Scientia Africana, Vol. 13 (No.1), June 2014. Pp 72-76
 ISSN 1118 - 1931

BOUNDARY CONDITIONS IN THE GINZBURG LANDAU FORMULATION IN HEAVY FERMIONS SUPERCONDUCTORS

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Received:30-09-13
Accepted:28-01-14

ABSTRACT
The linearized gap equation is the basis for the microscopic derivation of the second order terms in the Ginzburg-Landau free energy expansion. However, close to the boundary these second order terms do not have the same form, since the kernel is changed due to quasi-particle scattering. In addition, these boundary corrections in their most general form to the Ginzburg-Landau functional, a group theoretical method is used. The boundary lowers locally the spatial symmetry of the system.

INTRODUCTION
The linearized gap equation in the form is the basis for the microscopic derivation of the second order terms in the Ginzburg-Landau free-energy Abrikosov, A. A., et al (1963). Excluding the gradient and fourth order term, we find that the corresponding part of the Ginzburg landau equation is

$$\eta(r) = \sum_j \int kij\ (r, r)\ d^3\ r'\eta_j\ (r)$$

$$= \sum_j Qij\ \eta_j\ (r) \qquad 1.1$$

This is a local limit, assuming that the variation of η is slow compared to the range ξ_o of the kernel $\{\xi_o << \xi(T)\}$. In the homogeneous region, Q_{ij} is always diagonal and proportional to the unit matrix for one single representation. However, close to the boundary these second order terms do not have the same form, since the kernel is changed due to quasi-particle scattering. To add these boundary corrections in their most general form to the Ginzbury Landau functional, we shall again use a group theoretical method. The boundary lowers locally the spatial symmetry of the system. The remaining symmetry G'is a subgroup of the bulk symmetry group G, which we represent further simply by the corresponding point groups G(G'). This means that we can add further terms to the Ginzburg Landau free energy which are invariant under this lower symmetry and are restricted to the boundary.

A convenient way to find the invariant terms is to derive the coupling terms of the order parameter to the normal vector n of the surface for the strain tensor Gor'kov, L. P, (1987). Since the normal vector n(written in the crystal lattice basis) belongs to the vector representation $D_{(G)}$ (Γ_4 for O_h, $\Gamma_2 \otimes \Gamma_5$ for D_{4h} and D_{6h}), we can derive these terms by the decomposition of

$$D^*_{(G)}{}^{(m)} \otimes \Gamma^* \otimes \Gamma \qquad 1.2$$

where Γis the representation of the order parameter. Because the vector representation has negative parity, the exponent m has to be an even integer.

In table 1 a list of these terms is given their restriction to the surface is represented by a δ function located there. The real extension is of the order of ξ_o which is negligibly small compared to the length scale ξ (T) in the Ginzbury-Landau regime close to Tc. We should mention that invariant terms of the form

$$D^{*}_{(G)}{}^{(m)} \otimes \Gamma^* \otimes \Gamma' + c.c, \qquad 1.3$$

also exit, combining two different representations and these can lead to admixtures of the order representations. However, for simplicity, we neglect them in further consideration without loss of the main surface properties we want to describe. To complete the boundary conditions we have to consider the variation of the Ginzbury-Landau theory (H_{ext} in the external magnetic field, however, we shall concentrate on the case of zero field). This condition is obtained from varitational minimization if we add the term $-(^1/_{4\pi})\int d^3r\, H_{ext}-$ B to the free energy.

Table I: Surface terms of the Ginzburg-Landau theories in (a) Cubic symmetry, where n is the surface normal vector and g_1 are real constants describing the surface properties, (b) hexagonal symmetry and (c) tetragonal symmetry.

Irreducible representation Γ	$F_{sf}(\eta\ ;\ \eta)$
	(a)
$\Gamma_1^{\pm}$	$g_1\lvert\eta\rvert^2$
$\Gamma_2^{\pm}$	$[g_1 + g_2\{(n_x^2 - n_y^2)(n_y^2 - n_z^2)(n_z^2 - n_x^2)\}^2]\lvert\eta\rvert^2$
$\Gamma_3^{\pm}$	$g_1(\lvert\eta_1\rvert^2 + \lvert\eta_2\rvert^2) + g_2[(2n_z^2 - n_x^2 - n_y^2)(\lvert\eta_2\rvert^2 - \lvert\eta_1\rvert^2)$
	$+ 3(n_x^2 - n_y^2)(\eta_1^*\eta_2 + \eta_1\eta_2^*)$
$\Gamma_{4,5}^{\pm}$	$g_1(\lvert\eta_1\rvert^2 + \lvert\eta_2\rvert^2 + \lvert\eta_3\rvert^2)$
	$+ g_2[n_x^2(2\lvert\eta_1\rvert^2 - \lvert\eta_2\rvert^2 - \lvert\eta_3\rvert^2) + n_y^2(2\lvert\eta_2\rvert^2 - \lvert\eta_1\rvert^2 - \lvert\eta_3\rvert^2)$
	$+ n_z^2(2\lvert\eta_3\rvert^2 - \lvert\eta_1\rvert^2 - \lvert\eta_2\rvert^2)]$
	$+ g_3[n_y n_z^2(\eta_2^*\eta_3 + \eta_2\eta_3^*) + n_z n_x(\eta_3^*\eta_1 + \eta_3\eta_1^*)$
	$+ n_x n_y(\eta_1^*\eta_2 + \eta_1\eta_2^*)$
	(b)
$\Gamma_1^{\pm}$	$[g_1(n_x^2 + n_y^2) + g_2n_z^2]\lvert\eta\rvert^2$
$\Gamma_2^{\pm}$	$[g_1(n_x^2 + n_y^2) + g_2n_z^2 + g_3(n_x n_y (n_x^2 - 3n_y^2))^2]\lvert\eta\rvert^2$
$\Gamma_3^{\pm}$	$[g_1(n_x^2 + n_y^2) + g_2n_z^2 + g_3(n_x n_y (n_x^2 - 3n_y^2))^2]\lvert\eta\rvert^2$
$\Gamma_4^{\pm}$	$[g_1(n_x^2 + n_y^2) + g_2n_z^2 + g_3(n_y n_z (n_y^2 - 3n_x^2))^2]\lvert\eta\rvert^2$
$\Gamma_{5,6}^{\pm}$	$[g_1(n_x^2 + n_y^2) + g_2n_z^2](\lvert\eta_1\rvert^2 + \lvert\eta_2\rvert^2) + g_3[(n_x^2 - n_y^2)(\lvert\eta_1\rvert^2 + \lvert\eta_2\rvert^2)$
	$+ 2n_x n_y(\eta_1^*\eta_2 + \eta_1\eta_2^*)]$
	(c)
$\Gamma_1^{\pm}$	$[g_1(n_x^2 + n_y^2) + g_2n_z^2]\lvert\eta\rvert^2$
$\Gamma_2^{\pm}$	$[g_1(n_x^2 + n_y^2) + g_2n_z^2 + g_3(n_x n_y (n_x^2 - n_y^2))^2]\lvert\eta\rvert^2$
$\Gamma_3^{\pm}$	$[g_1(n_x^2 + n_y^2) + g_2n_z^2 + g_3(n_x^2 - n_y^2)^2]\lvert\eta\rvert^2$
$\Gamma_4^{\pm}$	$[g_1(n_x^2 + n_y^2) + g_2n_z^2 + g_3\, n_x^2 - n_y^2]\lvert\eta\rvert^2$
$\Gamma_5^{\pm}$	$[g_1(n_x^2 + n_y^2) + g_2n_z^2](\lvert\eta_1\rvert^2 + \lvert\eta_2\rvert^2) + g_3(n_x^2 - n_y^2)(\lvert\eta_1\rvert^2 + \lvert\eta_2\rvert^2)$
	$+ g_4n_x n_y(\eta_1^*\eta_2 + \eta_1\eta_2^*)]$

Scientia Africana, Vol. 13 (No.1), June 2014. Pp 72-76
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THEORETICAL CONSIDERATION AND CALCULATION

The surface free energy has the form

$$F_{sf} = \{[g_1(n_x^2 + n_y^2) + g_2 n_z^2](\,|\eta_1|^2 + |\eta_2|^2\,) + g_3(n_x^2 - n_y^2)(\,|\eta_1|^2 + |\eta_2|^2\,) + g_4(n_x n_y)(\eta_1^*\eta_2 + \eta_1\eta_2^*)]\}\,\delta[n.(r - r_o)], \qquad 1.4$$

where r_o is a point on the boundary. It is easy to see that the choice of coefficient $g_1 = g_3 = g_4|2\rangle\ 0$ and $g_1 = a'\xi o > 0$ reproduces the result for specular scattering,[a' has the dimension of energy per unit volume and is defined by the second order coefficient A (T) =a'(T/Tc – 1); ξ_o takes the spatial extension of the kernel K into account],

For a surface perpendicular to n= (1, 0, 0) we find

$$F_{sf} = 2g_1/\eta_1/^2\delta(x) \qquad 1.5$$

The component η_1 is suppressed at the surface. To give an approximate solution of the boundary problem in the Ginzburg-Landau region we consider a superconductor with the homogeneous phase $\Delta(k) = i_{\sigma y}\ k_z\ (k_x \pm i_{ky})\ \eta_o\ (T)$. The magnitude of η_o derived from the minimization of the corresponding free energy is

$$|\eta_0(T)|^2 = \frac{-A(T)}{4(\beta_1 - \beta_2) + \beta_3} \qquad 1.6$$

with the free energy density

$$f_o = A(T)\,|\eta_0(T)|^2 \qquad 1.7$$

Approximation η_2 by $i|\eta_0|$ = constant, and varying the free energy with respect to $|\eta_1(x)|$, including the gradient terms, we obtain the differential equation

$$\delta^2 x|\eta_1| + \frac{2\beta_1}{k_1}|\eta_1|(|\eta_0|^2 - |\eta_1|^2) = 0 \quad 1.8$$

With the surface terms we find the boundary conditions.

$$[-k_1\delta x|\eta_1| + 2g_1|\eta_1|(|\eta_0|^2 - |\eta_1|) = 0,\ \left[-K_1|\eta_1|\ \delta x\ \phi_1 - \frac{2eAx}{c}\ \right] = 0 \quad 1.9$$

We parameterized the order parameter $\eta_j = |\eta_1|\exp(i\varnothing j)$ and separated it into a real and an imaginary part. The second equation corresponds to the natural condition well know from the conventional Ginzburg-Landau theory that no supercurrent is allowed to flow perpendicular to the surface for the complete expression of the current. The first equation with equation (1.8) gives the analytic solution

$$|\eta_1(x)| = |\eta_o|\tanh\left|\frac{x - x_o}{\sqrt{2}\xi}\right.$$

and

$$x_o = \frac{\bar{\xi}}{\sqrt{2}}\sinh^{-1}\left[\frac{k_1}{\sqrt{2}\xi g_1}\right] \quad 1.10$$

with $\bar{\xi}^{-2}\ (T) = 2\beta_1|\eta_0(T)|^2/k_1$ as the coherence length in the x-direction. This result is restricted to the range $|x| >> \xi_o$[5]. In this analysis $|\eta_1(o)|$ is finite and can be connected with an extrapolation length b defined by $\delta x|\eta_1(o)| = |\eta_1(o)|/b$, which leads to $b = k_1/2g_1 = k_1/2a\xi_o$. The length b is of the order ξ_o and therefore negligibly small compared with $\xi(T)$. Langner, A. D, et al (1988).

To calculate the surface energy F, per unit area we insert equation (1.10) in the free energy. By a partial integration and using equation (1.8) and (1.9), we find

$$F_s = \int_o^\infty (f - f_o)dx = \beta_1\int_o^\infty (|\eta_o|^4 - |\eta_1|^4)dx = {}^2/_3\beta_1\xi|\eta_o|^4 \quad 1.10$$

Generally, the surface energy is proportional to $|\eta_o(T)|^3$ – $|T - Tc|,^{3/2}$ whereas the bulk energy has a quadratic temperature dependence $|T - Tc|,^{3/2}$. This different T dependence is due to the fact that the region of reduced condensation energy at the surface is confined within a length $\xi - |\eta_o|^{-1}$, which changes with temperature $|T - Tc|,^{1/2}$. Kumar, P, and Wolfle, (1987).

This solution does not take into account that the two order parameter components are coupled by the fourth order terms $(2\beta_1 - 4\beta_2 + \beta_3)|\eta_1|^2 \; |\eta_2|^2$ for $\Delta\varnothing = {}^{4\pi}/_2$. Hence in general the component η_2 also varies at the surface. Roughly we can say that its modulus is lowered if $(2\beta_1 - 4\beta_2 + \beta_3) < 0$ and enhanced if $(2\beta_1 - 4\beta_2 + \beta_3) > 0$. The analytic solution of the complete problem is more complicated. However, the given solution is a good approach under the condition $[2\beta_1 - 4\beta_2 + \beta_3] << 2\beta_1$ [note that $2\beta_1 < (2\beta_1 - 4\beta_2 + \beta_3 < 2\beta_1$ is required for the stability of the state in equation (1.6).

RESULTS AND DISCUSSION

Considering the direction n= $(1, 1, 0)/\sqrt{2}$, it is useful to diagonalize the bilinear form in equation (1.4) by

$$\eta'_1 = \frac{1}{\sqrt{2}}(\eta_1 + \eta_2) \text{ and } \eta'_2 = \frac{1}{\sqrt{2}}(\eta_1 - \eta_2) \qquad 1.12$$

This yields the basis gap functions

$$\overline{\Delta}^1_{(1)}(k) = i\sigma_y k_z (k_x + k_y)/\sqrt{2}$$

and

$$\overline{\Delta}^1_{(2)}(k) = i\sigma_y k_z (k_x - k_y)/\sqrt{2}, \qquad 1.13$$

which are the states classified by the parity operation p(n). The component $\eta_1'$is suppressed, and η'_2 has similar properties to these of η_2 above. Finally, in the case of n=(0, 0, 1), the surface term treats both components equally, reconfirming the earlier result. These last two examples can be treated similarly to the first case. However, one has to keep in mind that in unconventional superconductors the coherence length $\xi(n)$ is in general direction dependent. Hess, D, W., et al (1989).

As we have seen, the group theoretical treatment is appropriate for analyzing the problem of specularly reflecting surfaces. It is, however, more general, since it is based only on the symmetry properties of the surface. Hence this formulation can be used for all surfaces with scattering properties that do not further lower its symmetry. This is the case if the scattering behaviour is homogeneous parallel to the surface, considered on a length scale ξ_o. Therefore diffuse scattering may also be included. The phenomenological parameters g_1 depend on the quality of the surface and describe the scattering of the Cooper pairs of the surface.

In the A phase of superfluid. He the geometry of the confining vessel has a significant influence on the superfluid phase. At the wall the angular momentum is aligned parallel to the surface normal vector n. Since the direction of the angular momentum is continuously degenerate, the bulk phase is determined by the shape of the surface. A similar effect is not expected in anisotropic superconducts.

The degeneracy of the superconducting phases discrete and therefore a certain phase is fixed in the bulk region. Thus no defect, and so no surface, can have a long-range influence except just at the phase transition. Additionally, in the case of heavy fermion superconductors, the range of the surface influence is rather short, because the zero temperature coherence length ξ_o is of the order of 10x the lattice constant, so no essential effect on the superconducting phase is expected, except for very thin films. On the other hand, the boundary

Scientia Africanca, Vol. 13 (No.1), June 2014. Pp 72-76
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conditions derived here can lead to magnetic effects if the superconducting phase breaks time-reversal symmetry.

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