Is the term “type-1.5 superconductivity” warranted by Ginzburg-Landau theory?

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It is shown that within the Ginzburg-Landau (GL) approximation the order parameters \(\Delta_1(r,T)\) and \(\Delta_2(r,T)\) in two-band superconductors vary on the same length scale, the difference in zero-\(T\) coherence lengths \(\xi_{\nu} \sim \hbar v_F / \Delta_{\nu}(0)\), \(\nu = 1, 2\) notwithstanding. This amounts to a single physical GL parameter \(\kappa\) and the classic GL dichotomy: \(\kappa < 1/\sqrt{2}\) for type-I and \(\kappa > 1/\sqrt{2}\) for type-II.

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I. INTRODUCTION

The physics of all superconductors near their critical temperature, \(T_c\), is based on the GL theory.\(^1\) This includes multi-band superconductors with distinct sheets of the Fermi surface. A number of recent papers deal with two-band materials with coefficients of the GL free energy (for the field-free state),

\[
F = \sum_{\nu=1,2} \left( a_{\nu} \Delta_{\nu}^2 + b_{\nu} |\Delta_{\nu}|^4 / 2 \right) - 2 \gamma \Delta_1 \Delta_2 ,
\]

introduced phenomenologically, see, e.g., Ref.\(^2\). Choosing these coefficients in various ways, one could arrive to a number of the choice dependent conclusions.\(^3,4\) However, the coefficients can be derived from microscopic theory; they are certain functions of the microscopic coupling constants responsible for superconductivity and of temperature \(T\). This has been done time ago by Tilley\(^5\) and later by Zhitomirsky and Dao\(^6\) who have shown, within a weak-coupling model, that the coefficients \(a_{\nu}\) do not have the familiar GL form \(\alpha(T - T_c)\). Instead, they acquire a constant part, \(const + \alpha(T - T_c)\), which is intimately related to the constant \(\gamma\) of the mixed Josephson-type term to ensure \(\Delta_\nu \sim \sqrt{T_c - T}\) near \(T_c\).

We argue in this work that the ratio of the order parameters is \(T\) independent in the GL domain,

\[
\Delta_1(r,T) / \Delta_2(r,T) = const ,
\]

with the constant depending on interactions responsible for superconductivity. The one-dimensional version of Eq.\(^2\) has first been obtained while solving the GL problem of the interface energy between superconducting and normal phases relevant for the distinction between type-I and type-II superconductors.\(^2\) For the strong intraband scattering (the dirty limit), the result \(^2\) has been obtained by Koshelev and Golubov provided the interband scattering could be disregarded.\(^2\) Here, we establish this result for any problem in the GL domain.

We show that the equations for \(\Delta_1(r,T)\) and \(\Delta_2(r,T)\) are reduced to one independent GL equation. In other words, there is a single complex order parameter describing the two-band superconductor in the GL domain and, as a consequence, a single length scale \(\xi\) for spatial variation of both \(\Delta_1(r,T)\) and \(\Delta_2(r,T)\).

Our results, along with the earlier critique\(^9\) and a comprehensive review by Brandt and Das\(^10\) question validity of publications discussing properties of MgB\(_2\) within the GL framework where each band is attributed with its own coherence length and sometimes even with its own penetration depth, see, e.g., Ref.\(^11\) and references therein.

We stress that our claim that the gap functions \(\Delta_\nu(r,T)\) change on the same length scale relates exclusively to the temperature domain, however narrow it could be, where the GL theory is valid. Out of this domain and at low temperatures in particular, different length scales \(\sim \hbar v_F / \Delta_{\nu}(0)\) may enter and result in properties substantially different from those in the GL region. Still, as long as the GL energy functional is used, the assumption of two coherence lengths cannot be justified.

Below, we discuss the phenomenologic two-band GL theory and later confirm our conclusions within a weak-coupling microscopic scheme.

II. TWO-BAND GL IN FIELD

The two-band GL functional reads:

\[
\mathcal{F} = \int dV \left\{ \sum_{\nu=1,2} \left( a_{\nu} |\Delta_{\nu}|^2 + b_{\nu} |\Delta_{\nu}|^4 / 8 \nu^2 \right) + K_{\nu} |\Pi|\Delta_{\nu}^2 \right\} - \gamma \left( \Pi \Delta_1^2 + \Pi \Delta_2^2 \right) + \frac{B^2}{8\pi} \}
\]

where \(\Pi = \nabla + 2\pi i A / \phi_0\) and the constant \(\gamma\) along with the coefficients \(a, b, K\) will be given later. The GL equations are minimum conditions for the functional \(\mathcal{F}\). One obtains varying \(\mathcal{F}\) with respect to \(\Delta_{\nu}^*\):

\[
a_1 \Delta_1 + b_1 \Delta_1 |\Delta_1|^2 - \gamma \Delta_2 - K_1 \Pi^2 \Delta_1 = 0 , \quad (4)
\]

\[
a_2 \Delta_2 + b_2 \Delta_2 |\Delta_2|^2 - \gamma \Delta_1 - K_2 \Pi^2 \Delta_2 = 0 . \quad (5)
\]

We now recall that in the one-band GL equation,

\[
a \Delta + b |\Delta|^2 - K \Pi^2 \Delta = 0 ,
\]

all terms are of the same order \(1 - T / T_c)^{3/2} = \tau^{3/2}\) \((\Delta \propto \tau^{1/2}, a \propto \tau, \text{and } \Pi^2 \propto \xi^{-2} \propto \tau)\). This is not so for Eqs.\(^4, 5\) because \(\gamma\) is a constant and \(a_{\nu}\) may contain constant parts.
Having this in mind, we express $\Delta_2$ in terms of $\Delta_1$ from Eq. (24) and substitute the result in Eq. (5) keeping only terms up to the order $\tau^{3/2}$:

$$
(a_1 a_2 - \gamma^2) \Delta_1 + (b_1 a_2 + b_2 a_1 \gamma^2) \Delta_1 |\Delta_1|^2
- (a_1 K_2 + a_2 K_1) \Pi^2 \Delta_1 = 0.
$$

Similarly, one obtains an equation for $\Delta_2$:

$$
(a_1 a_2 - \gamma^2) \Delta_2 + (b_1 a_2 + b_2 a_1 \gamma^2) \Delta_2 |\Delta_2|^2
- (a_1 K_2 + a_2 K_1) \Pi^2 \Delta_2 = 0.
$$

In zero field, one has $\Delta_2^2 \propto (a_1 a_2 - \gamma^2)$, so that at $T_c$, $a_1 a_2 - \gamma^2 = 0$, and therefore $a_\nu$ must contain constant parts,

$$
a_\nu = a_\nu c - a_\nu r,
$$

such that $a_1 c a_2 c = \gamma^2$.

Eqs. (7) and (8) for $\Delta_\nu$ can now be written as:

$$
- \alpha \tau \Delta_1 + \beta_1 \Delta_1 |\Delta_1|^2 - K \Pi^2 \Delta_1 = 0,
$$

$$
- \alpha \tau \Delta_2 + \beta_2 \Delta_2 |\Delta_2|^2 - K \Pi^2 \Delta_2 = 0,
$$

with

$$
\alpha = a_1 + a_2, \quad K = a_1 c K_2 + a_2 c K_1, \quad \beta_1 = b_1 a_2 c + b_2 a_1 c / \gamma^2, \quad \beta_2 = b_2 a_1 c + b_1 a_2 c / \gamma^2.
$$

We note that within the accuracy of the GL theory, up to $O(\tau^{3/2})$, the equations for $\Delta_1$ and $\Delta_2$ are coupled only via the vector potential.

In particular, in zero field we have

$$
\Delta_\nu^2 = \alpha \tau / \beta_\nu,
$$

so that the ratio

$$
\frac{\Delta_\nu^2 (T)}{\Delta_\nu^2 (0)} = \frac{\beta_2}{\beta_1},
$$

comes out to be $T$ independent in the GL domain.

Furthermore, one easily checks that for any solution $\Delta_1(r, T)$ of Eq. (10), Eq. (11) is satisfied by

$$
\Delta_2 (r, T) = \Delta_1 (r, T) \sqrt{\beta_2 / \beta_1}.
$$

In particular, this implies that in equilibrium $\Delta_1 (r, T)$ and $\Delta_2 (r, T)$ must have either the same phases or the phases differing by $\pi/2$. It is found in Ref. 6 that for small $\gamma$ the ratio $\Delta_2 / \Delta_1$ changes away of $T_c$; we note, however, that this deviation is beyond the GL accuracy. Reliable results beyond GL can be obtained only within microscopic approaches like Gor’kov or Bogolyubov - de Gennes theories.

Moreover, introducing the order parameters normalized on their zero-field values,

$$
\frac{\Delta_1}{\Delta_{10} (T)} = \frac{\Delta_2}{\Delta_{20} (T)} = \Psi,
$$

both Eq. (10) and (11) are reduced to one:

$$
\Psi (1 - |\Psi|^2) = - \frac{K}{\alpha \tau} \Pi^2 \Psi.
$$

Thus, the length scale of the space variation of both $\Delta_1$ and $\Delta_2$, the coherence length, is given by

$$
\xi^2 = K / \alpha \tau.
$$

III. MICROSCOPIC WEAK-COUPLING TWO-BAND MODEL NEAR $T_c$.

To establish connection of GL equations with the two-band microscopic theory we turn to a weak-coupling model for clean and isotropic materials (not because these restrictions are unavoidable, but rather due to the model simplicity).

Perhaps, the simplest formally weak-coupling approach is based on the Eilenberger quasiclassical formulation of the Gor’kov equations valid for general anisotropic order parameters and Fermi surfaces. Eilenberger functions $f, g$ for clean materials in zero-field obey the system:

$$
0 = \Delta g - \hbar \omega f,
$$

$$
g^2 = 1 - f^2,
$$

$$
\Delta (k) = 2 \pi T N (0) \sum_{\omega > 0} \langle V (k, k') f (k', \omega) \rangle_{k'}.
$$

Here, $k$ is the Fermi momentum; $\Delta$ is the order parameter that may depend on the position $k$ at the Fermi surface. Further, $N(0)$ is the total density of states (DoS) at the Fermi level per spin; the Matsubara frequencies are given by $\hbar \omega = \pi T (2n + 1)$ with an integer $n$, and $\omega_D$ is the Debye frequency; $\langle ... \rangle$ stands for averages over the Fermi surface.

Consider a model material with the gap given by

$$
\Delta (k) = \Delta_{1,2}, \quad k \in F_{1,2},
$$

where $F_1, F_2$ are two sheets of the Fermi surface. The gaps are assumed constant at each band. Denoting DoS on the two parts as $N_{1,2}$, we have for a quantity $X$ constant at each Fermi sheet:

$$
\langle X \rangle = \langle X (1, N_{1,2} / N (0)) = n_1 X_1 + n_2 X_2,
$$

where $n_{1,2} = N_{1,2} / N (0)$; clearly, $n_1 + n_2 = 1$.

Equations (19) and (20) are easily solved:

$$
f_\nu = \Delta_\nu / \beta_\nu, \quad g_\nu = \hbar \omega / \beta_\nu, \quad \beta_\nu^2 = \Delta_\nu^2 + \hbar^2 \omega^2,
$$

where $\nu = 1, 2$ is the band index. The self-consistency equation (21) takes the form:

$$
\Delta_\nu = \sum_{\mu=1,2} n_{\mu} \lambda_{\nu \mu} \Delta_\mu \sum_{\omega} \frac{2 \pi T}{\rho_\mu} \frac{2 \pi T}{\rho_\mu}.
$$

where $\lambda_{\nu \mu} = N (0) V_{\nu \mu}$ are dimensionless effective interaction constants. The notation commonly used in literature, $\lambda_{\mu \nu}^{(i)} = n_{\mu} \lambda_{\nu \mu}$, includes DoS. We find our notation convenient since, being related to the coupling potential, our coupling matrix is symmetric: $\lambda_{\mu \nu} = \lambda_{\nu \mu}$.

It is seen from the system (25) that $\Delta_{1,2}$ turn zero at the same temperature $T_c$ unless $\lambda_{12} = 0$ and equations (25) decouple, the property that has been noted in earlier work. As $T \rightarrow T_c$, $\Delta_{1,2} \rightarrow 0$, and $\beta \rightarrow \hbar \omega$. The sum over $\omega$ in Eq. (25) is readily evaluated:

$$
S = \sum_{\omega} \frac{2 \pi T}{\hbar \omega} \bigg|_{T_c} = \ln \frac{2 \hbar \omega_D}{T_c \pi e^{-\gamma}} = \ln \frac{2 \hbar \omega_D}{1.76 T_c},
$$

(26)
\( \gamma = 0.577 \) is the Euler constant. This relation can also be written as
\[
1.76 T_c = 2 \hbar \omega_D e^{-\gamma} .
\] (27)

The system (25) at \( T_c \) is linear and homogeneous:
\[
\Delta_1 = S(n_1 \lambda_1 \delta_1 + n_2 \lambda_2 \delta_2) , \quad \Delta_2 = S(n_1 \lambda_1 \delta_1 + n_2 \lambda_2 \delta_2) . \quad (28)
\]
The zero determinant gives \( S \) and, therefore, \( T_c \):
\[
S^2 n_1n_2 \eta - S(n_1 \lambda_1 + n_2 \lambda_2) + 1 = 0 , \quad \eta = \lambda_1 \lambda_2 - \lambda_2^2 .
\] (29)

The roots of this equation are:
\[
S = \frac{n_1 \lambda_1 + n_2 \lambda_2 \pm \sqrt{(n_1 \lambda_1 - n_2 \lambda_2)^2 + 4n_1n_2 \lambda_2^2}}{2n_1n_2 \eta} . \quad (31)
\]

Various possibilities that arise depending on values of \( \lambda_{\mu \nu} \) are discussed, e.g., in Refs.14-18. Introducing \( T \)-independent quantities,
\[
S_1 = \lambda_{22} - n_1 \eta \sigma , \quad S_2 = \lambda_{11} - n_2 \eta \sigma ,
\] (32)
we write Eq. (29) as
\[
S_1 S_2 = \lambda_2^2 , \quad (33)
\]
the form useful for manipulations below.

If \( \lambda_{12} = 0 \), Eq. (31) provides two roots \( 1/n_1 \lambda_{11} \) and \( 1/n_2 \lambda_{22} \). The smallest one gives \( T_c \), whereas the other corresponds to the temperature at which the second gap turns zero. We note that this situation is unlikely; it implies that the ever present Coulomb repulsion is exactly compensated by the effective interband attraction.

Since the determinant of the system (25) is zero, the two equations are equivalent and give at \( T_c \):
\[
\left( \frac{\Delta_2}{\Delta_1} \right)_{T_c} = \frac{1 - n_1 \lambda_{11} S}{n_2 \lambda_{22} S} . \quad (34)
\]

When the right-hand side is negative, \( \Delta \)’s are of opposite signs. Within the one-band BCS, the sign of \( \Delta \) is a matter of convenience; for two bands, \( \Delta_1 \) and \( \Delta_2 \) may have equal or opposite signs.\(^{19}\)

After simple algebra, Eq. (34) can be manipulated to
\[
\left( \frac{\Delta_2}{\Delta_1} \right)_{T_c}^2 = \frac{S_1}{S_2} . \quad (35)
\]

We thus obtain by comparing with Eq. (10) or (11) the ratio of phenomenological coefficients in terms of microscopic couplings: \( \beta_1 / \beta_2 = S_1/S_2 \). We have seen above that within the GL approximation this ratio remains the same at any \( T \) in the GL domain not only for a uniform field-free state (or for \( \gamma \rightarrow \infty \) as in Ref. 20) but for any situation with \( \Delta \)’s depending on coordinates in the presence of magnetic fields.

We note that the proportionality of \( \Delta_1 \) and \( \Delta_2 \) has also been shown to hold within microscopic weak-coupling theory in the dirty limit by Koshelev and Golubov.\(^{21}\) It is also worth mentioning here that the above proof of this proportionality based on the GL approach is quite general and holds for any scattering, gap anisotropies etc.

In the following we use the GL coefficients obtained in Refs. 5 and 6. In our notation they read:
\[
a_\nu = \frac{N(0)}{\eta} (S_\nu - \eta n_\nu), \quad b_\nu = \frac{N(0)}{W^2} n_\nu, \quad W = \frac{8\pi^2 T^2}{7\xi(3)} ,
\] (36)

where the energy scale \( W \sim \pi T_c \) is introduced for brevity and \( n_\nu \) are the Fermi velocities in two bands which for simplicity are assumed isotropic. We, in fact, confirmed Eqs. (30) of Zhitomirsky and Dao employing different methods (except our \( b_\nu \) is by a factor of 2 larger than that of Ref. 6). It is worth noting that the microscopically derived \( a_\nu \) are not proportional to \( \tau \) as in the standard one-band GL unless one of the parameters \( S_\nu \) is zero; given the condition (33) this may happen only if \( \lambda_{12} = 0 \). This feature of the two-band GL is sometimes overlooked.\(^{21,22}\)

As stressed in Ref. 6 the term \( K_\nu |\Pi \Delta_\nu|^2 \) with order parameters gradients is the only possible in the GL energy, although the symmetry may allow for other combinations of gradients.

The coefficients entering the GL Eqs. (10) and (11) are:
\[
\alpha = \frac{N(0)^2 C}{\eta} , \quad K = \frac{\hbar^2 v^2 N(0)^2}{6W^2} , \quad \beta_\nu = \frac{N(0)^2 D S_\nu}{\eta W^2 \lambda_1^2} , \quad (37)
\]
where
\[
\hat{v}^2 = n_1 S_2 v_1^2 + n_2 S_1 v_2^2 \quad (38)
\]
has the dimension of a squared velocity and
\[
C = n_1 S_2 + n_2 S_1 , \quad D = n_1 S_2^2 + n_2 S_1^2 \quad (39)
\]
are constants.

Hence, we can express the length scale (18) of the space variation of both \( \Delta_1 \) and \( \Delta_2 \) in the GL domain in terms of microscopic parameters:
\[
\xi^2 = \frac{\hbar^2 \hat{v}^2}{2W^2 C \tau} . \quad (40)
\]

The upper critical field follows: \( H_{c2} = \phi_0/2\pi \xi^2 \). The one-band limit is obtained by setting \( n_1 = 1, n_2 = 0 \) so that \( C = S_2 \) and \( \hat{v}^2 = S_2 v^2/3 \) that yields \( \xi^2 = 7(3)\hbar^2 v^2/48\pi^2 T^2 \tau \) as it should.

Variation of the free energy \( \mathcal{F} \) with respect to the vector potential \( \mathbf{A} \) gives the current density. Following the standard procedure we obtain for the penetration depth of a weak magnetic field:
\[
\frac{1}{\lambda^2} = \frac{32\pi^3}{\phi_0^2} \sum_{\nu=1,2} \Delta_\nu^2 K_\nu = \frac{16\pi CN(0)\nu^2 \hat{v}^2}{e^2 D} \tau . \quad (41)
\]
In the one-band limit this yields the correct result: \( \lambda^{-2} = (16\pi e^2 N(0)v^2/3c^2)\tau \).
A straightforward calculation yields the equilibrium zero-field free energy:

\[ F_0 = -N(0)W^2C^2/2D \tau^2. \]  

(42)

The thermodynamic field \( H_c \) follows: \( H_c^2/8\pi = -F_0 \). One can show that the relative specific heat jump at \( H_c \) differs from the one-band value 12/\( T \zeta(3) \) = 1.43 by a factor \( C^2/D < 1.22 \).

One can now form the dimensionless GL parameter,

\[ \kappa^2 = \frac{\lambda^2}{\xi^2} = \frac{c^2W^2D}{8\pi N(0)e^2\hbar^2D^4}, \]  

and verify the standard relation \( H_{c2}/H_c\sqrt{2} = \kappa \).

Finally, the \textit{equilibrium energy} is evaluated by substituting the solutions of the GL equations to the functional [3]:

\[ F = \frac{H_c^2}{4\pi} \int dV \left\{ \delta^2 - \frac{1}{2} |\psi|^4 \right\}. \]  

(44)

where \( b = B/H_c\sqrt{2} \) is the dimensionless field. Thus, the theory of a two-band superconductor near \( T_c \) is mapped onto the standard one-order parameter GL scheme.

In particular, this mapping means that the GL problem of the interface energy between normal and superconducting phases has the same solution, i.e., \( \kappa = 1/\sqrt{2} \) separates type-I and type-II superconductors. This has been demonstrated in Ref. 7 by solving numerically the nonlinear system of GL equations [1] [3] without discarding terms \( O(\tau^2) \) employed here.

A. Remark on boundary conditions

The solution [15] for the two gap functions of the GL Eqs. [10] and [11] holds indeed provided the boundary conditions for \( \Delta_2 \) are the same as for \( \Delta_1 \) multiplied by the factor \( \sqrt{\beta_1/\beta_2} \). This is clearly the case for the 1D problem of the S-N interface energy. The same is true for the problem of the single vortex structure: both \( \Delta \)'s are zero at the vortex center and approach \( \Delta_{v,0} \) with the correct ratio at infinity.

However, for, e.g., proximity situations with a two-band superconductor on one side of the contact with a normal metal, the condition on the superconducting side far from the boundary is satisfied, whereas the question of boundary conditions at the boundary remains open. In this case, one cannot claim that \( \Delta(x)'s \) are proportional. Nevertheless, as is seen from Eqs. [10] and [11], the length scale \( \xi = \sqrt{K/\alpha\tau} \) is still the same for both order parameters.

IV. DISCUSSION

Two-band GL equation have been used in a number of publications where the coefficients in the GL energy functional \( a, b, K_c \) and \( \gamma \) were varied and possible consequences were discussed. Moreover, different \( \xi' \)s and even \( \lambda' \)s were assigned to the two bands along with two different \( \kappa' \)s. This led to speculations that situations may exist where one of the bands behaves as a type-II superconductor with \( \kappa_1 > 1/\sqrt{2} \), while the other may have \( \kappa_2 < 1/\sqrt{2} \) and behave near \( T_c \) as the type-I; the superconductivity in such situations was called “type-1.5”.

MgB\(_2\) has been suggested as such an example, see, e.g., Ref. [1] and references therein.

The present work argues that such situations do not exist. The point is that the GL equations are derived from the microscopic theory within certain approximations that lead to the free energy near \( T_c \) being proportional to \( (1 - T/T_c)^2 \) and the order parameter (or parameters) varying as \( (1 - T/T_c)^{1/2} \). Formally, the nonlinear system of GL equations [1] [3] for two-band materials can be solved with any accuracy. However, physically there is no point in going to accuracy higher than that of equations themselves; whatever results obtained along these lines will be absolutely unreliable. To get a near-\( T_c \) description more accurate than GL, one should go back to microscopic theory that generates many extra terms in the free energy expansion even for the one-band situation, see, e.g., Ref. [24] so that the multi-band generalization of such an approach is unlikely to produce a useful theory. It is demonstrated on a one-dimensional problem of Ref. [7] and is shown for a general case in this paper that \textit{within the GL accuracy} both order parameters of a two-band superconductor vary on the same length scale \( \xi \) of Eq. [13] contrary to requirements of “1.5 type superconductivity”.

We note that this conclusion holds for the “GL domain” defined as the temperature interval near \( T_c \) where the GL expansion can be justified. We do not specify this domain explicitly because its size may vary from one case to another. E.g., it is argued in Ref. [8] that for two dirty bands (with no inter-band scattering) of MgB\(_2\), the domain of GL applicability shrinks practically to zero. However, whatever this size is, within this domain the two order parameters vary on the same length scale. Therefore, attempts to employ the GL functionals - on hand - and to assume different length scales - on the other - cannot be justified.

Moreover, we show that - within the GL accuracy - the two GL equations for the two-band case are reduced to a single equation for the normalized order parameter; in other words, the two-band superconductor is described by a single complex order parameter. This excludes possibilities of having “fractional vortices” with exotic properties such as those discussed in Refs. [25] [26].

Microscopically, our results were derived within a weak coupling theory of clean superconductors. We believe, however, our conclusions go beyond that. For our results to hold it is crucial that due to the finite interband Josephson coupling \( \gamma \), the coefficients a, in the GL energy remain finite at \( T_c \). Once this is guaranteed our qualitative conclusions remain unchanged, even if
assumptions of the weak coupling, no-scattering, and isotropy do not apply.

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