Ginzburg–Landau functional for superconductors with anisotropic pairing

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Limitations are found on the values of the phenomenological constants in the gradient terms in the Ginzburg–Landau functional. A layered superconducting phase arises in a certain region of parameter values in a zero magnetic field. The usual Landau picture of second-order phase transitions is disrupted in the case of a superconducting transition of this sort.

The diverse properties of superconductors with a nontrivial pairing can be studied through the use of a Ginzburg–Landau expansion, as in the usual case. Of primary interest are superconductors which are described near T_c by a multicomponent order parameter which is transformed by one of the multidimensional representations of the point group of the crystal. The corresponding types of Ginzburg–Landau functionals were first discussed in Refs. 1–3. The simplest is an energy functional for a vector order parameter $\Delta(\vec{k},\vec{r}) = \eta_x(\vec{r})\phi_x(\vec{k}) + \eta_y(\vec{r})\phi_y(\vec{k})$, which arises in the case of the representation E_1 of the group D_6 (the particular nature of the spin state is unimportant here):

$$\mathcal{F} = \int dV \left\{ \alpha\tau\eta_i^*\eta_i + \beta_1(\eta_i^*\eta_i)^2 + \beta_2|\eta_i\eta_i|^2 + K_1 D_i^*\eta_j^* D_i\eta_j + K_2 D_i^*\eta_i^* D_j\eta_j \right.$$
$$\left. + K_3 D_i^*\eta_j^* D_j\eta_i + K_4 D_z^*\eta_i^* D_z\eta_i + \frac{\vec{h}^2}{8\pi} - \frac{\vec{h}\vec{H}}{4\pi} \right\};$$

$$\tau = \frac{T}{T_c} - 1;\quad i,j = x,y,;\quad D_k = \partial_k - i\frac{2e}{\hbar c}A_k. \tag{1}$$

Before we use an energy of this type to study specific physical properties of a superconductor, we need to establish the limitations imposed on the values of the phenomenological constants in the Landau theory. In the present letter we examine these limitations exclusively for the energy in (1). There is no difficulty in generalizing the method proposed here to functionals of other symmetries.

All the limitations which we are seeking arise because in a zero external magnetic field ($\vec{H} = 0$) the Ginzburg–Landau functional must describe a transition from a symmetric high-temperature phase ($\vec{\eta}=0$) to a superconducting phase ($\vec{\eta}\neq 0$) as T is lowered. It follows in turn that the terms of fourth degree must be positive definite.[1-3] With respect to the energy in (1), we thus conclude $\beta_1>0$, $\beta_2>-\beta_1$. Depending on the sign of β_2, two types of homogeneous states, differing in symmetry, are possible below T_c:

$$\vec{\eta}\sim(1,0), \quad \text{if} \quad \beta_2<0; \tag{2a}$$

$$\vec{\eta}\sim(1,i), \quad \text{if} \quad \beta_2>0. \tag{2b}$$

We also need to impose some restrictions on the constants K_n with which the gradient terms appear in energy (1). So far, only two types of such conditions have been discussed.

We set $\vec{A}(\vec{r})=0$. In this case the derivatives reduce to an ordinary differentiation. When the expansion is carried out on the basis of a correctly selected representation, gradient terms of this sort must be positive definite. As a result, we find the necessary conditions.

$$K_1>0, \quad K_4>0, \quad K_{123}>0 \quad (K_{n\ldots m}=K_n+\ldots+K_m). \tag{3}$$

Conditions (3) are furthermore sufficient conditions if the order parameter does not interact with the magnetic field ($e=0$). We will show that this is not the case for functional (1).

Sufficient conditions can be found if the requirement of positive definiteness is imposed on the gradient terms for an arbitrary $\vec{A}(\vec{r})$, i.e., if we assume that these terms increase the energy for an arbitrary choice of $D_i\eta_j$ at each point in space. Along with the condition $K_4>0$, of which we are already aware, we thus find the stronger restrictions[4]

$$K_1>|K_3|; \tag{4a}$$

$$K_{123}>|K_2|. \tag{4b}$$

Conditions (4) guarantee that a transition occurs at $T=T_c$ from a normal state with $\vec{\eta}=0$ to one of the states in (2) and that these states are stable with respect to the appearance of inhomogeneities of any sort. They exhibit a Meissner effect and the usual sign of the slope of the $H_{c2}(T)$ curve at $T=T_c$. Nevertheless, we need to understand the extent to which these properties of the superconducting state stem from conditions (4) and also the extent to which it is necessary that these conditions themselves be satisfied. For example, in a weak-coupling theory we would have $K_1=K_2=K_3$, and even minor effects associated with the electron–hole asymmetry or with impurities could reverse the sign of inequality (4a). The results of Ref. 5, where a "magnetic" instability of state (2a) was found, also lead to this question.

We switch to some new units, putting the functional in dimensionless form. We set $\alpha=1$, $\beta_1=1$, and $K_1=1$. We then have

$$\frac{\vec{h}^2}{8\pi}\rightarrow\vec{h}^2,\ \ D_k\rightarrow D_k=\frac{1}{k}\partial_k+iA_k,\ \ \beta_2\rightarrow\beta_2/\beta_1,\ \ K_n\rightarrow K_n/K_1,$$

where k is the Ginzburg–Landau parameter. For brevity, we will use the old notation for these new dimensionless constants.

The symmetry group of functional (1) includes continuous translations, continuous rotations around the $\vec{z}$ axis, and the gauge group. The irreducible representations of this group are characterized by the wave vector $\vec{q}$ (below we assume $\vec{q}$, $\vec{A} \perp \vec{z}$, and $\vec{h} \parallel \vec{z}$), by the star of the wave vector (by its neighborhood in the $\vec{x}\vec{y}$ plane), and by the index of the representation of its small group, C_2. Accordingly, expanding the order parameter and the magnetic field in plane waves,

$$\eta_i(\vec{r}) = \sum \eta_{iq} \exp(i\vec{q}\vec{r}), \quad \vec{A}(\vec{r}) = \sum \vec{A}_q \exp(i\vec{q}\vec{r}), \quad \vec{A}_q = \vec{A}^*_{-q}, \quad \vec{h}_q = i(\vec{q} \times \vec{A}_q), \tag{5}$$

we find the quadratic terms

$$\tau(|\eta_{10}|^2 + |\eta_{20}|^2) + \sum_{q \neq 0} \left[\left(\tau + \frac{K_{123}}{\kappa^2} \vec{q}^{\,2} \right) |\eta_q^{\parallel}|^2 + \left(\tau + \frac{1}{k^2} \vec{q}^{\,2} \right) |\eta_q^{\perp}|^2 \right]. \tag{6}$$

A new feature of the Landau theory for transitions of this sort with a complex order parameter is the existence of invariants which are quadratic in η, which are linear in the magnetic field, and which are made up of basis functions of different irreducible representations:

$$\frac{2}{k} \left(\sum_{k=p+q} p_i A_{iq} \eta^*_{ik} \eta_{jp} \right) + \frac{K_2}{k} \left(\sum_{k=p+q} p_j A_{iq} \eta^*_{ik} \eta_{jp} + \text{c.c.} \right)$$
$$+ \frac{K_3}{k} \left(\sum_{k=p+q} p_j A_{iq} \eta^*_{jk} \eta_{ip} + \text{c.c.} \right). \tag{7}$$

The first invariant, which also arises in the case of scalar superconductors, vanishes identically since the magnetic field is transverse. The second and third sums in (7) give rise to a layered superconducting phase at $\vec{H} = \vec{0}$. An analytic solution of the Ginzburg–Landau equations is possible only in certain limiting cases. Before we look at them, let us review the various symmetry types of a layered structure. A magnetic field which varies in accordance with $h = h\cos(\vec{q}\vec{r})$ has the following symmetry group [the generating elements are given in braces (curly brackets); $\vec{q} \parallel \vec{x}$]:

$$G = \{L_{2z}, RT_{\vec{a}/2}, T_{\vec{b}}, RU_{2x}, \sigma_h\},$$

where $\vec{a} \parallel \vec{x}$, $a = 2\pi/q$, $\vec{b} \parallel \vec{y}$, and R is time reversal. For the group G, there can be several types of superconducting structures with the maximal symmetry, which are definitely extremals of the Ginzburg–Landau functional:

$$\eta_x \sim i, \quad \eta_y \sim \cos(\vec{q}\vec{r}) \quad \{\exp(i\pi)L_{2z}, \ \exp(i\pi)RT_{\vec{a}/2}, \ T_{\vec{b}}, \ \exp(i\pi)RU_{2x}\}, \tag{8a}$$

$$\eta_x \sim \cos(\vec{q}\vec{r}), \quad \eta_y \sim i \quad \{\exp(i\pi)L_{2z}, \ \exp(i\pi)RT_{\vec{a}/2}, \ T_{\vec{b}}, RU_{2x}\}, \tag{8b}$$

$$\eta_x \sim \sin(\vec{q}\vec{r}), \quad \eta_y = 0 \quad \{L_{2z}, \ \exp(i\pi)RT_{\vec{a}/2}, \ T_{\vec{b}}, RU_{2x}\}, \tag{8c}$$

$$\eta_x = 0, \quad \eta_y \sim \sin(\vec{q}\vec{r}) \quad \{L_{2z}, \ \exp(i\pi)RT_{\vec{a}/2}, \ T_{\vec{b}}, \exp(i\pi)RU_{2x}\}. \tag{8d}$$

If conditions (4a) and (4b) are violated, there are two paths along which an instability of homogeneous states to states (8a) and (8b), respectively, can occur.

All the symmetry elements in (8) must of course be represented by magnetic operators, which were introduced in Ref. 6 for the case of periodic magnetic fields. For magnetic translations the following relation holds:

$$T_{\vec{a}}T_{\vec{b}} = T_{\vec{b}}T_{\vec{a}} \exp\left(i\frac{2e}{\hbar c}\oint \vec{A}d\vec{s}\right), \tag{9}$$

where the integral is over the boundary of the unit cell. For the superconducting order parameter, the periodicity condition takes the form

$$T_{\vec{a}}\Delta(\vec{k},\vec{r}) = \exp(i\varphi_1)\Delta(\vec{k},\vec{r}), \quad T_{\vec{b}}\Delta(\vec{k},\vec{r}) = \exp(i\varphi_2)\Delta(\vec{k},\vec{r}).$$

These conditions mean that magnetic translations over the basic periods are commutative. In addition to (9), we draw the conclusion that a layered superconducting structure, symmetric under continuous translations along one direction and under discrete translations along another direction, can arise only if there is a zero magnetic flux through the sample. As in the usual case, the layered phases in (8a) and (8b) are disrupted by a magnetic field as the result of a penetration of vortices (or chains of vortices) with a finite energy. The result should be a Meissner effect.

Let us assume that condition (4a) alone is violated. Let us examine the appearance of an inhomogeneous structure of the corresponding symmetry, (8a). Near the transition point, the amplitudes η_{iq} with wave vectors which are multiples of $2\pi/a$ are small with respect to the amplitude of the fundamental mode. We thus substitute $\eta_x \sim \mu$, $\eta_y \sim i\nu\sqrt{2}\cos(\vec{q}\vec{r})$, and $h = h\cos(\vec{q}\vec{r})$ into (1). The energy becomes

$$\mathcal{F}/V = \tau\mu^2 + \left(\tau + \frac{q^2}{k^2}\right)\nu^2 + 2h^2\left(1 + \frac{\lambda^2}{q^2}\right) + \frac{2\sqrt{2}}{k}K_3 h\mu\nu + \beta_{12}\left(\mu^4 + \frac{3}{2}\nu^4\right)$$
$$+2(\beta_1 - \beta_2)\mu^2\nu^2, \quad \lambda^2 = \left(\mu^2 + \frac{1}{2}K_{123}\nu^2\right). \tag{10}$$

Minimizing the terms which depend on the magnetic field through h, we find

$$\Delta\mathcal{F}_h/V = -\frac{K_3^2}{k^2}\frac{q^2\mu^2\nu^2}{q^2+\lambda^2}, \quad h = -\frac{K_3 q^2\mu\nu}{\sqrt{2}k(q^2+\lambda^2)}. \tag{11}$$

We then minimize with respect to q:

$$\Delta\mathcal{F}_{qh}/V = -\frac{\nu^2}{\kappa^2}(|K_3|\mu - \lambda)^2, \quad q^2 = |K_3|\mu\lambda - \lambda^2 \quad \text{for} \quad |K_3|\mu > \lambda;$$
$$\Delta\mathcal{F}_{qh}/V = 0, \quad q^2 = 0 \quad \text{for} \quad |K_3|\mu < \lambda. \tag{12}$$

We combine (12) with the terms in (10) which are independent of h and q:

$$\mathcal{F}/V = \tau(\mu^2 + \nu^2) + \beta_{12}(\mu^2 + \nu^2)^2 + \frac{1}{2}\beta_{12}\nu^4 - 4\beta_2\mu^2\nu^2 - \frac{\nu^2}{k^2}(|K_3|\mu - \lambda)^2. \tag{13}$$

For negative values of β_2 which are large in absolute value, the minimum in (13), with (12), leads to the phase in (2a): $\nu^2 = 0$, $\mu^2 = |\tau|/2\beta_{12}$. However, as was mentioned in Ref. 5, this phase becomes unstable at $|K_3| \geqslant 2\kappa\sqrt{\beta}_2 + 1$. Analysis of the energy in (13) shows that a superconducting transition is still a second-order transition in this region of parameter values, and it goes to phase (8a) in the case $\tau = 0$. Assuming $\kappa \gg 1$ and, correspondingly, $|K_3| \gg 1$, to satisfy this condition, we find

$$\Delta^2 = |\tau| \Big/ \left(2\beta_{12} - \left(\frac{K_3^2}{k^2} + 4\beta_2\right)\zeta\right),$$

$$\zeta = \frac{1}{2}\left(\frac{K_3^2}{k^2} + 4\beta_2\right) \Big/ \left(\frac{K_3^2}{k^2} + 4\beta_2 + \frac{1}{2}\beta_{12}\right), \quad \mu^2 = \Delta^2(1 - \zeta), \quad \nu^2 = \Delta^2\zeta. \tag{14}$$

Along with (11) and (12), this result means that in a layered phase we have q^2, $h \sim |\tau|$, and the symmetry of this phase varies continuously with q with increasing distance from the transition point.

It is convenient to imagine the following picture, which is interesting from the experimental standpoint. On a diagram (e.g., in the P, T plane), the superconducting and normal phases are separated by a curve which may intersect the line $\beta_2(P,T) = 0$. If condition (4a) is also violated, and the condition $|K_3|/k \ll 1$ holds, then the phase in (8a) will arise in the region with

$$-\frac{(|K_3| - 1)^2}{4k^2} \leqslant \beta_2(P,T) \leqslant \frac{K_3^4}{2k^4}. \tag{15}$$

The boundary at the left corresponds to a line of second-order phase transitions with a specific-heat discontinuity

$$\Delta C = T_c\left(\frac{\partial\beta_2}{\partial T}\right)^2 \frac{4\tau^2}{\beta_{12}^2(\beta_{12} + (|K_3| - 1)K_{123}/k^2)}. \tag{16}$$

The intersection of this line with the line of the superconducting transitions gives rise to a polycritical point at which three curves of second-order transitions converge. The disappearance of the specific-heat discontinuity in (16) as T_c is approached accounts for an intersection of this sort.

The presence of invariants (7) in the energy functional disrupts the standard Landau scheme for second-order phase transitions. Although a second-order transition does occur at $\tau = 0$ for a certain representation ($q = 0$), the symmetry of the superconducting phase at $\tau < 0$ in the parameter region in (15) cannot be determined through a minimization of exclusively the invariants of fourth degree, constructed on the basis of this representation.

The boundary on the right (found in the approximation $|K_3| \gg 1$) corresponds to a first-order transition between phases (8a) and (2b), with a latent heat

$$Q = T_c \frac{\partial \beta_2}{\partial T} \frac{\tau^2}{4}.$$

Substituting the more general expressions for η_x and η_y into (1), we can show that no other layered phases with a symmetry lower than the maximal symmetry at small values of $|K_3|/k$ (small values of β_2) arise. At $|K_3|/k \gg 1$, on the other hand, the stability condition for phase (8a) is violated before the transition to phase (2b):

$$\frac{K_3^2}{k^2} + 3\beta_2 > \beta_2^2.$$

A phase with a lower symmetry $\{\exp(i\pi)L_{2x}, T_{\vec{a}}, T_{\vec{b}}\}$ arises in the process.

Some necessary limitations supplementing (3) are found from the condition that the fourth-degree terms in (13) be positive definite:

$$\frac{(|K_3| - 1)^2}{k^2} < (-4\beta_2 + (2 + \sqrt{6})\beta_{12}). \tag{17}$$

Corresponding results for phase (8b) can be found by replacing $|K_3| - 1$ by $|K_2| - K_{123}$ in all the equations above. In particular, one more necessary condition arises:

$$\frac{(|K_2| - K_{123})^2}{k^2} < (-4\beta_2 + (2 + \sqrt{6})\beta_{12}). \tag{18}$$

If conditions (4a) and (4b) are violated simultaneously, phases of a lower symmetry arise. There are similar limitations on these phases, but they cannot be written out explicitly.

When the actual values of the constants are taken into account (for UPt_3, for example, we would have $k \sim 20$–40 and $\beta_2 \sim 0.2\beta_1$), limitations of the type in (17) and (18) on the coefficients in functional (1) are not much stronger than conditions (3).

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