Fe-based superconductors: role of the magnetic impurities

Maxim M. Korshunov

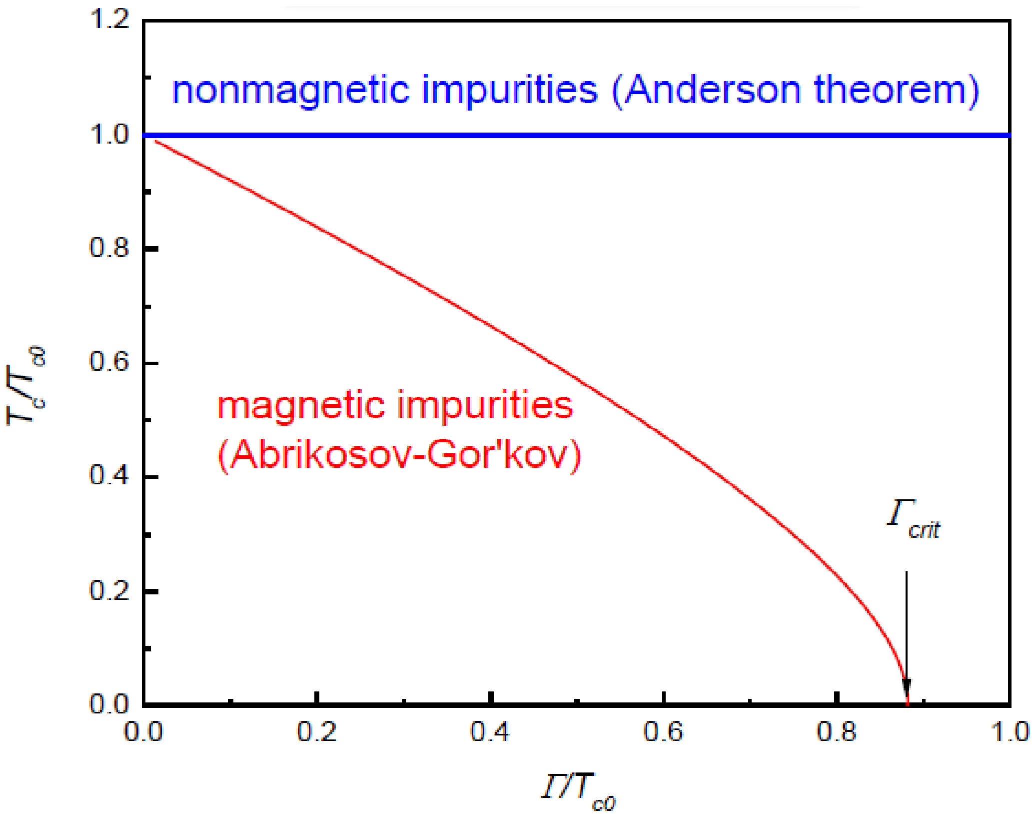
L.V. Kirensky Institute of Physics, Krasnoyarsk, Russia

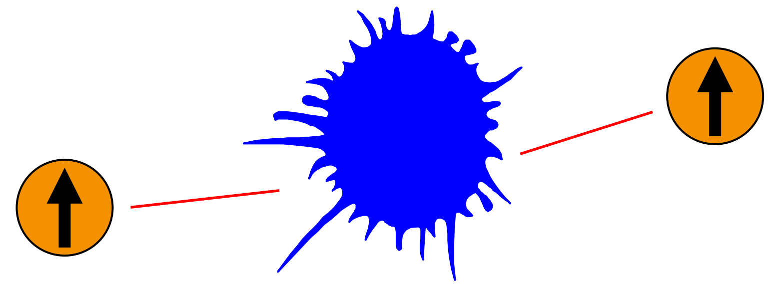
In collaboration with

- **Oleg Dolgov (MPI FKF Stuttgart)**
- **Alexander Golubov (University of Twente)**
- **Dima Efremov (IFW Dresden)**

[ICTP EXS-October-2014]

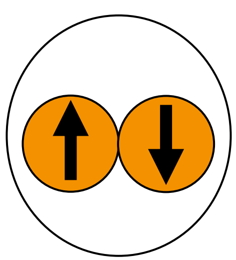
Effect of impurity scattering: single-gap *s*-wave system

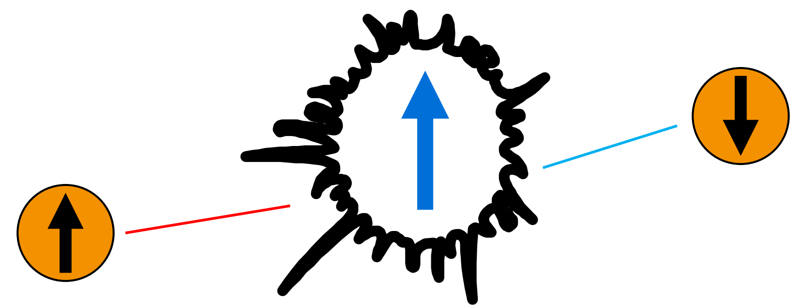




nonmagnetic impurity

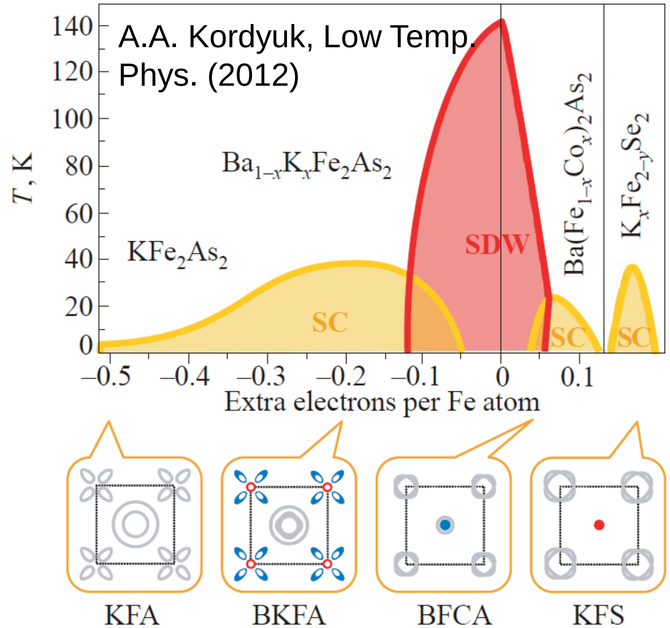
Singlet cooper pair



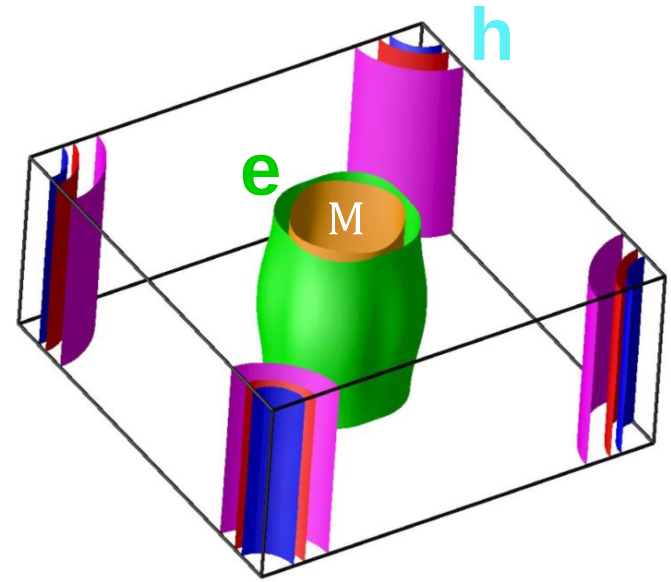


magnetic impurity

Fe-based superconductors



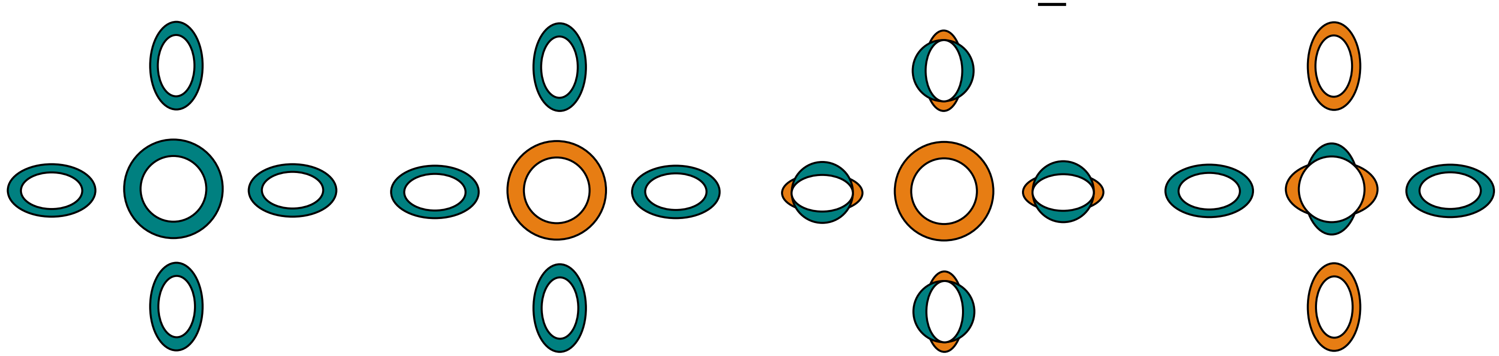
DFT result: Fe^{2+} $3d^6$-states form the FS



Weak CEF splitting: all 5 orbitals ($d_{x^2-y^2}$, $d_{3z^2-r^2}$, d_{xy}, $d_{xz}+d_{yz}$) are near the Fermi level

Symmetry proposals for FeBS

s_{++}	$s_{\pm}$	nodal $s_{\pm}$	d



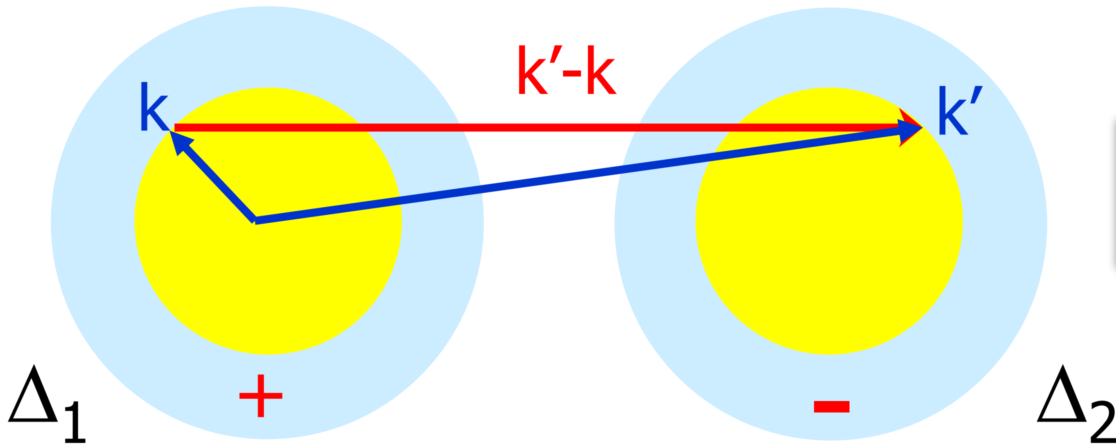
Orbital fluctuations, Phonons	Spin fluctuations	“Realistic” Spin fluctuations	Mott-Hubbard-type theories

P.J. Hirschfeld, MMK, and I.I. Mazin, Rep. Prog. Phys. 74, 124508 (2011)

Inter- and intraband nonmagnetic impurity scattering in the 2-band $s_{\pm}$ system

Inter-

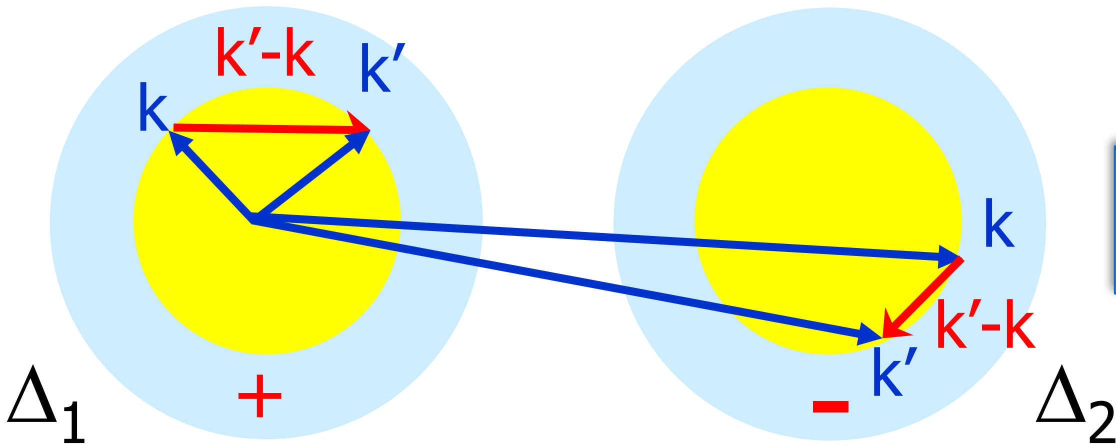
u



mixes + and –
gaps, breaks pairs

Intra-

v

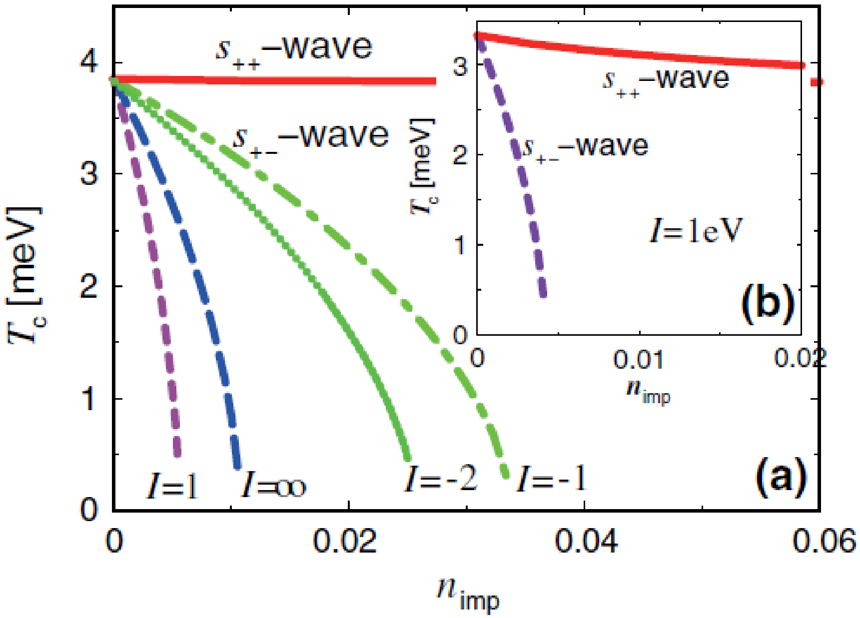


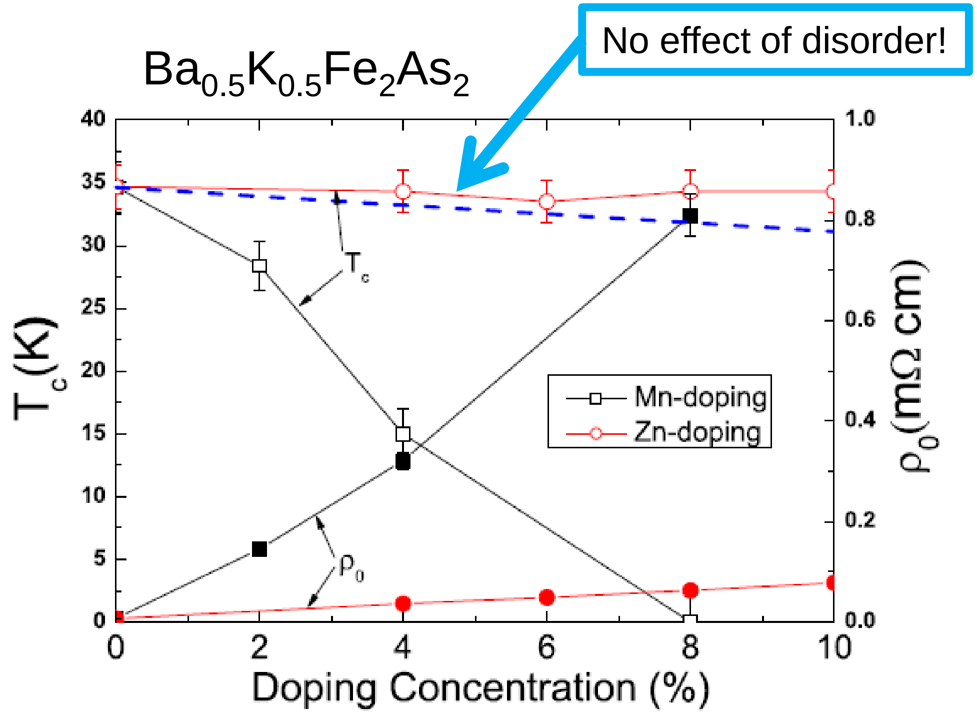
no mixing of +/-
no pairbreaking

A.A. Golubov and I.I. Mazin, PRB 55, 15146 (1997), Physica C 243, 153 (1995)

P.J. Hirschfeld, MMK, and I.I. Mazin, Rep. Prog. Phys. 74, 124508 (2011)

Non-magnetic vs. magnetic impurities





Theory: suppression of T_C by non-magnetic impurities

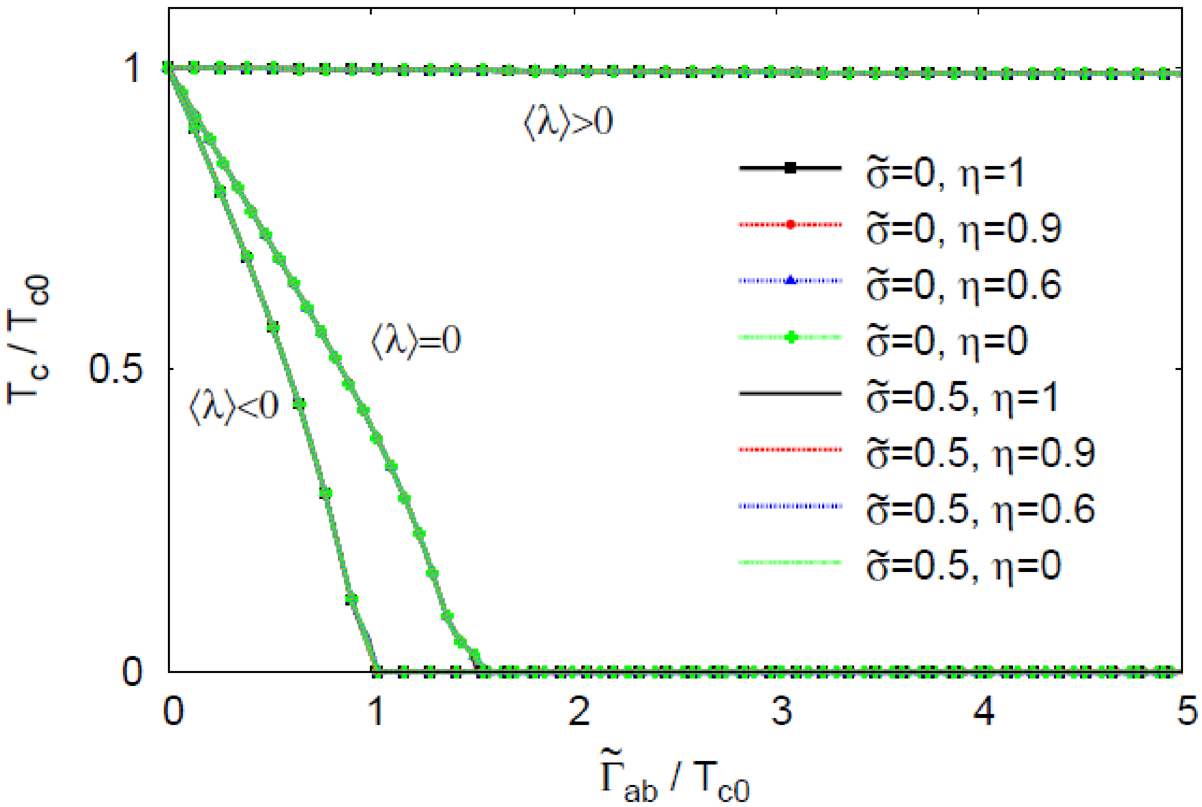
S. Onari, H. Kontani, PRL 103, 177001 (2009)

For Zn (non-magnetic impurity) the suppression of T_c is negligible

Magnetic impurities (Mn) suppress T_c, $\Delta T_c/(1\%\text{Mn}) = -4.2\text{K}$

P. Cheng et al., PRB 81, 174529 (2010)

Non-magnetic impurities in a two-band $s_{\pm}$ state: universal scattering rate



Interband and intraband impurities
$v^2 = u^2\eta$

Impurity strength
$$\tilde{\sigma} = \frac{\pi^2 N_a N_b u^2}{1 + \pi^2 N_a N_b u^2}$$

$\tilde{\sigma} \to 0$: Born limit
$\tilde{\sigma} \to 1$: unitary limit

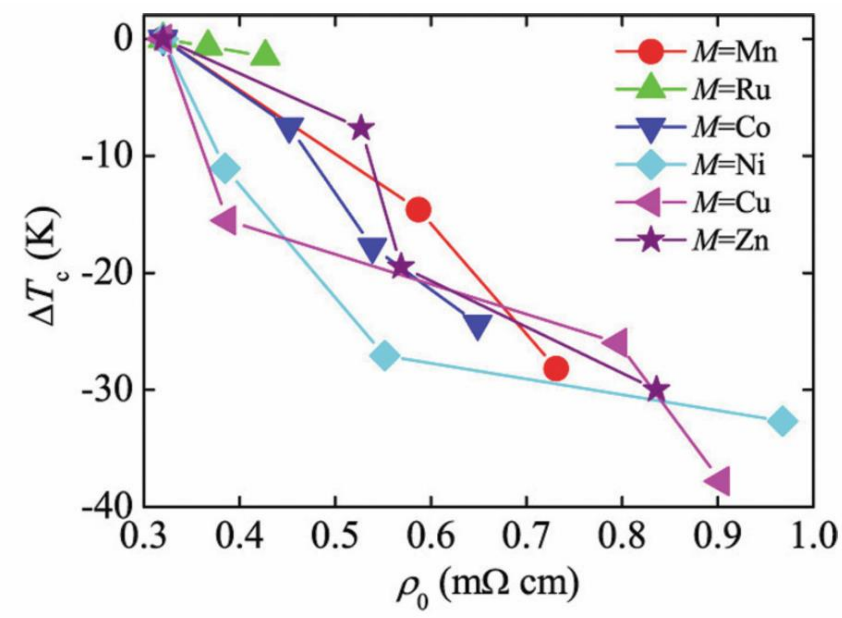
Scattering rate
$$\Gamma_{a(b)} = n_{\text{imp}} \pi N_{b(a)} u^2 (1 - \tilde{\sigma})$$

Averaged coupling constant
$$\langle\lambda\rangle_{FS} = \frac{N_a}{N}(\lambda_{aa} + \lambda_{ab}) + \frac{N_b}{N}(\lambda_{ba} + \lambda_{bb})$$

D.V. Efremov, MMK, O.V. Dolgov, A.A. Golubov, and P.J. Hirschfeld, PRB 84, 180512(R) (2011)

Experiment: disorder

$Ba_{0.5}K_{0.5}Fe_{2-2x}M_{2x}As_2$



J. Li et al., PRB 85, 214509 (2012)

Irradiation studies

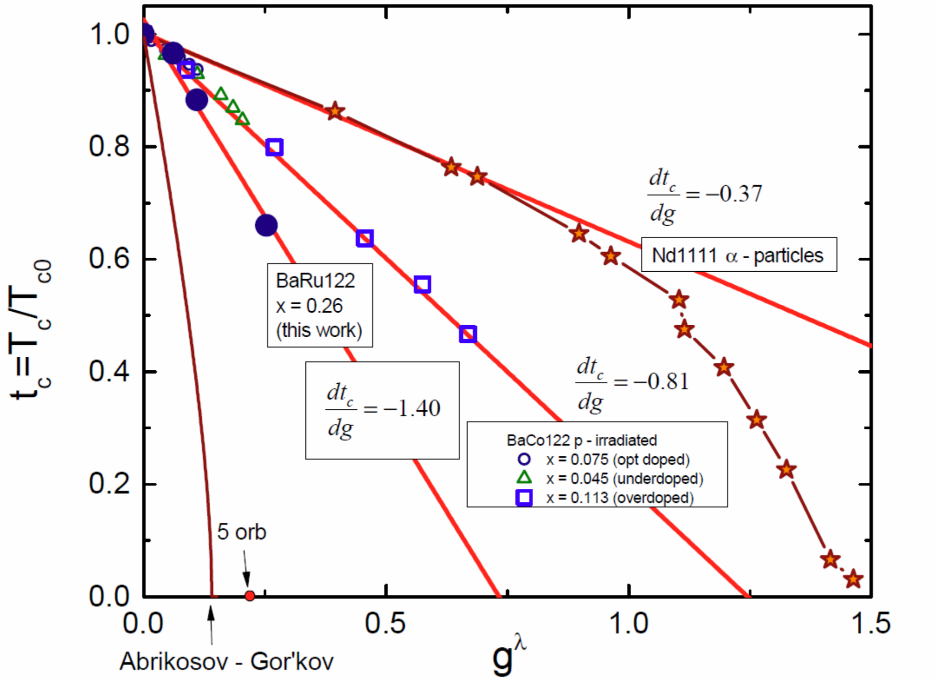


FIG. 3. (Color online) Comparison of the T_c suppression by three irradiation techniques used to introduce artificial disorder in iron - pnictides. The single effective dimensionless scattering rate, g^λ, was calculated from the penetration depth and resistivity, see text for description. Abrikosov - Gor'kov theory for an isotropic $s-$wave superconductor with magnetic impurities (solid line) and a critical scattering rate within 5 band $s_\pm$ model [6] are also shown.

R. Prozorov et al., arXiv:1405.3255v1

Effect of impurity scattering: Born limit

Single-band case: $1 = 2T_c \lambda \pi N_0 \sum_{0<\omega_n \le \omega_D} \left(\frac{\tilde{\phi}_n}{\Delta} \frac{1}{\tilde{\omega}_n} \right)_{T_c}$

Nonmagnetic (magnetic) impurities:

$$\begin{cases} \tilde{\omega}_n = \omega_n + \frac{\Gamma_a}{2} \frac{\tilde{\omega}_n}{\sqrt{\tilde{\omega}_n^2 + \tilde{\phi}_n^2}} \\ \tilde{\phi}_n = \Delta \pm \frac{\Gamma_a}{2} \frac{\tilde{\phi}_n}{\sqrt{\tilde{\omega}_n^2 + \tilde{\phi}_n^2}} \end{cases}$$

Nonmagnetic: $\left(\frac{\tilde{\phi}_n}{\Delta} \frac{1}{\tilde{\omega}_n} \right)_{T_c} = \frac{1}{\omega_n}$ → $T_c = 1.13 \omega_D e^{-1/\lambda N_0}$

Anderson's theorem
impurities cancel out!

Magnetic: $\left(\frac{\tilde{\phi}_n}{\Delta} \frac{1}{\tilde{\omega}_n} \right)_{T_c} = \frac{1}{\omega_n + \Gamma_a}$

impurity scattering rate $\Gamma_a = \pi N_0 n_{\mathrm{imp}} u^2$

T_c is suppressed compared to the clean case (T_{c0})! $\ln \frac{T_{c0}}{T_c} = \Psi\left(\frac{1}{2} + \frac{\Gamma_a}{2\pi T_c} \right) - \Psi\left(\frac{1}{2} \right)$

Magnetic interband-only impurities in the 2-band case:

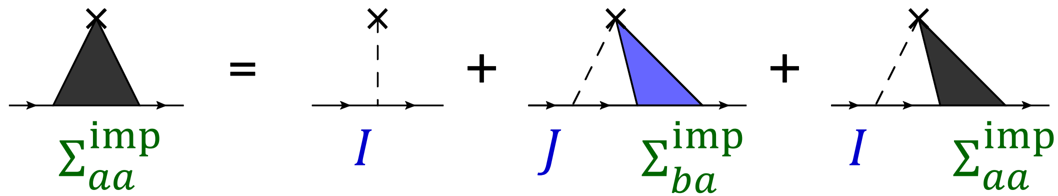
if $\Delta_a = -\Delta_b$ then $\left(\frac{\tilde{\phi}_{\alpha n}}{\Delta_\alpha} \frac{1}{\tilde{\omega}_{\alpha n}} \right)_{T_c} = \frac{1}{\omega_n}$ → T_c is not suppressed ($s_\pm$)

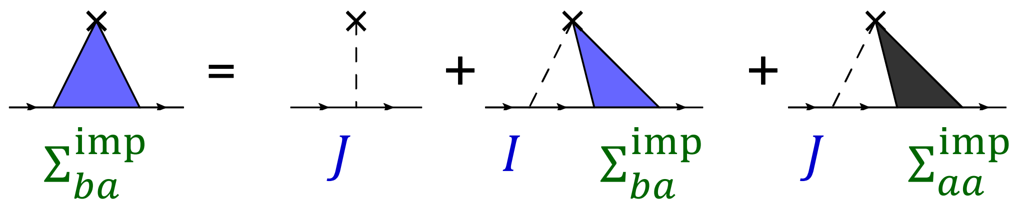
A.A. Golubov and I.I. Mazin, PRB 55, 15146 (1997), Physica C 243, 153 (1995)

T-matrix approximation for the impurity self-energy

$$i\tilde{\omega}_{an} = i\omega_n - \Sigma_{0a}(\omega_n) - \Sigma_{0a}^{\mathrm{imp}}(\omega_n), \quad \tilde{\phi}_{an} = \Sigma_{2a}(\omega_n) + \Sigma_{2a}^{\mathrm{imp}}(\omega_n)$$

$$\hat{\boldsymbol{\Sigma}}^{\mathrm{imp}}(\omega_n) = n_{\mathrm{imp}}\,\hat{\mathbf{U}} + \hat{\mathbf{U}}\,\hat{\mathbf{g}}(\omega_n)\hat{\boldsymbol{\Sigma}}^{\mathrm{imp}}(\omega_n)$$





n_{imp} is the impurity concentration

I and J are the impurity potentials

Impurity potential $\hat{\mathbf{U}} = \begin{pmatrix} I\hat{S} & J\hat{S} \\ J\hat{S} & I\hat{S} \end{pmatrix}$

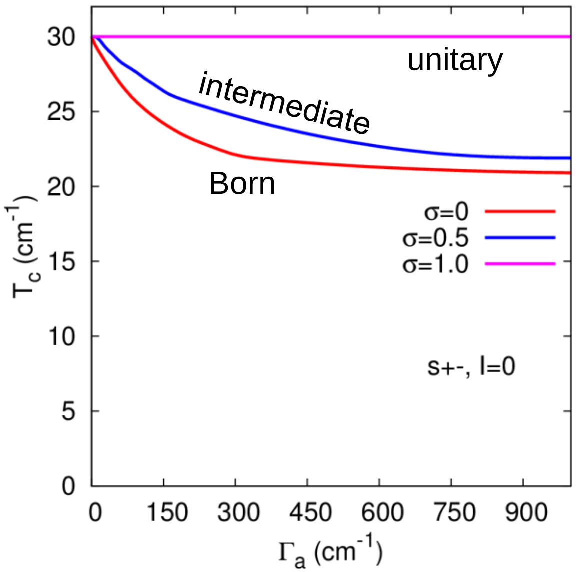
Generalized cross-section parameter (helps to control the approximation)

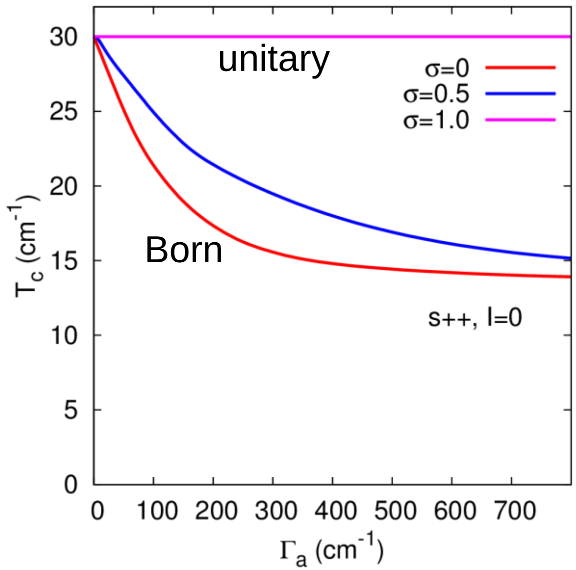
$$\sigma = \frac{\pi^2 J^2 s^2 N_a N_b}{1 + \pi^2 J^2 s^2 N_a N_b} \to \begin{cases} 0, & \text{Born} \\ 1, & \text{unitary} \end{cases}$$

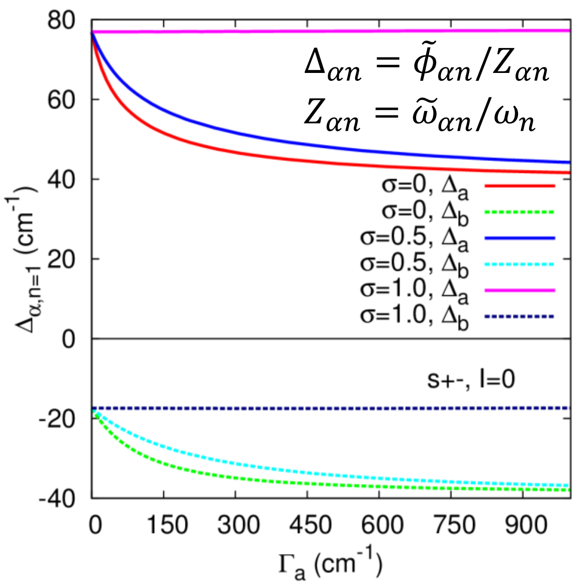
Effective impurity scattering strength

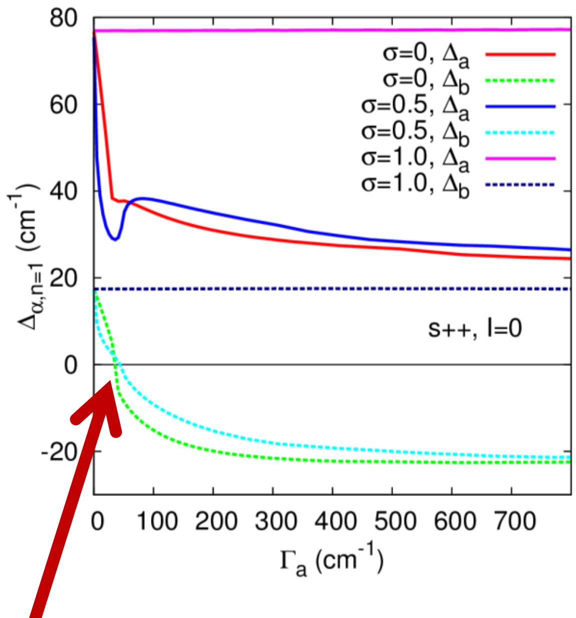
$$\Gamma_{a,b} = \frac{2 n_{\mathrm{imp}}\sigma}{\pi N_{a,b}} \to \begin{cases} 2\pi J^2 s^2 n_{\mathrm{imp}} N_{b,a}, & \text{Born} \\ \dfrac{2 n_{\mathrm{imp}}}{\pi N_{a,b}}, & \text{unitary} \end{cases}$$

Interband magnetic impurities: results for the $s_{\pm}$ and s_{++} systems









Smaller gap changes sign for $\Gamma > 40\ \mathrm{cm}^{-1}$!

Interband-only impurities **do not** destroy $s_{\pm}$ superconductivity

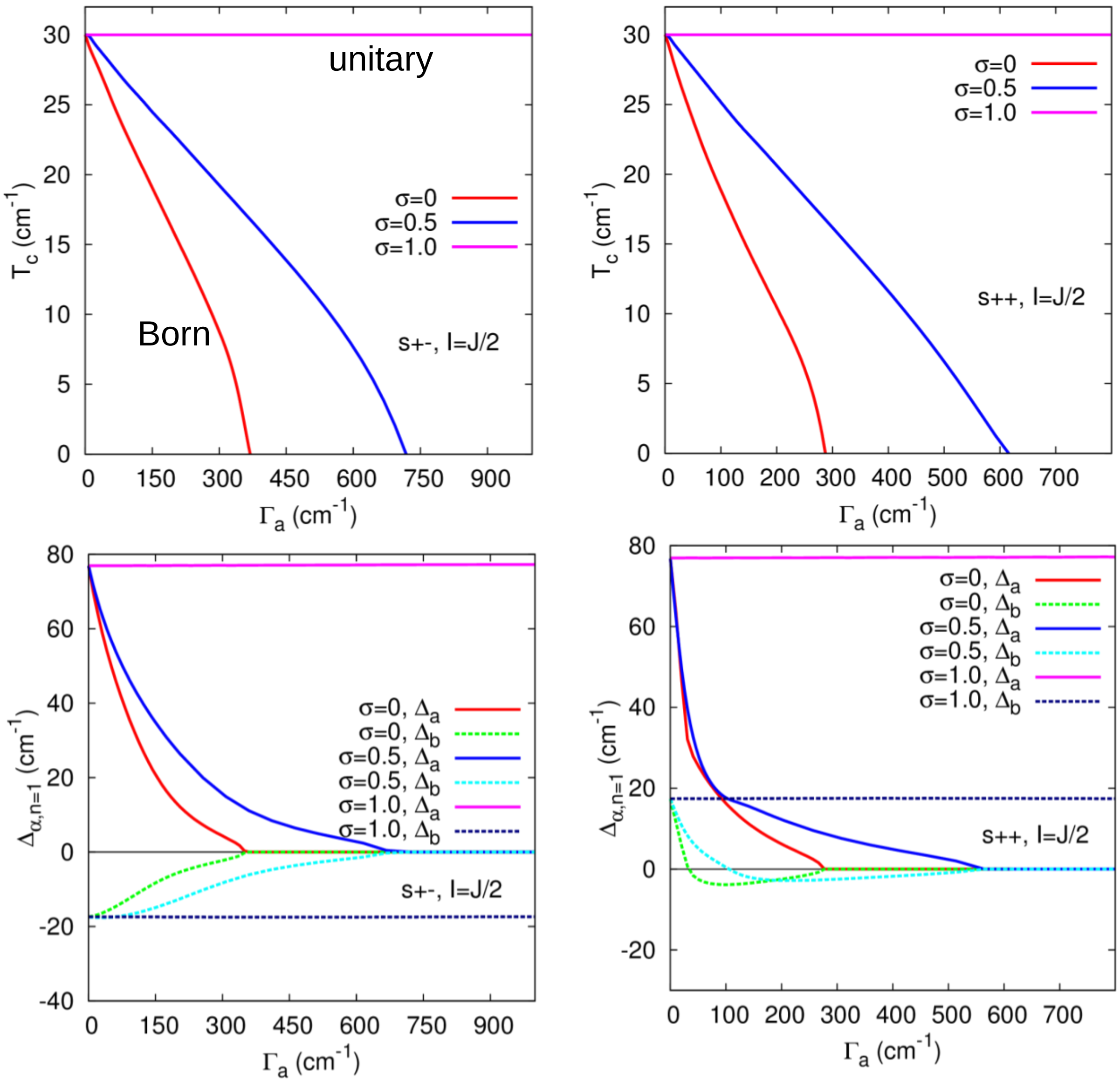
This confirms qualitative arguments that $s_{\pm}$ state with magnetic disorder behave like the s_{++} state with non-magnetic impurities [Golubov, Mazin (1995,1997)] and agrees with the Born limit results [Li, Wang, EPL 88, 17009, (2009)].

$s_{++} \to s_{\pm}$ transition!

Then T_c **saturates** since the **interband-only impurities do not** destroy $s_{\pm}$ state.

It is the only way for the s_{++} state to be robust against the magnetic disorder.

Finite intraband magnetic disorder: $s_{\pm}$ and s_{++} systems



Interband-only impurities **do not** destroy $s_{\pm}$ superconductivity, but **intraband do**!

Finite intraband disorder finally suppress T_c to zero.

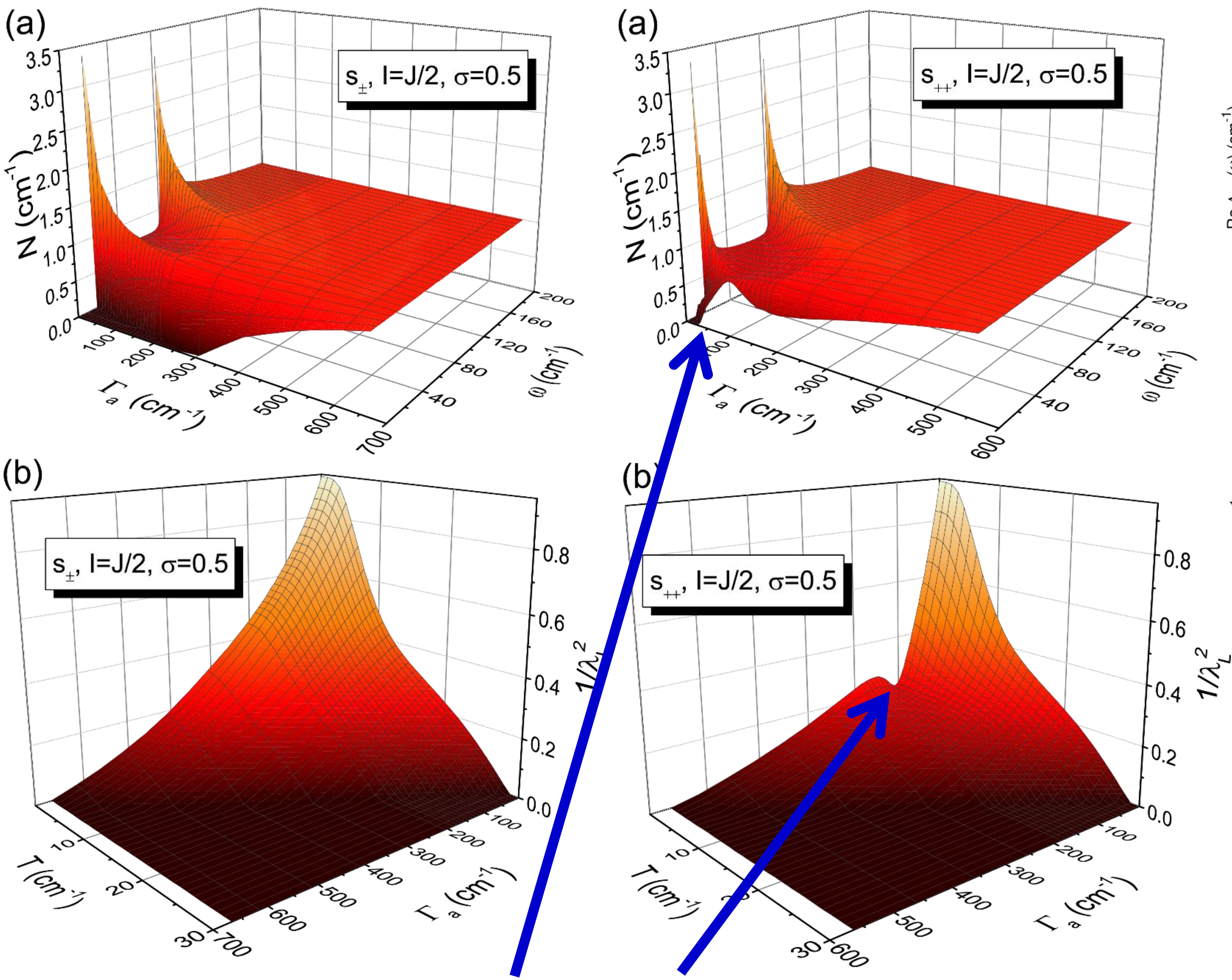
$\boldsymbol{s_{++}} \to \boldsymbol{s_{\pm}}$ transition can't save s_{++} state from being destroyed.

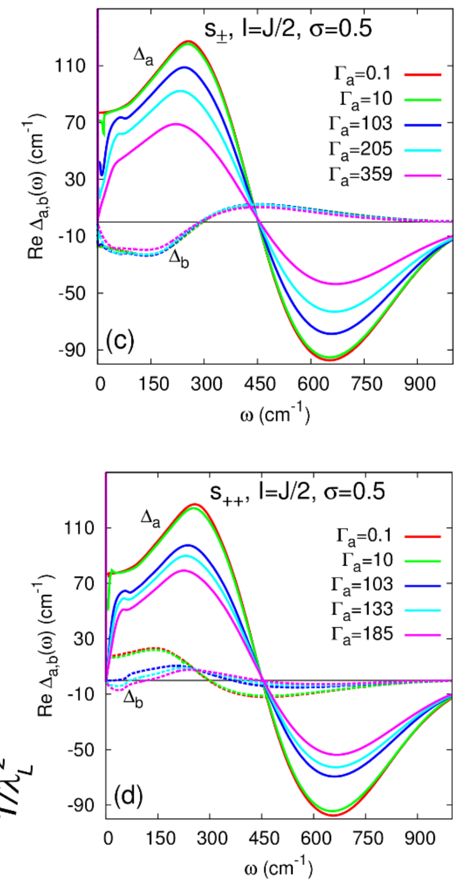
The only exception here is the unitary limit ($\sigma = 1$). At $T \to T_c$:

$$\tilde{\omega}_{an} = \omega_n + \mathrm{i}\Sigma_{0a}(\omega_n) + \frac{\Gamma_a}{2}\mathrm{sgn}(\omega_n)$$

$$\tilde{\phi}_{an} = \Sigma_{2a}(\omega_n) + \frac{\Gamma_a}{2}\frac{\tilde{\phi}_{an}}{|\tilde{\omega}_{an}|}$$

DOS and penetration depth in $s_{\pm}$ and s_{++} systems





$s_{++} \rightarrow s_{\pm}$ transition

$$\hat{V} = \begin{pmatrix} J/2 & J \\ J & J/2 \end{pmatrix}$$

$\sigma \rightarrow 0$: Born limit

$\sigma \rightarrow 1$: unitary limit

Conclusions

- **The T_c suppression is much slower than suggested in AG theory**
- **There are few exceptional cases with the saturation of T_c for the finite amount of magnetic impurities:**
- **(1) $s_{\pm}$ superconductor with the purely interband impurity scattering potential.**
- **(2) s_{++} state with the interband-only scattering due to the $s_{++} \rightarrow s_{\pm}$ transition.**
  Since this transition goes through the gapless regime, there should be clear signatures in the thermodynamics of the system. Therefore, it may manifest itself in optical and tunneling experiments, as well as in a photoemission and thermal conductivity on Fe-based superconductors and other multiband systems.
- **(3) the unitary scattering limit**

MMK, D.V. Efremov, A.A. Golubov, O.V. Dolgov, PRB 90, 134517 (2014)