Quasiclassical theory of superconductivity: a multiple interface geometry

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In many cases of interest such as a multilayer mesoscopic structure (e.g. a superlattice) or the grain boundaries network in high-$T_c$'s, one deals with the situation where electrons traverse many partially transparent interfaces without losing coherence. Then, the consequent reflection/transmission events require a simultaneous consideration. Theoretically, even an isolated interface poses certain difficulties: Since abrupt changes violate the quasiclassical condition, the theory of superconductivity in terms of the quasiclassical matrix Green’s function $\hat{g}_R$ is invalid at interfaces. The interface is included via the boundary condition derived by Zaitsev \cite{5} – a cubic matrix relation.

In case of many interfaces, one comes to a system of nonlinear matrix equations solution of which is far from simple if possible. Moreover, some authors argue \cite{6} that the normalization condition is violated in the multiple interface case so that the quasiclassical scheme fails. The purpose of this paper is to consider the multiple interface case so that the quasiclassical equation Eq.(1) is valid, whereas the knots are included via the boundary matching condition. The latter is formulated for the “wave functions” $\phi = (\begin{pmatrix} \phi_+ \\ \phi_- \end{pmatrix})$, $\bar{\phi} \equiv (\begin{pmatrix} \nu \\ -\nu \end{pmatrix})$ factorizing $\hat{g}_R$, $\hat{g}_R(x+0,x) = \phi_+(x)\bar{\phi}_-(x)$, found from the linear equations,

$$(iv\frac{\partial}{\partial x} + \hat{H}_R(x))\phi = 0, \phi_\pm(x \to \pm \infty) = 0, \quad (2)$$

and normalized, $\bar{\phi}_-\phi_+ = 1$.

A general interface is partially diffusive, mixing states within a continuum of momenta. As a model, one allows mixing a finite number of states, $N$ incoming and $N$ outgoing, at a knot. The knot value of the wave functions $\phi_i (\phi_{k'})$ in the in-coming (out-going) channels, $i, k' = 1, \ldots, N$ are related to each other by the unitary scattering matrix $\hat{S}$:

$${\phi_{k'}} = \sum_{i=1}^{N} S_{ki} \phi_i. \quad (3)$$

The energy independent matrix $S$, the normal state property, is considered as a given input.

In this scheme, one finds the “wave function” $\phi$ by solving Eq.(2) on the pieces of the trajectory in between the knots and uses Eq.(3) to tailor the pieces. The scheme allows one to consider the usual and Andreev reflections on equal footing, simultaneously with (in)elastic scattering processes included via the self-energy $\Sigma_R$.

Here we restrict ourselves to the simplest case of $N = 2$ (corresponding e.g. to a partially transparent specular interface) when the $S$-matrix takes the form $$(r, t) \rightarrow \begin{pmatrix} r_t & t_r \\ -t_r & r_t \end{pmatrix}, \quad R \equiv |r|^2, T = |t|^2, R + T = 1.$$ Analysis \cite{1} shows that Eq.(3) leads to the following relation among the knot values of the 1-point Green’s functions $\hat{g}_1^R$ and $\hat{g}_1^T$ on the trajectories 1 and $1'$:

$${\hat{g}_1^R} = M \hat{g}_1^R M^{-1} \quad (4)$$

where the transfer matrix $M$ reads

$${M} = \frac{1}{2tr} \left( 1 + R \right) \left( 1 - \frac{T}{1 + R} \hat{g}_2^T \hat{g}_2^R \right), \quad (5)$$

here $\hat{g}_2^{R*T}$, the “across the interface” propagator, is

$${\hat{g}_2^{R*T}} = \frac{1}{1 + \frac{1}{2} [\hat{g}_2^R, \hat{g}_2^R]_+} \left( \hat{g}_2^R + \hat{g}_2^T + \frac{1}{2} [\hat{g}_2^R, \hat{g}_2^R] \right), \quad (6)$$

where $[\ldots]_\pm$ denotes (anti)commutator.
Eqs. (11) being equivalent to Zaitsev’s boundary conditions, seem to be more convenient for numerical calculations. Besides, they can be easily generalised to the case of a diffusive interface modelled by a knot \( N > 2 \).

To illustrate the method, we calculate the density of states and the superfluid density for a system with 3 planes of reflection: a sandwich made of two superconducting layers \( L \) and \( R \) separated by a partially transparent interface; the layers occupy the regions \(-d_L < z < 0\) and \(0 < z < d_R\) and the order parameter is \( \Delta_L \) and \( \Delta_R \), respectively.

Consider the periodic zig-zag trajectory in the \( R \)-layer, formed by reflections from the boundary at \( z = d_R \) and the interface at \( z = 0 \); it is specified by the angle \( \theta \) and the period \( a_\theta = 2d_R/\cos \theta \). Knots are the points where the zig-zag touches the interface. Because of the periodicity, each of the regular solutions \( \phi_\pm(x) \) is proportional to one of the eigenvectors of the evolution matrix \( \hat{U}_x \), defined via \( \phi(x + a_\theta) = \hat{U}_x \phi(x) \). The evolution matrix reads,

\[
\hat{U}_x = \hat{U}^{(0)}(x,0) M \hat{U}^{(0)}(0,x-a_\theta),
\]

where \( M \) is the transfer matrix Eq. (6), and \( \hat{U}^{(0)} \) is the bulk evolution operator corresponding to Eq. (3): \( \hat{U}^{(0)}(x+y,y) = \exp[iz\hat{H}^R/v] \). One can show that the 1-point Green’s function for the direction \( n_z = \pm \cos \theta \) can be calculated as

\[
\hat{g}^R(x) = \hat{U}_x' \left/ \sqrt{\left( \hat{U}_x \right)^2} \right.,
\]

where \( \hat{U}_x' \) stands for \( \hat{U}_x - \left( \frac{1}{2} \text{Tr} \hat{U}_x \right) \mathbb{1} \).

Given the interface value of the Green’s function in the \( L \)-layer, one finds the transfer matrix from Eqs. (3-11), and Eqs. (11) give the \( R \)-layer Green’s function. Equations analogous to (11) can be written for the \( L \)-layer. Numerical iteration of the system of the equations, allows one to evaluate the physical properties of the system.

Motivated by the recent idea about the paramagnetic instability at normal-metal - superconductor interfaces in the situation where the proximity induced order parameter in the normal metal is negative (repulsion), we consider the case when \( \Delta_L = -\Delta_R \) (questions related to the self-consistency equation are left aside here). The angular resolved density of states (DOS), i.e. \( \text{Re} \langle \hat{g}^R \rangle_{11} \) for the almost transparent interface \( R = 0.1 \) is presented in Fig. 1. Note the zero value of DOS at small energies: DOS is extremely sensitive to reflection which leads to the splitting of the zero energy Andreev levels. Accordingly, the superfluid density \( \rho_s(T) \) (i.e. \( \rho_s < 0 \)) being strong for ideal interface, \( R = 0 \), disappears when the probability of reflection is as low as 0.04. These findings confirm the theoretical possibility of the paramagnetic effect, and at the same time indicate that the effect is very sensitive to the interface reflection inevitable in the experiment.

In conclusion, a new method which allows one to describe a system with multiple interfaces in the framework of the quasiclassical theory is presented.

![Figure 1: Angle resolved DOS vs (energy/\( \Delta \)); \( \Delta_L = -\Delta_R = \Delta, d_L/\cos \theta = d_R/\cos \theta = v/\Delta \).](image1)

![Figure 2: Space averaged superfluid density vs temperature for the reflection \( R = 0, 0.01, 0.04 \).](image2)

### References

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