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Multiband quasi-1D systems as high-temperature mean field superconductors

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Outline

- Introduction: multiband quasi-1D (Q1D) superconductors
- Minimal model: mean-field and fluctuation-shifted critical temperatures
- Results: multiband fluctuation ``screening” at the Lifshitz transition
- Conclusions

Introduction

It is well-known that the **off-diagonal long range order** is not possible in 1D

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This means that the **spontaneous breakdown of the continuous symmetry** does not take place for 1D case (including the breakdown of $U(1)$ symmetry, associated with the superconducting order parameter).

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In other words, fluctuations **fully suppress superconductivity** in 1D

The superconducting state **can still be achieved** when several 1D structures (parallel chains of molecules or atoms) are coupled one to another [see e.g. K. B. Efetov and A. I. Larkin, Sov. Phys. JETP **39**, 1129 (1974); L. P. Gor'kov L. P. and I. E. Dzyaloshinskii I. E., Sov. Phys. JETP **40**, 198 (1975)]

However, such Q1D superconductors are still affected by strong fluctuations diminishing the coherence temperature.

Material	T_C (K)	p_{ext} (kbar)
$(TMTSF)_2SbF_6$	0.36	10.5
$(TMTSF)_2PF_6$	1.1	6.5
$(TMTSF)_2AsF_6$	1.1	9.5
$(TMTSF)_2ReO_4$	1.2	9.5
$(TMTSF)_2TaF_6$	1.35	11
$(TMTTF)_2Br$	0.8	26

These predictions were confirmed by the discovery of the **low-temperature superconductivity in Fabre and Bechgaard salts** - organic Q1D superconductors

Bechgaard salts are derived from tetramethyltetraselenafulvalene (TMTSF)

Subsequent theoretical efforts were focused on finding the conditions under which **the critical temperature of the Q1D superconductors could be increased** rather than reduced.

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It was suggested that such an increase can be achieved in the vicinity of the **Lifshitz transition** near the edge of the Q1D single-particle energy band. [See e.g. A. Perali, A. Bianconi, A. Lanzara, N. L. Saini, Solid State Commun. **100**, 181 (1996); A. Bianconi, A. Valletta, A. Perali, N. L. Saini, Solid State Commun. **102**, 369 (1997); A. A. S. and M. D. Croitoru, Phys. Rev. B **73**, 012510 (2006); A. A. S., M. D. Croitoru, A. Vagov, and F. M. Peeters, Phys. Rev. B **82**, 104524 (2010).]

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However, the fluctuations, that are already very large in the presence of the Q1D effects, are additionally enhanced due to the Bose-like character of the pairing.

The enhancement of T_c was found for weakly interacting stripes, formed due to a particular transformation of the antiferromagnetic insulator. [S. A. Kivelson, E. Fradkin, and V. J. Emery, Nature **393**, 550 (1998); E. Arrigoni, E. Fradkin, and S. A. Kivelson, Phys. Rev. B **69**, 214519 (2004).]

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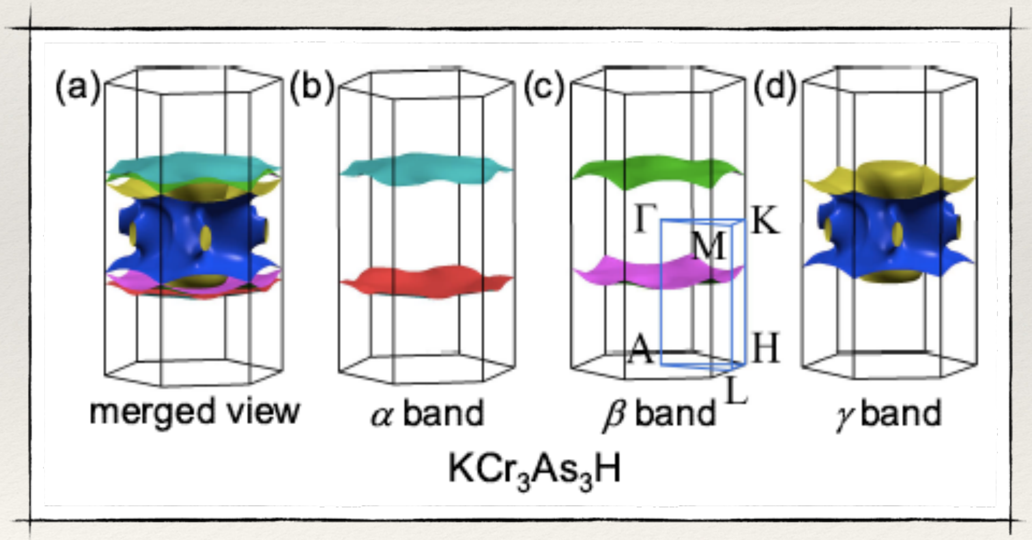
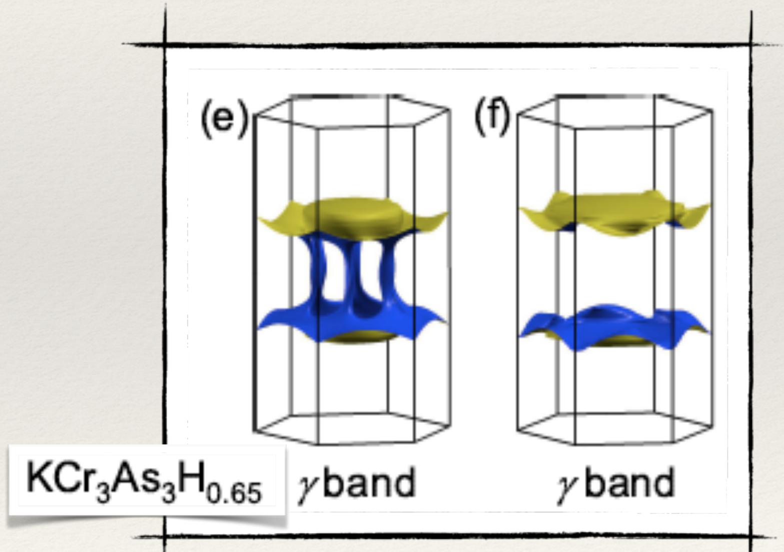
The effect requires, however, a **subtle balance** of different interplaying physical mechanisms, relevant for superconducting cuprates.

Recently the interest in Q1D superconductors has been boosted by the discovery of Cr_3As_3 -chain based materials. [J.-K Bao et al. , Phys. Rev. X **5**, 011013 (2015); Z.-T. Tang et al., Phys. Rev. B **91**, 020506 (2015); Z.-T. Tang et al., Sci. China Mater. **58**, 16 (2015); H. Jiang et al., Scientific Reports **5**, 16054 (2015)S.-Q. Wu et al., Phys. Rev. B **100**, 155108 (2019).]

First-principle calculations demonstrate that these superconductors are **multiband materials, where the quasi-1D bands coexist with conventional 3D bands**



Fermi surface

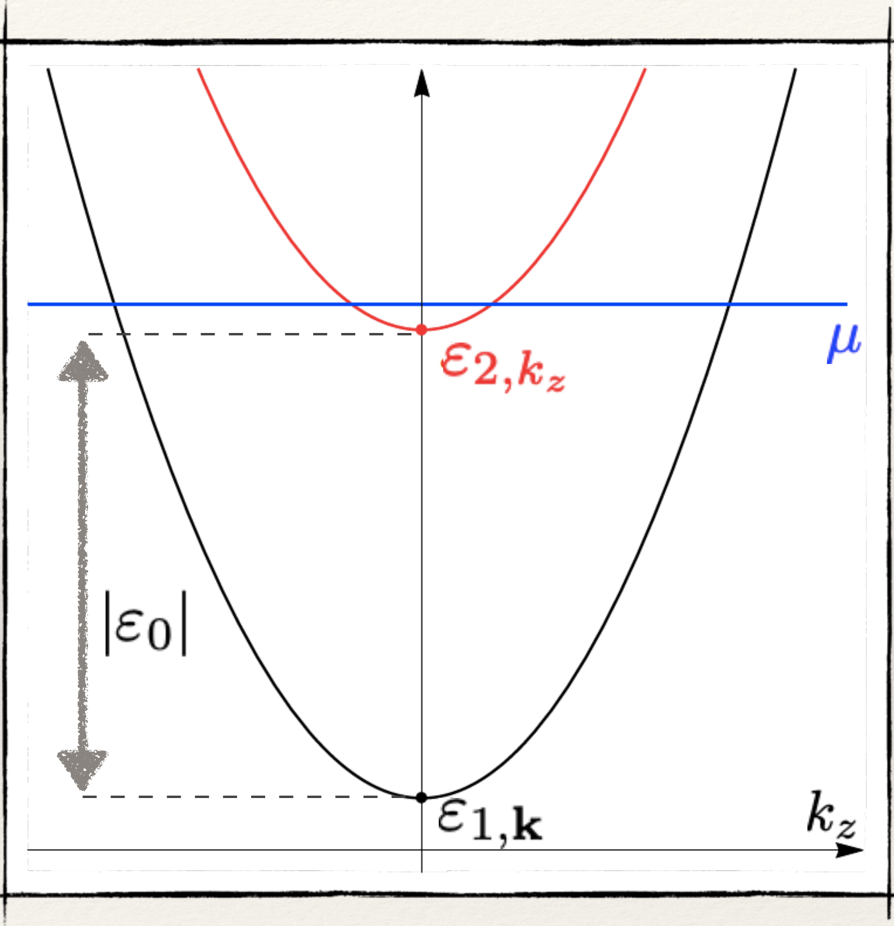


Fermi surface of γ-band: Lifshitz transition by changing the H-intercalation

How coupling to the stable 3D condensate changes the properties of Q1D condensate? Can it stabilize the system near the Lifshitz transition?

Minimal model and formalism

- We consider a **two-band** superconductor with **Q1D** and **3D** contributing bands
- The s-wave pairing is assumed for in both Q1D and 3D bands, coupled via the **Josephson-like interband transfer** of Cooper pairs.
- The intraband and interband pair-exchange couplings are determined by the **real matrix** $\check{g}$, with the elements $g_{\nu\nu'} = g_{\nu'\nu}$ $(\nu, \nu' = 1{,}2)$.
- For simplicity we consider the **parabolic single-particle dispersion** in both bands; the Fermi surface of the 3D band $\nu = 1$ is spherically symmetric. The principal axis of the Q1D band $\nu = 2$ is parallel to the z-axis.
- The system is in the **clean limit**



In the x and y directions the Q1D energy dispersion is **degenerate** and we assume the effective finite integral of the density of states (DOS) for both directions:

$$\varepsilon_{1,\mathbf{k}} = \varepsilon_0 + \frac{\hbar^2 \mathbf{k}^2}{2m_1}, \quad \varepsilon_{2,k_z} = \frac{\hbar^2 k_z^2}{2m_2}$$

Lower-edge energy of the 3D band $\varepsilon_0 < 0$

$m_{1,2}$ are the effective masses and $\mathbf{k} = (k_x, k_y, k_z)$, the energies and the chemical potential μ are **measured relative to the bottom of the Q1D band**. Our study is focused on the superconducting state near the Lifshitz transition at $\mu = 0$.To have a BCS-like condensate in the 3D band, we assume that $|\varepsilon_0|$ is much larger than the characteristic pairing energy in the 3D band.

The **mean-field Hamiltonian**, introduced by H. Suhl with coauthors and independently by V. A. Moskalenko, reads

$$\mathcal{H} = \int \mathrm{d}^3\mathbf{r} \Big\{ \sum_{\nu=1,2} \Big[\sum_{\sigma} \hat{\psi}^{\dagger}_{\nu\sigma}(\mathbf{r})\, T_\nu(\mathbf{r})\, \hat{\psi}_{\nu\sigma}(\mathbf{r}) + \big(\hat{\psi}^{\dagger}_{\nu\uparrow}(\mathbf{r}) \hat{\psi}^{\dagger}_{\nu\downarrow}(\mathbf{r})\, \Delta_\nu(\mathbf{r}) + \mathrm{h.c.} \big) \Big] + \langle \vec{\Delta}, \check{g}^{-1} \vec{\Delta} \rangle \Big\}$$

$T_\nu(\mathbf{r})$ - the single-particle Hamiltonian, $\Delta_\nu(\mathbf{r})$ - the band-dependent superconducting gap function; $\check{g}^{-1}$ - the inverse coupling matrix; $\overrightarrow{\Delta} = (\Delta_1, \Delta_2)^T$ and $\langle , \rangle$ - the scalar product of vectors in the band space.

Self-consistency requires

$$\vec{\Delta} = \check{g}\vec{R} \quad \rightarrow \quad \begin{pmatrix} \Delta_1 \\ \Delta_2 \end{pmatrix} = \begin{pmatrix} g_{11} & g_{12} \\ g_{12} & g_{22} \end{pmatrix} \begin{pmatrix} R_1 \\ R_2 \end{pmatrix}$$

$$R_\nu = \langle \hat{\psi}_{\nu\uparrow}(\mathbf{r}) \hat{\psi}_{\nu\downarrow}(\mathbf{r}) \rangle$$

Two critical temperatures

Our strategy: the model based on the above equations is used to calculate and compare the mean-field critical temperature T_{c0} with the fluctuation-shifted critical temperature T_c:

(1) T_{c0} is obtained by solving the **linearized variant of the matrix gap equation** (self-consistency equation).

(2) Thermal fluctuations are investigated by using the expansion for the **free energy functional** for the two-band system with respect to the band superconducting gap functions, which essentially gives the two-band Ginzburg-Landau free energy functional.

When $T_c \approx T_{c0}$ - thermal fluctuations are insignificant

If $T_c \ll T_{c0}$ - thermal fluctuations suppress the coherence

To calculate both T_{c0} and T_c, we employ the **expansion**

$$R_\nu[\Delta_\nu] = (\mathcal{A}_\nu - a_\nu)\Delta_\nu - b_\nu \Delta_\nu |\Delta_\nu|^2 + \sum_{i=x,y,z} \mathcal{K}_\nu^{(i)} \nabla_i^2 \Delta_\nu$$

$$\mathcal{A}_\nu,\ a_\nu,\ b_\nu,\ K_\nu^{(i=x,y,z)}$$

depend on the microscopic model

For **3D band**

$$\mathcal{A}_1 = N_1 \ln\left(\frac{2e^\gamma \hbar\omega_c}{\pi T_{c0}}\right),\ a_1 = -\tau N_1,\ b_1 = \frac{7\zeta(3)}{8\pi^2}\frac{N_1}{T_{c0}^2}, \mathcal{K}_1^{(x)} = \mathcal{K}_1^{(y)} = \mathcal{K}_1^{(z)} = \frac{\hbar^2 v_1^2}{6} b_1,$$

with $\tau = 1 - T/T_{c0}$, $N_1 = m_1 k_F / 2\pi^2\hbar^2$ - 3D DOS, ω_c - the cut-off frequency, γ - the Euler constant, and $v_1 = \hbar k_F / m_1$ - the Fermi velocity in 3D band.

For **Q1D band** the coefficients are given by integrals and can be calculated only numerically. For $|\mu| < \hbar\omega_c$ one gets

$$\mathcal{A}_2 = N_2 \int_{-\tilde{\mu}}^{1} \mathrm{d}y \, \frac{\tanh\left(y/2\tilde{T}_{c0}\right)}{y\sqrt{y+\tilde{\mu}}}, \; a_2 = -\tau \frac{N_2}{2\tilde{T}_{c0}} \int_{-\tilde{\mu}}^{1} \mathrm{d}y \, \frac{\mathrm{sech}^2\left(y/2\tilde{T}_{c0}\right)}{\sqrt{y+\tilde{\mu}}},$$

$$b_2 = \frac{N_2}{4\hbar^2\omega_c^2} \int_{-\tilde{\mu}}^{1} \mathrm{d}y \, \frac{\mathrm{sech}^2\left(y/2\tilde{T}_{c0}\right)}{y^3\sqrt{y+\tilde{\mu}}} \left[\sinh\left(\frac{y}{\tilde{T}_{c0}}\right) - \frac{y}{\tilde{T}_{c0}}\right],$$

$$\mathcal{K}_2^{(z)} = \hbar^2 v_2^2 \frac{N_2}{8\,\hbar^2\omega_c^2} \int_{-\tilde{\mu}}^{1} \mathrm{d}y \, \frac{\sqrt{y+\tilde{\mu}}}{y^3} \, \mathrm{sech}^2\left(y/2\tilde{T}_{c0}\right) \times \left[\sinh\left(\frac{y}{\tilde{T}_{c0}}\right) - \frac{y}{\tilde{T}_{c0}}\right], \quad \mathcal{K}_2^{(x,y)} = 0,$$

where $\tilde{T}_{c0} = T_{c0}/\hbar\omega_c$ and $\tilde{\mu} = \mu/\hbar\omega_c$; $v_2 = \sqrt{2\hbar\omega_c/m_2}$ - the characteristic velocity; and $N_2 = \sigma_{xy}/4\pi\hbar v_2$ - the 1D DOS at the cut-off energy, with the factor σ_{xy} accounting for the states in x and y directions.

Mean-field critical temperatures

The **linearized** matrix gap equation

$$\check{L}\vec{\Delta} = 0, \quad \check{L} = \check{g}^{-1} - \begin{pmatrix} \mathcal{A}_1 & 0 \\ 0 & \mathcal{A}_2 \end{pmatrix}.$$

The determinant of $\check{L}$ is zero:

$$(g_{22} - G\mathcal{A}_1)(g_{11} - G\mathcal{A}_2) - g_{12}^2 = 0$$

$$G = g_{11}g_{22} - g_{12}^2$$

$$\mathcal{A}_1 = \mathcal{A}_1(T_{c0})$$

$$\mathcal{A}_2 = \mathcal{A}_2(T_{c0})$$

T_{c0} - the solution

In addition, the linearized matrix gap equation yields

$$\check{L}\vec{\Delta} = 0, \quad \check{L} = \check{g}^{-1} - \begin{pmatrix} \mathcal{A}_1 & 0 \\ 0 & \mathcal{A}_2 \end{pmatrix}$$

$$\vec{\Delta} = \psi(\mathbf{r})\vec{\eta} \qquad \longleftarrow \qquad \check{L}\vec{\eta} = \check{L}\begin{pmatrix} \eta_1 \\ \eta_2 \end{pmatrix} = 0$$

$$\vec{\eta} = \begin{pmatrix} S \\ 1 \end{pmatrix}, \; S = \frac{g_{11} - G\mathcal{A}_2}{g_{12}}.$$

normalization is not necessary

$\check{L}$ and $\overrightarrow{\eta}$ are not position dependent; $\psi(\mathbf{r})$ controls the spatial profiles of both condensates (Landau order parameter) in the **mean-field approach immediately near the critical temperature**

$$\Delta_1(\mathbf{r}) \propto \Delta_2(\mathbf{r}) \propto \psi(\mathbf{r})$$

Fluctuation-shifted critical temperature

The actual critical temperature T_c is lower than T_{c0} due to fluctuations. The fluctuation-induced correction to T_{c0} is obtained by using the standard Gibbs distribution $e^{-F/T}$, with the free energy functional

$$F = \int d^3\mathbf{r}\Big[\sum_{\nu=1,2} f_\nu + \langle \vec{\Delta}, \check{L}\vec{\Delta}\rangle\Big],\; f_\nu = a_\nu\,|\Delta_\nu|^2 + \frac{b_\nu}{2}\,|\Delta_\nu|^4 + \sum_{i=x,y,z} \mathcal{K}_\nu^{(i)}\,|\nabla_i \Delta_\nu|^2 .$$

The stationary condition for this functional yields the matrix gap equation, discussed above.

Expansion

$$\vec{\Delta}(\mathbf{r}) = \psi(\mathbf{r})\vec{\eta} + \varphi(\mathbf{r})\vec{\xi}$$

$\varphi(\mathbf{r})$ - the second fluctuation mode

$$\langle \vec{\eta}, \vec{\xi}\rangle = 0 \qquad \vec{\eta} = (S,1)^T \;\; \vec{\xi} = (1,-S)^T$$

The free energy functional $\varphi(r)$ is then expressed in terms of ψ and φ as

$$F = \int d^3\mathbf{r}(f_\psi + f_\varphi + f_{\psi\varphi}),$$

where

$$f_\psi = a_\psi \left|\psi\right|^2 + \frac{b_\psi}{2} \left|\psi\right|^4 + \sum_{i=x,y,z} \mathcal{K}_\psi^{(i)} \left|\nabla_i \psi\right|^2$$

and

$$f_\varphi = a_\varphi \left|\varphi\right|^2 + \frac{b_\varphi}{2} \left|\varphi\right|^4 + \sum_{i=x,y,z} \mathcal{K}_\varphi^{(i)} \left|\nabla_i \varphi\right|^2$$

with $f_{\psi\varphi}$ the interaction between the two modes and the coefficients are averages over the contributing bands.

The dependence of the coefficients associated with the two fluctuations modes plays an important role and should be discussed in more details:

$$a_\psi = S^2 a_1 + a_2,\ b_\psi = S^4 b_1 + b_2,\ \mathcal{K}_\psi^{(i)} = S^2 \mathcal{K}_1^{(i)} + \mathcal{K}_2^{(i)},$$

$$a_\varphi = a_\varphi^{(0)} + a_1 + S^2 a_2,\ b_\varphi = b_1 + S^4 b_2,\ \mathcal{K}_\varphi^{(i)} = \mathcal{K}_1^{(i)} + S^2 \mathcal{K}_2^{(i)}.$$

↓

$$a_\varphi^{(0)} = \frac{(1+S^2)^2}{SGg_{12}} \neq 0\ (T \to T_{c0});\ a_1, a_2 \propto \tau \to 0\ (T \to T_{c0})$$

↓

The mode ψ is **critical** as its characteristic length is divergent, the mode φ is **not critical** as its lengths is finite, it gives only minor corrections to the contribution of thermal fluctuations.

The mode φ describes non-critical fluctuations and can be safely omitted, i.e.

$$F = \int d^3\mathbf{r} \left[a_\psi |\psi|^2 + \frac{b_\psi}{2} |\psi|^4 + \sum_{i=x,y,z} \mathcal{K}_\psi^{(i)} |\nabla_i \psi|^2 \right].$$

Coefficients in front of the spatial gradient term read

$$\mathcal{K}_\varphi^{(x)} = \mathcal{K}_1^{(x)},\ \mathcal{K}_\varphi^{(y)} = \mathcal{K}_1^{(y)},\ \mathcal{K}_\varphi^{(z)} = \mathcal{K}_1^{(z)} + S^2 \mathcal{K}_2^{(z)}.$$

We obtain that the thermal fluctuations of the two-band system, made of the Q1D and 3D bands, are controlled by the anisotropic single-component Ginzburg-Landau theory. The anisotropy axis is along the z-direction, the principal axis of the Q1D band.

For thermal fluctuations

$$\vec{\Delta}(\mathbf{r}) = \psi(\mathbf{r})\vec{\eta} + \varphi(\mathbf{r})\vec{\xi} \longrightarrow \begin{pmatrix} \Delta_1(\mathbf{r}) \\ \Delta_2(\mathbf{r}) \end{pmatrix} = \psi(\mathbf{r}) \begin{pmatrix} S \\ 1 \end{pmatrix}$$

$$\Delta_1(\mathbf{r}) = S\psi(\mathbf{r}),\ \Delta_2(\mathbf{r}) = \psi(\mathbf{r}).$$

Coupling to a stable 3D condensate gives rise to a single critical mode that controls the thermal fluctuations of the condensate gap functions Δ_1 and Δ_2. In other words **``light''** excitations of the Q1D condensate are always accompanied by **``heavy''** excitations of the stable 3D condensate. This is the **multiband fluctuation screening mechanism**.

L. Salasnich, A. A. S., A. Vagov, J. Albino Aguiar, and A. Perali, Phys. Rev. B **100**, 064510 (2019)

Using the **renormalization group** approach for single-component Ginzburg-Landau theory (e.g., see Larkin and Varlamov fluctuation textbook), one obtains

$$\frac{T_{c0}-T_c}{T_c}=\frac{8}{\pi}\sqrt{Gi},$$

with the Ginzburg number (or the Ginzburg-Levanyuk parameter)

$$Gi=\frac{1}{32\pi^2}\frac{T_{c0}b_\psi^2}{a'_\psi\mathcal{K}_\psi^{(x)}\mathcal{K}_\psi^{(y)}\mathcal{K}_\psi^{(z)}},$$

and $a'_\psi = da_\psi/dT$. Gi can be rewritten as

$$Gi=Gi_{3D}\frac{\left(b_2/b_1+S^4\right)^2}{\left(a_2/a_1+S^2\right)\left(\mathcal{K}_2^{(z)}/\mathcal{K}_1^{(z)}+S^2\right)S^4}.$$

Gi_{3D} - the Ginzburg number for standalone 3D band

The scheme of calculations

$$T_{c0}$$

↓

$$\mathcal{A}_2(T_{c0}),\ S = (g_{11} - G\mathcal{A}_2)/g_{12}$$

↓

$$a_\psi = S^2 a_1 + a_2,\ b_\psi = S^4 b_1 + b_2,\ \mathcal{K}_\psi^{(i)} = S^2 \mathcal{K}_1^{(i)} + \mathcal{K}_2^{(i)}$$

↓

$$Gi,\ T_c$$

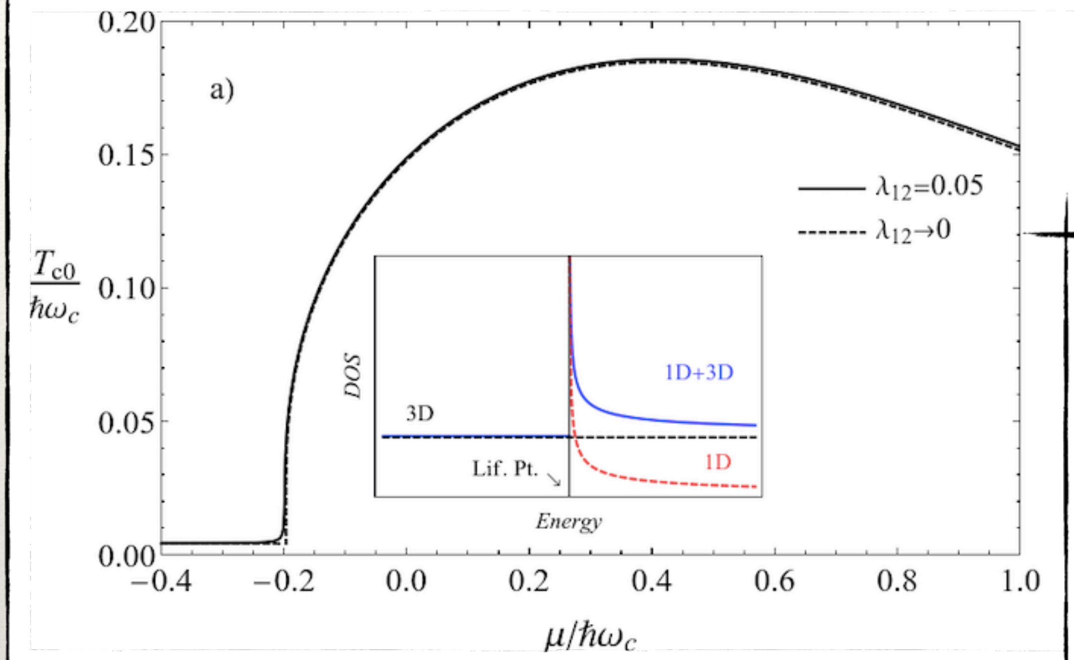
Relevant parameters

Essential parameters of the model are the couplings $g_{11}, g_{22}, g_{12} = g_{21}$ and the DOSs N_1 and N_2, while the cutoff $\hbar\omega_c$ sets the energy scale. Below it is convenient to introduce the dimensionless coupling constants $\lambda_{\nu\nu'} = g_{\nu\nu'}\sqrt{N_\nu N_{\nu'}}$ (Q1D -band 2, 3D -band 1).

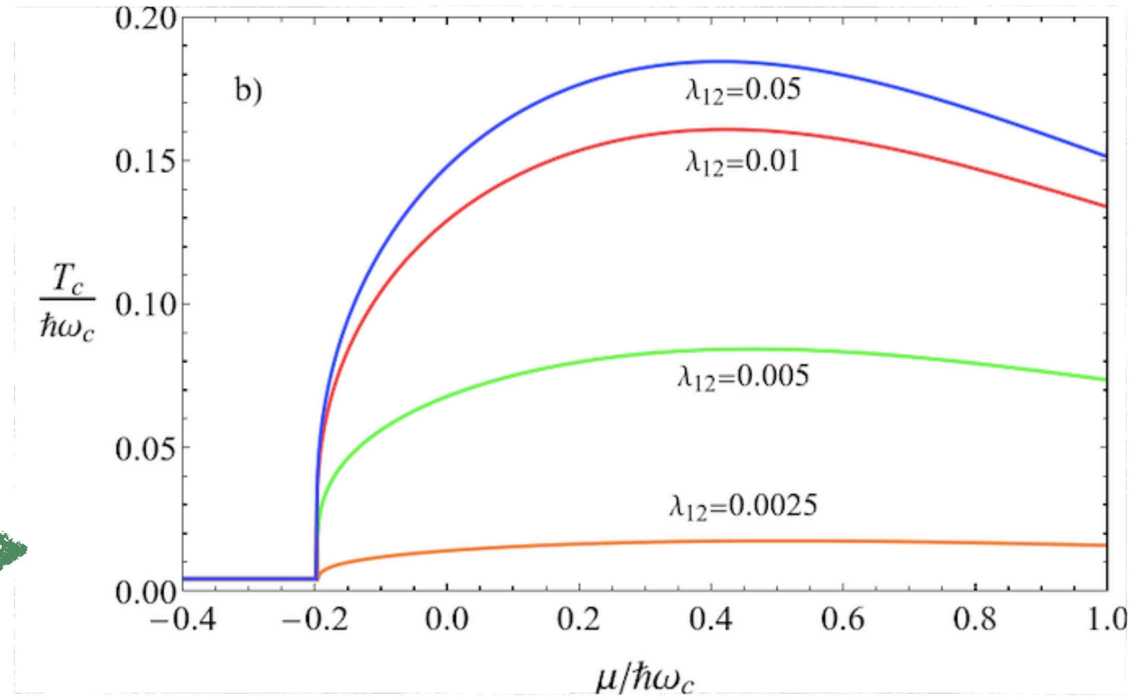
The parameter S, which controls T_{c0} , depends on $\lambda_{11}, \lambda_{22}, \lambda_{12}$ and on the DOSs ratio N_1/N_2 (the latter is 1 for simplicity). The interband pair-exchange coupling λ_{12} is considered as a variable. For intraband couplings we assume $\lambda_{22} = 0.2$, $\lambda_{11} = 0.18$ (standalone 3D band is active) and $\lambda_{22} = 0.2$, $\lambda_{11} = -0.05$ (standalone 3D band is passive).

The fluctuation-shifted T_c depends on S and Gi_{3D}. To find Gi_{3D} one needs to choose N_1. However, we follow a different path and use an estimate $Gi_{3D} \sim 10^{-10}$. Recall, that the Ginzburg number of most conventional 3D superconductors is in the range $10^{-6} \div 10^{-16}$, see Ketterson and Song textbook.

Results $\lambda_{11} = 0.18, \lambda_{22} = 0.2$

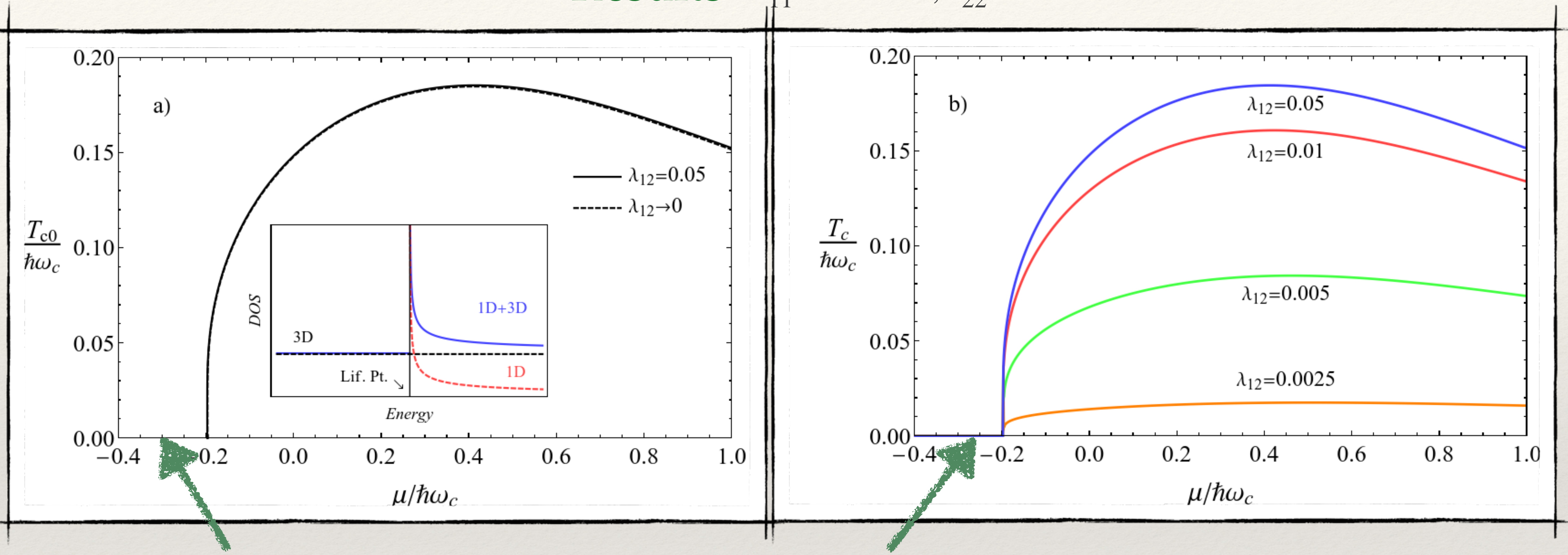


Mean-field near the Lifshitz transition



Fluctuation driven critical temperature near the Lifshitz transition; taking $\hbar\omega_c \approx 400\,\mathrm{K}$ (like in Al), one obtains $T_{c,max} \approx 70\,\mathrm{K}$

Results $\lambda_{11} = -0.05, \lambda_{22} = 0.2$



quasi-1D band does not contribute - superconductivity disappears due to the passive 3D band

Results are almost the same as previously for the active 3D band: the critical temperature is mainly controlled by quasi-1D band; fluctuation "screening" takes place even in the presence of the passive 3D band.

Conclusions

- Our calculations demonstrate that coupling to a stable 3D condensate ``screens" out the severe thermal Q1D fluctuations.
- The ``screening” is so effective that even in the vicinity of the Lifshitz transition (the chemical potential is near the edge of the Q1D band) the system is a mean-field high-T_c superconductor.
- The thermal fluctuations are suppressed at very small intraband pair-exchange couplings, i.e. almost for nearly decoupled bands.
- The results are not sensitive to the character of the 3D band: it can be passive so that the condensate appears there only due to Josephson-like coupling between bands.
- Our results are obtained for the s-wave pairing but they hold also for d-wave symmetry. We also expect a similar scenario of ``screening” in the presence of the triplet superconductivity, as well (related investigations are underway).

Thank you for your attention