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High-T_c Multiband Superconductors with a Quasi-1D and a 3D Bands

Tiago T. Saraiva

tteixeirasaraiva@hse.ru
https://www.hse.ru/en/staff/tiago

Moscow Institute of Mathematics and Electronics
Higher School of Economics (Moscow)

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Thanks to my coauthors!

Please check our current version of this work at:

arXiv.org > cond-mat > arXiv:2002.01989

Condensed Matter > Superconductivity

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Quasi-one-dimensional system as a high-temperature superconductor

T. T. Saraiva, P. J. F. Cavalcanti, A. Vagov, A. S. Vasenko, A. Perali, L. Dell'Anna, A. A. Shanenko

Recently, the discovery of Cr_2As_3-chains and organic compounds such as potassium-doped p-terphenyl ($K_xC_{18}H_{14}$) have raised the attention of our community due to intriguing experimental results, showing high superconducting critical temperatures (up to 120K).

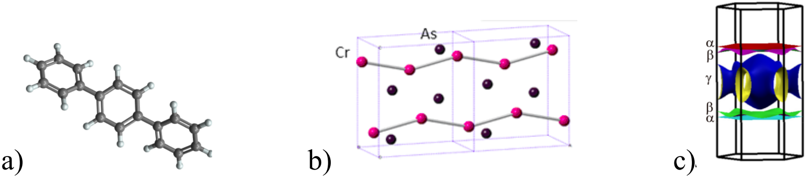

Figure: Molecular structures of the a) p-terphenyl and b) Cr_2As_3 chains. c) Fermi surfaces of Cr_2As_3 with quasi-1D and 3D Fermi sheets [PRB **92**, 104511 (2015)].

Multiband Sytems

Consider the multiband system with two gaps given in terms of the anomalous averages [PRL **3**, 12 (1959)]

$$\Delta_i = \sum_{j=1}^{2} g_{ij} \left\langle \psi_{\downarrow j} \psi_{\uparrow j} \right\rangle , \tag{1}$$

where $i = 1, 2$. The coupling matrix g is considered symmetric. The gap expansion is given in terms of the band-dependent unperturbed Green functions:

$$\mathcal{G}^{(0)}_{\omega i}(\vec{x}, \vec{y}) = \int \frac{d^3 k}{2\pi} \frac{\exp[-i\vec{k} \cdot (\vec{x} - \vec{y})]}{i\hbar\omega - \xi_{ki}} \tag{2}$$

and $\bar{\mathcal{G}}^{(0)}_{\omega i}(\vec{x}, \vec{y}) = -\mathcal{G}^{(0)}_{-\omega i}(\vec{y}, \vec{x})$. They are dependent on the fermionic Matsubara frequencies $\omega_n = \pi T(2n+1)/\hbar$ (in our notation $k_b = 1$).

Dispersion Relations

The strongest band (labeled $i = 1$) has quasi-1D Fermi surfaces, in such a way that the dispersion relation has very large effective electronic masses in two directions, say, $m_y, m_z \gg m_x$, in such a way that one can approximate:

$$\xi_{k1} = \sum_{l=x,y,z} \frac{\hbar^2 k_l^2}{2m_l} - \mu \approx \frac{\hbar^2 k_x^2}{2m_x} - \mu. \tag{3}$$

The weaker band (labeled $i = 2$) is the usual 3D band:

$$\xi_{k2} = \frac{\hbar^2 k^2}{2m} - \mu. \tag{4}$$

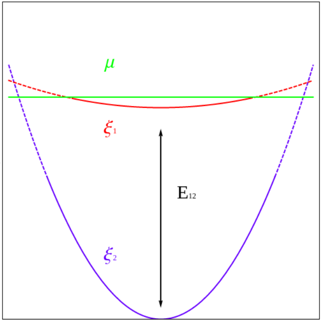

Figure: Sketch of the band-dependent single-electron energies ξ_1 and ξ_2 as function of the momentum.

The Gorkov equations produce the following expansion for the gap in terms of $\mathcal{G}^{(0)}_{\omega i}$ and $\bar{\mathcal{G}}^{(0)}_{\omega i}$ [PRB **85**, 014502 (2012)]:

$$\sum_j \gamma_{ij}\Delta_j(\vec{x}) = \int d^3y K_{ai}(\vec{x},\vec{y})\Delta_i(\vec{y}) + \int \prod_{l=1}^{3} d^3y_l K_{bi}(\vec{x},\vec{y}_1,\vec{y}_2,\vec{y}_3)\Delta_i(\vec{y}_1)\bar{\Delta}_i(\vec{y}_2)\Delta_i(\vec{y}_3) + ..., \quad (5)$$

where $\gamma = g^{-1}$ and we have defined the kernels

$$K_{ai}(\vec{x},\vec{y}) = -gT\sum_\omega \mathcal{G}^{(0)}_{\omega i}(\vec{x},\vec{y})\bar{\mathcal{G}}^{(0)}_{\omega i}(\vec{y},\vec{x}), \quad (6)$$

$$K_{bi}(\vec{x},\vec{y}_1,\vec{y}_2,\vec{y}_3) = -gT\sum_\omega \mathcal{G}^{(0)}_{\omega i}(\vec{x},\vec{y}_1)\bar{\mathcal{G}}^{(0)}_{\omega i}(\vec{y}_1,\vec{y}_2)\times \times \mathcal{G}^{(0)}_{\omega i}(\vec{y}_2,\vec{y}_3)\bar{\mathcal{G}}^{(0)}_{\omega i}(\vec{y}_3,\vec{x}) \quad (7)$$

Critical Temperature in the Uncoupled Regime

Let us start in the limit $g_{12} = 0$. In this case the so-called *mean-field critical temperature*, T_{c0}, can be obtained by neglecting spatial variations of the gaps and terms $\mathcal{O}(\Delta_i^3)$. The gap expansion becomes

$$-g_{ii} T \sum_{\omega} \int \mathrm{d}^3 z \frac{\mathrm{d}^3 k}{(2\pi)^3} \frac{\mathrm{d}^3 k'}{(2\pi)^3} \frac{\exp[-i(\vec{k} - \vec{k}') \cdot \vec{z}]}{(i\hbar\omega - \xi_{ki})(i\hbar\omega + \xi_{k'i})} = 1. \tag{8}$$

The 3D band produces the standard value for

$$\frac{T_{c0}}{\hbar\omega_c} = \frac{2e^{\Gamma}}{\pi} \exp[-1/g_{22} N_2(0)] \tag{9}$$

where $N_2(0) = mk_F/2\pi^2\hbar^2$ is the DOS at the Fermi level of band 2 and $\Gamma \approx 0.577$.

The equation for the q1D band results in:

$$\lambda_1 \int_0^{1+\tilde{\mu}} \mathrm{d}e \, \frac{\tanh[(e-\tilde{\mu})/(2\tilde{T}_{c0})]}{(e-\tilde{\mu})e^{1/2}} = 1, \tag{10}$$

where $\tilde{X} = X/\hbar\omega_c$ ($\hbar\omega_c$ is the cutoff energy) and

$$\lambda_1 = g_{11}N_1 = g_{11}\sigma^{(yz)}\sqrt{\frac{m_x}{32\pi^2\hbar^3\omega_c}}, \tag{11}$$

where it is defined the constant

$$\sigma^{(yz)} = \left(\int \frac{dk_y}{2\pi}\frac{dk_z}{2\pi}\right) \sim (a_y a_z)^{-1}, \tag{12}$$

the inverse product of the lattice parameters in the y and z directions, respectively.

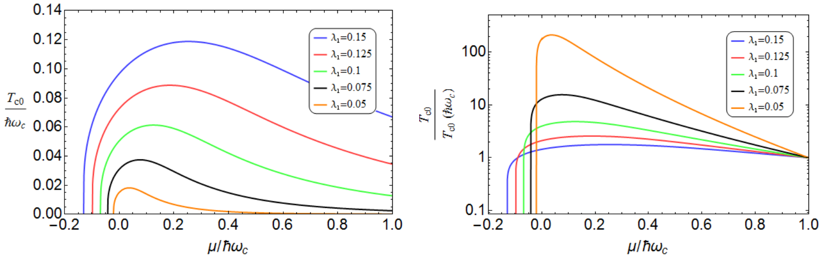

Figure: Left: plot of the mean-field critical temperature of the q1D system as function of the chemical potential (in units of $\hbar\omega_c$). Right: relative T_{c0} with respect to its value at the deep-band regime, $\mu = \hbar\omega_c$. Each contour line correspond to a different value of the dimensionless coupling, λ_1.

Ginzburg-Landau Coefficients

In order to include the effect of fluctuations of the gap, we need to calculate the GL coefficients for the q1D system. Expanding the gap in Taylor series,

$$\Delta_1(\vec{x}) \approx \int d^3z K_{a1}(\vec{z}) \left[\Delta_1(\vec{x}) + \frac{(\vec{z}\cdot\vec{\nabla})^2}{2}\Delta_1(\vec{x}) \right] + \\ + \Delta_1(\vec{x})^3 \int d^3y_1 d^3y_2 d^3y_3 K_{b1}(\vec{x}, \vec{y}_1, \vec{y}_2, \vec{y}_3) \tag{13}$$

$$\Rightarrow a_1 \Delta_1(\vec{x}) + b_1 \Delta_1(\vec{x})^3 - \mathcal{K}_1^{(x)} \partial_x^2 \Delta_1(\vec{x}) = 0 \tag{14}$$

In this case, $\mathcal{K}_1^{(y)} = \mathcal{K}_1^{(z)} \approx 0$.

$$a_1 = -\tau \frac{N_1}{2\tilde{T}_{c0}} \int\limits_0^{1+\tilde{\mu}} \frac{\mathrm{d}e}{e^{1/2}\left\{1+\cosh\left[\frac{(e-\tilde{\mu})}{\tilde{T}_c}\right]\right\}} \tag{15}$$

$$b_1 = \frac{N_1}{4\hbar^2\omega_c^2} \int\limits_0^{1+\tilde{\mu}} \mathrm{d}e \frac{\mathrm{sech}^2\left[(e-\tilde{\mu})/2\tilde{T}_{c0}\right]}{e^{1/2}(e-\tilde{\mu})^3} \times \left[\frac{e-\tilde{\mu}}{\tilde{T}_{c0}} - \sinh\left(\frac{e-\tilde{\mu}}{\tilde{T}_{c0}}\right)\right], \tag{16}$$

$$\mathcal{K}_1^{(x)} = \frac{\hbar^2}{m_x} \frac{N_1}{4\hbar^2\omega_c^2} \int\limits_0^{1+\tilde{\mu}} \mathrm{d}e\sqrt{e} \frac{\mathrm{sech}^2\left[(e-\tilde{\mu})/2\tilde{T}_{c0}\right]}{(e-\tilde{\mu})^3} \times \left[\frac{e-\tilde{\mu}}{\tilde{T}_{c0}} - \sinh\left(\frac{e-\tilde{\mu}}{\tilde{T}_{c0}}\right)\right], \tag{17}$$

where $\tau = 1 - T/T_c$.

Ginzburg-Levanyuk Parameter

The Ginzburg-Levanyuk parameter, Gi, gives the temperature $T^* = T_{c0}(1 - Gi)$ where the specific heat in the presence of fluctuations dominates over the specific heat without fluctuations.

$$Gi^{3D} = \frac{1}{32\pi^2} \frac{T_{c0} b^2}{a \mathcal{K}^{(x)} \mathcal{K}^{(y)} \mathcal{K}^{(z)}} \tag{18}$$

$$Gi^{2D} = \frac{b}{4\pi a \sqrt{\mathcal{K}^{(x)} \mathcal{K}^{(y)}}} \tag{19}$$

$$Gi^{1D} = \sqrt[3]{\frac{b^2}{128 \mathcal{K}^{(x)} T_{c0} a^3}} \tag{20}$$

[Phys. Rev. B **100**, 064510 (2019)]

Inserting the GL parameters derived previously at the expresion for Gi^{1D}, we obtain:

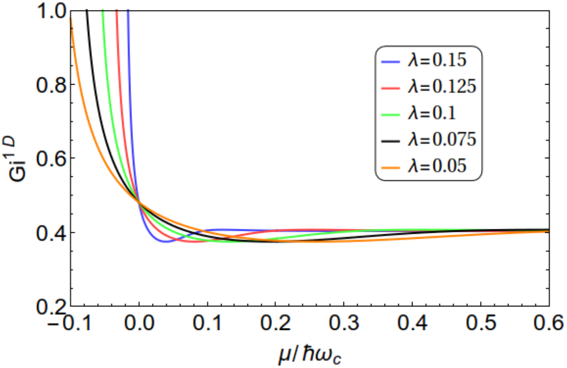

Figure: Ginzburg number for a quasi-1D band as function of the chemical potential for different values of coupling.

T_{c0} for Quasi-1D + 3D Bands

Now let us see the case $g_{12} \neq 0$:

$$\sum_j \gamma_{ij}\Delta_j = \int \mathrm{d}^3 z K_{ai}(\vec{z})\Delta_i \tag{21}$$

$$\sum_j L_{ij}\Delta_j = \sum_j (\gamma_{ij} - I_{ai}\delta_{ij})\Delta_j = 0, \tag{22}$$

where $I_{ai} = \int d^3 z K_{ai}(\vec{z})$.

$$I_{a1} = N_1 \int_0^{1+\tilde{\mu}} de \frac{\tanh[(e-\tilde{\mu})/2\tilde{T}_c]}{(e-\tilde{\mu})e^{1/2}}, \quad N_1 = \sigma^{(yz)}\sqrt{\frac{m_x}{32\pi^2\hbar^2}}$$

$$I_{a2} = N_2(0)\ln\left(\frac{2e^{\Gamma}}{\pi}\frac{1}{\tilde{T}_c}\right), \quad N_2(0) = mk_F/2\pi^2\hbar^2$$

The matrix L produces non-trivial solutions for $\vec{\Delta}$ when

$$\det(L) = (g_{11} - GI_{a1})(g_{11} - GI_{a2}) - g_{12}^2 = 0, \tag{23}$$

where $G = g_{11}g_{22} - g_{12}^2$. The dimensionless couplings are defined as

$$\lambda_1 = g_{11}N_1, \tag{24}$$

$$\lambda_2 = g_{22}N_2(0), \tag{25}$$

$$\lambda_{12} = g_{12}\sqrt{N_1 N_2(0)}. \tag{26}$$

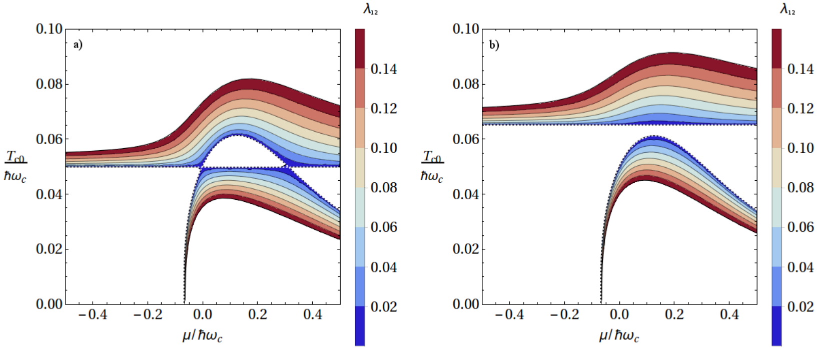

Figure: Contour lines of T_{c0} for different inter-band couplings, λ_{12}, in the cases when a) $\lambda_1 = 0.1$ and $\lambda_2 = 0.32$ and b) $\lambda_1 = 0.1$ and $\lambda_2 = 0.35$. The dashed black lines corresponds to solutions for T_{c0} in the decoupled regime, $\lambda_{12} = 0$.

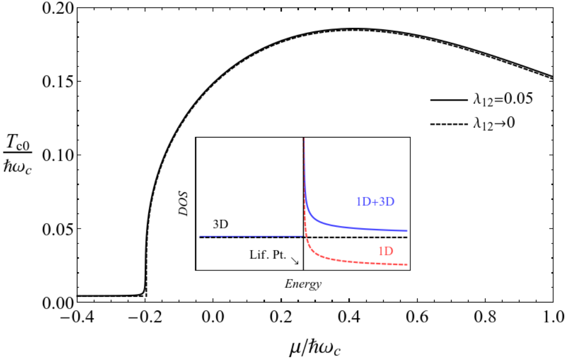

Figure: mean-field critical temperature for the two-band system with $\lambda_1 = 0.2$ and $\lambda_2 = 0.18$.

Effective dimension of the system

First one must solve the eigenvalue equation $L\vec{\Delta} = 0$:

$$\zeta_+ = 0 \qquad \vec{\eta}_+ = \begin{pmatrix} 1 \\ S \end{pmatrix}, \tag{27}$$

$$\zeta_- \neq 0 \qquad \vec{\eta}_- = \begin{pmatrix} -S \\ 1 \end{pmatrix}, \tag{28}$$

where

$$S = [g_{22} - GN_1 I_{a1}]/g_{12} = [\lambda_{22} - \Lambda I_{a1}]/\chi^{1/2}\lambda_{12}, \tag{29}$$

$\Lambda = \lambda_1\lambda_2 - \lambda_{12}^2$ and $\chi = N_1/N_2$. Obviously,

$$\vec{\Delta} = \Psi(\vec{x})\vec{\eta}_+. \tag{30}$$

By substituting this simplified expression at the gap expansion and selecting only $\tau^{3/2}$ contributions we obtain that $\Psi(\vec{x})$ obeys the GL equation

$$a\Psi + b\Psi^3 + \sum_{l=x,y,z} \mathcal{K}_l \partial_l^2 \Psi = 0 \tag{31}$$

with redefined coefficients

$$a = a_1 + a_2 S^2, \tag{32}$$

$$b = b_1 + b_2 S^4, \tag{33}$$

$$\begin{cases} \mathcal{K}^{(x)} = \mathcal{K}_1^{(x)} + \mathcal{K}_2 S^2 \\ \mathcal{K}^{(y)} = \mathcal{K}^{(z)} = \mathcal{K}_2 S^2, \end{cases} \tag{34}$$

where $a_2 = -\tau N_2(0)$, $b_2 = 7\zeta(3)N_2(0)/8\pi^2$ (remember that $\mathcal{K}_1^{(y)} = \mathcal{K}_1^{(z)} = 0$).

The the effective dimension of the two-band system is 3!!

The Effect of Fluctuations

$$Gi = \frac{1}{32\pi^2}\frac{T_{c0}b^2}{a\mathcal{K}^{(x)}\mathcal{K}^{(y)}\mathcal{K}^{(z)}} \tag{35}$$

$$= Gi_2^{3D}\frac{T_{c0}}{T_{c02}}\frac{\left(\frac{b_1}{b_2}+S^4\right)^2}{\left(\frac{a_1}{a_2}+S^2\right)\left(\frac{\mathcal{K}_1^{(x)}}{\mathcal{K}_2}+S^2\right)S^4} \tag{36}$$

where

$$Gi_2^{3D} = \frac{1}{32\pi^2}\frac{T_{c02}b_2^2}{a_2\mathcal{K}_2^3}. \tag{37}$$

In the limit of infinite deep band, $E_{12}\to\infty$, $\mathcal{K}_1^{(x)} \ll \mathcal{K}_2$, we have

$$Gi = Gi_2^{3D}\frac{T_{c0}}{T_{c02}}\frac{\left(\frac{b_1}{b_2}+S^4\right)^2}{\left(\frac{a_1}{a_2}+S^2\right)S^6}. \tag{38}$$

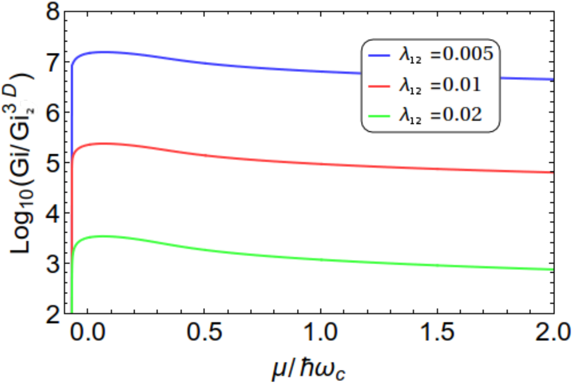

Figure: Ginzburg number for the case of two-bands with respect to the isolated 3D band. $\lambda_1 = 0.1$ and $\lambda_2 = 0.05$.

Renormalized Critical Temperature

With renormalization group technique, one can derive the critical temperature of the system in the presence of fluctuations:

$$T_c = \frac{T_{c0}}{1 + 8\pi\sqrt{Gi}}. \tag{39}$$

[Larkin and Varlamov, *Theory of FLuctuations in Superconductors*, 2005.]

Enhancement of the Critical Temperature

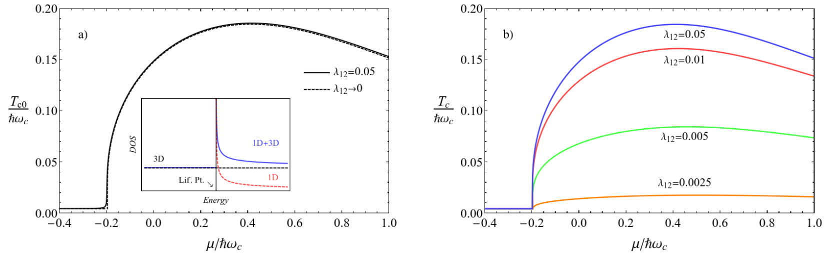

Figure: a) The mean-field critical temperature, T_{c0}, for the 2-band case of q1D and 3D bands. b) Renormalized critical temperature, T_c. In both plots, $\lambda_1 = 0.2$ and $\lambda_2 = 0.18$. $Gi^{3D} = 10^{-10}$.

Conclusion

- Even though isolated q1D systems have high mean-field critical temperatures, the effect of fluctuations is too strong which prevents these systems to achieve high-T$_c$.
- The combination of a q1D and a 3D bands forms an effective 3D system with high mean-field critical temperature and lower effect of fluctuations over T_c.
- This simple model gives a clear approach for explaining High-T_c's measured in those recently discovered chain-like materials with quasi-1D bands.