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

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(Dated: February 7, 2020)

It is well-known that quasi-one-dimensional superconductors suffer from the pairing fluctuations that significantly reduce the superconducting temperature or even completely suppress any coherent behavior. Here we demonstrate that a coupling to a robust pair condensate changes the situation dramatically. In this case the quasi-one-dimensional system can be a high temperature superconductor governed by the proximity to the Lifshitz transition at which the Fermi level approaches the lower edge of the single-particle spectrum.

I. INTRODUCTION

It is a textbook issue that the superconducting order is suppressed in a one-dimensional system due to fluctuations. The situation is slightly improved when one-dimensional conducting filaments (parallel chains of molecules/atoms) are coupled to one another. Theoretical studies demonstrated that a resulting quasi-one-dimensional (quasi-1D) system can superconduct but its coherent properties are still affected by fluctuations. The related superconducting transition temperature is typically much smaller than the critical temperature obtained within the BCS approximation unless a strong coupling between filaments abandon quasi-1D features. The theoretical results were confirmed by observations of low-temperature superconductivity in organic quasi-1D superconductors known as the Bechgaard salts.

Recently interest in quasi-1D systems was renewed due to the discovery of Cr₂As₂-chain based quasi-1D superconductors. The results of the first principle calculations of the electronic band structure make is possible to expect that the new quasi-1D superconductors are actually multiband compounds with contributing quasi-1D bands. In particular, there are two quasi-1D Fermi surface sheets coexisting with one 3D sheet in K₂Cr₃As₃ and also in KCr₃As₂Hₓ. Furthermore, it is demonstrated that the Fermi level in KCr₃As₂Hₓ is lifted by changing the H-intercalation which results in reconstructions of the Fermi surface topology (Lifshitz transitions).

One can expect that the coupling between quasi-1D and a robust pair condensate can diminish the pairing fluctuations due to the screening mechanism investigated in Ref. Then, the important question arises if it is possible to boost the superconductivity by approaching the Lifshitz transition at which the chemical potential crosses the lower edge of the quasi-1D band. The answer is far not trivial because though the mean-field temperature can significantly increase in the proximity of the Lifshitz point, the fluctuations tend to severely enhance due to the Bose character of the pairing in this regime. Since the fluctuations are already very strong in the presence of the quasi-1D effects, their further enhancement may compromise any expectation based on the mean-field arguments.

In the present paper, motivated by recent experiments with multiband quasi-1D superconductors, we investigate the quasi-1D and BCS condensates, coexisting in one system and coupled via the Josephson-like pair transfer. Our consideration reveals that such a two-band material is a BCS superconductor whose superconducting properties are determined by the quasi-1D system. Remarkably, its critical temperature increases by orders of magnitude when the chemical potential crosses the lower edge of the quasi-1D band.

The paper is organized as follows. In Sec. II we derive the Ginzburg-Landau (GL) functional of the quasi-1D band considered as a separate superconductors. The related coefficients of the GL theory are necessary in the subsequent consideration of the two-band system. In Sec. III we investigate a two-band superconductor with quasi-1D and 3D contributing bands. For simplicity, we consider the s-wave superconductor but our conclusions are not sensitive to the pairing symmetry, e.g., the same results hold for the d-wave pairing, as well. The conclusions are given in Sec. IV.

II. QUASI-1D BAND

It is known that the GL theory in the vicinity of the mean-field critical temperature Tc0 is obtained from the BCS microscopic formalism via the Gor’kov derivation. Below, for the reader convenience, we outline this derivation, specifying important features of the quasi-1D band in the vicinity of the Lifshitz transition (shallow quasi-1D...
The normal-state temperature Green functions are expressed as
g_\omega(x,y) = \int d^3k \frac{e^{-i(k\cdot(x-y))}}{(2\pi)^3 i\hbar\omega - \xi_k} \tag{4}
and \bar{g}_\omega(x,y) = -g_\omega(y,x). The integral kernels involve, as usual, the summation over the fermionic Matsubara frequencies \omega_n = \pi T(2n + 1)/\hbar (here the Boltzmann constant k_B is set to 1). The magnetic field is zero in the present consideration.

The quasi-1D Fermi surface is modelled 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. Then the related single-particle energy becomes

\xi_k = \frac{\sum_{i=1}^{3} \hbar^2 k_i^2}{2m_i} - \mu \approx \frac{\hbar^2 k_x^2}{2m_x} - \mu, \tag{5}

with \mu the chemical potential (the Fermi level) and m_x set to the free electron mass m.

A. Mean-field critical temperature

To obtain \T_{c0}, one considers only the linear contribution to the gap equation given by Eq. (1). As the order parameter is not position dependent, one obtains

\frac{1}{g\T_{c0}} = \sum_\omega \int d^3z d^3k d^3k' \frac{e^{-i(k-k')z}}{(2\pi)^3 (i\hbar\omega - \xi_k)(i\hbar\omega + \xi_{k'})}, \tag{6}

where z = x - y. This equation is reduced to

\frac{1}{\lambda_s} = \int_0^{1+\bar{\mu}} dx \frac{\tanh[(x - \bar{\mu})/2\T_{c0}]}{x^{1/2}(x - \bar{\mu})}, \tag{7}

where \T_{c0} = \T_{c0}/\hbar\omega_c, \bar{\mu} = \mu/\hbar\omega_c (\omega_c is the cut-off frequency) and the dimensionless coupling \lambda is defined as

\lambda_s = gN_s = g\sigma(yz) \sqrt{\frac{m}{32\pi^2\hbar^3\omega_c}}. \tag{8}

Here \sigma(yz) is given by

\sigma(yz) = \left( \int \frac{dk_y}{2\pi} \frac{dk_z}{2\pi} \right) \sim (a_y a_z)^{-1}, \tag{9}

and introduced to account for the states in y and z directions. It is proportional to the inverse product of the lattice parameters a_y and a_z. The auxiliary quantity N_s is the DOS in the quasi-1D band at the energy \hbar\omega_c.

The numerical results for \T_{c0} are given in Fig. 1 for different values of the dimensionless coupling \lambda_s. The dependence of \T_{c0} on \mu is similar for all given couplings, demonstrating a significant increase of \T_{c0} in the vicinity of \mu = 0, reflecting the Lifshitz transition. It is also demonstrated in Fig. 2 that the relative increase of the
mean-field critical temperature (as compare to its value at $\mu = 2\hbar \omega_c$) is more pronounced for lower values of the dimensionless coupling. Generally, for all couplings $\lambda_s < 0.1$ it is more than by an order of magnitude.

**B. The GL functional and Ginzburg number**

The increase of $T_{c0}$ near the Lifshitz point is remarkable but, as it is known, the mean-field approach for quasi-1D systems is compromised due to a significant role of fluctuations. To estimate such fluctuations, we derive the corresponding GL free energy functional as

$$F = \int d^3x \left[ a_s |\Delta|^2 + \frac{b_s}{2} |\Delta|^4 + \sum_i K^{(i)}_s |\partial_x \Delta_i|^2 \right],$$

where $i = x, y, z$, $\tau = 1 - T/T_{c0}$ and the coefficients $a_s$, $b_s$, and $K^{(i)}_s$ are given by

$$a_s = \frac{N_s}{2T_{c0}} \int_0^{\infty} dx x^{1/2} \left[ 1 + \cosh \left( \frac{x - \mu}{T_{c0}} \right) \right],$$

$$b_s = \frac{N_s}{8(\hbar \omega_c)^2} \int_0^{\infty} dx x^{1/2} \left[ \frac{\text{sech}^2 \left( (x - \mu)/2T_{c0} \right)}{(x - \mu)^3/2} \right] \left[ \sinh \left( \frac{x - \mu}{T_{c0}} \right) - \frac{x - \mu}{T_{c0}} \right],$$

$$K^{(i)}_s = \frac{\hbar^2 N_s}{2m(\hbar \omega_c)^2} \int_0^{\infty} dx x^{1/2} \left[ \frac{\text{sech}^2 \left( (x - \mu)/2T_{c0} \right)}{(x - \mu)^3/2} \right] \left[ \sinh \left( \frac{x - \mu}{T_{c0}} \right) - \frac{x - \mu}{T_{c0}} \right],$$

where the integration limits are extended as $\hbar \omega_c + \mu \to \infty$ because all the integrands are fast-decaying functions of $x$. Note that the stiffness, $K^{(i)}_s$, is zero for $y$ and $z$ directions due to the infinitely large effective electron mass.

The Ginzburg number (Ginzburg-Levanyuk parameter $G_{1D}$ for the functional $F$) reads

$$G_{1D} = \frac{T_{c0} - T^*}{T_{c0}} = \sqrt{\frac{T_{c0}^2 b_s^2 a_s^2}{128K^{(x)}_s a_s^3}},$$

where $T^*$ is the temperature above which the mean-field theory is not applicable due to significant thermal fluctuations. The results for $G_{1D}$ as a function of $\mu/\hbar \omega_c$ are given in Fig. 3. One can see that $G_{1D}$ is of the order of 1, which means that the mean-field theory is totally ruled out by fluctuations for any value of the chemical potential, in agreement with the previous results. Furthermore, one can see that the role of fluctuations increases in the vicinity of the Lifshitz point.

**III. TWO-BAND SUPERCONDUCTOR WITH QUASI-1D AND 3D BANDS**

Now we consider the two-band superconductor with the coupled shallow quasi-1D and deep 3D bands. The gaps $\Delta_s$ and $\Delta_d$ associated with quasi-1D and 3D bands, respectively, are components of the gap vector defined in the band space as

$$\vec{\Delta} = \left( \begin{array}{c} \Delta_s \\ \Delta_d \end{array} \right).$$

The gap equation is written in the matrix form

$$\gamma \vec{\Delta} = \vec{R},$$

where the components of the band-space vector $\vec{R}$ are given by ($i = s, d$)

$$R_i = \int d^3y K_{si}(x, y) \Delta_i(y) + \int \prod_{i=1}^3 d^3y_i K_{bi}(x, y_1, y_2, y_3) \Delta_i(y_1)\Delta_j(y_2)\Delta_k(y_3),$$

where we define the $2 \times 2$ coupling matrix $\tilde{\gamma}$ as

$$\tilde{\gamma} = \left( \begin{array}{cc} g_{ss} & g_{sd} \\ g_{ds} & g_{dd} \end{array} \right),$$

where $g_{sd} = g_{ds}$ and its inverse is $\gamma_{ij} = (\tilde{\gamma}^{-1})_{ij}$. The band-dependent integral kernels are given by Eqs. (2) and (3), where $G^{(0)}_{ij}$ is replaced by the band-dependent normal-state Green function $G^{(0)}_{ij}$ with the corresponding band-dependent single-particle energy. The 3D band dispersion relation assumes the spherical Fermi surface, i.e.,

$$\xi_{kd} = \sum_{i=1}^3 \frac{\hbar^2 k_i^2}{2m} - \mu_d = \frac{\hbar^2 k_i^2}{2m} - (\mu + E_{sd}),$$
with $E_{sd}$ the energy interval between the lower edges of the the 3D and quasi-1D bands. For the quasi-1D band we utilize the same single-particle energy as previously.

### A. The two-band mean-field temperature

In order to find the critical temperature, the gap equation (10) is linearized

$$\sum_j L_{ij} \Delta_j = \sum_j (\gamma_{ij} - I_{ai} \delta_{ij}) \Delta_j = 0,$$  \hspace{1cm} (20)

where $I_{ai} = \int d^2 z K_{ai}(z)$. Using the results obtained in section IV for the quasi-1D band we have

$$I_{as} = N_s \int_0^{\hbar \omega_c + \mu} dE \frac{\tanh[(E - \mu)/2T_c]}{(E - \mu)^{1/2}}.$$ \hspace{1cm} (21)

For the deep 3D band one finds

$$I_{ad} = N_d \ln \left( \frac{2e^\tau \hbar \omega_c}{\pi T_c} \right),$$ \hspace{1cm} (22)

where $N_d = mk_F/2\pi^2\hbar^2$ is the 3D DOS at the Fermi level.

The matrix $\tilde{L}$ [with its elements $L_{ij}$ given by Eq. (20)] yields a non-trivial solution for the gap functions only when $\det(\tilde{L}) = 0$, i.e.,

$$\begin{pmatrix} \lambda_{dd} - \Lambda \frac{I_{as}}{N_s} & \lambda_{ss} - \Lambda \frac{I_{ad}}{N_d} - \lambda_{sd}^2 \end{pmatrix} = 0 \hspace{1cm} (23)$$

where the dimensionless coupling $\lambda_{ij}$ are defined as $\lambda_{ss} = g_{ss} N_s$, $\lambda_{dd} = g_{dd} N_d$, and $\lambda_{sd} = g_{sd} \sqrt{N_s N_d}$ and $\Lambda = \lambda_{ss} \lambda_{dd} - \lambda_{sd}^2$. It is important to notice that due to the appearance of $N_s$ and $N_d$ in the definitions of $I_{as}$ and $I_{ad}$ in Eqs. (21) and (22), the mean-field critical temperature of the two-band system depends only on the dimensionless couplings $\lambda_{ss}$, $\lambda_{dd}$, and $\lambda_{sd}$ and the chemical potential.

The results for the two-band mean-field critical temperature $T_{c0}$, calculated for $\lambda_{ss} = 0.1$, $\lambda_{dd} = 0.05$, and the interband couplings $\lambda_{sd} \leq 0.05$, are shown in Fig. 4. One sees that $T_{c0}$ is not sensitive to the presence of the 3D band for the interband couplings $\lambda_{sd} < 0.05$. In this case the two-band system exhibits the same mean-field critical temperature as the quasi-1D band taken as a separate superconductor. The qualitative character of these results does not depend on the choice of the intraband couplings. For any choice of $\lambda_{ij}$, the transition temperature is not sensitive to the presence of the 3D band when $\lambda_{sd} < \lambda_{dd}$.

### B. Two-band Ginsburg-Landau theory and Ginzburg number

The solution to the linearized gap equation (20) is written in the form [10,17]

$$\tilde{\Delta}(\mathbf{x}) = \Psi(\mathbf{x}) \tilde{\eta},$$ \hspace{1cm} (24)

where $\tilde{\eta}$ is the eigenvector of the matrix $\tilde{L}$ corresponding to its zero eigenvalue and $\Psi(\mathbf{x})$ is the Landau order parameter. The eigenvector $\tilde{\eta}$ can be chosen as (normalization is not important)

$$\tilde{\eta} = \begin{pmatrix} 1 \\ S \end{pmatrix},$$ \hspace{1cm} (25)

with

$$S = \frac{1}{\lambda_{sd}^2 - \lambda_{as} \lambda_{dd} - \lambda_{ss} \lambda_{sd}^2} \left( \lambda_{dd} - \Lambda \frac{I_{as}}{N_s} \right) = \frac{1}{\lambda_{sd}^2 - \lambda_{as} \lambda_{dd} - \lambda_{ss} \lambda_{sd}^2} \left( \lambda_{dd} - \Lambda \frac{I_{as}}{N_s} \right).$$ \hspace{1cm} (26)

The Landau order parameter $\Psi(\mathbf{x})$ obeys the standard GL equation [10,17]

$$a \tau \Psi + b \Psi^3 + \sum_{i=x,y,z} \mathcal{K}^{(i)} \nabla_i^2 \Psi = 0,$$ \hspace{1cm} (27)

where $\tau = 1 - T/T_{c0}$ and the coefficients are averages over the contributing bands

$$a = a_s + a_d S^2, \quad b = b_s + b_d S^4,$$ \hspace{1cm} (28)

$$\mathcal{K}^{(i)}(i = x, y, z),$$ \hspace{1cm} (29)

and we recall that $\mathcal{K}^{(y)} = \mathcal{K}^{(z)} = 0$.

Using the standard procedure, we calculate the Ginzburg number for the resulting 3D anisotropic GL theory as

$$Gi = Gi^{3D} \frac{(b_s/b_d + S^4)^2}{(a_s/a_d + S^2) \left( \mathcal{K}_{ss}^{(x)} / \mathcal{K}_{dd}^{(x)} + S^2 \right) S^4}$$ \hspace{1cm} (30)
where

\[ G_{i}^{3D} = \frac{1}{32\pi^{2}} \frac{T_{c0}b_{d}^{2}}{a_{d}K_{d}^{(x)}K_{d}^{(y)}}, \]

Assuming that 3D band is infinitely deep, i.e., \( E_{sd} \to \infty \), we use \( K_{xx}/K_{d}^{(x)} \to 0 \), one obtains

\[ G_{i} = G_{i}^{3D} \left( \frac{b_{s}/b_{d} + S^{4}}{(a_{s}/a_{d} + S^{2})S^{2}} \right)^{2}. \]

In this case, the parameter \( G_{i} \) can be obtained using Eqs. (11) and (12) and

\[ a_{d} = -N_{d}, b_{d} = N_{d} \frac{7\zeta(3)}{8\pi^{2}T_{c0}}, \]

\[ K_{d}^{(x)} = K_{d}^{(y)} = K_{d}^{(z)} = \frac{\hbar^{2}v_{F}^{2}}{6N_{d}} \frac{7\zeta(3)}{8\pi^{2}T_{c0}}, \]

where \( v_{F} \) is the 3D band Fermi velocity.

The numerical data for the two-band Ginzburg number are given in Fig. 3 as calculated for \( \lambda_{ss} = 0.1, \lambda_{sd} = 0.05, N_{s}/N_{d} = 1 \) and different values of the interband coupling \( \lambda_{sd} \). Assuming the conservative estimate of the 3D Ginzburg number as \( G_{i}^{(3D)} \sim 10^{-16} \), we find that \( G_{i} \) of the resulting system is much smaller than 1 even for almost negligible values of the interband coupling. In this case the critical temperature of the system is determined by the quasi-1D band and significantly increases when approaching the Lifshitz point. This increase is not compromised by the fluctuations due to the stabilizing influence of the 3D band condensate.

### IV. CONCLUSIONS

We demonstrate that a quasi-1D superconducting condensate coupled to a stable 3D BCS condensate via the Josephson-like Cooper pair transfer between the two condensates, becomes a mean-field superconductor whose temperature can increase by orders of magnitude when the chemical potential approaches the lower edge of the quasi-1D band.

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