Physical Properties of $s_{\pm}$ Superconductors as a Model of Iron Pnictides

Alexander Golubov

University of Twente, The Netherlands

In collaboration with

A. Brinkman, University of Twente, Netherlands

O.V. Dolgov, Max Planlk Institute, Stuttgart, Germany

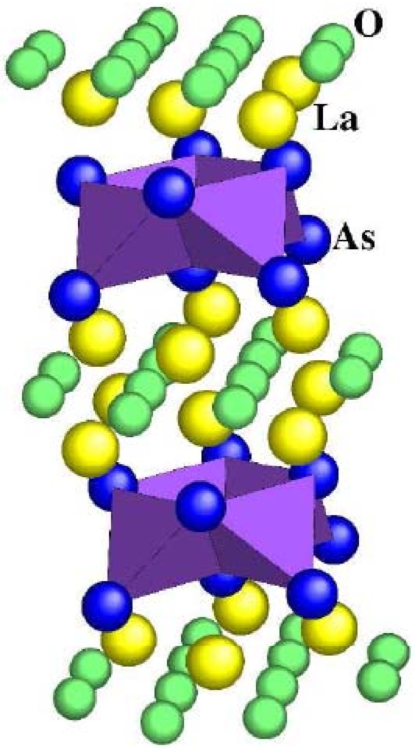
I.I. Mazin, *D. Parker*, Naval Research Lab, Washington, USA

Y. Tanaka, Nagoya University, Japan

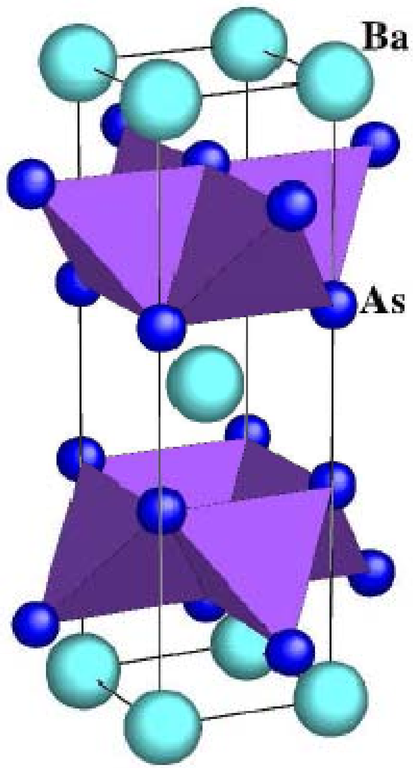
Outline

- Introduction
- $s_{\pm}$ pairing and impurity scattering
- Absence of the *Hebel-Slichter* peak in NMR relaxation and *T*-dependence of $1/T_1$
- Electromagnetic response in the $s_{\pm}$ model
- Tunneling in the $s_{\pm}$ model

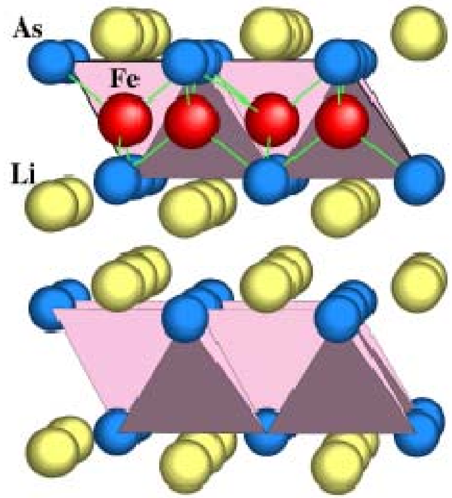
Crystal structure of FeAs superconductors



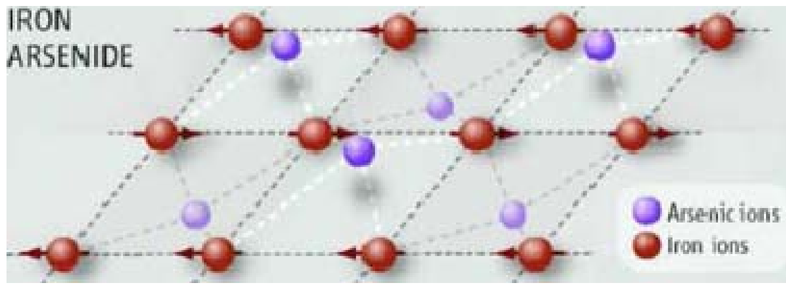
LaOFeAs



$BaFe_2As_2$



LiFeAs



FeAs tetrahedra form two-dimensional layers surrounded by LaO, Ba or Li.
Fe ions inside tetrahedra form a square lattice.

Basic Experiments on FeAs

J|A|C|S COMMUNICATIONS

February 2008

Published on Web 02/23/2008

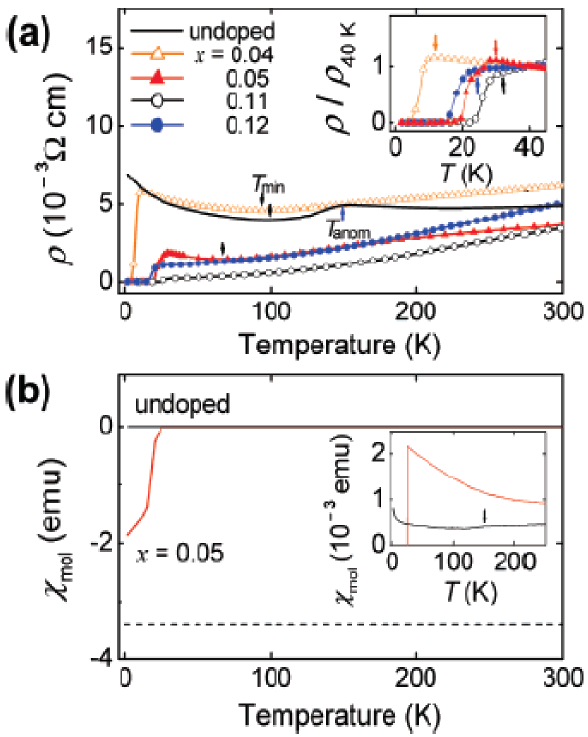
Iron-Based Layered Superconductor La[$O_{1-x}F_x$]FeAs ($x = 0.05-0.12$) with $T_c = 26$ K

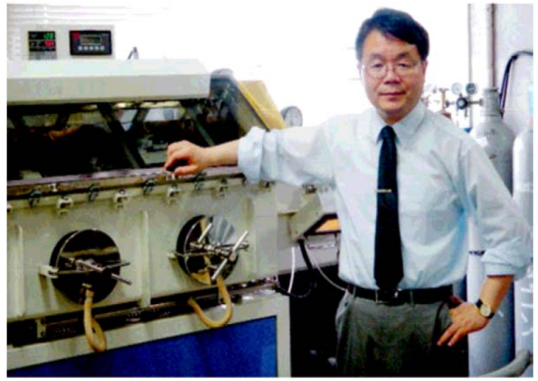
Yoichi Kamihara,*,† Takumi Watanabe,‡ Masahiro Hirano,†,§ and Hideo Hosono†,‡,§

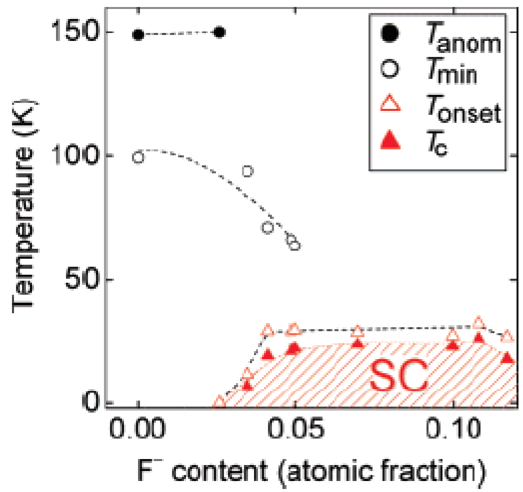
ERATO-SORST, JST, Frontier Research Center, Tokyo Institute of Technology, Mail Box S2-13, Materials and Structures Laboratory, Tokyo Institute of Technology, Mail Box R3-1, and Frontier Research Center, Tokyo Institute of Technology, Mail Box S2-13, 4259 Nagatsuta, Midori-ku, Yokohama 226-8503, Japan

Received January 9, 2008; E-mail: hosono@msl.titech.ac.jp

■ J. AM. CHEM. SOC. 2008, 130, 3296−3297

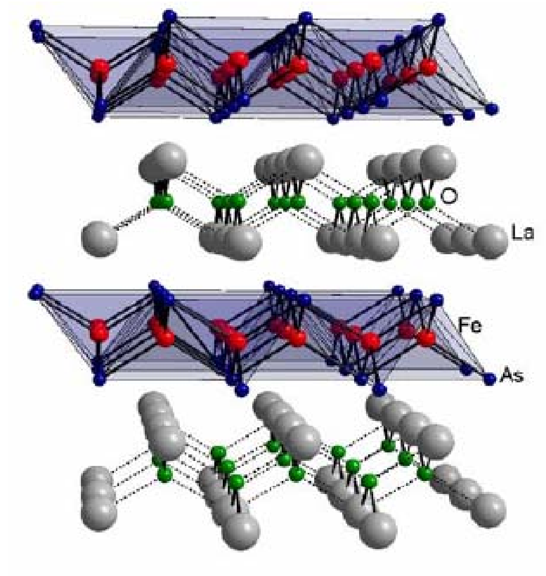




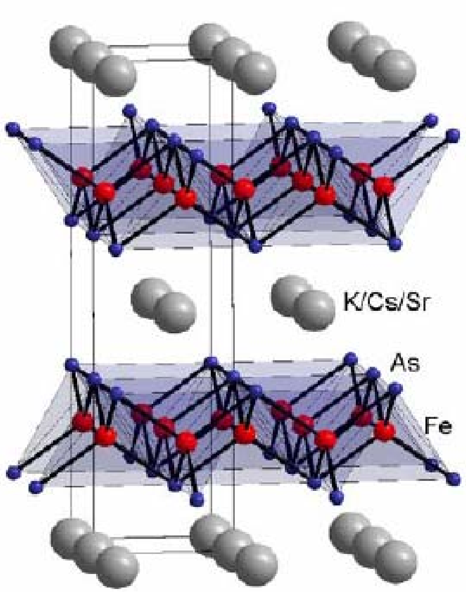


Electron doping!

Basic crystal structure of FeAs superconductors

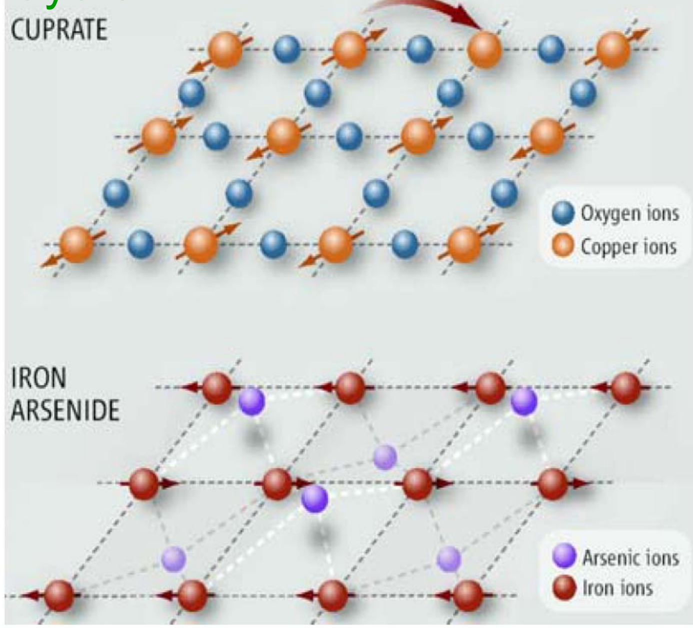


$$(RE)^{+3}O^{-2}Fe^{+2}As^{-3}$$



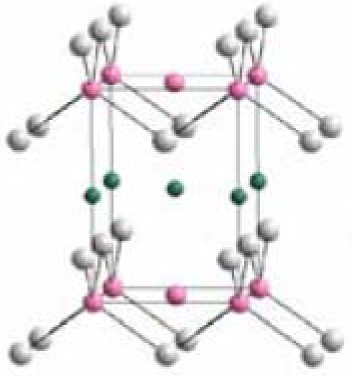
$$Ba^{+2}(Fe^{+2})_2(As^{-3})_2$$

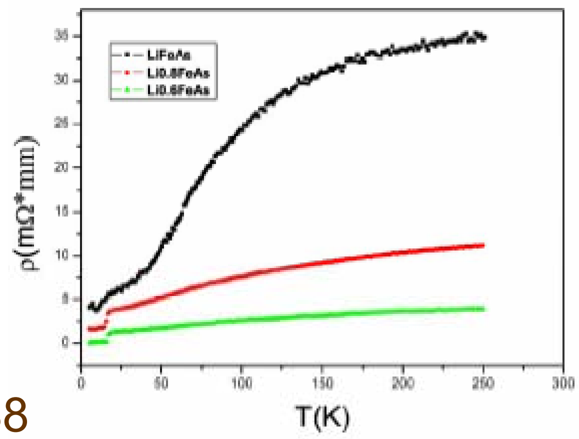
CuO_2 as compared with FeAs layers:



The superconductivity at 18 K in $Li_{1-x}FeAs$ compounds

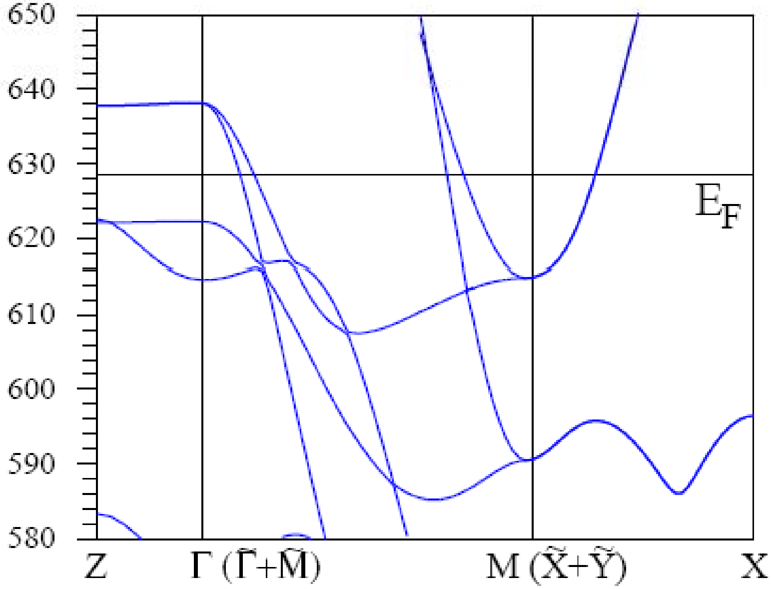
X.C.Wang, Q.Q. Liu, Y.X. Lv, W.B. Gao, L.X.Yang, R.C. Yu, F.Y.Li, C.Q. Jin*

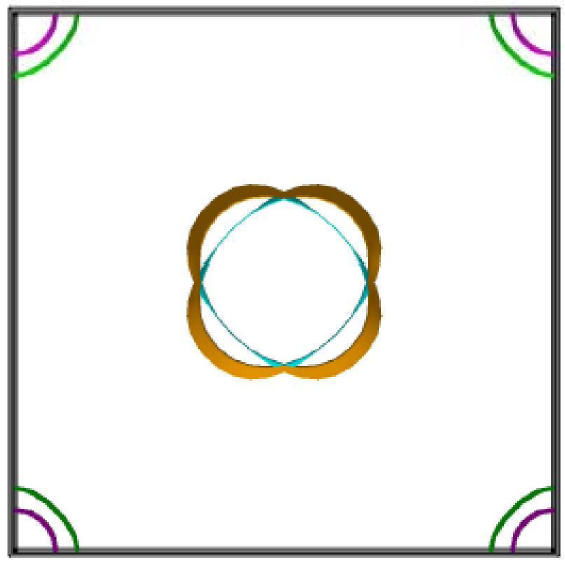




arXiv: 0806.4688

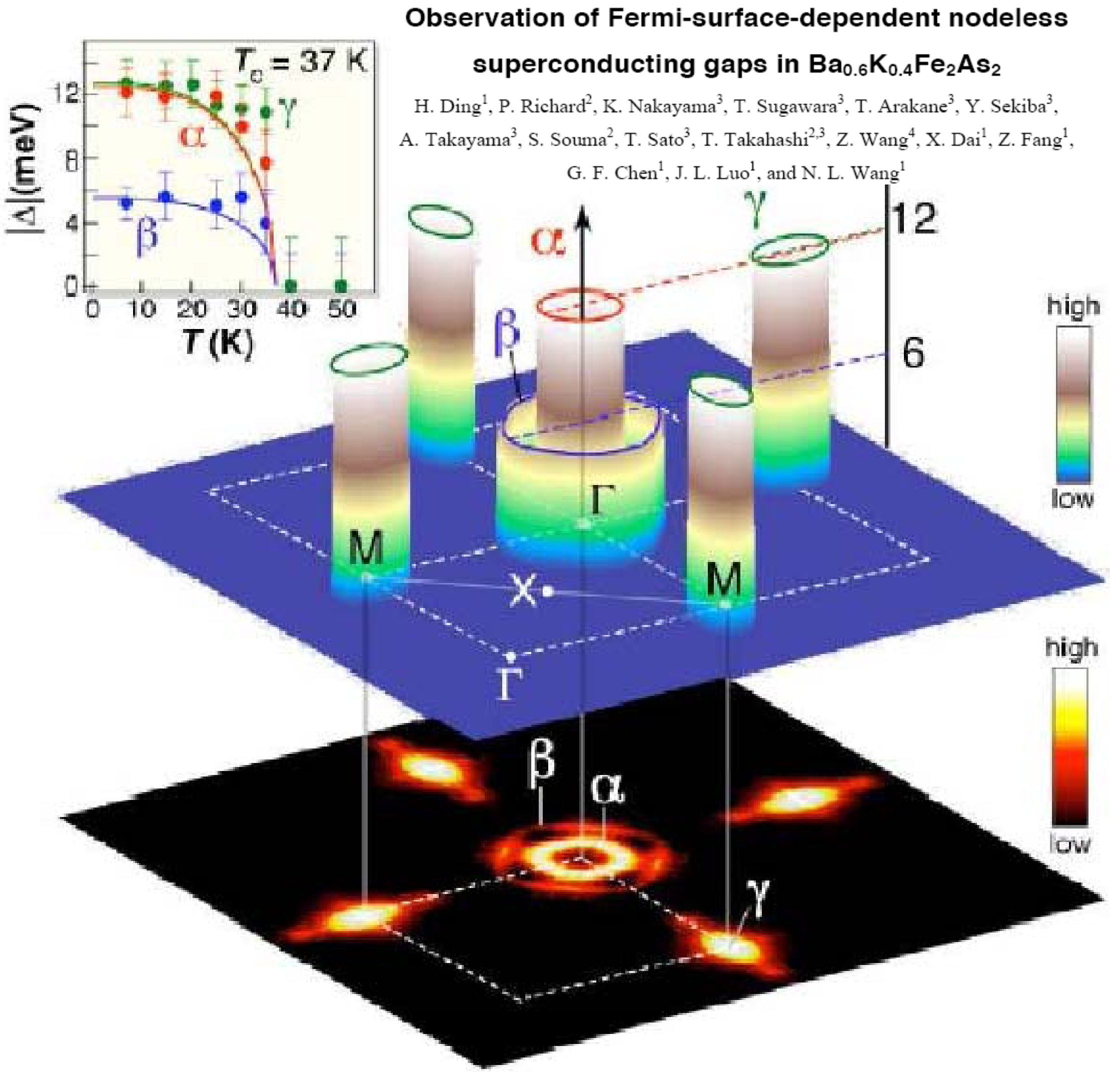
Band structure





Superconducting gap – ARPES data

arXiv: 0807.0419



Schematic picture of superconducting gaps in $Ba_{0.6}K_{0.4}Fe_2As_2$. Lower picture represents Fermi surfaces (ARPES intensity), upper insert – temperature dependence of gaps at different Sheets of the Fermi surface.

Spin fluctuations

$$\chi(\mathbf{q},\omega) = \frac{\chi_0(\mathbf{q},\omega)}{1 - J(\mathbf{q},\omega)\ \chi_0(\mathbf{q},\omega)}$$

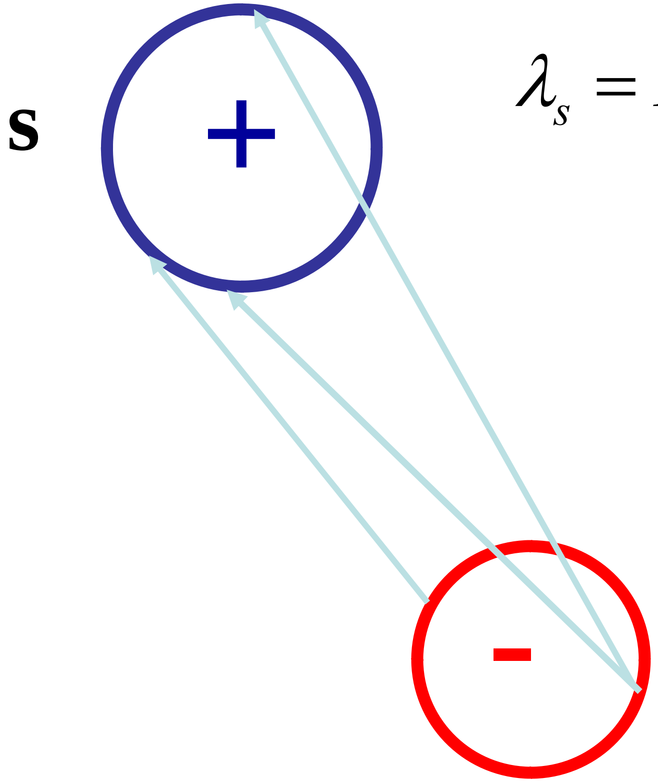
For a Mott-Hubbard system, $J(\mathbf{q},\omega)$ -magnetic interaction is *local in real space*

$$\chi_0(\mathbf{q},\omega) = \sum_{\mathbf{k}} \frac{f(\varepsilon_{\mathbf{k+q}}) - f(\varepsilon_k)}{(\varepsilon_{\mathbf{k+q}} - \varepsilon_k - \omega - i\delta)}$$

the *s/c* physics is just the same as old Berk-Schrieffer physics

1) Interaction is repulsive and peaked at $(\pi,\pi) \rightarrow$ pairing in $s\pm$ channel
2) Mass renormalization expected up to the energy of spin fluctuations

Repulsive pairing interactions in the $s_{+/-}$ channel:



$$\lambda_s = N(0)\langle\langle V(\mathbf{q})\rangle\rangle_{FS}$$

<u>s-wave:</u>
V>0 for all **q**

SF exchange repulsive, but pairing for all q's!

Simple model: spin sluctuations with spectral function

$$B_{ij}(\omega) = \lambda_{ij}\pi\omega\Omega_{sf} / (\Omega_{sf}^2 + \omega^2)$$

Parameters: $\Omega_{sf} = 25meV, \lambda_{11} = \lambda_{22} = 0.5, \lambda_{12} = \lambda_{21} = -2$ Tc=27K

Some properties of the $s_{+/-}$ state

1. Thermodynamics is exponential in clean limit (weak coupling)
   C/T, penetration depth, NMR $1/TT_1$. Singlet K
2. Reversed role of magnetic/nonmagnetic interband impurity scattering
   See next slides
3. Coherence factors: depend on the probing wave vector, BCS at $q \approx 0$, anti-BCS at $q \approx (\pi,\pi)$.
   - *suppressed Hebel-Slichter peak*

   suppressed Hebel-Slichter peak

4. Andreev bound states at finite energies
   See next slides
5. Enhancement of spin susceptibility near $q \approx (\pi,\pi)$ below T_c
   observed
7. Full gap(s) in tunneling
   Full gaps in ARPES, Andreev conductance ?

Experiments: symmetry of the superconducting order parameter

Fully gapped superconducting state:

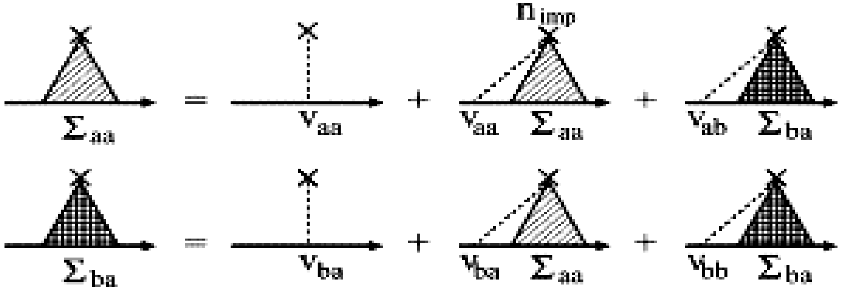
- PCAR: Y.Y. Chen et al., Nature 453, 1224 (2008); K.A. Yates et al., Supercond. Sci. Technol. 21, 092003 (2008); R.S. Gonnelli et al., arXiv:0807.3149.
- ARPES: L. Zhao et al., arXiv:0807.0398; H. Ding et al., EPL 83, 47001 (2008); T. Kondo et al., arXiv:0807.0815.
- Penetration depth: C. Martin et al., arXiv:0807.0876; K. Hashimoto et al., arXiv:0806.3149; L. Malone et al., arXiv:0806.3908

NMR – Lines of nodes at the FS:

- ^{75}As NMR: $1/T_1$ with a T^3 behavior below T_c (line of nodes?)
  Y. Nakai et al., JPSJ 77, 073701 (2008)
- ^{19}F NMR: $1/T_1$ can be explained by a two d-wave gap scenario, $\Delta=\Delta_1+\Delta_2$, $\Delta_1=3.5\ k_BT_c$, $\Delta_2=1.1k_BT_c$
  K. Matano et al., EPL 83, 57001 (2008)

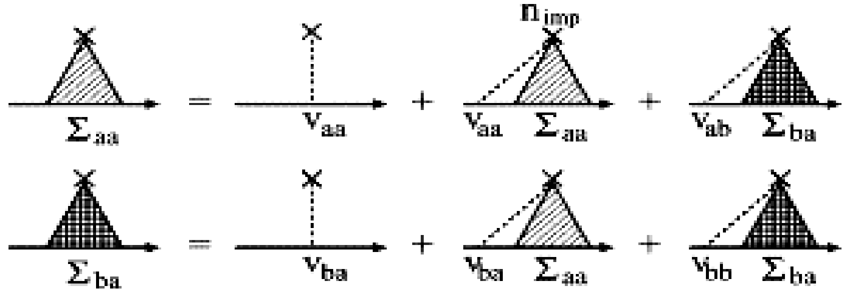
Effect of impurities

$$\hat{G} = \hat{G}_0 - \hat{\Sigma}_{imp}$$



Effect of impurities

$$\hat{G} = \hat{G}_0 - \hat{\Sigma}_{imp} \qquad \hat{v} = \begin{pmatrix} 0 & v \\ v & 0 \end{pmatrix}$$



Interband impurities

$$\Sigma_{aa}^{(0)} = -i\gamma_a \frac{\sigma\bar{\omega}_{an}\sqrt{\bar{\Delta}_{bn}^2 + \bar{\omega}_{bn}^2} - (\sigma - 1)\,\bar{\omega}_{bn}\sqrt{\bar{\Delta}_{an}^2 + \bar{\omega}_{an}^2}}{\det a}$$

$$\Sigma_{aa}^{(1)} = \gamma_a \frac{\sigma\bar{\Delta}_{an}\sqrt{\bar{\Delta}_{bn}^2 + \bar{\omega}_{bn}^2} + (\sigma - 1)\,\bar{\Delta}_{bn}\sqrt{\bar{\Delta}_{an}^2 + \bar{\omega}_{an}^2}}{\det a},$$

where $\gamma_i = \frac{n_{imp}\sigma}{\pi N_i(0)}$, and $\sigma = \frac{\pi^2 N_a(0) N_b(0) u^2}{1+\pi^2 N_a(0) N_b(0) u^2}$.

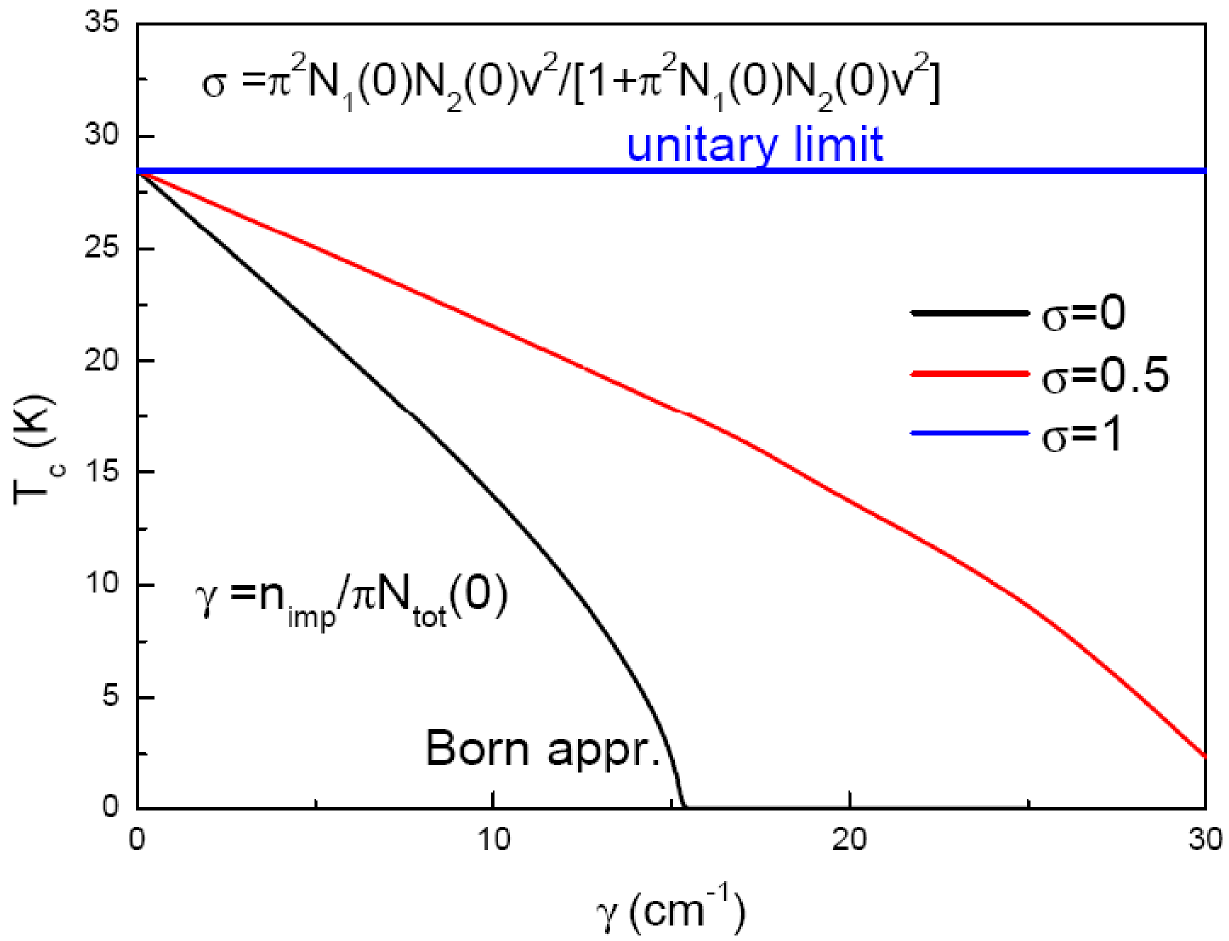
$$\det a =$$

$$\left[2\sigma(\sigma - 1)\left(\sqrt{\bar{\Delta}_{an}^2 + \bar{\omega}_{an}^2}\sqrt{\bar{\Delta}_{bn}^2 + \bar{\omega}_{bn}^2} - \bar{\omega}_{an}\bar{\omega}_{bn} + \bar{\Delta}_{an}\bar{\Delta}_{bn}\right) + \sqrt{\bar{\Delta}_{an}^2 + \bar{\omega}_{an}^2}\sqrt{\bar{\Delta}_{bn}^2 + \bar{\omega}_{bn}^2}\right].$$

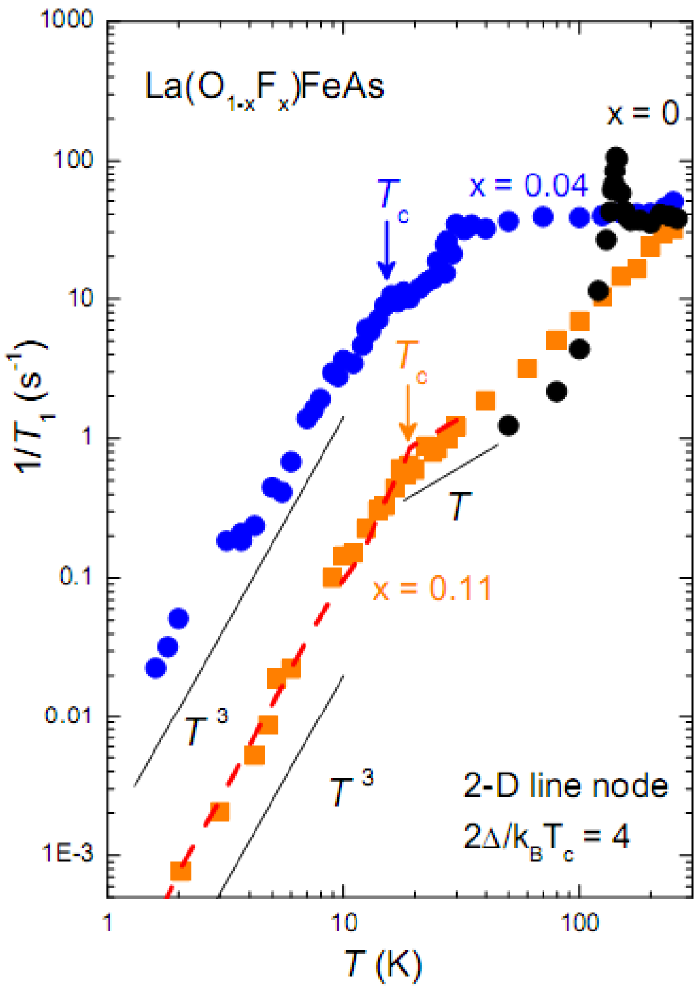
M.L.Kulić, OVD, PRB, **60**, 13062 (1999), Y. Ohashi, Physica C, **412-414**, 41(2004)

Robustness of T_c in the presence of impurities

$$\bar{\omega}_{an} = \omega_n + \gamma_{ab} sign\omega_n$$
$$\bar{\Delta}_{an} = \Delta_{an} + \gamma_{ab}\left[\sigma\bar{\Delta}_{an}/\bar{\omega}_{an} - (1-\sigma)\,\bar{\Delta}_{bn}/\bar{\omega}_{bn}\right] sign\omega_n$$

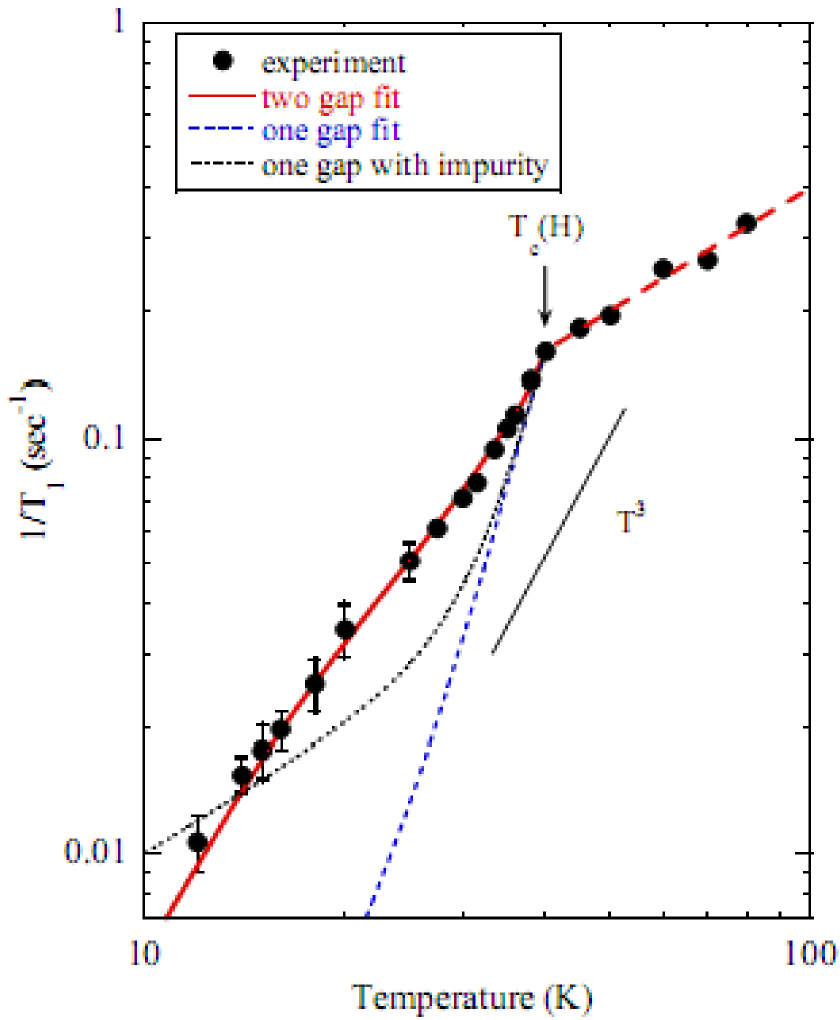


NMR experiments: superconductivity



^{75}As NMR: $1/T_1$ with a T^3 behavior (line of nodes?)

Y. Nakai et al., JPSJ 77, 073701 (2008)



^{19}F NMR: $1/T_1$ can be explained by a two d-wave gap scenario,

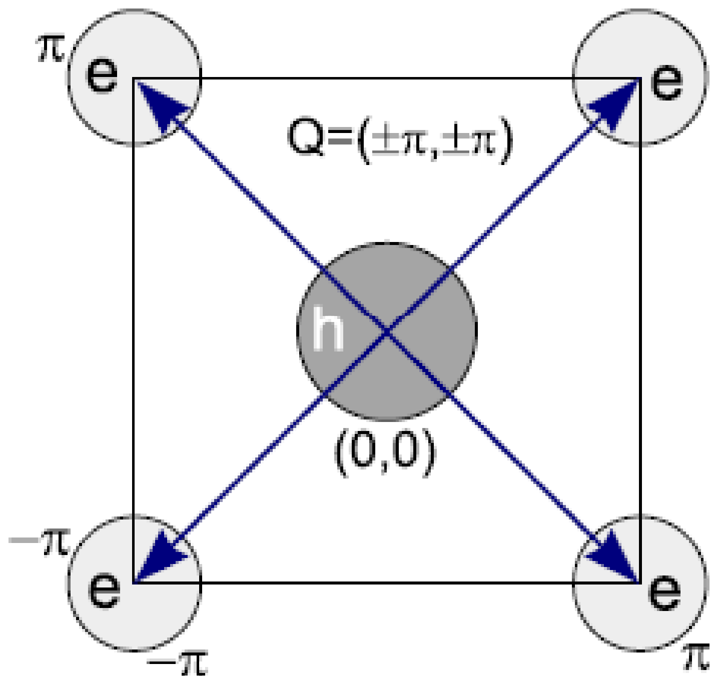
$\Delta = \Delta_1 + \Delta_2$, $\Delta_1 = 3.5\ k_B T_c$, $\Delta_2 = 1.1 k_B T_c$

K. Matano et al., EPL 83, 57001 (2008)

How to reconcile $s_{\pm}$ model with NMR $1/T_1$?

Use simplest model

Two types of pockets (h and e) at the Fermi surface in the *folded* BZ, reproduce LDA topology



Obtain spin-lattice relaxation rate using interband susceptibility χ_{12}:

$$1/T_1 T \propto \lim_{\omega \to 0} \mathrm{Im}\, \chi_{12}(\omega)/\omega$$

Absence of the Hebel-Slichter peak

Weak coupling:

$$\frac{1}{T_1 T} \propto \sum_{\mathbf{k}\mathbf{k}'} \left(1 + \frac{\Delta_1 \Delta_2}{E_{\mathbf{k}} E_{\mathbf{k}'}}\right) \left[-\frac{\partial f(E_{\mathbf{k}})}{\partial E_{\mathbf{k}}}\right] \delta(E_{\mathbf{k}} - E_{\mathbf{k}'})$$

s-wave

$\Delta_1 = \Delta_2 = \Delta$

$$\frac{1}{T_1} \propto \int_{\Delta(T)}^{\infty} dE \frac{E^2 + \Delta^2}{E^2 - \Delta^2} \mathrm{sech}^2\left(\frac{E}{2T}\right)$$

Hebel-Slichter peak

Absence of the Hebel-Slichter peak

Weak coupling: $$\frac{1}{T_1 T} \propto \sum_{\mathbf{k}\mathbf{k}'} \left(1 + \frac{\Delta_1 \Delta_2}{E_{\mathbf{k}} E_{\mathbf{k}'}}\right) \left[-\frac{\partial f(E_{\mathbf{k}})}{\partial E_{\mathbf{k}}}\right] \delta(E_{\mathbf{k}} - E_{\mathbf{k}'})$$

s-wave

$\Delta_1 = \Delta_2 = \Delta$

$$\frac{1}{T_1} \propto \int_{\Delta(T)}^{\infty} dE \frac{E^2 + \Delta^2}{E^2 - \Delta^2} \operatorname{sech}^2\left(\frac{E}{2T}\right)$$

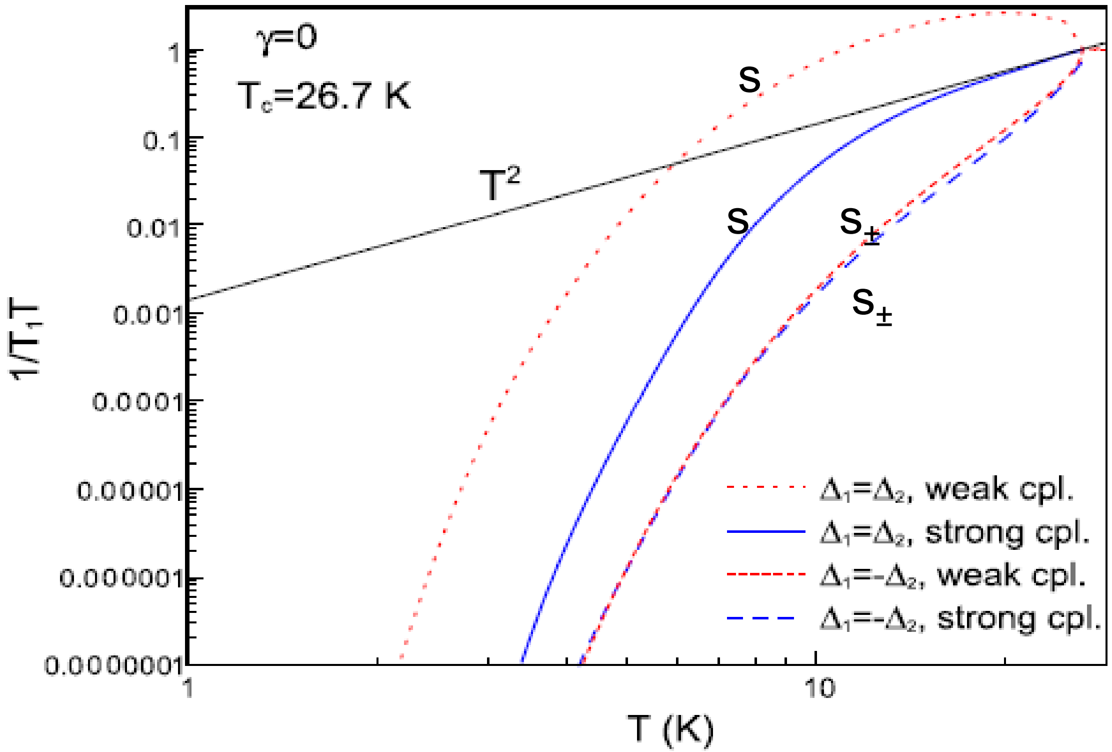
Hebel-Slichter peak

simplest $s_{\pm}$-wave

$\Delta_1 = -\Delta_2 = \Delta$

$$\frac{1}{T_1} \propto \int_{\Delta(T)}^{\infty} dE \frac{E^2 - \Delta^2}{E^2 - \Delta^2} \operatorname{sech}^2\left(\frac{E}{2T}\right) = \int_{\Delta(T)}^{\infty} dE \operatorname{sech}^2\left(\frac{E}{2T}\right)$$

No Hebel-Slichter peak!



Strong-coupling limit

$$\frac{1}{T_1 T} \propto \int_0^{\infty} d\omega \left(-\frac{\partial f(\omega)}{\partial \omega} \right) \{ [\mathrm{Re} g_1^Z(\omega) + \mathrm{Re} g_2^Z(\omega)]^2 + [\mathrm{Re} g_1^{\Delta}(\omega) + \mathrm{Re} g_2^{\Delta}(\omega)]^2 \}.$$

Here

$$g_i^Z(\omega) = n_i(\omega) Z_i(\omega)\omega / D_i(\omega)$$

$$g_i^{\Delta}(\omega) = n_i(\omega) \phi_i(\omega) / D_i(\omega)$$

$$D_i(\omega) = \sqrt{[Z_i(\omega)\omega]^2 - \phi_i^2(\omega)},$$

$$\phi_i(\omega) = Z_i(\omega)\Delta_i(\omega)$$

$Z_i(\omega)$ is the mass renormalization
$n_i(\omega)$ is a partial density of states

complex order parameter

EEliashberg equations:

$$\phi_i(\omega) = \sum_j \int_{-\infty}^{\infty} dz K_{ij}^{\Delta}(z,\omega) \mathrm{Re} g_j^{\Delta}(z) + i\gamma \frac{g_1^{\Delta}(\omega) - g_2^{\Delta}(\omega)}{2\mathcal{D}}$$

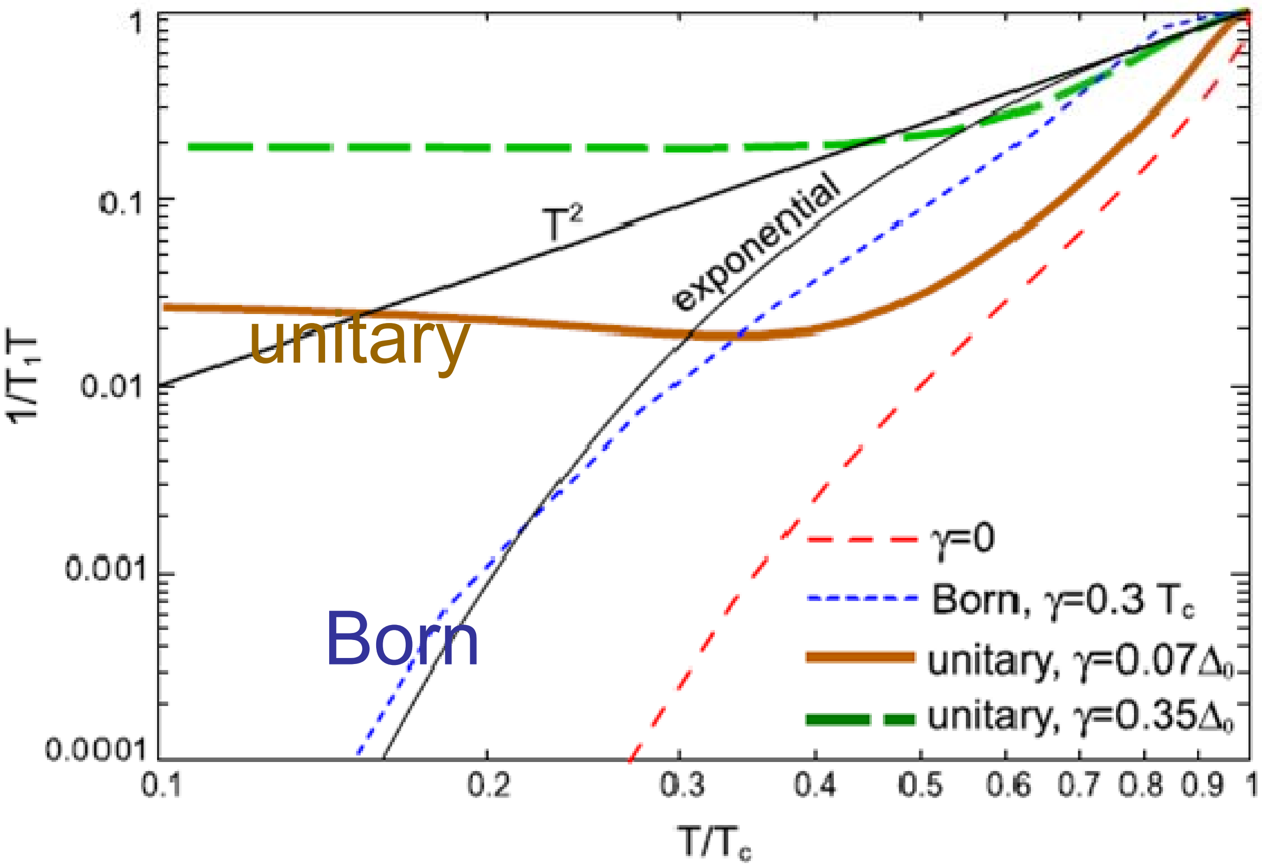
$$(Z_i(\omega) - 1)\omega = \sum_j \int_{-\infty}^{\infty} dz K_{ij}^{Z}(z,\omega) \mathrm{Re} g_j^{Z}(z) + i\gamma \frac{g_1^{Z}(\omega) + g_2^{Z}(\omega)}{2\mathcal{D}}$$

$$\sigma = \frac{[\pi N(0) v]^2}{1 + [\pi N(0) v]^2}$$

$$\mathcal{D} = 1 - \sigma + \sigma\{[g_1^Z(\omega) + g_2^Z(\omega)]^2 - [g_1^{\Delta}(\omega) - g_2^{\Delta}(\omega)]^2\}$$

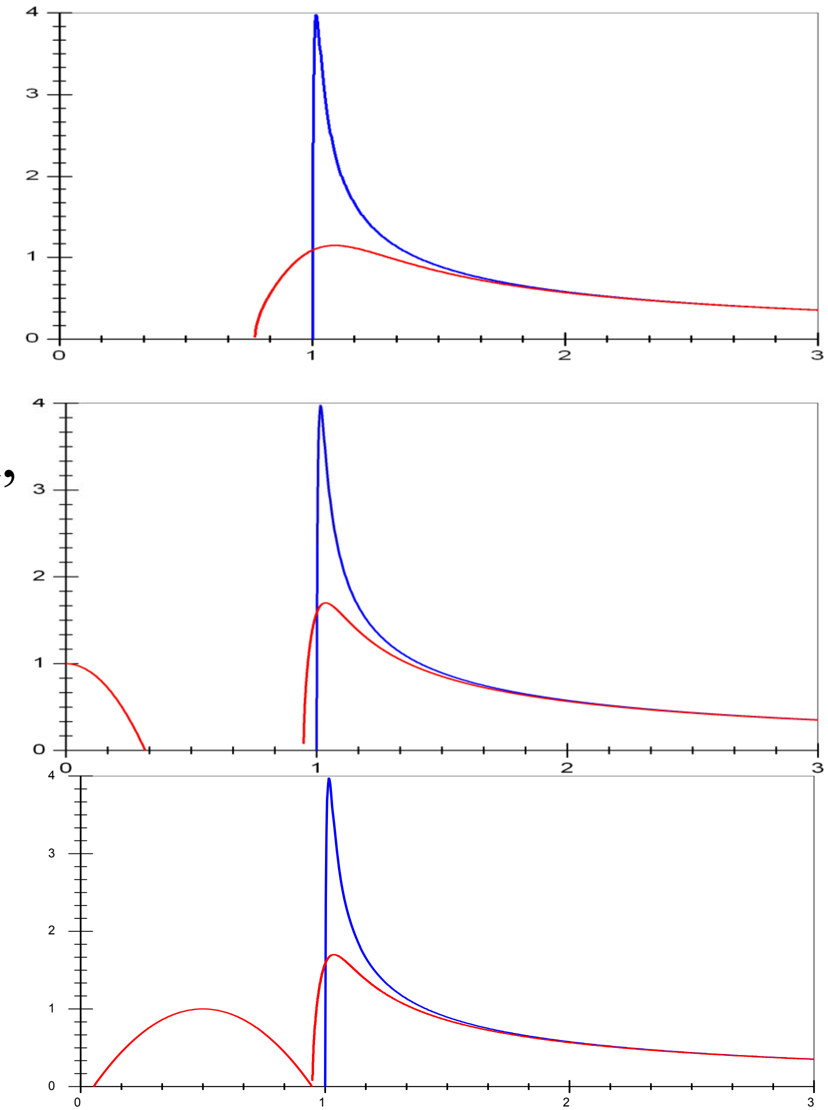
$\gamma = 2c\sigma/N(0)$ is the normal-state scattering rate,
c is the impurity concentration, v is the impurity potential, σ is the impurity strength ($\sigma \to 0$: Born limit, $\sigma = 1$: unitary limit)

The dependence of 1/T1 is not reproduced in both Born and unitary limits:

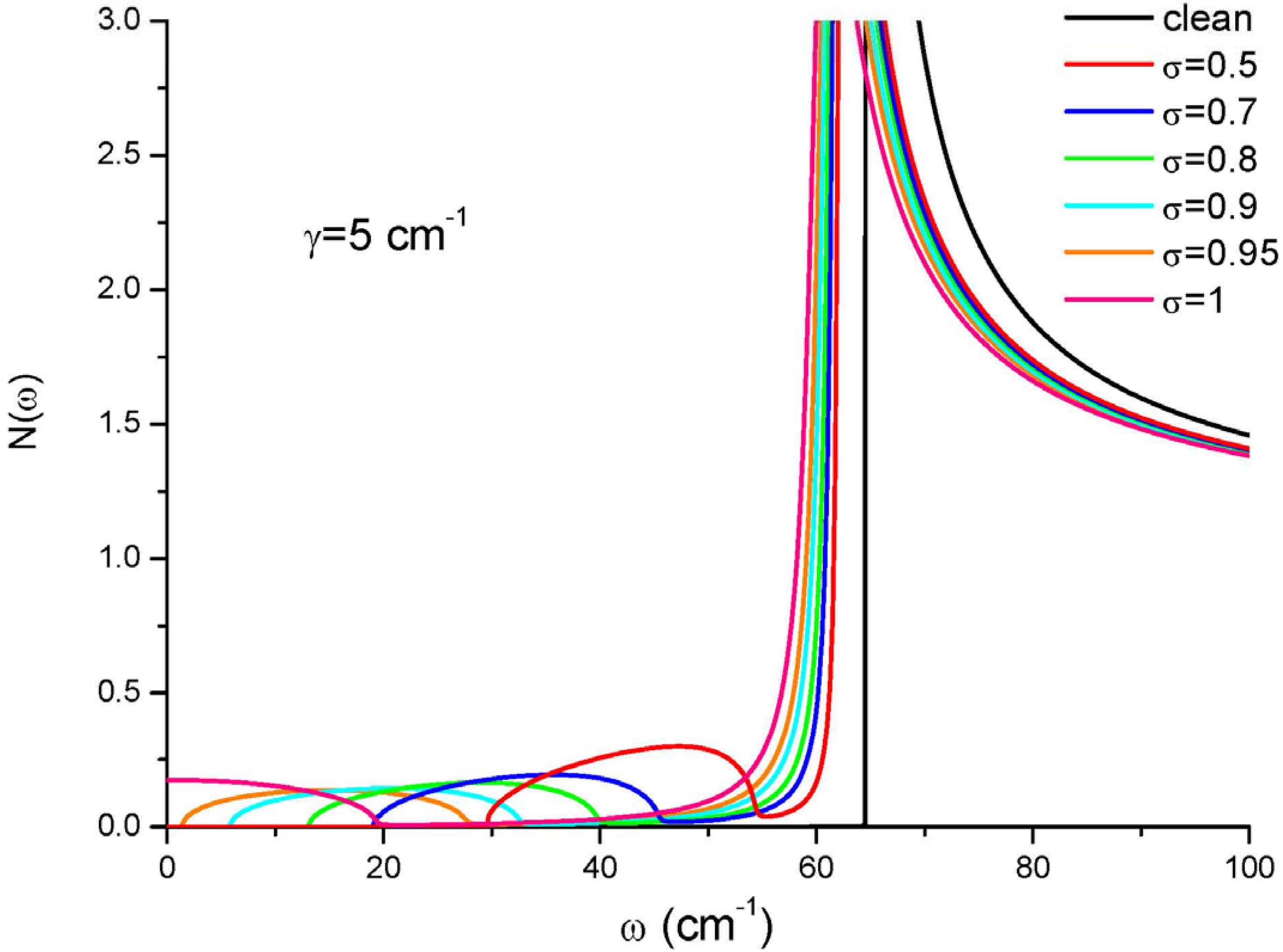


Impurity scattering: intermediate regime

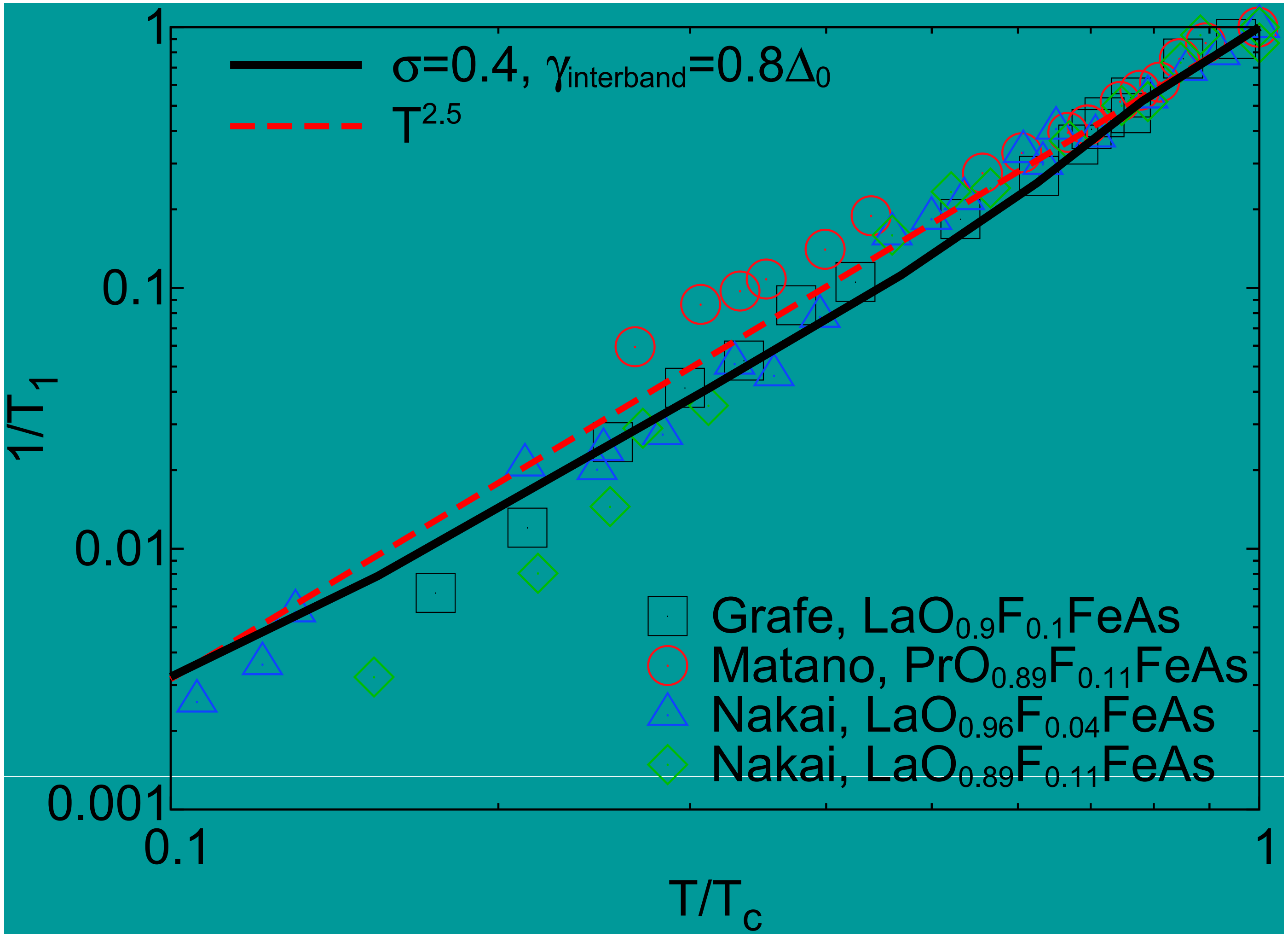
1. Nonmagnetic impurities are pair breaking
2. Born limit: no coherence peak, exponential at low T
3. Unitary limit: weak Tc suppression, zero-energy bound state
4. Intermediate limit: finite energy bound state, simulates power law



Impurity scattering: densities of states

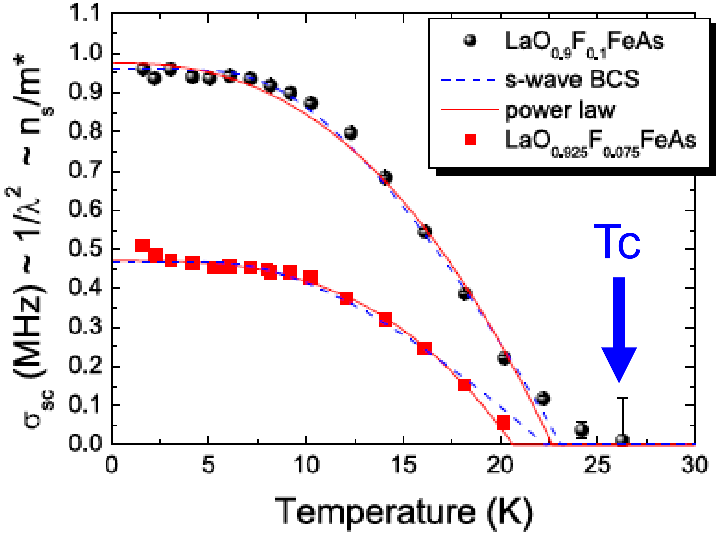


NMR: possible explanation of low-T behavior

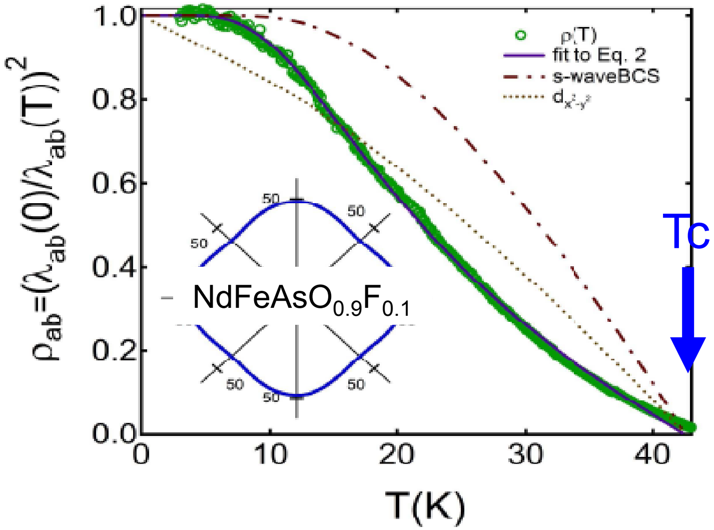


Superfluid density n_s : experiment

μSR: Luetkens, arXiv:0804.3115



μSR: Martin et al, arXiv:0807.0876



Superfuid density: the model

$$1/\lambda^2_{L,\alpha\beta}(T) \equiv (\omega^{sf}_{p,\alpha\beta}(T)/c)^2 =$$

$$\sum_{i=\sigma,\pi}\left(\frac{\omega^{\alpha\beta}_{p,i}}{c}\right)^2 \pi T \sum_{n=-\infty}^{\infty} \frac{\tilde{\Delta}^2_i(n)}{[\tilde{\omega}^2_i(n)+\tilde{\Delta}^2_i(n)]^{3/2}}$$

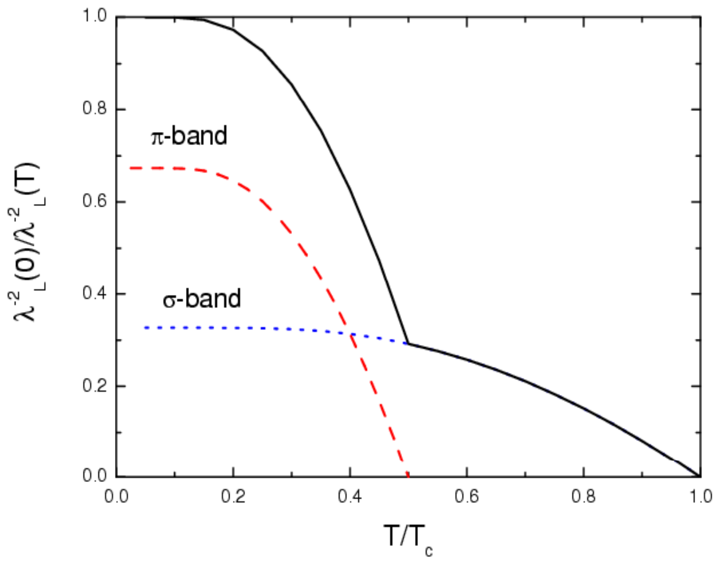
where $\tilde{\omega}(n) = \omega_n Z(\omega_n)$ and $\tilde{\Delta}(\omega_n) = \Delta(\omega_n) Z(\omega_n)$ are the solutions of the Eliashberg equations.

The case of weakly coupled bands (MgB2)

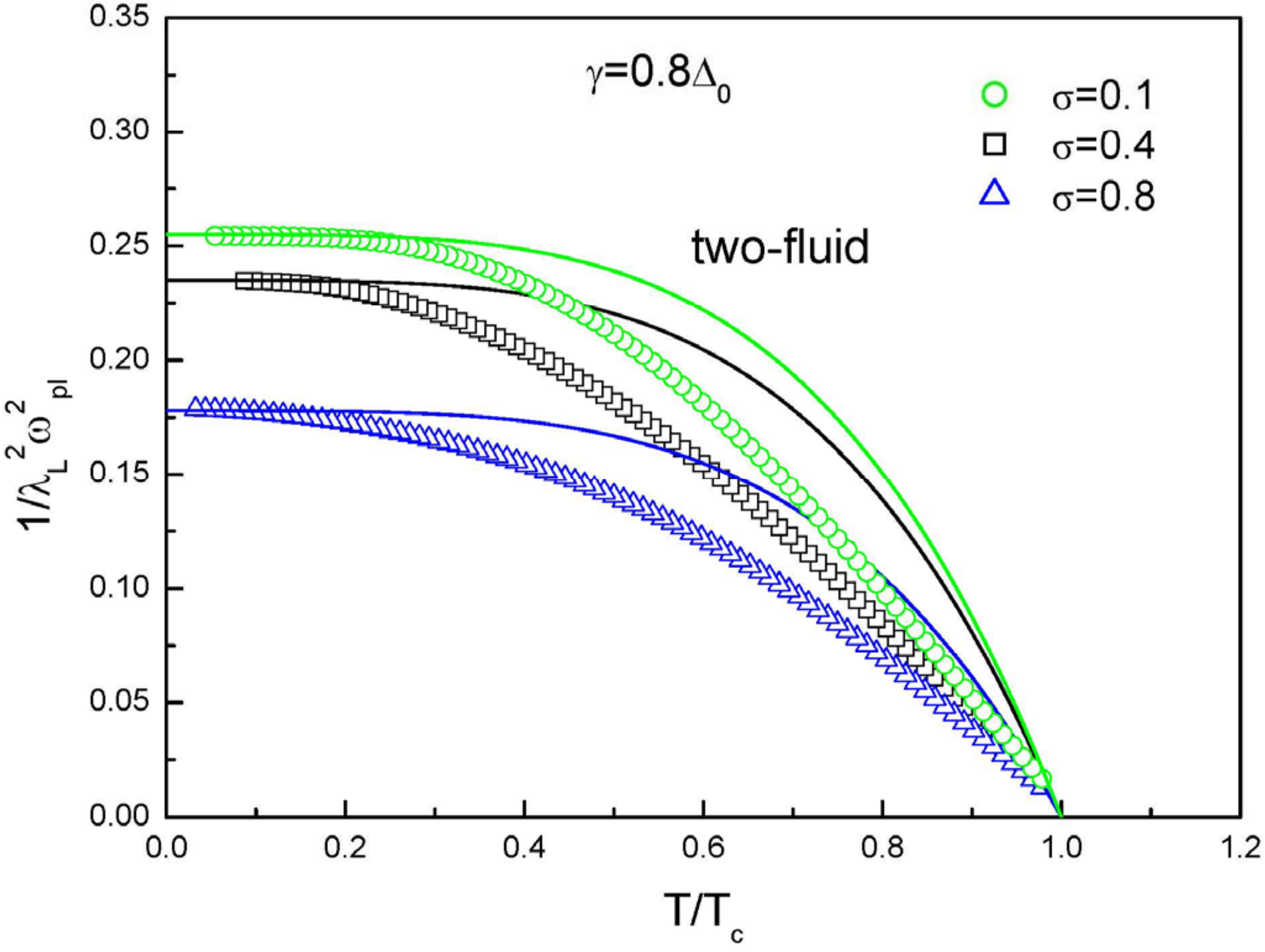
Effects of impurities

$$\Delta_i \to \Delta^0_i + \sum_j \gamma_{ij}\Delta_j/2\sqrt{\omega^2_n+\Delta^2_j}\ ,$$

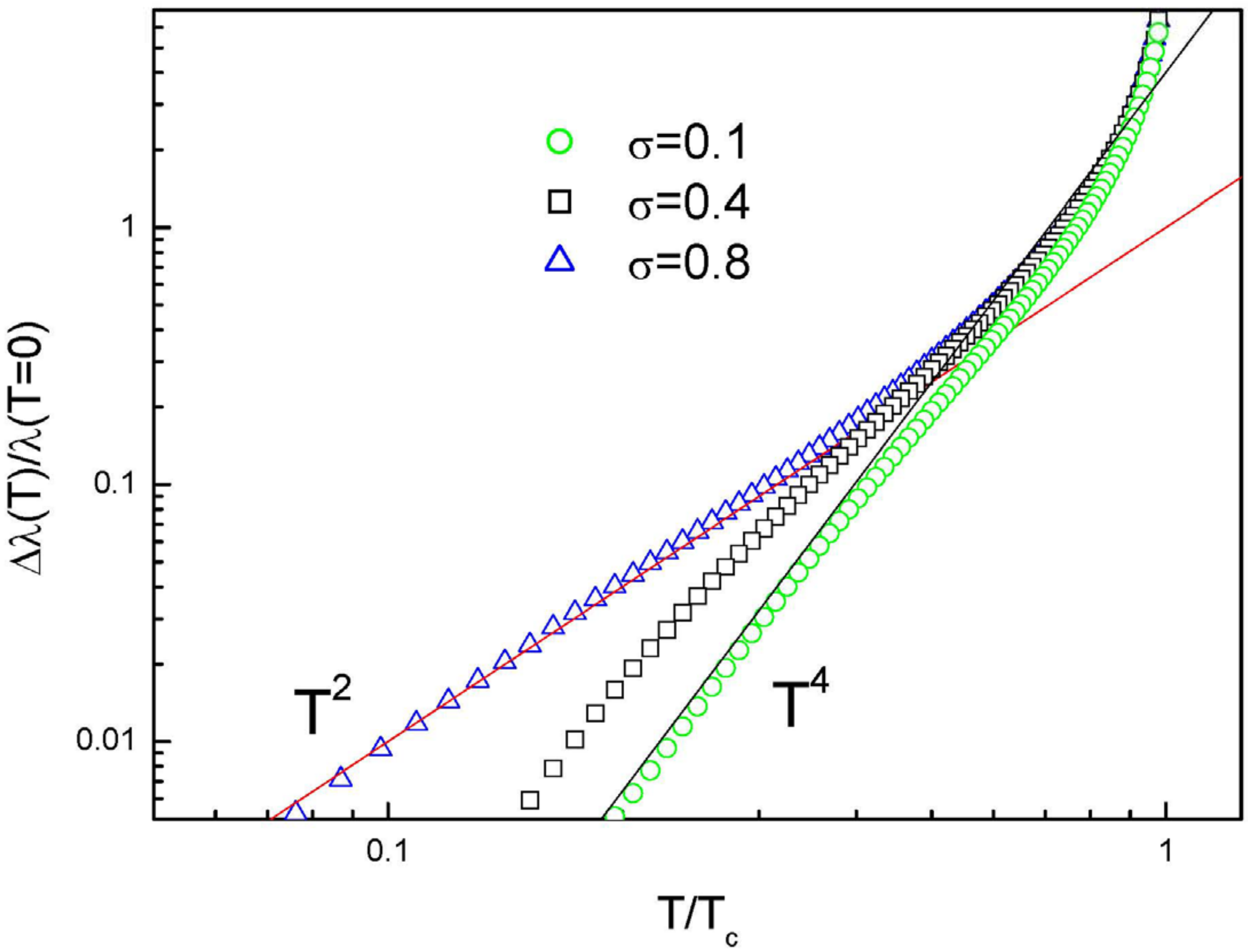
$$Z(\omega_n) \to Z^0(\omega_n) + \sum_j \gamma_{ij}/2\sqrt{\omega^2_n+\Delta^2_j}$$



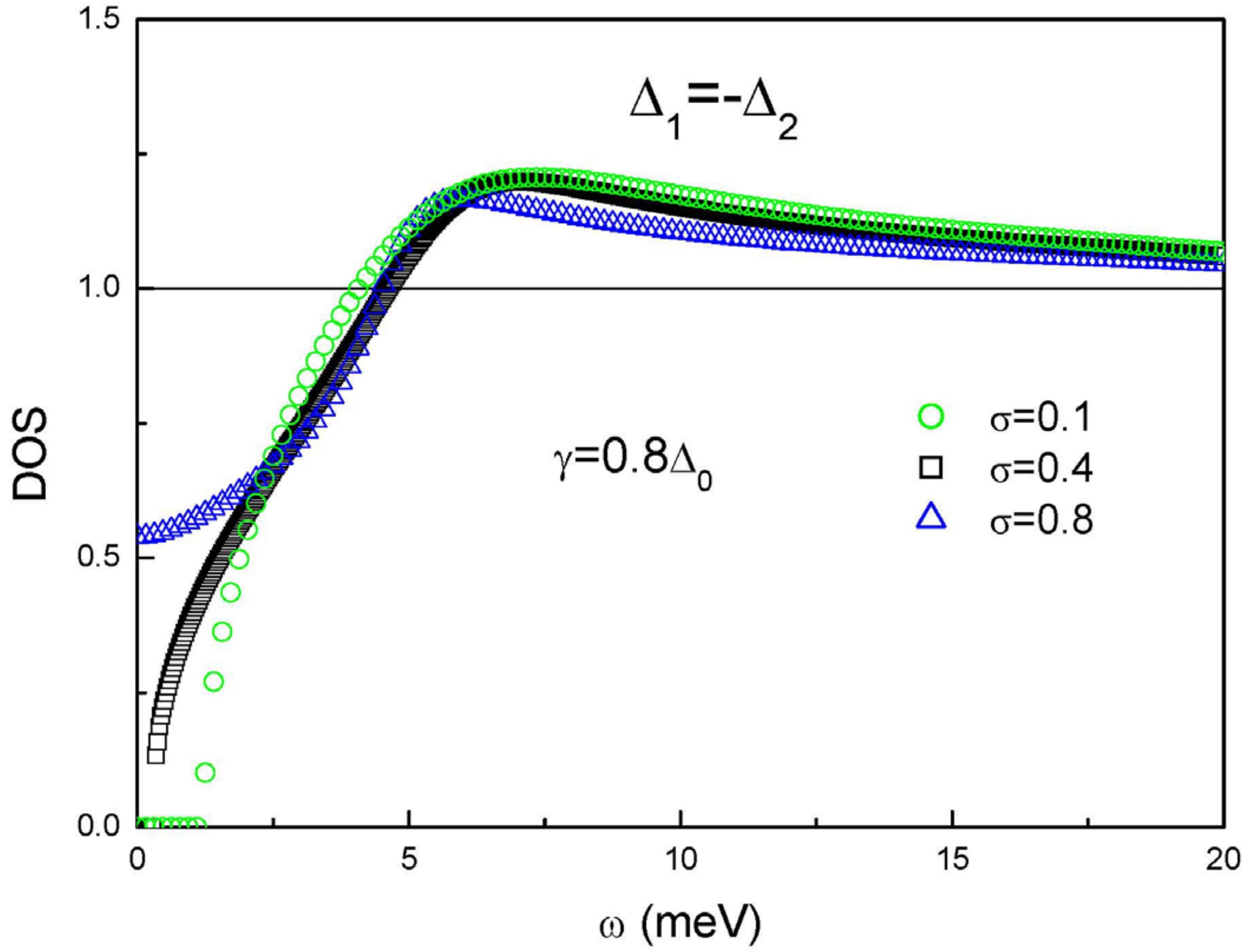
Magnetic field penetration depth:
calculations for various scattering rates



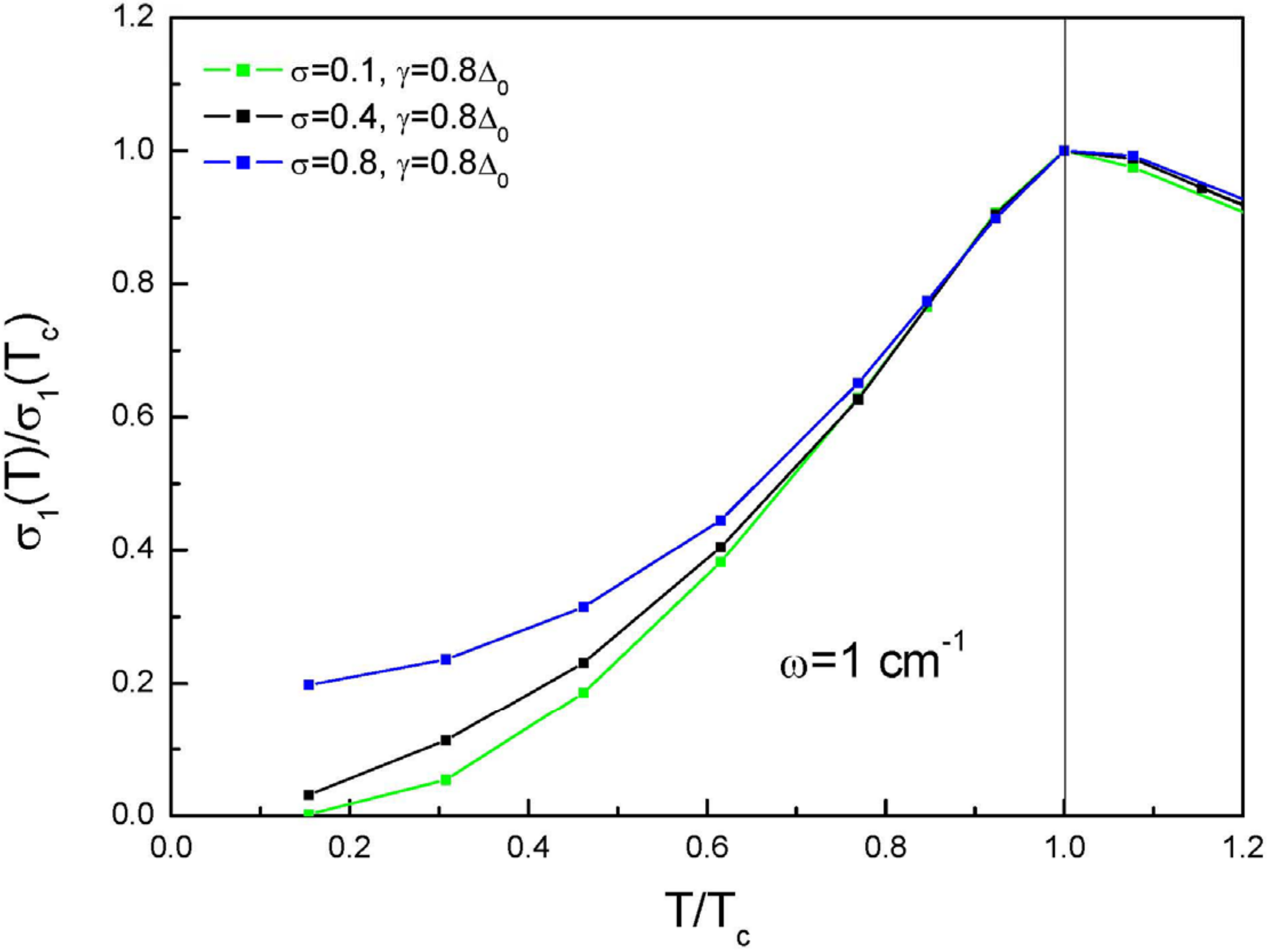
Magnetic field penetration depth: low T



Low energy density of states



The microwave conductivity $\sigma_1(T)$



Tunneling in N/S junction: extending Andreev reflection formalism (the BTK model) to two bands

A.A. Golubov et al, PRL 103, 077003 (2009)

$$\Psi = \Psi_N \theta(-x) + \Psi_S \theta(x),$$

$$\Psi_N = \psi_k \begin{pmatrix} 1 \\ 0 \end{pmatrix} + a\,\psi_k \begin{pmatrix} 0 \\ 1 \end{pmatrix} + b\,\psi_{-k} \begin{pmatrix} 1 \\ 0 \end{pmatrix},$$

$$\Psi_S = c\left[\phi_p \begin{pmatrix} u_1 \\ v_1 e^{-i\varphi_1} \end{pmatrix} + \alpha\phi_q \begin{pmatrix} u_2 \\ v_2 e^{-i\varphi_2} \end{pmatrix}\right]$$

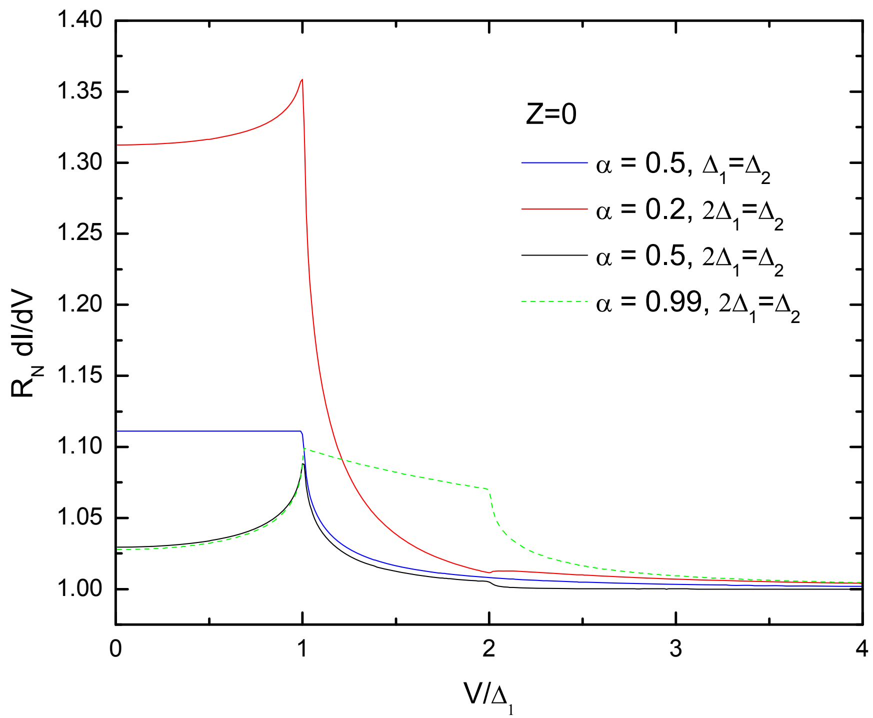
$$+\, d\left[\phi_{-p} \begin{pmatrix} v_1 \\ u_1 e^{-i\varphi_1} \end{pmatrix} + \alpha\phi_{-q} \begin{pmatrix} v_2 \\ u_2 e^{-i\varphi_2} \end{pmatrix}\right]$$

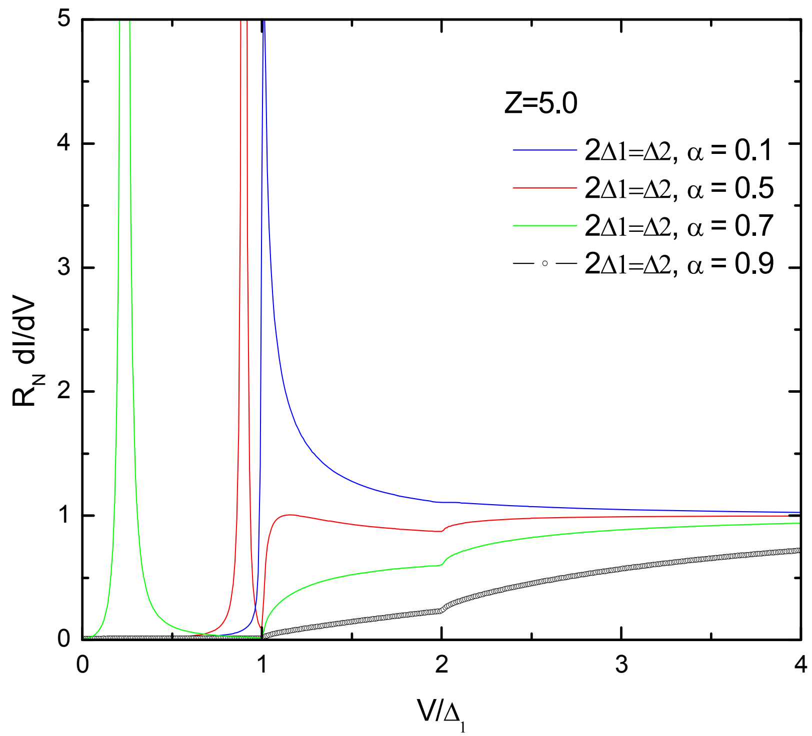
S_{++} model: $\varphi_1 = \varphi_2$ S_{+-} model: $\varphi_1 = \varphi_2 + \pi$

α is the mixing coefficient between electron and hole bands

Tunneling conductance in the $s_{\pm}$ case

$$Z = H / \hbar v_{FN}$$ **H – the barrier height**

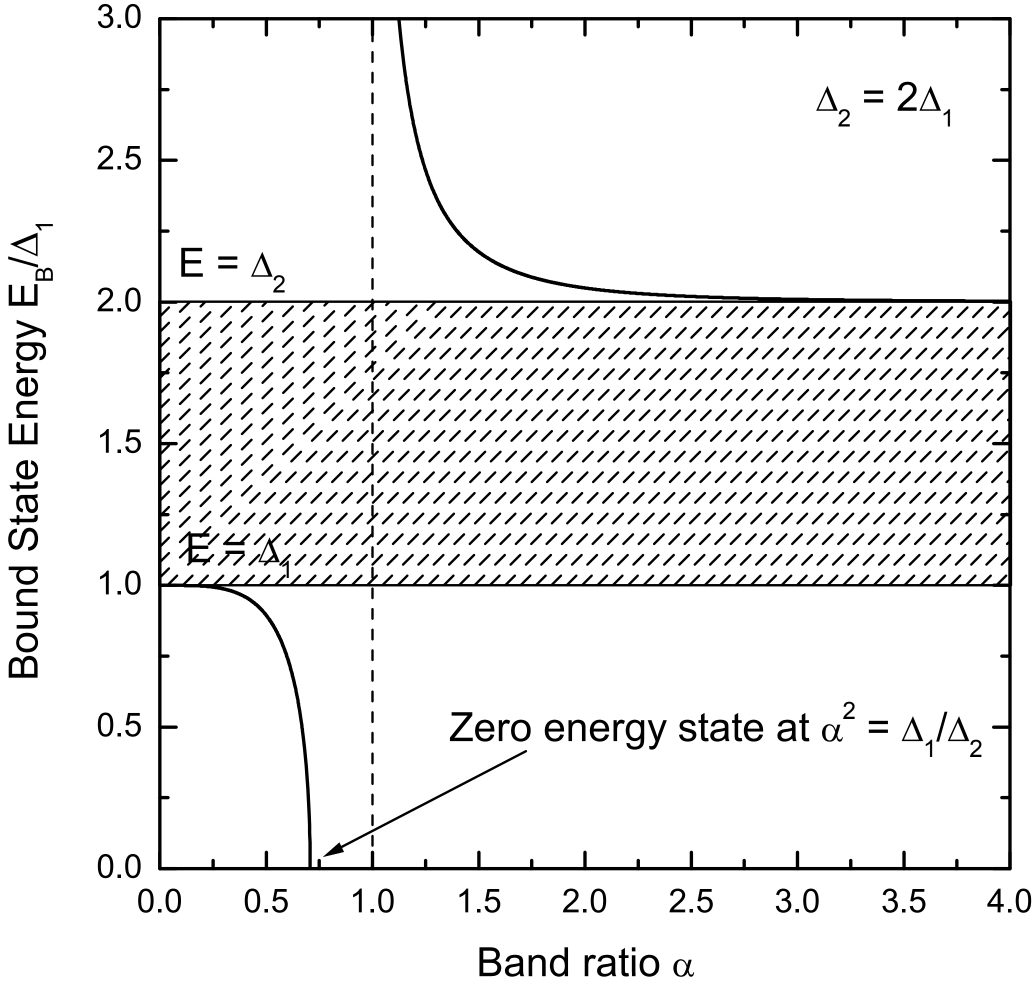




Andreev conductance is suppressed due to destructive interband interference

Bound states appear at finite energy for large Z

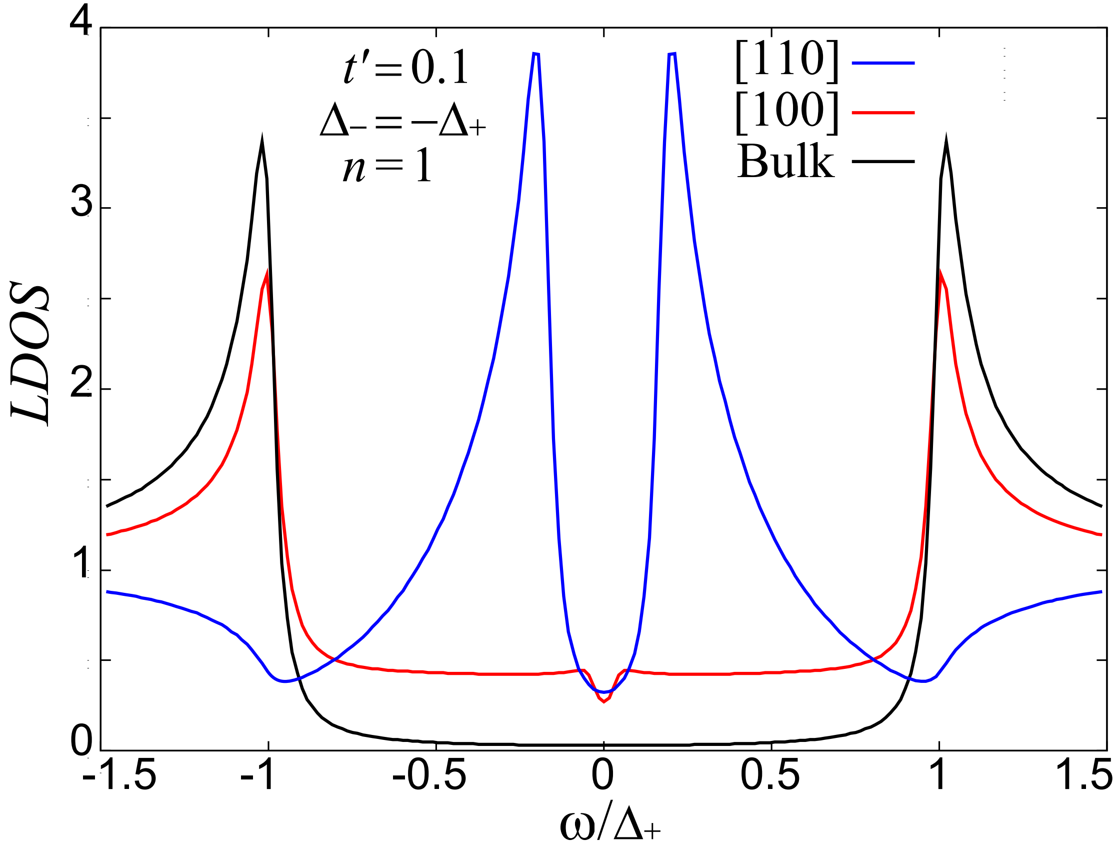
Tunneling regime: Surface bound states

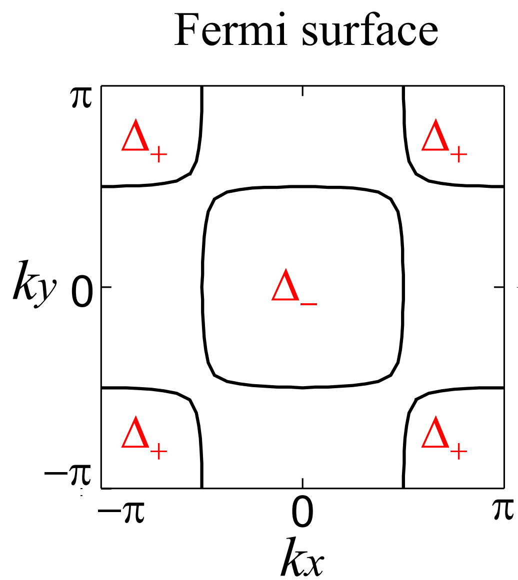


LDOS at surface

s+−wave

$\Delta_{+(-)}=+(-)0.1$





Andreev bound state with non zero energy (Onari and Tanaka)

Conclusions

- ***s*±** pairing can explain some properties of superconducting *Fe-pnictides*.
- T_c is robust against *unitary* interband scattering.
- The lack of an NMR Hebel-Slichter peak is consistent with the nodeless ***s*±** wave symmetry of the order parameter (whether in the clean or dirty limit).
- The low-temperature power-law behavior of $1/T_1$ can be also explained in the framework of the s± model but requires the impurity scattering beyond the Born limit.
- *Conductance Peak* can appear in *Andreev* and tunneling experiments, but, unlike nodal superconductors, at finite energy.