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Extrapolation lengths of unconventional superconductors

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Abstract. Boundary conditions for unconventional superconducting order parameters at a superconductor-to-insulator boundary with a combination of diffusive and specular scattering are derived from quasiclassical weak-coupling theory for a general Fermi surface. The resulting variational result for the extrapolation length is compared to recent numerical results for a d-wave order parameter and good agreement is found.

The starting point for the analysis of the effects of a superconductor-to-insulator surface within the Ginzburg–Landau theory of superconductivity is the introduction of a phenomenological surface free energy for the order parameter ($\eta_{\gamma,i}$) of the following form [1]:

$$F_{\rm surface} = \sum_{\gamma,i,j} g_{\gamma,i,j}(\boldsymbol{n}) \int {\rm d}S \;\; \eta_{\gamma,i}\eta^*_{\gamma,j} \tag{1}$$

where $\boldsymbol{n}$ is the surface normal, γ represents an irreducible representation of the relevant group and i, j span the basis of this representation. Including this surface free energy with the bulk free energy allows a study of the form of the order parameter at a superconductor-to-insulator boundary [1], a study of the surface superconductivity [2–5], and a study of the upper critical field as a function of sample thickness [6]. To gain an insight into what constitute reasonable values for the coefficients g, a microscopic calculation is desirable. This can be done via the calculation of a related quantity known as the extrapolation length. For an isotropic superconductor the extrapolation length is given by $b = \kappa/g$ [7] and κ is defined through the bulk Ginzburg–Landau free energy

$$F = \alpha_0(T - T_c)|\psi|^2 + \beta|\psi|^4 + \kappa \sum_i ({\rm D}_i\psi)({\rm D}_i\psi)^* \tag{2}$$

where ${\rm D}_i = \partial_i - ({\rm i}\,2e/\hbar c)A_i$ and $\boldsymbol{A}$ is the vector potential. Microscopic calculations have been made to determine b. Such calculations were originally performed for a spherical Fermi surface in the presence of specular and diffusive boundaries for isotropic and p-wave order parameters within a weak-coupling model [7–9]. More recently such calculations have been performed for general order parameter symmetries in the presence of a specular reflecting surface in a weak-coupling model with a spherical Fermi surface [3] and a general Fermi surface [6], and for a diffusive scattering surface in the presence of a spherical Fermi surface for general order parameter symmetries [2]. Efforts have also been made to study the form of the order parameter at a superconductor–insulator boundary beyond the Ginzburg–Landau regime for spherical and cylindrical Fermi surfaces and for both specular and diffusive scattering [10, 11]. Here an analytical formula for the extrapolation length for general order

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parameter symmetries with a general Fermi surface in the presence of a boundary with mixed specular and diffusive boundary conditions is presented. The analogous formulae for cylindrical and spherical Fermi surfaces are also presented. In the case of a d-wave order parameter in the presence of a cylindrical Fermi surface the formula is compared to the recent numerical results of Alber *et al* [12].

The correlation function method developed by de Gennes [7, 8] and extended to unconventional superconductors by Sigrist and Ueda [1] is used. A weak-coupling model with a general Fermi surface and no spin-flip scattering at the surface is assumed. The development of the formalism initially parallels that of Sigrist and Ueda [1]. The starting point is the following equation for the order parameter $\eta_i(\boldsymbol{R})$ (see reference [1] for details):

$$\eta_i(\boldsymbol{R}) = \int \mathrm{d}^3R' \; K_{ij}(\boldsymbol{R}, \boldsymbol{R}')\eta_j(\boldsymbol{R}') \tag{3}$$

with $K_{ij}(\boldsymbol{R}, \boldsymbol{R}')$ given by [1]

$$K_{ij}(\boldsymbol{R}, \boldsymbol{R}') = gk_BT \sum_{\omega_n} \sum_{\nu,\mu} \frac{\langle \mu|\mathrm{tr}\, \hat{\Delta}_i^\dagger[\boldsymbol{J}(\boldsymbol{R})]|\nu\rangle\langle\nu|\hat{\Delta}_j[\boldsymbol{J}(\boldsymbol{R})]|\mu\rangle}{(\mathrm{i}\omega_n - \epsilon_\nu)(-\mathrm{i}\omega_m - \epsilon_\mu)} \tag{4}$$

where

$$\langle\nu|\hat{\Delta}_j[\boldsymbol{J}(\boldsymbol{R})]|\mu\rangle = [\Delta_{s,s'}[(\boldsymbol{\nabla}_r - \boldsymbol{\nabla}_{r_1})/2\mathrm{i}]\phi^*_{\nu s}(r)\phi_{\mu s'}(r_1)]_{r_1\to r} \tag{5}$$

and $\hat{\Delta}_i(\boldsymbol{p})$ is related to the gap function $\hat{\Delta}(\boldsymbol{R}, \boldsymbol{p})$ by $\hat{\Delta}(\boldsymbol{R}, \boldsymbol{p}) = \sum_i \eta_i(\boldsymbol{R})\hat{\Delta}_i(\boldsymbol{p})$, the hat in $\hat{\Delta}$ indicates a 2×2 matrix in spin space that corresponds to the four allowed spin pairings of the paired quasiparticles, and 'tr' indicates a trace over this spin matrix (see reference [1] for details). A feature that is important in later considerations is that $K_{i,j}(\boldsymbol{R}, \boldsymbol{R}') = K_{j,i}(\boldsymbol{R}', \boldsymbol{R})$. After manipulating the kernel and using the semiclassical and weak-coupling approximations, which entail

$$\sum_\nu \langle \mathrm{tr}\, \hat{\Delta}_i^\dagger \hat{\Delta}_j\rangle \delta(\epsilon_\nu - \epsilon) \approx N(0)\langle \mathrm{tr}\, \hat{\Delta}_i^\dagger \hat{\Delta}_j\rangle_{\epsilon=\epsilon_F,\mathrm{classical}}$$

[7, 8] where $N(0)$ is the density of states at the Fermi surface, the following form for the kernel is found [1]:

$$K_{ij} = gN(0)\pi k_BT \sum_{\omega_n} \int_0^\infty \mathrm{d}t \;\; \exp(-2|\omega_n|t)\langle \mathrm{tr}\, \hat{\Delta}_i^\dagger[\boldsymbol{J}(\boldsymbol{R})]\hat{\Delta}_j[\boldsymbol{J}(\boldsymbol{R}', t)]\rangle_{\epsilon_F,\mathrm{classical}} \tag{6}$$

where the expectation value is an average in a canonical ensemble for an electron with momentum on the Fermi surface.

In the following it is assumed that the surface normal lies along a direction where $\epsilon_F(p_x, p_y, p_z) = \epsilon_F(p_x, p_y, -p_z)$; this will ensure that a quasiparticle reflected specularly from the boundary will have a momentum that lies on the Fermi surface. This restriction limits the analysis to high-symmetry directions where the off-diagonal components in the kernel are typically zero; therefore only the diagonal components are considered from here on. It is further assumed that there is homogeneity in the plane orthogonal to the surface normal.

Using the method of quasiclassical trajectories [13, 9, 7] it can be shown that the kernel takes the form (this is a simple extension of the work of Shapoval [9])

$$K_{ii}(z, z') = K_{ii}^{\mathrm{bulk}}(z - z') + K_{ii}^{\mathrm{surf}}(z, z') \tag{7}$$

where

$$K_{ii}^{\mathrm{bulk}}(z-z') = \left\langle \sum_{\omega_n} \exp\left(-2\frac{|\omega_n||z-z'|}{v_z}\right) \frac{\mathrm{tr}[\hat{\Delta}_i^\dagger(\boldsymbol{p})\hat{\Delta}_i(\boldsymbol{p})]}{v_z} \right\rangle \tag{8}$$

$$K_{ii}^{\mathrm{surf}}(z,z') = \left\langle \sum_{\omega_n} \int_{p'_z>0} \mathrm{d}^3p'\ S(\boldsymbol{p}\to\boldsymbol{p}') \exp\left(-2\frac{|\omega_n|z'}{v'_z} - 2\frac{|\omega_n|z}{v_z}\right) \frac{\mathrm{tr}[\hat{\Delta}_i^\dagger(\boldsymbol{p})\hat{\Delta}_i(\boldsymbol{p}')]}{v'_z} \right\rangle \tag{9}$$

where $\langle A\rangle$ means the average of A over the portion of the Fermi surface with $v_z > 0$, and $S(\boldsymbol{p} \to \boldsymbol{p}')$ gives the probability density for scattering from momentum $\boldsymbol{p}$ to momentum $\boldsymbol{p}'$ (this distribution satisfies $\int_{p_z>0} S(\boldsymbol{p}' \to \boldsymbol{p})\ \mathrm{d}^3p = 1$). The first term of the kernel corresponds to the contribution from the bulk (which remains when no surface is present), and the second contribution arises from the scattering of the quasiparticles from the surface. This scattering is characterized by the probability density $S(\boldsymbol{p} \to \boldsymbol{p}')$. For specular reflection

$$S_{ref}(\boldsymbol{p}\to\boldsymbol{p}') = \delta^3(\boldsymbol{p}' - 2(\boldsymbol{n}\cdot\boldsymbol{p})\boldsymbol{n}).$$

For diffusive scattering $S_{diff}(\boldsymbol{p} \to \boldsymbol{p}')$ is independent of $\boldsymbol{p}$ and the condition $K_{ii}(z,z') = K_{ii}(z',z)$ implies

$$S_{diff}(\boldsymbol{p}\to\boldsymbol{p}') = v'_z\delta(\epsilon(\boldsymbol{p}') - \epsilon_F)/\langle v_z\rangle.$$

Here the form

$$S(\boldsymbol{p}\to\boldsymbol{p}') = (1-P)S_{ref}(\boldsymbol{p}\to\boldsymbol{p}') + PS_{diff}(\boldsymbol{p}\to\boldsymbol{p}')$$

is used, which corresponds to a probability $1-P$ of being specularly reflected. The transition temperature is eliminated via the relation

$$\int \mathrm{d}z\ K_{ii}^{\mathrm{bulk}}(z) = 1.$$

The equation that the order parameter satisfies is given by

$$\eta_i(z) = \int_0^\infty \mathrm{d}z'\ K_{ii}(z,z')\eta_i(z'). \tag{10}$$

It can be verified that $\eta_i = \eta_{i0}(1 + x/b_i)$ is a solution to equation (10) as $x \to \infty$. This allows the use of the variational approach of Svidzinsky [14] to determine the coefficient b. Substituting $\eta = C(x + q(x))$ (then $b = \lim_{x\to\infty} q(x)$) into equation (10) gives

$$q(x) = \frac{E(x)}{2} + \int_0^\infty K(x,x')q(x')\ \mathrm{d}x' \tag{11}$$

with

$$E(x) = 2\int_0^\infty x'K(x,x')\ \mathrm{d}x' - 2x.$$

The above equation can be found by minimizing the functional

$$\Psi[q] = \left(\int_0^\infty \mathrm{d}x\ q(x)\left[q(x) - \int_0^\infty \mathrm{d}x'\ K(x,x')q(x')\right]\right)\Big/\left[\int_0^\infty \mathrm{d}x\ q(x)E(x)\right]^2. \tag{12}$$

The minimum value of $\Psi[q]$ is given by

$$\Psi_{min} = 1\Big/\left(2\int_0^\infty \mathrm{d}x\ q(x)E(x)\right). \tag{13}$$

The coefficient b can be expressed in terms of Ψ_{min} as

$$b = \left(\frac{1}{2}\int_0^\infty \mathrm{d}x\ xE(x) + \frac{1}{4\Psi_{min}}\right) \times \left(\frac{1}{2}\int_0^\infty \mathrm{d}x\ E(x) - \int_0^\infty \mathrm{d}x'\ x'\left[\int_0^\infty \mathrm{d}x\ K(x',x) - 1\right]\right)^{-1}. \quad (14)$$

Using a constant for $q(x)$ gives the following result:

$$b_i = \frac{(14\zeta(3)k_BT_c)^{-1}}{\langle \mathrm{tr}\,\Delta_i^\dagger\Delta_i v_z^2\rangle + P\,\mathrm{tr}\,[\langle\Delta_i^\dagger v_z\rangle\langle\tilde{\Delta}_i v_z^2\rangle - \langle\Delta_i^\dagger v_z^2\rangle\langle\tilde{\Delta}_i v_z\rangle]/2\langle v_z\rangle} \times \left\{\frac{(7\zeta(3))^2}{2\pi^3}\frac{[\langle \mathrm{tr}\,\Delta_i^\dagger\Delta_i v_z^2\rangle + (1-P)\langle \mathrm{tr}\,\Delta_i^\dagger\tilde{\Delta}_i v_z^2\rangle + P\,\mathrm{tr}\,\langle\Delta_i v_z\rangle\langle\tilde{\Delta}_i v_z^2\rangle/\langle v_z\rangle]^2}{\langle \mathrm{tr}\,\Delta_i^\dagger\Delta_i v_z\rangle - (1-P)\langle \mathrm{tr}\,\Delta_i^\dagger\tilde{\Delta}_i v_z\rangle - P\,\mathrm{tr}\,\langle\Delta_i v_z\rangle\langle\tilde{\Delta}_i v_z\rangle/\langle v_z\rangle} + \frac{\pi^3}{24}[\langle \mathrm{tr}\,\Delta_i^\dagger\Delta_i v_z^3\rangle + (1-P)\langle \mathrm{tr}\,\Delta_i^\dagger\tilde{\Delta}_i v_z^3\rangle + P\,\mathrm{tr}\,\langle\Delta_i^\dagger v_z^2\rangle\langle\tilde{\Delta}_i v_z^2\rangle/\langle v_z\rangle]\right\} \quad (15)$$

where $\Delta = \hat{\Delta}(\boldsymbol{p})$, $\tilde{\Delta} = \hat{\Delta}(\tilde{\boldsymbol{p}})$, $\tilde{\boldsymbol{p}} = (p_x, p_y, -p_z)$, and $\zeta(3) = \sum_{n\geqslant 0} 1/(n+1)^3$.

For a spherical Fermi surface and for a Fermi surface with cylindrical symmetry in the effective-mass approximation (when the axis of symmetry is orthogonal to the surface normal) the extrapolation length can be written as

$$\frac{b_i}{\xi_0} = \left((7\zeta(3))^{-1}\Big/\left\{\int_0^1 s^2F_-(s)\ \mathrm{d}s + P\frac{1}{2\pi}\,\mathrm{tr}\left[\left(\int_0^1 s\hat{\Delta}_i^\dagger(s)\right)\left(\int_0^1 s^2\hat{\Delta}_i(-s)\right) - \left(\int_0^1 s^2\hat{\Delta}_i^\dagger(s)\right)\left(\int_0^1 s\hat{\Delta}_i(-s)\right)\right]\right\}\right) \times \left\{\frac{\pi^4}{24}\left[\int_0^1 s^3F_-(s)\ \mathrm{d}s + (1-P)\int_0^1 s^3F_+(s)\ \mathrm{d}s + P\pi^{-1}\,\mathrm{tr}\left(\int_0^1 s^2\hat{\Delta}_i^\dagger(s)\right)\left(\int_0^1 s^2\hat{\Delta}_i(-s)\right)\right] + \frac{(7\zeta(3))^2}{2\pi^2}\left[\int_0^1 s^2F_-(s)\ \mathrm{d}s + (1-P)\int_0^1 s^2F_+(s)\ \mathrm{d}s + P\pi^{-1}\,\mathrm{tr}\left(\int_0^1 s\hat{\Delta}_i^\dagger(s)\right)\left(\int_0^1 s^2\hat{\Delta}_i(-s)\right)\right]^2\Big/\left[\int_0^1 sF_-(s)\ \mathrm{d}s - (1-P)\int_0^1 sF_+(s)\ \mathrm{d}s - P\pi^{-1}\,\mathrm{tr}\left(\int_0^1 s\hat{\Delta}_i^\dagger(s)\right)\left(\int_0^1 s\hat{\Delta}_i(-s)\right)\right]\right\} \quad (16)$$

where

$$\xi_0 = v_F/2\pi k_BT_c$$

$$F_-(s) = (1/2)\mathrm{tr}\int_0^{2\pi} \mathrm{d}\phi\ [\hat{\Delta}_i^\dagger(s,\phi)\hat{\Delta}_i(s,\phi) + \hat{\Delta}_i^\dagger(-s,\phi)\hat{\Delta}_i(-s,\phi)]$$

$$F_+(s) = (1/2)\mathrm{tr}\int_0^{2\pi} \mathrm{d}\phi\ [\hat{\Delta}_i^\dagger(s,\phi)\hat{\Delta}_i(-s,\phi) + \hat{\Delta}_i^\dagger(s,\phi)\hat{\Delta}_i(-s,\phi)]$$

$$\hat{\Delta}_i(s) = \int_0^{2\pi} \mathrm{d}\phi\ \hat{\Delta}_i(s,\phi)$$

and $\hat{\Delta}_i(\phi, s)$ is given by setting $\boldsymbol{p} = (\sqrt{1-s^2}\cos\phi, \epsilon^{1/2}\sqrt{1-s^2}\sin\phi, s)$ in $\hat{\Delta}(\boldsymbol{p})$, where $\epsilon = m_\perp/m_c$, and m_c and $m_\perp$ are the effective masses along and perpendicular to the axis of cylindrical symmetry.

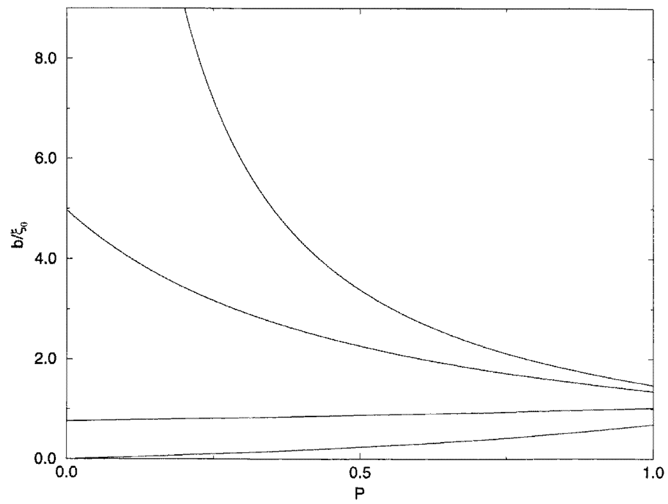

Figure 1. The extrapolation length for a $d_{x^2-y^2}$ superconductor with a cylindrical Fermi surface. P represents the probability of diffusive scattering, and θ is the angle that the surface normal makes with the $\hat{x}$-direction. The curves form top to bottom correspond to $\theta = 0, \pi/18, \pi/8$, and $\pi/4$ respectively.

As a particular example, the extrapolation length for a d-wave superconductor with a cylindrical Fermi surface takes the form

$$\frac{b}{\xi_0} = \frac{4}{7\pi\zeta(3)} \left\{ \frac{\pi^4}{24} \left[\frac{2}{3} + \frac{2}{35}\cos(4\theta) + (1-P)\left(\frac{2}{35} + \frac{2}{3}\cos(4\theta) \right) + P\frac{\pi^2}{32}\cos^2(2\theta) \right] \right.$$
$$\left. + \frac{49\zeta^2(3)}{32} \frac{[1 + (1-P)\cos(4\theta) + P\,\frac{1}{3}\cos^2(2\theta)]^2}{1 - \frac{1}{15}\cos(4\theta) - (1-P)(\cos(4\theta) - \frac{1}{15}) - P\,\frac{2}{9}\cos^2(2\theta)} \right\} \tag{17}$$

where θ is the angle between the surface normal (which lies in the basal plane) and the crystallographic $\boldsymbol{a}$-direction. The extrapolation length in this case has been studied numerically [12] and this provides a good test of the variational principle used to find equations (15), (16), and (17). Figure 1 shows the results from equation (17); this figure should be compared to figure 6 of reference [12]. The numerical values given in reference [12] for $b/\xi_0 < 4.0$ all agree to within less than five per cent with those found using equation (17). For $b/\xi_0 > 4.0$ the values found by using equation (17) are greater than those found numerically. The worst agreement is found for $\theta = 0$ and $P = 0.2$, where equation (17) gives $b/\xi_0 = 9.0$, while the result of reference [12] is $b/\xi_0 = 7.4$ (this is the largest value that they compute for b/ξ_0). This discrepancy is presumably due to finite-size effects that will arise in the numerical approach of reference [12]. Note that the variational approach used here gives a lower bound for the actual value of b/ξ_0.

In conclusion, a formula has been found for the extrapolation length within a weak-coupling quasiclassical theory for general order parameter symmetries, general Fermi surfaces, and a combination of specular and diffusive boundary conditions. This formula is valid only along high-symmetry directions for a general Fermi surface. For the case of d-wave pairing, the formula gives values that agree well with values found numerically [12]. Furthermore, the variational approach gives the correct values for b/ξ_0 in the solvable limits for all order parameter symmetries [3, 2], indicating that the approach used here to find the extrapolation length is reliable.

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