Effects of in-gap impurity levels and impurity bands in superconducting ferropnictides

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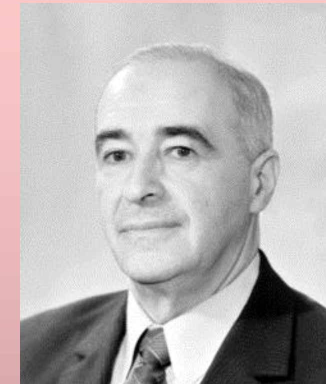
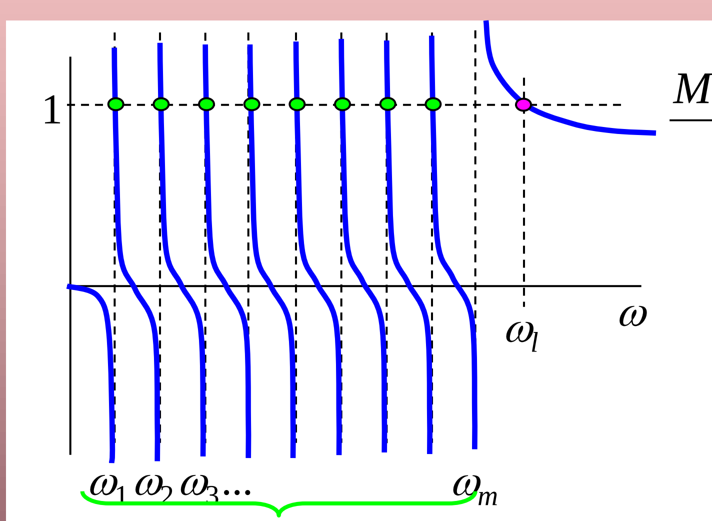
1. Introduction: impurity states in solids by Green function approach

Studies of impurity states in solids ascend to the early works by I.M. Lifshitz on local vibrations by light impurity atoms in crystalline lattices (done in 1941).

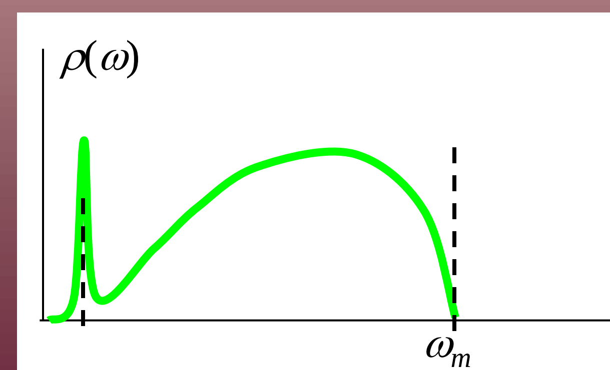




$$\frac{M-M'}{M}\frac{1}{N}\mathrm{Re}\sum_j \frac{\omega^2}{\omega^2-\omega_j^2}$$

[1] I. M. Lifshitz, JETP **12**, 117 (1942).
[2] I. M. Lifshitz, JETP **12**, 137 (1942).
[3] I. M. Lifshitz, JETP **12**, 156 (1942).

Next, the quasilocal (resonance) vibrations by heavy impurities were indicated by Yu. Kagan and Ya. Iosilevskii (JETP, 1963)



Since then, a lot of different impurity states were discovered in vibrational, magnetic, electronic, etc. excitation spectra with important applications, only to mention the donor and acceptor states in semiconductors.

The most consistent theoretical description of disorder effects in crystalline systems is generally considered in the framework of Green functions (GF's), beginning from their simplest temporal formulation. For electronic excitations in crystal with 2nd quantization Heisenberg operators a_k, the basic GF:

$$G_{\mathbf{k},\mathbf{k}'}(\varepsilon) = -i\int_0^\infty dt e^{i\varepsilon t/\hbar} \left\langle \left\{ a_{\mathbf{k}}(t), a_{\mathbf{k}'}^\dagger(0) \right\} \right\rangle \equiv \left\langle \left\langle a_{\mathbf{k}} \mid a_{\mathbf{k}'}^\dagger \right\rangle \right\rangle$$

assuming $\varepsilon \to \varepsilon + i0$

obeys the Heisenberg equation of motion:

$$\varepsilon G_{\mathbf{k},\mathbf{k}'}(\varepsilon) = \left\langle \left\{ a_{\mathbf{k}}(t), a_{\mathbf{k}'}^\dagger \right\} \right\rangle - i\int_0^\infty dt e^{i\varepsilon t/\hbar} \left\langle \left\{ \left[a_{\mathbf{k}}(t), H \right], a_{\mathbf{k}'}^\dagger(0) \right\} \right\rangle,$$

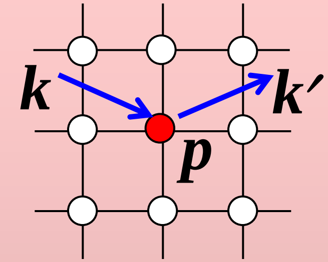
where the Hamiltonian $H = H_0 + H'$ involves:

$$H_0 = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}}$$

and some perturbation H'.

The sample case of Lifshitz perturbation in electronic spectrum (1963):

$$H' = \frac{V}{N} \sum_{\mathbf{k},\mathbf{p}} \mathrm{e}^{i\mathbf{k}\cdot\mathbf{p}} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}'},$$



leads to the solution for the diagonal GF:

$$G_{\mathbf{k},\mathbf{k}}(\varepsilon) \equiv G_{\mathbf{k}}(\varepsilon) = \left[g_{\mathbf{k}}(\varepsilon)^{-1} - \Sigma_{\mathbf{k}}(\varepsilon) \right],$$

with the non-perturbed GF:

$$g_{\mathbf{k}}(\varepsilon) = \frac{1}{\varepsilon - \varepsilon_{\mathbf{k}}},$$

and the self-energy function as a group expansion, GE (M.A. Ivanov, 1971):

$$\Sigma_{\mathbf{k}}(\varepsilon) = \frac{cV}{1 - Vg(\varepsilon)} \left[1 + c \sum_{\mathbf{n} \neq 0} \frac{A_{\mathbf{n}} \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{n}} + A_{\mathbf{n}} A_{-\mathbf{n}}}{1 - A_{\mathbf{n}} A_{-\mathbf{n}}} + \ldots \right],$$

single-impurity T-matrix — impurity pairs — impurity triples. etc.

Lifshitz equation: $1 - V \operatorname{Re} g(\varepsilon) = 0$

The basic elements of GE are:

$$g(\varepsilon) = N^{-1}\sum_{\boldsymbol{k}} g_{\boldsymbol{k}}(\varepsilon),$$ and $$A_{\boldsymbol{n}} = \frac{V}{1 - Vg(\varepsilon)}\sum_{\boldsymbol{k}} \mathrm{e}^{i\boldsymbol{k}\cdot\boldsymbol{n}} g_{\boldsymbol{k}}(\varepsilon),$$

local GF **inter-impurity interaction**

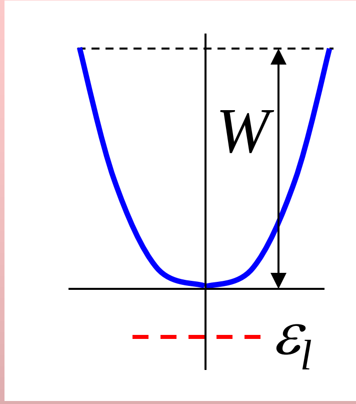
This so called renormalized GF defines band-like states with quasimomentum *k*,

dispersion law: $$\varepsilon(\boldsymbol{k}) = \varepsilon_{\boldsymbol{k}} + \mathrm{Re}\Sigma_{\boldsymbol{k}}(\varepsilon(\boldsymbol{k}))$$

and linewidth: $$\Gamma_{\boldsymbol{k}} = \mathrm{Im}\Sigma_{\boldsymbol{k}}(\varepsilon(\boldsymbol{k}))/[1 - d\mathrm{Re}\Sigma_{\boldsymbol{k}}(\varepsilon)/d\varepsilon]_{\varepsilon(\boldsymbol{k})},$$

provided the GE converges.

GE convergence can be roughly estimated by a comparison of the pair term to unity, using the explicit form of the interaction function A_r.



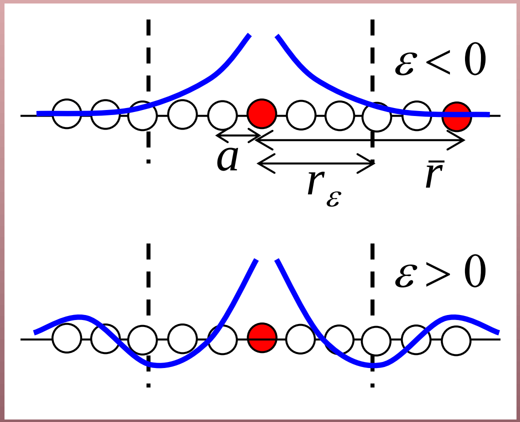
E.g., for parabolic dispersion $\varepsilon_k = \hbar^2 k^2/2m$ and negative energy range $\varepsilon < 0$, it reads:

$$A_{\boldsymbol{r}}(\varepsilon) \approx \frac{aW\mathrm{e}^{-r/r_\varepsilon}}{(\varepsilon - \varepsilon_l)\,r}$$

where

$$-\varepsilon_l \approx W(1+3V/W)^2 \ll W,$$ **impurity level**

$$r_\varepsilon = a\sqrt{-W/\varepsilon} \gg a$$ **impurity state range**



The pair term at $\varepsilon < 0$ evaluates as:

$$\frac{c}{a^3}\int_{r>a} \frac{A_{\boldsymbol{r}}\mathrm{e}^{-i\boldsymbol{k}\cdot\boldsymbol{r}} + A_{\boldsymbol{r}}^2}{1 - A_{\boldsymbol{r}}^2}\, d\boldsymbol{r} \approx \frac{c r_\varepsilon^3}{a^3} \sim \frac{r_\varepsilon^3}{\bar{r}^3},$$

so GE converges at:

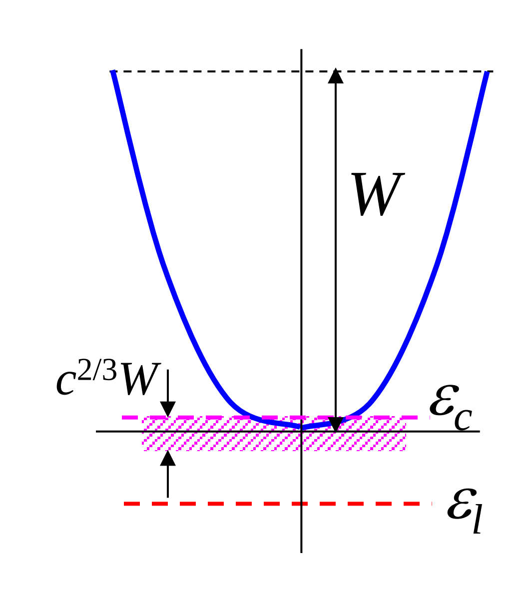
$$-\varepsilon > c^{2/3} W$$

Summation of pair interactions turns more complicated at $\varepsilon > 0$ (oscillating A_r function) but here a simpler test for band-like states is obtained from the Ioffe-Regel-Mott, IRM criterion (A.F. Ioffe, A.R. Regel, 1960; N.F. Mott, 1967):

$$\boldsymbol{k} \cdot \nabla_{\boldsymbol{k}} \varepsilon(\boldsymbol{k}) > \Gamma_{\boldsymbol{k}},$$

giving a similar estimate for the Mott's mobility edge:

$$\varepsilon > \varepsilon_c \sim c^{2/3} W.$$



Otherwise, if neither IRM nor renormalized group expansion apply, the states are localized and cannot be described with quasimomentum.

A special interest is in formation of specific **impurity band** in the disordered crystal.

$$\varepsilon - \varepsilon_{\mathbf{k}} - \mathrm{Re}\Sigma_{\mathbf{k}}(\varepsilon) = 0$$

Besides the common solution of slightly perturbed principal band:

$$\varepsilon_{pr,\mathbf{k}} \approx \varepsilon_{\mathbf{k}} + \frac{cW}{3c_0^{1/3}}$$

with the linewidth

$$\Gamma_{pr,\mathbf{k}} \approx \begin{cases} c c_0^{-2/3}\sqrt{\varepsilon W}, & \varepsilon < \varepsilon_l, \\ cW^{3/2}/\sqrt{\varepsilon}, & \varepsilon > \varepsilon_l, \end{cases}$$

$$c_0 = \left(\frac{\pi^2 \varepsilon_l}{4W}\right)^{3/2} \ll 1,$$

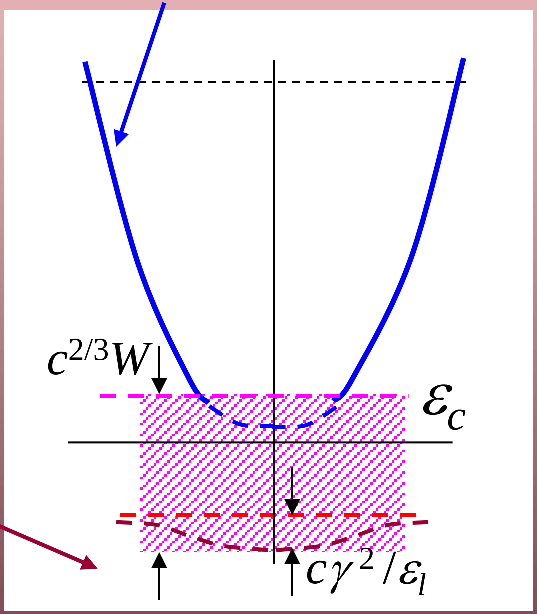
the characteristic concentration

also a formal solution for impurity band exist:

$$\varepsilon_{imp,\mathbf{k}} \approx \varepsilon_l - \frac{c\gamma^2}{\varepsilon_{\mathbf{k}} - \varepsilon_l}.$$

with the effective coupling constant :

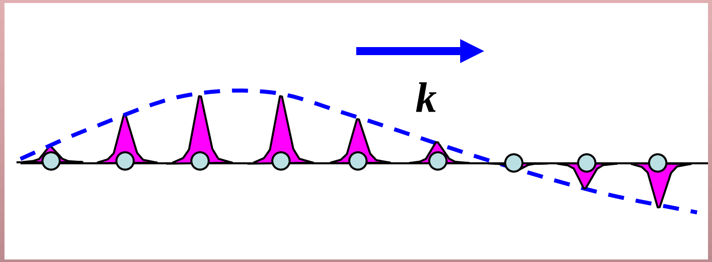
$$\gamma^2 = \frac{4W^{3/2}\varepsilon_l^{1/2}}{3\pi}$$



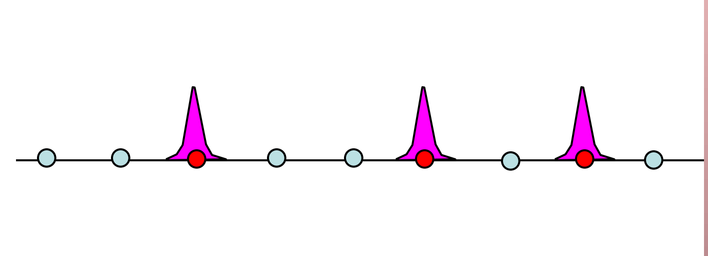
But this γ is too high, so that IRM and GE criteria does not hold for impurity band.

However, impurity bands turn possible in impurity systems with weak enough coupling γ , as in the Anderson *s-d* model (Ivanov, Pogorelov, 1979) or in some antiferromagnetic systems with impurities (Ivanov, Pogorelov, Loktev, 1981).

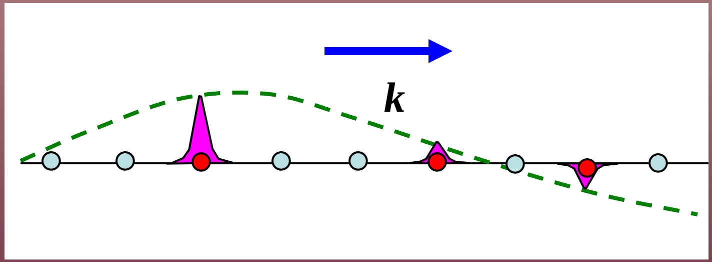
Note essential distinctions between localized and different types of band-like states in crystals with impurities.



common Bloch wave



impurity localized states



impurity band state

They cause differences in observable properties of such systems.

Impurities in superconductors: Anderson's theorem and all that

The description of superconducting systems requires passing to normal and anomalous GF's (L.P. Gor'kov, 1962), suitably combined into Nambu matrices:

$$\hat{G}_{\mathbf{k}}(\varepsilon) = \begin{pmatrix} \langle\langle a_{\mathbf{k}\uparrow} | a_{\mathbf{k}\uparrow}^{\dagger} \rangle\rangle & \langle\langle a_{\mathbf{k}\uparrow} | a_{-\mathbf{k}\downarrow} \rangle\rangle \\ \langle\langle a_{-\mathbf{k}\downarrow}^{\dagger} | a_{\mathbf{k}\uparrow}^{\dagger} \rangle\rangle & \langle\langle a_{-\mathbf{k}\downarrow}^{\dagger} | a_{-\mathbf{k}\downarrow} \rangle\rangle \end{pmatrix}$$

with a BCS Hamiltonian:

$$H_0 = \sum_{\mathbf{k}} \psi_{\mathbf{k}}^{\dagger} \left(\xi_{\mathbf{k}} \hat{\tau}_3 + \Delta_{\mathbf{k}} \hat{\tau}_3 \right) \psi_{\mathbf{k}}$$

involving Nambu spinors:

$$\psi_{\mathbf{k}} = \begin{pmatrix} a_{\mathbf{k},\uparrow} \\ a_{-\mathbf{k},\downarrow}^{\dagger} \end{pmatrix}, \qquad \psi_{\mathbf{k}}^{\dagger} = \begin{pmatrix} a_{\mathbf{k},\uparrow}^{\dagger} & a_{-\mathbf{k},\downarrow} \end{pmatrix}$$

The non-perturbed GF matrix:

$$\hat{g}_{\mathbf{k}} = \left(\varepsilon - \xi_{\mathbf{k}} \hat{\tau}_3 - \Delta_{\mathbf{k}} \hat{\tau}_1 \right)^{-1} = \frac{1}{\varepsilon^2 - E_{\mathbf{k}}^2} \begin{pmatrix} \varepsilon + \xi_{\mathbf{k}} & \Delta_{\mathbf{k}} \\ \Delta_{\mathbf{k}} & \varepsilon - \xi_{\mathbf{k}} \end{pmatrix}$$

with gapped spectrum:

$$E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^{\ 2} + \Delta_{\mathbf{k}}^{\ 2}}$$

Impurity perturbation Hamiltonian:

$$H' = \frac{1}{N}\sum_{\boldsymbol{k},\boldsymbol{k}',\boldsymbol{p}} \mathrm{e}^{i(\boldsymbol{k}-\boldsymbol{k}')\boldsymbol{p}} \psi^{\dagger}_{\boldsymbol{k}} \hat{V} \psi_{\boldsymbol{k}'}$$

with perturbation matrix: $\hat{V} = V_i \hat{\tau}_3$ **(non-magnetic impurity).**

Full GF matrix (renormalized):

$$\hat{G}_{\boldsymbol{k}} = \left(\hat{g}_{\boldsymbol{k}}^{-1} + \hat{\Sigma}_{\boldsymbol{k}}\right)^{-1}$$

$$\hat{\Sigma}_{\boldsymbol{k}} = c\hat{T}\left[1 + c\sum_{\boldsymbol{n}\neq 0}\left(\hat{A}_{\boldsymbol{n}}\mathrm{e}^{-i\boldsymbol{k}\cdot\boldsymbol{n}} + \hat{A}_{\boldsymbol{n}}^{2}\right)\left(1-\hat{A}_{\boldsymbol{n}}^{2}\right)^{-1} + \cdots\right].$$

$$\hat{T} = -\hat{V}\left(1+\hat{g}\hat{V}\right)^{-1}$$

T- matrix

$$\hat{A}_{\boldsymbol{n}} = N^{-1}\sum\nolimits_{\boldsymbol{k}} \mathrm{e}^{i\boldsymbol{k}\cdot\boldsymbol{n}} \hat{g}_{\boldsymbol{k}} \hat{T}$$

interaction matrix

Calculating GE for the simplest case of *s*-wave, $\Delta_{\mathbf{k}} = \Delta = \text{const}$, present the local GF matrix as:

$$\hat{g} = \frac{1}{N}\sum_{\mathbf{k}} \hat{g}_{\mathbf{k}} = \left(\varepsilon + \Delta\hat{\tau}_1\right) g_0 - g_3 \hat{\tau}_3$$

$$g_0(\varepsilon) = \frac{\pi\rho_{\mathrm{F}}}{2\sqrt{\Delta^2 - \varepsilon^2}}$$

$$g_3(\varepsilon) = \frac{1}{N}\sum_{\mathbf{k}} \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}^{\ 2} - \varepsilon^2} \approx \frac{1}{N}\sum_{\mathbf{k}} \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}^{\ 2}} = \text{const}$$

Then the explicit T-matrix:

$$\hat{T} = \frac{2}{\pi\rho_{\mathrm{F}}} \frac{v}{1+v^2} \left(\hat{\tau}_3 + v \frac{\varepsilon + \Delta\hat{\tau}_1}{\sqrt{\Delta^2 - \varepsilon^2}} \right), \qquad v = \frac{\pi}{2} \frac{\rho_{\mathrm{F}} V_i}{1 - V_i g_3},$$

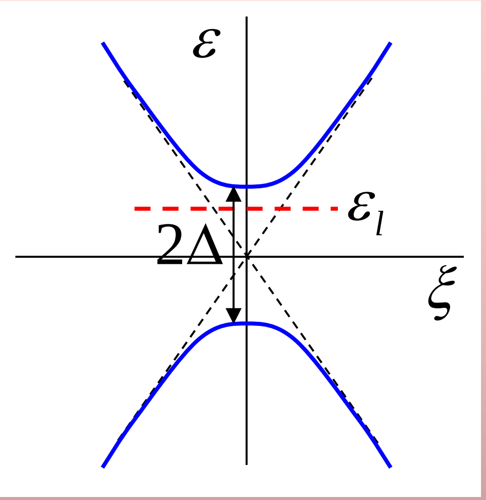
has no poles within the gap $\rightarrow$ Anderson's theorem.

This defines relative insensitivity of traditional superconductors to impurities.

Anderson's theorem limitation can be lifted by various mechanisms:

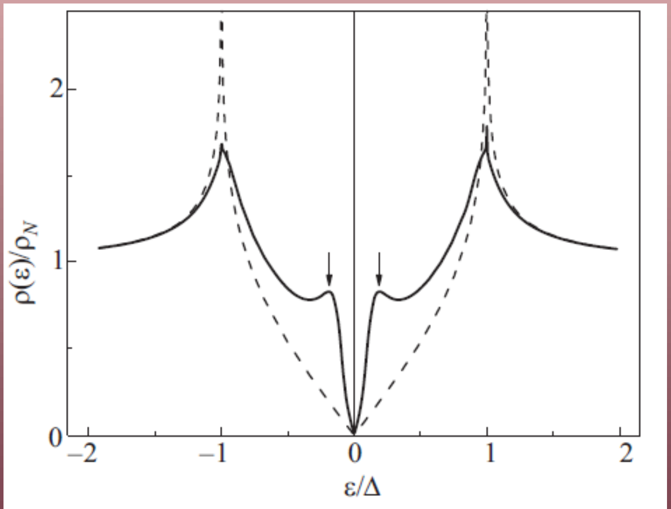
i) Perturbation by magnetic impurities (Shiba, 1968) :

$$\hat{V} = V_m$$



$$\hat{T}_m = V_m v_m \frac{2\left(1 - V_m g_3\right)\sqrt{\Delta^2 - \varepsilon^2} / \left(\pi \rho_F V_m\right) - \varepsilon + \Delta \hat{\tau}_1}{\sqrt{\Delta^2 - \varepsilon^2} - v_m \varepsilon},$$

ii) Non-magnetic impurities in *d*-wave superconductors: $\Delta_{\mathbf{k}} = \Delta \cos 2\varphi_{\mathbf{k}}$ (Balatsky, 1995; Pogorelov, 1995):

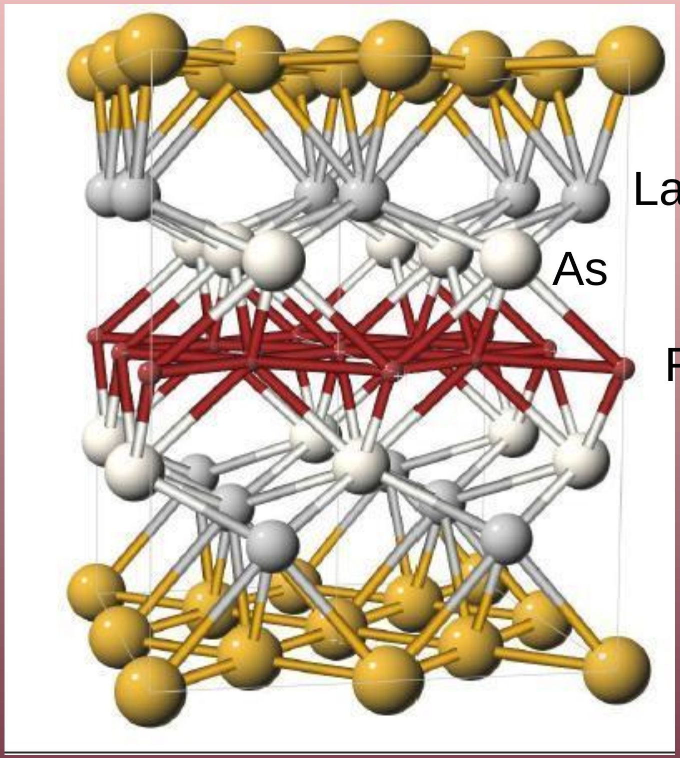


$$\hat{T}_d = V \frac{v g_d - \hat{\tau}_3}{1 - v^2 g_d^{\;2}},$$

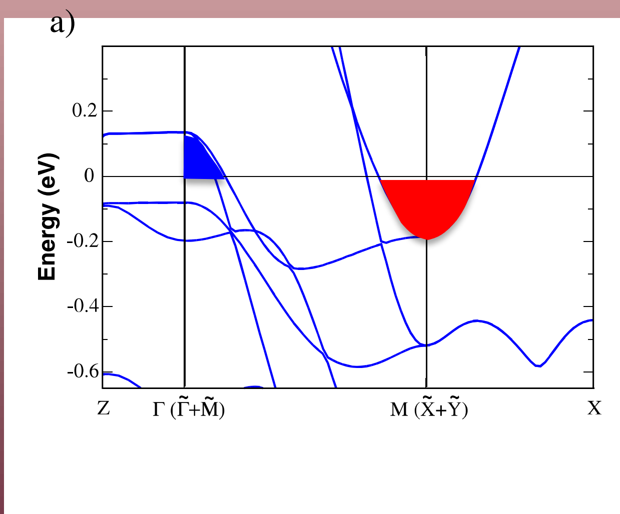
This permits quasilocal resonances but not impurity banding.

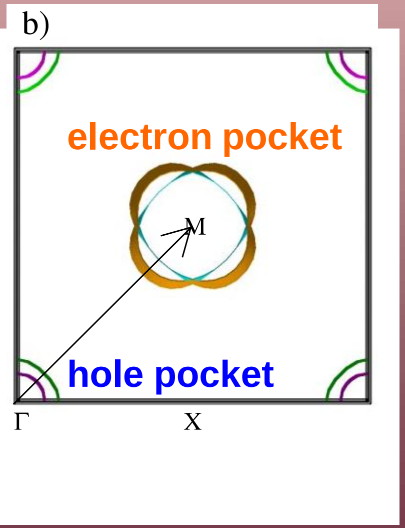
SC ferropnictides and in-gap impurity levels

The discovery of superconductivity (SC) with a high critical temperature in doped ferropnictide compounds by Y. Kamihara et al., J. Am. Chem. Soc. 128, 10012 (2006); J. Am. Chem. Soc. 130, 3296 (2008), has motivated a great interest to these materials.



The first principles numeric calculations show the importance of Fe d-orbitals for SC in these materials. The dominance of Fe 3d orbitals in LaOFeAs near its Fermi surface was demonstrated by LDA calculations.





Extended s-wave SC symmetry:

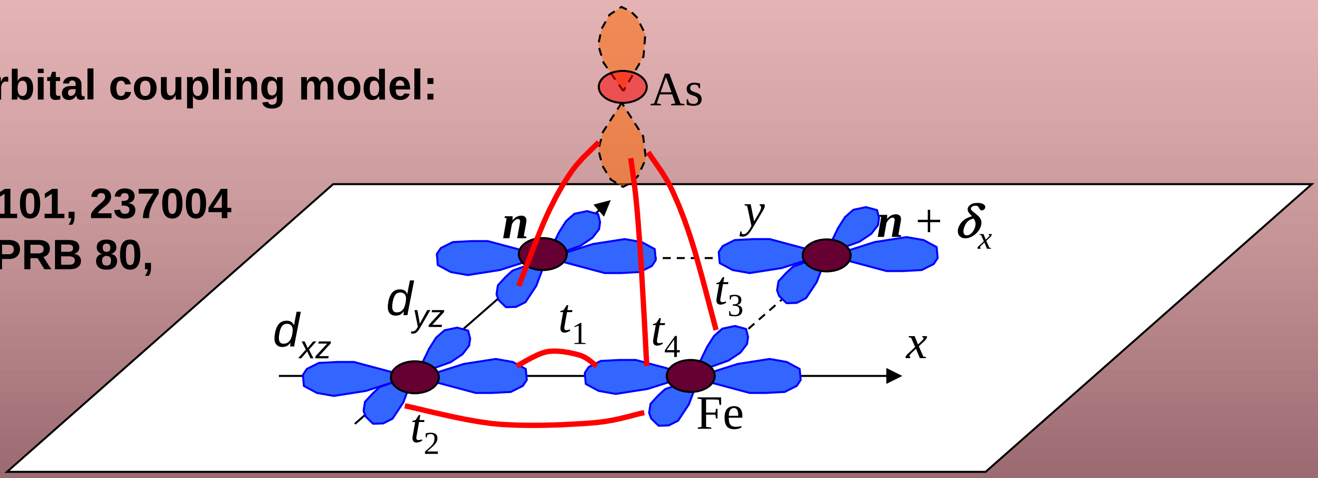
$$\Delta_e = -\Delta_h.$$

I.I. Mazin et al, PRL 101, 057003 (2008).

In general, the total of 5 atomic orbitals for each iron in LaOFeAs can be involved, however the ways to reduce this basis are sought, in order to simplify analytical and computational work.

Minimum two-orbital coupling model:

M. Daghofer et al, PRL 101, 237004 (2008); W.-F. Tsai et al, PRB 80, 064513 (2009).



A possibility for localized impurity levels within SC gaps in doped LaOFeAs was indicated.

D. Zhang, PRL 103, 186402 (2009);
Y.-Y. Zhang et al, PRB 80, 094528 (2009).

Impurity perturbation and Green functions

After diagonalization from 2 orbitals to 2 subbands, a non-perturbed 4×4 SC Hamiltonian reads:

$$\mathrm{H}_s = \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^{+} \hat{h}_s \Psi_{\mathbf{k}},$$

$$\Psi_{\mathbf{k}} = \begin{pmatrix} \alpha_{\mathbf{k},\sigma} \\ \alpha_{-\mathbf{k},\sigma}^{+} \\ \beta_{\mathbf{k},\sigma} \\ \beta_{-\mathbf{k},\sigma}^{+} \end{pmatrix}$$

Nambu indices

band indices

with

$$\hat{h}_s(\mathbf{k}) = \begin{pmatrix} \varepsilon_{e,\mathbf{k}} & \Delta_{\mathbf{k}} & 0 & 0 \\ \Delta_{\mathbf{k}} & -\varepsilon_{e,\mathbf{k}} & 0 & 0 \\ 0 & 0 & \varepsilon_{h,\mathbf{k}} & -\Delta_{\mathbf{k}} \\ 0 & 0 & -\Delta_{\mathbf{k}} & -\varepsilon_{h,\mathbf{k}} \end{pmatrix}$$

Full GF

$$\hat{G}_{\boldsymbol{k},\boldsymbol{k}'} = \left\langle\left\langle \Psi_{\boldsymbol{k}} \middle| \Psi_{\boldsymbol{k}}^{+} \right\rangle\right\rangle,$$

non-perturbed GF

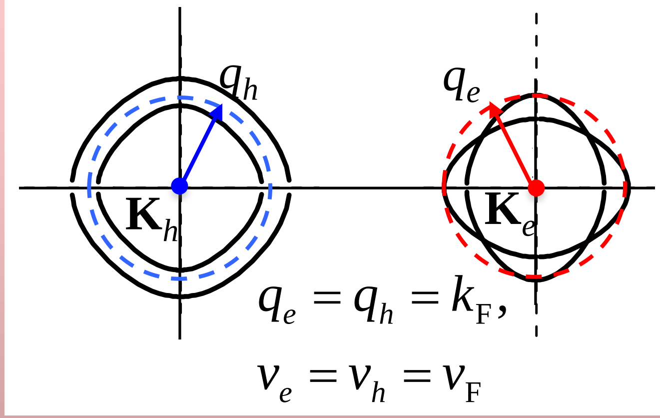
$$\hat{g}_{\boldsymbol{k}} = \begin{pmatrix} \frac{1}{2D_{e,\boldsymbol{k}}}\begin{pmatrix} \varepsilon + \varepsilon_{e,\boldsymbol{k}} & \Delta \\ \Delta & \varepsilon - \varepsilon_{e,\boldsymbol{k}} \end{pmatrix} & 0 \\ 0 & \frac{1}{2D_{h,\boldsymbol{k}}}\begin{pmatrix} \varepsilon + \varepsilon_{h,\boldsymbol{k}} & -\Delta \\ -\Delta & \varepsilon - \varepsilon_{h,\boldsymbol{k}} \end{pmatrix} \end{pmatrix},$$

with:

$$D_{i,\mathbf{k}} = \varepsilon^2 - \varepsilon_{i,\mathbf{k}}^2 - \Delta^2.$$

Use linearized and unified dispersion laws around Fermi level:

$$\varepsilon_{i,\mathbf{k}} = \varepsilon_{\mathrm{F}} + \xi_{i,\mathbf{k}},$$
$$\xi_{i,\mathbf{k}} \approx \hbar v_i \left(\left| \mathbf{k} - \mathbf{K}_i \right| - q_i \right)$$



Impurity perturbation (non-magnetic)

$$H' = V \sum_{\boldsymbol{p},\sigma} \left(x^{+}_{\boldsymbol{p},\sigma} x_{\boldsymbol{p},\sigma} + y^{+}_{\boldsymbol{p},\sigma} y_{\boldsymbol{p},\sigma} \right) = \frac{1}{N} \sum_{\boldsymbol{p},\boldsymbol{k},\boldsymbol{k}'} \mathrm{e}^{i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{p}} \Psi^{+}_{\boldsymbol{k}} \hat{V}_{\boldsymbol{k},\boldsymbol{k}'} \Psi_{\boldsymbol{k}'}$$

$$\hat{V}_{\mathbf{k},\mathbf{k}'} = V \hat{U}^{+}_{\mathbf{k}} \hat{U}_{\mathbf{k}'} \otimes \hat{\tau}_3$$

$$\hat{U}_{\mathbf{k}} = \mathrm{e}^{-i\hat{\sigma}_2 \theta_{\mathbf{k}}/2}, \qquad \theta_{\mathbf{k}} = \arctan \frac{\varepsilon_{xy,\mathbf{k}}}{\varepsilon_{-,\mathbf{k}}}.$$

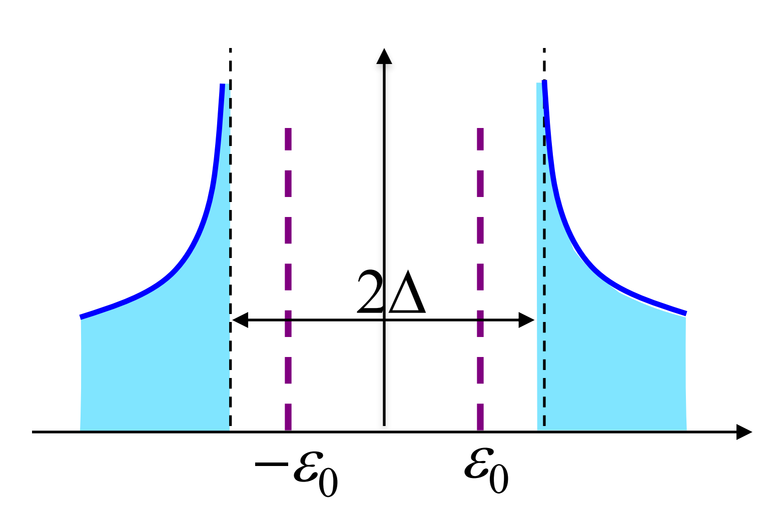
In the present model, T-matrix is: $\hat{T} = \hat{V}\left(1 - \hat{g}\hat{V}\right)^{-1},$

where $\hat{V} = V\hat{\sigma}_0 \otimes \hat{\tau}_3,$ $\hat{g} = \frac{1}{N}\sum_{\boldsymbol{k}} \hat{U}_{\boldsymbol{k}} \hat{g}_{\boldsymbol{k}} \hat{U}_{\boldsymbol{k}}^{+} = \varepsilon \begin{pmatrix} g_e \otimes \hat{\tau}_0 & 0 \\ 0 & g_h \otimes \hat{\tau}_0 \end{pmatrix},$

and $g_i(\varepsilon) \approx \frac{-\pi\rho_i}{\sqrt{\Delta^2 - \varepsilon^2}},$

obtains explicit form $\hat{T} = V\frac{v\varepsilon\sqrt{\Delta^2 - \varepsilon^2} - \left(\Delta^2 - \varepsilon^2\right)\hat{\tau}_3}{\left(1 + v^2\right)\left(\varepsilon^2 - \varepsilon_0{}^2\right)},$

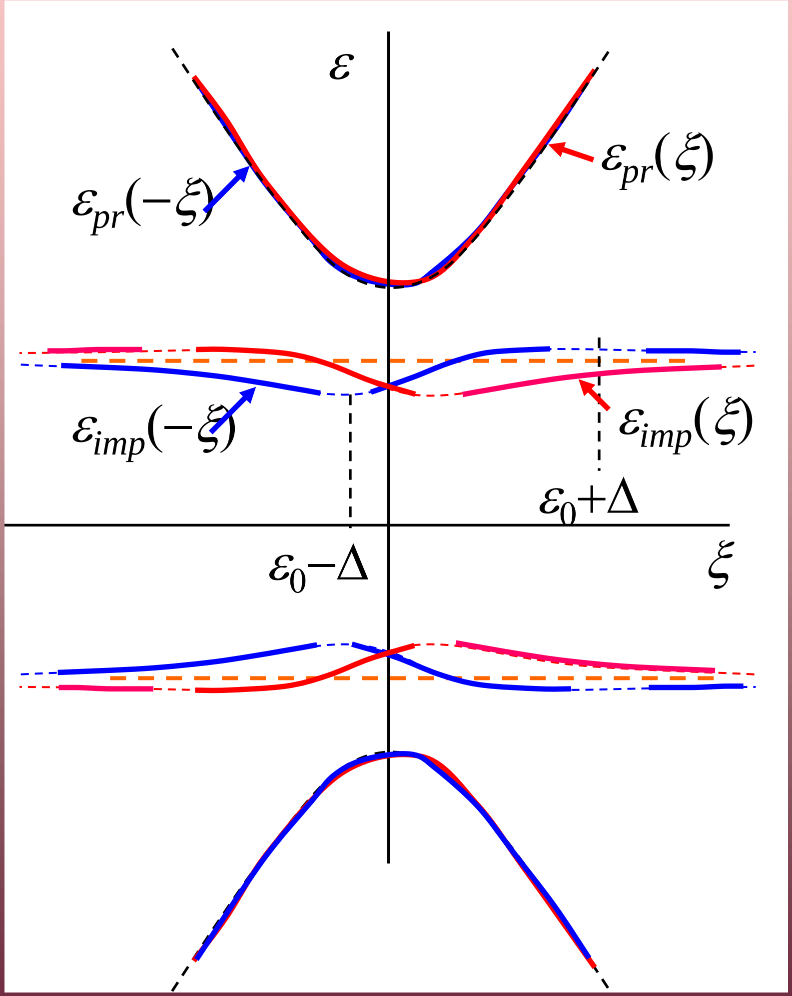
and near the impurity levels: $\pm\varepsilon_0 = \pm\frac{\Delta}{\sqrt{1 + v^2}},$



approximates as $\hat{T} = \gamma^2 \frac{\varepsilon - \varepsilon_0\hat{\tau}_3}{\varepsilon^2 - \varepsilon_0^2},$

with $v = \pi\rho_{\text{F}}V,$ $\gamma^2 = \frac{v^2 V \varepsilon_0^2}{\Delta},$

At finite *c*, the formal dispersion equation (up to 8 bands) results from the condition: det $\hat{G}_{\mathbf{k}}^{-1}(\varepsilon) = 0$ (but neglecting the energy level broadening by the effects of interaction between impurities), which can be expressed through the quasiparticle energy ξ:



four, modified from the principal bands:

$$\varepsilon_{pr}\left(\xi\right) \approx \sqrt{\Delta^2 + \xi^2},$$

and four narrow "impurity" bands:

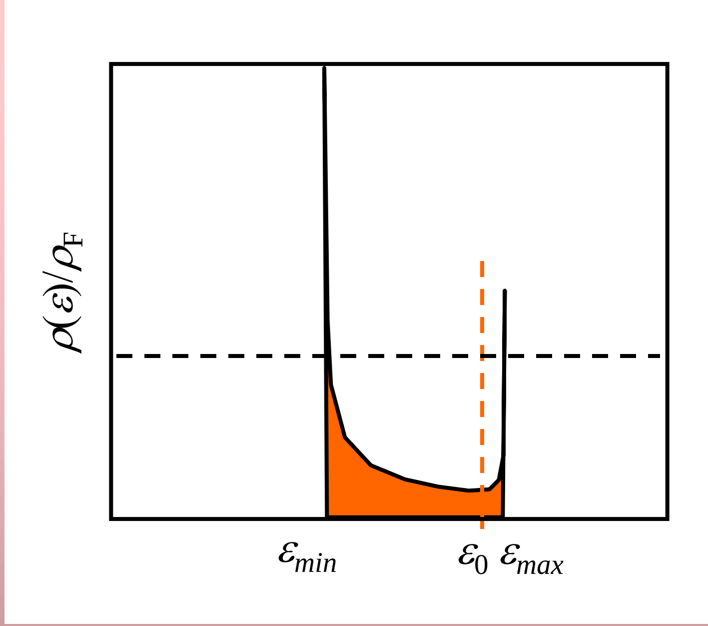
$$\varepsilon_{imp}\left(\xi\right) \approx \varepsilon_0 + c\gamma^2 \frac{\xi - \varepsilon_0}{\xi^2 + \xi_0^{\ 2}}.$$

All these bands contribute to the overall density of states (DOS) by the related quasiparticles:

$$\rho\left(\varepsilon\right) = \frac{1}{4\pi N} \operatorname{Im} \operatorname{Tr} \sum_{\mathbf{k}} \hat{G}_{\mathbf{k}}$$

Most peculiar are the contributions to DOS from the *imp*-bands

$$\rho_{imp}\left(\varepsilon\right) \approx \frac{\rho_{\mathrm{F}}}{v}\frac{\varepsilon^2-\varepsilon_0{}^2-c\gamma^2}{\sqrt{\left(\varepsilon_{\max}{}^2-\varepsilon^2\right)\left(\varepsilon^2-\varepsilon_{\min}{}^2\right)}},$$



Here the edge singularities are in fact smeared out at mobility edges where GE ceases to converge.

To estimate the GE convergence, calculate its pair term that will add a finite imaginary part $\Gamma_i(\xi)$ to the dispersion law $\varepsilon = \varepsilon_i(\xi)$.

Then apply the IRM criterion:

$$\varepsilon_{\max} - \varepsilon >> \Gamma_i\left(\varepsilon\right).$$

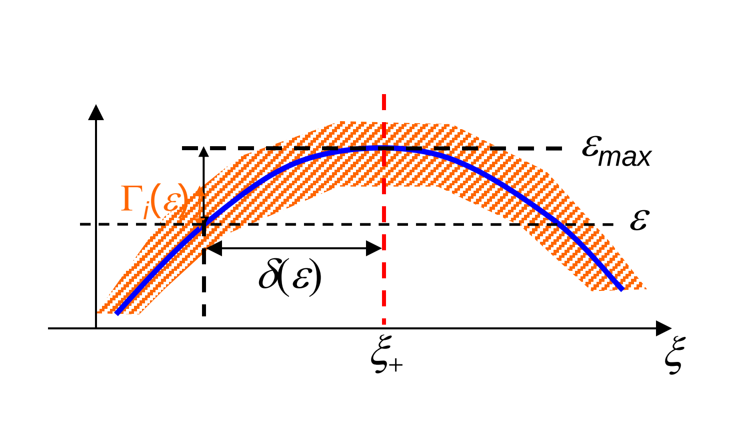
Localized vs band-like impurity states, group expansion analysis

To simplify calculation of $\Gamma_i(\varepsilon)$, fix the energy argument in the numerators of T-matrix and A-matrices at ε_0, getting their forms:

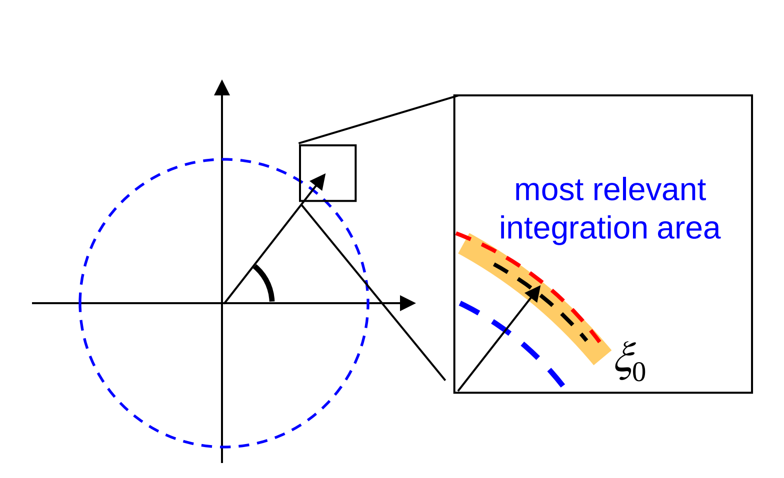
$$\hat{T}(\varepsilon) \approx \frac{\gamma^2 \varepsilon_0}{\varepsilon^2 - \varepsilon_0^2}\hat{m}_+,$$

$$\hat{m}_+ = \sigma_0 \otimes (\hat{\tau}_0 + \hat{\tau}_3),$$

$$\hat{A}_{\boldsymbol{n}}^0 = \hat{T}(\varepsilon)\frac{\varepsilon_0}{N}\sum_{\boldsymbol{k}} \frac{\mathrm{e}^{i\boldsymbol{k}\cdot\boldsymbol{n}}}{D_{\boldsymbol{k}}(\varepsilon)}\hat{g}_{\boldsymbol{k}},$$

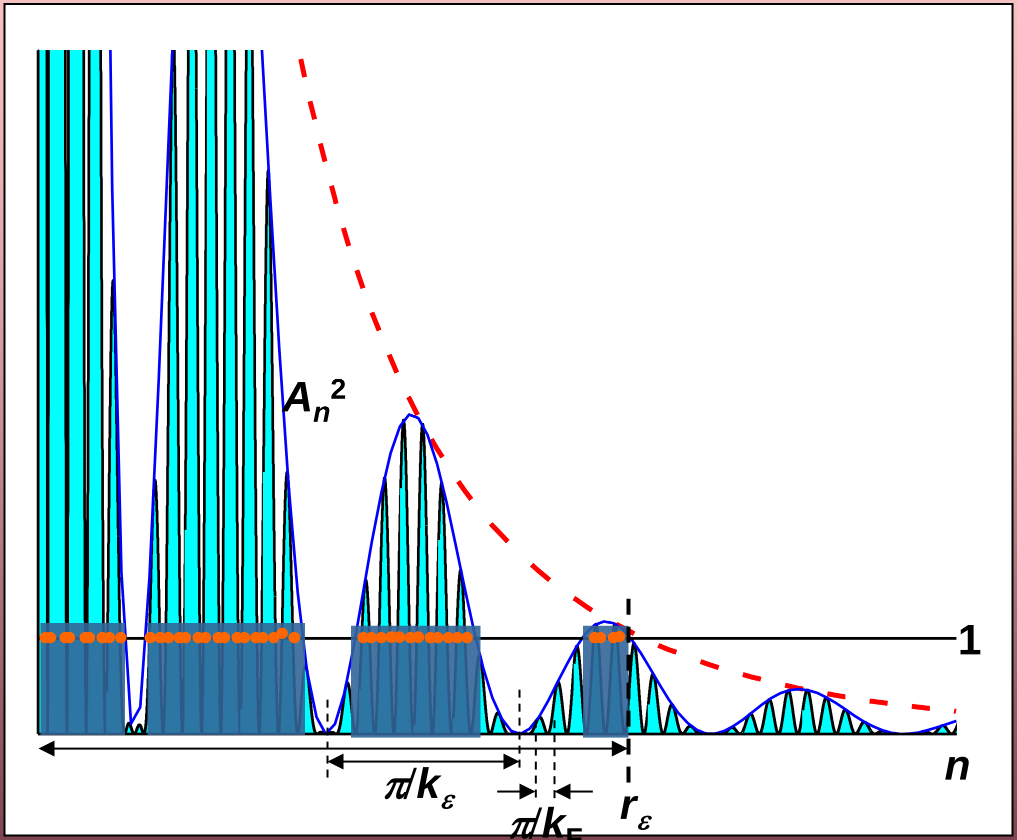


$$D_\xi(\varepsilon) \approx (\xi - \xi_+)^2 - \delta^2(\varepsilon)$$



The interaction matrix depends on the distance *n* between impurities as

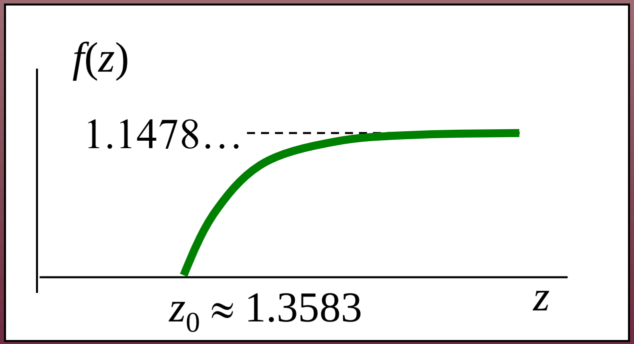
$$\hat{A}^0_{\mathbf{n}} = A_n(\varepsilon)\hat{m}_+, \qquad A_n(\varepsilon) \approx \sqrt{\frac{r_\varepsilon}{n}} \sin k_\varepsilon n \cos k_\mathrm{F} n,$$



$$r_\varepsilon \approx \frac{2\pi}{k_\mathrm{F}}\left[\varepsilon_0\rho_\mathrm{F}\frac{\Delta+\varepsilon_0}{c\delta(\varepsilon)}\right]^2, \qquad k_\varepsilon \approx \frac{\delta(\varepsilon)}{\hbar v_\mathrm{F}}$$

Integration in *n* over multiple poles is done in three steps: i) in fast oscillations, ii) in slow oscillations, iii) in monotonous envelope, resulting in:

$$\mathrm{Im}\, B \approx \frac{r_\varepsilon^2}{a^2} f(k_\varepsilon r_\varepsilon)$$



If $f(k_\varepsilon r_\varepsilon)$ is taken ~ 1, the IRM criterion reads:

$$\varepsilon_{\max} - \varepsilon >> \frac{c^2\gamma^2}{\varepsilon_{\max} - \varepsilon_0}\frac{r_\varepsilon^{\ 2}}{a^2}$$

and the (concentration independent) condition for existence of extended states in the impurity band would be

$$\varepsilon_{\max} - \varepsilon >> \Gamma_0 = \frac{(v\varepsilon_0)}{ak_{\mathrm{F}}}\sqrt{\frac{2\pi\rho_{\mathrm{F}}}{1+v^2}}$$

From comparison with the full extension of this band:

$$\varepsilon_{\max} - \varepsilon_{\min} = c\gamma^2\frac{1+v^2}{v^2\Delta},$$

such extended states can really exist if the impurity concentration surpasses the characteristic (small) value

$$c >> c_0 = \frac{(\pi\rho_{\mathrm{F}}\varepsilon_0)^{3/2}}{ak_{\mathrm{F}}}\sqrt{\frac{2v}{1+v^2}}$$

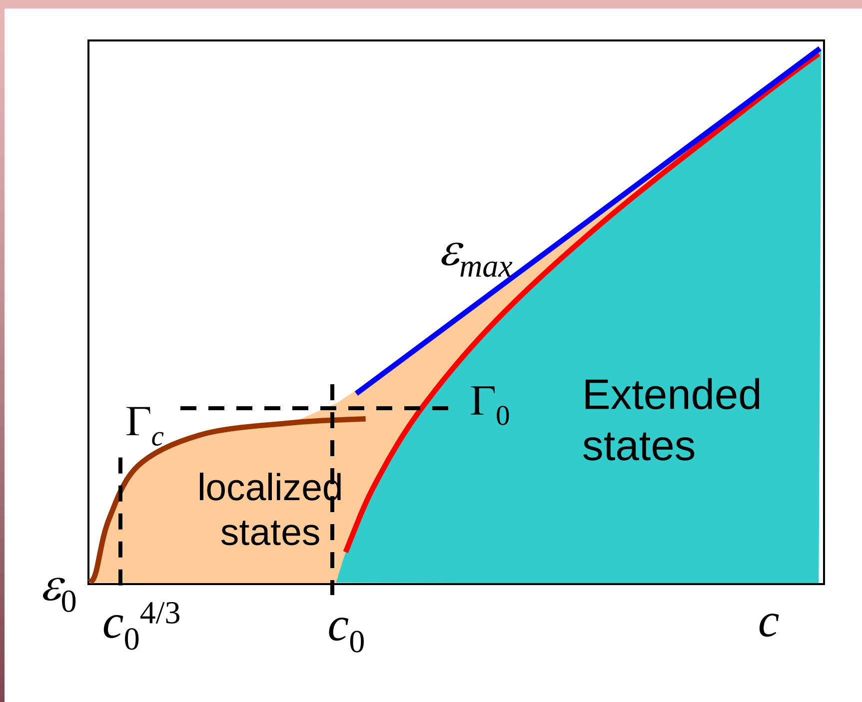
But since $f(k_\varepsilon r_\varepsilon)$ vanishes at $k_\varepsilon r_\varepsilon < z_0$, the broadening by the pair term at $c > c_0$ is even smaller:

$$\varepsilon_{\max} - \varepsilon > \left(\frac{c_0}{c}\right)^3\Gamma_0$$

Otherwise, for $c \lesssim c_0$, the impurity band does not exist, then we analyze the energy range near the impurity level with the so-called non-renormalized GE using the non-renormalized interaction function

$$A_n^{\ 0}(\varepsilon) \approx \sqrt{\frac{R_\varepsilon}{n}} e^{-n/r_0} \cos k_F n,$$

$$R_\varepsilon = \frac{2\pi}{k_F}\left(\frac{\varepsilon_0}{|\varepsilon - \varepsilon_0|}\right)^2, \qquad r_0 = \frac{2\varepsilon_F}{\xi_0 k_F}.$$



to give exponentially narrow concentration width of impurity level:

$$\Gamma_c = \Gamma_0 \exp\left(-\frac{c_0^{\ 4/3}}{c}\right).$$

DOS beyond Γ_c is estimated as:

$$\rho_{loc}(\varepsilon) \approx \frac{c^2}{c_0^{\ 4/3}|\varepsilon - \varepsilon_0|},$$

$$\text{at} \quad \Gamma_c << |\varepsilon - \varepsilon_0| << \Gamma_0,$$

$$\rho_{loc}(\varepsilon) \approx \frac{c^2 \varepsilon_0^{\ 4}}{|\varepsilon - \varepsilon_0|^5},$$

$$\text{at} \quad \Gamma_0 << |\varepsilon - \varepsilon_0|.$$

Observable impurity effects: thermodynamics

The fundamental SC order parameter is estimated from the modified gap equation:

$$\lambda^{-1} = \int_0^{\varepsilon_D} \rho(\varepsilon) d\varepsilon, \qquad \lambda = \rho_F V_{SC}$$

For *c* = 0, the unperturbed value:

$$\lambda^{-1} = \text{arcsinh}\,\frac{\varepsilon_D}{\Delta_0} \Rightarrow \Delta_0 \approx \varepsilon_D \mathrm{e}^{-1/\lambda}.$$

For *c* > 0, the main contribution comes from:

$$\int_0^{\varepsilon_D} \rho_{pr}(\varepsilon) d\varepsilon \approx \text{arcsinh}\,\frac{\varepsilon_D}{\Delta_c} - c\gamma^2 \int_{\Delta_c}^{\varepsilon_D} \frac{d\varepsilon}{(\varepsilon - \varepsilon_0)^2 \sqrt{\Delta_c{}^2 - \varepsilon^2}},$$

$$\int_{\Delta_c}^{\varepsilon_D} \frac{d\varepsilon}{(\varepsilon - \varepsilon_0)^2 \sqrt{\Delta_c{}^2 - \varepsilon^2}} \approx \frac{1}{\Delta_c{}^2} F\left(\frac{\Delta_c}{\varepsilon_0}\right),$$

$$F(z) = z\,\frac{\sqrt{z^2 - 1} + z \arccos(-1/z)}{(z^2 - 1)^{3/2}}.$$

Modified gap equation becomes

$$\operatorname{arcsinh}\frac{\Delta_c-\Delta_0}{\Delta_0}\approx\frac{cv^2}{c_1\left(1+v^2\right)}F\left(\frac{\Delta_c}{\varepsilon_0}\right).$$

and its approximated solution:

$$\frac{\Delta}{\Delta_0}\approx 1-\frac{c}{c_1}\frac{1+v^2F\left[\sqrt{1+v}\left(1+c/c_1\right)\right]}{\left(1+v^2\right)},$$

$$c_1=\frac{\pi\rho_{\mathrm{F}}\Delta}{v},$$

implies Δ to vanish at

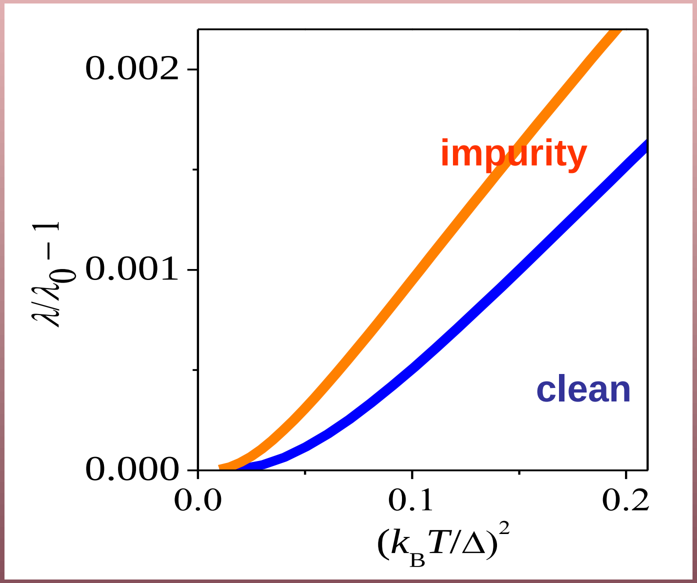
$$c\to c_1\frac{1+v^2}{1+v^2F\left[\sqrt{1+v}\left(1+c/c_1\right)\right]},$$

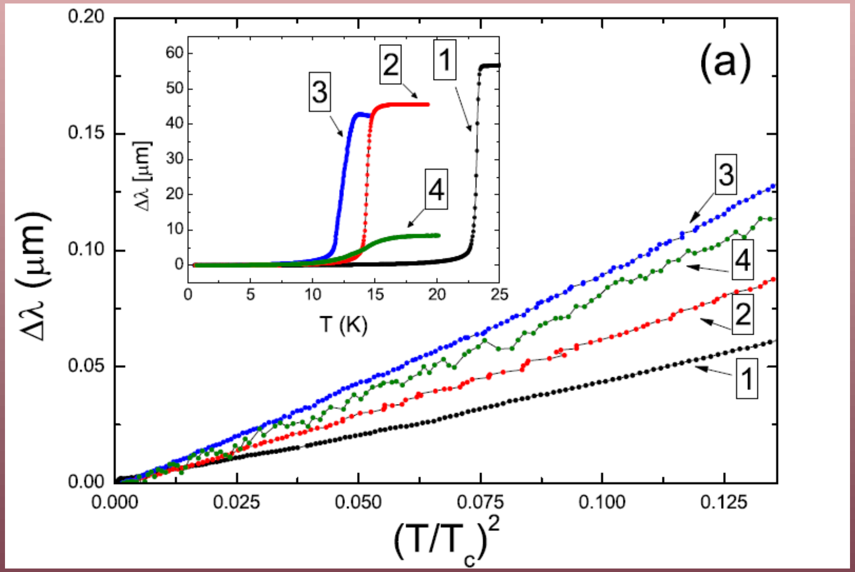
though such concentration is rather too high for the used approximations (of narrow impurity band *vs* gap parameter itself).

Impurity effect on the superfluid density n_s related to the London penetration depth $\lambda_L \sim (c/e)\sqrt{m/n_s}$:

$$n_s(T) = \int_0^\infty \frac{\rho(\varepsilon)d\varepsilon}{e^{\varepsilon/k_B T}+1} \approx \frac{c}{e^{\varepsilon_0/k_B T}+1} + \left(1 - \frac{c\gamma^2}{\Delta^2 - \varepsilon_0{}^2}\right) n_s{}^0(T),$$

shows a sizeable slowering down of its low-temperature decay:





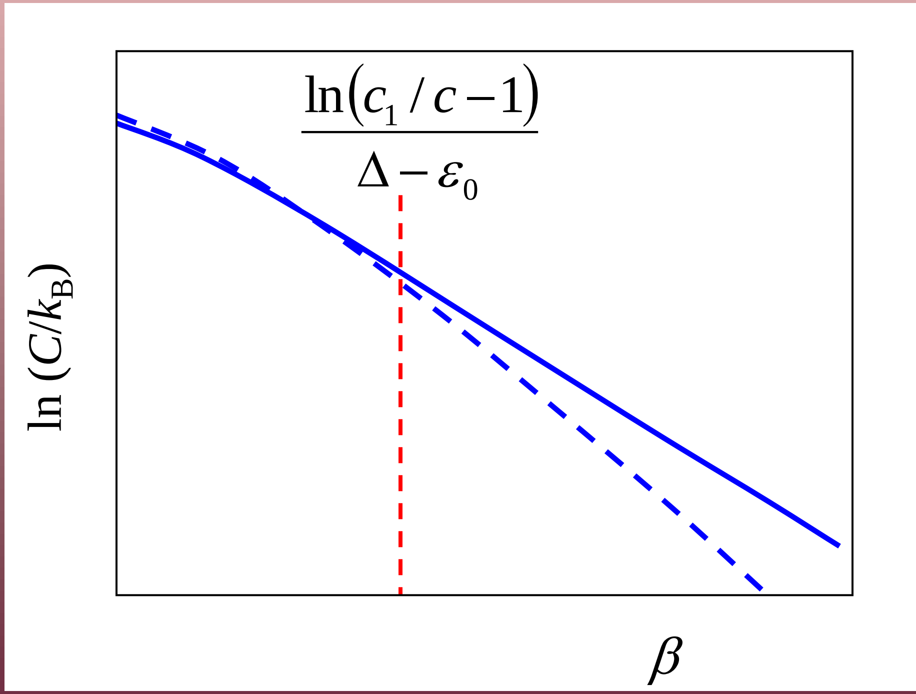
alike the experimental data on SC ferropnictides under disorder (R. T. Gordon et al, PRB 81, 180501R, 2010).

Impurity effect on the electronic specific heat in the SC state also follows from its contribution to DOS:

$$C(\beta) = \frac{\partial}{\partial T} \int_0^\infty \frac{\varepsilon \rho(\varepsilon) d\varepsilon}{e^{\beta\varepsilon} + 1},$$

changing the decay exponent $\Delta/k_B T$ at low temperatures $T < T^* = \frac{\Delta - \varepsilon_0}{k_B \ln(c_1/c - 1)}$

for a slower one: $\varepsilon_0/k_B T$.



Observable impurity effects: kinetics

Impurity effects on transport, e.g., optical conductivity, follow from the Kubo-Greenwood formula for a multiband superconductor:

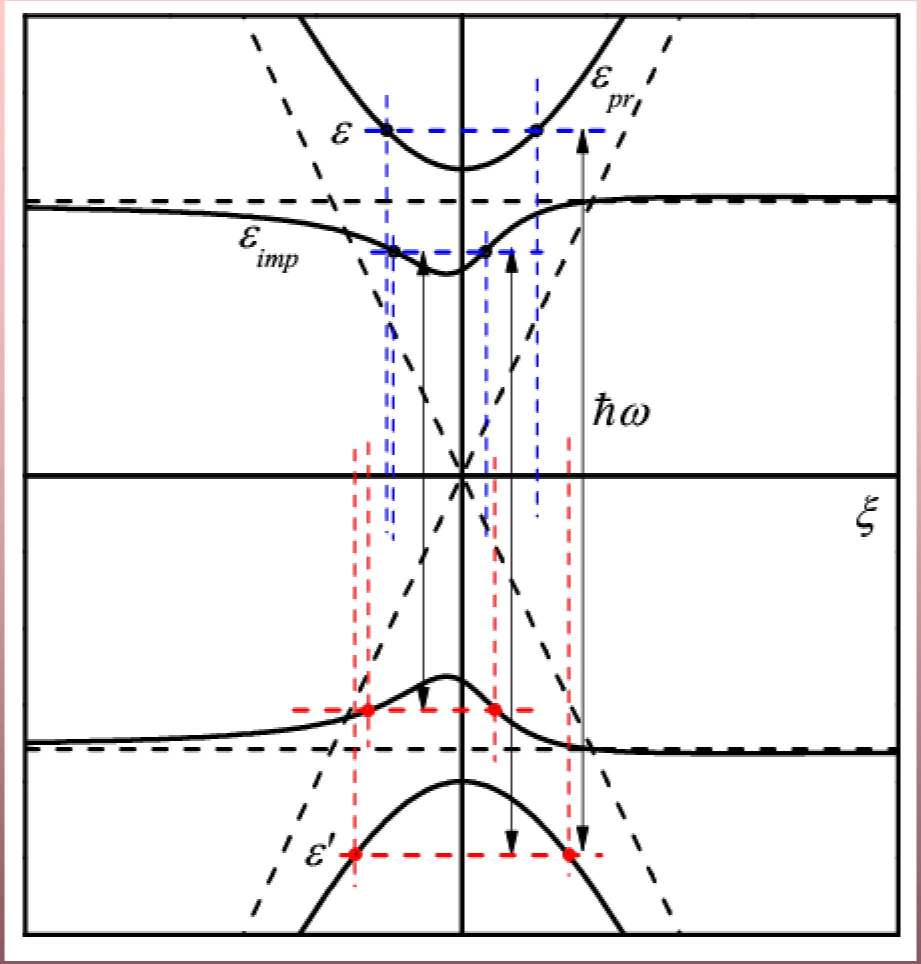
$$\sigma(\omega, T) = \frac{e^2}{\pi} \int d\varepsilon \frac{f(\varepsilon) - f(\varepsilon')}{\omega} \int d\mathbf{k} v_x(\mathbf{k}, \varepsilon) v_x(\mathbf{k}, \varepsilon') \times \mathrm{Tr}\left[\mathrm{Im}\hat{G}_{\mathbf{k}}(\varepsilon)\mathrm{Im}\hat{G}_{\mathbf{k}}(\varepsilon')\right],$$

with $\varepsilon' = \varepsilon - \hbar\omega,$ **for optical frequency** ω**, and the generalized velocity:**

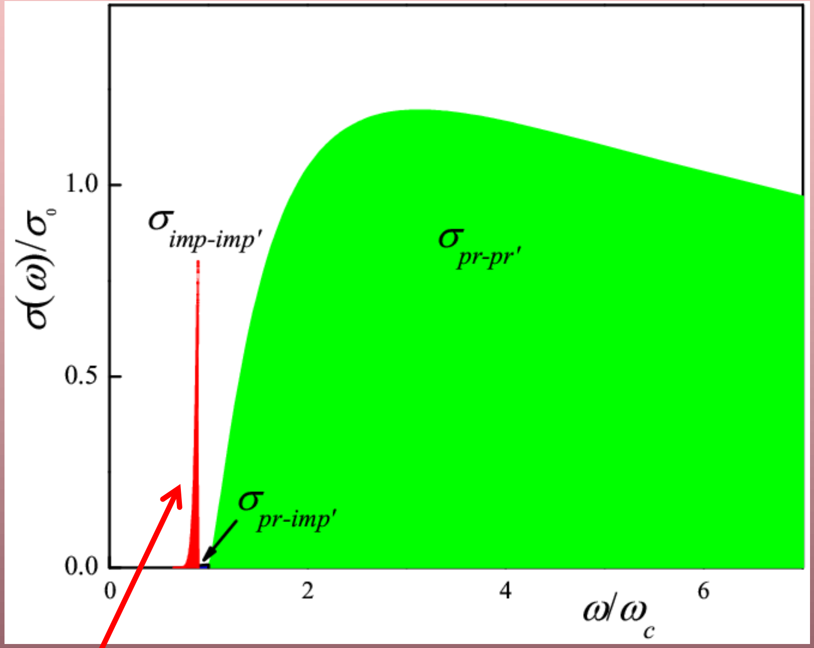
$$\mathbf{v}(\mathbf{k}, \varepsilon) = \left(\hbar \frac{\partial \mathrm{Re} D_{\mathbf{k}}(\varepsilon)}{\partial \varepsilon}\right)^{-1} \nabla_{\mathbf{k}} \mathrm{Re} D_{\mathbf{k}}(\varepsilon).$$

Unlike thermodynamics, this impurity effect is only due to the band-like states with well defined velocities

For the given band structure, 3 types of contributions are possible:



pr-pr, **for** $\omega > 2\Delta/\hbar$,
pr-imp, **for** $\omega > (\Delta + \varepsilon_0)/\hbar$,
imp-imp, **for** $\omega \approx 2\varepsilon_0/\hbar$,



At low temperatures, a special interest may pertain to the narrow *imp-imp* peak, for instance, as a narrow-band resonance element in the Terahertz range.

More detailed calculation results in explicit formulas:

$$\sigma_{pr-pr'}(\omega,0) \approx \sigma_0 \frac{2\omega_c}{\omega^2}\left\{\sqrt{4\omega^2-\omega_c^2}\ln\left[2\frac{\omega(2\omega-\omega_c)+\sqrt{\omega(\omega-\omega_c)(4\omega^2-\omega_c^2)}}{\omega_c^2}-1\right] + 2\omega\ln\left[2\frac{\omega-\sqrt{\omega(\omega-\omega_c)}}{\omega_c}-1\right]-2\sqrt{\omega(\omega-\omega_c)}\right\},$$

zero-temperature limit

$$\sigma_{pr-pr',T}(\omega) \approx \sigma_0 \frac{2\omega_c^2 e^{-\beta\Delta}}{\beta\hbar(\omega-\omega_c)\omega\sqrt{\Delta}}\left[\frac{\sqrt{\hbar\omega}}{\Delta}\left(1-\frac{F(\sqrt{\beta\hbar(\omega-\omega_c)})}{\sqrt{\beta\hbar(\omega-\omega_c)}}\right) + \frac{\sqrt{2\Delta}}{\hbar\omega-\Delta}\left(\frac{\sqrt{\pi}}{2}\frac{\mathrm{erf}(\sqrt{\beta\hbar(\omega-\omega_c)})}{\sqrt{\beta\hbar(\omega-\omega_c)}}-e^{-\beta\hbar(\omega-\omega_c)}\right)\right],$$

termic contribution

the Dawson function $F(z)=\sqrt{\pi}e^{-z^2}\mathrm{erf}(iz)/(2i)$

$$\sigma_{imp-imp'}(\omega,0) \approx \sigma_0 \frac{16c^{7/2}\gamma^7}{3\sqrt{2}\xi_-^7}\left(\frac{\omega-\omega_-}{\omega_-}\right)^{3/2},$$

Caution: the above results for an idealized case of full *e-h* symmetry and unsplitted SC gaps can be essentially modified for a more realistic band structure, however keeping a qualitative similarity of effects

Conclusions and prospects

- Studying of quasiparticle spectra in SC ferropnictides with impurities using Green functions permits description of in-gap local levels and appearance, with growing impurity concentration, of special type of band-like excitations mainly propagating over impurity sites in the lattice.
- Explicit dispersion laws and density of states are obtained either for main and impurity bands.
- Criteria of localization are built and the mobility edges for each band are determined.
- Found expressions for GF's are effective for observable thermodynamical and transport properties of SC ferropnictides with impurities.
- Practical applications of the found impurity resonance effects are expected in microelectronics.

Thank you