Superconductivity vs bound state formation in Fe-based superconductors

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Theoretische Physik III, Ruhr-Uni Bochum

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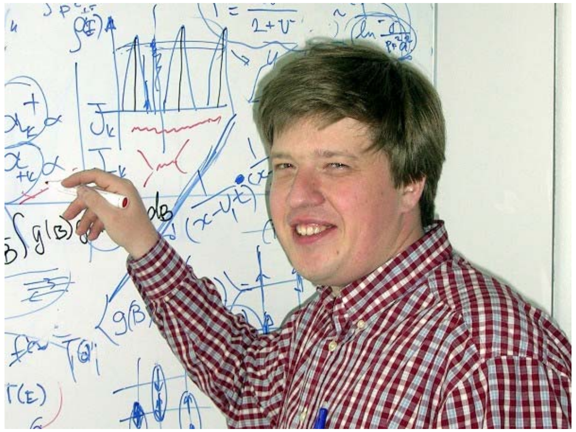
Collaborators:



Dmitry Efremov
(IFW Dresden)

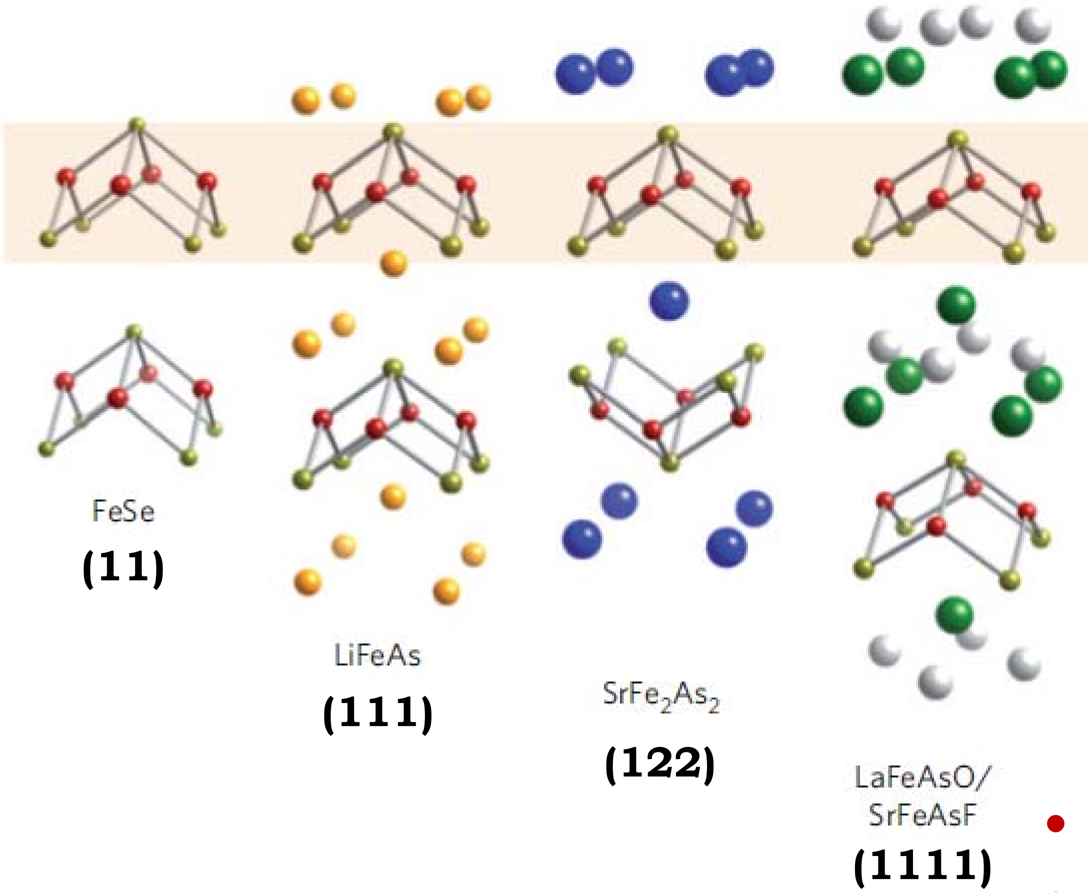
Andrey Chubukov
(Minnesota)

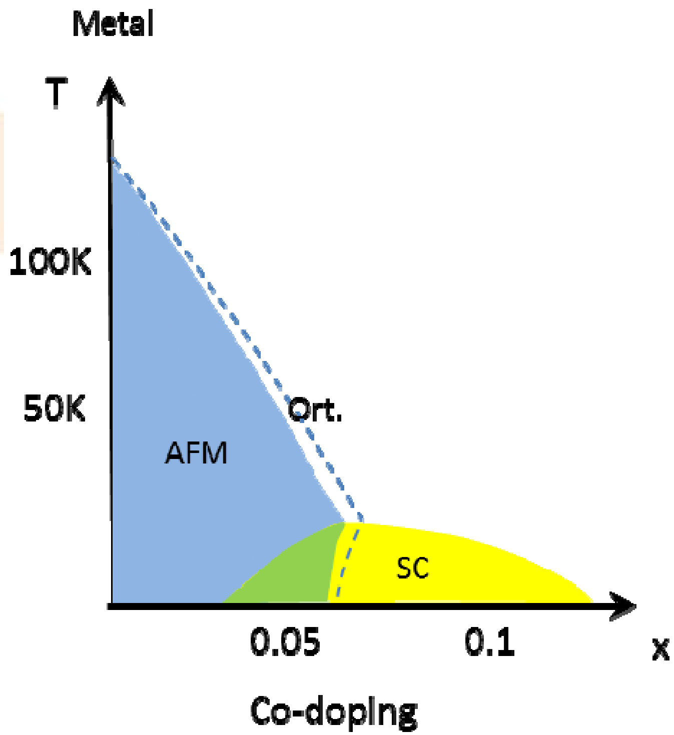
Jakob Böker
(Bochum, RUB)

Iron-based superconductors: materials

FeAs, FeSe layers; T_c up to 56K

N. Ni et al., Phys. Rev. B 78 (2008);
X.F. Wang et al., New Jour. Phys. 11 (2009)

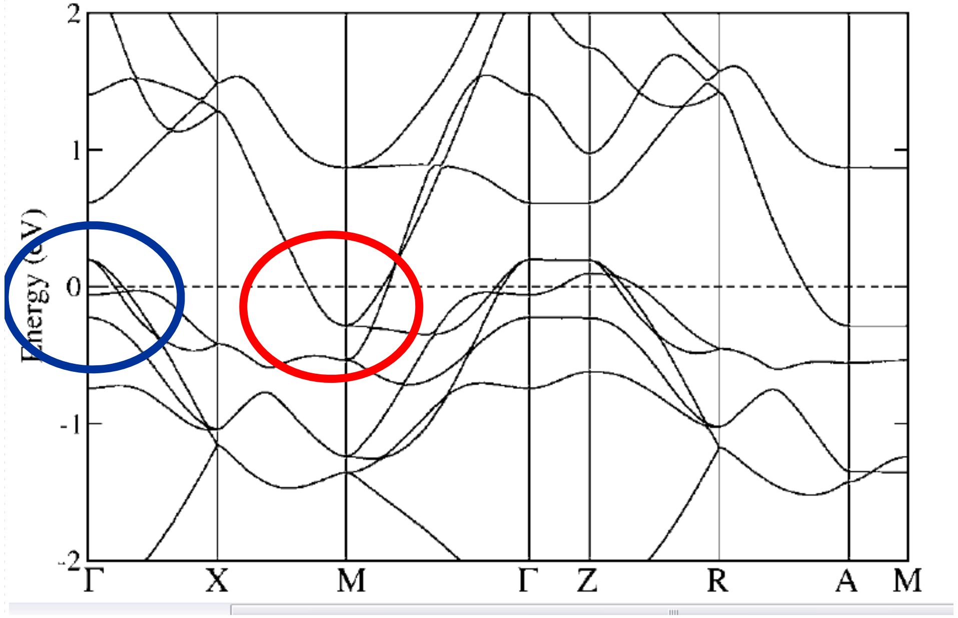




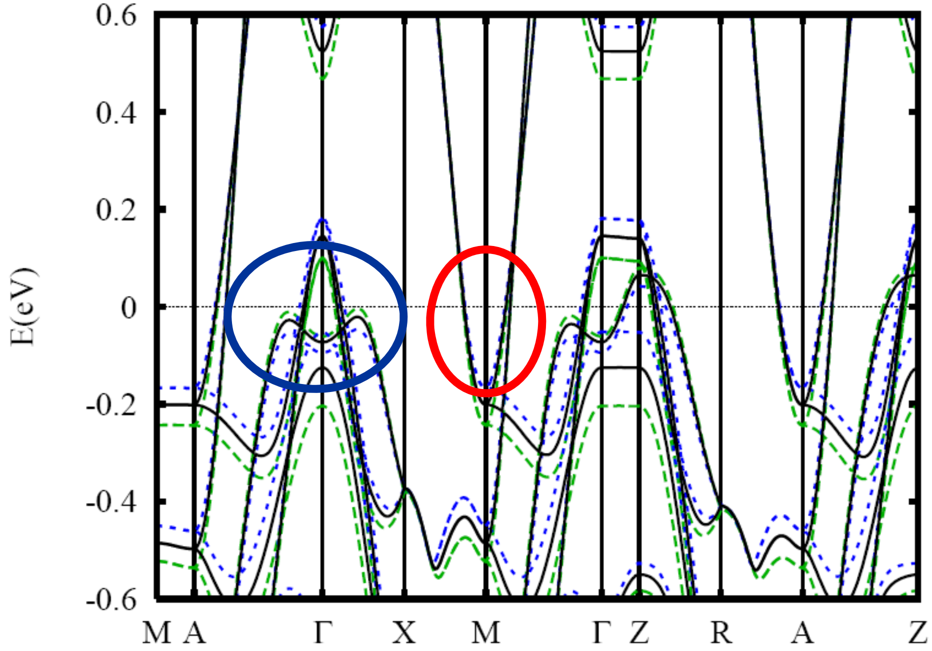
- Magnetic order (AFM)
- Nematic (struct.) order
- Superconductivity

DFT: common electronic structure

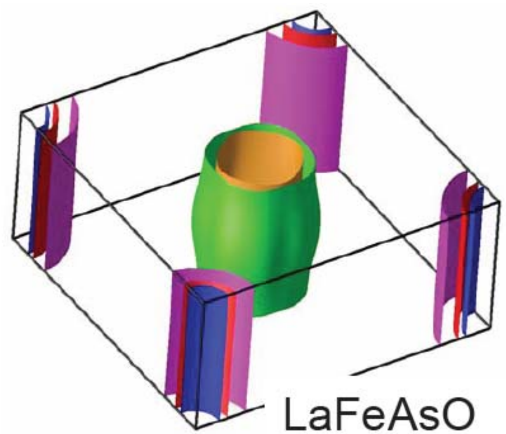
LOFP **Lebegue 2007** **(T_c=6K)**



LOFA **Singh & Du 2008** **(T_c=26K)**



Band structures for 2 materials nearly identical!
Hole pocket near Γ, electron pocket near M

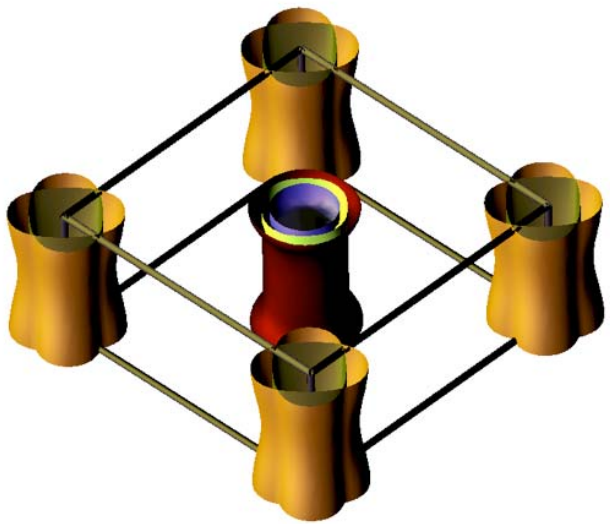


2D!

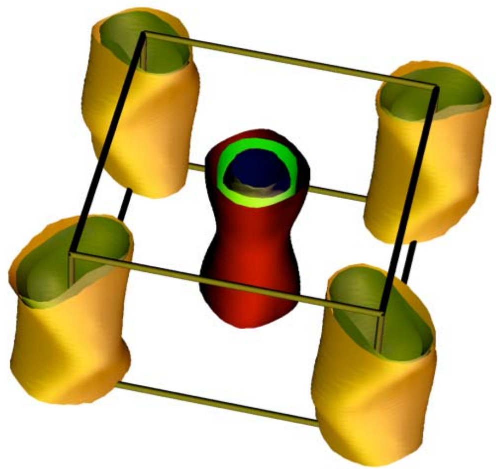
Comparison with other materials

Hole pockets near (0,0)
Electron pockets near (π,π)

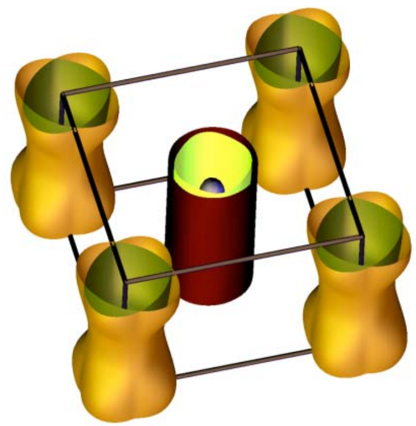
La-1111



Ba-122

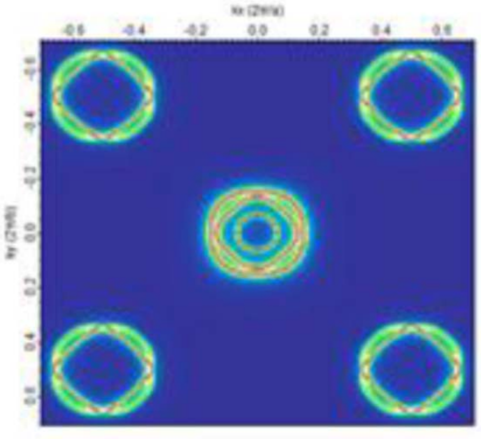


FeTe

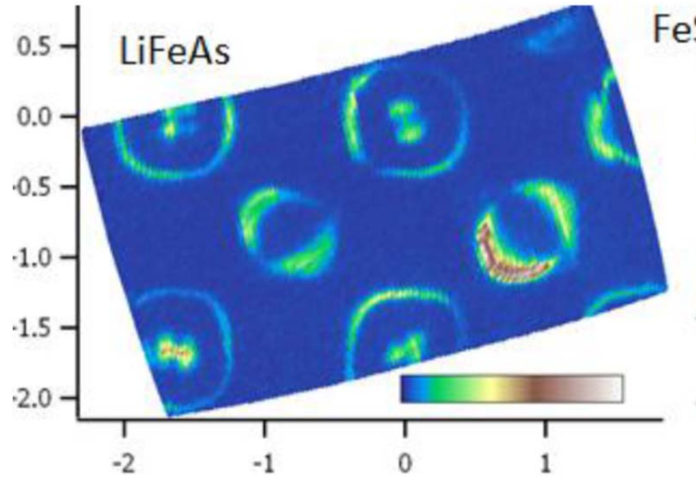


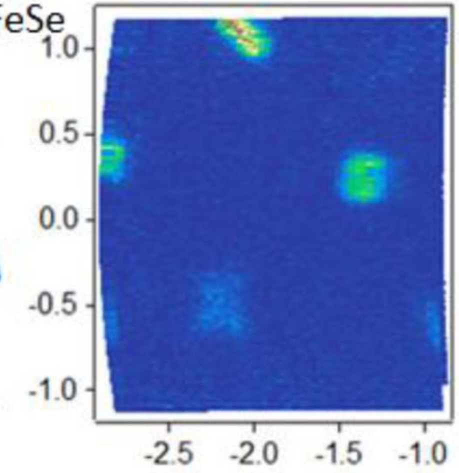
What is in reality?

Theory

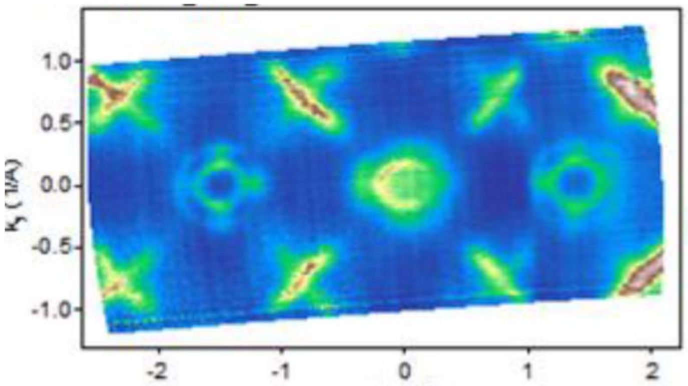


Experiments (ARPES and dHvA)

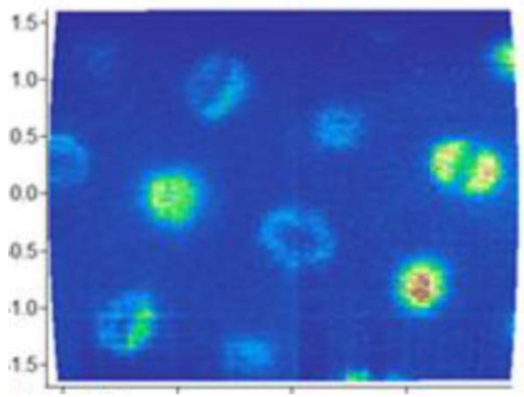




$Ba_{1-x}K_xFe_2As_2$



Co-$BaFe_2As_2$

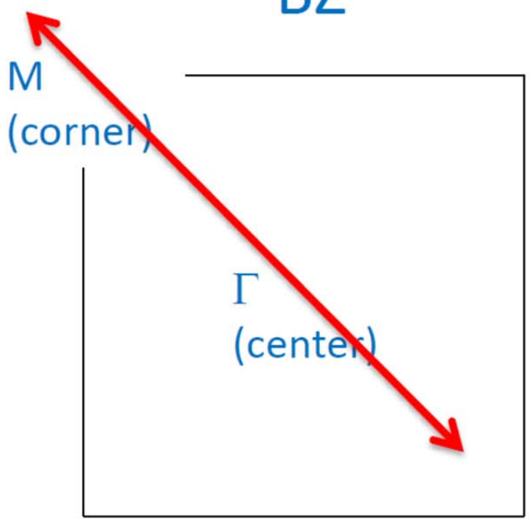


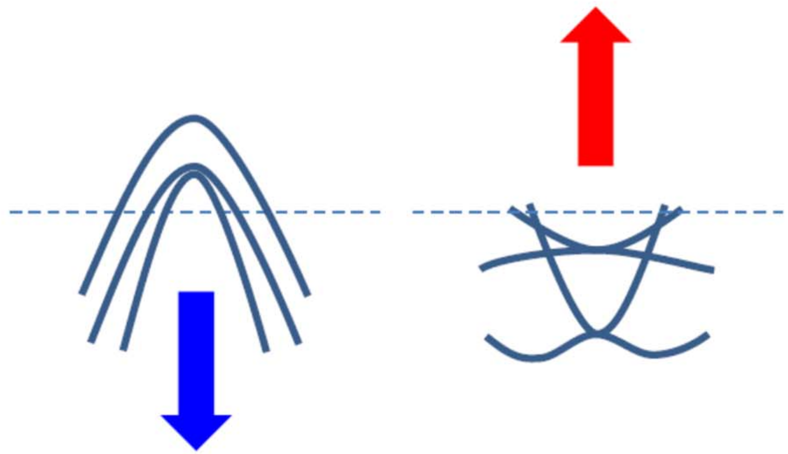
Borisenko group (IFW Dresden)

Peculiar renormalization effects in Fe-based SC

Summary of the experimental data

BZ





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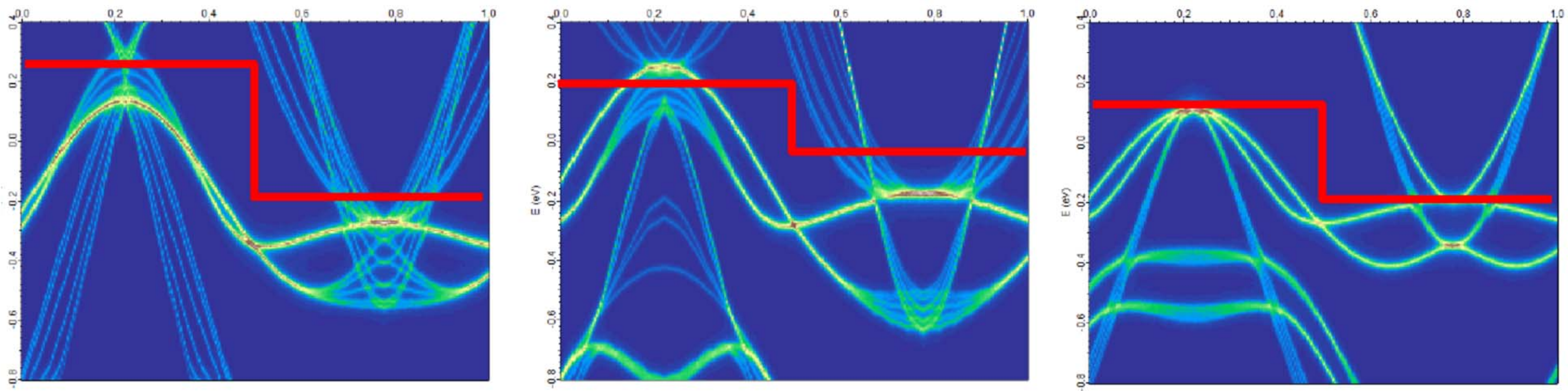
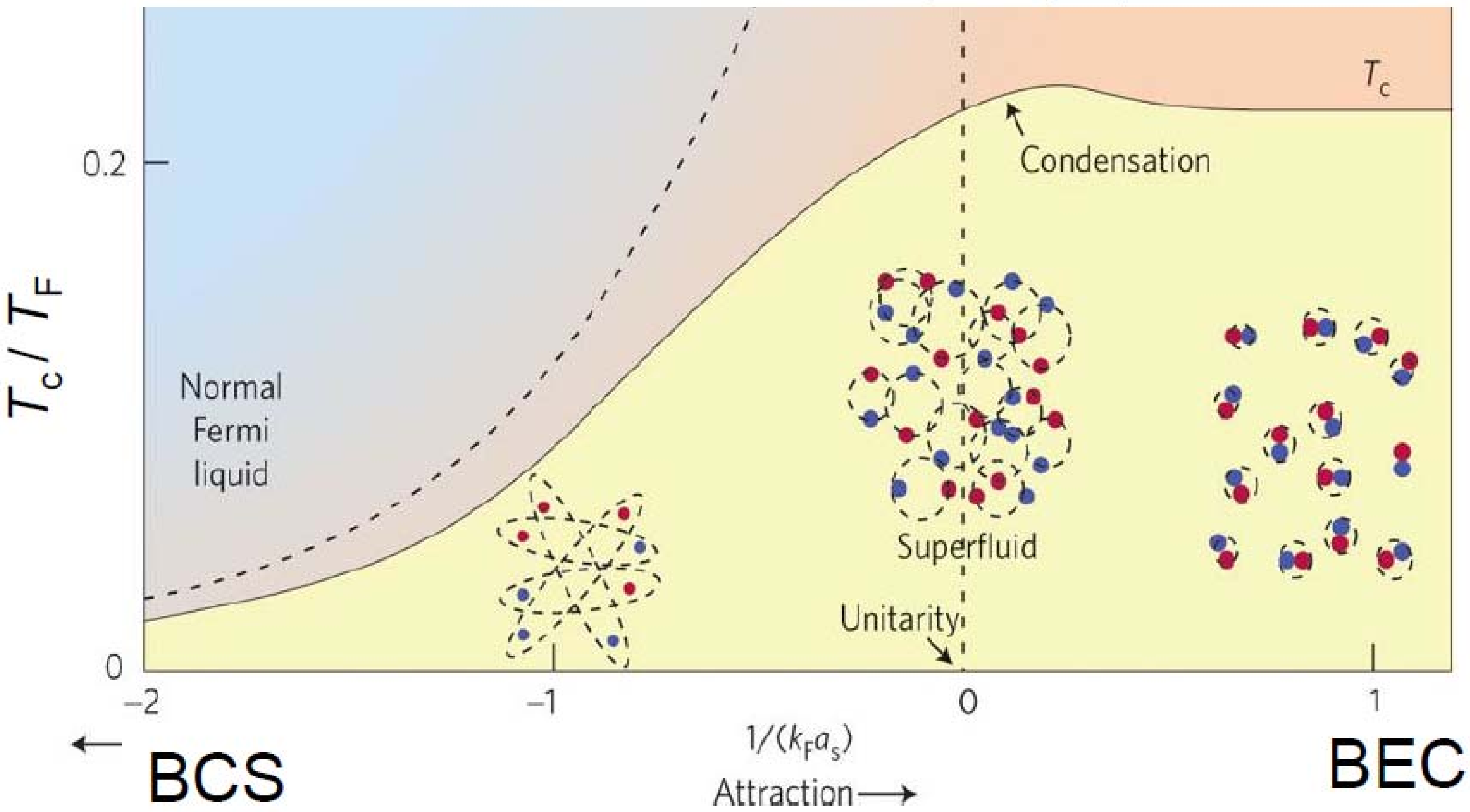


ARPES: A. Charnukha et al., Sci. Rep. 5, 18273 (2015)

BCS-BEC Crossover in Fe-based SC ?

M. Randeria, E. Taylor, Annu. Rev. Condens. Matter Phys. (14)



$k_F\xi \gg 1$	$k_F\xi \sim 1$	$k_F\xi \ll 1$
Cooper pairs	strongly interacting pairs	diatomic molecules

What should be the consequences of lowering the Fermi energies for the Cooper-pairing in Fe-based SC?

1) multiband character of superconductivity with electron and hole bands

2) One has to distinguish situations when

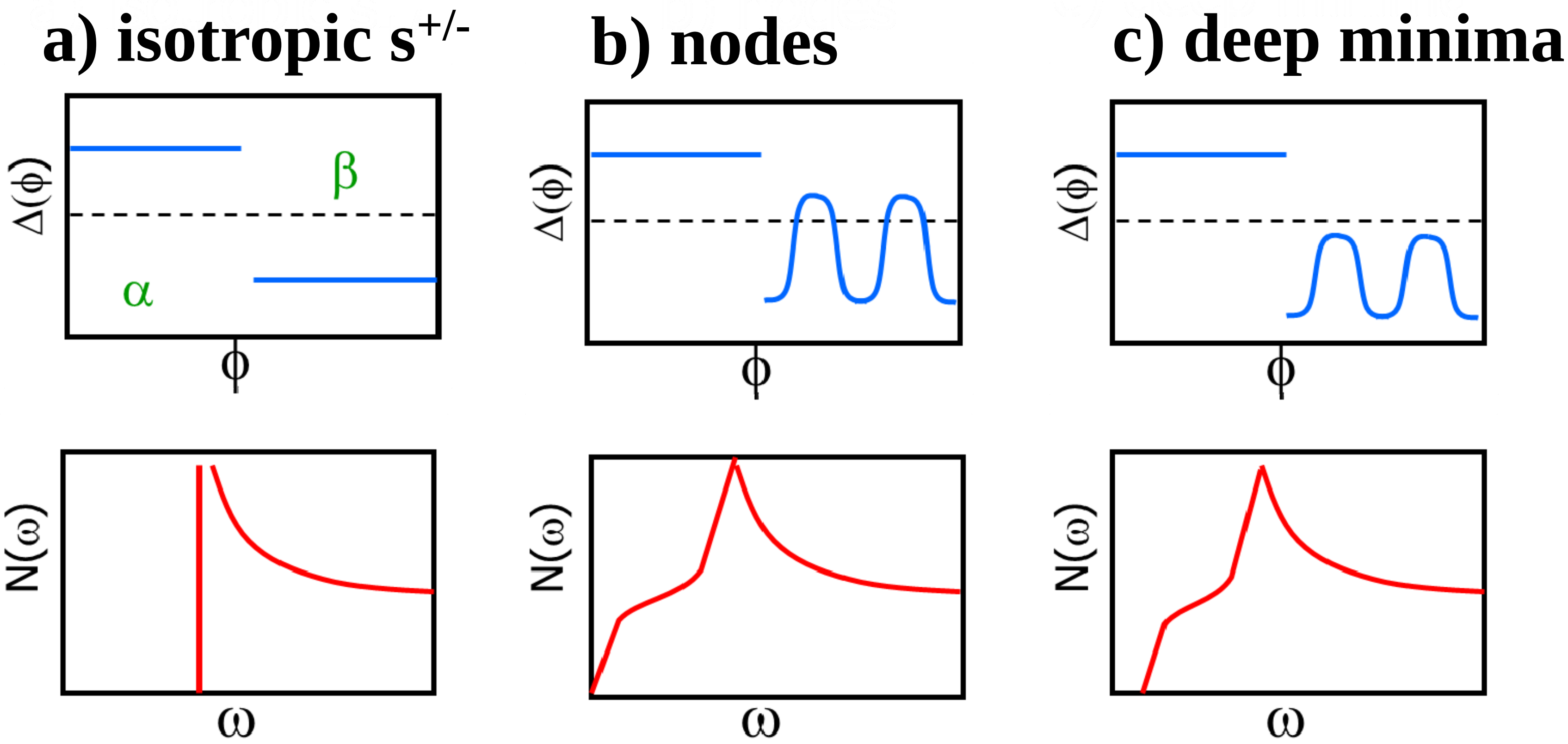
(i) only one band has low E_F, while others have much larger E_F

(ii) all Fermi energies are small

2D: two-particle bound state forms at arbitrary weak interaction

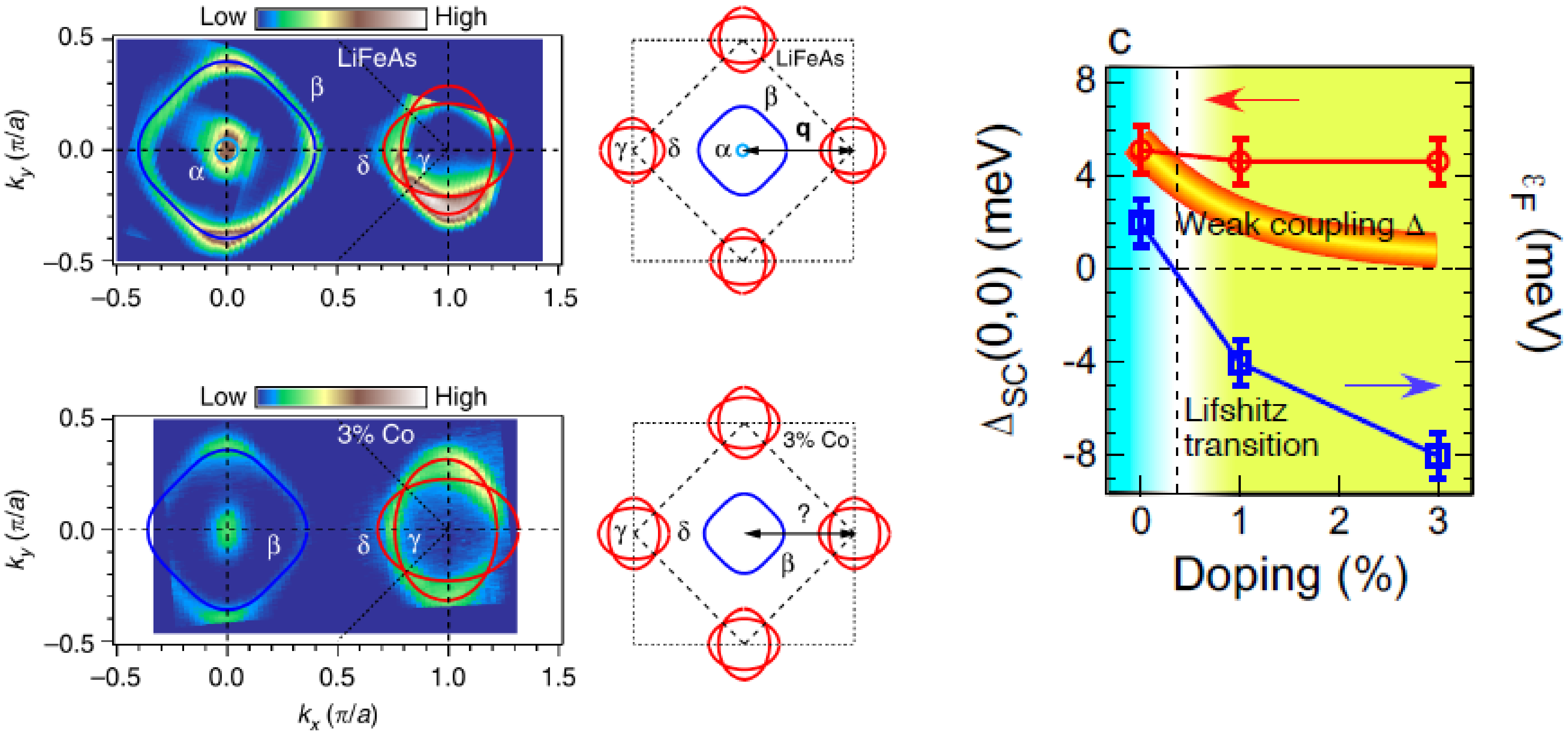
1) Common paradigm for Cooper-pairing in ferropnictides

Once both the electron and the hole pockets are present, enhanced **inter-band scattering** leads to a sign change of the gap between some pockets $s^{+/-}$ **state**



$$\Delta_1 = \Delta_2 e^{-i\pi} \quad \text{or} \quad \Delta_k = \Delta_0 \left(\cos k_x + \cos k_y\right)$$

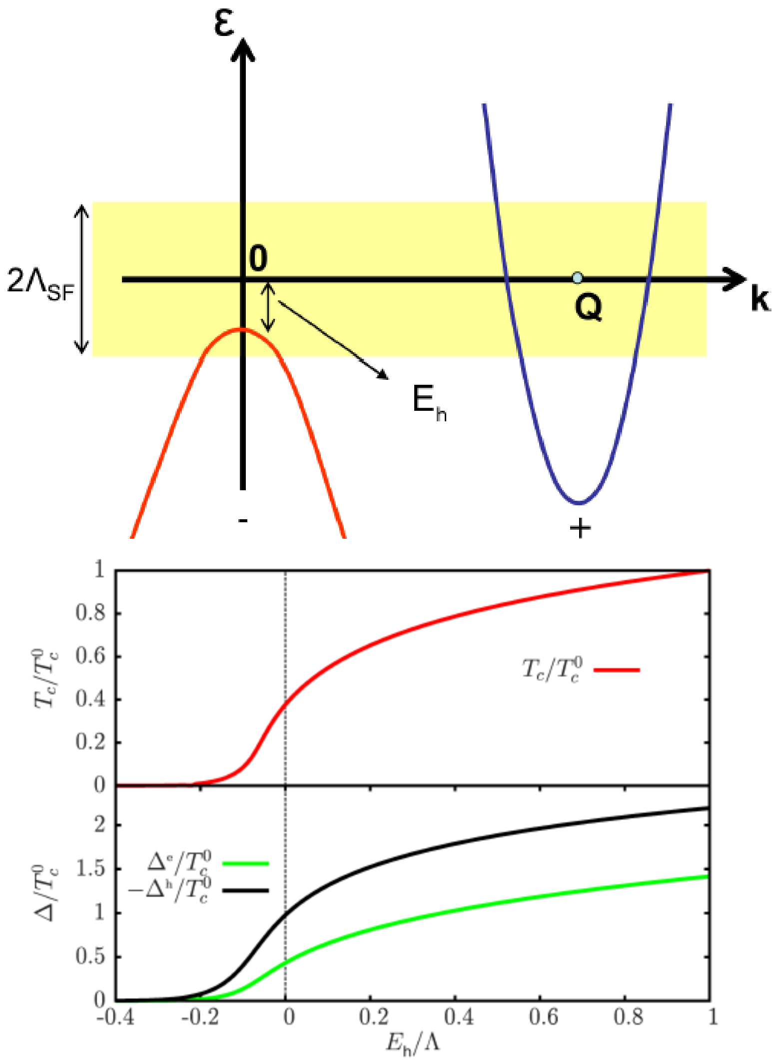
Case (i): 'incipient' bands



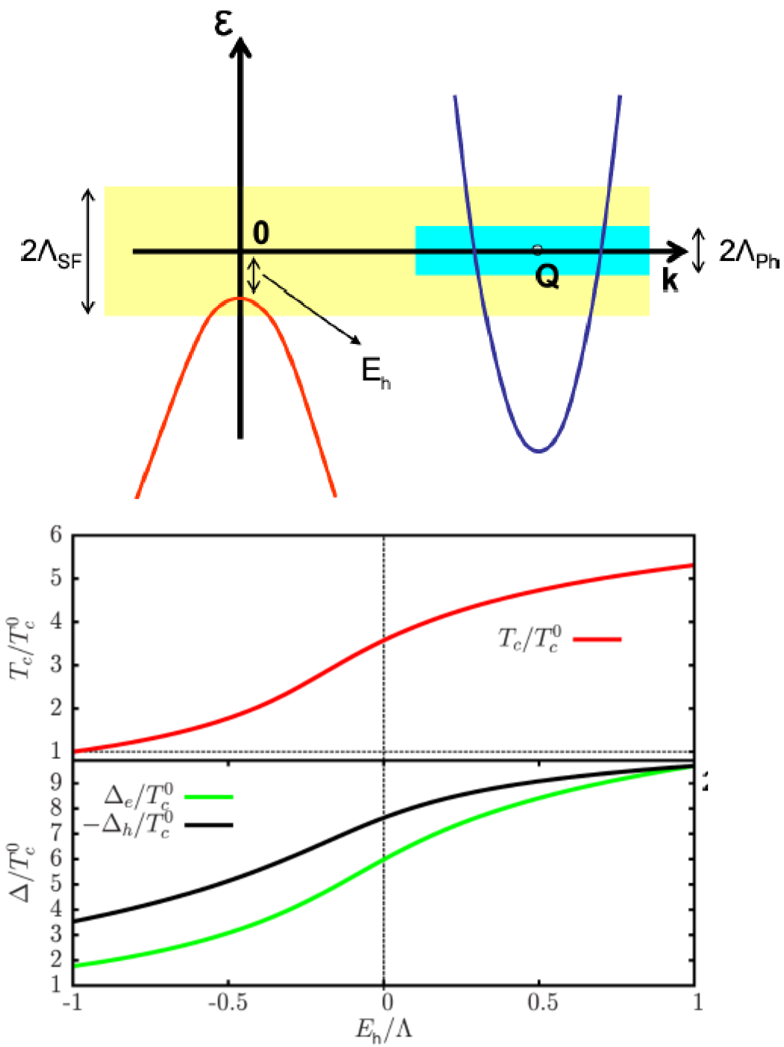
H. Miao *et. al*, Nat. Com. **6**, 6056 (2015)

(i) Incipient bands: BCS analysis

$s_\pm$ pairing with incipient band



Incipient + FL based SC



Xiao Chen, S. Maiti, AL, P. J. Hirschfeld PRB 92, 224514 (2015)

All Fermi energies are small: FeSe

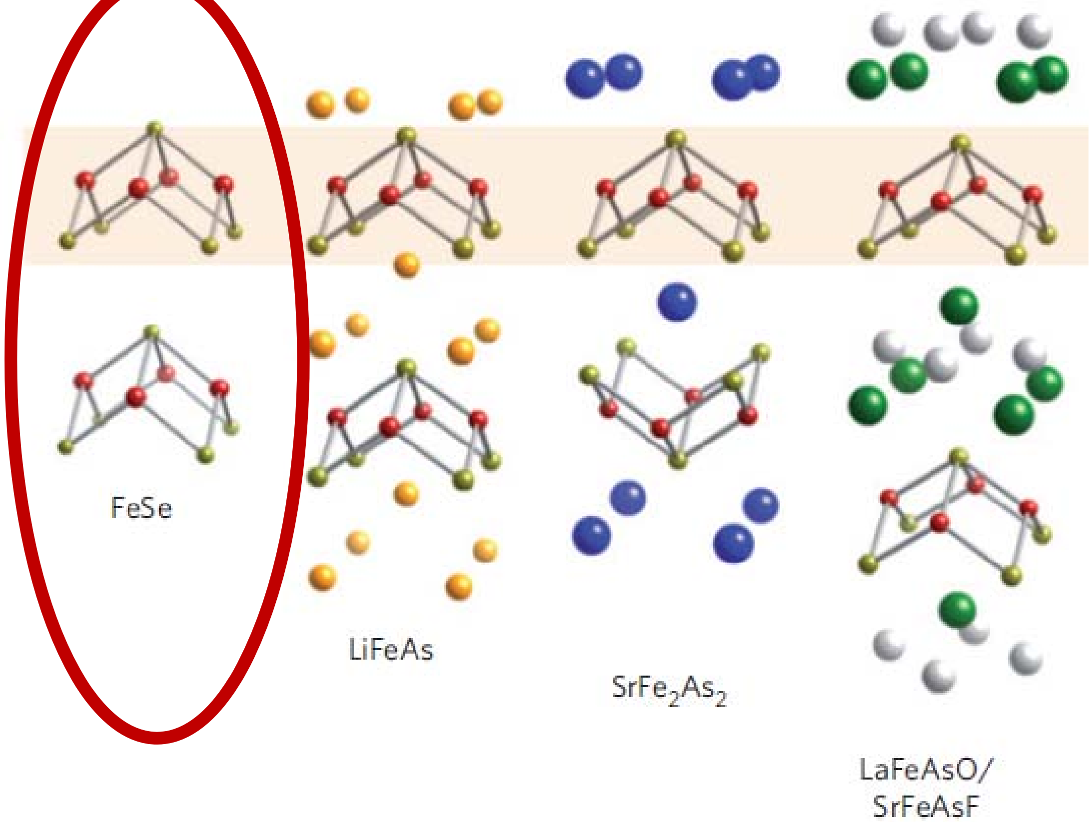
$$\frac{\Delta}{\varepsilon_F} \sim \frac{T_c}{T_F} \sim \frac{1}{\xi k_F}$$

Conventional superconductors

$\Delta/\varepsilon_F \sim 10^{-4} - 10^{-5}$

High-T_c cuprates

$\Delta/\varepsilon_F \sim 10^{-2} - 10^{-3}$



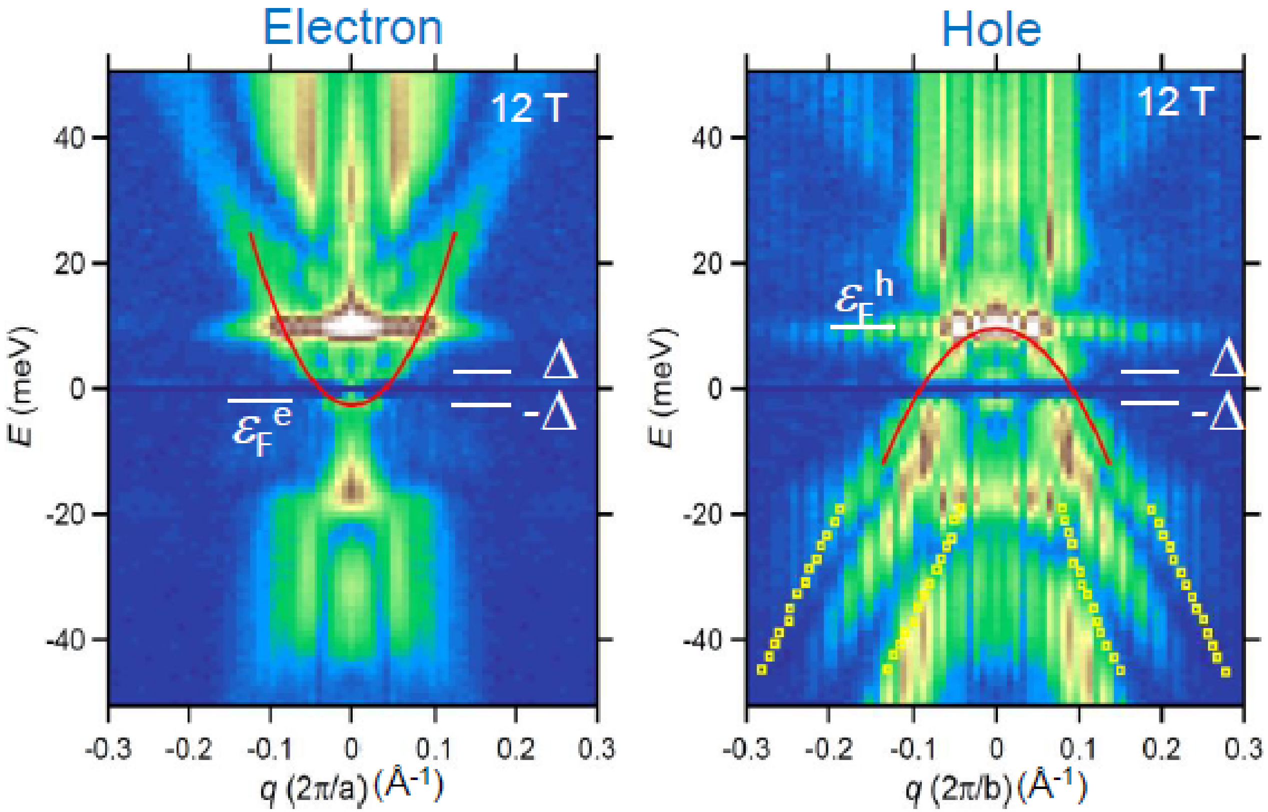
De Haas-van Alphen effect

k_F (Å^{-1})	E_F (meV)
0.043	3.5
0.078	5.1
0.13	9.4
0.14	16

T. Terashima et al, PRB 90, 144517 (2014)

FeSe: $\varepsilon_F \sim \Delta$

Superconducting gaps from Fourier –Transfromed STM



$\Delta/\varepsilon_F^e \sim 1$

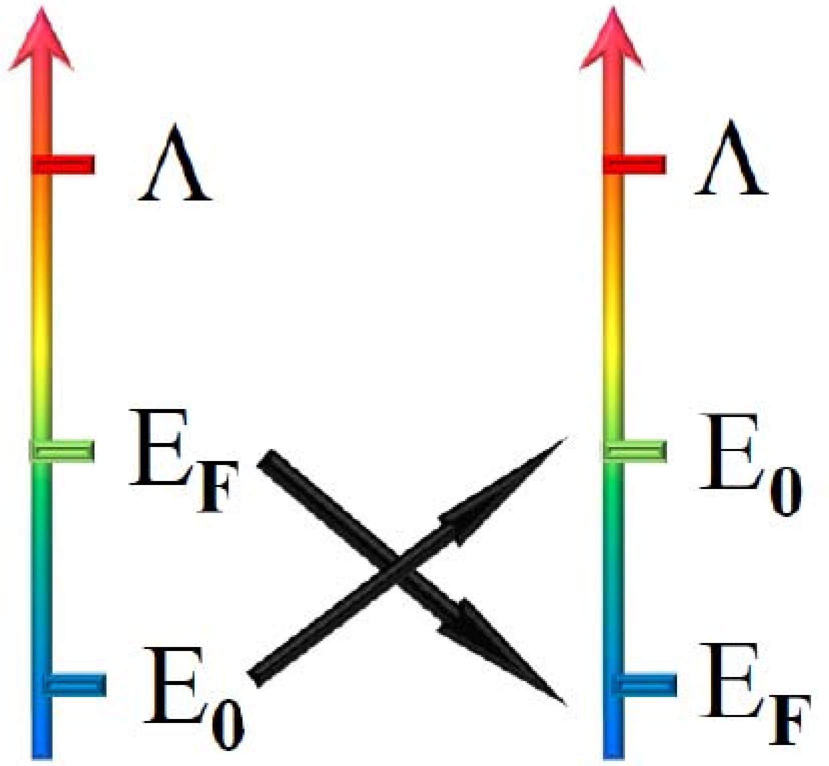
$\Delta/\varepsilon_F^h \sim 0.3$

$\Delta \sim 2.5$ meV

Conventional superconductors
$\Delta/\varepsilon_F \sim 10^{-4}$ - 10^{-5}
High-T_c cuprates
$\Delta/\varepsilon_F \sim 10^{-2}$ - 10^{-3}

S. Kasahara et al, PNAS 111, 16309 (2014)

FeSe: All E_F are small



Λ - upper energy cutoff

E_0 – energy of the bound state in vacuum

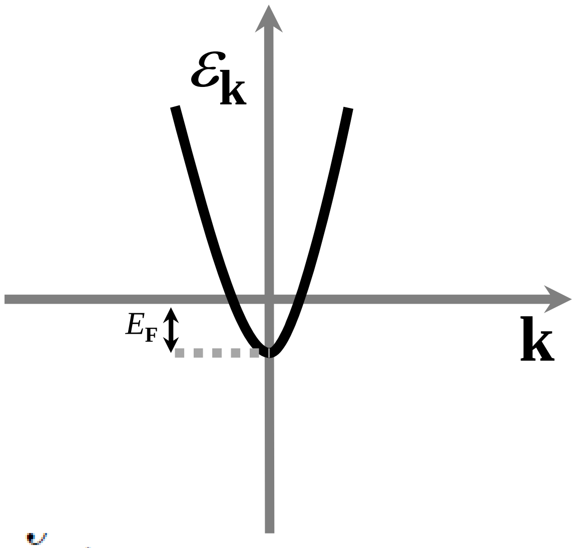
$$E_0 \sim \Lambda e^{-2/\lambda}$$

$$\lambda = mU/(2\pi)$$

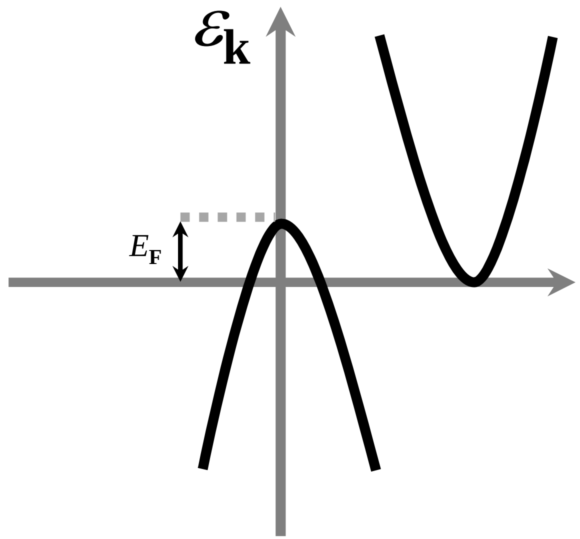
2D: two-particle bound state forms at arbitrary weak interaction

FeSe: all E_F are small

I



II



$\log \frac{\Lambda}{T_{ins}}$ ladder series of renormalizations $T_{ins} \ll \Lambda$

variation of the chemical potential cannot be neglected $\sim O\left(\frac{T_{ins}}{E_F}\right)$

Single band case

Variation of the chemical potential with temperature $\frac{T_{ins}}{E_F}$

$$1 = \frac{\lambda}{2}\int_0^{\Lambda} d\varepsilon \frac{\tanh\frac{\varepsilon-\mu}{2T_{ins}}}{\varepsilon-\mu}$$

$$= \frac{\lambda}{2}\left(\int_0^{\mu} dx \frac{\tanh\frac{x}{2T_{ins}}}{x} + \int_0^{\Lambda} dx \frac{\tanh\frac{x}{2T_{ins}}}{x}\right)$$

$$E_F = \int_0^{\Lambda} d\varepsilon \frac{1}{e^{(\varepsilon-\mu)/T_{ins}}+1} = T_{ins}\log\left(1+e^{\mu/T_{ins}}\right)$$

$E_F >> E_0$

$$T_{ins} = 1.13(\Lambda E_F)^{1/2} e^{-\frac{1}{\lambda}}$$

$$\mu(T_{ins}) \approx E_F$$

$E_F << E_0$

$$T_{ins} = \frac{E_0}{\log\frac{E_0}{E_F}}$$

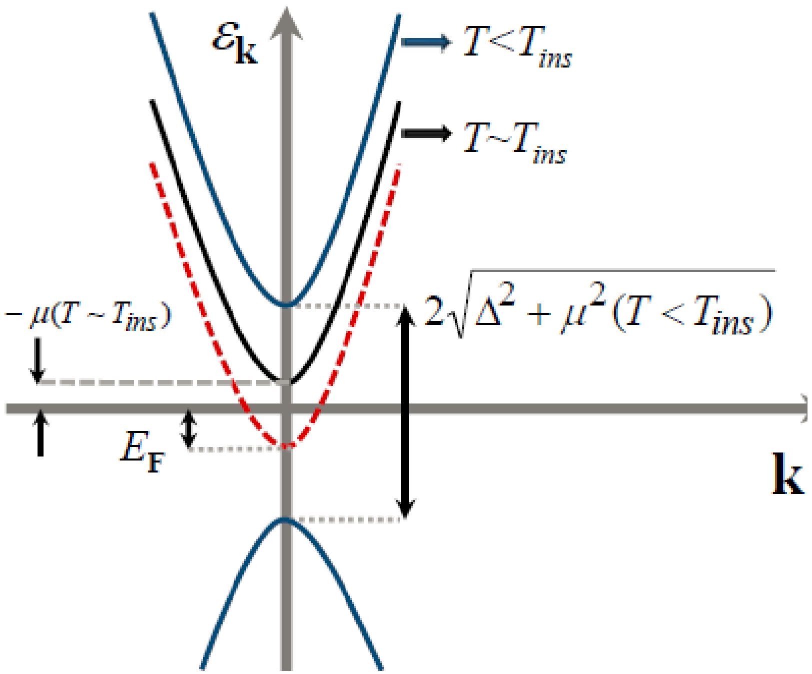
$$\mu(T_{ins}) \approx -E_0$$

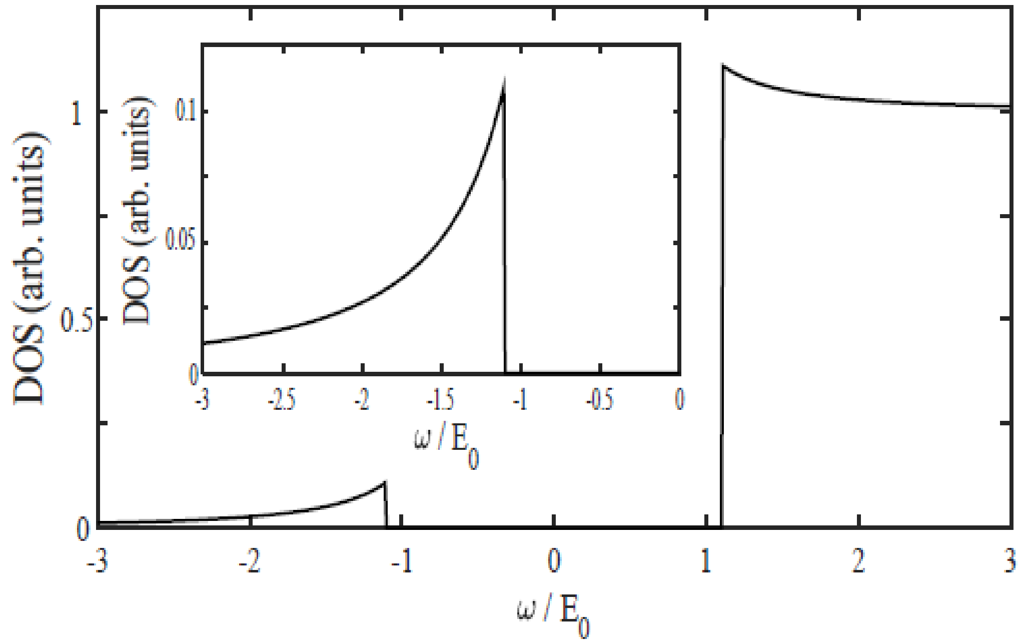
Single band case

$E_F << E_0$

$$\mu \approx -E_0$$

$$\Delta \sim T_{ins}\left(\frac{E_F}{E_0}\right)^{1/2} \log\frac{E_0}{E_F}.$$





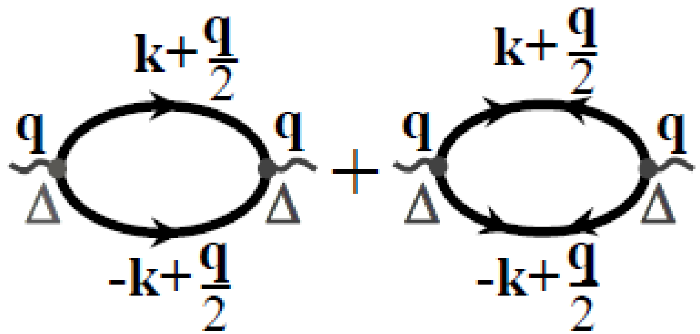
$$u_k^2 = \frac{1}{2}\left(1+\frac{\varepsilon_k-\mu}{\sqrt{(\varepsilon_k-\mu)^2+\Delta^2}}\right)$$

$$v_k^2 = \frac{1}{2}\left(1-\frac{\varepsilon_k-\mu}{\sqrt{(\varepsilon_k-\mu)^2+\Delta^2}}\right)$$

Single band case

Superconducting temperature, Tc

$E_{kin} =$ 

$E_{pot} =$ 

Comparison of the condensation energy (E_{kin}+E_{pot}(q=0))

$$E_{cond} = -N_0 \frac{\Delta^2}{2} = -N_0 E_0 E_F$$

and energy costs of the phase fluctuations (prefactor in front q^2 ~ superfluid stiffness)

$$\rho_s = \frac{E_F}{4\pi}$$

Single band case

Superconducting temperature, T_c

$$E_{cond} = -N_0 \frac{\Delta^2}{2} = -N_0 E_0 E_F \qquad \rho_s = \frac{E_F}{4\pi}$$

$$E_F >> E_0 \qquad\qquad E_F << E_0$$

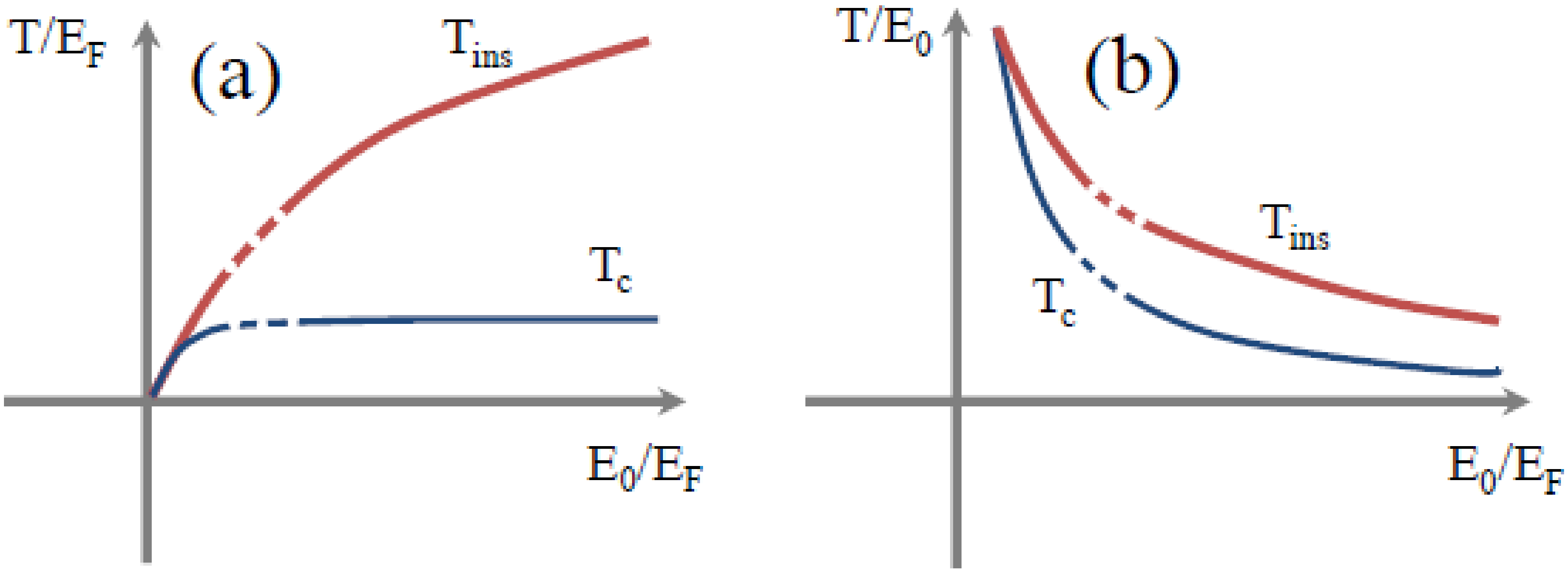
Phase fluctuatuations
too costly

$$T_c \approx \frac{\pi}{2} \rho(T=0)$$

$$T_c = T_{ins} \qquad\qquad T_c << T_{ins}$$

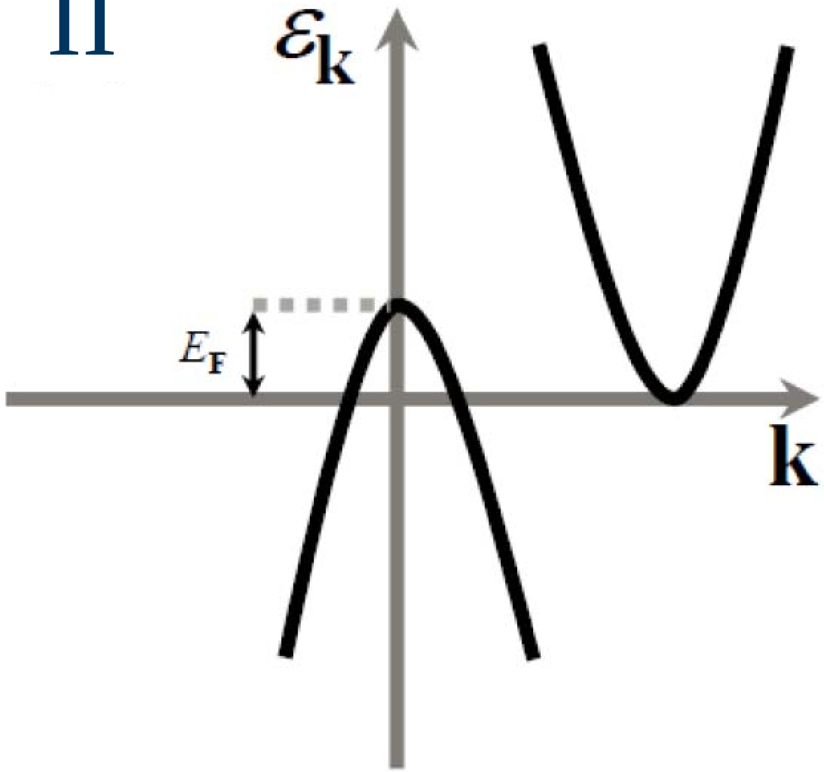
Single band case

Superconducting temperature, T_c



Two-band case: FeSe and s+- scenario

II



$$\Delta_e = -\frac{\lambda}{2}\Delta_h \int_{-\mu_h}^{\Lambda} \frac{dx}{x} \tanh\frac{x}{2T_{ins}}$$

$$\Delta_h = -\frac{\lambda}{2}\Delta_e \int_{-\mu_e}^{\Lambda} \frac{dx}{x} \tanh\frac{x}{2T_{ins}}$$

$$\mu_e = T\log\frac{1+e^{-\mu_h/T}}{1+e^{\mu_e/T}}$$

$$\mu_e + \mu_h = E_F.$$

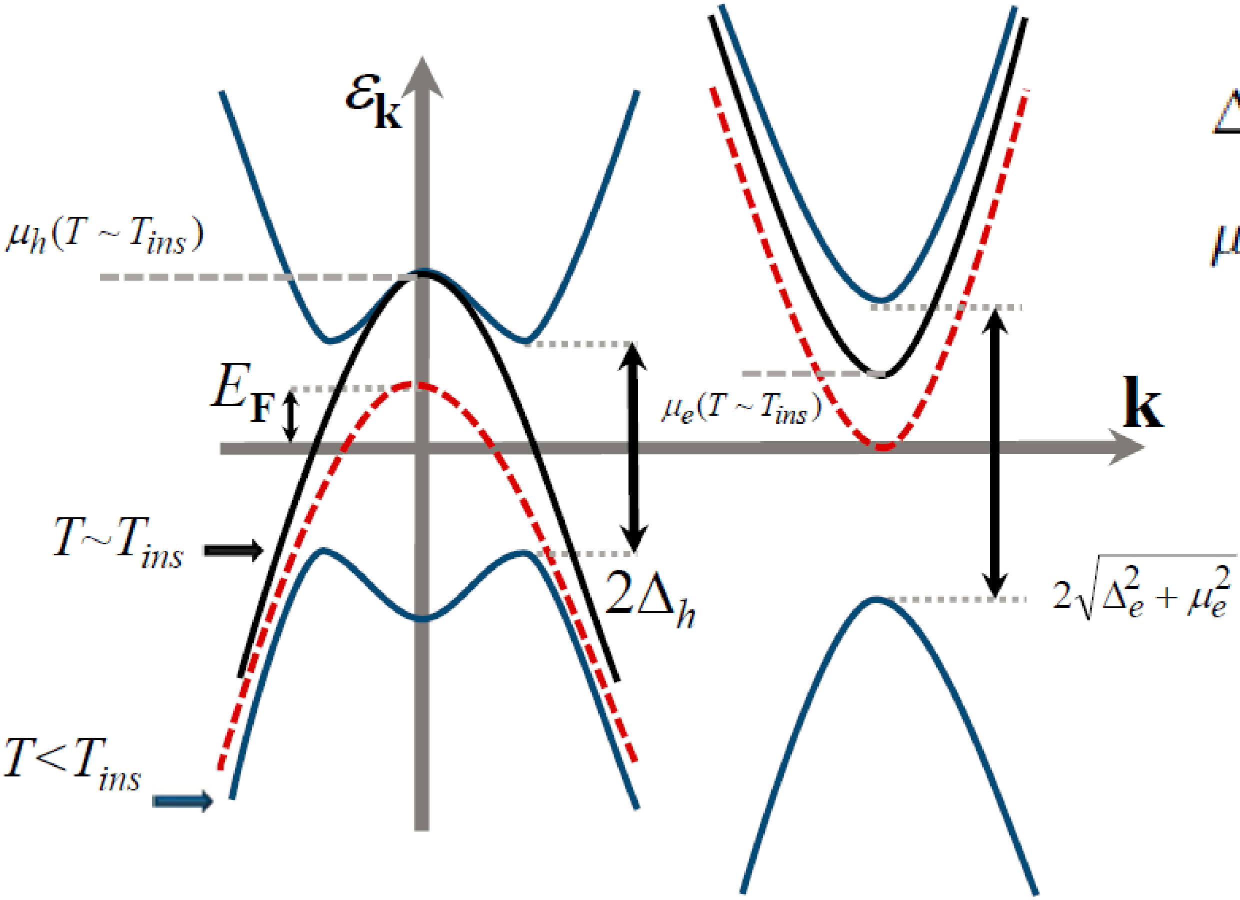
$$E_F << E_0$$

$$\Delta = 1.76 T_{ins} \gg E_F$$

$$\mu_h \approx \frac{3E_F}{2}, \quad \mu_e \approx -\frac{E_F}{2}$$

$$T_{ins} = 1.13 E_0 \left(1 + 0.22\frac{E_F}{E_0}\right)$$

Two-band case: evolution of the electron structure

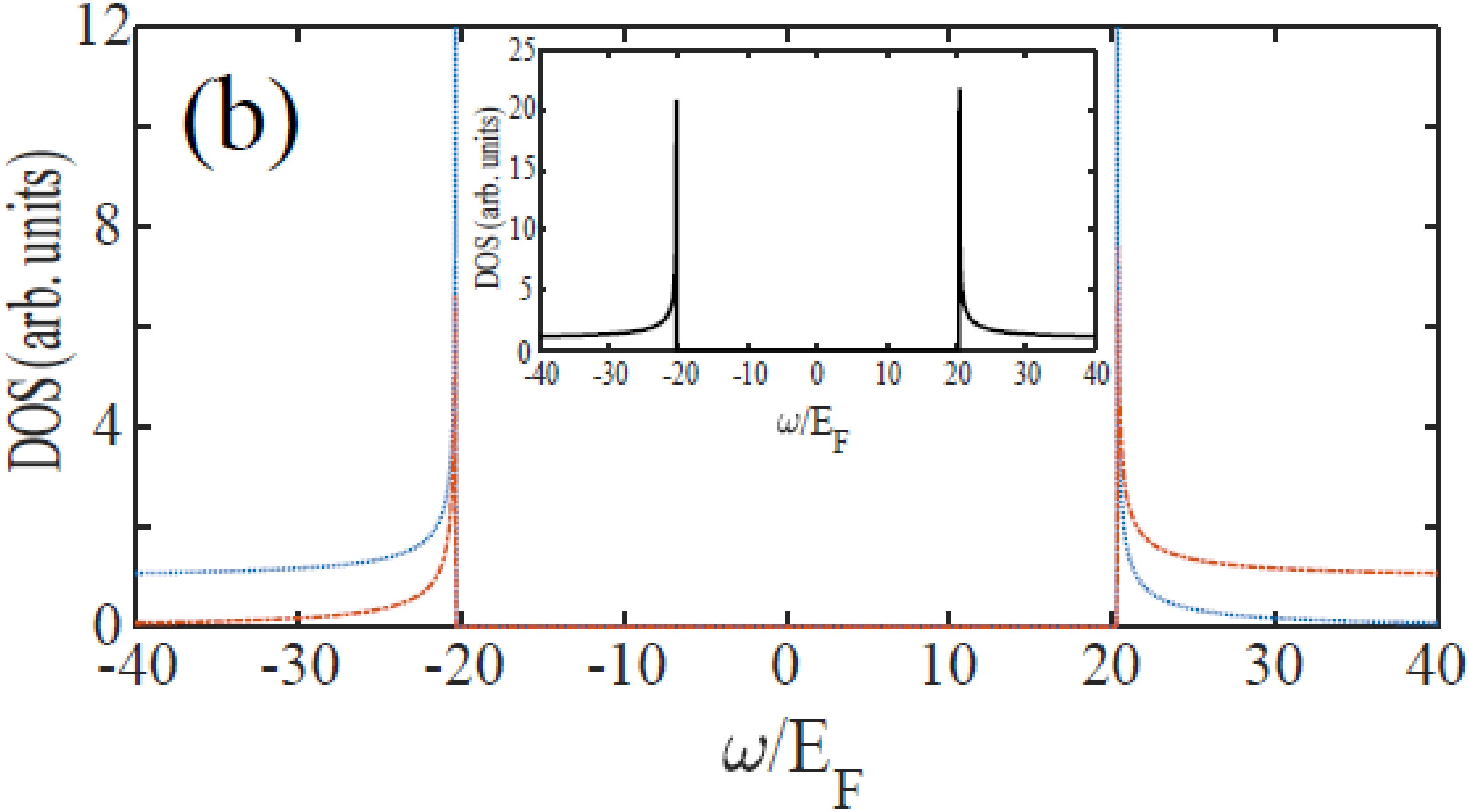


$$\Delta = 1.76 T_{ins} \gg E_F$$

$$\mu_h \approx \frac{3E_F}{2}, \quad \mu_e \approx -\frac{E_F}{2}$$

One chemical potential is negative but the other is always positive

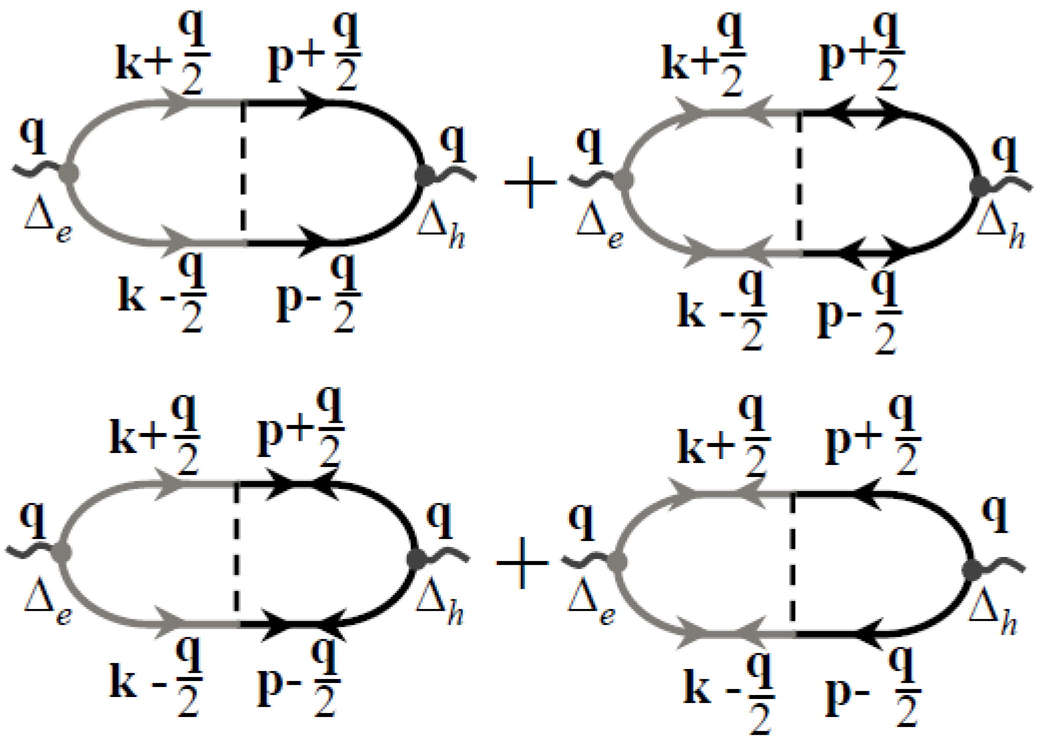
Two-band case: evolution of the electron structure



Below T_{ins} DOS looks rather symmetric

Two-band case: FeSe

Superconducting temperature, T_c



$$\delta E_{fl} = \frac{1}{2}\left[\rho_s^h(\nabla\tilde{\phi}_h)^2 + \rho_s^e(\nabla\tilde{\phi}_e)^2 + \frac{\Delta^2}{U}\left(\tilde{\phi}_e - \tilde{\phi}_h\right)^2\right]$$

T_c is determined by the combined stiffness

Two-band case: FeSe

Superconducting temperature, T_c

$$\delta E_{fl} = \frac{1}{2}\left[\rho_s^h(\nabla\tilde{\phi}_h)^2 + \rho_s^e(\nabla\tilde{\phi}_e)^2 + \frac{\Delta^2}{U}\left(\tilde{\phi}_e - \tilde{\phi}_h\right)^2\right]$$

$$\langle|\tilde{\phi}_e(k)|^2\rangle = \frac{T\left(k^2\rho_s^h + \frac{\Delta^2}{U}\right)}{k^4\rho_s^e\rho_s^h + \frac{\Delta^2}{U}k^2\left(\rho_s^e + \rho_s^h\right)}$$

$$\langle|\tilde{\phi}_h(k)|^2\rangle = \frac{T\left(k^2\rho_s^e + \frac{\Delta^2}{U}\right)}{k^4\rho_s^e\rho_s^h + \frac{\Delta^2}{U}k^2\left(\rho_s^e + \rho_s^h\right)}$$

Ordering of one phase produces mass term in the fluctuation of the other

Two-band case: FeSe

The total superfluid stiffness is also related to the total number of fermions

$$\frac{N_e}{N_0} = 8\pi\rho_s^e, \quad \frac{N_h}{N_0} = 2\Lambda - 8\pi\rho_s^h$$

$$E_F << E_0 \qquad T_c \approx (\pi/2)\rho_{comb}(T) = 1.57\rho_{comb}(0)$$

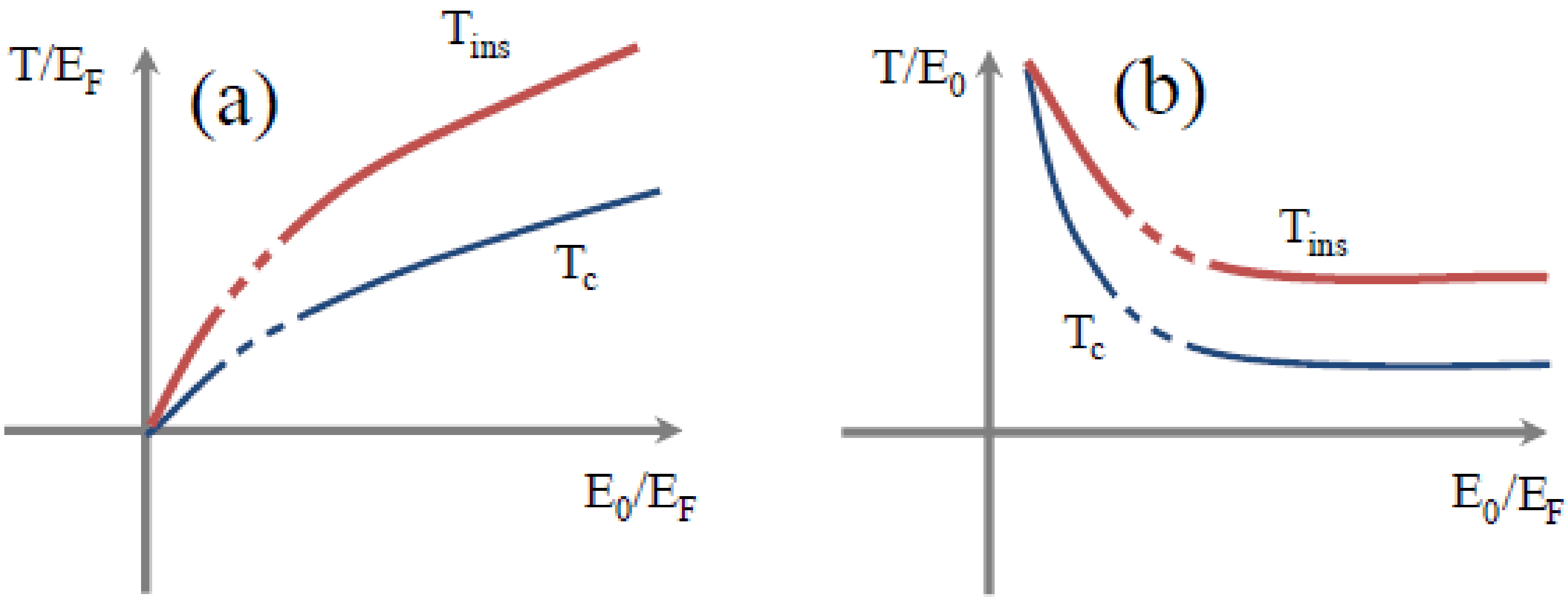
$$\rho_s^h \approx \rho_s^e \approx \frac{\Delta^2}{8\pi}\int_0^\infty d\varepsilon \frac{\varepsilon}{(\varepsilon^2 + \Delta^2)^{3/2}} = \frac{\Delta}{8\pi} = 0.07T_{ins}.$$

$$\rho_{comb} = 0.14T_{ins}, \quad T_c \approx 0.22T_{ins}$$

T_c however is still numercially smaller than T_{ins}

Two-band case: FeSe

T_c however is still numerically smaller than T_{ins}



There is a room for a BCS-BEC crossover regime in this case

Conclusions:

BCS-BEC crossover in neraly compensated metals

- Much harder (yet possible) to realize even for small E_F
- Superconductivity appears even if both $E_F=0$

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