Ginzburg-Landau theory of vortices in a multi-gap superconductor

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The Ginzburg-Landau functional for a two-gap superconductor is derived within the weak-coupling BCS model. The two-gap Ginzburg-Landau theory is, then, applied to investigate various magnetic properties of MgB$_2$ including an upturn temperature dependence of the transverse upper critical field and a core structure of an isolated vortex. Orientation of vortex lattice relative to crystallographic axes is studied for magnetic fields parallel to the c-axis. A peculiar 30°-rotation of the vortex lattice with increasing strength of an applied field observed by neutron scattering is attributed to the multi-gap nature of superconductivity in MgB$_2$.

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I. INTRODUCTION

Superconductivity in MgB$_2$ discovered a few years ago has attracted a lot of interest both from fundamental and technological points of view. Unique physical properties of MgB$_2$ include $T_c = 39$ K, the highest among s-wave phonon mediated superconductors, and the presence of two gaps $\Delta_1 \approx 7$ meV and $\Delta_2 \approx 2.5$ meV evidenced by the scanning tunneling microscope and the point contact spectroscopies and by the heat capacity measurements. The latter property brings back the concept of a multi-gap superconductivity formulated more than forty years ago for materials with large disparity of the electron-phonon interaction for different pieces of the Fermi surface.

Theoretical understanding of normal and superconducting properties of MgB$_2$ has been advanced in the direction of first-principle calculations of the electronic band structure and the electron-phonon interaction, which identified two distinct groups of bands with large and small superconducting gaps. Quantitative analysis of various thermodynamic and transport properties in the superconducting state of MgB$_2$ was made in the framework of the two-band BCS model. An outside observer would notice, however, a certain lack of effective Ginzburg-Landau or London type theories applied to MgB$_2$. This fact is explained by of quantitative essence of the discussed problems, though effective theories can often give a simpler insight. Besides, new experiments constantly raise different types of questions. For example, recent neutron diffraction study in the mixed state of MgB$_2$ has found a strange 30°-reorientation of the vortex lattice with increasing strength of a magnetic field applied along the c-axis. Such a transition represents a marked qualitative departure from the well-known behavior of the Abrikosov vortex lattice in single-gap type-II superconductors. Nature and origin of phase transitions in the vortex lattice are most straightforwardly addressed by the Ginzburg-Landau theory.

In the present work we first derive the appropriate Ginzburg-Landau functional for a two-gap superconductor from the microscopic BCS model. We, then, investigate various magnetic properties of MgB$_2$ using the Ginzburg-Landau theory. Our main results include demonstration of the upward curvature of $H_c^2(T)$ for transverse magnetic fields, investigation of the vortex core structure, and explanation of the reorientational transition in the vortex lattice. The paper is organized as follows. Section 2 describes the two-band BCS model and discusses the fit of experimental data on the temperature dependence of the specific heat. Section 3 is devoted to derivation of the Ginzburg-Landau functional for a two-gap weak-coupling superconductor. In Section 4 we discuss various magnetic properties including the upper critical field and the structure of an isolated vortex. Section 5 considers the general problem of an orientation of the vortex lattice in a hexagonal superconductor in magnetic field applied parallel to the c-axis and, then, demonstrates how the multi-gap nature of superconductivity in MgB$_2$ determines a reorientational transition in the mixed state.

II. THE TWO-BAND BCS MODEL

A. General theory

In this subsection we briefly summarize the thermodynamics of an s-wave two-gap superconductor with the aim to extract subsequently microscopic parameters of the model from available experimental data for MgB$_2$. We write the pairing interaction as

$$
\hat{V}_{BCS} = - \sum_{n,n'} g_{nn'} \int dx \Psi^\dagger_{n\uparrow}(x) \Psi^\dagger_{n\downarrow}(x) \Psi_{n'\downarrow}(x) \Psi_{n'\uparrow}(x),
$$

where $n = 1, 2$ is the band index. A real space representation (1) is obtained from a general momentum-space form of the model under assumption of weak momentum dependence of the scattering amplitudes $g_{nn'}$. We also assume that the active band has the strongest pairing interaction $g_{11} = g_1$ compared to interaction in the passive band $g_{22} = g_2$ and to interband scattering.
of the Cooper pairs $g_{12} = g_{21} = g_3$. Defining two gap functions
\[ \Delta_n(x) = -\sum_{n'} g_{nn'} \langle \Psi_{n'}(x) \Psi_{n'}(x) \rangle \tag{2} \]
the total Hamiltonian is transformed to the mean-field form
\[ \tilde{H}_{\text{MF}} = E_{\text{const}} + \sum_n \int dx \left[ \psi_n^\dagger(x) \tilde{\hat{h}}(x) \psi_n(x) + \Delta_n(x) \right], \tag{3} \]
\[ \tilde{\hat{h}}(x) \] being a single-particle Hamiltonian of the normal metal. The constant term is a quadratic form of anomalous averages $\langle \psi_{n'}(x) \psi_n(x) \rangle$. Using Eq. (2) it can be expressed via the gap functions
\[ E_{\text{const}} = \frac{1}{G} \int dx \left[ g_2 |\Delta_1|^2 + g_1 |\Delta_2|^2 - g_3 (\Delta_1^2 + \Delta_1^2 + \Delta_1^2) \right] \tag{4} \]
with $G = \det \{ g_{nn'} \} = g_1 g_2 - g_3^2$. The above expression has to be modified for $G = 0$. In this case the two equations (2) are linearly dependent. As a result, the ratio of the two gaps is the same for all temperatures and magnetic fields $\Delta_1(x)/\Delta_1(0) = g_1/g_3$, while the constant term reduces to $E_{\text{const}} = \int dx \left| \Delta_1(x) \right|^2 / g_1$.

The standard Gorkov’s technique can then be applied to derive the Green’s functions and energy spectra in uniform and nonuniform states with and without impurities. In a clean superconductor in zero magnetic field the two superconducting gaps are related via the self-consistent gap equations
\[ \Delta_n = \sum_{n'} \lambda_{nn'} \Delta_n', \int_0^{\omega_0} \frac{d\varepsilon}{\sqrt{\varepsilon^2 + \Delta_n^2}} \tanh \frac{\varepsilon^2 + \Delta_n^2}{2T} \tag{5} \]
with dimensionless coupling constants $\lambda_{nn'} = g_{nn'} N_n$, $N_n$ being the density of states at the Fermi level for each band. The transition temperature is given by $T_c = (2\omega_D C / \pi) e^{-1/\lambda}$, where $\omega_D$ is the Debye frequency, $C$ is the Euler constant and $\lambda$ is the largest eigenvalue of the matrix $\lambda_{nn'}$:
\[ \lambda = (\lambda_{11} + \lambda_{22})/2 + \sqrt{(\lambda_{11} - \lambda_{22})^2/4 + 4 \lambda_{12} \lambda_{21}} \tag{6} \]
Since $\lambda > \lambda_{11}$, the interband scattering always increases the superconducting transition temperature compared to an instability in a single-band case. The ratio of the two gaps at $T = T_c$ is $\Delta_2/\Delta_1 = \lambda_{22}/(\lambda - \lambda_{22})$. At zero temperature the gap equations (5) are reduced to
\[ \Delta_n = \sum_{n'} \lambda_{nn'} \Delta_n', \ln \frac{2 \omega_D}{\Delta_n} \tag{7} \]
By substituting $\Delta_n = 2 \omega_D r_n e^{-1/\lambda}$ the above equation is transformed to
\[ r_n = \sum_{n'} \lambda_{nn'} r_{n'} \left( \frac{1}{\lambda} - \ln r_{n'} \right) \tag{8} \]
For $1/\lambda \gg \ln r_n$, one can neglect logarithms on the right hand side and obtain for the ratio of the two gaps the same equation as at $T = T_c$, implying that $\Delta_2/\Delta_1$ is temperature independent. This approximation is valid only for $r_n \approx 1$, i.e., if all the coupling constants $\lambda_{nn'}$ have the same order of magnitude. (For $g_3^2 = g_1 g_2$ the above property is an exact one: the gap ratio does not change neither with temperature nor in magnetic field.) However, for $g_1 \ll g_2 \ll g_1$, the passive gap $\Delta_2$ is significantly smaller than the active gap $\Delta_1$ and $r_2 \ll 1$ so that the corresponding logarithm cannot be neglected. It follows from Eq. (5) that the ratio $\Delta_2/\Delta_1$ decreases between $T = T_c$ and $T = 0$ for small $g_3$. Such variations become more pronounced in superconductors with larger values of $\lambda$, which are away from the extreme weak-coupling limit $\lambda \ll 1$. Ab-initio calculations indicate that MgB$_2$ has an intermediate strength of the electron-phonon coupling with $\lambda_{12}(21) \ll \lambda_{11} \ll 1$, making this superconductor an ideal system to observe effects related to variations of the ratio of two gaps.

The jump in the specific heat at the superconducting transition can be expressed analytically as
\[ \Delta C = \frac{12}{7 \zeta(3)} \left( N_1 \Delta_1^2 + N_2 \Delta_2^2 \right)^2 \tag{9} \]
where the limit $T \to T_c$ has to be taken for the ratio of the two gaps. The specific heat jump is always smaller than the single-band BCS result $\Delta C / C = 12/7 \zeta(3) \approx 1.43$, unless $\Delta_1 = 2 \Delta_2$.

B. Fit to experimental data

One of the striking experimental evidences of the double-gap behavior in MgB$_2$ is an unusual temperature dependence of the specific heat with a shoulder-type anomaly around 0.25 $T_c$. We use here the multi-band BCS theory to fit the experimental data for $C(T)$. The Fermi surface in MgB$_2$ consists of four sheets: two nearly cylindrical hole sheets arising from quasi two-dimensional $p_{x,y}$ boron bands and two sheets from three-dimensional $p_z$ bonding and antibonding bands. The electronic structure of MgB$_2$ is now well understood from a number of density-functional studies, which generally agree with each other, though differ in certain details. Specifically, we choose as a reference the work of Kong et al., where the tight-binding fits for all Fermi surface sheets in MgB$_2$ are provided. Using these fits we have calculated various Fermi surface averages for each band. The density of states at the Fermi level is $N(0) = 0.41$ states/eV/cell/spin, which includes $N_e(0) = 0.16 + 0.049 + 0.0411$ states/eV/cell/spin in light and heavy $\sigma$-bands and $N_e(0) = 0.25 + 0.124 + 0.126$ states/eV/cell/spin in the two $\pi$-bands. Note, that the obtained $N_e(0)$ is somewhat larger than the number 0.205 cited by Kong et al., while the results for the $\sigma$-bands agree. Because of a strong mismatch in the electron-phonon coupling between two group of
III. THE GINZBURG-LANDAU FUNCTIONAL

We use the microscopic theory formulated in the previous section to derive the Ginzburg-Landau functional of a two-gap superconductor. In the vicinity of $T_c$, the anomalous terms in the mean-field Hamiltonian \( \hat{H}_a \) are treated as a perturbation \( V_a \). Then, the thermodynamic potential of the superconducting state is expressed as

\[
\Omega_s = E_{\text{const}} - \frac{1}{\beta} \ln \left( T_r \exp \left[ - \int_0^\beta V_a(\tau) d\tau \right] \right) ,
\]

where \( \beta = 1/T \). Expansion of Eq. 11 in powers of \( V_a \) yields the Ginzburg-Landau functional. Since the normal-state Green’s functions are diagonal in the band index, the Wick’s decoupling of \( V_a \) in \( \Omega_s \) does not produce any mixing terms between the gaps. As a result, the weak-coupling Ginzburg-Landau functional has a single Josephson-type interaction term:

\[
F_{\text{GGL}} = \int dx \left[ \alpha_1 |\Delta_1|^2 + \alpha_2 |\Delta_2|^2 - \gamma (\Delta_1^* \Delta_2 + \Delta_2^* \Delta_1) \right] + \frac{1}{2} \beta_1 |\Delta_1|^4 + \frac{1}{2} \beta_2 |\Delta_2|^4 + K_{11} |\nabla_1 |\Delta_1|^2 + K_{22} |\nabla_2 |\Delta_2|^2 \right] ,
\]

where \( \alpha_1, \alpha_2, \gamma, \beta_1, \beta_2, K_{11}, K_{22} \) are the coefficients, and \( |\Delta_1|^2 \) and \( |\Delta_2|^2 \) are the gap amplitudes in the \( \sigma \)-bands.

The gradient term coefficients depend in a standard way on the averages of Fermi velocities \( v_F \), over various sheets of the Fermi surface. Numerical integration of the tight-binding fits\(^{16}\) yields the following results: for the \( \sigma \)-band \( v_{1F}^2 = 2.13 \) (3.55, 1.51) and \( v_{2F}^2 = 0.05 \) (0.05, 0.05); for the \( \pi \)-band \( v_{1F}^2 = 1.51 \) (1.47, 1.55) and \( v_{2F}^2 = 2.96 \) (2.81, 3.10) in units of \( 10^5 \) cm\(^2\)/s, numbers in parentheses correspond to each of the constituent bands. The effective masses of the quasi-two-dimensional \( \sigma \)-band exhibit a factor of 40 anisotropy between in-plane and out of plane directions. In contrast, the three-dimensional \( \pi \)-band has a somewhat smaller mass along the c-axis. Using \( N_2/N_1 = 1.5 \) we find that the in-plane gradient constants for the two bands are practically the same \( K_{21}/K_{11} \approx 1.06 \), while the c-axis constants differ by almost two orders of magnitude \( K_{2z}/K_{1z} \approx 90 \).

A very simple form of the two-gap weak-coupling Ginzburg-Landau functional is somewhat unexpected. On general symmetry grounds, there are possible various types of interaction in quartic and gradient terms between two superconducting condensates of the same symmetry, which have been considered in the literature.\(^{35,46,37} \) The above form of the Ginzburg-Landau functional is, nevertheless, a straightforward
extension of the well-known result for unconventional superconductors. For example, the quartic term for a momentum-dependent gap is $|\Delta(k)|^4$ in the weak-coupling approximation. In the two-band model $\Delta(k)$ assumes a step-like dependence between different pieces of the Fermi surface, which immediately leads to the expression [12].

The Ginzburg-Landau equations for the two-gap superconductor, which are identical to those obtained from Eq. (12), have been first derived by an expansion of the gap equations in powers of $\Delta$ [38,39]. Recently, a similar calculation has been done for a dirty superconductor, with only intraband impurity scattering and the corresponding form of the Ginzburg-Landau functional has been guessed, though with incorrect sign of the coupling term. Here, we have directly derived the free energy of the two-gap superconductor. The derivation can be straightforwardly generalized to obtain, e.g., higher-order gradient terms, which are needed to find an orientation of the vortex lattice relative to crystal axis (see below). We also note that strong-coupling effects, e.g., dependence of the pairing interactions on the gap amplitudes, will produce other, generally weaker, mixing terms of the fourth order in $\Delta$. The interband scattering by impurities can generate a mixing gradient term as well.

Finally, for $G = (g_1g_2 - g_3^2) < 0$ a number of spurious features appears in the theory: the matrix $\lambda_{nn'}$ and the quadratic form acquire negative eigenvalues, while a formal minimization of the Ginzburg-Landau functional [12] leads to an unphysical solution at high temperatures. Sign of $\Delta_2/\Delta_1$ for such a solution is opposite to the sign of $g_3$. The origin of this ill-behavior lies in the approximation of positive integrals on the right-hand side of Eq. (5) by logarithms, which can become negative. Therefore, negative eigenvalues of $\lambda_{nn'}$ and $E_{\text{const}}$ yield no physical solution similar to the case when the BCS theory is applied to the Fermi gas with repulsion. The consequence for the Ginzburg-Landau theory [12] is that one should keep the correct sign of $\Delta_2/\Delta_1$ and use the Ginzburg-Landau equations, i.e., look for a saddle-point solution rather than seeking for an absolute minimum.

IV. THE TWO-GAP GINZBURG-LANDAU THEORY

In order to discuss various properties of a two-gap superconductor in the framework of the Ginzburg-Landau theory we write $\alpha_1 = -a_1 t$ with $a_1 = N_1$, $t = \ln(T_1/T) \approx (1 - T/T_1)$ and $T_1 = (2\omega d e^{\frac{G}{2}}/\pi e^{-g_2/GN_1})$ for the first active band and $\alpha_2 = \alpha_2 - a_2 t$ with $a_2 = N_2$, $\alpha_2 = (\lambda_1 - \lambda_2)/GN_1$ for the passive band.

A. Zero magnetic field

For completeness, we briefly mention here the behavior in zero magnetic field. The transition temperature is found from diagonalization of the quadratic form in Eq. (12):

$$t_c = \frac{\alpha_2}{2a_2} - \frac{\alpha_2^2}{4a_2^2} \frac{\gamma^2}{a_1a_2}.$$  \hspace{1cm} (13)

For small $\gamma$, one finds $t_c \approx -\gamma^2/\alpha_2$. Negative sign of $t_c$ means that the superconducting transition takes place above $T_1$, which is an intrinsic temperature of superconducting instability in the first band. The ratio of the two gaps $\rho = \Delta_2/\Delta_1 = \gamma/(\alpha_2 - a_2 t_n)$. Below the transition temperature, the gap ratio $\rho$ obeys

$$\alpha_2\rho - \gamma + \frac{\beta_2^2}{\beta_1^2} \rho^2 (a_1 t + \gamma \rho) = 0.$$ \hspace{1cm} (14)

For small $\gamma$, one can approximate $\rho \approx \gamma/\alpha_2$ and due to a decrease of $\alpha_2$ with temperature, small to large gap ratio $\rho$ increases away from $t_c$.

B. The upper critical field

1. Magnetic field parallel to the $c$-axis

Due to the rotational symmetry about the $c$-axis, the gradient terms in the $a$-$b$ plane are isotropic and can be described by two constants $K_{a1} = K_a$. The linearized Ginzburg-Landau equations describe a system of two coupled oscillators and have a solution in the form $\Delta_1 = c_0 f_0(x)$ and $\Delta_2 = d_0 f_1(x)$, where $f_0(x)$ is a state on the zeroth Landau level. The upper critical field is given by $H_{c2} = h_{c2} f_0/2\pi$

$$h_{c2} = \frac{a_1 t}{2K_1} - \frac{\alpha_2}{2K_2} + \sqrt{\left(\frac{a_1 t}{2K_1} + \frac{\alpha_2}{2K_2}\right)^2 + \frac{\gamma^2}{K_1K_2}}.$$ \hspace{1cm} (15)

The ratio of the two gaps $\rho = d_0/c_0$ along the upper critical line is

$$\rho = \frac{\gamma}{\alpha_2 + K_2 h_{c2}}.$$ \hspace{1cm} (16)

The above expression indicates that an applied magnetic field generally tends to suppress a smaller gap. Whether this effect overcomes an opposite tendency to an increase of $\Delta_2/\Delta_1$ due to a decrease of $\alpha_2$ with temperature depends on the gradient term constants. For example, in the limit $\gamma \ll \alpha_2$ we find from (10) $\rho \approx \gamma/\alpha_2 - (a_2 - a_1 K_2/K_1) t$. If $K_2$ is significantly larger than $K_1$, while $a_2 \approx a_1$, the smaller gap is quickly suppressed along the upper critical field line. However, for MgB$_2$ one finds $K_2/K_1 \approx 1$ for in-plane gradient terms. Therefore, the ratio $\Delta_2/\Delta_1$ continues to grow along $H_{c2}(T)$, though slower than in zero field.

2. Transverse magnetic field

We assume that $H \parallel \hat{y}$ and consider a homogeneous superconducting state along the field direction. The gradient terms in two transverse directions $\hat{x}$ and $\hat{z}$ have
The upper critical field is entirely determined by the ac-
(15), where $\lambda$ is given by the same expression as in the isotropic case parameter $K$. The critical field is, then, obtained from maximizing the two temperature regimes. At low temperatures $t$, $\lambda$ can be done numerically. Analytic expressions are possible in two similar cases. The vector potential is chosen in the Landau gauge $z \rightarrow z(K_z/K_x)^{1/4}$ and $a$ variational approach, which is known to give a good accuracy in similar cases. The vector potential is chosen in the Landau gauge $A = (Hz, 0, 0)$ and we look for a solution in the form

$$\left( \begin{array}{c} \Delta_1 \\ \Delta_2 \\ \end{array} \right) = \left( \begin{array}{c} \lambda \\ \pi \\ \end{array} \right)^{1/4} e^{-\lambda z^2/2} \left( \begin{array}{c} c \\ d \\ \end{array} \right), \tag{17}$$

where $\lambda$, $c$, and $d$ are variational parameters. After spatial integration and substitution $\lambda = h/\mu$, $h = 2\pi H/\Phi_0$, the quadratic terms in the Ginzburg-Landau functional become

$$F_2 = (-a_1 t + h\tilde{K}_1)|c|^2 + (a_2 + h\tilde{K}_2)|d|^2 - \gamma(c^*d + d^*c), \quad \tilde{K}_n = \frac{1}{2}(K_n\mu + K_{nz}/\mu) \tag{18}$$

The determinant of the quadratic form vanishes at the transition into superconducting state. Transition field is given by the same expression as in the isotropic case $16$, where $K_n$ have to be replaced with $\tilde{K}_n$. The upper critical field is, then, obtained from maximizing the corresponding expression with respect to the variational parameter $\mu$. In general, maximization procedure has to be done numerically. Analytic expressions are possible in two temperature regimes. At low temperatures $t \gg |t_c|$, the upper critical field is entirely determined by the active band and

$$h_{c2} = \frac{a_1 t}{\sqrt{K_1 K_{1z}}} \tag{19}$$

In the vicinity of $T_c$, an external magnetic field has a small effect on the gap ratio $\rho = d/c \approx \gamma/\alpha_{20}$ and an effective single-gap Ginzburg-Landau theory can be applied. The upper critical field is given by a combination of the gradient constants $K_{ni}$ weighted according to the gap amplitudes:

$$h_{c2} = \frac{a_1(t - t_c)}{\sqrt{(K_1 + \rho^2 K_2)(K_{1z} + \rho^2 K_{2z})}} \tag{20}$$

Since, in MgB$_2$ one has $K_{1z} \approx 0.01K_{2z}$ and $\rho^2 \approx 0.1$, the slope of the upper critical field near $T_c$ is determined by an effective gradient constant $K_{eff} \approx \rho^2 K_{2z} > K_{1z}$ (while $(K_1 + \rho^2 K_2) \approx K_1$). Thus, the upper critical field line $H_{c2}(T)$ shows a marked upturn curvature between the two regimes $20$ and $19$. Such a temperature behavior has been recently addressed in a number of theoretical works based on various forms of the two-band BCS theory $24,25,26,27$. We suggest here a simpler description of the above effect within the two-gap Ginzburg-Landau theory.

Finally, we compare the Ginzburg-Landau theory with the experimental data on the temperature dependence of the upper critical field for magnetic field parallel to the basal plane $20$. We choose ratios of the gradient term constants and the densities of states in accordance with the band structure calculations $16$ and change parameters $\gamma$ and $\alpha_{20}$, which are known less accurately, to fit the experimental data. The best fit shown in Fig. 2 is obtained for $\alpha_{20}/\alpha_1 = 0.65$ and $\gamma/\alpha_1 = 0.4$. The prominent upward curvature of $H_{c2}(T)$ takes place between $t_c = -0.18$ ($T_c = 36$ K) and $t \approx 0.2$ ($T = 26$ K), i.e. well within the range of validity of the Ginzburg-Landau theory. The above values of $\alpha_{20}$ and $\gamma$ can be related to $g_2/g_1$ and $g_3/g_1$ and they appear to be closer to the second choice of $g_n$ used for Fig. 1. The ratio of the two gaps, as it changes along the $H_{c2}(T)$ line, is shown on the inset in Fig. 2. It varies from $\Delta_1/\Delta_2 \approx 2.3$ near $T_c = 36$ K to $\Delta_1/\Delta_2 \approx 45$ at $T = 18$ K, where the Ginzburg-Landau theory breaks down. Due to a large difference in the $c$-axis coherence lengths between the two bands, the smaller gap is quickly suppressed by transverse magnetic field. Also, the strong upward curvature of $H_{c2}(T)$ leads to temperature variations of the anisotropy ratio $\gamma_{an} = H_{c2}(T)/H_{c2}(T)$, which changes from $\gamma_{an} = 1.7$ near $T_c$ to $\gamma_{an} = 4.3$ at $T = 18$ K. These values are again consistent with experimental observations $16$ as well as with theoretical studies $24,25,26$.

C. Structure of a single vortex

The structure of an isolated superconducting vortex parallel to the $c$-axis has been studied in MgB$_2$ by the
an azimuthal angle and $\Delta$ gaps are parametrized as $\Delta_{\theta}$ along the $c$-axis oriented parallel to the hexagonal perconductor in the framework of the Ginzburg-Landau equations. The obtained spectra provide information about a small passive gap. A large vortex core size of about 5 coherence lengths $\xi_c = \sqrt{\Phi_0/2\pi H_c2}$ was reported and attributed to a fast suppression of a passive gap by magnetic field, whereas the $c$-axis upper critical field is controlled by a large gap in the $\sigma$-band. The experimental observations were confirmed within the two-band model using the Bogoliubov-de Gennes equations. We have, however, seen in the previous Subsection that a $\pi$-gap in MgB$_2$ is not suppressed near $H_c2(T)$ for fields applied along the $c$-axis. To resolve this discrepancy we present here a systematic study of the vortex core in a two-gap superconductor in the framework of the Ginzburg-Landau theory.

We investigate the structure of a single-quantum vortex oriented parallel to the hexagonal $c$-axis. The two gaps are parametrized as $\Delta_n(r) = \psi_n(r)e^{-i\theta}$, where $\theta$ is an azimuthal angle and $r$ is a distance from the vortex axis. Since the Ginzburg-Landau parameter for MgB$_2$ is quite large $\kappa \approx 25$, magnetic field can be neglected inside vortex core leading to the following system of the Ginzburg-Landau equations

$$\alpha_n \psi_n - \gamma \psi_n + \beta_n \psi_n^3 - K_n (\psi_n' + \psi_n/r - Q^2 \psi_n) = 0 \quad (21)$$

for $n = 1, 2$ ($n' = 2, 1$) and $Q \approx 1/r$. Away from the center of a vortex, the two gaps approach their asymptotic amplitudes $\psi_{0n}$

$$\psi_{01} = \sqrt{\frac{\alpha_1 + \gamma \rho}{\beta_1}}, \quad \psi_{02} = \sqrt{\frac{\gamma / \rho - \alpha_2}{\beta_2}} \quad (22)$$

with $\rho$ obeying Eq. (21). All distances are measured in units of a temperature-dependent coherence length derived from the upper critical field Eq. (13). In order to solve Eq. (21) numerically, a relaxation method has been used on a linear array of 4000 points uniformly set on a length of 80$\xi$ from the vortex center. An achieved accuracy is of the order of $10^{-6}$.

The obtained results are shown in Figures 3–5, where amplitudes $\psi_n(r)$ are normalized to the asymptotic value of the large gap $\psi_{01}$. To quantify the size of the vortex core for each component we determine the distance $d_n$, where $\psi_n(r)$ reaches a half of its maximum value $\psi_{0n}$. In the case of a single-gap superconductor such a distance is given within a few percent by the coherence length. In a two-gap superconductor the characteristic length scale for the large gap $d_1$ remains close to $\xi$, while $d_2$ can substantially vary. Size of the vortex core is given by $d_v = \max(2d_1, 2d_2)$.

Results for temperature dependence of the vortex core are presented in Fig. 4. The parameters $\alpha_20$ and $\gamma$ are taken the same as in the study of the upper critical field, while we choose $K_2/K_1 = 9$ in order to amplify effect for the small gap. As was discussed above, the equilibrium ratio of the two gaps $\psi_{02}/\psi_{01}$ grows with decreasing temperature (increasing $t$). Simultaneously, the small gap becomes less constrained with its interaction to the large gap and the half-amplitude distance $d_2$ shows a noticeable growth. For $K_2 \approx K_1$ such a less constrained behavior of $\psi_2(r)$ at low temperatures does not lead to an increase of the core size because both gaps have similar intrinsic coherence lengths.

This trend becomes more obvious if the coupling constant $\gamma$ is changed for fixed values of all other parameters, see Fig. 4. For vanishing $\gamma$, the distance $d_2$ approaches asymptotically an intrinsic coherence length in the passive band. This length scale depends on $K_2$ ($d_2/d_1|_{\gamma=0} \approx \sqrt{K_2/K_1} = 3$), but is not directly related to an equilibrium value of the small gap: the small gap is reduced by a factor of 7 between $\gamma = 0.6$ and $\gamma = 0.03$, while the core size increases by 50% only. Therefore, the single-band BCS estimate $\xi_2 = v_F/(\pi \Delta_2)$ for the char-
a peculiar behavior is determined by the two-gap nature of superconductivity in MgB$_2$.

A. Single-gap superconductor

An orientation of the flux line lattice in tetragonal and cubic superconductors has been theoretically studied by Takanaka. Recently, similar crystal field effects were found to be responsible for the formation of the square vortex lattices in the borocarbides. The case of a single-gap hexagonal superconductor is treated by a straightforward generalization of the previous works. Symmetry arguments suggest that coupling between the superconducting order parameter and a hexagonal crystal lattice appears at the sixth-order gradient terms in the Ginzburg-Landau functional. For simplicity, we assume that gap anisotropy is negligible. Then, the six-order gradient terms derived from the BCS theory are

$$F_6 = \frac{\zeta(7)N_0}{32\pi^6T_c^6} \left(1 - \frac{1}{2^6}\right) (\psi_F \psi_F \psi_F \psi_F \psi_F \psi_F) \times (\nabla \nabla \nabla \nabla \nabla) .$$

The above terms can be split into isotropic part and anisotropic contribution, the latter being

$$F_6^{an} = \frac{\zeta(7)N_0}{64\pi^6T_c^6} \left(1 - \frac{1}{2^6}\right) (\psi_F^2 - (\psi_F^2)) \times \Delta^4 \left[\nabla_x^2 - 15\nabla_y^4 + 15\nabla_x^2 \nabla_y^2 - \nabla_y^6 \right] \Delta$$
$$= -\frac{1}{2}K_6 \Delta^4 \left[(\nabla_x + i\nabla_y)^6 + (\nabla_x - i\nabla_y)^6 \right] \Delta .$$

In this expression $\hat{x}$ is fixed to the $a$-axis in the basal plane. (An alternative choice is the $b$-axis.) If $\hat{x}$ and $\hat{y}$ are simultaneously rotated by angle $\varphi$ about the $c$-axis, $(\nabla_x \pm i\nabla_y)^6$ acquires an extra factor $e^{\pm 6i\varphi}$. In the following we always make such a rotation in order to have $\hat{x}$ pointing between nearest-neighbor vortices. Periodic Abrikosov solutions with chains of vortices parallel to the $x$-axis are most easily written in the Landau gauge $A = (-Hy, 0, 0)$.

The higher order gradient terms Eq. 24 give a small factor $H^2 \sim (1 - T/T_c)^2$ and can be treated as a perturbation in the Ginzburg-Landau regime. The Landau levels expansion yields $\Delta(x) = c_0f_0(x) + c_0f_0(x) + \ldots$, where the coefficient for the admixed sixth Landau level is $c_6/c_0 \approx -\sqrt{(6^6/3)}h^2e^{6i\varphi}K_6/K$. When substituted into the quartic Ginzburg-Landau term, this expression produces the following angular dependent part of the free energy:

$$\delta F(\varphi) = -\frac{2\sqrt{6}\xi K_6^2}{3K} h^2 e^{6i\varphi} |c_0|^2 (|f_0|/f_0)^2 f_0 \cos(6\varphi) ,$$

with $|c_0|^2 = K(h_{c2} - h)(|f_0|^2)/(|\beta|(|f_0|^4))$. Spatial averaging of the combination of the Landau levels is done in

![FIG. 5: Spatial dependencies of the gaps for various values of $K_2/K_1$ for $t = 0.3$.](image-url)
a standard way
\[
\frac{\langle |f_{0}|^2 f_0 f_0 \rangle}{\langle |f_{0}|^2 \rangle^2} = \frac{\sqrt{\sigma}}{12\sqrt{3}} \sum_{n,m} \cos(2\pi \rho mn) e^{-\pi \sigma (n^2 + m^2)}
\times \left[ \frac{\pi^2 \sigma (n-m)^6 - \frac{15}{2} \pi^2 \sigma^2 (n-m)^4}{4 \pi \sigma (n-m)^2 - \frac{15}{8}} \right],
\]
where summation goes over all integer \(n\) and \(m\) and parameters \(\rho\) and \(\sigma\) describe an arbitrary vortex lattice. For a hexagonal lattice \((\rho = 1/2, \sigma = \sqrt{3}/2)\), the numerical value of the lattice factor is \(\langle |f_{0}|^2 f_0 f_0 \rangle / \langle |f_{0}|^2 \rangle = -0.279\). Hence, \(\delta F(\varphi) \simeq + K_6 \cos(6\varphi)\) and for \(\langle v_{F x}^6 \rangle > \langle v_{F y}^6 \rangle \) \((K_6 > 0)\) the equilibrium angle is \(\varphi = \pi/2\) \((\pi/6)\), which means that the shortest spacing between vortices in a triangular lattice is oriented perpendicular to the \(a\)-axis, while for the other sign of anisotropy the shortest side of a vortex triangle is along the \(a\)-axis. Thus, the Fermi surface anisotropy fixes uniquely the orientation of the flux line lattice near the upper critical field.

**B. Two-gap superconductor**

In a multiband superconductor effect of crystal anisotropy may vary from one sheet of the Fermi surface to another. We apply again the tight-binding representation to obtain a quantitative insight about such effects in MgB\(_2\). Explicit expressions for dispersions of the two hole \(\sigma\)-bands are presented in the Appendix. Hexagonal anisotropy in the narrow \(\sigma\)-cylinders is enhanced by a nonanalytic form of the hole dispersions. Combined anisotropy of the \(\sigma\)-band is \(\langle v_{F x}^6 \rangle = 4.608\), \(\langle v_{F y}^6 \rangle = 4.601\), while for the \(\pi\)-band \(\langle v_{F x}^6 \rangle = 1.514\), \(\langle v_{F y}^6 \rangle = 1.776\) in units of \(10^{56}\) \(\text{cm/s}^5\). According to the choice of the coordinate system the \(\hat{x}\)-axis is parallel to the \(b\)-direction and the \(\hat{y}\)-axis is parallel to the \(a\)-direction in the boron plane. The above values might not be very accurate due to uncertainty of the LDA results, however, they suggest two special qualitative features for MgB\(_2\). First, relative hexagonal anisotropy of the Fermi velocity \(v_{F n}(\varphi)\) differs by almost two orders of magnitude between the two sets of bands. Second, corresponding hexagonal terms have different signs in the two bands. In Appendix, we have shown that the sign difference is a robust feature of the tight-binding approximation and cannot be changed by a small change of the tight-binding parameters.

We investigate equilibrium orientation of the vortex lattice in MgB\(_2\) within the two-gap Ginzburg-Landau theory. Anisotropic sixth-order gradient terms of the type \(2\alpha_5 d_0 d_6\) have to be added to the functional for each of the two superconducting order parameters. As was discussed in the previous paragraph the anisotropy constants have different signs \(K_{61} > 0\) and \(K_{62} < 0\) and obey \(|K_{61}| \ll |K_{62}|\). In the vicinity of the upper critical field the two gaps are expanded as \(\Delta_1(x) = c_0 f_0(x) + c_6 f_6(x)\) and \(\Delta_2(x) = d_0 f_0(x) + d_6 f_6(x)\). Solution of the linearized Ginzburg-Landau equations yields the following amplitudes for the sixth Landau levels:

\[
c_6 = -4\sqrt{6} h^3 e^{6\varphi} \frac{K_{61} d_0 c_0 + K_{62} \gamma d_0}{\alpha_1 d_2 - \gamma^2},
\]
\[
d_6 = -4\sqrt{6} h^3 e^{6\varphi} \frac{K_{61} d_0 c_0 + K_{62} \gamma c_0}{\alpha_1 d_2 - \gamma^2}
\]

with \(\alpha_{1,2} = \alpha_{1,2} + 13K_{1,2}h\). Subsequent calculations follow closely the single-gap case from the preceding subsection. The angular dependent part of the free energy is obtained by substituting \(\alpha_{1,2}\) into the fourth-order terms:

\[
\delta F(\varphi) = \left[ \beta_1 c_0^2 + \beta_2 d_0^2 (d_4 + d_6^2) \right] \frac{\langle |f_0|^2 f_0^2 \rangle}{\langle |f_0|^2 \rangle^2} \cos(6\varphi).
\]

The resulting expression can be greatly simplified. If one uses \(\Delta_2/\Delta_1^2 \sim 0.1\) as a small parameter. With accuracy \(O(|\Delta_2/\Delta_1|^4)\) we can neglect the angular dependent part determined by the small gap. This yields in a close analogy with Eq. \(\beta_{1,2}\) the following anisotropy energy for the vortex lattice near \(H_{c2}\):

\[
\delta F(\varphi) = -\frac{2\sqrt{6}}{3K_1} \frac{h^2 \beta_1 |c_0| \langle |f_0|^2 f_0^2 \rangle}{\langle |f_0|^2 \rangle^2 K_{61} + K_{62} \gamma^2 (\alpha_2 + K_2 h) \gamma (\alpha_2 + K_2 h)}.
\]

Despite the fact that we have omitted terms \(\sim \delta d_0 d_6\), the Fermi surface anisotropy of the second band still contributes to the effective anisotropy constant \(K_{61}^\text{eff}\) via linearized Ginzburg-Landau equations. Along the upper critical line this contribution decreases suggesting the following scenario for MgB\(_2\).

In the region near \(T_c\), the second band makes the largest contribution to \(K_{61}^\text{eff}\): a small factor \(\gamma^2 \sim 0.1\) is outweighed by \(|K_{61}|/K_{62} < 0.1\). As a result, \(K_{61}^\text{eff}\) is negative and \(\varphi = 0\), which means that the shortest inter-vortex spacing is parallel to the \(b\)-axis. At lower temperatures and higher magnetic fields the second term in \(K_{61}^\text{eff}\) decreases and the Fermi surface anisotropy of the first band starts to determine the (positive) sign of \(K_{61}^\text{eff}\). In this case, \(\varphi = \pi/2\) \((\pi/6)\) and the side of the vortex triangle is parallel to the \(a\)-axis. The very small \(|K_{61}|/K_{62}| = 1.8 \cdot 10^{-2}\) which follows from the band structure data is insufficient to have such a reorientation transition in the Ginzburg-Landau region. Absolute values of anisotropy coefficients are, however, quite sensitive to the precise values of the tight-binding parameters and it is reasonable to assume that experimental values of \(K_{6n}\) are such that the reorientation transition is allowed.

The derived sequence of the orientations of the flux line lattice in MgB\(_2\) completely agrees with the neutron scattering data, though we have used a different scan line in the \(H-T\) plane in order to demonstrate the presence of the 30°-orientational transformation, see Fig. 6. Condition \(K_{61}^\text{eff} = 0\), or similar one applied to Eq. \(\beta_{1,2}\), defines a line \(H^*(T)\) in the \(H-T\) plane, which has a negative
slope at the crossing point with $H_{c2}(T)$. The six-fold anisotropy for the vortex lattice vanishes along $H^*(T)$ and all orientations with different angles $\varphi$ become degenerate in the adopted approximation. The sequence of orientational phase transition in such a case depends on weaker higher-order harmonics. One can generally write

$$\delta F(\varphi) = K_6 \cos(6\varphi) + K_{12} \cos(12\varphi) , \quad (30)$$

where the higher-order harmonics comes with a small coefficient $|K_{12}| \ll |K_6|$. Depending on the sign of $K_{12}$ transformation between low-field $\varphi = 0$ and high-field $\varphi = \pi/6, \pi/2$ orientations, when $K_6$ changes sign, goes either via two second-order transitions ($K_{12} > 0$) or via single first-order transition ($K_{12} < 0$). In the former case the transitions take place at $K_6 = \pm 4K_{12}$, whereas in the latter case the first-order transition is at $K_6 = 0$. These conclusions are easily obtained by comparing the energy of a saddle-point solution $\cos(6\varphi) = -K_6/(4K_{12})$ for Eq. (30), which is $\delta F_{ap} = -K_6^2/(8K_{12})$, to the energies of two extreme orientations.

In order to determine sign of the higher-order harmonics for a two-gap superconductor we expand the fourth-order terms in the Ginzburg-Landau functional (22) to the next order

$$\delta F'(\varphi) = \frac{1}{2} \left[ \beta_1 c_0^2 (c_0^2 + c_0^2) + \beta_2 d_0^2 (d_0^2 + d_0^2) \right] (f_0^2 f_0^2) . \quad (31)$$

These terms are responsible for a $\cos(12\varphi)$ anisotropy introduced before. Similar angular dependence is also induced by higher-order harmonics of the Fermi velocity $v_F(\varphi)$, though our estimate shows that even for the $\pi$-bands corresponding modulations are very small.\textsuperscript{20} Sign of $\cos(12\varphi)$ term in Eq. (31) depends only on a geometric factor, spatial average of the Landau levels wave functions. We find for a perfect triangular lattice

$$\langle f_0^2 f_0^2 \rangle / \langle |f_0| \rangle^2 = 0.804.$$  Thus, the twelfth-order harmonics in Eq. (31) has a positive coefficient and transformation between the low-field state with $\varphi = 0$ and the high-field state $\varphi = \pi/6$ goes via a phase with intermediate values of $\varphi$ separated by two second order transitions.

The anisotropy terms of the type (21) also produce a six-fold modulation of the upper critical field in the basal plane. Sign of the corresponding modulations of $H_{c2}(\varphi)$ should also change at a certain temperature, which is determined by a suppression of the small gap in transverse magnetic field and is not, therefore, related to the intersection point of $H_{c2}(T)$ and $H^*(T)$ lines on the phase diagram for $H \parallel c$, Fig. 6.

VI. CONCLUSIONS

We have derived the Ginzburg-Landau functional of a two-gap superconductor within the weak-coupling BCS theory. The functional contains only a single interaction term between the two superconducting gaps (condensates). This property allows a meaningful analysis of various magnetic properties of a multi-gap superconductor in the framework of the Ginzburg-Landau theory. Apart from confirming the previous results on an unusual temperature dependence of the transverse upper critical field in MgB$_2$, we have presented detailed investigation of the vortex core structure and have shown that the orientational phase transitions observed in the flux line lattice in MgB$_2$ is a manifestation of the multi-band nature of superconductivity in this material. The proposed minimal model for the $30^\circ$-rotation of the vortex lattice includes only anisotropy of the Fermi surface. An additional source of six-fold anisotropy for the vortex lattice can arise from angular dependence of the superconducting gap. It was argued that the latter source of (four-fold) anisotropy is essential for physics of the square to distorted triangular lattice transition in the mixed state of borocarbides.\textsuperscript{50} For phonon-mediated superconductivity in MgB$_2$, the gap modulations should be quite small, especially for the large gap on the narrow $\sigma$-cylinders of the Fermi surface. Experimentally, the role of gap anisotropy can be judged from the position of $H^*(T)$ line in the $H-T$ plane. $H^*(T)$ does not cross $H_{c2}(T)$ line in scenarios with significant gap anisotropy.\textsuperscript{50} A further insight in anisotropic properties of different Fermi surface sheets in MgB$_2$ can be obtained by studying experimentally and theoretically the hexagonal anisotropy of the upper critical field in the basal plane.

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APPENDIX: ANISOTROPY IN $\sigma$-BANDS

We give here expressions for the dispersions and Fermi surface anisotropies in the two $\sigma$-bands, which are derived from the tight-binding fits of Kong et al.\(^{16}\) The in-plane $p_{x,y}$ boron orbitals in MgB$_2$ undergo an $sp^3$-hybridization with $s$-orbitals and form three bonding bands. At $k_{\perp} = 0$ these bands are split into a non-degenerate $A$-symmetric band and doubly-degenerate $E$-symmetric band, which lies slightly above the Fermi level. Away from the $k_{\perp} = 0$-line the $E$-bands splits into light and heavy hole bands. Their dispersions obtained by expansion of the tight-binding matrix\(^{15}\) in small $k_{\perp}$ are

$$
\varepsilon_{l}(k) = \varepsilon(k_z) - 2t_{\perp} \left[ \frac{k_x^2}{2} + 2g(k) \right]
\left[ \frac{1}{2}k_{\perp}^2 + dk_{\perp}^4 \frac{2g(k) + 7 + 9d}{384(1+d)} \right],
$$

$$
\varepsilon_{h}(k) = \varepsilon(k_z) - 2t_{\perp} \left[ \frac{k_x^2}{2} + 2g(k) \right]
\left[ \frac{1}{2}k_{\perp}^2 - dk_{\perp}^4 \frac{2g(k) + 7 + 9d}{384(1+d)} \right],
$$

where $\varepsilon(k_z) = \varepsilon_0 - 2t_{\perp} \cos k_z$ and $g(k) = \left( k_x^6 - 15k_x^4k_y^2 + 15k_x^2k_y^4 - k_y^6 \right)/k_y^6$. The tight-binding parameters are presented in Ref.\(^ {16}\) are $\varepsilon_0 = 0.58$ eV, $t_{\perp} = 5.69$ eV, $t_z = 0.094$ eV, and $d = 0.16$. The six-fold anisotropy is given by unusual nonanalytic terms, which are formally of the fourth order in $k$. Appearance of such nonanalytic terms is a direct consequence of the degeneracy of the two bands at $k = 0$. For example, a nonanalytic form of $\varepsilon(k)$ is known for four-fold degenerate hole bands of Si and Ge\(^{41}\) which have cubic anisotropy already in $O(k^2)$ order. Nonanalyticity of $\varepsilon_{l,h}(k)$ leads to a relative enhancement of the hexagonal anisotropy on two narrow Fermi surface cylinders. This anisotropy has opposite sign in light- and heavy-hole bands. The net anisotropy of the combined $\sigma$-band is determined mostly by the light-holes, which have larger in-plane Fermi velocities.

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