Impurity effects in ferropnictide superconductors: localization vs banding

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Impurities in superconductors: Anderson's theorem and all that

The quasiparticle spectra of superconducting systems are commonly related to normal and anomalous Green functions (L.P. Gor'kov, 1962), combined into Nambu matrices:

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

Using the BCS Hamiltonian (without impurity perturbation):

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

with Nambu spinors:

$$\psi_{\mathbf{k}}^{\dagger} = \left(a_{\mathbf{k},\uparrow}^{\dagger} \quad a_{-\mathbf{k},\downarrow}\right)$$

one arrives at 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:

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

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

Leads to a full GF matrix (renormalized): $\hat{G}_{\boldsymbol{k}} = \left(\hat{g}_{\boldsymbol{k}}^{-1} + \hat{\Sigma}_{\boldsymbol{k}} \right)^{-1}$

with a self-energy matrix as a group expansion (GE) (M.A. Ivanov 1971)

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

$$\hat{T} = -\hat{V}\left(1 + \hat{g}\hat{V} \right)^{-1} \qquad \hat{A}_{\boldsymbol{n}} = N^{-1}\sum\nolimits_{\boldsymbol{k}} \mathrm{e}^{i\boldsymbol{k}\cdot\boldsymbol{n}} \hat{G}_{\boldsymbol{k}} \hat{T}$$

T- matrix interaction matrix

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

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

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

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

Then the explicit T-matrix:

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

$$v = \frac{\pi}{2}\frac{\rho_{\mathrm{F}} V_i}{1 - V_i g_3},$$

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

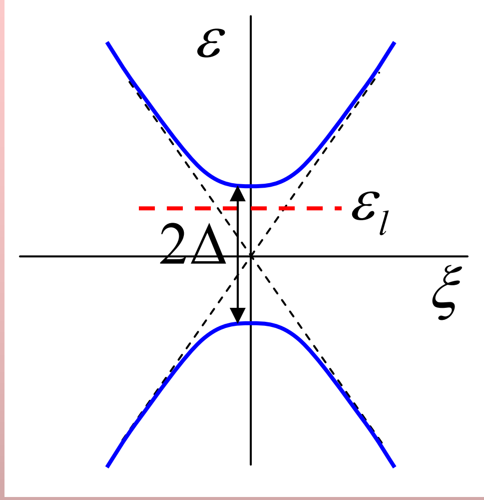
This defines relative insensitivity of traditional superconductors to impurities.

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

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

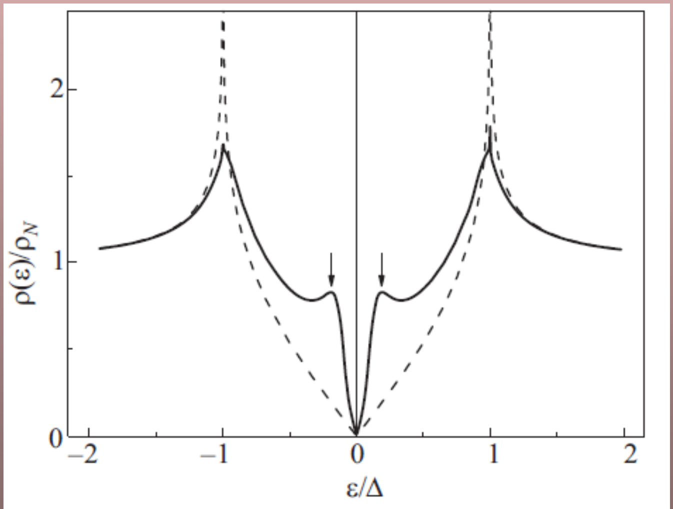
$$\hat{V} = V_m$$

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



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

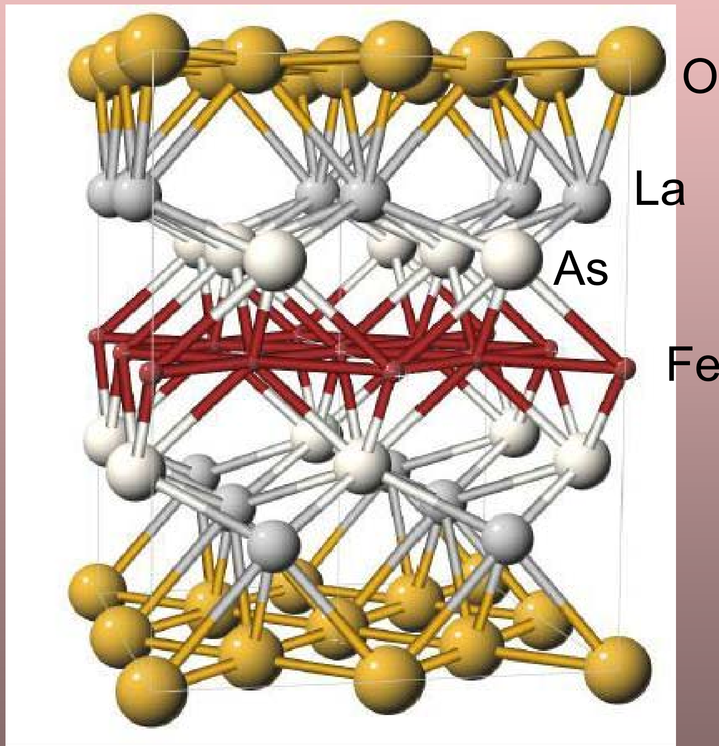
$$\hat{T}_d = V \frac{v g_d - \hat{\tau}_3}{1 - v^2 g_d^{\ 2}},$$



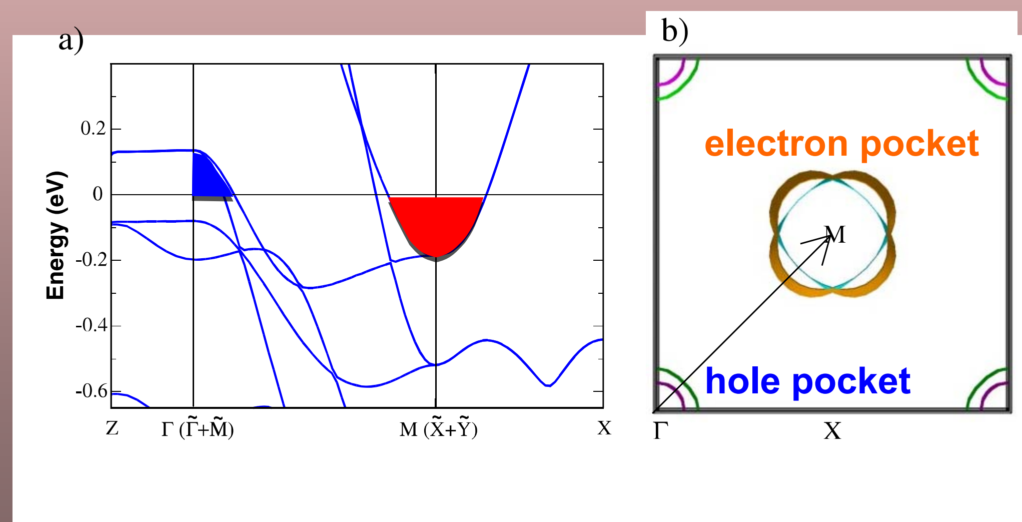
This permits quasilocal resonances but not impurity banding.

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).

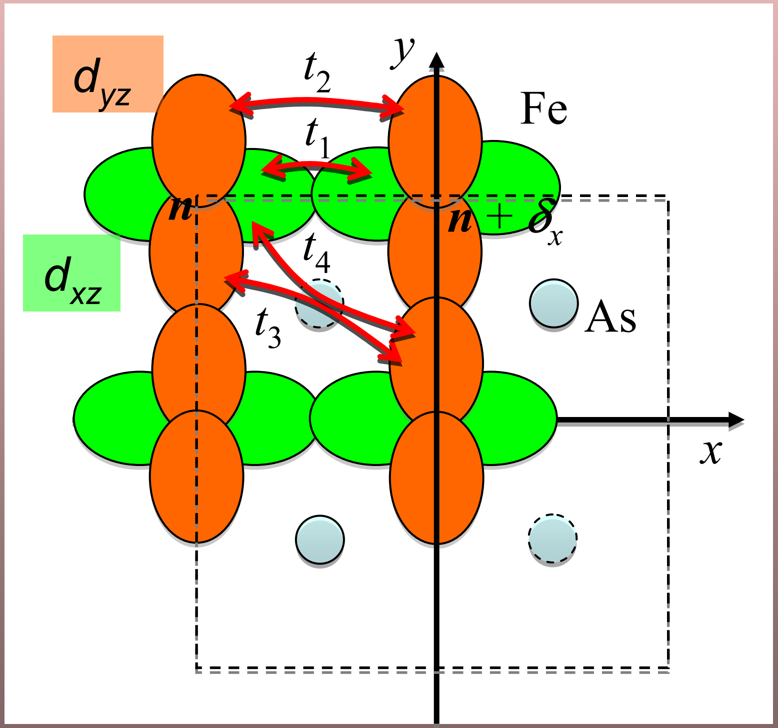
In general, the total of 5 atomic orbitals for each iron in LaOFeAs can be involved, however the ways to reduce this basis are sought, in order to simplify analytical and computational work.

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:

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

with

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

Nambu indices

band indices

and

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

Full GF $\hat{G}_{k,k'} = \langle\langle \Psi_k | \Psi_k^{+} \rangle\rangle,$

non-perturbed GF

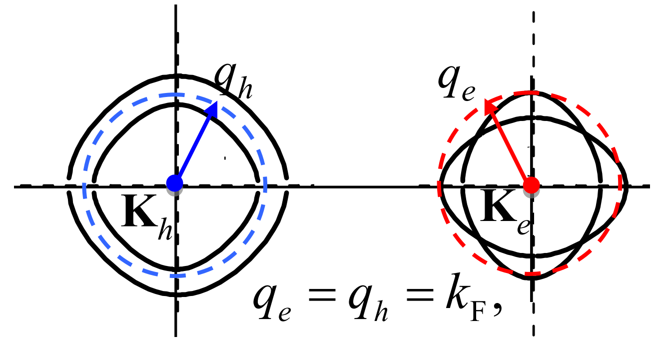
$$\hat{g}_k = \begin{pmatrix} \frac{1}{2D_{e,k}} \begin{pmatrix} \varepsilon + \varepsilon_{e,k} & \Delta \\ \Delta & \varepsilon - \varepsilon_{e,k} \end{pmatrix} & 0 \\ 0 & \frac{1}{2D_{h,k}} \begin{pmatrix} \varepsilon + \varepsilon_{h,k} & -\Delta \\ -\Delta & \varepsilon - \varepsilon_{h,k} \end{pmatrix}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

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

Use linearized and unified dispersion laws around Fermi level:

$$\varepsilon_{i,\mathbf{k}} = \varepsilon_{\mathrm{F}} + \xi_{i,\mathbf{k}},$$

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



$$q_e = q_h = k_{\mathrm{F}},$$

$$v_e = v_h = v_{\mathrm{F}}$$

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

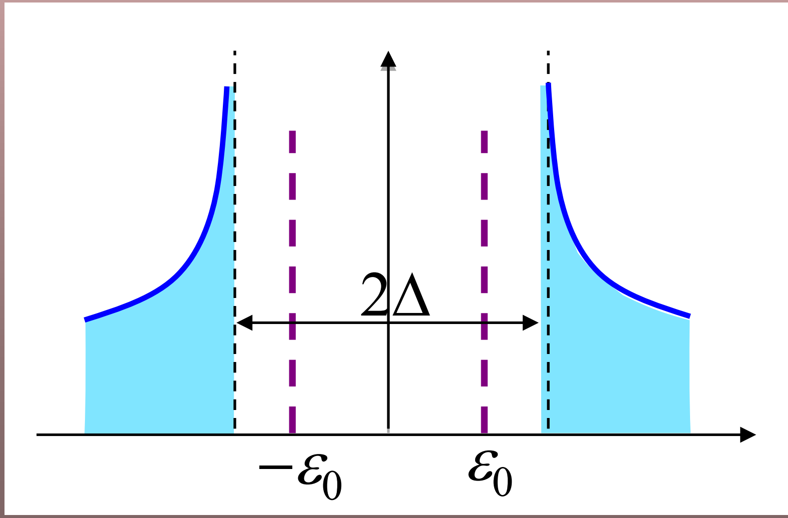
and $g_i\left(\varepsilon\right) \approx \frac{-\pi\rho_i}{\sqrt{\Delta^2 - \varepsilon^2}},$

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

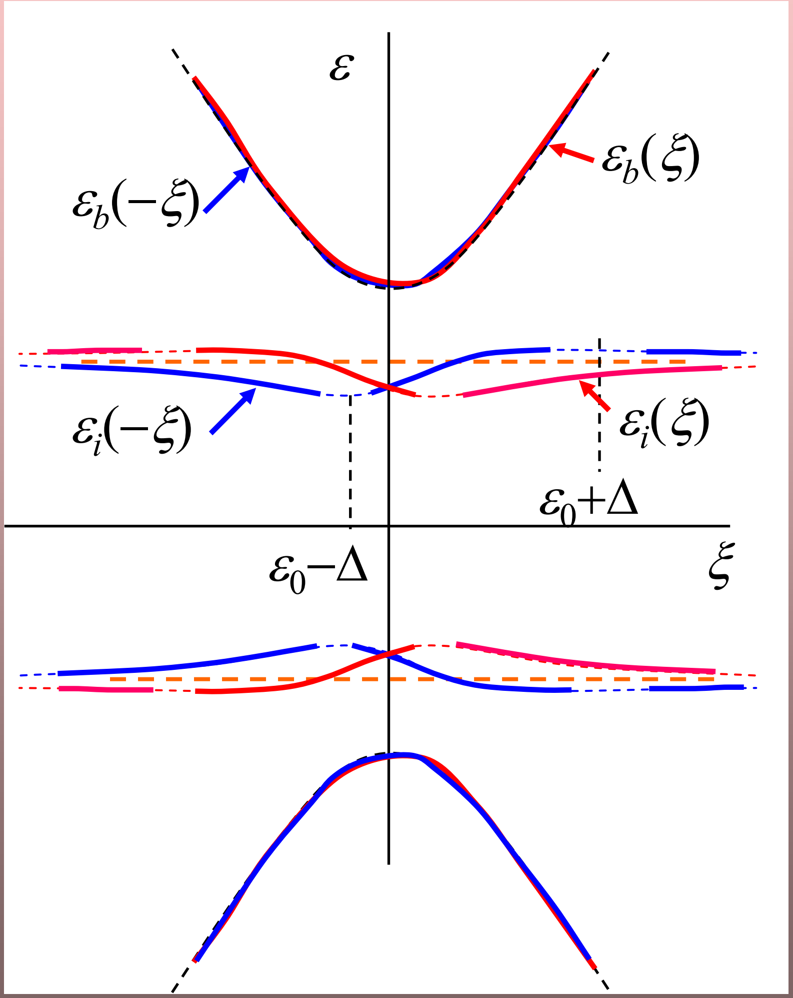
and near the impurity levels: $\pm\varepsilon_0 = \pm\frac{\Delta}{\sqrt{1 + v^2}},$

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

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



At finite c, the formal dispersion equation (up to 8 bands) results from the condition: det $\hat{G}_{\mathrm{k}}^{-1}(\varepsilon) = 0$ (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 unperturbed bands:

$$\varepsilon_b(\xi) \approx \sqrt{\Delta^2 + \xi^2},$$

and four narrow "impurity" bands:

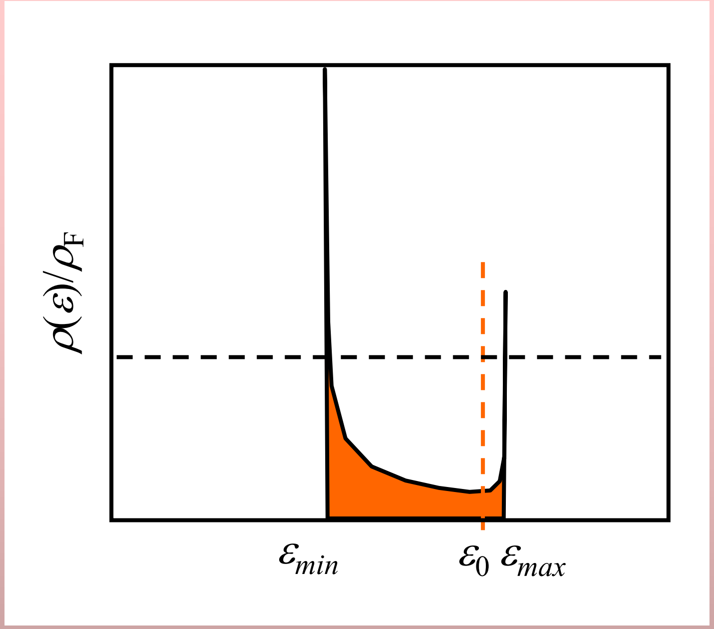
$$\varepsilon_i(\xi) \approx \varepsilon_0 + c\gamma^2 \frac{\xi - \varepsilon_0}{\xi^2 + \xi_0^{\,2}}.$$

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

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

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

$$\rho_i(\varepsilon) \approx \frac{\rho_F}{v} \frac{\varepsilon^2 - \varepsilon_0{}^2 - c\gamma^2}{\sqrt{(\varepsilon_{\max}{}^2 - \varepsilon^2)(\varepsilon^2 - \varepsilon_{\min}{}^2)}},$$



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 Ioffe-Regel-Mott (IRM) criterion for band-like states:

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

A.F. Ioffe and A.R. Regel (1960); N.F. Mott (1967)

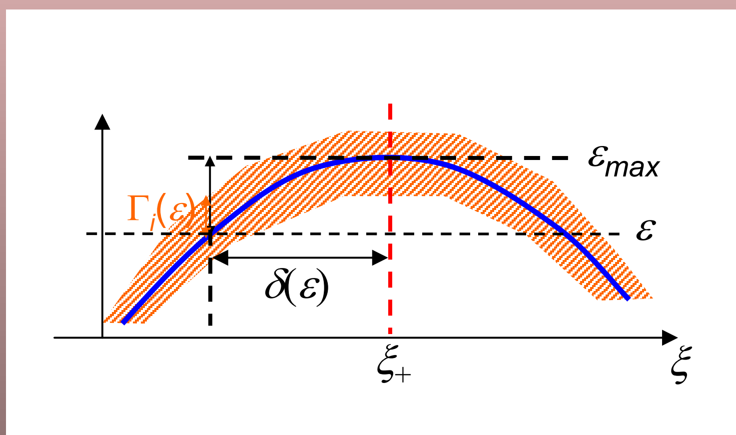
Localized vs band-like impurity states, group expansion analysis

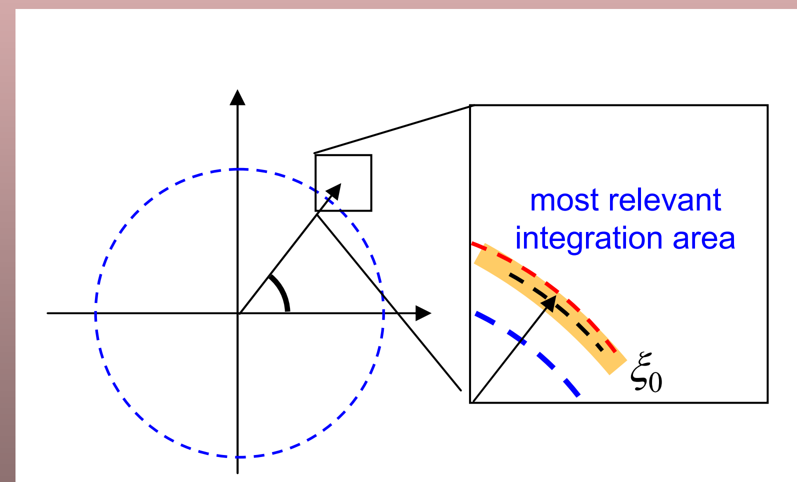
To simplify calculation of $\Gamma_i(\varepsilon)$, fix the energy argument in the numerators of T-matrix and A-matrices at ε_0, getting their forms:

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

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

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





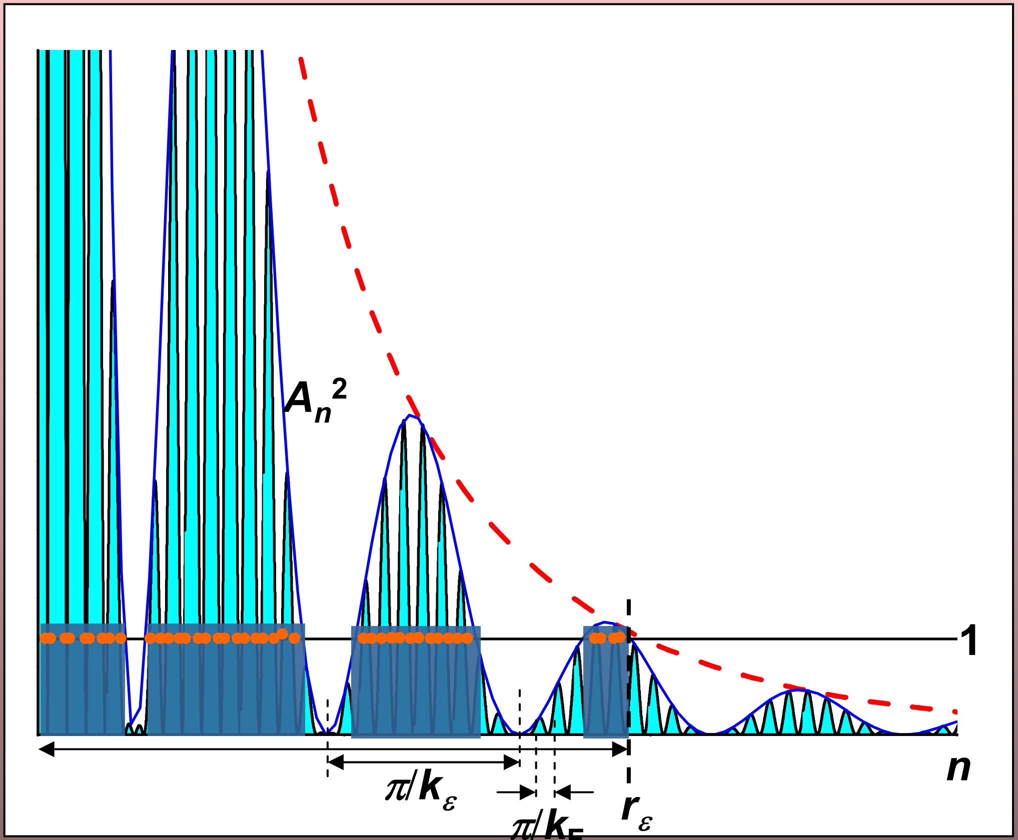
$$D_\xi(\varepsilon) \approx (\xi - \xi_+)^2 - \delta^2(\varepsilon)$$

The interaction matrix depends on the distance n between impurities as

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

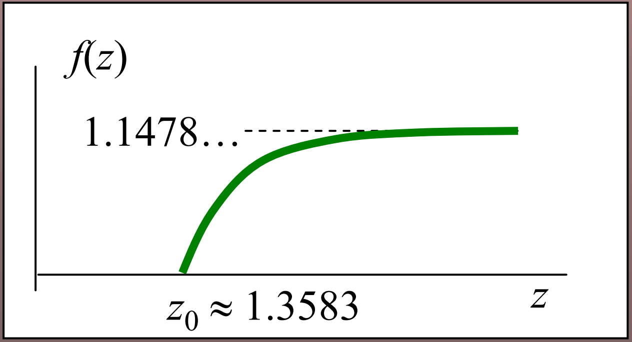
$$r_\varepsilon \approx \frac{2\pi}{k_{\mathrm{F}}}\left[\varepsilon_0 \rho_{\mathrm{F}} \frac{\Delta + \varepsilon_0}{c\delta(\varepsilon)}\right]^2,$$

$$k_\varepsilon \approx \delta(\varepsilon)/\hbar v_{\mathrm{F}}$$



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

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

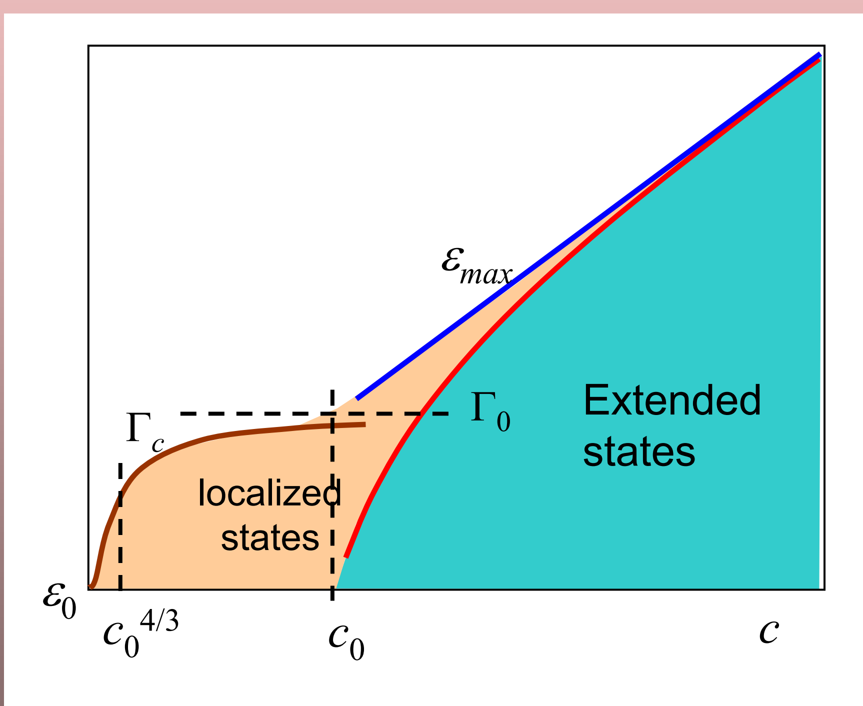
But since $f(k_\varepsilon r_\varepsilon)$ vanishes at $k_\varepsilon r_\varepsilon < z_0$, the broadening by the pair term at $c > c_0$ is even smaller:

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

Otherwise, for c ♎ 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

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

$$R_\varepsilon = \frac{2\pi}{k_\mathrm{F}}\left(\frac{\varepsilon_0}{|\varepsilon-\varepsilon_0|}\right)^2, \qquad r_0 = \frac{2\varepsilon_\mathrm{F}}{\xi_0 k_\mathrm{F}}.$$



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:

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

For $c = 0$, the unperturbed value:

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

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

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

$$\int_{\Delta_c}^{\varepsilon_D} \frac{d\varepsilon}{(\varepsilon - \varepsilon_0)^2 \sqrt{\Delta_c^{\,2} - \varepsilon^2}} \approx \frac{1}{\Delta_c^{\,2}} F\left(\frac{\Delta_c}{\varepsilon_0}\right), \qquad F(z) = z \frac{\sqrt{z^2 - 1} + z \arccos(-1/z)}{\left(z^2 - 1\right)^{3/2}}.$$

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:

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

implies Δ to vanish at

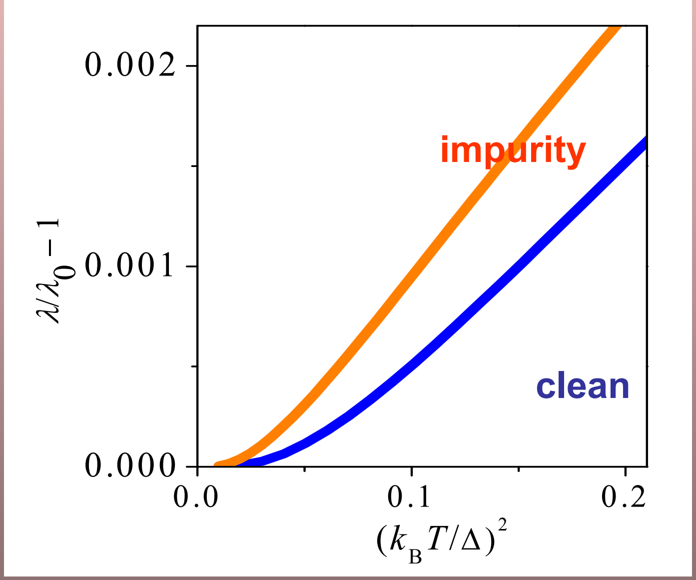
$$c\to c_1\frac{1+v^2}{1+v^2F\left[\sqrt{1+v}\left(1+c/c_1\right)\right]},$$

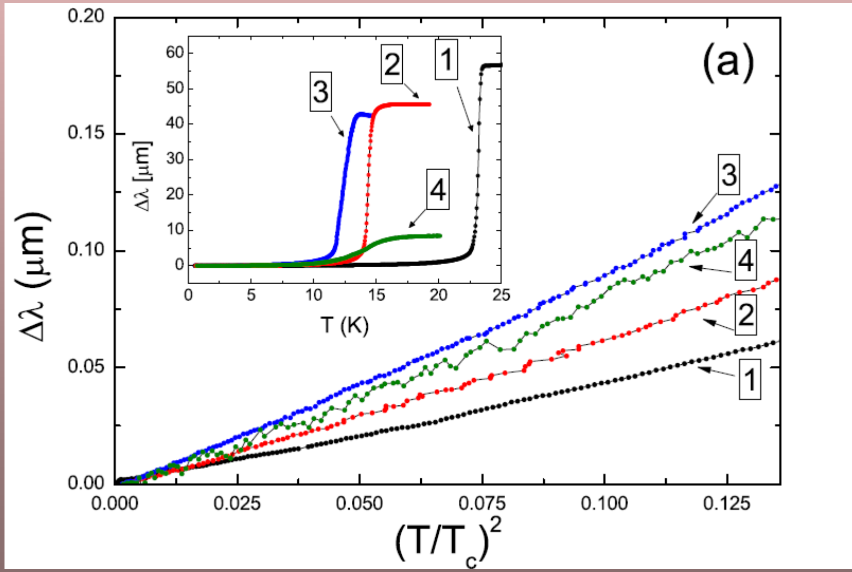
though such concentration is rather too high for the used approximations (of narrow impurity band *vs* gap parameter itself).

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).

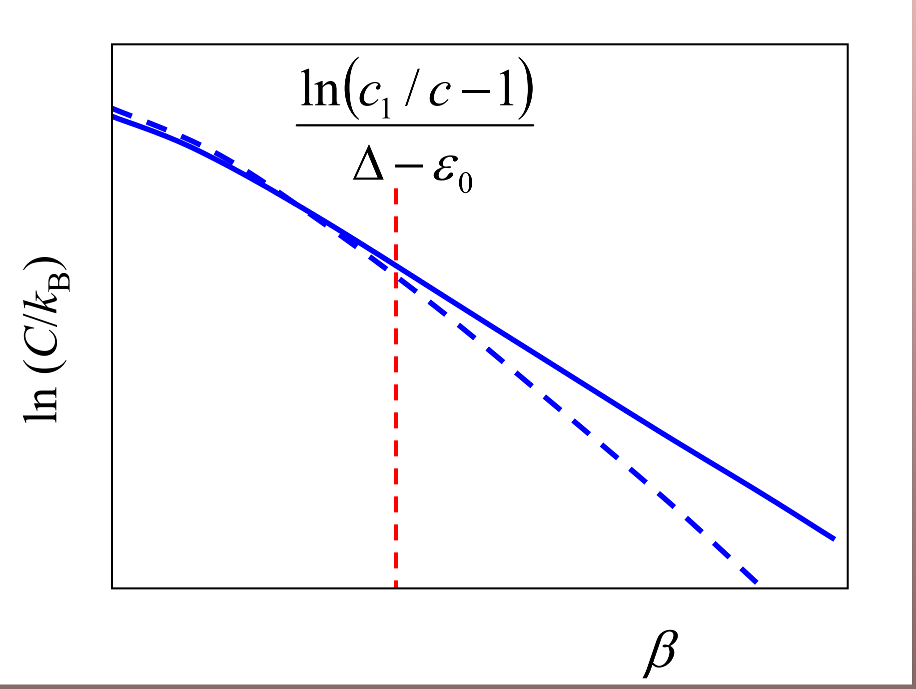
Impurity effect on the electronic specific heat in the SC state also follows from its contribution to DOS:

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

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:

$$\sigma(\omega,T)=\frac{e^2}{\pi\omega}\int d\varepsilon\left[f(\varepsilon,T)-f(\varepsilon',T)\right]$$

$$\times\int d\boldsymbol{k}v_x(\boldsymbol{k},\varepsilon)v_x(\boldsymbol{k},\varepsilon')\mathrm{Tr}\left[\mathrm{Im}\hat{G}_{\boldsymbol{k}}(\varepsilon)\right]\left[\mathrm{Im}\hat{G}_{\boldsymbol{k}}(\varepsilon')\right]$$

with the Fermi occupation function: $f(\varepsilon,T)=\left(\mathrm{e}^{\varepsilon/k_\mathrm{B}T}+1\right)^{-1},$

energy shift: $\varepsilon'=\varepsilon-\hbar\omega,$

and the generalized velocity function:

$$\boldsymbol{v}(\boldsymbol{k},\varepsilon)=\frac{\nabla_{\boldsymbol{k}}\,\mathrm{Re}\,D_{\boldsymbol{k}}(\varepsilon)}{\hbar\partial\,\mathrm{Re}\,D_{\boldsymbol{k}}(\varepsilon)/\partial\varepsilon},$$

that coincides with common subband velocities along the corresponding dispersion laws:

$$\boldsymbol{v}\left(\boldsymbol{k},\varepsilon_j(\boldsymbol{k})\right)=\hbar^{-1}\nabla_{\boldsymbol{k}}\varepsilon_j(\boldsymbol{k})=\boldsymbol{v}_j(\boldsymbol{k}).$$

j = *b*, *i*

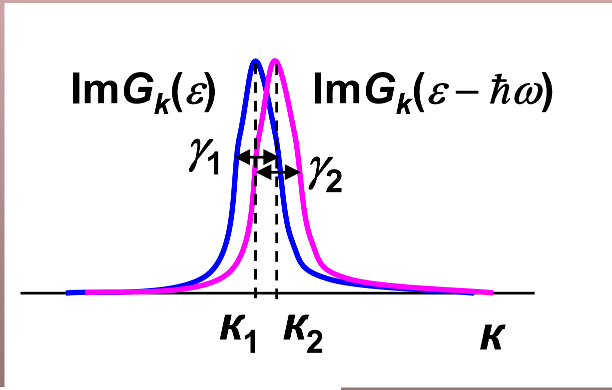
Unlike those in thermodynamics, this impurity effect is only due to the band-like states, with well defined velocities, Practical calculation of this formula is done through a decomposition by the most relevant trace of the matrix product Im$G_k(\varepsilon)$ Im$G_k(\varepsilon - \hbar\omega)$ in a sum of sharp peaks in quasimomentum over all the subbands:

$$\mathrm{Tr}\left[\mathrm{Im}\hat{G}_{\boldsymbol{k}}(\varepsilon)\right]\left[\mathrm{Im}\hat{G}_{\boldsymbol{k}}(\varepsilon')\right] = 2\sum_j \frac{\xi^2 + z^2}{\xi - \xi_j}\prod_{j'\neq j}\frac{1}{\xi_{j'} - \xi_j},$$

with ξ_j being the roots of

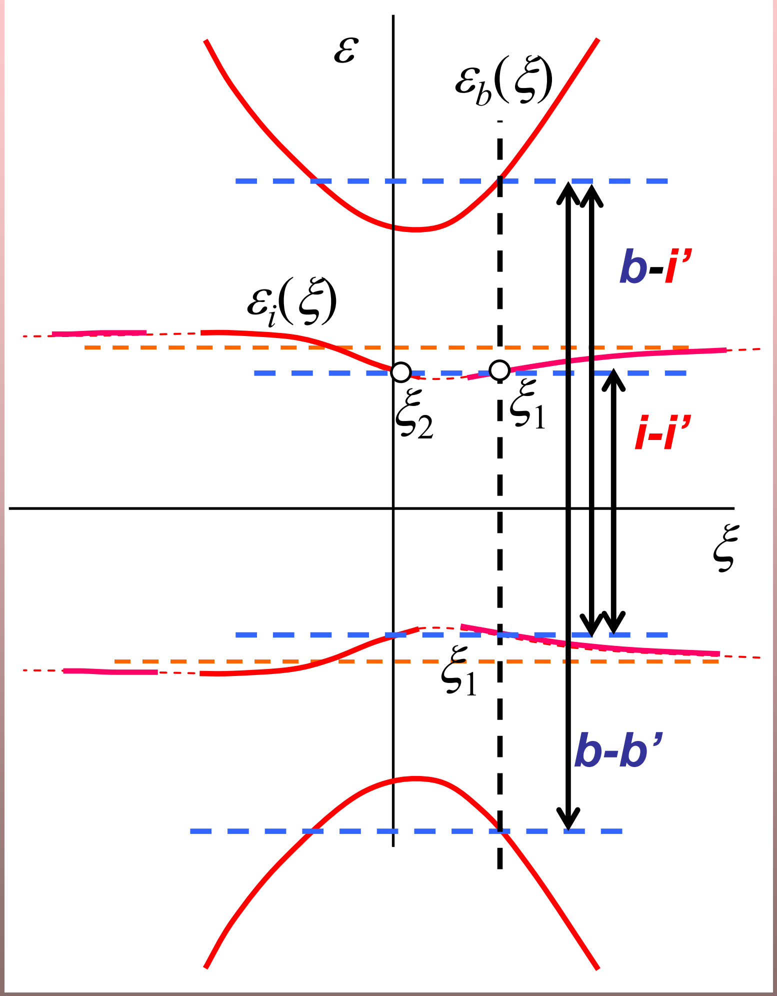
$$D_{\boldsymbol{k}}(\varepsilon) = \varepsilon^2 - \xi^2 - \Delta^2 - 2c\gamma^2\frac{\varepsilon^2 - \varepsilon_0\xi}{\varepsilon^2 - \varepsilon_0^{\,2}} \quad \text{and} \quad z^2 = \Delta^2 - \varepsilon^2\left(1 - \frac{c\gamma^2}{\varepsilon^2 - \varepsilon_0^{\,2}}\right).$$

Main contributions to the quasimomentum integral come from coinciding peaks of Im$G_k(\varepsilon)$ and Im$G_k(\varepsilon')$ (within to their widths), as seen from the simple Lorentzian approximation:

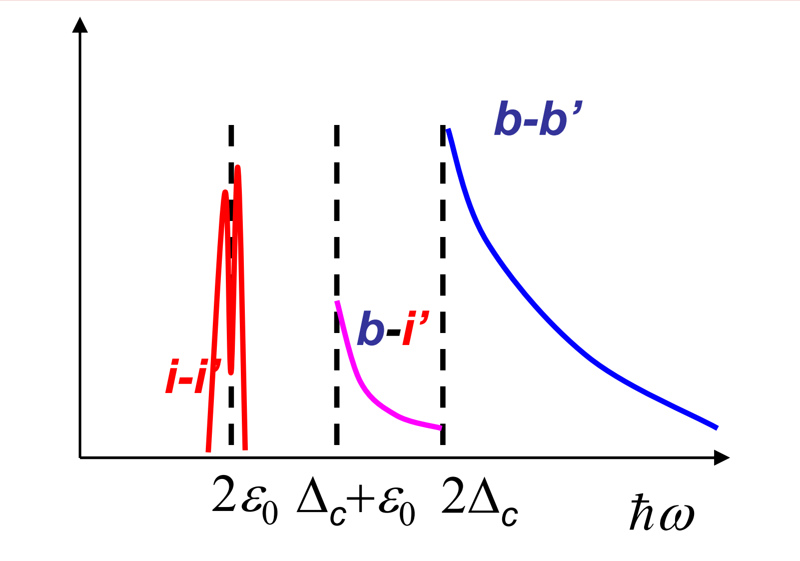


$$\int dk \frac{\gamma_1\gamma_2}{\left[(k-k_1)^2 + \gamma_1^{\,2}\right]\left[(k-k_2)^2 + \gamma_2^{\,2}\right]} = \frac{\pi(\gamma_1+\gamma_2)}{(k_1-k_2)^2 + (\gamma_1+\gamma_2)^2}.$$

For given band structure, 3 types of coinciding momenta in different subbands and corresponding contributions to optical conductivity are possible:



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

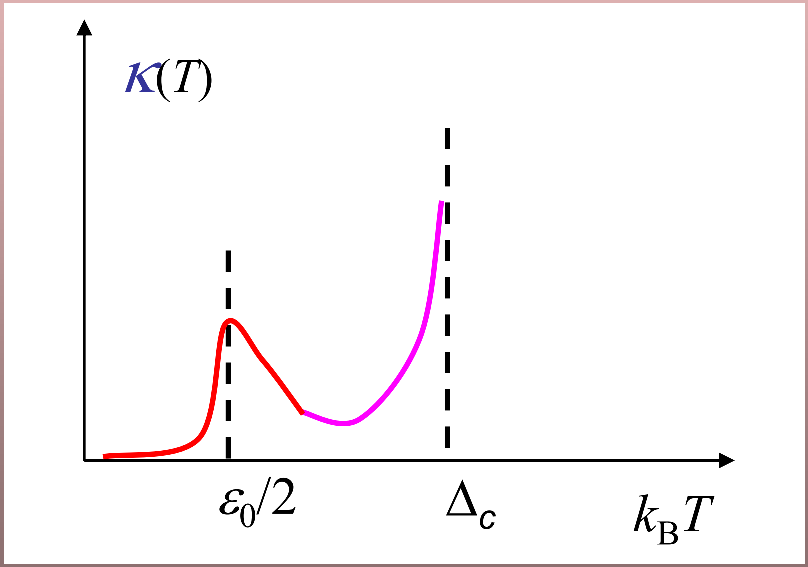


At low temperatures, a special interest may pertain to the narrow *i-i'* peak, for instance, as permitting a narrow-band resonance element in the Terahertz range.

Another type of impurity kinetic effects emerges in d.c. transport characteristics, as the heat conductivity, by the corresponding Kubo-Greenwood formula:

$$\kappa(T) = \frac{\hbar}{\pi}\int d\varepsilon \frac{\partial f(\varepsilon,T)}{\partial\varepsilon}\varepsilon^2 \int d\boldsymbol{k} v_x(\boldsymbol{k},\varepsilon)^2 \mathrm{Tr}\left[\mathrm{Im}\hat{G}_{\boldsymbol{k}}(\varepsilon)\right]^2 .$$

Here the energy integration of the coinciding peaks within the narrow impurity band produces an additional contribution to $\kappa(T)$ that attains maximum at temperatures about $\varepsilon_0/2k_B$, and, unlike the before mentioned impurity effect in the specific heat, is only possible at impurity concentrations above the critical value c_0.



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