Screening of pair fluctuations in two-band superconductors

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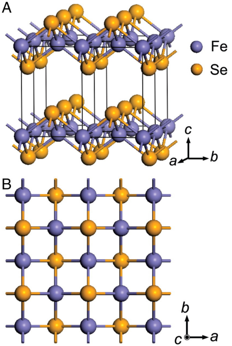
Summary

- Two-band superconductivity
- Ginzburg-Landau for two-band superconductivity
- Beyond-mean-field critical temperature
- Pseudo-gap suppression by inter-band coupling
- Conclusions

Two-band superconductivity (I)

Magnesium diboride (MgB_2) and iron-based superconductors ($FeSe$, $FeTe$) are examples of multi-band superconductors,[1] where multiple Fermi surfaces can be effectively controlled by doping or by applying pressure.



For iron-based superconductors the superconducting state is generally a coherent mixture of pair condensates in deep and shallow bands.

[1] M.V. Milošević and A. Perali, Supercond. Sci. Technol. **28**, 060201 (2015).

Two-band superconductivity (II)

Let us consider the microscopic model of a 2D two-band superconductor[2] characterized by a **symmetric s-wave coupling matrix** with elements g_{ij}:

$$\hat{H} = \sum_{i=1,2} \sum_{\sigma=\uparrow,\downarrow} \int d^2\mathbf{r} \Big\{ \hat{\psi}^{+}_{i,\sigma}(\mathbf{r}) \left[-\frac{\hbar^2}{2m_i} \nabla^2 + \epsilon_i - \mu \right] \hat{\psi}_{i,\sigma}(\mathbf{r}) \Big\}$$
$$+ \sum_{i=1,2} \int d^2\mathbf{r} \Big\{ \hat{\psi}^{+}_{i,\uparrow}(\mathbf{r}) \hat{\psi}^{+}_{i,\downarrow}(\mathbf{r}) \Delta_i(\mathbf{r}) + \hat{\psi}_{i,\uparrow}(\mathbf{r}) \hat{\psi}_{i,\downarrow}(\mathbf{r}) \Delta^{*}_{i}(\mathbf{r}) \Big\} , \quad (1)$$

where $\hat{\psi}_{i,\sigma}(\mathbf{r})$ is the fermionic field operator which destroys a fermion of spin σ and band i at the position $\mathbf{r}$, ϵ_i and m_i are depth and effective mass of band i, μ is the chemical potential, while the energy gaps are

$$\Delta_1(\mathbf{r}) = g_{11} \langle \hat{\psi}_{1,\uparrow}(\mathbf{r}) \hat{\psi}_{1,\downarrow}(\mathbf{r}) \rangle + g_{12} \langle \hat{\psi}_{2,\uparrow}(\mathbf{r}) \hat{\psi}_{2,\downarrow}(\mathbf{r}) \rangle , \quad (2)$$
$$\Delta_2(\mathbf{r}) = g_{21} \langle \hat{\psi}_{1,\uparrow}(\mathbf{r}) \hat{\psi}_{1,\downarrow}(\mathbf{r}) \rangle + g_{22} \langle \hat{\psi}_{2,\uparrow}(\mathbf{r}) \hat{\psi}_{2,\downarrow}(\mathbf{r}) \rangle . \quad (3)$$

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[2] H. Suhl, B. T. Matthias, and L. R. Walker, Phys. Rev. Lett. **3**, 552 (1959).

Two-band superconductivity (III)

The model crucially depends on the mixing parameter

$$S = \frac{1}{2\lambda_{12}} \left[\lambda_{22} - \frac{\lambda_{11}}{\chi} \pm \sqrt{\left(\lambda_{22} - \frac{\lambda_{11}}{\chi}\right)^2 + 4\frac{\lambda_{12}^2}{\chi}} \right] , \qquad (4)$$

where $\chi = N_2/N_1$, $\lambda_{ij} = g_{ij}(N_1 + N_2)$, and $N_i = m_i/(2\pi\hbar^2)$ is the 2D density of states of the i-th band.

The corresponding mean-field critical temperature reads[3]

$$T_{c0} = \frac{2e^{\gamma}}{\pi} \hbar\omega_c \exp\left[-\frac{(1+\chi)(\lambda_{22} - \lambda_{12} S)}{\lambda_{11}\lambda_{22} - \lambda_{12}^2} \right] , \qquad (5)$$

where $\hbar\omega_c$ denotes the energy cutoff (the same for both bands), and $\gamma \approx 0.577$ is the Euler-Mascheroni constant.

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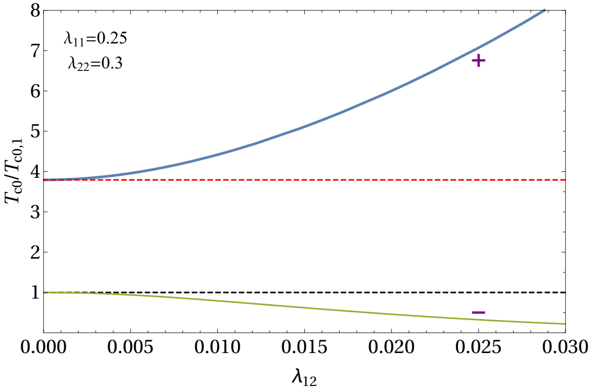
[3] H. Suhl, B. T. Matthias, and L. R. Walker, Phys. Rev. Lett. **3**, 552 (1959).

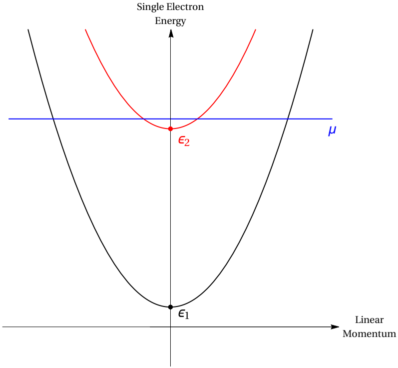
Two-band superconductivity (IV)



In the presence of inter-band coupling λ_{12} the mean-field critical temperature T_{c0} of the two-band system has two branches ($+$ and $-$): the higher one ($+$) gives the physical mean-field critical temperature. Here $T_{c0,1}$ is the mean-field critical temperature of the band 1 in the absence of inter-band coupling λ_{12}.

Ginzburg-Landau for two-band superconductivity (I)

In the case of a two-band system with a deep band ($i = 1$) and a shallow band ($i = 2$) one must have $0 < \epsilon_1 \ll \epsilon_2 \simeq \mu$,



In our calculations, in the absence of inter-band coupling λ_{12}, the shallow band 2 has a larger mean-field critical temperature $T_{c0,2}$ with respect to the mean-field critical temperature $T_{c0,1}$ of the deep band 1, i.e. $T_{c0,2} > T_{c0,1}$.

Ginzburg-Landau for two-band superconductivity (II)

Near T_{c0}, from the two-component Ginzburg-Landau (GL) functional[4] or from the two-band BCS model[5] one derives a single-component GL functional

$$F = \int \left\{ a(T)|\psi(\mathbf{r})|^2 + \frac{b}{2}|\psi(\mathbf{r})|^4 + \mathcal{K}|\nabla\psi(\mathbf{r})|^2 \right\} d^2\mathbf{r} \ , \qquad (6)$$

where $\psi(\mathbf{r})$ is the single order parameter and moreover

$$a(T) = \alpha(T - T_{c0}) \quad \text{with} \quad \alpha = \left(\frac{N_1}{S} + N_2 S\right)\frac{1}{T_{c0}} \qquad (7)$$

$$b = 2\left(\frac{N_1}{S^2} + N_2 S^2\right)\frac{7\zeta(3)}{8\pi^2 T_{c0}^2} \qquad (8)$$

$$\mathcal{K} = \left(\frac{7\zeta(3)N_1 v_1^2}{4S} + 3\zeta(2)N_2 v_T^2 S\right)\frac{\hbar^2}{8\pi^2 T_{c0}^2} \qquad (9)$$

with $v_1 = \sqrt{2(\mu - \epsilon_1)/m_1}$ Fermi velocity of the deep band, $v_T = \sqrt{2T_{c0}/m_2}$ thermal velocity, and $\zeta(x)$ the Riemann zeta function.

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[4] B. T. Geilikman, R. O. Zaitsev, and V. Z. Kresin, Sov. Phys. Solid State **9**, 642 (1967).

[5] M.E. Zhitomirsky and V.H. Dao, Phys. Rev. B **69**, 054508 (2004).

Beyond-mean-field critical temperature (I)

In the superconducting state, where $T < T_{c0}$, the characteristic length of the Ginzburg-Landau functional is the coherence length

$$\xi(T) = \sqrt{\frac{\mathcal{K}}{|a(T)|}} = \sqrt{\frac{\mathcal{K}}{\alpha(T_{c0} - T)}} \; . \tag{10}$$

The Ginzburg-Levaniuk number Gi defines the interval in the vicinity of T_{c0} where the mean field theory is compromised by fluctuations.[6] It can be written in terms of the parameters of the Ginzburg-Landau functional

$$Gi = \frac{b}{4\pi\alpha\mathcal{K}} \; , \tag{11}$$

and the corresponding Ginzburg-Levaniuk temperature is

$$T_{Gi} = T_{c0}(1 - Gi) \; . \tag{12}$$

Within the Gaussian beyond-mean-field approach, at T_{Gi} the mean-field specific heat $c_{s,mf}$ is equal to the beyond-mean-field one $c_{s,bmf}$, which diverges at T_{c0}.

[6] A. Larkin and A. Varlamov, Theory of Fluctuations in Superconductors (Clarendon Press, 2007).

Beyond-mean-field critical temperature (II)

It follows that there are two relevant scales:
i) A small length

$$\xi(0) = \sqrt{\frac{\mathcal{K}}{\alpha T_{c0}}} , \tag{13}$$

with a corresponding large wavenumber

$$\Lambda_{max} = \frac{1}{\xi(0)} . \tag{14}$$

ii) A large(r) length

$$\xi(T_{Gi}) = \sqrt{\frac{\mathcal{K}}{\alpha T_{c0} Gi}} \tag{15}$$

with a corresponding small(er) wevenumber

$$\Lambda_{min} = \frac{1}{\xi(T_{Gi})} . \tag{16}$$

Beyond-mean-field critical temperature (III)

Extremizing the Ginzburg-Landau functional with respect to $\psi^*(\mathbf{r})$ one gets the Euler-Lagrange equation

$$a(T)\,\psi + b\,|\psi|^2\psi - \mathcal{K}\,\nabla^2\psi = 0 \; . \tag{17}$$

It is important to stress that the mean-field theory assumes a uniform order parameter.

Here we write the space-dependent order parameter $\psi(\mathbf{r})$ in the following way

$$\psi(\mathbf{r}) = \psi_0 + \eta(\mathbf{r}) \; , \tag{18}$$

where $\eta(\mathbf{r})$ represents a fluctuation with respect to the real and uniform configuration ψ_0 with the condition

$$\langle \eta(\mathbf{r}) \rangle_T = \langle \eta^*(\mathbf{r}) \rangle_T = 0 \; , \tag{19}$$

where $\langle \cdots \rangle_T$ is the thermal average.

Beyond-mean-field critical temperature (IV)

Inserting Eq. (18) into Eq. (17), and after thermal averaging we obtain

$$\left[a(T) + 2b\,\langle|\eta|^2\rangle_T + b\,\langle\eta^2\rangle_T\right]\,\psi_0 + b\,\psi_0^3 + b\,\langle|\eta|^2\eta\rangle_T = 0\;. \qquad (20)$$

Clearly, only removing all thermal averages one recovers the familiar mean-field result

$$\psi_0 = \begin{cases} 0 & \text{for } T \geq T_{c0} \\ \sqrt{-\frac{a(T)}{b}} & \text{for } T < T_{c0} \end{cases}\;. \qquad (21)$$

We take into account thermal fluctuations of the order parameter keeping $\langle|\eta|^2\rangle_T$ but neglecting the anomalous averages $\langle\eta^2\rangle_T$ and $\langle|\eta|^2\eta\rangle_T$. We then obtain[7]

$$\left(a(T) + 2b\,\langle|\eta|^2\rangle_T\right)\,\psi_0 + b\,\psi_0^3 = 0\;, \qquad (22)$$

and consequently the beyond-mean-field result

$$\psi_0 = \begin{cases} 0 & \text{for } T \geq T_c \\ \sqrt{-\frac{a(T)+2b\langle|\eta|^2\rangle_T}{b}} & \text{for } T < T_c \end{cases}\;. \qquad (23)$$

[7] LS, A. Shanenko, A. Vagov, J. Albino Augiar, and A. Perali, e-preprint arXiv:1810.03321

Beyond-mean-field critical temperature (V)

In this case the uniform order parameter ψ_0 becomes different from zero only below the beyond-mean-field critical temperature T_c given by the equation

$$a(T_c) + 2b\,\langle|\eta(\mathbf{r})|^2\rangle_{T_c} = 0\,. \tag{24}$$

After some calculation based on statistical mechanics we get

$$\langle|\eta(\mathbf{r})|^2\rangle_T = \frac{1}{L^2}\sum_{\mathbf{q}} \frac{1}{\beta\left(a(T) + 2b\langle|\eta(\mathbf{r})|^2\rangle_T + \mathcal{K}q^2\right)}\,, \tag{25}$$

and consequently we find the beyond-mean-field critical temperature[8]

$$T_c = T_{c0} - \frac{2b\langle|\eta(\mathbf{r})|^2\rangle_{T_c}}{\alpha}, \tag{26}$$

where

$$\langle|\eta(\mathbf{r})|^2\rangle_{T_c} = \int_{\Lambda_{min}<q<\Lambda_{max}} \frac{d^2\mathbf{q}}{(2\pi)^2}\,\frac{T_c}{\mathcal{K}q^2} = \frac{T_c}{2\pi\mathcal{K}}\ln\left(\frac{\Lambda_{max}}{\Lambda_{min}}\right). \tag{27}$$

[8] LS, A. Shanenko, A. Vagov, J. Albino Augiar, and A. Perali, e-preprint arXiv:1810.03321

Beyond-mean-field critical temperature (VI)

By using $\Lambda_{min} = 1/\xi(T_{Gi})$ and $\Lambda_{max} = 1/\xi(0)$, after some further algebric manipulations we obtain the following shift of the mean-field critical temperature due to fluctuations of the paring order parameter

$$\frac{\delta T_c}{T_c} \equiv \frac{T_{c0} - T_c}{T_c} = 2\, Gi \, \ln\left(\frac{1}{4Gi}\right) \ , \tag{28}$$

where T_{c0} is the mean-field critical temperature of the two-band system, T_c is the beyond-mean-field critical temperature, and Gi the Ginzburg-Levaniuk number of the two-band system.

This result[9] is fully consistent with an alternative derivation based on the Renormalization Group.[10]

[9] LS, A. Shanenko, A. Vagov, J. Albino Augiar, and A. Perali, e-preprint arXiv:1810.03321

[10] A. Larkin and A. Varlamov, Theory of Fluctuations in Superconductors (Clarendon Press, 2007).

Pseudo-gap suppression by inter-band coupling (I)

To investigate the sensitivity of the pair fluctuations to the inter-band coupling, we consider the regime $v_T \ll v_1$ namely $\mathcal{K}_2 \ll \mathcal{K}_1$, and also $N_2/N_1 \simeq 1$ which implies $b_2/b_1 \simeq \alpha_2/\alpha_1 \simeq 1$.
In this way, we find that the Ginzburg-Levaniuk number can be written as[11]

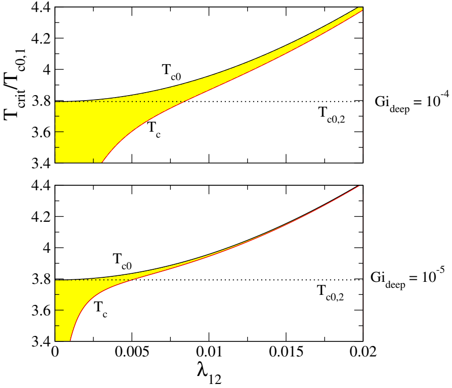
$$Gi = \frac{b}{4\pi\alpha\mathcal{K}} = \frac{b_1}{4\pi\alpha_1\mathcal{K}_1} \frac{1 + \frac{b_2}{b_1}S^4}{(1 + \frac{\alpha_2}{\alpha_1}S^2)(1 + \frac{\mathcal{K}_2}{\mathcal{K}_1}S^2)} \simeq Gi_{\mathrm{deep}} \frac{1 + S^4}{1 + S^2} , \quad (29)$$

where $Gi_{\mathrm{deep}} = b_1/(4\pi\alpha_1\mathcal{K}_1)$ is the Ginzburg-Levaniuk number of the deep band and S is the mixing parameter previously introduced.

In the next slide we plot the mean-field critical temperature T_{c0} and beyond-mean-field critical temperature T_c as a function of the inter-band coupling λ_{12}, for two values of the Ginzburg-Levaniuk number Gi_{deep}.
In the plot the mean-field transition temperature of the uncoupled deep band $T_{c0,1}$ is taken as reference value.

[11] LS, A. Shanenko, A. Vagov, J. Albino Augiar, and A. Perali, e-preprint arXiv:1810.03321

Pseudo-gap suppression by inter-band coupling (II)



Mean-field critical temperature T_{c0} (black curves) and beyond-mean-field critical one T_c (red curves) vs inter-band coupling λ_{12}. The **yellow area** is the pseudo-gap region.[12] Remarkbly, pseudo-gap suppression in FeSe has been recently observed.[13]

[12] LS, A. Shanenko, A. Vagov, J. Albino Augiar, and A. Perali, e-preprint arXiv:1810.03321

[13] T. Hanaguri et al., Phys. Rev. Lett. **122**, 077001 (2019).

Conclusions

- We have considered the Ginzburg-Landau fuctional of a 2D two-band superconductor with a deep band and a shallow band.
- The macroscopic parameters of the Giunzburg-Landau functional and the mean-field critical temperature T_{c0} crucially depend on the couplings of the microscopic two-band model and their mixing parameter.
- We have derived a beyond-mean-field critical temperature T_c which takes into account thermal fluctuations of the order parameter. We have found that T_c depends on the Ginzburg-Levaniuk number Gi of the two-band system.
- Usually, in 2D systems thermal fluctuations make T_c much smaller than T_{c0}. However, in our case, we have shown that a small tunneling coupling of Cooper pairs between the two bands strongly suppress the difference between T_{c0} and T_c. In other words, there is an efficient screening of pair fluctuations.

Acknowledgements

Thank you for your attention!

Announcement

International Conference "Superfluctuations 2019"

Fluctuations and Highly Non Linear Phenomena
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2-4 September 2019 at the University of Padova (Italy)

Organizers: L. Dell'Anna, A. Perali, and L. Salasnich

webpage: www.multisuper.org/superfluctuations-2019/