$$

But **Tc decreases** with sunken band for a given V_{AFM} (Q)



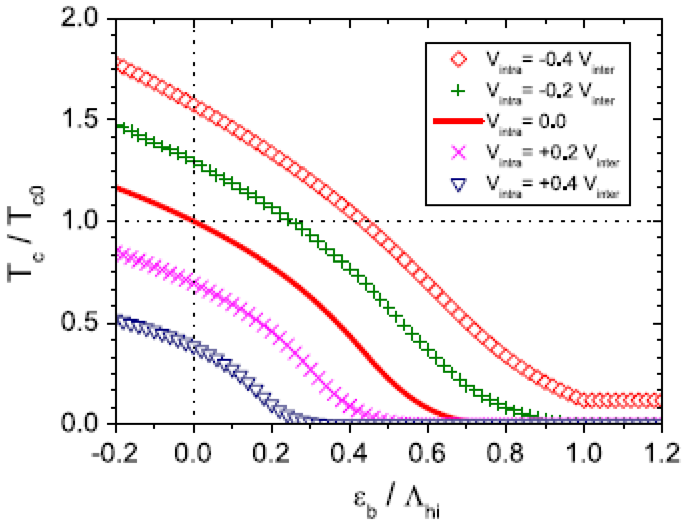


$$\tilde{\lambda}_{eff} = [\bar{V}_{he} N_e \bar{V}_{eh} N_h] \cdot \ln\left[\frac{1.14\Lambda_{hi}}{\epsilon_b}\right]$$

$$\tilde{\lambda}_{eff} = \sqrt{\bar{V}_{he} N_e \bar{V}_{eh} N_h}$$

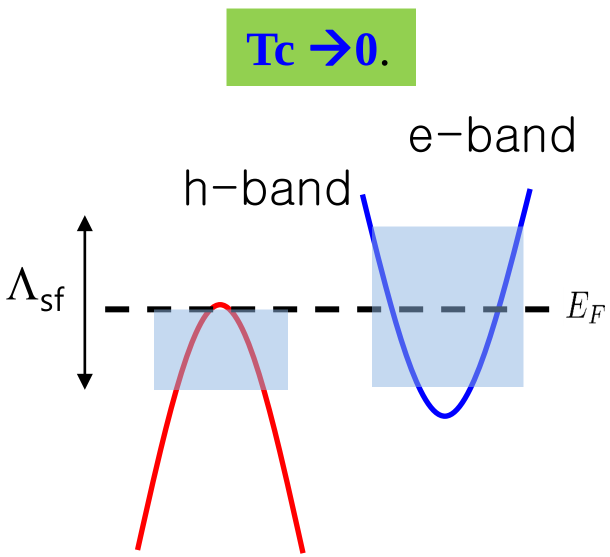
Assuming only interband V_{he}

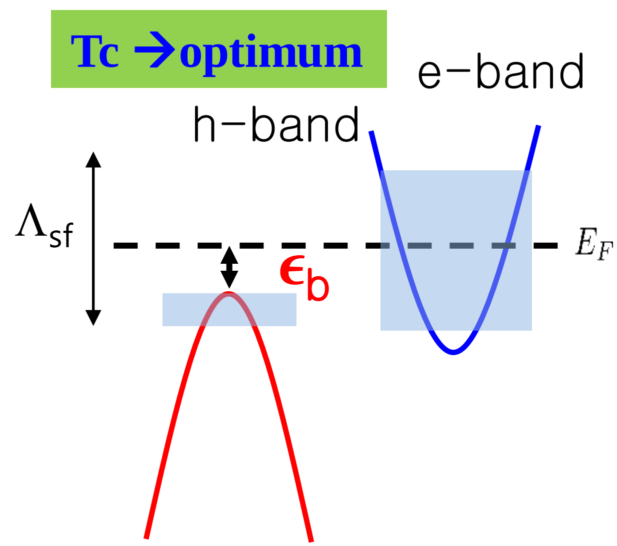
$$T_c(\epsilon_b) \approx 1.14\Lambda_{hi} \exp\left[-1/\tilde{\lambda}_{eff}(\epsilon_b)\right]$$



One problem of this incipient band model: optimal ϵ_b ~ 60-80 meV ?

In real materials, Tc →0 as ϵ_b →0 ?
Opposite trend to the incipient band pairing scenario.





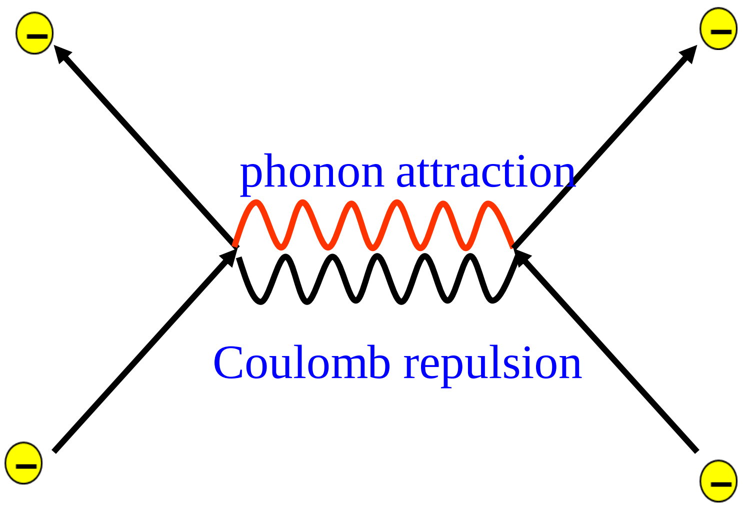
1. **±S-gap** solution with higher Tc without impurity
2. but impurity pair-breaking effect severely suppresses **Tc →0**.

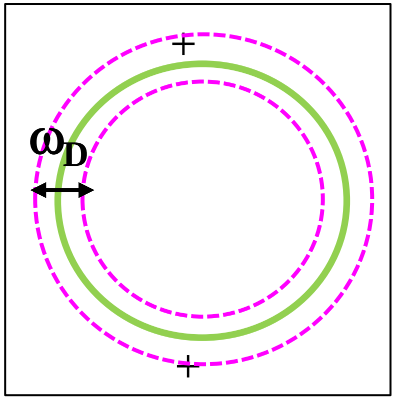
1. Without impurity, T_c is lower.
2. **±S-gap** and **++S_{ee}-gap** solutions are degenerate, with the same Tc
3. **++S_{ee}-gap** solution is robust against impurities.

New Concept:

Dynamical Tuning of pairing Cutoff

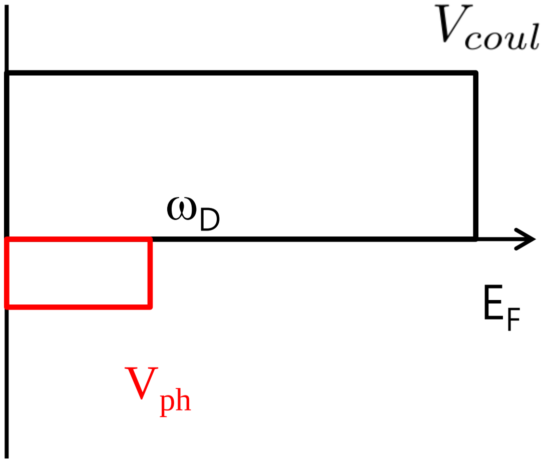
BCS theory:





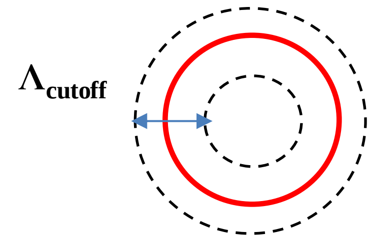
S-wave gap

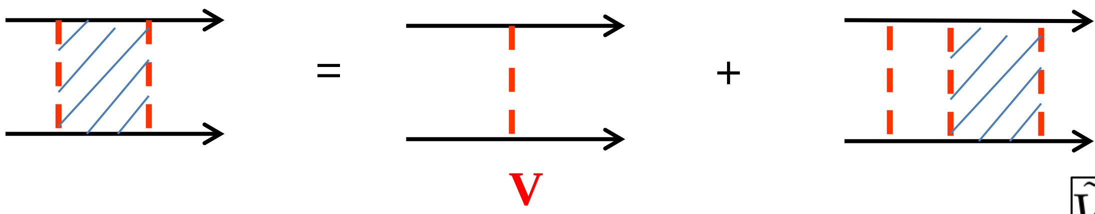
Bare elec-elec int. is strongly repulsive.



RG scaling for **S_{ee}-wave gap solution**

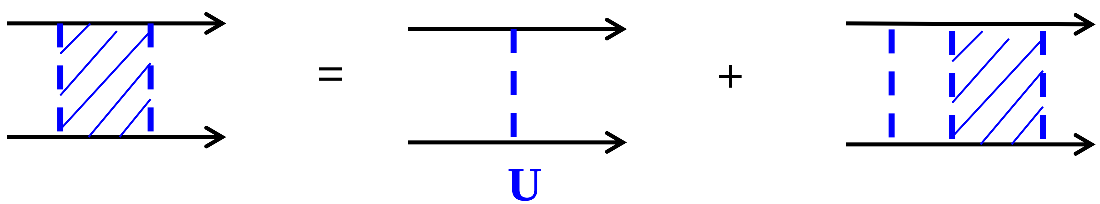
pairing interaction : Cooperon propagator

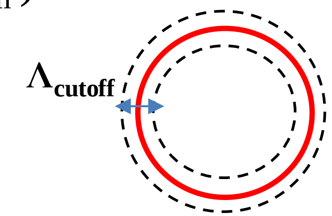




$$\tilde{V} = \frac{V}{1+VN(0)\log\frac{E_F}{T}}$$

RG process of pairing interaction (reduce Λ_{cutoff} from E_f to ω_m)





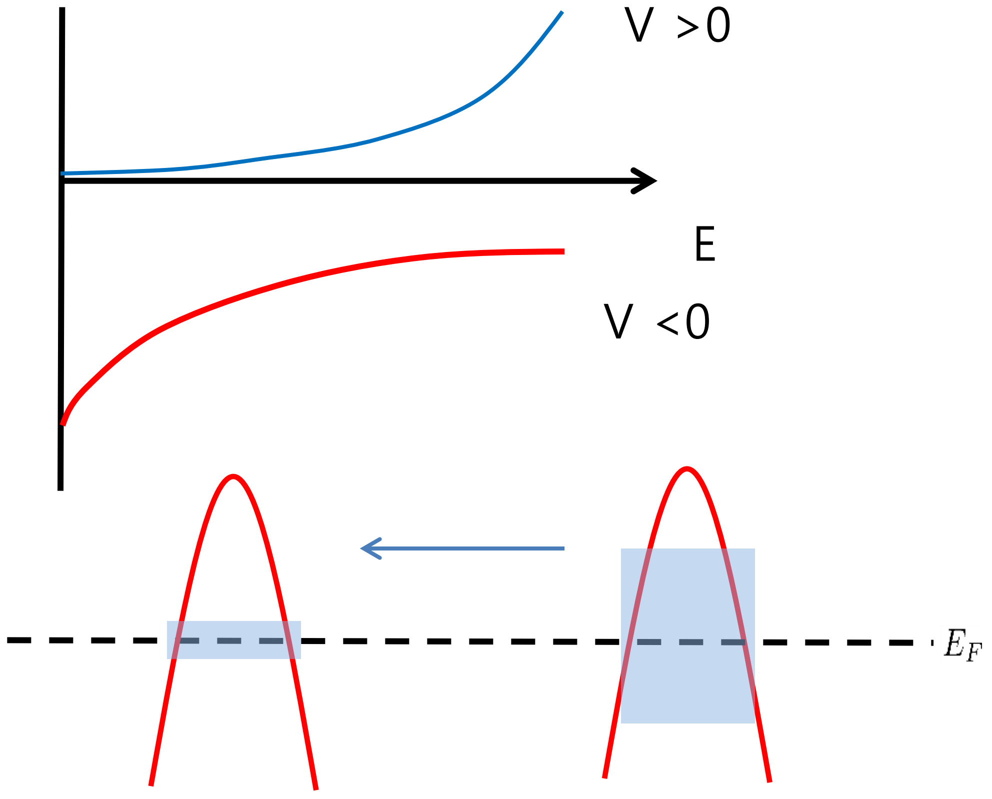
$$V_{tot} = \frac{V}{1+VN(0)\log\frac{E_F}{T}} = \frac{U}{1+UN(0)\log\frac{\omega_m}{T}}$$

with $\omega_m < E_F$

$$U = \frac{V}{1+VN(0)\log\frac{E_F}{\omega_m}}$$

Renormalized int. **U** from original **V**.

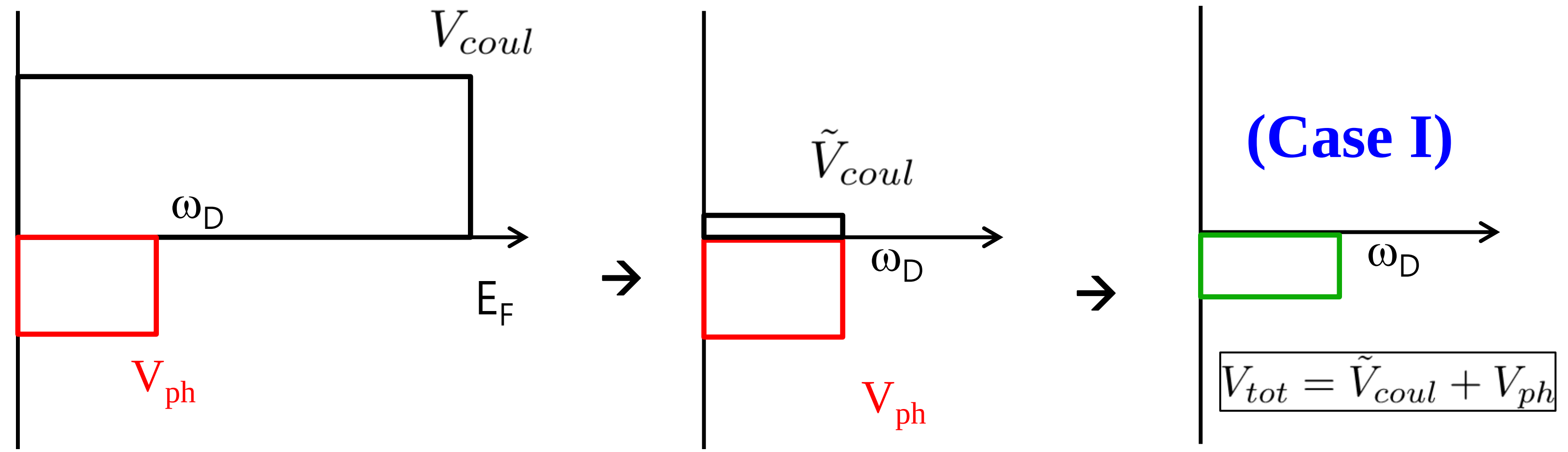
$$U = \frac{V}{1+VN(0)\log\frac{E_F}{\omega_m}}$$

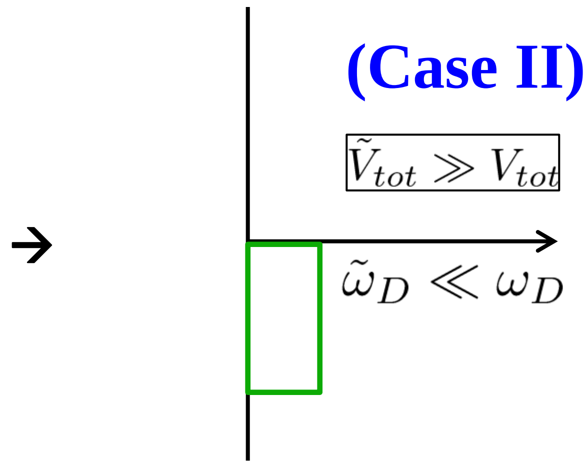


Lowering cutoff energy Λ_{cut}

$$U = \frac{V}{1+VN(0)\log\frac{E_F}{\omega_m}}$$

V_{tot} <0 for low energy of E< ω_D



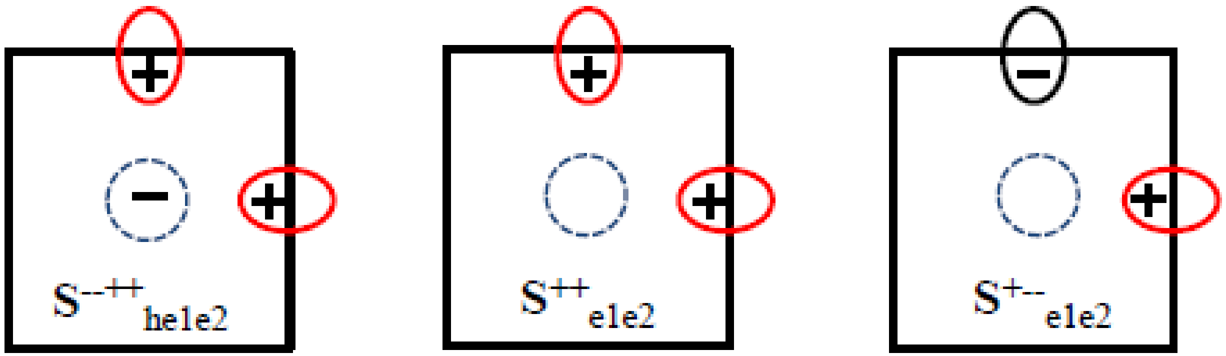


$$T_c = 1.14\omega_D e^{-1/N_0 V_{tot}}$$

$$T_c = 1.14\tilde{\omega}_D e^{-1/N_0 \tilde{V}_{tot}}$$

Case I and **Case II** have the same Tc.

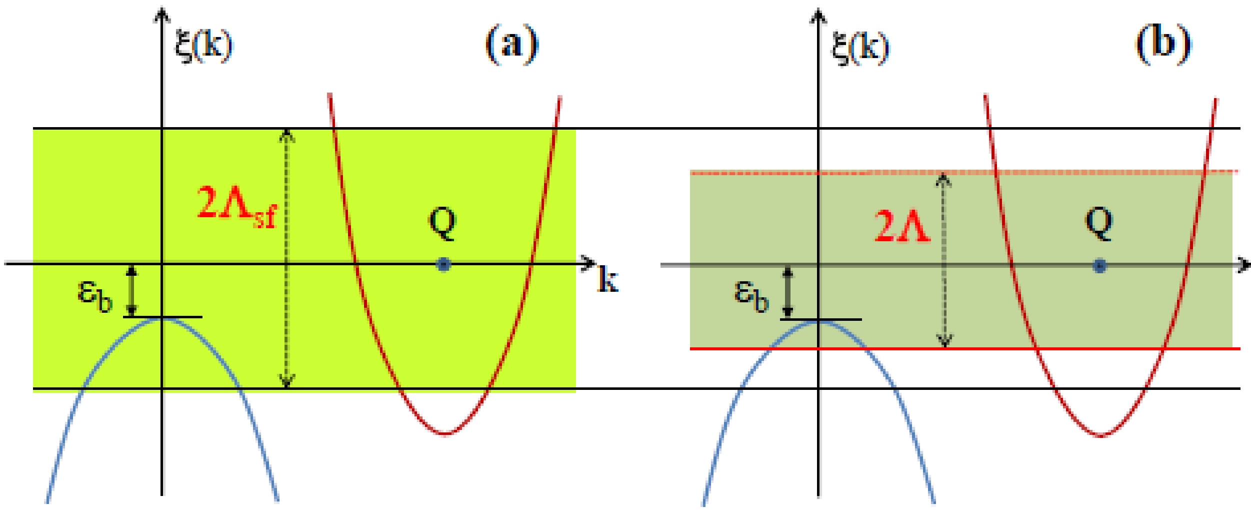
Possible pairing solutions in Incipient band model

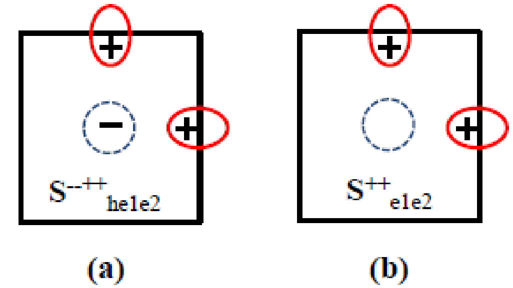


(a) (b) (c)

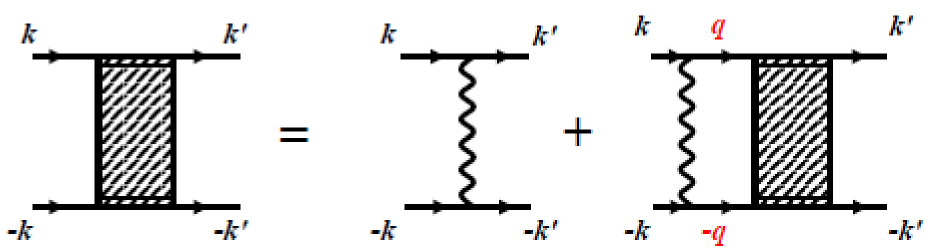
First, compared the solutions **(a)** and **(b).**

Scaling the cutoff Λ





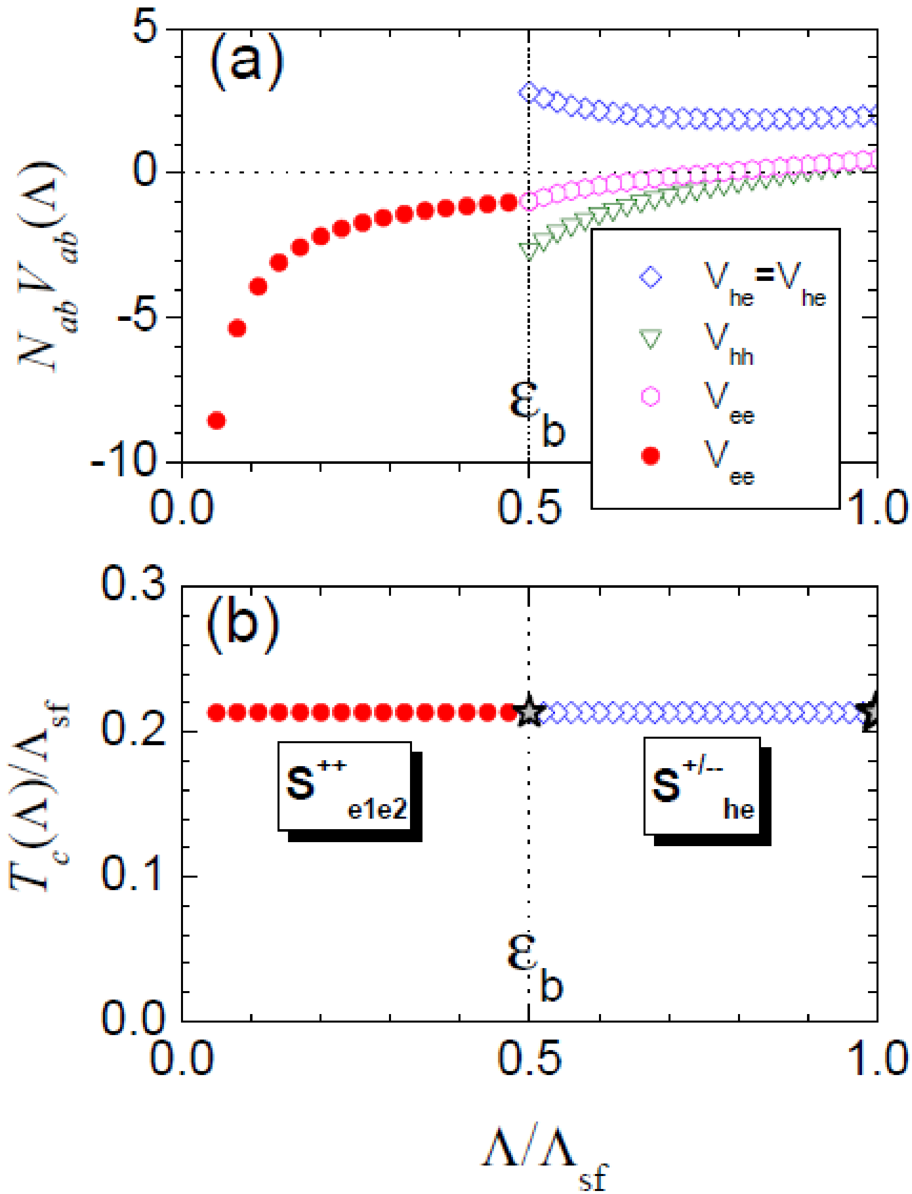
RG of V_{ab} (Λ)

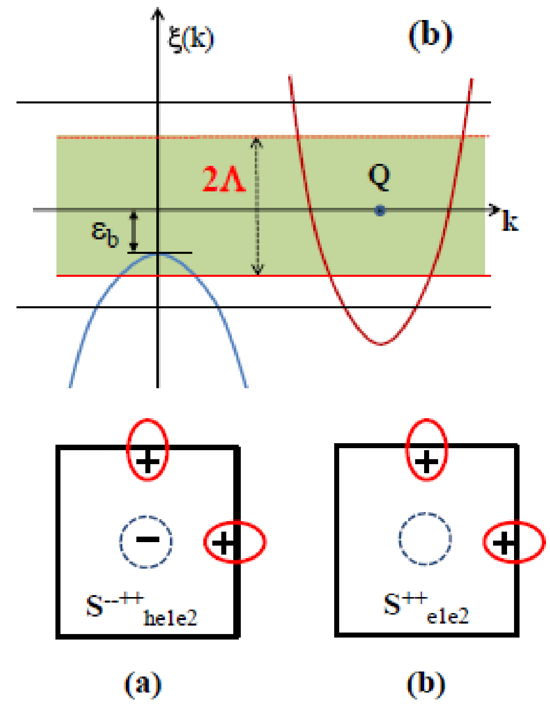


$$\hat{V}(\Lambda) = \hat{V}^0 + \hat{V}^0 \cdot \hat{\chi}(\Lambda_{sf};\Lambda) \cdot \hat{V}(\Lambda)$$

$$\hat{V}^0 = \begin{pmatrix} V^0_{hh} & V^0_{he} \\ V^0_{eh} & V^0_{ee} \end{pmatrix}$$

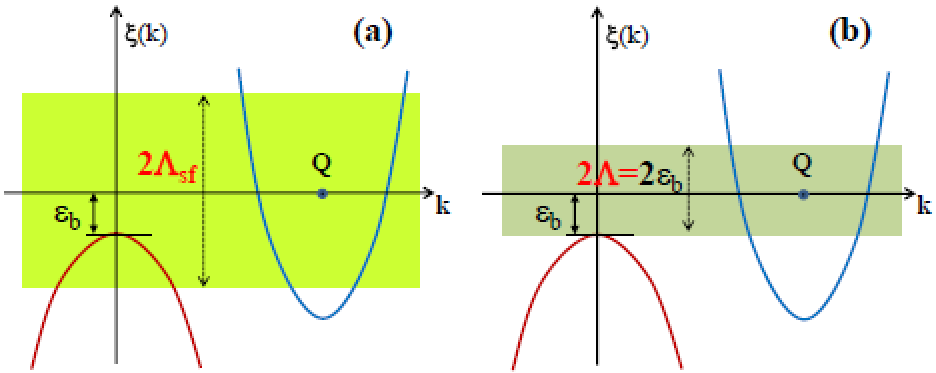
$$\hat{\chi}(\Lambda_{sf};\Lambda) = \begin{pmatrix} \chi_h & 0 \\ 0 & \chi_e \end{pmatrix}$$



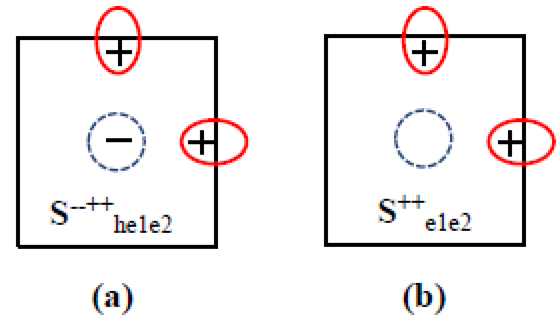


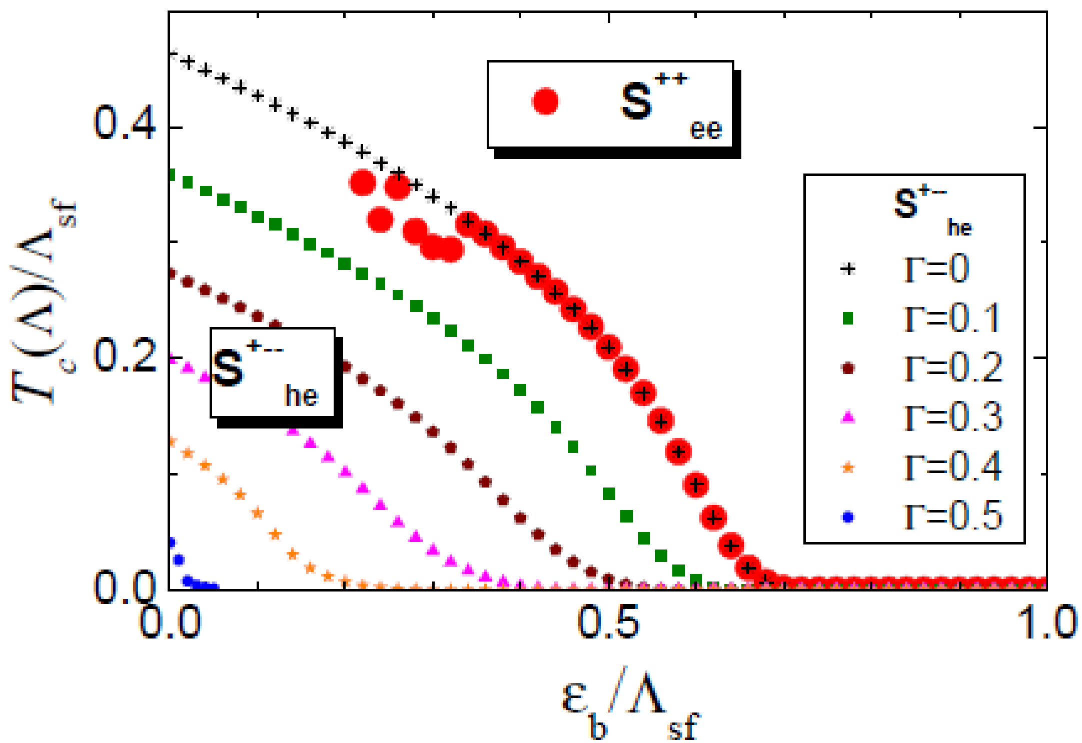
Tc is the same !!

Pairing solution changes across ε_b.



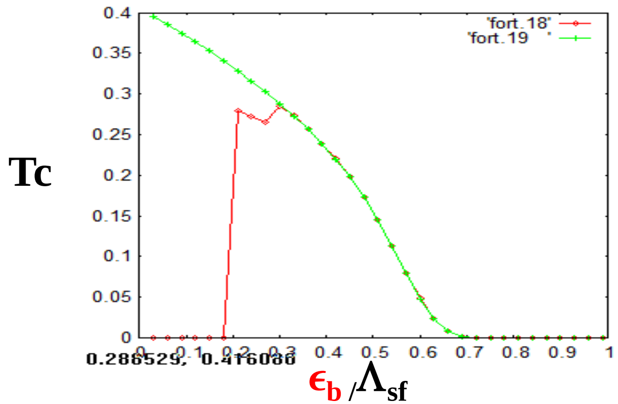
Now consider only two solutions:



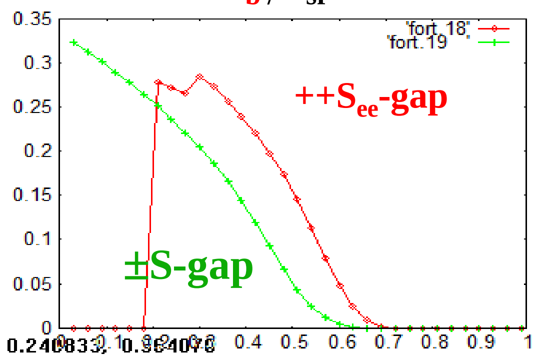


Non-mag impurities kill only $S+-_{he}$ –state.

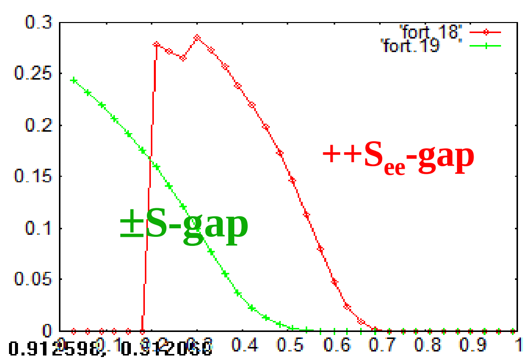
Imp. Effect on ±S-gap n ++S_{ee}-gap



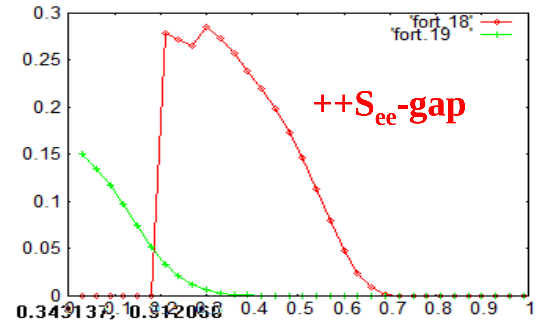
Imp.
Γ=0.0



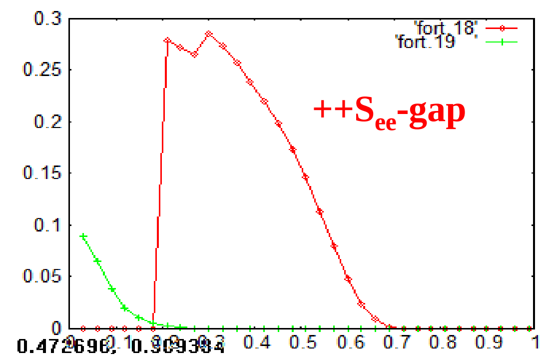
Imp.
Γ=0.1



Imp.
Γ=0.2



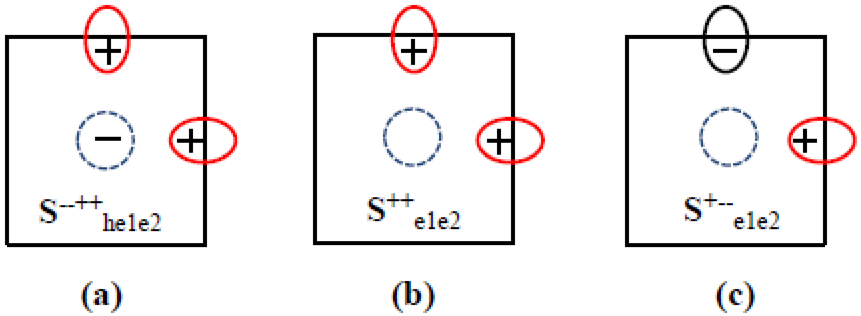
Imp.
Γ=0.3

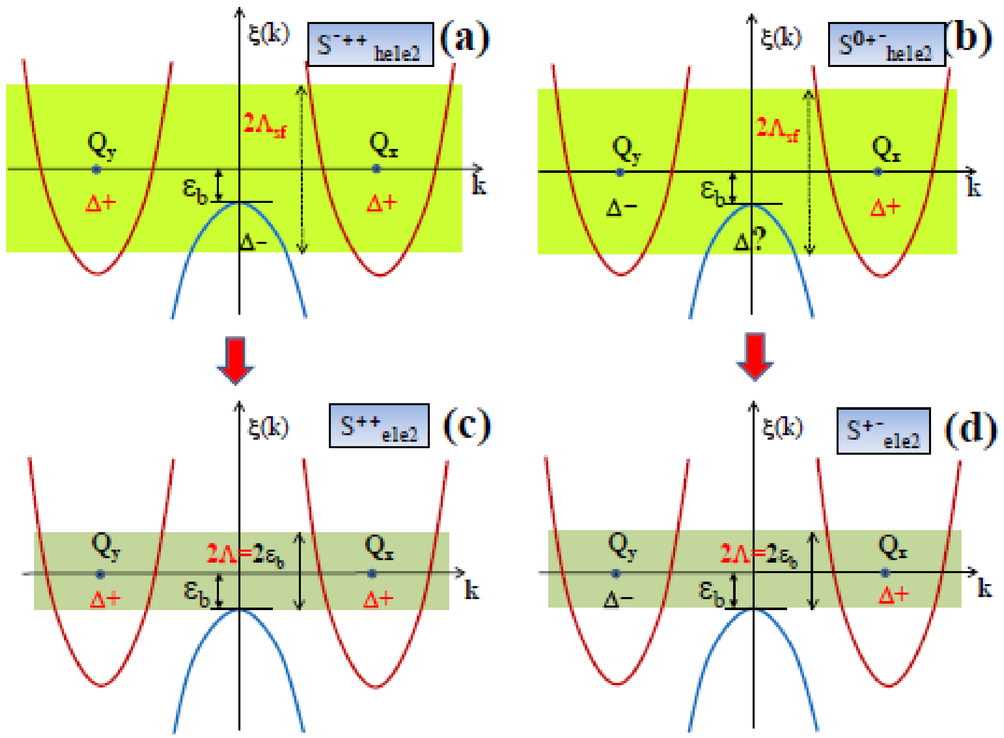


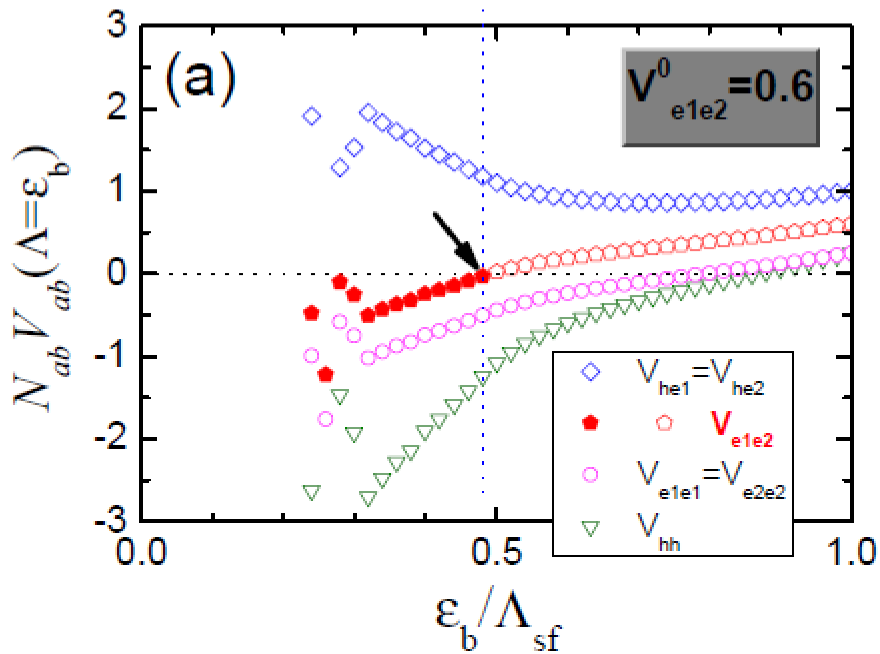
Imp.
Γ=0.35

Impurity pair-breaking only for ±S-gap,
++S_{ee}-gap is robust against imp. scattering.

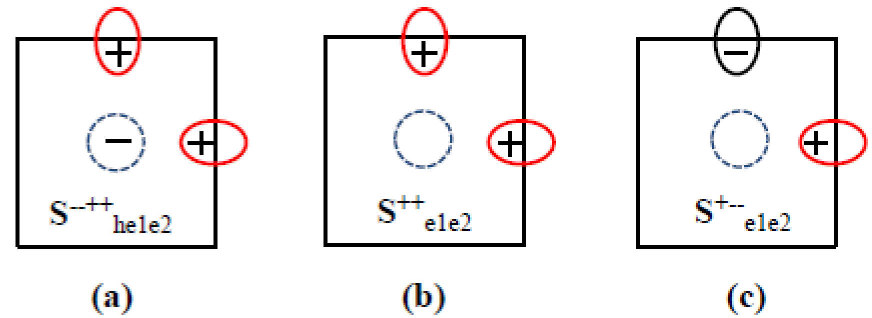
Three band model

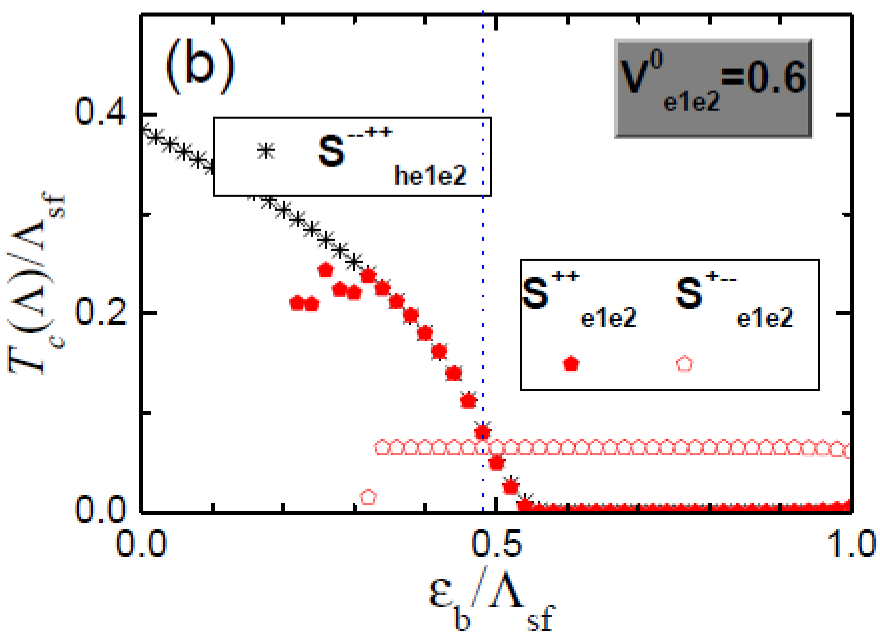


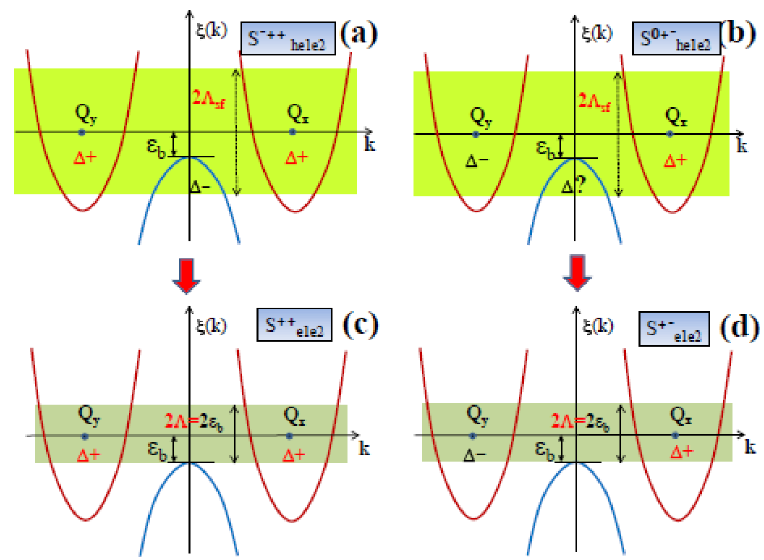




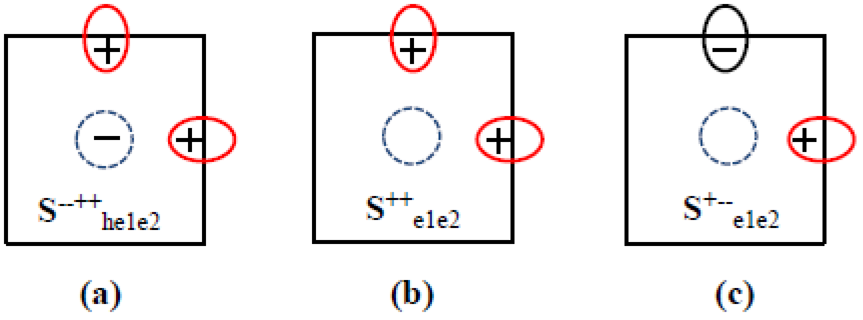
$$V = \begin{bmatrix} V_{hh} & V_{he_1} & V_{he_2} \\ V_{e_1h} & V_{e_1e_1} & V_{e_1e_2} \\ V_{e_2h} & V_{e_2e_1} & V_{e_2e_2} \end{bmatrix}$$

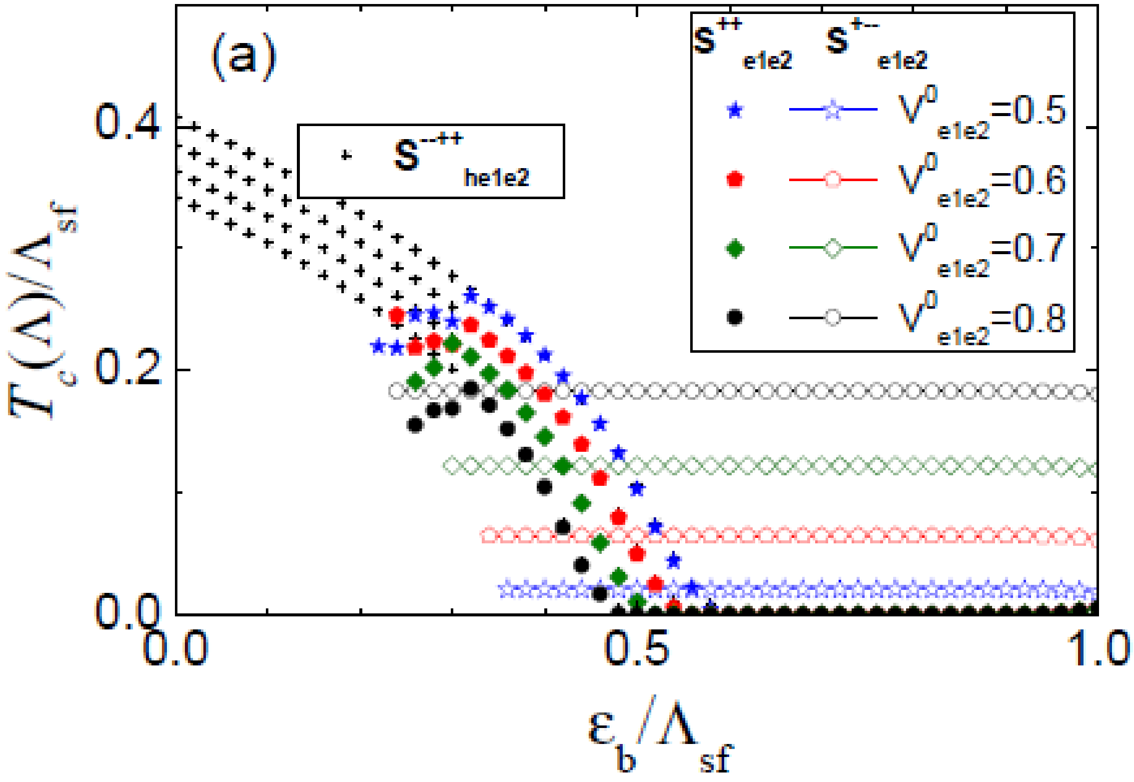


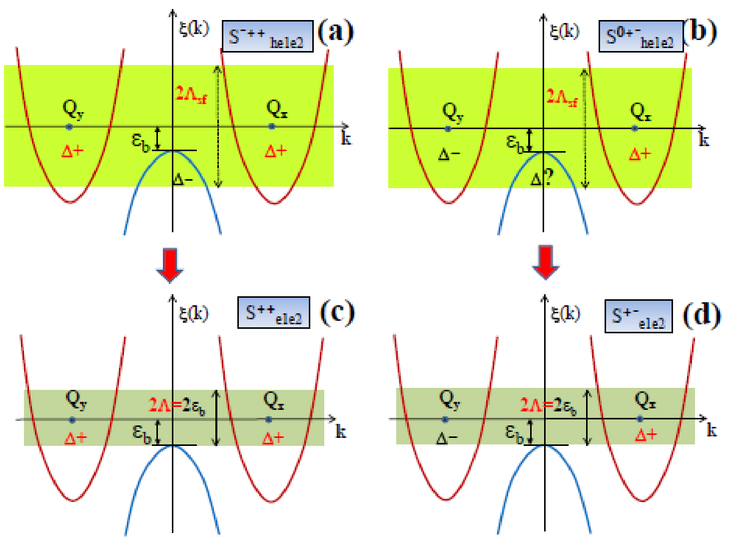




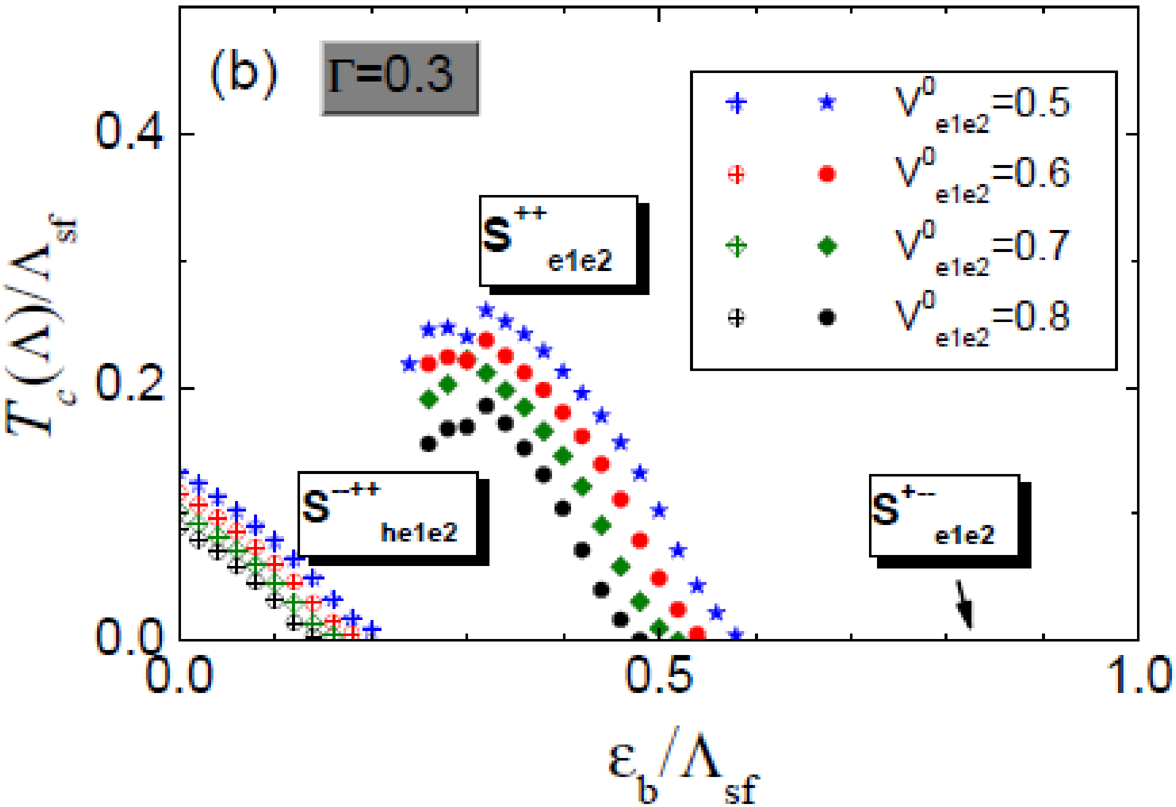
Varying V_{e1e2}

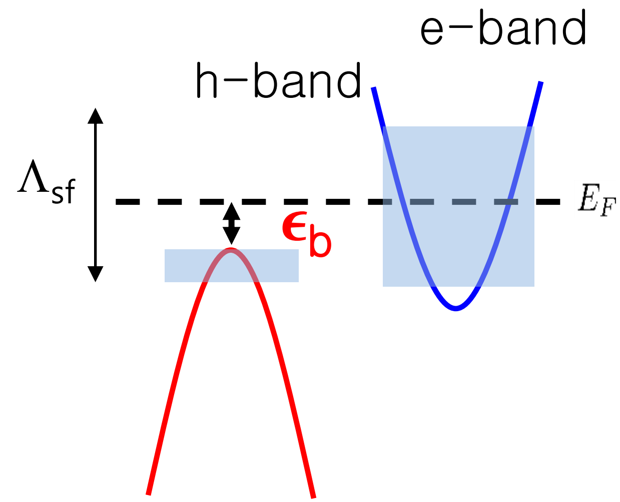






With non-magnetic impurities.





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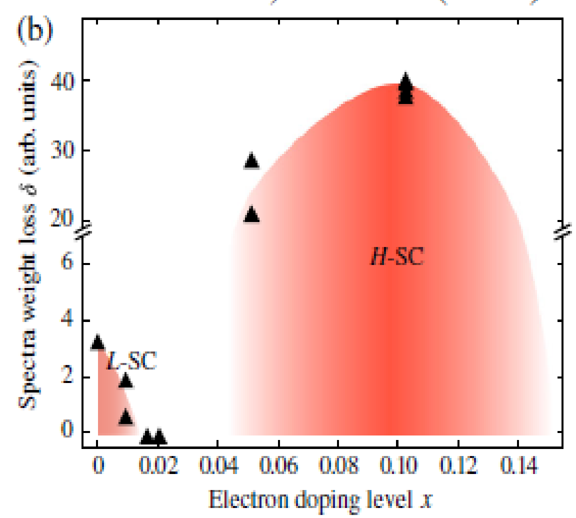

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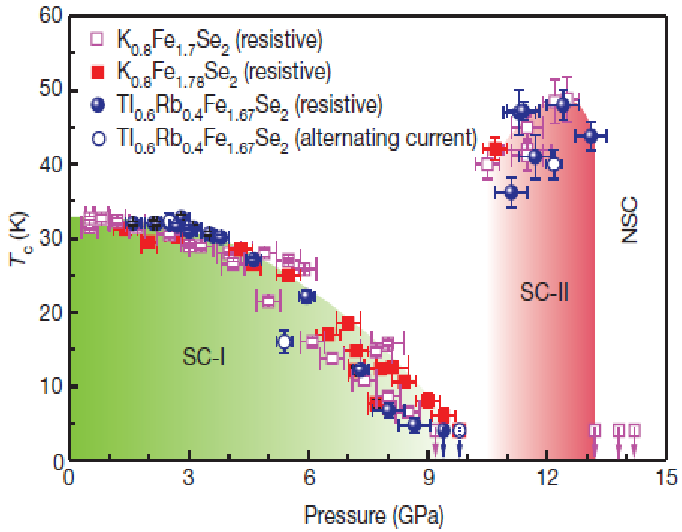
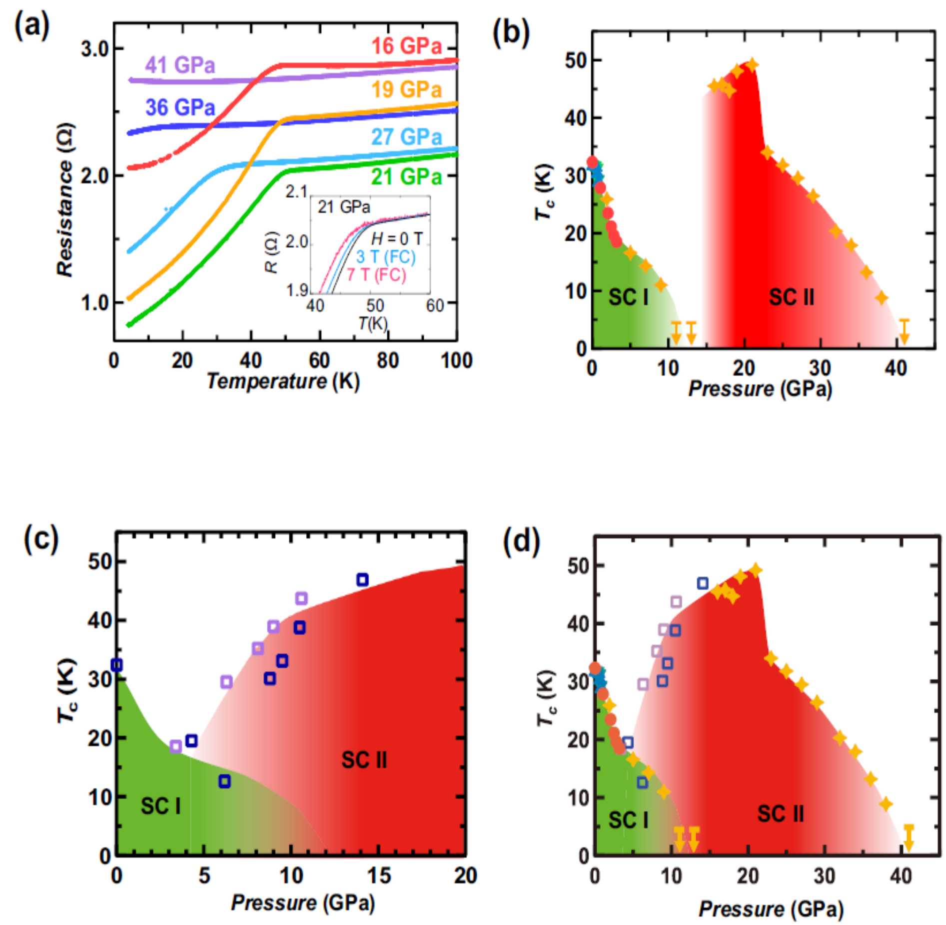


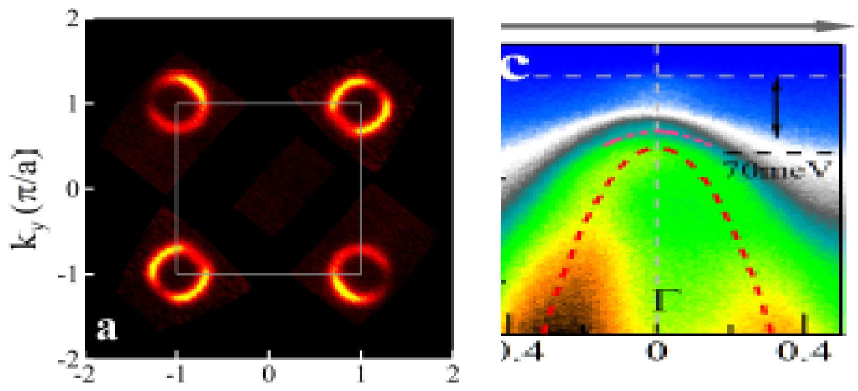
Figure 4 | Pressure dependence of the T_c for $Tl_{0.6}Rb_{0.4}Fe_{1.67}Se_2$, $K_{0.8}Fe_{1.7}Se_2$ and $K_{0.8}Fe_{1.78}Se_2$. The symbols represent the pressure–temperature

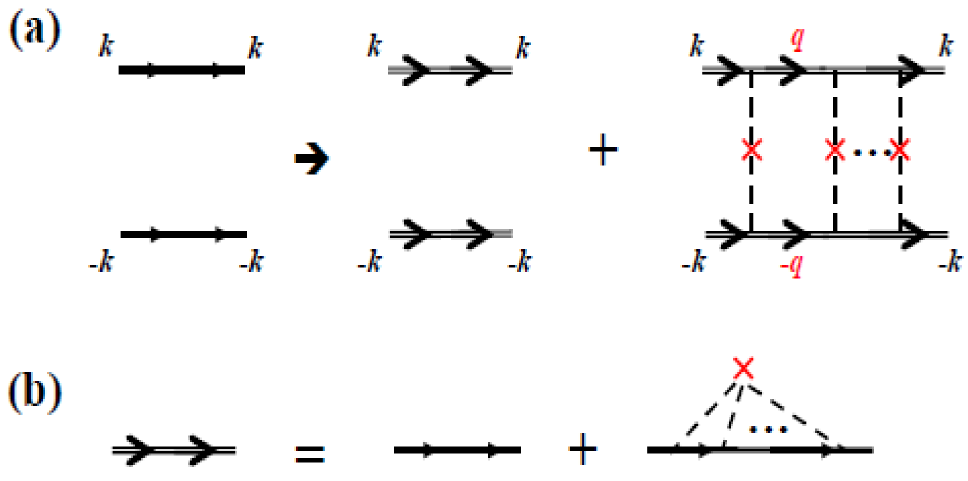
SCIENTIFIC REPORTS | 5 : 9477 | DOI: 10.1038/srep09477



Conclusions:

1. All HEDIS system with only electron pockets has **$++S_{ee}$-gap**
2. FeSe monolayer is special. Need small angle phonon boost
3. Pairing cutoff energy is dynamically tuned by RG to ϵ_b .
4. **$\pm S_{he}$-pairing** paradigm still governs FeSe system.

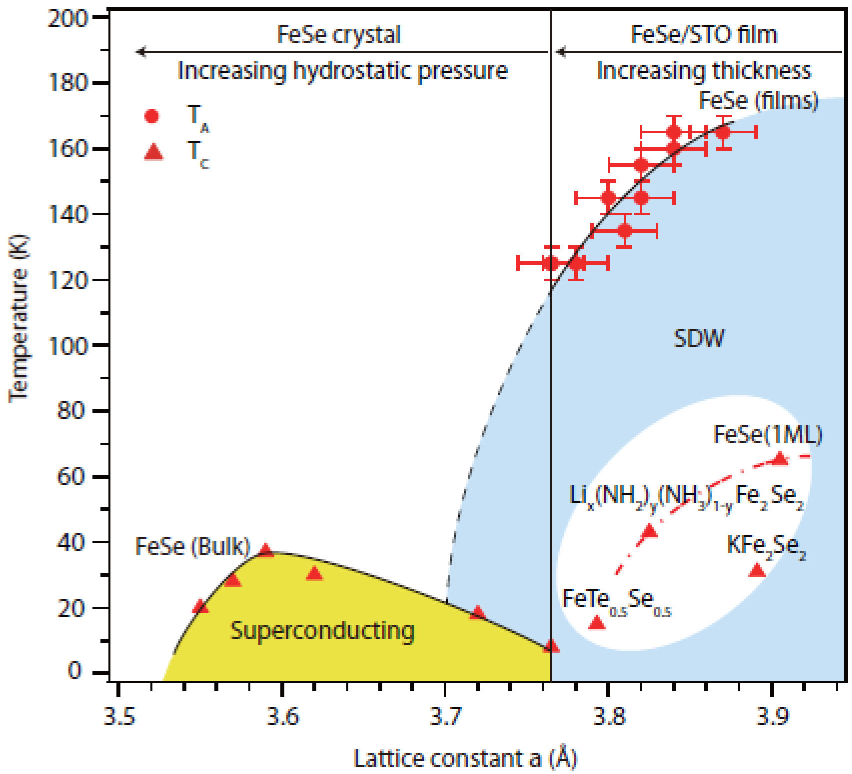




$$\tilde{\chi}_e(\Lambda_{sf};\Lambda) = -T_c \sum_n 2N_e \int_{\Lambda}^{\Lambda_{sf}} d\xi \frac{\eta_v}{\tilde{\omega}_n^2 + \xi^2},$$

$$\tilde{\chi}_h(\Lambda_{sf};\Lambda) = -T_c \sum_n N_h \int_{-\Lambda_{sf}}^{-\Lambda} d\xi \frac{\eta_v}{\tilde{\omega}_n^2 + \xi^2}.$$

When $\eta_v = \eta_1$, Cooperon is invariant w.r.t non-mag. Impurity scatt.



FeSe crystal
Increasing hydrostatic pressure
FeSe/STO film
Increasing thickness
FeSe (films)
T_A
T_C
SDW
FeSe(1ML)
Li_x(NH_2)_y(NH_3)_1-y Fe_2Se_2
KFe_2Se_2
FeSe (Bulk)
Superconducting
FeTe_0.5Se_0.5
Temperature (K)
Lattice constant a (Å)
200
180
160
140
120
100
80
60
40
20
0
3.5
3.6
3.7
3.8
3.9