Superconductivity in Multiple Interface Geometry: 
Applicability of Quasiclassical Theory

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The method of two-point quasiclassical Green’s function is reviewed and its applicability for description of multiple reflections/transmissions in layered structures is discussed. The Green’s function of a sandwich built of superconducting layers with a semi-transparent interface is found with the help of recently suggested quasiclassical method [A. Shelankov, and M. Ozana, Phys. Rev. B 61, 7077 (2000)], as well as exactly, from the Gor’kov equation. By the comparison of the results of the two approaches, the validity of the quasiclassical method for the description of real (non-integrable) systems is confirmed.

1. INTRODUCTION

One of the most efficient tools in the superconductivity theory is the method of the quasiclassical Green’s function. In recent decades, the quasiclassical technique has been successfully applied to a broad variety of problems. Efficiency of the quasiclassical theory is due to the fact that it allows one to get description directly on the large spatial and temporal scales relevant for superconductivity, completely eliminating from the theory short “quantum” scales given by the Fermi wave length. Ignoring fine features on the quantum scale, the theory gives a closed set of equations for smoothly varying envelopes.

The quasiclassical approximation is applicable in superconductors because the order parameter \( \Delta \) varies on the coherence length \( \xi \sim v_F/\Delta \), which usually much exceeds the Fermi wave length \( \hbar/\bar{p}_F \), \( v_F \) and \( p_F \) being the Fermi velocity and momentum, respectively. As first discussed by Andreev, the slow spatial modulations of the order parameter cannot significantly change the momentum. Then, the two-component wave function...
\( \psi \) can be presented as \( \psi = e^{i \hbar p_F \cdot r (u)} \) where \( u \) and \( v \) are functions which slowly vary along a straight line, a classical trajectory corresponding to the momentum \( p_F \). After the factorization, the Fermi wave length does not enter the theory anymore.

The quasiclassical condition is violated if the potential energy varies on a scale of order of \( \lambda_F \) e.g. when disorder (impurities) or interfaces are present. Disorder does not pose any difficulty as long as one is interested only in the impurity averaged properties: On average, disorder enters the equations via the self-energy, acting like a smooth effective potential. Scattering by an isolated interface also does not create conceptionsal difficulties to the quasiclassical theory: one can include the reflection and transmission events by an appropriate boundary condition for the Andreev wave function \( \delta \) or the Green's function \( \eta \). It is worthwhile to notice at this point that the quasiclassical scheme does not give correct results for quantities local in the 2D phase space. For instance, a particle with the momentum \( k_{Fx} \) reflected from a wall creates the density, \( |\Psi|^2 = |e^{i k_{Fx} x} + re^{-i k_{Fx} x}|^2 \), which oscillates on the Fermi wave length due to the interference term \( 2 \text{Re} re^{-2ik_{F}x} \). However, the interference pattern, which is very sensitive to the value of \( k_{Fx} \), i.e. the direction of incidence, disappears after integration in a small region of the incidence angle. Although the quasiclassical technique ignores the interference of the incident and reflected wave, it gives correct predictions for coarse-grained averages: Observables like e.g. the electric current density, are given by the integral over the momentum space, and the low resolution description suffices.

In many interesting cases such as domains in the high-T\(_c\) oxides or artificial mesoscopic structures, a few partially reflecting interfaces are present. In a multi-layer geometry, the quasiclassical method meets severe difficulties as noted in Ref. \( \delta \). The purpose of this paper is to identify the physics behind the difficulties and check the validity of the recently suggested quasiclassical scheme by a numeric comparison with exact results for a double-layer structure.

We attribute the difficulties in the theory to the existence of interfering paths formed by sequential reflections in a multi-layer structure. Consider, for instance, a sandwich built of two superconductors, left and right, of finite thicknesses, \( a^{(l,r)} \) with a partially transparent interface, Fig. \( \delta \)(a). We assume that the outer walls and the interface are ideal so that all the reflections and transmissions are specular. A fragment of a classical trajectory for a symmetric sandwich is shown in Fig. \( \delta \)(b).

Various processes of the Andreev reflection of an electron-like excitation coming on the knot \( A \) are shown in Fig. \( \delta \). In the present context, the most interesting is the process shown in Fig. \( \delta \)(c) where the particle makes a loop.
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Fig. 1. (a) Sandwich build of two superconductor layers with the order parameters $\Delta^{(l,r)}$ and thicknesses $a^{(l,r)}$ separated by a partially transparent interface. (b) The semiclassical wave which corresponds to a particle hitting the interface at the point (knot) $A$, is split by the interface into the left and right beams. If the left and right layers have the same thickness, the beams meet each other again at the knot $B$ after the reflection by the outer walls.

The amplitude of the process, unlike the processes in Fig. 2(a),(b) contains the phase shift $\exp[ip_F(L^{(r)} - L^{(l)})]$ where $L^{(r)}$ and $L^{(l)}$ are the lengths of the left and right arms, respectively. As a result, the total amplitude given by the sum of various contributions, non-trivially depends on the value $p_F$. One comes to the conclusion that the Andreev factorisation, $\psi = e^{ip_F r(u)}$, which is the essence of the quasiclassical method, becomes impossible.

It is clear that the loop contribution is very sensitive to geometry and surface roughness. Indeed, (independent) variations of $L^{(l,r)}$ on the scale of $\lambda_F$ destroy the interference. Besides, loops exist only if the trajectories which are split by knot $A$ in Fig. meet again on knot $B$. This may happen only in an ideal structure; any imperfection on a scale $\gtrsim \lambda_F$ would not allow this “accidental” event to happen. (In other words, any real physical system is non-integrable.) In a real system, multiple reflections/transmissions lead to the formation of single-connected tree-like trajectories as has been discussed in Ref. 9. The quasiclassical technique is expected to be applicable if one solves the equations on the tree rather than on straight line trajectories.

Below, we compare exact and quasiclassical theories. For definiteness, we consider the trajectory resolved density of states (DOS) obtained by both approaches. It is clear from the very beginning, that agreement may be present only on a low resolution level: strong microscopic variations of the exact DOS in the $p - r$ space must be smoothen by integration in a small region of the phase space. Even then, disagreement is expected. The point is that the exact calculations are manageable only for an ideal geometry.
Fig. 2. (a) and (b) Examples of processes included into quasiclassical theory. An electron is Andreev reflected back as a hole and follows the original trajectory. The loops are not formed in these cases. (c) The simplest example of a loop-forming process. An electron is scattered in the right arm and then Andreev reflected as a hole in the left arm. Such a process is not included in the quasiclassical approach which considers only tree-like (simply connected) trajectories.

whereas the quasiclassical theory is expected to be valid only when some roughness is present. In the ideal geometry, there are always loops which survive averaging in the phase space, and their contribution may spoil the agreement.

The paper is organised as follows. In Sec. 2, we review the quasiclassical approach to the multi-layer systems. We introduce the trajectory Green’s function and its factorization. The Green’s function in the double layer system is found using both quasiclassical theory (Sec. 3) as well as Gor’kov equations (Sec. 4). In Sec. 5, the exact approach is compared with the quasiclassical theory. The applicability and the limits of quasiclassics are discussed. The results are summarised in Sec. 6.

2. QUASICLASSICAL TECHNIQUE

After Eilenberger, the quasiclassical Green’s (retarded) function $\hat{g}_n^R(r)$, which is a $2 \times 2$ matrix in a spin-singlet Cooper pair superconductor, is introduced as

$$\hat{g}_n^R(r) = \frac{i}{\pi} \int d\xi \hat{G}_{p}^R(r) ,$$

(1)
Applicability of the quasiclassical theory ... where \( \hat{G}_p(r) \) is the Green’s function \( \hat{G}(r_1, r_2) \) in the Wigner representation

\[
\hat{G}_p^R(r) = \int \hat{G}^R(r + \frac{p}{2}, r - \frac{p}{2}) e^{ip\cdot\rho}. \tag{2}
\]

The Green’s function for a given direction of the momentum \( n \) obeys a differential equation which couples the spatial points along a straight line parallel to \( n \) (or, more precisely parallel to the Fermi velocity \( v_F \) corresponding the selected point of the Fermi surface in case of anisotropic spectrum). The line is the classical trajectory of the electron (hole).

Alternatively, to Eq. (1), one may use the formulation of the quasiclassical technique in terms of the 2-point Green’s function on classical trajectories. The 2-point Green’s function obeys the following equations

\[
\left( iv \frac{\partial}{\partial x_1} + \hat{H}^R_{\varepsilon, n}(r_1) \right) \hat{g}^R_{\varepsilon}(x_1, x_2|n, R) = iv\delta(x_1 - x_2), \quad r_1 = R + x_1 n, \tag{3}
\]

\[
\hat{g}^R_{\varepsilon}(x_1, x_2|n, R) \left( -iv \frac{\partial}{\partial x_2} + \hat{H}^R_{\varepsilon, n}(r_2) \right) = iv\delta(x_1 - x_2), \quad r_2 = R + x_2 n, \tag{4}
\]

where the derivative in Eq. (4) operates backwards. The \( 2 \times 2 \) traceless matrix \( \hat{H}^R_{\varepsilon, n} \) reads,

\[
\hat{H}_{\varepsilon, n} = \hat{h}_{\varepsilon, n} - \hat{\Sigma}^R_{\varepsilon, n},
\]

\[
\hat{h}_{\varepsilon, n} = \begin{pmatrix}
\varepsilon - v \cdot p_s & \Delta_n \\
-\Delta^*_n & -\varepsilon + v \cdot p_s
\end{pmatrix}, \quad v = vn, \tag{5}
\]

where \( \Delta_n \) is the order parameter (which may depend on the direction \( n \)), and \( p_s = -\frac{\varepsilon}{e} A, A \) being the vector potential, and \( \hat{\Sigma}^R \) is built of the impurity self-energy and the part of the electron-phonon self-energy not included to the self-consistent field \( \Delta \). (Below, we omit \( R, n \) and \( \varepsilon \) for brevity and use the notation \( \hat{g}^R_{\varepsilon}(x_1, x_2) \).

The propagator \( \hat{g}^R \) tends to zero at \( |x_1 - x_2| \to \infty \), and \( \hat{g}^R \) is an analytic function of \( \varepsilon \) in the upper half plane for any \( x_{1,2} \) including \( |x_1 - x_2| = \infty \).

Although the observables can be expressed via the quasiclassical 1-point Green’s function \( (x_1 = x_2) \), the 2-point Green’s function turns out to be a useful intermediate object. It gives a full physical description of the system in the approximation where part of the orbital degree of freedom is treated classically (no quantum broadening in the plane \( \perp n \)), with a complete quantum treatment of the electron-hole degree of freedom.

It is important that the construction based on the notion of smooth classical trajectories remains valid in the presence of disorder (or phonons), in the standard approximation when the scattering is included on the average via the self-energy (provided \( p_F l \gg 1, l \) being the mean free path).
2.1. Constructing 2-point Green’s function

The two-point matrix Green’s function on the trajectory \((n, R)\), is conveniently built from column “wave functions” \(\phi, \phi = (u^v)\) which satisfy the equation

\[
\left( iv \frac{\partial}{\partial x} + \hat{H}^R(x) \right) \phi = 0 ,
\]

(6)

here \(\hat{H}^R(x)\) stands for \(\hat{H}^R_{\xi,n}(r)\) at the trajectory point \(r = xn + R\).

Denote \(\bar{\phi}\) the row built from a column \(\phi\) by the following rule:

\[
\bar{\psi} \equiv \psi^T \tau_y \frac{1}{t} \Rightarrow \left( u^v \right) \Rightarrow \left( v , -u \right) .
\]

By virtue of the identity \((\hat{H}^R)^T = -\tau_y \hat{H}^R \tau_y\), the row \(\bar{\phi}(x)\) built from a solution to Eq. (6), satisfies the conjugated equation

\[
\bar{\phi}(x) \left( -iv \frac{\partial}{\partial x} + \hat{H}^R(x) \right) = 0 .
\]

(7)

It follows from Eq. (6) combined with (7), that

\[
\frac{d}{dx} (\phi_a \phi_b) = 0 .
\]

(8)

This relation is valid for any pair of solutions \(\phi_a\) and \(\phi_b\).

The Green’s function is built of the regular solutions to Eq. (6), i.e. solutions satisfying the following boundary conditions

\[
\phi_+(x) \to 0, \quad x \to +\infty , \quad \phi_-(x) \to 0, \quad x \to -\infty .
\]

(9)

Denote \(\phi^{(N)}_{\pm}\) the normalized solutions,

\[
\overline{\phi}^{(N)}_-(x) \phi^{(N)}_+(x) = 1 .
\]

(10)

The normalization is possible because the l.h.s. is a (finite) constant as it is seen from Eq. (8).

The Green’s function reads

\[
\hat{g}^R(x_1, x_2) = \left\{ \begin{array}{ll}
\phi^{(N)}_+(x_1) \phi^{(N)}_-(x_2) , & x_1 > x_2 ; \\
\phi^{(N)}_-(x_1) \phi^{(N)}_+(x_2) , & x_1 < x_2 .
\end{array} \right.
\]

(11)

Indeed, it satisfies Eq. (3) and Eq. (4) at \(x_1 \neq x_2\), and is regular at \(|x_1-x_2| \to \infty\) by virtue of Eq. (7). Besides, the normalization in Eq. (10) ensures that the discontinuity at \(x_1 = x_2\),

\[
\hat{g}^R(x + 0, x) - \hat{g}^R(x - 0, x) = \hat{1} ,
\]

(12)

has the value required by the \(\delta\)-function source in Eqs.(3), and (4).
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2.2. 1-point Green’s function

To find observables like the electric current or charge density, one needs the Green’s functions with coinciding spatial arguments, i.e. the 1-point Green’s function.

The 1-point Green’s functions, \( \hat{g}_R^R(x) = \hat{g}^R(x \pm 0, x) \), can be expressed via the normalized waves (see Eq. (11))

\[
\hat{g}_R^R(x) = \phi_+^{(N)}(x)\overline{\phi}_-^{(N)}(x) \quad \hat{g}_-^R(x) = \phi_-^{(N)}(x)\overline{\phi}_+^{(N)}(x).
\]

(13)

This expression can be identically written in the form,

\[
\hat{g}_R^R(x) = \frac{1}{\phi_-(x)\phi_+(x)} \phi_+(x)\overline{\phi}_-(x) \quad \hat{g}_-^R(x) = \frac{1}{\phi_-^-(x)\phi_+^+(x)} \phi_-(x)\overline{\phi}_+^+(x),
\]

(14)

where the normalization of the wave functions \( \phi_{\pm} \) is arbitrary.

Note the projecting properties:

\[
\hat{g}_\pm^R \hat{g}_\pm^R = \pm \hat{g}_\pm^R, \quad \hat{g}_\pm^R \hat{g}_\mp^R = 0, \quad \text{Sp} \hat{g}_\pm^R = \pm 1.
\]

(15)

Tagging electron- and hole-like excitations in accordance with the direction of their propagation (\( \pm x \) directions) and considering examples, e.g. the normal state, one concludes that \( \hat{g}_+^R \) can be identified as the (quasi)electron part of the Green’s function, and \( \hat{g}_-^R \) is the (quasi)hole one (and vice versa for \( \hat{g}_-^R \)).

Denoting

\[
a \equiv \frac{u_-}{v_-}, \quad b \equiv \frac{v_+}{u_+},
\]

(16)

where \( u_{\pm} \) and \( v_{\pm} \) are the components of \( \phi_{\pm} \),

\[
\phi_{\pm}(x) = \begin{pmatrix} u_{\pm}(x) \\ v_{\pm}(x) \end{pmatrix},
\]

Eq. (14) becomes

\[
\hat{g}_+^R = \frac{1}{1 - ab} \begin{pmatrix} 1 \\ b \end{pmatrix} \begin{pmatrix} 1 & -a \end{pmatrix}, \quad \hat{g}_-^R = \frac{1}{1 - ab} \begin{pmatrix} a \\ 1 \end{pmatrix} \begin{pmatrix} b & -1 \end{pmatrix}.
\]

(17)

As shown in Ref. 10, the 1-point Green’s function of the quasiclassical theory (“\( \xi \)-integrated”), \( \hat{g}^R \), is given by

\[
\hat{g}^R = \hat{g}_+^R + \hat{g}_-^R.
\]

(18)

i.e.

\[
\hat{g}^R = \phi_+^{(N)}\overline{\phi}_-^{(N)} + \phi_-^{(N)}\overline{\phi}_+^{(N)}.
\]

(19)
In terms of $\hat{g}^R$, 
\begin{equation}
\hat{g}^R_{\pm} = \frac{1}{2} \left( \hat{g}^R \pm 1 \right),
\end{equation}
and the relations in Eq. (15) lead to the well-known normalization condition 
\begin{equation}
\left( \hat{g}^R \right)^2 = \hat{1}.
\end{equation}
and
\begin{equation}
\text{Sp} \, \hat{g}^R = 0.
\end{equation}
Combining Eqs. (18) and (17), one gets
\begin{equation}
\hat{g}^R = \frac{1}{1 - ab} \begin{pmatrix} 1 + ab & -2a \\ 2b & -(1 + ab) \end{pmatrix}.
\end{equation}

This parameterisation of the Green’s function has been recently suggested by Schopohl and Maki (see, also Ref. 12). The present derivation leads quite naturally to this decomposition, and clearly shows the physics behind it. Seeing that $a$ and $b$ may be interpreted as the “local” amplitudes of the Andreev reflection for electron and hole (see below), we call them the Andreev amplitudes. The amplitudes $a$ and $b$ obey the nonlinear Riccati equation. From the Bogoliubov - de Gennes equation for $\psi = (u \, v)$, the Riccati equation for the ratio $u/v$ has been derived by Nagato et al.

### 2.3. Knot matching conditions

In the quasiclassical picture, particles move on smooth trajectories, usually, straight lines characterised by the direction of velocity $n$ (and the initial position $R$). On interfaces, where potentials change on atomic scales, the quasiclassical condition is violated, and the quasiclassical wave function spreads from the original trajectory to those coupled by quantum scattering. Following Ref. 9, we call a “knot” the point where classical trajectories are tied together.

In a general case, the knot ties together $N$ in- and $N$ out-trajectories. The in-trajectories (or channels) are those which have the the Fermi velocity directed towards the knot; the out-trajectory is characterised by the velocity directed from the knot. The in- and out-trajectories are somehow numbered, $l = 1, \ldots, N$; we mark the outgoing trajectories with $l$ so that $k'$ stands for the $k$-th outgoing channels.

On the quasiclassical scale $\sim v_F/\Delta$, the knot is point-like, and one can define the knot value of the trajectory wave function. Denote $\psi_i$ the 2-component wave function on the $i$-th in-coming trajectory, $i = 1, \ldots, N$
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at the point where it enters the knot, and analogously $\psi_{k'}$ the knot value on the $k$–th outgoing trajectory.

The knot matching conditions suggested in Ref. 9 read

$$\psi_{k'} = \sum_{i=1}^{N} S_{k'i} \psi_i , \quad \overline{\psi}_{k'} = \sum_{i=1}^{N} S_{k'i}^{\ast} \overline{\psi}_i , \quad \text{(22)}$$

where $S_{k'i}$ are the elements of the unitary scattering matrix. In the spirit of the quasiclassical theory, $S_{k'i}$ is the normal metal property taken at the Fermi surface; it is an electron-hole scalar. This relation generalises the matching conditions of Ref. 6 to the many channels case.

Eq. (6) together with the matching conditions in Eq. (22) allows one to find the 2-component amplitudes on trajectories with knots, and, therefore, the Green’s functions.

2.4. Matching Green’s functions

First consider an isolated knot mixing semi-infinite trajectories (with no more knots on them). With the origin chosen at the knot, the trajectory coordinate $x_n$ extends from $-\infty$ to 0 on the $n$-th incoming trajectory, and $0 < x_{k'} < \infty$ on the $k'$-outgoing one. As before, the requirement,

$$\phi_{-,m}(-\infty) = 0 , \quad \phi_{+,k'}(\infty) = 0 , \quad m, k = 1, \ldots, N \; ; \quad \text{(23)}$$

uniquely defines the solutions $\phi_{-,n}(x_n)$ and $\phi_{+,k'}(x_{k'})$ (up to a normalization factor). The knot values of the regular solutions are conveniently written as

$$\phi_{-,m}(x_m = 0) = \begin{pmatrix} a_m \\ 1 \end{pmatrix} , \quad \phi_{+,k'}(x_{k'} = 0) = \begin{pmatrix} 1 \\ b_{k'} \end{pmatrix} , \quad m, k = 1, \ldots, N ; \quad \text{(24)}$$

the parameters $a_m$ or $b_{k'}$ are “bulk” properties independent on the knot.

The problem is to find the knot values

$$\phi_{+,l}(x_l = 0) \equiv \begin{pmatrix} 1 \\ b_l \end{pmatrix} , \quad \phi_{-,n'}(x_{n'} = 0) \equiv \begin{pmatrix} a_{n'} \\ 1 \end{pmatrix} , \quad l, n = 1, \ldots, N , \quad \text{(25)}$$

needed to evaluate $\phi_{+,l}(x_l < 0)$ and $\phi_{-,n'}(x_{n'} > 0)$ and, therefore, the Green’s functions on the trajectories tied by the knot. On each of the trajectories, the Green’s function in the immediate vicinity to the knot is expressed via the corresponding pair $a_l$ and $b_l$ or $a_{n'}$ and $b_{n'}$ by the relation in Eq. (21).

As has been shown in Ref. 9, the boundary condition for the Andreev amplitudes $a_{n'}$ and $b_l$ can be conveniently formulated in terms of the determinant

$$D(\{a\}, \{b\}) = \det \left| 1 - \hat{S} \hat{a} \hat{S}^{\dagger} \hat{b} \right| , \quad \text{(26)}$$
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built of the S-matrix and the diagonal matrices \( \hat{a} = \text{diag}(a_1, a_2, \ldots, a_N) \) and \( \hat{b} = \text{diag}(b_1, b_2, \ldots, b_{N'}) \); \( a_m \) and \( b_{k'} \) entering Eq. (24) are bulk parameters insensitive to the presence of the knot.

An important property of \( D \) is that it is a linear function of any of \( a \)'s and \( b \)'s, so that identically

\[
\mathcal{D} = \mathcal{D}^{(l)}_0 + a_l \mathcal{D}^{(l)}_1, \quad \mathcal{D} = \mathcal{D}^{(n')}_0 + b_{n'} \mathcal{D}^{(n')}_1, \quad n', l = 1, 2, \ldots, N,
\]

where

\[
\mathcal{D}^{(l)}_0 = \mathcal{D}|_{a_l=0}, \quad \mathcal{D}^{(l)}_1 = \frac{\partial}{\partial a_l} \mathcal{D}, \quad \mathcal{D}^{(n')}_0 = \mathcal{D}|_{b_{n'}=0}, \quad \mathcal{D}^{(n')}_1 = \frac{\partial}{\partial b_{n'}} \mathcal{D}.
\]

Also, \( D \) is a sum each terms of which is a product of an equal number of \( a \)'s and \( b \)'s. From this one concludes that

\[
\sum_l \mathcal{D}^{(l)}_0 = \sum_n \mathcal{D}^{(n')}_0.
\]

These identities are useful for transforming various expressions.

Rephrasing the procedure described in Ref. 9, the knot values of the Andreev amplitudes in Eq. (25) can be found by the following formulae:

\[
a_{n'} = -\mathcal{D}^{(n')}_1 \mathcal{D}^{(n')}_0, \quad b_l = -\mathcal{D}^{(l)}_1 \mathcal{D}^{(l)}_0.
\]

For the case \( N = 2 \), equivalent relations have been derived in Ref. 15.

Now, one is able to build the Green’s functions Eq. (17) on the \( l \)-th in- and \( n \)-th out trajectories.

\[
\hat{g}^{(l)}_+ = \frac{1}{\mathcal{D}} \begin{pmatrix} \mathcal{D}^{(l)}_0 & 1 \end{pmatrix} \begin{pmatrix} a_l & -1 \end{pmatrix}, \quad \hat{g}^{(n')}_- = \frac{1}{\mathcal{D}} \begin{pmatrix} -\mathcal{D}^{(n')}_1 \mathcal{D}^{(n')}_0 & b_{n'} \end{pmatrix} \begin{pmatrix} -1 & 1 \end{pmatrix}.
\]

With the help of the identities in Eq. (27) and Eq. (28), one can present Eq. (31) in the form,

\[
\hat{g}^{R(l)} = \begin{pmatrix} 2\gamma_l - 1 & -2\gamma_l a_l \\ \frac{2}{\alpha_l} (1 - \gamma_l) & -(2\gamma_l - 1) \end{pmatrix}, \quad \hat{g}^{R(n')} = \begin{pmatrix} 2\gamma_{n'} - 1 & \frac{2}{\beta_{n'}} (1 - \gamma_{n'}) \\ 2\gamma_{n'} b_{n'} & -(2\gamma_{n'} - 1) \end{pmatrix},
\]

where

\[
\gamma_l = \frac{\mathcal{D}^{(l)}_0}{\mathcal{D}}, \quad \gamma_{n'} = \frac{\mathcal{D}^{(n')}_0}{\mathcal{D}}.
\]

It follows from Eq. (28) that

\[
\sum_l \left( \hat{g}^{R(l)} \right)_{11} = \sum_n \left( \hat{g}^{R(n')} \right)_{11}.
\]
This identity is directly related to the current conservation.

Summarising, the Green’s functions on trajectories linked by a knot are calculated as follows. First, one solves Eq. (6) with the boundary condition in Eq. (23) on each of the trajectories and calculates “bulk” functions \( \phi_{-m}(x < 0) \) and \( \phi_{+k'}(x > 0) \). By this, one finds \( a_m \) and \( b_{k'} \) in Eq. (24). For a knot characterised by a scattering matrix \( S \), one is then able to find the determinant \( D \) Eq. (26). The next step is to calculate the knot values of \( b \)’s on the incoming trajectories and \( a \)’s on the outgoing ones using Eq. (30). Then, one solves Eq. (3) for \( \phi_{+l}(x < 0) \) on the incoming trajectories and \( \phi_{-l'}(x > 0) \) on the outgoing ones with the boundary condition \( \phi_{+l}(0) = (1 \quad b_l) \) and \( \phi_{-l'}(0) = (0 \quad l') \), respectively. The 1-point Green’s function is then built from \( \phi_{\pm} \) using the representation in Eq. (19). The knot values of the Green’s functions can be also found from Eqs. (31), or (32).

This scheme is also applicable when the trajectories connected by the knot under consideration may enter other knots, in a tree-like trajectory (see Fig. 3). As a matter of principle, one assumes that the system under consid-

Fig. 3. An example of a tree-like trajectory. Pieces of the straight lines show the trajectories before or after they enter a knot (filled circles), i.e. before or after a collision with an interface. There is only one path connecting any two points on the tree so that the tree is effectively 1-dimensional.

eration is finite, and it is surrounded by a “clean” material where trajectories are infinite lines without knots. Then, one solves the problem for the knots on the boundary and moves inwards towards the knot of interest. In the one-dimensional topology of the tree with only one path connecting any two knots, the procedure is unique.
3. SANDWICH: QUASICLASSICAL GREEN’S FUNCTION

In this section we calculate the quasiclassical Green’s function in a double layer system depicted on Fig. 1. The real space classical trajectory of a particle in a two layer system is formed by multiple reflections on the outer surface and the interface between the layers (see Fig. 4).

The Green’s function can be found using Eq. (32). In this simple case with only two in- and out-trajectories, determinant $D$ reads

$$D = R(1 - a_1b_1')(1 - a_2b_2') + T(1 - a_1b_2')(1 - a_2b_1'), \quad (35)$$

where $R$ and $T$ are the reflection and transmission coefficients.

The problem is to find the amplitudes $a_m$ on the incoming legs of a certain knot and $b_k'$ on the outgoing legs. Since none of the legs lead to infinity the situation is slightly different than in the previous chapter and the procedure has to be modified.

![Fig. 4. The trajectories of a particle in a two layer system.](image)

The argument used to find the equations for the amplitudes $a_m$ and $b_{k'}$ is the invariance with respect to translation parallel to the interface. Suppose we know a transfer matrix which relates the wave function $\phi$ in the legs say "2" and "4". Because of the translational invariance these two functions can differ only by a prefactor. In another words $\phi$ is eigenfunction of the transfer matrix and the ratio of the components of $\phi$ must be the same in both corresponding legs. Thus the amplitudes $a$ in legs "2" and "4" are equal $a_2 = a_4$. One can argue in the same way to show that $a_1 = a_3, b_1' = b_3'$ and so on.
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We can proceed in the following manner. First we find the transfer matrix as a product of knot transfer matrix and propagator across the layer. Then we relate the amplitudes in corresponding legs. We get a set of 4 equations for 4 unknowns $a_1, a_2, b_1'$ and $b_2'$ (see Fig. 4 for notations).

The knot transfer matrix connecting the wave function in the incoming and outgoing legs on a knot can be written as follows

$$M_{2'\rightarrow 2} \propto \begin{pmatrix} 1 & a_1 \\ b_{1'} & 1 \end{pmatrix} \begin{pmatrix} R & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & a_1 \\ b_{1'} & 1 \end{pmatrix}^{-1}. \quad (36)$$

The transfer matrix for the channels on the right side is a function of the amplitudes only on the left side.

The propagator across the layer is found by integration of Eq. (6). For homogeneous superconductor the expression reads:

$$U(x) \propto \begin{pmatrix} 1 & a_0^{(r)} \\ b_0^{(r)} & 1 \end{pmatrix} \begin{pmatrix} e^{-i\xi^{(r)}_x} & 0 \\ 0 & e^{i\xi^{(r)}_x} \end{pmatrix} \begin{pmatrix} 1 & a_0^{(r)} \\ b_0^{(r)} & 1 \end{pmatrix}^{-1}. \quad (37)$$

Here, $a_0^{(r)} = \Delta^{(r)}/(\varepsilon + \xi^{(r)})$ and $b_0^{(r)} = \Delta^{(r)*}/(\varepsilon + \xi^{(r)})$ are the bulk values of $a$ and $b$ in the right layer, and $\xi^{(r)} = \sqrt{\varepsilon^2 - |\Delta^{(r)}|^2}$ (Im $\xi^{(r)} > 0$).

Once the transfer matrices for both sides are known, one can write down the 4 equations for the four unknown amplitudes $a_{1,2}$ and $b_{1',2'}$. Solving the equations and using the expressions relating $a$'s and $b$'s in the in/out going channels from the previous chapter one finds the amplitudes in every leg. Thus the Green’s function can be constructed and the density of states calculated.

When the numerical calculations are carried out, it is easier to use an iterative procedure instead of solving the set of four nonlinear equations. One starts with the bulk values of $a$ and $b$ in, say, right side and calculates the corresponding amplitudes on the left. These values are then used to calculate back $a$ and $b$ on the right side. This process is continued until self-consistency is reached.

4. SANDWICH: EXACT GREEN’S FUNCTION

In this section we calculate the exact Green’s function for a sandwich. Consider a sandwich formed by two homogeneous layers with thicknesses $a^{(l,r)}$ and order parameters $\Delta^{(l,r)}$; here and below, the superscript $(l)$ and $(r)$ label quantities which refer to the left and right layer, respectively, see Fig. 3(a).
The left (right) layer occupies the region $-a^{(l)} < x < 0$ ($0 < x < a^{(r)}$). The interface is characterised by the scattering $S$-matrix,

$$S = \begin{pmatrix} t & r \\ r & t \end{pmatrix},$$

with the transmission and reflection amplitudes $t$ and $r$ for the case of $\delta$-function interface potential. The outer walls are impenetrable. The goal is to find the exact Green’s function $G(r, r')$ from the Gor’kov equation.

Due to the translational invariance in the direction parallel to the layers, the problem is effectively one-dimensional. For a given value of the parallel momentum $p_{||}$, the Green’s function, $\hat{G} = \hat{G}_{\varepsilon, p_{||}}(x, x')$, depends on the two coordinates $x$ and $x'$ as well as the energy $\varepsilon$. The Gor’kov equation reads:

$$(\varepsilon - \hat{H}) \hat{G}(x, x') = \mathbb{1}\delta(x - x') \quad \hat{H} = \begin{pmatrix} \hat{\xi} & \Delta \\ \Delta^* & -\hat{\xi} \end{pmatrix}.$$  \hspace{1cm} (39)

For the parabolic spectrum, $\hat{\xi} = \hat{p}_{x}^{2}/2m - p_{Fx}^{2}/2m$, where $p_{Fx}$ is $x$-proiection of the Fermi momentum $p_{F}^{2} = p_{F}^{2} - p_{||}^{2}$. The Green’s function is continuous at $x = x'$: $\hat{G}(x^{+}, x) = \hat{G}(x^{-}, x)$. Its derivatives suffer a jump generated by the delta-function on the r.h.s. of Eq. (39):

$$\hat{p}_{x} \hat{G}(x, x') \bigg|_{x=x'^{+}}^{x=x'^{-}} = 2m/\hbar.$$  \hspace{1cm} (40)

The boundary conditions at $x = 0$ corresponding to the semi-transparent interface are conveniently written as

$$\hat{P}^{\sigma} \hat{G}(0^{+}, x') = \sum_{\sigma' = \pm} M_{\sigma\sigma'} \hat{P}^{\sigma'} \hat{G}(0^{-}, x') \quad \sigma = \pm,$$  \hspace{1cm} (41)

where the projectors $\hat{P}^{\pm}$,

$$\hat{P}^{\pm} = \frac{1}{2}(1 \pm \hat{p}_{x}/p_{Fx}) \hspace{1cm} (42)$$

and the transfer matrix $M$,

$$M = \begin{pmatrix} 1/t^{*} & r/t \\ r^{*}/t^{*} & 1/t \end{pmatrix}.$$  \hspace{1cm} (43)

It is convenient to express the Green’s function in terms of two-component functions $\Phi_{\nu, \sigma}(x)$ and $\overline{\Phi}_{\nu, \sigma}(x')$ defined as follows:

$$\Phi_{\nu, \sigma}(x) = \phi_{\nu} e^{i\sigma p_{\nu} x} \quad ; \quad \overline{\Phi}_{\nu, \sigma}(x') = \overline{\phi}_{\nu} e^{-i\sigma p_{\nu} x'}.$$  \hspace{1cm} (44)
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Here $\sigma = \pm$, $p_\nu = p_{Fx} + \nu \xi/m$ is the electron ($\nu = +$) or hole ($\nu = -1$) momentum, and $\phi_\nu$ is the solutions to matrix equation

$$
\begin{pmatrix}
\nu \xi \\
\Delta \\
\Delta^* \\
-\nu \xi
\end{pmatrix} \phi_\nu = \varepsilon \phi_\nu,
$$

(45)

and $\bar{\phi}_\nu$ is the adjoint row-vector defined in such a way that $\bar{\phi}_\nu \phi_\mu = \delta_{\nu\mu}$.

The Green’s function can be then written as:

$$i \hbar v_{Fx} \hat{G}(x,x') \sigma_z = \begin{cases}
\sum_{\nu,\nu',\sigma,\sigma'} \Phi_{\nu,\sigma}(x) \langle \nu,\sigma|Q^>||\nu',\sigma'\rangle \overline{\Phi}_{\nu',\sigma'}(x') & \text{for } x > x' \\
\sum_{\nu,\nu',\sigma,\sigma'} \Phi_{\nu,\sigma}(x) \langle \nu,\sigma|Q^<|\nu',\sigma'\rangle \overline{\Phi}_{\nu',\sigma'}(x') & \text{for } x < x'.
\end{cases}
$$

(46)

The $4 \times 4$ matrices $\hat{Q}^<,>$ are constants. It has different form for $x > x'$ and $x < x'$.

Inserting the Green’s function into Eqs. (39-40) and using the matching condition at the interface in Eq. (41) one gets $\langle \nu,\sigma|Q^<|\nu',\sigma'\rangle$. After straightforward but lengthy calculations, we have found the following rather simple result:

$$
\begin{pmatrix}
\tau_z Q_{11}^> & \tau_z Q_{12}^> \\
\tau_z Q_{21}^> & \tau_z Q_{22}^>
\end{pmatrix} = \frac{1}{D} 
\begin{pmatrix}
w_+ - A_+ A_- w_+ w_- & A_- w_+ (w_- - 1) \\
A_+ w_- (w_+ - 1) & w_- - A_+ A_- w_+ w_+
\end{pmatrix},
$$

(47)

$$D = 1 - A_+ A_- \text{Tr}(w_+ w_-).
$$

(48)

Here, $w_\pm$ is a $2 \times 2$ matrix, $w_\pm = W_\pm/\text{Tr}W_\pm$,

$$W_\nu = \begin{pmatrix}
1 \\
\exp(2i \eta \rho(r) a(r)) \cdot \left(r^* + |r|^2 e^{2i \eta \rho(l) a(l)} + |r|^2 + r e^{2i \eta \rho(l) a(l)}\right)
\end{pmatrix},
$$

(49)

and $A_\pm$ are (scalar) coefficients,

$$A_\pm = \frac{\overline{\phi}_\pm^{(r)} \phi_\pm^{(l)}}{\bar{\phi}_\pm^{(r)} \phi_\pm^{(l)}},
$$

(50)

which have the physical meaning of the Andreev reflection amplitudes for a transparent interface.

The Gor’kov Green’s function for a sandwich is known from the literature. Eq. (47) agrees with the previous work, giving simple and concise form for the Green’s function.
4.1. Coarse-grained Green’s function

As have been already mentioned in the Introduction, the quasiclassical theory does not attempt to give any good description on the truly microscopically local level. Instead, it supplies knowledge about coarse-grained observables. Accordingly, one should derive the coarse-grained Green’s function corresponding to the exact theory before comparing it with the quasiclassical counterpart.

![Figure 5: Discrete energy levels in the sandwich Fig. 1(a)](image)

Fig. 5. Discrete energy levels in the sandwich Fig. 1(a) corresponding to eigenstates with a definite momentum \( p_{||} \). The curves show how the position of the level \( \varepsilon \) changes under small variations of the angle \( \Theta \), \( \cos \Theta = p_{||}/p_F \). The sandwich with \( a^{(l)} = v_F/\Delta^{(l)} \) is thick on the scale of the Fermi wavelength: \( a^{(l)} = 1000/p_F \); the transparency of the interface \( T = 0.9 \). Other parameters of the sandwich: \( a^{(r)} = 3a^{(l)} \), \( \Delta^{(r)} = -2\Delta^{(l)} \).

The space averaging of the partial (i.e., momentum resolved) density of states is rather simple. For a given \( p_{||} \), the density of states is proportional to the imaginary part \( G_{p_{||}}(x, x' \rightarrow x) \). It is seen from Eq. (44) that the elements of the \( Q \)-matrix which are off-diagonal in \( \sigma \), create rapidly oscillating terms. Therefore, space averaging amounts to ignoring the off-diagonal terms.

Even reduced to a low spatial resolution, the Green’s function remains to be a fast function of the momentum direction. For instance, the density of states is non-zero only at those discrete values of \( p_{||} \) where the energy variable \( \varepsilon \) equals to the energy of the bound state for the finite motion in the \( x \)-direction. Fig. 5 shows the fast periodic motion of the energy level
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positions under a small variation of $p_\parallel$. An integration within a small interval of the angles is required to transform the density of states from a sequence of the $\delta$-function spikes into a smooth function of the momentum direction.

Fig. 6. The energies of the bound states as a function of angle (full line) superimposed on the quasiclassical angular resolved density of states (dashed line). The parameters of the double layer are $\Delta^{(r)} = -2\Delta^{(l)}, a^{(l)} = v_F/\Delta^{(l)}, a^{(r)} = 3v_F/\Delta^{(l)}, T = 0.9, \Theta = \pi/4$.

In the next section we compare the coarse-grained density of states extracted from the exact Green’s function with the quasiclassical trajectory resolved DOS.

5. DOS: QUASICLASSICAL VS. EXACT

In the most simple case where the order parameter is the same in the left and right layers, the both theories reproduce the BCS density of states for any transparency of the interface (as a consequence of the Anderson theorem). Nontrivial comparison requires an inhomogeneous order parameter.

First, we analyze a generic “sample”, parameters of which are in no special relation to each other. In Fig. 7, the energy of the bound states of the exact theory are superimposed on the quasiclassical DOS.

One sees that indeed the periodic motion of the levels occurs in the allowed bands predicted by the quasiclassics. From Fig. 8, which shows the
DOS as a function of energy, one may conclude that the quasiclassical theory gives correct energy dependence, excepting perhaps some very fine details.

In Fig. 7, the angular resolved density of states calculated using both exact (dashed line) and quasiclassical (full line) methods. The parameters of the double layer are \( \Delta^{(r)} = -2\Delta^{(l)}, a^{(l)} = v_F/\Delta^{(l)}, a^{(r)} = 3v_F/\Delta^{(l)}, T = 0.9, \Theta = \pi/4 \).

In Fig. 8, we show the DOS for a specially selected “sample” for which non-classical effects are expected to be most pronounced. The sample is left-right symmetric except that \( \Delta^{(l)} = -\Delta^{(r)} \). Because of the symmetry, the contribution of the loop in Fig. 2(c) survives the coarse-grained angular averaging. Besides, the knot scattering matrix \( S \) of the “sample” is intentionally chosen as “\( \sqrt{NOT} \)”, i.e.

\[
S = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}, \quad S^2 = i \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},
\]

(51)

In this case due to the quantum interference of reflected and transmitted, the interface is fully transparent if the particle hits it twice (provided the sandwich is symmetric). The quasiclassical theory misses this phase sensitive effect since only the probabilities enter the theory.

As clearly seen from Fig. 8, the two approaches show distinct result for this “sample”. We attribute the disagreement to the loop contribution. This point of view is supported by Fig. 9 where DOS is shown for the sample...
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Fig. 8. The quasiclassical (full line) and exact (dashed line) angular resolved density of states for $\sqrt{NOT}$ case. The parameters of the double layer are $\Delta^{(r)} = -\Delta^{(l)}$, $a^{(t)} = 4v_F/\Delta^{(l)}$, $a^{(r)} = 4v_F/\Delta^{(l)}$, $T = 2/3$, $\Theta = \pi/4$.

differing from the previous one only in a slight violation of the left-right symmetry. For this sample, the disagreement is much less pronounced. This can be understood since in an asymmetric sample, the simple loop contribution averages to zero.

6. CONCLUSIONS

The main goal of the study has been to check the validity of the quasiclassical scheme suggested in Ref. 9 for the description of multiple reflections in layered superconducting systems. For this, we have compared the angular (trajectory) resolved density of states obtained from the full Gor’kov equation and the quasiclassical theory. From the comparison, we conclude that the approach based on the notion of quasiclassical tree-like trajectories is in qualitative agreement with the exact theory. Some quantitative disagreement which comes as no surprise, seems to be under control. The point here is that the assumption about the tree-like character of classical trajectories can be justified only for rough interfaces when the system becomes non-integrable, whatever small the disorder. However, the exact Green's function is calculated in the ideal geometry where the trajectories have loops (as in Fig. 1). We ascribe the disagreement to the loop contribution. Choosing the geometry, we able to control to some extent the loop
Fig. 9. The angular resolved density of states for “almost” $\sqrt{N\Omega T}$ case. The parameters of the double layer are $\Delta^{(r)} = -\Delta^{(l)}, a^{(l)} = 4v_F/\Delta^{(l)}, a^{(r)} = 4.1v_F/\Delta^{(l)}, T = 2/3, \Theta = \pi/4$. The full line corresponds to the quasiclassical theory, the dashed line to the exact calculation.

contribution. Indeed, the disagreement is most pronounced in the symmetric “sample” (see Fig. 8) where the contribution of the simplest loops shown in Fig. 1(b) survives coarse-grained averaging. A small asymmetry, which destroys their contribution, considerably reduces the disagreement (see Fig. 9). Note that loops always exist in the ideal specular geometry: even for an asymmetric sandwich, $a^{(l)} \neq a^{(r)}$, a loop is formed after every second collision with the interface. These higher order loops are not destroyed by either the angular averaging or the averaging with respect to the layer thickness as in Ref. 13 and 14. In our opinion, the difficulties with the quasiclassical theory reported in Ref. 13 and 14 originate in the contribution of the high order loops.

Finally, our conclusion about the validity of the quasiclassical theory is as follows. The theory is applicable for the description of a typical real sample where some roughness of the interfaces and surfaces is inevitably present. Since real typical samples are most probably non-integrable, the trajectories are tree-like, and the scheme suggested in Ref. 9 is valid. However, the scheme does not include certain physics which may be of importance in some situations where the sample is manufactured to enhance the role of interfering paths. Then, one should use the full version of the Gor’kov equations for the description of such a special system.
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