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# Microscopic derivation of two-component Ginzburg-Landau model and conditions of its applicability in two-band systems

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We report a microscopic derivation of two-component Ginzburg-Landau (GL) field theory and the conditions of its validity in two-band superconductors. We also investigate the conditions when microscopically derived or phenomenological GL models fail and one should resort to a microscopic description. We show that besides being directly applicable at elevated temperatures, a version of a minimal two-component GL theory in certain cases also gives accurate description of certain aspects of a two-band system even substantially far from  $T_c$ . This shows that two-component GL model can be used for addressing a wide range of questions in multiband systems, in particular vortex physics and magnetic response. We also argue that single Ginzburg-Landau parameter cannot in general characterize magnetic response of multiband systems.

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## I. INTRODUCTION

Ginzburg-Landau theory of single-component superconductors has historically proven its strong predicting power and its extraordinary value as a phenomenological tool. This is despite the fact that *formally* it can be justified only in some cases in a very narrow band of temperatures. The temperature on the one hand should be high enough to permit an expansion in a small order parameter. On the other hand the temperature should not be too high because the mean-field theory becomes invalid near  $T_c$  due to critical fluctuations. Nonetheless the great success of the GL theory is due to the fact that it yields a qualitatively correct picture in extremely wide range of temperatures even when its application cannot be justified on formal grounds.

Shortly after the theoretical proposal of two-band superconductivity and more recently, two-component GL (TCGL) expansions were done in application to two-band systems, see e.g.<sup>1</sup>. However in contrast to single-component GL theory, the conditions under which TCGL model is valid is still widely believed to be an open question. In this work, we resolve this question. By taking advantage of the recently calculated normal modes and length scales in two-band Eilenberger model<sup>8</sup> we present the first self-consistent microscopic analysis of the applicability of TCGL theories to describe both linear and nonlinear responses of two-component superconductors. The results validate applicability to TCGL for studying of a wide spectrum of physical questions, including aspects of physics in low-temperatures regimes.

**The problem:** the temperature range of validity of TCGL model is bounded from below by a requirement that the field amplitudes should be small. More important bound follows from the observed, under certain conditions, disappearance of one of two fundamental length scales governing the asymptotical behavior of the superfluid density in microscopic theories<sup>8</sup>. This implies that

classical two-component field theory obtained in power-law expansion does fail at low temperatures or at substantially strong interband couplings<sup>8</sup>. Also, like for its single-component counterpart, the region of validity of TCGL expansion is bounded from above by a fluctuation region.

The key difference between TCGL and single-component GL theory is the fact that the former has several coherence lengths. The existence of multiple length scales which arise from hybridized normal modes of the linearized TCGL theory, can dramatically affect the magnetic response of the system<sup>7</sup>. Under certain conditions it results in situations where the London penetration length falls between two coherence lengths<sup>5</sup>, which was recently termed “type-1.5” regime<sup>6</sup> (for a recent brief review see<sup>9</sup>). However because the condensates in the bands are not independently conserved, in the limit  $T \rightarrow T_c$  there should be indeed only one divergent length scale associated with density variations. This in turn implies that in certain cases there also could be a temperature range close to  $T_c$  where long-wavelength physics is well approximated by a single-component GL theory (although this regime is not generic since its width is controlled by different parameters than the fluctuation region and thus it can be non-existent because of critical fluctuations). Therefore the conditions of the applicability of TCGL are quite different from that of single-component GL theory and warrant a careful investigation, which we present below.

## II. MODEL AND BASIC EQUATIONS

Expansion in powers of gradients and gap functions of microscopic equations yields the two-component

Ginzburg-Landau (TCGL) free energy density:

$$F = \left\{ \sum_{j=1,2} \left( a_j |\Delta_j|^2 + \frac{b_j}{2} |\Delta_j|^4 + K_j |\mathbf{D}\Delta_j|^2 \right) - \gamma (\Delta_1 \Delta_2^* + \Delta_2 \Delta_1^*) + \frac{B^2}{8\pi} \right\}. \quad (1)$$

where  $\mathbf{D} = \nabla + i\mathbf{A}$ ,  $\mathbf{A}$  and  $\mathbf{B}$  are the vector potential and magnetic field and  $\Delta_{1,2}$  are the gap functions in two different bands. Despite the fields  $\Delta_{1,2}$  are often called “two order parameters” in the literature, below we avoid this terminology since it is not quite accurate. First there is only  $U(1)$  local symmetry in this model in spite of the presence of two components, since the other global  $U(1)$  symmetry is explicitly broken by the terms  $\gamma (\Delta_1 \Delta_2^* + \Delta_2 \Delta_1^*)$ . Second, and more important circumstance is that the applicability of the Ginzburg-Landau or Gross-Pitaevskii classical field theory does not in general require any broken symmetries. The simplest example being two-dimensional superfluids at finite temperature: they can be indeed be described by Gross-Pitaevskii classical complex field, yet they do not possess spontaneously broken symmetry. Likewise in superfluid turbulence there is even no algebraic long-range order yet the system can be described by a classical complex field. Indeed in some cases, like e.g. in  $U(1) \times U(1)$  superconductors or superfluids one can write down two-component classical field theory on symmetry grounds. A  $U(1)$  system such as two-band superconductors can also under certain conditions be described by two-component classical field theory, although it does not automatically follows from its symmetry. The main aim of this paper is to analyze under which conditions two-band superconductors are described by TCGL theory.

To verify applicability of TCGL theory we present a comparative study of linear response and non-linear regime in TCGL and exact microscopic theories. We consider the microscopic model of clean superconductor with two overlapping bands at the Fermi level<sup>8</sup>. Within quasiclassical approximation the band parameters characterizing the two different cylindrical sheets of the Fermi surface are the Fermi velocities  $V_{Fj}$  and the partial densities of states (DOS)  $\nu_j$ , labelled by the band index  $j = 1, 2$ .

It is convenient to normalize the energies to the critical temperature  $T_c$  and length to  $r_0 = \hbar V_{F1}/T_c$ . The vector potential is normalized by  $\phi_0/(2\pi r_0)$ , the current density normalized by  $c\phi_0/(8\pi^2 r_0^3)$  and therefore the magnetic field is measured in units  $\phi_0/(2\pi r_0^2)$  where  $\phi_0 = \pi\hbar c/e$  is the magnetic flux quantum. In these units the Eilenberger equations for quasiclassical propagators take the form

$$\begin{aligned} v_{Fj} \mathbf{n}_p \mathbf{D} f_j + 2\omega_n f_j - 2\Delta_j g_j &= 0, \\ v_{Fj} \mathbf{n}_p \mathbf{D}^* f_j^+ - 2\omega_n f_j^+ + 2\Delta_j^* g_j &= 0. \end{aligned} \quad (2)$$

Here  $v_{Fj} = V_{Fj}/V_{F1}$ ,  $\omega_n = (2n+1)\pi T$  are Matsubara frequencies, the vector  $\mathbf{n}_p = (\cos\theta_p, \sin\theta_p)$  parameterizes the position on 2D cylindrical Fermi surfaces. The

quasiclassical Green’s functions in each band obey normalization condition  $g_j^2 + f_j f_j^+ = 1$ .

The self-consistency equation for the gaps is

$$\Delta_i = T \sum_{n=0}^{N_d} \int_0^{2\pi} \lambda_{ij} f_j d\theta_p. \quad (3)$$

The coupling matrix  $\lambda_{ij}$  satisfies the symmetry relations  $n_1 \lambda_{12} = n_2 \lambda_{21}$  where  $n_i$  are the partial densities of states normalized so that  $n_1 + n_2 = 1$ . The vector potential satisfies the Maxwell equation  $\nabla \times \nabla \times \mathbf{A} = \mathbf{j}$  where the current is

$$\mathbf{j} = -T \sum_{j=1,2} \sigma_j \sum_{n=0}^{N_d} \text{Im} \int_0^{2\pi} \mathbf{n}_p g_j d\theta_p. \quad (4)$$

The parameters  $\sigma_j$  are given by  $\sigma_j = 4\pi\rho n_j v_{Fj}$  and

$$\rho = (2e/c)^2 (r_0 V_{F1})^2 \nu_0.$$

The derivation of the TCGL functional (1) from the microscopic equations<sup>1</sup> formally follows the standard scheme (we present it in the Appendix A). First we find the solutions of Eqs.(2) in the form of the expansion by powers of the gap functions amplitudes  $\Delta_{1,2}$  and their gradients. Then these solutions are substituted to the self-consistency equation for the gap functions which yields the TCGL theory. The derivation of coefficients in the expansion (1) is presented in the Appendix A. Here we denote the values of coefficients obtained from microscopic theory as  $\bar{a}_\nu$ ,  $\bar{b}_\nu$ ,  $\bar{K}_\nu$  and  $\bar{\gamma}$  which are given by the expressions

$$\begin{aligned} \bar{a}_i &= \rho n_i (\bar{\lambda}_{ii} + \ln T - G_c) \\ \bar{\gamma} &= \rho n_1 n_2 \lambda_J / \text{Det} \hat{\Lambda} \\ \bar{b}_i &= \rho n_i X / T^2 \\ \bar{K}_i &= \rho v_{Fi}^2 \bar{b}_i / 4 \end{aligned} \quad (5)$$

where  $\lambda_J = \lambda_{21}/n_1 = \lambda_{12}/n_2$ . Here  $X = \zeta\zeta(3)/8\pi^2$ ,  $\bar{\lambda}_{ij} = \lambda_{ij}^{-1}$  and  $G_c = [\text{Tr} \hat{\lambda} - \sqrt{\text{Tr} \hat{\lambda}^2 - 4 \text{Det} \hat{\lambda}}] / (2 \text{Det} \hat{\lambda})$ .

Note that in general the derivation of the TCGL model is *not* implemented as an expansion in powers of a single small parameter  $\tau = (1 - T/T_c)$  but the outlined above procedure is based on the assumption of smallness of several parameters (gap functions and their gradients). Indeed the formal justification of these assumptions is not straightforward and to the present moment it has been absent<sup>1</sup>. In the present work we show under what conditions these assumptions are rigorously justified.

### III. ASYMPTOTIC BEHAVIOUR OF THE FIELDS AND COHERENCE LENGTHS.

First we investigate the asymptotical behaviour of the superconducting gaps formulated in terms of the linear modes of the density fields both in GL<sup>7</sup> and microscopic<sup>8</sup>

theories. To find the linear modes we rewrite the equations in terms of the deviations of the gap fields from their ground state values:  $\Delta_i = \Delta_{i0} + \bar{\Delta}_i$  where  $i = 1, 2$ . To illuminate the qualitatively important physics we consider a one-dimensional case in the absence of magnetic field. Let us rewrite the TCGL equations by keeping on the left hand side the terms linear in deviations  $\bar{\Delta}_i$  while collecting the higher-order nonlinear terms in the r.h.s.:

$$\begin{aligned} [K_1 d^2/dx^2 - a_1 - 3b_1 \Delta_{10}^2] \bar{\Delta}_1 + \gamma \bar{\Delta}_2 &= N_1 \\ [K_2 d^2/dx^2 - a_2 - 3b_2 \Delta_{20}^2] \bar{\Delta}_2 + \gamma \bar{\Delta}_1 &= N_2. \end{aligned} \quad (6)$$

The r.h.s. gives nonlinear source terms  $N_i = b_i(3\Delta_{i0}\bar{\Delta}_i^2 + \bar{\Delta}_i^3)$ . The solution of Eq.(6) can be found in Fourier representation to have the form

$$\bar{\Delta}_i(k) = \hat{R}_{ij}^{-1} N_j(k) \quad (7)$$

where

$$\begin{aligned} R_{12} &= R_{21} = \gamma \\ R_{ii} &= -[K_i k^2 + a_i + 3b_i \Delta_{i0}^2]. \end{aligned}$$

In this case the response function  $\hat{R}^{-1}$  has two poles in the upper complex half-plane  $k = i\mu_H$  and  $k = i\mu_L$  which determine the two inverse length scales or, equivalently, the two masses of composite gap functions fields<sup>7</sup>, which we denote as “heavy”  $\mu_H$  and “light”  $\mu_L$  (i.e.  $\mu_H > \mu_L$ ).

Let us set  $K_1 = K_2$  which can be accomplished by rescaling the fields  $\Delta_{1,2}$ . Then the matrix  $\hat{R}^{-1}(k)$  can be diagonalized with the  $k$ -independent rotation introducing the new linear modes of the fields  $\Phi_\beta = U_{\beta i} \bar{\Delta}_i$  and the sources  $N_\beta = U_{\beta i} N_i$  where  $\beta = L, H$  and  $i = 1, 2$ . The rotation matrix  $\hat{U}$  is characterized by the mixing angle<sup>7,8</sup> as follows:

$$\hat{U} = \begin{pmatrix} \cos \theta_L & \sin \theta_L \\ -\sin \theta_H & \cos \theta_H \end{pmatrix} \quad (8)$$

Using the diagonal form of the response function  $\hat{R}^{-1}(k)$  in the real-space domain we obtain

$$\Phi_\beta(x) = -\frac{1}{2\mu_\beta} \int_0^\infty dx_1 e^{-\mu_\beta |x_1 - x|} N_\beta(x_1) + C_\beta e^{-\mu_\beta x} \quad (9)$$

where  $C_\beta = \int_0^\infty [N_\beta(x) + 2N_\beta(0)] e^{-\mu_\beta x} dx / 2\mu_\beta$  is chosen so that to satisfy the boundary condition  $\Phi_\beta(0) = N_\beta(0) / \mu_\beta^2$  which corresponds to the condition  $\Delta_{1,2}(0) = 0$  at  $x = 0$ .

### A. The limit $\tau \rightarrow 0$ .

The expression (9) shows that two fields  $\Phi_{L,H}$  vary at distinct coherence lengths:  $\xi_H = 1/\mu_H$  and  $\xi_L = 1/\mu_L$ . They constitute fundamental length scales of the TCGL theory (1). They characterize the asymptotical relaxation of the linear combinations of the fields  $\Delta_{1,2}$ , the linear combinations are represented by the composite fields

$\Phi_{L,H}$ . Our calculation shows that these length scales behave qualitatively different in the limit  $\tau \rightarrow 0$ . Infinitesimally close to  $T_c$  the largest length diverges as  $\xi_L \sim \tau^{-1/2}$  while the smaller  $\xi_H$  remains finite. Similar behavior also follows from full microscopic calculation shown on Fig.(1)b,c,d where the temperature dependence of masses  $\mu_{L,H}$  is plotted. The presence of the non-diverging length scale  $\xi_H$  makes the qualitative difference with the single-band GL theory but indeed does not contradict the standard textbook picture that *in the limit*  $\tau \rightarrow 0$  the mean field theory of a  $U(1)$  system should be well approximated by single-component GL model. As we show below the amplitude of the “heavy” mode vanishes in the  $\tau \rightarrow 0$  limit faster than that of “light” mode. Neglecting the “heavy” mode contribution one indeed obtains a single-component GL theory.

We can use the Eq.(9) to evaluate the asymptotical amplitudes of  $\Phi_{H,L}(r)$  in terms of the powers of the expansion parameter  $\tau$ , in the limit  $\tau \rightarrow 0$ . The goal is to evaluate how the contributions from different length scales affect overall profile of the fields as they recover their ground state value away from  $x = 0$ . First we note that the source terms  $N_{L,H}(x)$  are confined at the region determined by the coherence length  $x < \xi_L$ . Inside this region the amplitude of the deviations of the gaps from the ground state values are large so that

$$\bar{\Delta}_i(x) \sim \Delta_{0i} \sim \tau^{1/2}.$$

Thus the amplitude of sources is of the order  $N_{L,H} \sim \tau^{3/2}$ . Let us consider the first term in the expression (9) for  $\beta = L$  at the asymptotical region  $x > \xi_L$ . In this case the integration is confined within  $x_1 < \xi_L$  and yields the following estimate  $\Phi_L \approx A_L e^{-\mu_L x}$  where

$$A_L \sim \xi_L \tau^{3/2} \sim \tau^{1/2}.$$

The second term in the Eq.(9) gives the contribution of the same order to the amplitude of the “light” mode.

The amplitude of the “heavy” mode is determined entirely by the first term in Eq.(9) for  $\beta = H$ . We consider the asymptotical region  $x \ll \xi_L$  therefore in this estimate we put  $N_H(x_1) \approx N_H(0)$  so that

$$\Phi_H(x) = N_H(0) (2e^{-\mu_H x} - 1) / \mu_H^2.$$

The function  $\Phi_H(x)$  has a characteristic scale  $\xi_H = 1/\mu_H$  and its overall amplitude is determined by the factor

$$A_H \sim N_H(0) / \mu_H^2 \sim \tau^{3/2}.$$

Thus in the limit  $\tau \rightarrow 0$  the “heavy” mode drops out because of the vanishing amplitude  $A_H \sim \tau^{3/2}$  as compared to the “light” mode  $A_L \sim \tau^{1/2}$ . Note that it is thus principally incorrect to attribute different exponents directly to the functions  $\Delta_i$  and to assume that they become equal in the limit  $\tau \rightarrow 0$  as claimed in<sup>2</sup> and followed in some other literature<sup>4</sup>.

On the qualitative level we give a less technical but on the other hand more intuitively transparent description

of the limiting behavior of the fields near  $T_c$ . We consider the situation where the coefficients of quadratic terms in Eq.(1) can be written in the form  $a_j(T) = \alpha_j(T - T_j)$  with  $\alpha_j > 0$ . Thus in the small  $\tau$  limit, first the weakest superconducting component becomes passive: it has nonzero superfluid density only because of the bilinear Josephson coupling  $\gamma(\Delta_1 \Delta_2^* + c.c.)$ . To elucidate what happens in the  $\tau \rightarrow 0$  limit one can redefine fields using the following transformation  $\mathbf{\Delta} = \mathbf{X}_D \Psi_D(\mathbf{r}) + \mathbf{X}_S \Psi_S(\mathbf{r})$  where  $\mathbf{X}_D = (\alpha_2(T_D - T_2), \gamma)^T$ ,  $T_D \equiv T_c$  is the critical temperature,  $\mathbf{X}_S = (\gamma, \alpha_1(T_S - T_1))^T$  and  $T_S = T_1 + T_2 - T_D < T_D$ . This transformation, mixes the gaps and produces a representation where the bilinear Josephson coupling between the new fields is eliminated at the cost of introducing mixed gradient and fourth-order couplings:

$$F = \sum_{i,j=D,S} K_{ij} \mathbf{D}\Psi_i (\mathbf{D}\Psi_j)^* + \beta_i(T - T_i) |\Psi_i|^2 + \sum_{i,j,k,l=D,S} \beta_{ijkl} \text{Re}(\Psi_i \Psi_j \Psi_k^* \Psi_l^*). \quad (10)$$

In the limit  $\tau \rightarrow 0$  the dominant component  $\Psi_D$  becomes single-component GL order parameter while the component  $\Psi_S$  is passive. However instead of being induced by the bilinear Josephson coupling,  $\Psi_S$  is induced by the terms like  $\Psi_S \Psi_D^* |\Psi_D|^2$ . Thus for  $\tau \rightarrow 0$  one has  $\Psi_D \sim \tau^{1/2}$ . From the fact that  $\beta_S(T - T_S)$  and  $\beta_{SDDD}$  are finite at  $\tau = 0$  it follows that in the same limit we have  $\Psi_D \gg \Psi_S \sim \tau^{3/2}$ . It means that *in the limit*  $\tau \rightarrow 0$  retaining only the terms containing  $\Psi_D$  is justified and it allows to approximate the model by a conventional single order parameter theory.

For infinitesimally small  $\tau$  there remains only single GL equation for the order parameter  $\Psi_D$

$$-K_{DD} \mathbf{D}^2 \Psi_D + \beta_D(T - T_c) \Psi_D + \beta_{DDDD} \Psi_D |\Psi_D|^2 = 0 \quad (11)$$

where  $\beta_{DDDD} = (a_{2D}^2 b_1 + a_{1D}^2 b_2) / \alpha_1$  and

$$\beta_D = \frac{T_D - T_S}{T_D - T_2} > 0 \quad (12)$$

$$K_{DD} = \frac{a_{1D} K_2 + a_{2D} K_1}{\alpha_1 \alpha_2 (T_D - T_2)},$$

where  $a_{1,2D} = a_{1,2}(T_D)$ .

Thus it is the disappearance of the amplitude of the subdominant mode which allows one to take a single-component GL limit in this mean-field theory. The ‘‘heavy’’ mode with finite mass even infinitesimally close to  $T_c$  is generated here by the presence of the term  $|\mathbf{D}\Psi_S|^2 \sim \xi_H^{-2} |\Psi_S|^2$  where  $\xi_H$  is a finite length not diverging at  $T_c$ . Therefore near  $T_c$  one has  $|\mathbf{D}\Psi_S|^2 \sim \xi_H^{-2} |\Psi_S|^2 \sim \tau^3$  which is of the same order as the other terms in the free energy functional. Note that the fields  $\Psi_{D,S}$  introduced here are not directly related to the normal modes of the system since the mixed gradient and quartic terms will lead to mode mixing<sup>7</sup> at finite  $\tau$ . Also note that despite there is a growing disparity of the coherence lengths at small but finite  $\tau$  when one approaches critical temperature, it does not imply that one necessary

falls into type-1.5 regime because  $\xi_1 < \lambda < \xi_2$  is only necessary but not sufficient condition for the appearance of this regime. That is, a system in some of these cases is type-I despite having  $\xi_1 < \lambda < \xi_2$ .

## B. GL theory at finite $\tau$ .

Unfortunately the limiting  $\tau \rightarrow 0$  analysis does not have much physical significance in a generic two-band system. First, the mean-field theory becomes invalid in the same limit  $\tau \rightarrow 0$  so the regime where the system is well described by single-component GL theory can be cutoff by critical fluctuations. More importantly, as we argue below, this analysis is in general inapplicable for an assessment of, e.g. magnetic response of the system. The magnetic response is a finite-length scale property and requires finite- $\tau$  theory. Finally, as shown in microscopic calculations the masses of the fields in two-band models in certain cases change rapidly and in a non-trivial way with decreasing temperature. Thus a limiting  $\tau \rightarrow 0$  analysis in general cannot give even an approximate physical picture even at very small  $\tau$ . In particular that implies that in a two-band system, a Ginzburg-Landau parameter (which one, may in principle construct in the  $\tau \rightarrow 0$  limit at a mean-field level) is not a useful characteristic. Rather it is required to make an accurate quantitative study of two-band theory at finite  $\tau$  to determine the conditions under which the model can be described by single- or two- component GL theory or does not allow a description by any such GL functionals at all. In order to do it we utilize the exact form of the response function  $\hat{R}^{-1}$  (i.e. valid at any  $T$ ) found from the linearized microscopic theory according to the procedure developed in<sup>8</sup>. In contrast to the GL theory, the microscopic response function  $\hat{R}^{-1}(k)$  has branch cuts along the imaginary axis starting at point  $\pm i k_{bc}$  where  $k_{bc} = 2\sqrt{\Delta_{02}^2 + (\pi T)^2}$  (we assume that  $\Delta_{02} < \Delta_{01}$ ). Inside the circle  $|k| < |k_{bc}|$  shown by the white area in Fig.(1)a the response function is meromorphic, i.e. its singular points are only poles shown by the red crosses. The non-meromorphic region is marked by the yellow shade in all panels of Fig.(1). In general inside the meromorphic circle there can be two poles of  $\hat{R}^{-1}(k)$  at  $\text{Im}(k) > 0$  shown by red crosses in Fig.(1)a. Analogously to TCGL these poles determine the masses  $\mu_{L,H}$  of the ‘‘heavy’’ and ‘‘light’’ modes, and thus the corresponding coherence lengths. The contribution of the branch cut contains the continuous spectrum of length scales shorter than  $1/k_{bc}$  which can not be described within GL theory. Moreover for some parameters (e.g. at strong Josephson coupling) one of the poles which corresponds to the ‘‘heavy’’ mode can disappear by merging with the branch cut. In this case there is only one fundamental length scale left since the contribution of the ‘‘heavy’’ mode can not be separated from the branch cut.

The microscopically calculated temperature dependen-

cies of masses of the modes in a superconductor with weak interband coupling are shown in Fig.(1)b by red solid lines. For a reference we also plot masses in  $U(1) \times U(1)$  theory which has two independently diverging coherence lengths at  $T = T_{c1}$  and  $T = T_{c2}$  (chosen to be  $T_{c2} = 0.5T_{c1}$ ). For coupled bands the hybridization of modes removes the divergence at  $T = T_{c2}$  and introduces the avoided crossing point of the “heavy” and “light” modes.

Let us now assess the applicability of minimal TCGL model Eq.(1) without using expansion in powers of  $\tau$ . Compared to the previous works<sup>1</sup>, we use more complicated temperature dependence of the coefficients derived in the Appendix A. Let us compare the behavior of the masses of the modes in the microscopically derived TCGL and a full microscopic theory. It is shown for the cases of weak and strong interband coupling in Fig.(1)c,d. We have found that TCGL theory describes the lowest characteristic mass  $\mu_L(T)$  with a very good accuracy near  $T_c$  [compare the blue and red curves in Fig. (1)c,d]. Remarkably, when interband coupling is relatively weak [Fig.(1)c] the “light” mode is quite well described by TCGL also at low temperatures down to  $T = 0.5T_c$  around which the weak band crosses over from active to passive (proximity-induced) superconductivity. Indeed the  $\tau$  parameter is large in that case and cannot be used at all to justify a GL expansion. Nonetheless if the interband coupling is small one does have a small parameter to implement a GL expansion for one of the components. Namely one can still expand, e.g. in the powers of the weak gap  $|\Delta_2|/\pi T \ll 1$ . On the other hand for the “heavy” mode we obtain some discrepancies even relatively close to  $T_c$ , although TCGL theory gives qualitatively correct picture for this mode when the interband coupling is not too strong. More substantial discrepancies between TCGL and microscopic theories appear only at lower temperatures or at stronger interband coupling [Fig.(1)d] where the microscopic response function has only one pole, while TCGL theory generically has two poles.

Comparison of the masses of normal modes of a  $U(1) \times U(1)$  (dotted blue lines) and a weakly coupled two-band  $U(1)$  model (red lines) shown in Fig.(1)d demonstrates that adding a Josephson coupling removes divergence of coherence length of the weak band. This is because the Josephson coupling represents explicit symmetry breakdown from  $U(1) \times U(1)$  to  $U(1)$  and thus eliminates one of the superconducting phase transitions at lower  $T_c$ . However when this coupling is weak one of the coherence lengths has a substantial peak around that temperature. The peaked behaviour of coherence length near the critical temperature of the weak superconducting band is has clear physical manifestation in the temperature dependence of the vortex core size. Let us note that to assess the overall size of core requires analysis of full nonlinear theory. In Fig.(2) we plot the sizes of the vortex cores in weak and strong bands calculated in the full nonlinear model according to the two alternative definitions. The

first one is the slope of the gap function distribution at  $r = 0$  which characterizes the width of the vortex core near the center  $R_{cj} = (d \ln \Delta_j / dr)^{-1}(r = 0)$  [Fig.(2)a]. The second one is the healing length  $L_{hj}$  defined as  $\Delta_j(L_{hj}) = 0.95\Delta_{0j}$  [Fig.(2)b] (i.e. this length is not directly related to exponents but quantifies at what length scales the gap functions almost recover their ground state values). Both definitions demonstrate the stretching of the vortex core in the weak component related to the peak of the coherence length shown in the Fig.(1)d. Note that the weak band healing length  $L_{h2}(T)$  in Fig.(2)b has maximum at the temperature slightly larger than  $T_{c2}$  which is consistent with the fact that the maximum of coherence length  $\xi_L$  (equivalently the minimum of the field mass  $\mu_L$ ) in Fig.(1)d is shifted to the temperature above  $T_{c2}$  ( $T_{c2}$  is defined as the lower critical temperature in the limit of no Josephson coupling).

### C. Effects of higher order gradient terms.

The origin of the small disagreement between the TCGL and microscopic masses of the “heavy” mode is the absence of higher-order gradient terms in the expansion (1). The inclusion of higher order gradients means adding more terms to the Taylor expansion of the function  $\hat{R}(k)$  which is known to converge inside the circle  $|k| < |k_{bc}|$ . Using this procedure one can get a better agreement with microscopic theory (compare green dashed and red solid lines in Fig.(1)c,d). However, such an extension is hardly useful because as a byproduct it generates unphysical artifacts such as many parasitic poles of the response function  $\hat{R}^{-1}(k)$  outside the circle  $|k| < |k_{bc}|$ . The position of parasitic poles appearing in the sixth-order gradient expansion is shown by green circles in the Fig.(1a). These parasitic poles lie outside the imaginary axis, thus yielding unphysical oscillating contributions to asymptotical behavior of the corresponding linear modes.

### D. Characteristic length scale of the phase difference variations.

In the  $U(1) \times U(1)$  system one has two massive modes associated with the modules of the complex fields and a Goldstone boson associated with the phase difference. If one adds a Josephson coupling there appears also the third mass parameter. When Josephson term is present the phase difference acquires a preferred value. Its deviations from the preferred value are characterized by a mass parameter. In the constant density approximation the terms of the TCGL functional which describe the phase difference mode are:

$$\frac{1}{2} \frac{K_1 K_2 \Delta_{10}^2 \Delta_{20}^2}{K_1 \Delta_{10}^2 + K_2 \Delta_{20}^2} (\nabla(\theta_1 - \theta_2))^2 - \gamma \Delta_{10} \Delta_{20} \cos(\theta_1 - \theta_2) \quad (13)$$

Expanding the second term gives the mass parameter for the phase difference mode

$$m_{(\theta_1-\theta_2)} = \sqrt{\gamma \frac{K_1 \Delta_{10}^2 + K_2 \Delta_{20}^2}{K_1 K_2 \Delta_{10} \Delta_{20}}}. \quad (14)$$

It is useful to consider the behavior of this mass in the limit  $T \rightarrow T_c$ . In that case we have  $\Delta_{10,20} \propto \sqrt{1 - T/T_c}$ . Thus

$$\lim_{T \rightarrow T_c} (m_{(\theta_1-\theta_2)}) \rightarrow const \quad (15)$$

To summarize this part we have shown that the TCGL model of the form given by Eq. (1) with microscopically derived temperature dependencies of coefficients is overall highly accurate at elevated temperatures. The small discrepancies with microscopic theory affect only short-length scale physics which implies that TCGL model gives the precise answer for long-range intervortex forces. Also we find that in some cases the TCGL model provides an accurate description of the large length scales physics at temperatures much lower than  $T_c$ . In Appendix A 1 we discuss the origin of the disagreements between these results and some of the recent literature<sup>4</sup>.

#### IV. VORTEX STRUCTURE: TCGL VS MICROSCOPIC THEORY.

For inhomogeneous situations, such as vortex solutions, the overall profiles of the fields is affected not only by fundamental length scales (i.e. coherence lengths) but also by nonlinear effects.

Let us now study non-linear effects case of vortex solutions. Obviously, because of the growing importance of nonlinear effects at lower temperatures the Eq.(1) cannot describe quantitatively well the total structure of vortices when  $T \ll T_c$ . In Fig.(3) we compare the vortex solutions in the self-consistent microscopic theory (red dotted curves) and in the corresponding TCGL theory with coefficients obtained by expansion (blue dashed-dotted curves). One can see that at elevated temperatures the agreement is very good but for lower temperatures there is a growing discrepancy. One of the reasons behind the discrepancy is the trivial shift of the ground state values of the fields by nonlinearities. Note that at the level of GL theory the inclusion of more nonlinear terms merely renormalizes masses and length scales but does not alter the form of linear theory<sup>7</sup>. Thus in the current example of the full nonlinear model it is also reasonable to check if one could get a better agreement with microscopic theory by treating the coefficients in the minimal TCGL model Eq.(1) phenomenologically. For all practical purposes this provides alternative route to the more restrictive approach of finding a refined microscopic expansion. A good agreement with the microscopic theory in this procedure will imply that the system does possess a description in terms of a classical two-component field theory.

$T$	0.98	0.8	0.7	0.5	0.4	0.2
$b_1$	$0.95\bar{b}_1$	$0.85\bar{b}_1$	$0.76\bar{b}_1$	$0.54\bar{b}_1$	$0.44\bar{b}_1$	$0.18\bar{b}_1$
$K_1$	$\bar{K}_1$	$0.8\bar{K}_1$	$0.65\bar{K}_1$	$0.5\bar{K}_1$	$0.4\bar{K}_1$	$0.15\bar{K}_1$
$b_2$	$\bar{b}_2$	$\bar{b}_2$	$\bar{b}_2$	$0.76\bar{b}_2$	$0.64\bar{b}_2$	$0.29\bar{b}_2$
$K_2$	$\bar{K}_2$	$0.55\bar{K}_2$	$0.35\bar{K}_2$	$0.3\bar{K}_2$	$0.15\bar{K}_2$	$0.08\bar{K}_2$

TABLE I: Fitting of TCGL coefficients to match the solutions of exact microscopic equations. Here we denote the values of coefficients obtained from microscopic theory as  $\bar{a}_\nu$ ,  $\bar{b}_\nu$ ,  $\bar{K}_\nu$  and  $\bar{\gamma}$ .

We compared the vortex solutions in the TCGL theory with fitted coefficients and the exact microscopic model for the particular example of the system with coupling constants  $\lambda_{11} = 0.5$ ,  $\lambda_{22} = 0.46$ ,  $\lambda_{12} = \lambda_{21} = 0.005$  and  $v_{F2}/v_{F1} = 5$ . The values of the coefficients which provide the best fit are listed in the table I.

By the green dashed lines we show the fits obtained by setting the values of the TCGL coefficients as listed in the table I. By doing it we find that the solutions of microscopic equations in a large region of parameters can be fitted with excellent accuracy by the effective TCGL theory, even at quite low temperatures. The main discrepancies at very low temperatures arise due to non-local effects which lead to the disappearance of the ‘‘heavy’’ asymptotic mode as well as due to Kramer-Pesch-like vortex core shrinking<sup>8,10</sup> in both components which cannot be captured in the TCGL field theory. Note however that even in the case where TCGL description starts breaking down, the discrepancy is mostly pronounced near the origin of the core, while the soft modes and long-range intervortex interaction can be well described by a phenomenological TCGL theory.

#### V. CONCLUSIONS

TCGL model is widely used for describing various aspects of multiband superconductivity. However the TCGL expansion has never been rigorously justified for two-band systems, and the current literature contains diametrically opposite claims regarding the validity of the expansion or such basic aspects as the form of TCGL functional and behavior of the coherence lengths near  $T_c$ <sup>1,2,4</sup>. We investigated under which conditions a two-band system can be described by a TCGL theory. First we obtained a TCGL model with a microscopically derived temperature dependence of coefficients (more general than what could be obtained in a straightforward  $\tau$  expansion) and demonstrated that it gives an accurate description of length scales and vortex solutions at elevated temperatures by a comparison with an exact microscopic theory. Second we have shown that, in a much wider range of temperatures, the minimal TCGL model with phenomenologically adjusted coefficients gives an accurate description of linear and nonlinear physics such

as vortex excitations and thus the magnetic response of the system.

The existence of two coherence lengths  $\xi_L, \xi_H$  along with the magnetic field penetration lengths  $\lambda$  in the TCGL model makes it impossible in general to define the Ginzburg-Landau parameter in two-band systems, unless one takes the limit  $\tau \rightarrow 0$ . In contrast to  $U(1) \times U(1)$  superconductors, the two-band systems have only  $U(1)$  symmetry, and as we discussed above it guarantees that one of the modes drops out of the mean field theory the limit  $\tau \rightarrow 0$  allowing one to define in that limit  $\kappa_{GL} = \xi_L(T \rightarrow T_c)/\lambda(T \rightarrow T_c)$ . However, even slightly away from the limit  $\tau \rightarrow 0$ , when interband coupling is weak the ratio  $\xi_L/\lambda$  has a very strong temperature dependence and the second mode develops with the coherence  $\xi_H$ . Thus in general  $\kappa_{GL}$  cannot be used as universal characteristic of magnetic response of two-band systems.

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## Appendix A: Microscopic model and derivation of TCGL

### 1. Ginzburg-Landau expansion.

To derive differential GL equations (6) from the microscopic theory, first we find the solutions of Eilenberger Eqs.(2) in the form of the expansion by the gap functions amplitudes  $|\Delta_{1,2}|$  and their gradients  $|(\mathbf{Dn}_p)\Delta_{1,2}|$ . Then these solutions are substituted to the self-consistency Eq.(3). Using this procedure we find the solutions of Eqs.(2) in the form:

$$f = \frac{\Delta}{\omega_n} - \frac{|\Delta|^2 \Delta}{2\omega_n^3} - \frac{v_F}{2\omega_n^2} (\mathbf{Dn}_p)\Delta + \frac{v_F^2}{4\omega_n^3} (\mathbf{Dn}_p)(\mathbf{Dn}_p)\Delta. \quad (\text{A1})$$

and  $f^+(\mathbf{n}_p) = f^*(-\mathbf{n}_p)$ . Note that a GL expansion is based on neglecting the higher-order terms in powers of  $|\Delta|$  and  $|(\mathbf{Dn}_p)\Delta|$ . Indeed this approximation naturally fails in a number of cases. In this work we determine the regimes when it can be justified, in particular by direct comparison with exact microscopic model. Let us determine microscopic coefficients in the GL expansion. Substituting to the self-consistency Eqs.(3) and integrating by  $\theta_p$  we obtain

$$\Delta_1 = (\lambda_{11}\Delta_1 + \lambda_{12}\Delta_2)G + (\lambda_{11}GL_1 + \lambda_{12}GL_2) \quad (\text{A2})$$

$$\Delta_2 = (\lambda_{21}\Delta_1 + \lambda_{22}\Delta_2)G + (\lambda_{21}GL_1 + \lambda_{22}GL_2) \quad (\text{A3})$$

where

$$G = 2 \sum_{n=0}^{N_d} \frac{\pi T}{\omega_n}; \quad X = \sum_{n=0} \frac{\pi T}{\omega_n^3} \quad (\text{A4})$$

$$GL_j = X \left( \frac{v_{Fj}^2}{4} \mathbf{D}^2 \Delta_j - |\Delta_j|^2 \Delta_j \right) \quad (\text{A5})$$

Expressing  $GL_i$  from the equations above we obtain

$$n_1 GL_1 = n_1 \left( \frac{\lambda_{22}}{\text{Det}\hat{\Lambda}} - G \right) \Delta_1 - \frac{\lambda_J n_1 n_2}{\text{Det}\hat{\Lambda}} \Delta_2 \quad (\text{A6})$$

$$n_2 GL_2 = n_2 \left( \frac{\lambda_{11}}{\text{Det}\hat{\Lambda}} - G \right) \Delta_2 - \frac{\lambda_J n_1 n_2}{\text{Det}\hat{\Lambda}} \Delta_1 \quad (\text{A7})$$

Comparing these Eqs with Eqs (6) we obtain the expression for the coefficients

$$\bar{a}_i = \rho n_i (\tilde{\lambda}_{ii} + \ln T - G_c) \quad (\text{A8})$$

$$\bar{\gamma} = \rho n_1 n_2 \lambda_J / \text{Det}\hat{\Lambda}$$

$$\bar{b}_i = \rho n_i X / T^2$$

$$\bar{K}_i = \rho v_{Fi}^2 \bar{b}_i / 4$$

where  $\lambda_J = \lambda_{21}/n_1 = \lambda_{12}/n_2$ . The temperature is normalized to the  $T_c$ . Here  $X = 7\zeta(3)/8\pi^2$ ,  $\tilde{\lambda}_{ij} = \lambda_{ij}^{-1}$  and

$$G_c = G(T_c) = \frac{\text{Tr}\lambda - \sqrt{\text{Tr}\lambda^2 - 4\text{Det}\lambda}}{2\text{Det}\lambda}.$$

We have used the expression  $G(T) = G(T_c) - \ln T$ . Near the critical temperature  $\ln T \approx -\tau$  and we obtain  $\bar{a}_i = n_i \lambda_J (T - T_i)$  where  $T_i = (1 + G_c - \tilde{\lambda}_{ii})$ .

### 2. Remark on $\tau$ -expansion

Here we comment on the origin of the qualitative disagreement of our result compared to the work<sup>4</sup> which aims at calculating higher order corrections in  $\tau = (1 - T/T_c)$ . First let us make a few general remarks: Note that in the derivation of TCGL theory we do not implement an expansion in powers of  $\tau = (1 - T/T_c)$ . Instead we retain more complicated temperature dependence of the coefficients. Also we stress that any approach to GL expansion depends on what parameters are assumed to be small, the question is always how and for what parameters such an assumption is justified. The origin of the principal difference in the behavior of the length scales (Ref.<sup>4</sup> asserts that there are two divergent length scales when  $\tau \rightarrow 0$ ). It originates in the adoption in<sup>4</sup> of a  $U(1) \times U(1)$  theory as the leading order in expansion following the erroneous derivation in<sup>2</sup> (see the discussion of the errors in that derivation in<sup>3</sup>). Another problem with a straightforward implementation of the expansion by  $\tau$  is that *in general* it is uncontrollable in the next to leading order in two-band theories, if one explicitly retains two gap fields. This is because in contrast to the single-component GL theory, in general it is not possible to classify different terms by powers of the parameter  $\tau$ . As shown in the main body of the paper, system contains a mode with non-diverging coherence length so that the spatial derivatives in general do not necessary add the power of  $\tau$ . Also since the work<sup>4</sup> uses as a leading order the incorrect derivation from<sup>2</sup> it requires adjustments.

## Appendix B: Asymptotic in two-dimensional vortex problem

The consideration of asymptotic modes in Sec.III can be generalized for the two-dimensional axially symmetric problem, which allows to treat the asymptotical behaviour of the gap functions far from the vortex core. First of all in this case one should substitute the  $d^2/dx^2$  by  $\nabla_r^2 = d^2/dr^2 + r^{-1}d/dr$  in Eq. (6).

Choosing the proper value of the mixing angle the l.h.s. of Eq. (6) can be diagonalized and the system acquires the form

$$(\nabla_r^2 - \mu_i^2) \bar{\Psi}_i = N_i \quad (\text{B1})$$

where the nonlinear  $N_{H,L}$  are obtained according to the rule (8).

Our interest is the asymptotical behaviour of the fields  $\bar{\Delta}_{L,H}$  determined by the equation above. The solution of Eq.(B1) can be found in Fourier representation  $\bar{\Delta}(k) = \int_{-\infty}^{\infty} \Delta(x)e^{ikx} dx$  to have the form (7). In this particular case the response function is a diagonal matrix:

$$\hat{R}(k) = \begin{pmatrix} (k^2 + \mu_H^2) & 0 \\ 0 & (k^2 + \mu_L^2) \end{pmatrix}$$

In the real-space domain the field components can be expressed with the help of Fourier-Bessel transform

$$\bar{\Psi}_i = \int_0^{\infty} J_0(kr_1) J_0(kr) \hat{R}_{ij}^{-1} N_j(r_1) k dk r_1 dr_1.$$

The integration by  $k$  in this expression can be performed by transforming the contour in the complex plane. Using the exact form of the response function the fields asymptotic is found to be given by the following expression

$$\bar{\Psi}_i(r) = \pi K_0(\mu_i r) \int_0^r r_1 dr_1 I_0(\mu_i r_1) N_i(r_1) + \pi I_0(\mu_i r) \int_r^{\infty} r_1 dr_1 K_0(\mu_i r_1) N_i(r_1) \quad (\text{B2})$$

where  $K_0$  and  $I_0$  are modified Bessel functions having the following asymptotics  $K_0, I_0(x) \approx e^{\mp x}/\sqrt{x}$ .

The expression (B2) yields a number of length scales characterizing the asymptotical relaxation of the gap fields. The largest length is the mean field coherence length  $\xi_L = 1/\mu_L \sim 1/\tau^{1/2}$ . However the presence of the another linear mode in the theory sets the scale which is proportional to  $\xi_H = 1/\mu_H$ . This scale remains finite even at  $T = T_c$  but its amplitude vanishes.

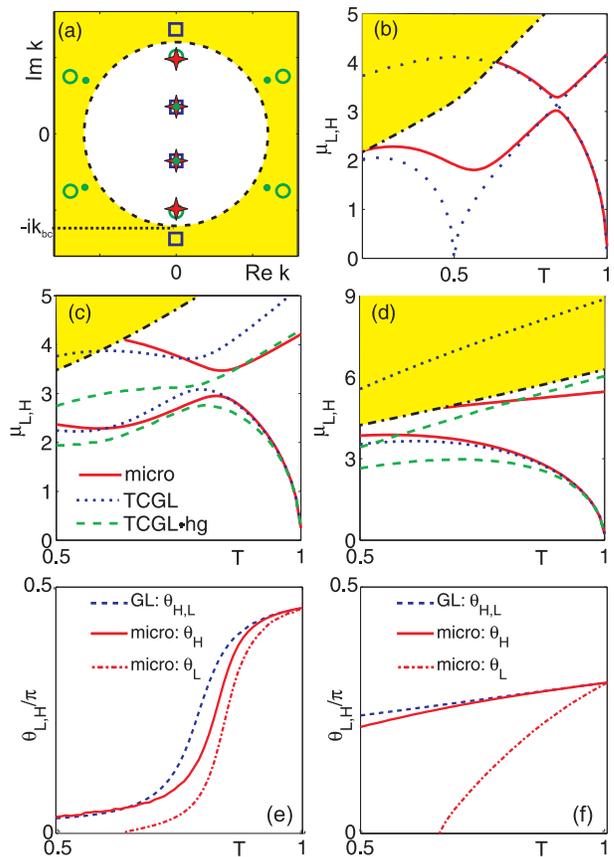


FIG. 1: (a) Comparison of the response function singularities in the complex  $k$  plane given by the exact microscopic and microscopically derived TCGL theories. Red crosses are the physical poles of microscopic theory. Blue squares correspond to the conventional TCGL theory while green circles show the parasitic poles appearing in TCGL expansion up to sixth order in gradients. The white circle is the area where  $\hat{R}(k)$  is analytical and  $\hat{R}^{-1}(k)$  is meromorphic. In all plots (a-d) the yellow shade indicates the area where the response function is not meromorphic. (b) Comparison of the masses of normal modes of a  $U(1) \times U(1)$  (dotted blue lines) and a weakly coupled two-band  $U(1)$  model (red lines). For the weak component in the  $U(1) \times U(1)$  we also plot the correlation length for superconducting fluctuations in the normal state for  $T > T_{c2}$ . As clearly seen in that plot, adding a Josephson coupling removes divergence of coherence length of the weak band. This is because the Josephson coupling represents explicit symmetry breakdown from  $U(1) \times U(1)$  to  $U(1)$  and thus eliminates the phase transition at lower  $T_c$ . However when this coupling is weak one of the coherence lengths has a peak around that temperature. (c) and (d) Comparison of field masses given by microscopic (solid lines), TCGL (dotted) and TCGL with sixth-order gradients (dashed lines) theories. The microscopic parameters are  $\lambda_{11} = 0.5$ ,  $\lambda_{22} = 0.426$  and  $\lambda_{12} = \lambda_{21} = 0.005$ ; 0.01; 0.1 for (b,c,d) correspondingly. (e-f) Comparison of the mixing angle behaviour given by the exact microscopic (red lines) and microscopically derived TCGL theories (blue line). Parameters are the same as on the panels (c-d) correspondingly. Panels (d) and (f) show a pattern how the TCGL theory starts to deviate from the microscopic theory at lower temperature when interband coupling is increased.

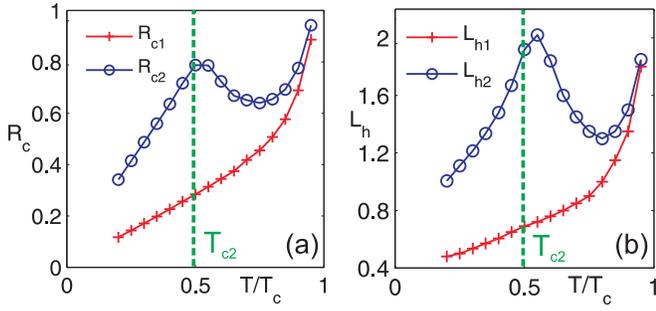


FIG. 2: (a) Sizes of the vortex cores  $R_{c1,2}$  and (b) healing lengths  $L_{h1,2}$  in weak (blue curve, open circles) and strong bands (red curve, crosses) as functions of temperature. The parameters are  $\lambda_{11} = 0.5$ ,  $\lambda_{22} = 0.426$ ,  $\lambda_{12} = \lambda_{21} = 0.0025$  and  $v_{F2}/v_{F1} = 1$ . In the low temperature domain, the vortex core size in the weak component grows and reaches a local maximum near the temperature  $T_{c2}$  (the temperature near which the weaker band crosses over from being active to having superconductivity induced by an interband proximity effect)<sup>8</sup>. In the absence of interband coupling there is a genuine second superconducting phase transition at  $T_{c2} = 0.5T_{c1}$  where the size of the second core diverges. When interband coupling is present it gives an upper bound to the core size in this temperature domain, nonetheless this regime is especially favorable for appearance of type-1.5 superconductivity<sup>8</sup>.

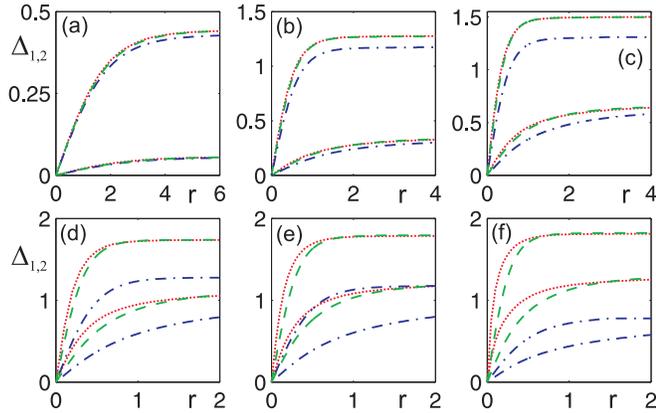


FIG. 3: Behavior of the gap functions  $\Delta_{1,2}(r)$  in a vortex solution. Comparison of the results of exact microscopic calculation (red dotted lines), TCGL with microscopically calculated coefficients (blue dash-dotted lines) and TCGL with phenomenologically fitted coefficients (green dashed lines) at (a)  $T = 0.98$ , (b)  $T = 0.8$ , (c)  $T = 0.7$ , (d)  $T = 0.5$ , (e)  $T = 0.4$ , (f)  $T = 0.2$ . Coupling constants are  $\lambda_{11} = 0.5$ ,  $\lambda_{22} = 0.46$ ,  $\lambda_{12} = \lambda_{21} = 0.005$  and  $v_{F2}/v_{F1} = 5$ .

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