Mesoscopic Superconductivity: Quasiclassical Approach

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Abstract

This Thesis is concerned with the quasiclassical theory of mesoscopic superconductivity. The aim of the Thesis is to introduce the boundary conditions for a quasiclassical Green’s function on partially transparent interfaces in mesoscopic superconducting structures and to analyze the range of applicability of the quasiclassical theory. The linear boundary conditions for Andreev amplitudes, factoring the quasiclassical Green’s function, are presented. The quasiclassical theory on classical trajectories is reviewed and then generalized to include knots with paths intersections. The main focus of the Thesis is on the range of validity of the quasiclassical theory. This goal is achieved by comparison of quasiclassical and exact Green’s functions. The exact Gor’kov Greens function cannot be directly used for the comparison because of its strong microscopic variations on the length-scale of $\lambda_F$. It is the coarse-grain averaged exact Green’s function which is appropriate for the comparison. In most of the typical cases the calculations show very good agreement between both theories. Only for certain special situations, where the classical trajectory contains loops, one encounters discrepancies. The numerical and analytical analysis of the role of the loop-like structures and their influence on discrepancies between both exact and quasiclassical approaches is one of the main results of the Thesis. It is shown that the terms missing in the quasiclassical theory can be attributed to the loops formed by the interfering paths. In typical real samples any imperfection on the scale larger than the Fermi wavelength disconnects the loops and the path is transformed into the tree-like graph. It is concluded that the quasiclassical theory is
fully applicable in most of real mesoscopic samples. In the situations where the conventional quasiclassical theory is inapplicable due to contribution of the interfering path, one can use the modification of the quasiclassical technique suggested in the Thesis.

*Keywords:* mesoscopic superconductivity, quasiclassical theory, boundary conditions, multi-layer structures, Gor’kov equations, quasiclassical Green’s function, Green’s function on classical trajectories.
Publications

This Thesis is based on the papers:


Paper outside the subject of the Thesis:

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I. INTRODUCTION

Small conductors whose dimensions are intermediate between the microscopic and the macroscopic are called mesoscopic. They are much larger than microscopic objects like atoms, but not large enough to possess bulk properties. During the last few years, substantial experimental and theoretical activities have been devoted to the study of electronic transport in mesoscopic systems. These include semiconductor nanostructures, structures in two-dimensional electron gases, normal or superconducting tunnel junctions, and heterostructures (see [1–4] and the references therein). The coming together of the so far separate fields of mesoscopic physics and superconductivity has led to the discovery of many new phenomena which appear to be unique to mesoscopic structures.

Quasiclassical technique [5–7] has become a widely used tool in the description of superconductivity in mesoscopic systems, such as restricted structures with many interfaces[8–11]. On the theoretical side, studying an interface using the quasiclassical theory is problematic since the quasiclassical condition is violated by fast change of potentials on the atomic distances in the vicinity of the interface. Another difficulties arise when one attempts to describe the coherent reflection/transmission by many interfaces, for example in a multi-layer mesoscopic structures. Moreover some authors [12, 13] doubt the very applicability of the quasiclassical scheme in restricted geometries. They argue that the quasiclassical normalization is violated in double layer systems with partially transparent interface. It is the purpose of the Thesis to present a consistent quasiclassical approach to mesoscopic superconductivity and to analyze its range of applicability.

This Thesis serves as an introduction to the series of articles [14–16] dealing with the quasiclassical approach to mesoscopic superconductivity. Below we outline some concepts used in the Thesis.

A. Quasiclassical theory

The main subject of the Thesis is the quasiclassical theory of mesoscopic superconductivity. In Sec.II we review of the quasiclassical theory following the approach from Ref.[17]. The basic assumption of the
theory is that the the Fermi wavelength, $\lambda_F = 1/p_F$, is much smaller than any other length-scale of the problem. This means that the Fermi momentum $p_F$ is much larger than a typical interval of momenta of electrons $\delta p$ around the Fermi surface $\delta p \ll p_F$. The quasiclassical approximation corresponds to an expansion into the powers of $\delta p/p_F$. In the main approximation all the terms of order of $\delta p/p_F$ and higher are neglected.

There are several alternative approaches to the quasiclassical theory of superconductivity. In this Thesis we are concerned with the theory based on the notion of classical trajectory[17, 18]. The idea is that electrons in a superconductor move along the classical path with the Fermi velocity $v_F$. In this approximation, the quantum coherence exists only along the classical trajectories without any coupling between neighboring paths. The quantum broadening occurs only along the line. The Green’s function on trajectory is introduced and a set of equations governing the particle propagation along the classical path is derived in Sec.II. The equations are then solved for the case of homogeneous superconductor.

The next step in the scheme, also presented in Sec.II, is to include interfaces into the calculations. The reflection on an isolated interface mixes together semi-infinite pieces of classical trajectories allowing a particle to scatter to several different channels. Such a scattering can be fully described by a phenomenological scattering matrix. The boundary conditions for the quasiclassical equations at such interfaces are the main topic of Paper I.

Having in mind the comparison with the exact theory, the case of double layer sandwich with partially transparent interface is analyzed at the end of Sec.II.

B. Exact microscopical theories

The quasiclassical theory of mesoscopic superconductivity reviewed in Sec.II proposes a simple way of dealing with multiple interface geometries. However the applicability of the quasiclassical theory has been recently questioned [12, 13]. It has been reported that in certain restricted geometries the quasiclassical normalization condition is violated. In order to justify the quasiclassical theory one must analyze
the region of validity of the quasiclassical approach. Sec.III has the following program. First to review the exact techniques and then to use them to compare the results with the quasiclassical calculations.

In Sec.III we first focus to the Green’s function approach based on Gor’kov equation. The formulation of the Green’s function theory used in this Thesis is due to Gor’kov [19]. It is based on a single particle \(2 \times 2\) matrix Green’s function \(G(x, x')\) satisfying the Gor’kov equation
\[
(\varepsilon - \hat{H}) \hat{G} = 1 ,
\]
where \(\varepsilon\) is energy and \(\hat{H}\) the “Hamiltonian” described in details in Sec.III. As an illustration of the technique the case of infinite homogeneous superconductor is considered. The Gor’kov Green’s function is factored using certain amplitudes \(\phi\) and \(\phi^\dagger\) which are also discussed in Sec.III. As another example of the technique the Gor’kov Green’s function in a homogeneous slab is found. Finally the expression for the Green’s function in double-layer sandwich with partially transparent interface is derived.

The second part of Sec.III is devoted to Bogolubov - de Gennes equation, which is essentially generalization of the ordinary Hartree-Fock equations to include the effects of the superconducting pairing potential \(\Delta(r)\) as well as of ordinary potentials. If the Hamiltonian depends on the coordinate, such as through variations of \(\Delta(r)\), the plane wave momentum eigenfunctions used in the original BCS theory are no longer appropriate. They must be replaced by suitable position-dependent functions \(\psi(r) = \begin{pmatrix} u(r) \\ v(r) \end{pmatrix}\). Note that for \(\Delta = 0\) the Bogolubov - de Gennes equation decouples into two Schrödinger equations for the functions \(u\) and \(v\). \(u(r)\) and \(v(r)\) are the ordinary electron and hole eigenfunctions of the normal state with energies \(\pm \varepsilon\) relative to the Fermi energy.

Solutions to Bogolubov - de Gennes equation in the case of homogeneous superconductors are considered in Sec.III. They are plane waves propagating across the metal. In case of an interface the solutions must be matched on both sides of the interface. It turns out that it is more convenient to use a extended representation, the wave functions with 4-component structure. The boundary conditions on the interface take then particularly simple form and a general formula for transfer matrix across a structure with several interfaces can be derived.
C. Discrepancies between quasiclassical and exact theories

In Sec.IV we look into the problems of applicability of the quasiclassical theory in restricted geometries. The main source of the problems may be described as follows: The trajectory considered in the quasiclassical technique has only tree-like structure. The reason being that the Andreev decomposition of the rapidly oscillating and slowly varying part of the Gor'kov Green's function cannot be performed if the loop-like structure would be present. However in certain geometries the loops can in principle appear. The loop-like structure is the consequence of a symmetry of the problem. It is, however, argued that in any real system with certain roughness of the interfaces the loops disconnect and the quasiclassical approach is valid. The quasiclassical theory in the formulation from Paper I is based only on the tree-like trajectories. If one nevertheless does include the loops, then certain problems with normalization condition for the quasiclassical Green's function can be met. Papers II and III deal numerically and analytically with these problems.

In order to determine the region of validity of the quasiclassical theory of superconductivity, we (in Sec.IV) analyze the simple situation when the loop-like trajectories may appear - the case of double layer sandwich. We employ results from both exact as well as quasiclassical calculations already collected in Secs.II-III and find out what processes are responsible for the discrepancies between both approaches. It is shown that while both methods give the same results (after the coarse grain average of the exact calculations, Sec.IV) in typical cases, there exist certain special symmetrical situations where both theories do not agree. This happens when the loop-like structures, absent in the quasiclassical theory, have significant contribution to the result. This situations are discussed in Sec.IV. At the end of Sec.IV the numerical comparisons of a current across a multi-layer structures are carried out.

D. Outline

The main goal of the Thesis is to present the quasiclassical theory of mesoscopic superconductivity and to analyze its range of validity.
This is achieved by calculating several measurable quantities, like the current density or the density of states, using both exact and quasiclassical techniques. The results are then compared and analyzed. The Thesis is built in the following way.

Sec.II presents a review of the quasiclassical theory of superconductivity on classical trajectories. It introduces the quasiclassical 2-point Green’s function on a trajectory, 1-point quasiclassical Green’s function and its factorization into solutions of Andreev-like equation. The method is illustrated on the case of homogeneous superconductor. The boundary conditions on an transparent interface are put forward. The calculations of the quasiclassical Green’s function in a double-layered sandwich with transparent interface between the two metals are presented at the end of the Sec.II.

In the next Sec.III the exact microscopical theories are reviewed. We start with Gor’kov equation for exact Green’s function and show its solution for several simple cases: an infinite homogeneous superconductor and a finite homogeneous slab. Then the approach based on Bogolubov - de Gennes equation, and its variant based on generalized wave function, is presented. This approach is particularly convenient for analyzing the multiple-planar structures. The transfer matrix for multi-layer structures is derived.

In Sec.IV we directly compare the exact and quasiclassical theories. We numerically analyze the local density of states in double layer sandwich and the current density in multi-layer planar structures.

The last section Sec.V reviews the attached papers - the basis for the Thesis.
II. QUASICLASSICAL THEORY

The exact calculations based on Gor’kov equation give results with space dependence on the length-scale of Fermi wavelength $\lambda_F$. However in the most of the practical situations the external fields, the geometry of the sample and all the other relevant lengths change only on the length-scale much larger than $\lambda_F$. If one wants to compare the theoretical predictions with experiment, certain space averaging, which cancels the rapidly oscillating parts, has to be always performed. This procedure, first calculating the exact solutions and afterwards throwing all the atomic degrees of freedom away, makes the calculations lengthy and tedious. An alternative to this procedure is the quasiclassical theory [5–7] which is based on the idea to exclude the irrelevant length-scales from very beginning. The main object of the theory, the quasiclassical Green’s function, is found from the Gor’kov Green’s function by performing the integration over momentum. In this section we review the approach based on Ref.[17]. First we introduce the Green’s function on the classical trajectory and then the equations for them. For the stationary case the equations are solved using factorization of the Green’s functions. This method is well suited for formulation of the quasiclassical boundary conditions on partially transparent interfaces and walls, which are also discussed. Instead of formulating the boundary conditions for the quasiclassical Green’s function [23] we (following Ref.[14]) introduce the boundary conditions for the Andreev “wave” functions. At the end of this section the theory is applied and the calculation of the quasiclassical Green’s function in double layer sandwich is presented.

A. Quasiclassical Green’s Function

The quasiclassical theory of superconductivity is based on the assumption that the Fermi momentum $p_F$ is much larger than any other relevant momentum $p_F \gg \delta p$. In another words the theory is neglecting all the terms of the order $\delta p/p_F$. The central object of the quasiclassical theory of superconductivity is the two point Green’s function $g_{\epsilon}(x_1,x_2|\mathbf{n},\mathbf{R})$ defined on a classical trajectory $\mathbf{r}_{1,2} = \mathbf{R} + x_{1,2}\mathbf{n}$. $\mathbf{R}$ is an arbitrary point on the trajectory and $\mathbf{n}$ an unit vector specify-
ing the direction. The quasiclassical Greens function is found from Gor’kov Green’s function in the following way

\[ \hat{g}_\varepsilon^R(x_1, x_2|n, R) = \frac{i}{2\pi} \int_{-\infty}^{\infty} v_F d(p-p_F) \hat{G}_\varepsilon^R(np, R)e^{i(p-p_F)(x_1-x_2)}, \quad (2.1) \]

where \( G_\varepsilon^R(np, R) \) is retarded Gor’kov Green’s function (discussed in more details in Sec.III) in the Wigner representation

\[ \hat{G}_\varepsilon^R(p, r) = \int \hat{G}_\varepsilon^R(r + \rho/2, r - \rho/2)e^{-i\rho \cdot p} d\rho. \quad (2.2) \]

For definiteness we consider here only the retarded Green’s functions \( \hat{G}_\varepsilon^R \). In the spirit of the quasiclassical approximation the fast “quantum” oscillations on the scale of \( \lambda_F \) are integrated out in Eq.(2.1). The slowly varying two point quasiclassical Green’s function obeys the first order differential equations, with the derivative which couples only the points along the classical trajectory. As shown in Refs.[14, 17, 18] the equations for the quasiclassical Green’s functions read

\[ \left( iv \frac{\partial}{\partial x_1} + \hat{H}_R^R(x_1) \right) g^R(x_1, x_2) = iv\delta(x_1 - x_2), \quad (2.3) \]

\[ g^R(x_1, x_2) \left( -iv \frac{\partial}{\partial x_2} + \hat{H}_R^R(x_2) \right) = iv\delta(x_1 - x_2), \quad (2.4) \]

where the derivative in Eq.(2.4) operates backwards. We omit \( R, n \) and \( \varepsilon \) for brevity and use the notation \( g^R(x_1, x_2) \) in Eqs.(2.3-2.4). The 2 \( \times \) 2 matrix \( \hat{H}_R^R \) has the following form,

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

\[ \hat{h}_{\varepsilon,n}^R = \begin{pmatrix} \varepsilon - v \cdot p_s & -\Delta_n \\ \Delta_n & -\varepsilon + v \cdot p_s \end{pmatrix}, \quad v = vn, \quad (2.5) \]

where \( \Delta_n \) is the order parameter (which may generally dependent on the direction \( n \)), and \( p_s = -\varepsilon n \), \( A \) being the vector potential. \( \hat{\Sigma}^R \) is built of the impurity self-energy and the part of the electron-phonon self-energy not included to the self-consistent field \( \Delta \).
The observable quantities are calculated from the limit of \( g^R(x_1, x_2) \) at the coinciding arguments. For example the local density of states at point \( R \) reads

\[
\nu_\varepsilon(R) = \frac{1}{2} \nu_0 \int \frac{d\Omega_n}{4\pi} \mathrm{Tr} \left( \tau_z \Re g^R(n, R) \right),
\]

where \( \nu_0 \) is the normal metal density of states and the integration is performed over all possible directions \( n \). The current density in the equilibrium is found from the following expression

\[
j(R) = \frac{m p_F}{4\pi} \mathrm{Tr} \int \frac{d\Omega_n}{4\pi} v_F n \tau_z \left( g^R(R) - g^A(R) \right) \tanh \frac{\varepsilon}{2T},
\]

where \( T \) is the temperature, \( \varepsilon \) is energy and \( \tau_z \) is Pauli matrix.

**B. Factorization of the Quasiclassical Green’s Function**

In this section we are going to build the Green’s function on the classical trajectory, satisfying Eqs.(2.3-2.4). We, following Refs.[14, 17], introduce “wave” functions \( \phi \), solutions to Andreev equation, which are then used to factor the quasiclassical Green’s function \( \hat{g}(x_1, x_2) \). This approach turns out to be very convenient for the derivation of the boundary conditions on partially transparent interfaces. Instead of writing the boundary conditions directly for the quasiclassical Green’s function one writes equivalent conditions for the “wave” functions \( \phi \). Such conditions are linear and have simpler physical interpretation then the cubic boundary conditions for \( \hat{g}(x_1, x_2) \) [23].

The quasiclassical Green’s function on the trajectory \((n, R)\) can be build from the solutions \( \phi \) to the Andreev equation [20, 21]

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

where \( \hat{H}^R(x) \) stands for \( \hat{H}_{n}^R(r) \) at the point \( r = x_n + R \). We also introduce “conjugated” functions \( \bar{\phi} \) which are solutions to equation

\[
\bar{\phi}(x) \left( -i v_F \frac{\partial}{\partial x} + \hat{H}^R(x) \right) = 0.
\]
It follows from the identity \( \left( \hat{H}^R \right)^T = -\tau_y \hat{H}^R \tau_y \) that the conjugated wave functions \( \overline{\phi} \) are directly related to \( \phi \)

\[
\overline{\phi} = \phi^T \frac{1}{i\tau_y} \, ,
\]  

(2.10)

where \( \tau_y \) is Pauli matrix and \((\cdot)^T\) denotes the transpose operation.

Eq.(2.8) is the first order differential equation for two component function \( \phi \). It has thus two linearly independent solutions. Denote \( \phi_{\pm} \) the solutions regular (going to zero) at \( x \to \pm \infty \). Using Eqs.(2.8-2.9) the following continuity equation can be derived

\[
\frac{d}{dx}(\overline{\phi}_{\nu} \phi_{\nu'}) = 0 \, .
\]

(2.11)

Since the derivative of the product \( \overline{\phi}_- \phi_+ \) is zero, the product itself is a constant independent on the coordinate \( x \). One can fix the normalization of the “wave” functions \( \phi(x) \) in the following way

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

(2.12)

Using the “wave” functions \( \phi(x) \) and \( \overline{\phi}(x) \) normalized according to Eq.(2.12) the quasiclassical Green’s function, solution to Eqs.(2.3-2.4) reads

\[
\hat{g}^R(x_1, x_2) = \begin{cases} 
\phi_+(x_1) \overline{\phi}_-(x_2) & x_1 > x_2 \\
\phi_-(x_1) \overline{\phi}_+(x_2) & x_1 < x_2
\end{cases} \, .
\]

(2.13)

The Green’s function in Eq.(2.13) satisfies Eqs.(2.3-2.4), is regular at \( |x_1 - x_2| \to \infty \) and has finite discontinuity at \( x_1 = x_2 \)

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

(2.14)

as required by the r.h.s. of Eqs.(2.3-2.4).

C. One-point Green’s Function

In this section we establish the relation between the two-point quasiclassical Green’s function on a classical trajectory and the one-point
Green’s function. The observable quantities like the current density, charge density or the local density of states, depend only on the Green’s function with coinciding spatial arguments.

As it is showed in Ref. [17] the one-point quasiclassical Green’s function can be expressed via \( \hat{g}^R(x_1, x_2) \)

\[
\hat{g}^R(x) = \hat{g}^R(x^+, x^-) + \hat{g}^R(x^-, x^+) .
\tag{2.15}
\]

The analysis of the equation for \( \hat{g}^R(x) \) shows that the equation does not determine \( \hat{g}^R(x) \) uniquely (see [17, 22] and references therein). It must be supplemented by the normalization condition \( \left( \hat{g}^R \right)^2 = 1 \).

The quasiclassical Green’s function \( \hat{g}^R(x) \) can be written using the solutions to Andreev equation (2.8)

\[
\hat{g}^R = \phi_+ \bar{\phi}_- + \phi_- \bar{\phi}_+ .
\tag{2.16}
\]

For numerical studies it is often convenient to introduce so called Andreev amplitudes \( a \) and \( b \). They are defined in the following way

\[
\phi_\pm = \left( \begin{array}{c} u_\pm \\ v_\pm \end{array} \right) ; \quad a = \frac{u_-}{v_-} ; \quad b = \frac{v_+}{u_+} .
\tag{2.17}
\]

The equation for \( a \) and \( b \) is of Riccati type. The one point quasiclassical Green’s function can be rewritten using the Andreev amplitudes \( a \) and \( b \)

\[
\hat{g}^R = \frac{1}{1 - ab} \begin{pmatrix} 1 + ab & -2a \\ 2b & -(1 + ab) \end{pmatrix} .
\tag{2.18}
\]

This parameterization has been recently suggested by Schopohl and Maki [29, 30]. The Riccati equation for the ratio \( u/v \) has been derived by Nagato et al [13].

**D. Homogeneous Superconductor**

As an illustration of the quasiclassical approach we calculate the quasiclassical Green’s function and a propagator in the case of clean homogeneous superconductor subject to no external fields.
The normalized solutions to Eq.(2.8) \( \phi_\pm \) and its conjugated counterparts \( \overline{\phi}_\pm \) in the case of clean homogeneous superconductor with the order parameter \( \Delta \) can be written in the following way

\[
\phi_\pm(x) = \psi_\pm e^{\pm \xi_R^R x},
\]

\[
\psi_+ = N \left( \frac{1}{\alpha} \right); \quad \psi_- = N \left( \frac{\alpha'}{1} \right)
\]

\[
\overline{\psi}_+ = N \left( \alpha, -1 \right); \quad \overline{\psi}_- = N \left( 1, -\alpha' \right),
\]

\[
\alpha = \frac{\Delta^*}{\varepsilon + \xi_R^R}; \quad \alpha' = \frac{\Delta}{\varepsilon + \xi_R^R}
\]

\[
N = (1 - \alpha \alpha')^{-1/2},
\]

where \( \xi_R^R = \sqrt{\varepsilon^2 - |\Delta|^2} \) and the branch of the square root is chosen so that \( \Im \xi_R^R > 0 \). Substituting the “wave” functions from Eq.(2.19) into the expression for the quasiclassical Green’s function Eq.(2.16) one gets

\[
g^R = \frac{1}{\xi_R^R} \left( \frac{\varepsilon}{\Delta^*} - \frac{-\Delta}{-\varepsilon} \right).
\]

The density of states of homogeneous superconductor is calculated from Eq.(2.6) and gives \( \nu(\varepsilon) = \nu_0 R \left( \varepsilon/\xi_R^R \right) \), where \( \nu_0 \) is the normal metal density of states.

It is often convenient to introduce a propagator along a path. It connects the solutions of Eq.(2.8) at points \( x \) and \( x + y \): \( \phi(x + y) = \hat{U}(y)\phi(x) \). In the homogeneous case the solutions to Eq.(2.8) are known and the propagator can be calculated

\[
\hat{U} = \hat{1} \cos \frac{\xi_R^R y}{v_F} + \frac{i}{\xi_R^R} \hat{H}^R \sin \frac{\xi_R^R y}{v_F}.
\]

Particularly for normal metal \( \Delta = 0 \) and the propagator is a diagonal matrix multiplying the electron part by \( e^{i \xi_R^R y/v_F} \) and the hole part by \( e^{-i \xi_R^R y/v_F} \).

E. Boundary Conditions

In the quasiclassical picture the quasiparticles move along classical trajectories characterized by the direction \( n \) (and the initial position
Since only the coordinates on the specified trajectory enter equation for quasiclassical Green’s function the trajectories are not mixed and the propagation of quasiparticles along different trajectories are completely independent. A presence of an interface, cutting the trajectory, completely changes this picture. First of all the basic assumption of the quasiclassical theory that the external fields change slowly on the length-scale of Fermi wavelength is not satisfied. Moreover on the interface the quasiparticle can change its direction and continue along different path, so several different trajectories are mixed.

It has been shown by Zaitsev [23] that the presence of an interface can be incorporated in the quasiclassical theory by boundary conditions for quasiclassical Green’s function (see also [24–26] and references therein). Zaitsev’s boundary conditions, being cubic equations for matrix Green’s function, are far too difficult to be used for more complicated geometries than just one interface. The alternative to Zaitsev’s boundary condition has been recently suggested [14]. The idea is to write the conditions not directly for quasiclassical Green’s function but rather for the “wave” functions $\phi(x)$ which factor the Green’s function on trajectories. The trajectories are mixed using normal state scattering matrix, which enters the theory as a phenomenological parameter. The scattering matrix can be in principle found out from a microscopic theory.

Consider an interface which couples $N$ incoming and $N$ outgoing trajectories. The in- and out- trajectories are numbered $l = 1, \cdots, N$; we mark the outgoing trajectories with prime thus $k'$ stands for the $k$-th outgoing channel. Denote $\psi_i$ the 2-component wave function on $i$-th in-coming trajectory and $\psi_{k'}$ the value of the wave function on the $k$-th outgoing trajectory. The boundary conditions suggested in [14] (see also [27, 28]) read

$$\psi_{k'} = \sum_{i=1}^{N} S_{k' i} \psi_i ,$$

(2.26)

where $S_{k' i}$ are the elements of the scattering matrix found in the normal metal case.

Eq.(2.8) together with the boundary conditions (2.26) allows one to find the 2-component amplitudes $\phi(x)$ along the trajectories including
FIG. 1: Specular scattering on a single partially transparent interface. The transfer matrix $M_{1' \leftarrow 1}$, which depends only on the amplitudes $\phi_{2,2'}$ on the right side of the interface and the scattering matrix $S_{ij}$, couples the amplitudes $\phi_1$ and $\phi_{1'}$ in the left superconductor: $\phi_{1'} = M_{1' \leftarrow 1} \phi_1$.

the scattering events on interfaces. Then the quasiclassical Green’s function can be also found.

The simplest situation is the specular reflection, depicted on Fig. 1, where one connects only two incoming and two outgoing channels. In this case the transfer matrix which connects the effective wave function $\psi_1$ in the incoming channel 1 with wave function $\psi_{1'}$ is found and expressed only using $\psi_2$ and $\psi_{2'}$. As derived in Ref. [14] the transfer matrix reads

$$M_{1' \leftarrow 1} = \frac{(1 + R)}{2r^*} \left( 1 - \frac{T}{1 + R} \hat{g}_{2'2} \right),$$

(2.27)

where $R$ and $T$ are the reflection and transmission probabilities. $\hat{g}_{2'2}$ is the Green’s function build from Andreev amplitudes $b_{2'}$ and $a_2$ using expression (2.18).

The typical calculation procedure reads: 1. integrate $\phi_{\pm}(x)$ from $\pm \infty$. 2. transfer across the interface using Eq. (2.27) till the point of interest. 3. evaluate the Andreev amplitudes and the Green’s function.
FIG. 2: A double layer sandwich with a partially transparent interface. It consists of two homogeneous superconductors with the order parameters $\Delta^{(l)}$ and $\Delta^{(r)}$. The thicknesses of the layers are $a^{(l)}$ and $a^{(r)}$. Because of the symmetry of the problem the amplitudes in corresponding legs, e.g. 2 and 4, are proportional, $\phi_2 \propto \phi_4$.

F. Green’s Function in a Sandwich

In this section we present the calculation of the quasiclassical Green’s function in a double layer sandwich depicted on Fig.2. Each (left / right) layer is described by the thickness $a^{(l)}/a^{(r)}$ and the constant order parameter $\Delta^{(l)}/\Delta^{(r)}$. As it is derived in [14] the quasiclassical Green’s function in each of the legs at the scattering center can be expressed using the Andreev amplitudes $a_{1,2}$ in the incoming channels and $b_{1',2'}$ in the outgoing channels. The knot values of the Green’s function on $k$-th in- or $k'$-th out-channel ($k = 1, 2$) read

$$\hat{g}^{(k)} = \frac{1}{D} \begin{pmatrix} 2D_0^{(k)} - D & -2a_kD_0^{(k)} \\ -2D_1^{(k)} & -2D_0^{(k)} + D \end{pmatrix} \quad (2.28)$$

$$\hat{g}^{(k')} = \frac{1}{D} \begin{pmatrix} 2D_0^{(k')} - D & 2D_1^{(k')} \\ -2D_0^{(k')}b_{k'} & -2D_0^{(k')} + D \end{pmatrix} \quad (2.29)$$

$$D = R(1 - a_1b_{1'})(1 - a_2b_{2'}) + T(1 - a_1b_{2'})(1 - a_2b_{1'}) \quad (2.30)$$

Here $D_0^{(k)} = D(a_k = 0)$, and $D_1^{(k)} = \frac{\partial}{\partial a_k} D$. $T$ and $R$ are transmission...
and reflection probabilities on the interface between the superconductors. The problem under consideration is to find Andreev amplitudes $a_{1,2}$ and $b_{1',2'}$.

Because of the translational symmetry of the problem the Andreev amplitudes $a_{1,2} = a_{3,4}$ and $b_{1',2'} = b_{3',4'}$. The problem now reads: How to calculate the amplitudes $a_{1,2}$ and $b_{1',2'}$ if none of the trajectories directly lead to infinity? The solution is to use an iterative procedure. One starts with the bulk values of the amplitudes $a_0 = \Delta / (\varepsilon + \xi)$ and $b_0 = \Delta^*/(\varepsilon + \xi)$. The evolution operators $M_{4-2}$ and $M_{4'-2'}$ are constructed and solving the eigenvalue equation Andreev amplitudes $a_2$ and $b_2$ in the first approximation are found. These values are then used to construct the evolution operators $M_{3-1}$ and $M_{3'-1'}$. So one finds also the first order values for $a_1$ and $b_{1'}$. The procedure continues until the self-consistency is reached.
III. EXACT THEORY

In the previous section the quasiclassical theory of superconductivity has been reviewed. In order to check the applicability of the quasiclassical technique we present the exact treatment in formulation convenient for further comparison between both exact and quasiclassical results. The exact microscopical theories of superconductivity appeared in 50’s starting with the BCS [31] paper. In this section we review two different techniques. First we present the Gor’kov Green’s function approach [19, 32–34] and show the solutions to Gor’kov equations in certain special cases. The next part of this section is devoted to Bogolubov - de Gennes (BdG) equation [35–37]. An extended version of BdG theory, suitable for description of planar multi-layer structures, is then presented. The comparison between both exact and quasiclassical techniques is left for Sec.IV.

A. Gor’kov Equation

The Green’s function technique is a widely used tool in the theory of superconductivity [19, 32–34]. In this section we write down the Gor’kov equation for the Green’s function $G^R$ and rewrite it to the form convenient for the calculation in planar multi-layer structures.

The two-point Gor’kov Greens function $G^R_{\epsilon}(\mathbf{r}_1, \mathbf{r}_2)$ satisfies the Gor’kov equation

$$
(\varepsilon - \mathbb{H}) G^R(\mathbf{r}_1, \mathbf{r}_2) = \mathbb{I} \delta(\mathbf{r}_1 - \mathbf{r}_2),
$$

$$
\mathbb{H} = \begin{pmatrix}
\xi(\hat{p}) & \Delta(\mathbf{r}) \\
\Delta^*(\mathbf{r}) & -\xi(\hat{p})
\end{pmatrix},
$$

where in the case of parabolic spectrum $\xi(\hat{p}) = \frac{\hat{p}^2}{2m} - \frac{p_F^2}{2m}$ and $\Delta(\mathbf{r})$ is the order parameter generally dependent on the coordinate $\mathbf{r}$. $p_F$ is the Fermi momentum.

One often deals with systems which are translational invariant along a plane. Typical example being multilayer structure. In this case it is convenient to choose the $x$ axis perpendicular to the interfaces. Due to the translational invariance in the direction parallel to
the layers the problem is effectively one-dimensional.

$$G(r_1, r_2) = \sum_{p|p} G_{p|}(x_1, x_2) e^{i p|p(r_1-r_2)|}$$ (3.3)

For a given value of the parallel momentum $p|p$, the Green’s function $G_{p|p}(x_1, x_2)$ depends on the two coordinates, energy $\varepsilon$ and momentum $p|p$. The Gor’kov equation for $G_{p|p}(x_1, x_2)$ then reads

$$(\varepsilon - \mathbb{H}) G^{R}(x_1, x_2) = \mathbb{1} \delta(x_1, x_2) ,$$ (3.4)

where $\varepsilon$ is the energy, which is a quantum number in the equilibrium case. The “Hamiltonian” $\mathbb{H}$ is a $2 \times 2$ matrix with the following structure

$$\mathbb{H} = \begin{pmatrix} \xi(\hat{p}) & \Delta \\ \Delta^* & -\xi(\hat{p}) \end{pmatrix} .$$ (3.5)

Here $\Delta$ is the order parameter and $\xi = p^2/2m - p^2_{F_x}/2m$, and $p_{F_x}$ is $x$-projection of the Fermi momentum $p^2_{F_x} = p^2_F - p^2|p|$. In the next section we show how to solve the Gor’kov equation in the simplest possible case: homogeneous superconductor.

**B. Homogeneous Superconductor**

We consider the case of one dimensional homogeneous superconductors in the absence of external fields. The order parameter does not depend on the space coordinate $\Delta(r) = \Delta$.

In the homogeneous case the Green’s function can be expanded into products of $\psi_\nu$ and $\psi^\dagger_\nu'$ which are solutions to the following equations:

$$(\varepsilon - \mathbb{H}) \psi_\nu e^{i \sigma p_\nu x} = 0 ; \quad e^{i \sigma p_\nu' x'} \psi^\dagger_\nu', (\varepsilon - \mathbb{H}) = 0 .$$ (3.6)

In homogeneous superconductor there are two propagating solutions with corresponding momenta $p^2_\pm = p^2_F \pm 2m\xi$. Here $p_F$ is the Fermi momentum, $m$ is mass and $\xi^2 = \varepsilon^2 - |\Delta|^2$, where $3\xi > 0$. By definition the real part of the momenta $p_\pm$ is positive, $\Re p_\pm > 0$. The solutions to Eq.(3.6), amplitudes $\psi$ and $\psi^\dagger$, can be conveniently presented in
the following form

$$\psi_+ = \left(\begin{array}{c} 1 \\ \alpha \end{array}\right); \quad \psi_- = \left(\begin{array}{c} \alpha' \\ 1 \end{array}\right)$$

(3.7)

$$\psi_+^\dagger = \left(\begin{array}{c} 1, -\alpha' \\ 1 - \alpha \alpha' \end{array}\right); \quad \psi_-^\dagger = \left(\begin{array}{c} -\alpha, 1 \\ 1 - \alpha \alpha' \end{array}\right)$$

(3.8)

$$\alpha = \frac{\Delta^*}{\varepsilon + \xi}; \quad \alpha' = \frac{\Delta}{\varepsilon + \xi}$$

(3.9)

The amplitudes $\psi$ and their “conjugated” counterparts $\psi^\dagger$ are directly related

$$\psi_+^\dagger \nu = \nu \psi_{\nu^T}^\dagger; \quad \psi_-^\dagger \nu = \psi_{\nu^T}$$

where $\tau_y$ is Pauli matrix and $(\cdot)^T$ stands for the transposing operation. The product of $\psi$ and $\psi^\dagger$ satisfies a normalization condition:

$$\psi_\nu^\dagger \psi_\nu = \delta_{\nu\nu'}.$$  

(3.10)

Using the above results one can write down the Gor’kov Green’s function for homogeneous bulk superconductor. The boundary conditions implies that the Green’s function has to go to zero at $x, x' \to \pm \infty$:

$$\hat{G}(x, x')\sigma_z = \left\{ \begin{array}{ll}
\sum_{\nu\nu'} G_{\nu\nu'}^r \psi_\nu \psi_\nu^\dagger e^{i\nu p_x} e^{-i\nu' p_{x'}} & \text{for } x > x' \\
\sum_{\nu\nu'} G_{\nu\nu'}^\langle \psi_\nu \psi_\nu^\dagger e^{-i\nu p_x} e^{i\nu' p_{x'}} & \text{for } x < x'
\end{array} \right.$$  

(3.11)

The unknown coefficients $G_{\nu\nu'}^\langle$ are found from the continuity of Green’s function at $x = x'$ and from the jump of derivatives at the same point:

$$\left[ \hat{G}(x, x') \right]_{x=x'+0} = 0; \quad \left[ \hat{p} \hat{G}(x, x') \right]_{x=x'-0} = \frac{2m}{\hbar} \mathbb{1}. $$

(3.12)

What gives that $G_{\nu, \nu^T}^\langle = 0$ and $G_{\nu\nu'}^r = \nu \frac{m}{\hbar \Delta \hbar}$. The retarded Gor’kov Green’s function for homogeneous superconductor can then be written as

$$\hat{G}(x, x')\sigma_z = \frac{m}{\hbar} \times \left\{ \begin{array}{ll}
\frac{1}{p_+} e^{ip_+ (x-x')} \psi_+ \psi_+^\dagger - \frac{1}{p_-} e^{-ip_- (x-x')} \psi_- \psi_-^\dagger, & x > x' \\
\frac{1}{p_+} e^{-ip_+ (x-x')} \psi_+ \psi_+^\dagger - \frac{1}{p_-} e^{ip_- (x-x')} \psi_- \psi_-^\dagger, & x < x'
\end{array} \right.$$  

(3.13)
Using Eq. (3.13) and expressions for the amplitudes in Eqs. (3.7-3.9) one can calculate the density of states in homogeneous superconductors and gets as expected: \( \nu(\varepsilon) = \nu_0 \Re \left( \frac{\varepsilon}{\sqrt{\varepsilon^2 - |\Delta|^2}} \right) \), here \( \nu_0 \) is the normal metal density of states.

### C. Finite Slab

We consider a homogeneous slab of the width \( a_L + a_R \). We choose the coordinate system so that the \( x \) axis is perpendicular to the walls. Let the left wall be located at \( x = -a_L \) and the right wall at \( x = a_R \). The notation has been chosen so to conveniently extend the calculations to the case of double layer sandwich. Our goal is to find the Gor'kov Green’s function \( \hat{G}(x, x') \). In order to simplify the notation we use \( \hat{G}_{p||}(x, x') \) as a shorthand for \( \hat{G}_{p||}(x, x') \).

The boundary conditions in the slab require that the Green’s function vanishes on the walls. This constraint is satisfied by the following form:

\[
\hat{G}^R(x, x') = \begin{cases} 
\sum_{\nu \nu'} G_{\nu \nu'}^> \psi_\nu \psi_{\nu'}^+ \sin p_\nu (x - a_R) \sin p_{\nu'} (x' + a_L) , x > x' \\
\sum_{\nu \nu'} G_{\nu \nu'}^< \psi_\nu \psi_{\nu'}^+ \sin p_\nu (x + a_L) \sin p_{\nu'} (x' - a_R) , x < x' 
\end{cases}.
\]

(3.14)

Then we have to take into consideration the matching conditions at \( x = x' \) in Eq. (3.12). The continuity of Green’s function at point \( x = x' \) gives \( G_{\pm \mp}^< = 0 \) and \( G_{\pm \mp}^> = G_{\pm \mp}^< \). That is only the amplitudes with the same quasi-particle index \( \nu \) survive. The value of the amplitudes is found from the jump of derivatives at point \( x = x' \). The Green’s function in the finite homogeneous slab finally reads

\[
\hat{G}(x, x') = \begin{cases} 
\frac{2m}{\hbar} \sum_{\nu} \frac{\sin p_\nu (x - a_R) \sin p_{\nu} (x' + a_L)}{p_\nu \sin p_{\nu} (a_L + a_R)} \psi_\nu \psi_{\nu'}^+ , & \text{for } x > x' \\
\frac{2m}{\hbar} \sum_{\nu} \frac{\sin p_\nu (x + a_L) \sin p_{\nu} (x' - a_R)}{p_\nu \sin p_{\nu} (a_L + a_R)} \psi_\nu \psi_{\nu'}^+ , & \text{for } x < x' 
\end{cases}.
\]

(3.15)

In the limit \( L \rightarrow \infty \) one can show that Eq. (3.15) transforms to form of the Green’s function in homogeneous superconductor from
Eq. (3.13). The Green’s function in finite slab has poles at energies where \( \sin p \pm (a_L + a_R) = 0 \). This is no surprise since the problem of an infinite well is being considered.

### D. Double Layer Sandwich

Consider a sandwich formed by two homogeneous layers with thicknesses \( a_{L,R} \) and order parameters \( \Delta_{L,R} \); here and below, the subscript \( L \) and \( R \) label quantities which refer to the left and right layer, respectively.

The left (right) layer occupies the region \(-a_L < x < 0 \) \((0 < x < a_R)\). The interface is characterized by the scattering \( S \)-matrix,

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

with the transmission and reflection amplitudes \( t \) and \( r \). The outer walls are impenetrable. The goal is to find the exact Green’s function \( G(x, x') \) from the Gor’kov equation.

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. (3.4):

\[
\hat{p}_x \bigg|_{x = x' + 0}^{x = x' - 0} = 2m/\hbar.
\]

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

\[
\hat{P}^\sigma \hat{G}(0^+, x') = \sum_{\sigma' = \pm} M_{\sigma\sigma'} \hat{P}^{\sigma'} \hat{G}(0^-, x') \quad \sigma = \pm,
\]

where the projectors \( \hat{P}^\pm \),

\[
\hat{P}^\pm = \frac{1}{2} (1 \pm \hat{p}_x/p_F)_x,
\]

and the transfer matrix \( M \),

\[
M = \begin{pmatrix} 1/t^* & r/t \\ r^*/t^* & 1/t \end{pmatrix}.
\]
It is convenient to express the Green’s function in terms of two-component functions $\Phi_{\nu,\sigma}(x)$ and $\Phi_{\nu,\sigma}(x')$ defined as follows:

$$
\Phi_{\nu,\sigma}(x) = \psi_{\nu} e^{i\sigma p_{\nu} x}; \quad \Phi_{\nu,\sigma}^\dagger(x') = \psi_{\nu}^* e^{-i\sigma p_{\nu} x'}.
$$

(3.21)

Here $\sigma = \pm$, $p_{\nu} = p_{F_\nu} + \nu \xi/m$ is the electron ($\nu = +$) or hole ($\nu = -1$) momentum, and $\psi_{\nu}$ are defined in Eqs.(3.7-3.8).

The Green’s function can be then written as:

$$
i\hbar v_{F_\nu} \hat{G}(x, x')_{\sigma z} = \sum_{\nu,\nu',\sigma,\sigma'} \Phi_{\nu,\sigma}(x) \langle \nu, \sigma | Q^> | \nu' \sigma' \rangle \Phi_{\nu',\sigma'}^\dagger(x') , \quad x > x'$$

and

$$
i\hbar v_{F_\nu} \hat{G}(x, x')_{\sigma z} = \sum_{\nu,\nu',\sigma,\sigma'} \Phi_{\nu,\sigma}(x) \langle \nu, \sigma | Q^< | \nu' \sigma' \rangle \Phi_{\nu',\sigma'}(x') , \quad x < x'$$

(3.22)

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

Inserting the Green’s function into Eq.(3.4) and Eq.(3.17) and using the matching condition at the interface in Eq. (3.18) one gets $\langle \nu, \sigma | Q^<,> | \nu' \sigma' \rangle$. After straightforward but lengthy calculations, we have found the following rather simple result:

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

(3.23)

$$
D = 1 - A_- A_+ Tr(w_+ w_-).
$$

(3.24)

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

$$
W_\nu = \begin{pmatrix}
1 & (r^* + |r|^2 e^{2ip_{\nu}\zeta} a^{(l)}) \\
e^{2ip_{\nu}\zeta} a^{(r)} & (|r|^2 + r e^{2ip_{\nu}\zeta} a^{(l)})
\end{pmatrix},
$$

(3.25)

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

$$
A_\pm = \frac{\psi_{\pm}^{(r)} \psi_{\mp}^{(l)}}{\psi_{\mp}^{(r)} \psi_{\pm}^{(l)}},
$$

(3.26)

which have the physical meaning of the Andreev reflection amplitudes for a transparent interface. The Green’s function for a sandwich is known from the literature [12]. Eq.(3.23) agrees with the previous work, giving simple and concise form of the Green’s function.
E. Bogolubov - de Gennes Equation

A general inhomogeneous superconductor can be described using the quasiparticle language. The motion of quasiparticles - excitations in the superconductor is governed by the Bogolubov - de Gennes (BdG) equation. The equation was originally introduced by Bogolubov [35] in 1958. The technique was further analyzed by de Gennes in his book [36]. In this section we first write down BdG equation and then analyze its solution in the case of homogeneous superconductor subject to no external fields.

BdG equation is Schrödinger equation for inhomogeneous superconductor. In the course of the derivation one first writes down the BCS Hamiltonian and then diagonalizes it. One ends up with the following equation

$$(\xi(\hat{p}) \Delta \Delta^* - \xi(\hat{p})) \psi(r) = \varepsilon \psi(r) .$$

(3.27)

Here $\psi(r)$ is the two-component wave function, and $\varepsilon$ is the excitation energy. Solving Bogolubov - de Gennes equation means finding the eigen-energies $\varepsilon_n$ (spectrum) and the two-component eigen-vectors $\psi_n$.

All the observable quantities can be expressed using the solutions to BdG equation $\psi_n = \begin{pmatrix} u_n \\ v_n \end{pmatrix}$, the eigen-energies $\varepsilon_n$ and the distribution function $f_n$ which describes the quasi-particle occupation of $n$’th level. As an example consider the current density. It is found as a sum of contributions of currents corresponding to each level times the occupation number $f_n$

$$j(r) = \sum_n f_n \cdot \Re (u_n^* \hat{v} u_n - v_n^* \hat{v}^* v_n) ,$$

(3.28)

where $\hat{v} = \frac{1}{m} \hat{p}$ is the velocity operator and $(\cdot)^*$ stands for the complex conjugation.

In the following we analyze solutions to Bogolubov - de Gennes equation in the case of a homogeneous superconductor, where the order parameter $\Delta(r)$ does not depend on the coordinate. Later in the Thesis we will be interested in the multi-layer structures which are translational invariant along a plane. In such situation it is convenient
to separate variables. We choose the $x$ axis perpendicular to the interfaces. A general coordinate vector $r$ can be written as $r = (x, r_\parallel)$. Using the coordinates $(x, r_\parallel)$ any solution to BdG equation can be rewritten in the following form

$$\psi(r) = e^{ip_\parallel r_\parallel} \psi(x).$$  \hfill (3.29)

Plugging the form of the wave function from (3.29) to Eq.(3.27) and considering the above simplifications we get the following one-dimensional version of BdG equation

$$\left(\begin{array}{cc} \hat{\xi} & \Delta \\ \Delta^* & -\hat{\xi} \end{array} \right) \psi(x) = \varepsilon \psi(x).$$  \hfill (3.30)

Eq.(3.30) has generally 4 linearly independent solutions. Two of them correspond to the propagation of an electron-like excitations (to the left and right) and two of them to the hole-like excitations. The eigen functions are plane waves $\propto \exp[\pm ipx]$ with the momenta $p_\pm$

$$p^2_\pm = p^2_F - p^2_\parallel \pm 2m\xi,$$  \hfill (3.31)

where $\xi = \sqrt{\varepsilon^2 - |\Delta|^2}$, $\Im\xi > 0$. We define the momenta $p_\pm$ with positive real part $\Re p_\pm > 0$.

The four linearly independent solutions corresponding to the fixed quantum numbers $\varepsilon$ and $p_\parallel$ can be then written

$$\psi_{\nu,\sigma}(\varepsilon, p_\parallel; r) = e^{ip_\parallel r_\parallel} e^{i\sigma p_\nu x} \psi_\nu, \quad \nu = \pm, \quad \sigma = \pm,$$  \hfill (3.32)

where $\psi_\nu$ are defined in Eq.(3.7). The indices $\nu$ and $\sigma$ can be interpreted in the following way (see Fig.(3.32)). The electron-like excitations $\nu = +$ propagates to the right for $\sigma = +$ and to the left for $\sigma = -$. For the hole-like excitation $\sigma = +$ describes propagation to the left and vice versa.

F. Extended Wave Functions

So far we have described the propagation in a homogeneous layer. Now we consider an interface between two half infinite superconductors with constant order parameters $\Delta_L$ and $\Delta_R$. We model the interface by the $\delta$-potential with a strength $\lambda$: $V(x) = \frac{\lambda}{m} \delta(x)$. Since
FIG. 3: 4 linearly independent solutions to BdG equation. Index $\nu$ describes the type of the quasiparticle $\nu = +$ is the electron-like and $\nu = -$ the hole-like excitation. $\sigma$ identifies the direction of the propagation.

BdG equation is the second order differential equation the wave functions are continuous at the interface and the derivatives have the finite jump there, proportional to $\lambda$. We shall not however proceed in this direction but rather introduce a 4-component object consisting of the wave function and its derivative. Then we show how to match this 4-component wave functions on the interface.

The 4-component wave functions are built out of the solutions to BdG equation in the following way

$$\Psi = \begin{pmatrix} \hat{p}\psi \\ \hat{p}\psi \end{pmatrix},$$

where $\psi$ is a solution to BdG equation and $\hat{p}$ is the momentum operator. The interface matching boundary conditions between the wave function $\Psi_L$ on the left and $\Psi_R$ on the right now read

$$\Psi_L = \mathcal{D}\Psi_R; \quad \mathcal{D} = \mathbb{1} \otimes \begin{pmatrix} 1 & 0 \\ 2i\lambda & 1 \end{pmatrix}.$$

(3.34)
Here $D$ is $4 \times 4$ matrix. The product $\hat{A} \otimes \hat{B}$ means that each of the components of the matrix $\hat{B}$ is multiplied by the matrix $\hat{A}$. Other way around, matrix $\hat{A}$ acts on the two component wave function $\psi$ while matrix $\hat{B}$ operates in $(\psi \varphi)$ space.

Inside of a layer with a constant order parameter $\Delta = const$ the wave function can be written as a linear combination of propagating plane waves. The 4-component plane wave solutions read:

$$
\Psi_{\nu\sigma}(x) = e^{i\sigma p_{\nu} x} \psi_{\nu} \otimes \phi_{\sigma,p_{\nu}} \quad ; \quad \phi_{\sigma,p_{\nu}} = \frac{1}{\sqrt{2p_{\nu}}} \left( \begin{array}{c} 1 \\ \sigma p_{\nu} \end{array} \right). \quad (3.35)
$$

It is also convenient to define the “conjugated” amplitudes $\Psi^\dagger$

$$
\Psi_{\nu\sigma}^\dagger(x) = e^{-i\sigma p_{\nu} x} \psi_{\nu}^\dagger \otimes \phi_{\sigma,p_{\nu}}^\dagger \quad ; \quad \phi_{\sigma,p_{\nu}}^\dagger = \sqrt{\frac{p_{\nu}}{2}} \left( \begin{array}{c} 1 \\ \sigma \end{array} \right). \quad (3.36)
$$

The following orthogonality and completeness relations hold

$$
\Psi_{\nu'\sigma'}^\dagger \Psi_{\nu\sigma} = \delta_{\nu'\nu} \delta_{\sigma'\sigma} \quad ; \quad \sum_{\nu,\sigma} \Psi_{\nu\sigma} \Psi_{\nu,\sigma}^\dagger = \mathbf{1}. \quad (3.37)
$$

The orthogonality relations can be now used to construct an evolution operator inside of an homogeneous layer $\hat{U}_{x+a-x}$. This is an operator which relates the 4-component wave functions at the point $x$ and $x+a$ (inside a homogeneous layer):

$$
\hat{U}(a) = \sum_{\nu,\sigma} e^{i\sigma p_{\nu} a} \Psi_{\nu\sigma} \Psi_{\nu\sigma}^\dagger. \quad (3.38)
$$

Knowing the wave function at left layer interface the wave function on the right is $\Psi(x+a) = \hat{U}(a)\Psi(x)$, where $a$ is the width of the layer.

### G. Transfer Matrix

Generally any wave function in homogeneous superconductor can be expressed as a linear combination of $\Psi_{\nu\sigma}$ with $\nu = \pm$, $\sigma = \pm$. The expansion coefficients can be interpreted as the probability amplitudes
for the propagation of a quasiparticle in corresponding channel

$$\Psi(x) = \sum_{\nu,\sigma} C_{\nu\sigma} \Psi_{\nu\sigma}(x)$$  \hspace{1cm} (3.39)

$$\begin{pmatrix} C_{+\,+} \\ C_{-\,-} \\ C_{+\,-} \\ C_{-\,+} \end{pmatrix} \rightarrow \begin{pmatrix} C_{e\,\rightarrow} \\ C_{h\,\rightarrow} \\ C_{e\,\leftarrow} \\ C_{h\,\leftarrow} \end{pmatrix}.$$  \hspace{1cm} (3.40)

Here $C_{e\,\rightarrow}$ is the amplitude of propagation of an electron-like quasiparticle to the right, $C_{e\,\leftarrow}$ amplitude of propagation the electron-like quasiparticle to the left and so on. Generally a wave function can be in each layer fully described by the four amplitudes $C_{\nu\sigma}$. This feature can be used establish a transfer matrix technique, which propagates a solution to BdG equation across several interfaces.

The problem of a charge transport through a planar multi-layer structure has already received considerable attention [38, 39]. In the following we consider the propagation through a multi-layer planar structure using the technique based on the extended BdG wave functions. The set-up is depicted on Fig.4. It consists of $N$ parallel layers which are interconnected via insulating barriers modeled by $\delta$-function potentials. The thicknesses of the slabs are $a_1, \ldots, a_N$ and the order parameters $\Delta_1, \ldots, \Delta_N$. The structure is surrounded by two half infinite superconductors with order parameters $\Delta_0$ and $\Delta_{N+1}$.

Each interface is fully described by its transfer matrix $D$. The problem now is to find the across-interface transfer matrix, analogy of $D$, which relates the amplitudes $C_{\nu\sigma}$ on the left and right sides of the structure. Inserting the expansion in Eq.(3.39) into boundary condition (3.34) we get

$$C_{\nu L,\sigma L} = \sum_{\nu R,\sigma R} D_{\nu L,\sigma L}^{\nu R,\sigma R} C_{\nu R,\sigma R}$$  \hspace{1cm} (3.41)

$$D_{\nu L,\sigma L}^{\nu R,\sigma R} = \Psi_{\nu L,\sigma L}^{\dagger} D \Psi_{\nu R,\sigma R}$$  \hspace{1cm} (3.42)

$D_{\nu L,\sigma L}^{\nu R,\sigma R}$ is the transfer matrix across a single interface. Lets now write down the total transfer matrix across the whole multi-layer structure. Such a matrix is found as a successive product of the transfer matrices
FIG. 4: A planar, multi-layer structure consisting of $N$ superconducting slabs surrounded by two half-space metals. The order parameters are denoted by $\Delta_0, \cdots, \Delta_{N+1}$. Thicknesses of the layers are $a_1, \cdots, a_N$. The interfaces are modeled by $\delta$-function potentials with strengths $\lambda_0, \cdots, \lambda_N$.

across each interface and the propagator through the layer. Thus combining Eqs.(3.38) and (3.41) we get

$$M_{\nu R, \sigma R} = \sum_{\nu_1, \sigma_1, \nu_{N+1}, \sigma_{N+1}} D_{\nu_1, \sigma_1} D_{\nu_2, \sigma_2} \cdots D_{\nu_N, \sigma_N} e^{-i p_{\nu_1} a_1} e^{-i p_{\nu_2} a_2} \cdots e^{-i p_{\nu_N} a_N}$$

(3.43)

$$C_{\nu L, \sigma L} = \sum_{\nu R, \sigma R} M_{\nu R, \sigma R} C_{\nu R, \sigma R}$$

(3.44)

This is the final expression for the transfer matrix across the $N$-layer structure depicted on Fig.(4). Here $a_i$ is the width of $i$’th layer $p_{\nu_i}$ is the momentum for a quasiparticle in the $i$’th layer and $D_{\nu_i, \sigma_i}$ is the transfer matrix across $i$’th interface.
IV. COMPARISON

The quasiclassical theory is powerful and widely used tool in mesoscopic superconductivity. However its validity in certain cases has been recently questioned [12]. Namely, it has been reported that the quasiclassical normalization condition is not valid in double layer sandwich.

The main goal of this section is to compare the quasiclassical and exact theories in the geometries where the problems have been met, and to point out the reasons for discrepancies between both approaches. We first analyze the loop-like structures in the classical path which are responsible the discrepancies. Then we show numerical results. We compare the density of states in a bi-layer structures and the currents through certain multi-layer structures.

A. Classical trajectories

When discussing the quasiclassical theory one often uses the notion of classical trajectory. It is said that the quasiclassical trajectories are the tree-like structures and the loops are always excluded[14]. One might thus ask a natural questions “where are the trajectories in the exact approaches?” Take, for example, the plane wave solutions to BdG equation. Any state is fully described by the momentum and the position of the particle (and so the trajectory) is completely unknown. This does not seem to be in accordance with the quasiclassical theory where the particles move along well specified trajectories. It is the purpose of this subsection to show how the classical trajectories enter the exact theory.

In order to get localized wave packets one has to build a wave packet from plane waves with parallel momenta around a certain mean value $q_{||}$. For convenience we choose the Gaussian wave packet with a typical width $\Delta q$:

$$
\phi_{q_{||}} \propto \int dp_{||} e^{-\frac{1}{2} \frac{(p_{||}-q_{||})^2}{(\Delta q)^2}} \psi_{p_{||}}
$$

(4.1)

Since in homogeneous superconductor any wave function with fixed parallel momentum $p_{||}$ can be written as a linear combination of the
plane waves (see Eq.(3.39), we build the wave packet out of one such wave. In the general case we would have to consider sum of 4 such wave packets:

$$\psi_{p||} = e^{ip||y}e^{ip_x(p||)(x+X)}.$$ (4.2)

Here $p_x(p||) = \sqrt{p_F^2 - p_{||}^2} \pm 2m\xi$, $X$ stands for the additional phase dependent on $p_x$ which can enter the amplitude of the plane wave [43]. The corresponding wave packet is found by substituting the expression for $\psi_{p||}$ from Eq.(4.2) into Eq.(4.1):

$$\psi_{q||} \propto e^{iq||y}e^{ip_x(q||)(x+X)} \exp \left[ -\frac{1}{2}(\Delta q)^2 \left( y - \frac{q_{||}}{p_x(q||)}(x + X) \right)^2 \right].$$ (4.3)

The integral was evaluated under condition $(\Delta q)^2 \ll p_F^2 - q_{||}^2$, thus we excluded the incidence almost parallel to the interface. The particle follows trajectory $y(x) = \tan \theta \cdot x + y_0$, where the angle is found from $\tan \theta = q_{||}/p_x$ and $y_0 = X \tan \theta$. The parameter $X$ shifts the beam along the $y$ axis. This is the case when the beam is reflected inside of a multilayer structure and reenters the layer again.

1. Single interface

Consider, as an example, an electron incident from left to a single interface located at $x = 0$. In this case $X = 0$. Since $|p^e_x| > |p^h_x|$ the angle of the Andreev reflected hole will be larger then the one for incident electron. Thus generally the Andreev reflected hole will go along different trajectory, as is depicted on Fig.(5). However in the quasiclassical limit, where $|p^e| - |p^h| \ll p_F$ the trajectories for incoming electron and outgoing hole “almost” coincide.

One more remark about the single interface. In the quasiclassical theory one specifies the interface by the scattering matrix containing the amplitudes of normal reflection and transmission through the interface. Using expression Eq.(3.41) for the transfer matrix on a single interface, one can relate the reflection and transmission amplitudes to the strength of the $\delta$-potential $\lambda$:

$$r = \frac{p_L - p_R - 2i\lambda}{p_L + p_R + 2i\lambda}; \quad t = \frac{2\sqrt{p_Lp_R}}{p_L + p_R + 2i\lambda},$$ (4.4)
where $p_L$ and $p_R$ are the momenta in the left and right normal metal. The amplitudes were calculated for the NIN case.

2. Reflection on a finite layer

In order to illustrate the re-entrance of the beam at several different $y$’s we consider, as another example, an one-layer system. The system consists of two half infinite metals which are sandwiching a finite layer. For the sake of simplicity we consider just normal metals. The plane wave solutions to BdG equation describing an electron incident from the left reads:

$$\psi_{p_{||}}(x, y) \propto e^{i p_{\parallel} y} \left( e^{i p_x x} + r e^{-i p_x x} \right), \quad (4.5)$$

where $p_x = \sqrt{p_F^2 - p_{||}^2 + 2m\varepsilon}$. Using the expression for $M$ in Eq.(3.43) one gets the following formula for the reflection amplitude

$$r = r_0 + r_1 t_0^2 \sum_{n=1}^{\infty} (r_0 r_1)^n e^{-i 2nap_x} \quad (4.6)$$

Here $a$ is the width of the layer and $\lambda_{i}$ is the strength of the $\delta$-potential on $i$’th interface. The parameters $r_{i}$ and $t_{i}$ are the reflection and transmission amplitudes on $i$’th interface defined in Eq.(4.4). The total
reflection amplitude is the sum of amplitudes of all the possible reflection processes. First of all it is the simple reflection, then transmission through the first interface, reflection on the second and transmission through the first interface again and so on.

Substituting Eq.(4.6) into Eq.(4.3) with $X_n = n \cdot 2a$ one gets (see Fig.(6)) that the beam is reflected back to the left metal always at $y_n = n \cdot 2a_{yi}^{22}$. As is seen in Fig.(6) the particle follows the classical tree-like trajectory.

3. Double - layer system

In the previous examples we have encountered only the tree-like trajectories. At each interface the particle was scattered into one of several channels which did not interfere with any other part of the trajectory. This absence of loops is essential for the quasiclassical theory. Now we shall analyze the double layer system where the different branches of the trajectory can meet again. Consider the total normal reflection amplitude for an electron incident from the left to the structure consisting of two normal layers as depicted on Fig.(7). Using the same procedure as before, that is constructing the transfer matrix from Eq.(3.43) and then building the total scattering matrix, one finds the total reflection amplitude to be

$$r = r_0 + r_0^2 \cdot \frac{r_1 e^{-i2ap_x} + r_2(t_1^2 - r_1^2)e^{-i4ap_x}}{1 - [r_1(r_0 + r_2)e^{-i2ap_x} + r_0r_2(t_1^2 - r_1^2)e^{-i4ap_x}]}$$

(4.7)
where \( r_i \) and \( t_i \) are the reflection and transmission amplitudes for \( i \)'th interface, \( a \) is the width of each layer and \( p_x \) is the electron momentum in the \( x \) direction.

The total amplitude can be written as a sum of amplitudes \( r = r^{(0)} + r^{(1)} + r^{(2)} + \ldots \) for the reflection of a beam at positions \( y_0, y_1, y_2, \ldots \) and so on. The first two amplitudes \( r^{(0)} \) and \( r^{(1)} \) are the same as in the case of the one layer scattering. The first non-trivial result is for \( r^{(2)} \).

Expanding Eq.(4.7) in terms of \( e^{-i2ap_x} \) and collecting all the terms in front of \( e^{-i4ap_x} \) we get

\[
r^{(2)} = t_0^2 r_0 r_1^2 + t_1^2 r_2.
\]

(4.8)

Thus the amplitude \( r^{(2)} \) is sum of the amplitudes corresponding to the two different processes depicted on Fig.(8) The quasiparticle current in the beam (2) is proportional to \( |r^{(2)}|^2 \). However if the same quantity is calculated using the quasiclassical technique the sum of the probabilities for each of the contributing process enters. Clearly we account for a discrepancy between the exact and quasiclassical theories even in this simple example. The difference originates from the presence of the loop-like structure which is not included in quasiclassical approach.
A Classical trajectories

B. Numerical comparison: double layer

If the loop-like structures indeed contribute to the exact Green’s function then it is plausible to expect that also the measurable quantities are affected. In order to check the influence of the loops on measurables we compare the results from both quasiclassical and exact approaches on double-layer sandwich. The quantity of interest being the local density of states at the interface.

Note that the quasiclassical theory does not even attempt to give any good description on the truly microscopical level. Instead, it supplies the knowledge about coarse grain observable quantities. One should derive the coarse-grain Green’s function corresponding to the exact theory before comparing it with its quasiclassical counterpart.

First of all one has to spatially average the exact Green’s function. This is done by throwing the rapidly oscillating terms away. On the low spatial resolution, the Green’s function remains to be a fast function of the trajectory angle (the direction of momentum). Moreover for a given fixed $p_\parallel$ the density of states consists only of peaks located at the eigen-energies of the corresponding infinite well problem. Fig.9 shows the periodic motion of the energy levels as a function of the trajectory angle.

One sees on Fig.9 that the periodic motion of the energy levels occurs in the allowed bands predicted by the quasiclassical theory. After the integration in a small interval of angles the exact density of states transforms from a sequence of the $\delta$-function spikes into a smooth function of energy.

The comparison of the angular resolved density of states after the coarse grain averaging of the exact Green’s function is depicted on Fig.10. Both numerical results well agrees.

The good agreement from Fig.10 would suggest that the loop-like structures do not significantly influence the result. This is, however, not always the case. One can consider highly symmetric, specially chosen, samples, where the disagreement is remarkable. Such case is depicted on Fig.11. Although in the gap the bound local density of states have the same behaviour for both theories, above the gap one reports significant discrepancies. For certain energies the peaks in the exact density of states correspond to a dips for quasiclassical curve.
FIG. 9: The energies of the bound states as a function of the trajectory angle superimposed on the graph of the quasiclassical angular resolved density of states. The parameters of the double layer are $\Delta_R = -2\Delta_L, a_R = 3a_L = 3v_F/\Delta_L$. The transparency of the interface $T = 0.9$.

FIG. 10: The angular resolved density of states calculated using both exact (dotted line) and quasi-classical (full line) methods. The parameters of the double layer are $\Delta^{(r)} = -2\Delta^{(l)}, a^{(l)} = v_F/\Delta^{(l)}, a^{(r)} = 3v_F/\Delta^{(l)}, T = 0.9, \Theta = \pi/4$. 
FIG. 11: The quasi-classical (full line) and exact (dotted line) angular resolved density of states for the symmetric case $a(l) = a(r)$. The parameters of the double layer are $\Delta(r) = -\Delta(l), a(l) = 4v_F/\Delta(l), a(r) = 4v_F/\Delta(l), T = 2/3, \Theta = \pi/4$.

Does Fig.11 mean that quasiclassical theory is not at all applicable? The answer is no. The discrepancies seen from Fig.11 are due to the perfect symmetry of the system. Even the slight variation of the symmetry rapidly changes the exact result, while changing the quasiclassical curve only slightly. On Fig.12 the small change in the thickness of only one of the layer is presented. The agreement of the results immediately improves.

Thus we can conclude that while the exact calculations are very sensitive to geometrical resonances, the quasiclassical results are robust and more faithfully reproduce the real experimental conditions where no symmetries cannot be present due to e.g. roughness of the walls.

C. Numerical comparison: multi-layer

In this section we compare another measurable quantity - current through a multi-layer planar structure. We show how the symmetry of the setup and thus the loop-like structures in/excluded from the
FIG. 12: The angular resolved density of states for “almost” symmetric 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 quasi-classical theory, the dotted line to the exact calculation.

calculations affect the results.

We start with the current density through a one-layer structure. The current is driven across the layer by a finite phase difference of the order parameters in the left and right superconductors. The energy dependence of the angular integrated current, calculated using both techniques, is plotted in Fig.(13). The solid line depicts the quasiclassical result. The crosses corresponds to the exact solution to BdG equation. While calculating the current one first finds the angular resolved current and then integrates it over all the direction. The angular resolved current calculated using the exact theory is a rapidly oscillating function of the angle. This feature is shown on Fig.(13) using the error-bars. They are defined as

$$\langle (\Delta j)^2 \rangle = \int d\theta (j_{\text{BdG}} - j_{\text{QC}})^2.$$ (4.9)

One sees that despite the fast variation of the angular dependent current the total currents perfectly agrees.

In the one layer structure any trajectory of a particle is always tree-like structure, thus there are no loops. In order to see the influence
of the loops on the current we consider a two layer system SISISIS. The thicknesses of the layers are the same $a = v_F/|\Delta_0|$. The order parameters are $\Delta_0 = \Delta_1 = \Delta_2$, $\Delta_3 = e^{i\pi/2}\Delta_0$. The transparencies of the interfaces are $T_0 = 0.8$, $T_1 = 0.5$, $T_2 = 0.8$. Since the reflection probabilities of the outer interfaces are rather small $R_{0,2} = 0.2$ the amplitudes of higher order processes (multiple reflections in the layers) are rapidly decaying with the order of the process. Thus the simple loops have, in this case, much higher influence on the result then the 8-shaped loops. Inspecting the total current dependence on energy depicted on Fig.(14) one indeed sees large discrepancies between the currents calculated using different approaches. This should be no surprise since the quasiclassical technique does not include the loops which contribute to the overall current. However the system under consideration is too ideal since the thicknesses of both layer are exactly the same. On the next Fig.(15) we plot the dependence of the current on the energy for the case when the thicknesses are slightly different (changed by 1%). We encounter perfect agreement
FIG. 14: Current through SISIS structure. The order parameters are $\Delta_0 = \Delta_1 = \Delta_2, \Delta_3 = e^{i\pi/2}\Delta_0$. The thicknesses of the layers are the equal $a = v_F/|\Delta_0|$. The transparencies are $T_0 = 0.8, T_1 = 0.5, T_2 = 0.8$.

FIG. 15: Current through SISIS structure. The order parameters are $\Delta_0 = \Delta_1 = \Delta_2, \Delta_3 = e^{i\pi/2}\Delta_0$. The thicknesses of the layers are the different $a_1 = 0.99v_F/|\Delta_0|$, $a_2 = 1.01v_F/|\Delta_0|$. The transparencies are $T_0 = 0.8, T_1 = 0.5, T_2 = 0.8$. 
between both techniques. The loops are disconnected and the exact calculations perfectly match the quasiclassical results.

The final question is about the influence of the 8-shaped loops on the current. Consider now the previous setup but decrease the transparencies of the outer interfaces to $T_{0.2} = 0.5$. This will increase the amplitudes of the higher order processes and thus enhance the discrepancies between the two approaches due to additional resonances.

As is seen from Fig.(16) and Fig.(17) the difference between the currents survives even the change of the thicknesses of the two layers. No rigid variation of layer thicknesses can possibly eliminate the higher order loops. Nevertheless the quasi-classics indeed does give the correct physical result, since any system with even microscopical roughness of the interfaces posses only trajectories with the tree-like structure.
V. SUMMARY OF THE PAPERS

A. Paper I: Quasiclassical Theory of Superconductivity

In many cases of interest one deals with the situation where quasiparticles transverses many partially transparent interfaces without losing coherence. 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 not valid at interfaces. Nevertheless the interface can be included into the theory using a boundary conditions derived by Zaitsev [23]. They are cubic matrix relation. In case of many interfaces, one comes to a system of nonlinear matrix equations, solutions of which is far not simple, if at all possible. The purpose of the presented paper [14] is to suggest a new method which allows one to study systems with multiple partially transparent interfaces SIS’ or SIN in the framework of the quasiclassical theory of superconductivity.

The main idea is to write a boundary conditions for the scattering on an interface not directly for the quasiclassical Green’s function $\hat{g}^R$. 

FIG. 17: Current through SISIS structure. The order parameters are $\Delta_0 = \Delta_1 = \Delta_2, \Delta_3 = e^{i\pi/2}\Delta_0$. The transparencies are $T_0 = 0.5, T_1 = 0.5, T_2 = 0.5$. The asymmetrical case $a_1 \neq a_2$. 
but rather for the “wave” functions $\phi_{\pm}(x)$ which factor $\hat{g}^R$ (see Chapter II). A general interface is partially diffusive, mixing states within a continuum of momenta. As a model, one allows only mixing of a finite number of states, $N$ incoming and $N$ outgoing at a scattering point - knot. The knot value of the wave functions $\phi_i (\phi_{k'})$ in the incoming (outgoing) channels, $i, k' = 1, \ldots, N$ are related to each other by the unitary scattering matrix $\hat{S}$

$$\phi_{k'} = \sum_{i=1}^{N} \hat{S}_{k'i} \phi_i . \tag{5.1}$$

The energy independent scattering matrix $\hat{S}$ is the normal state property and is considered as a given phenomenological parameter. Eq.(5.1) is used as a boundary condition for Andreev equation governing $\phi(x)$ on classical trajectory. In this scheme, one finds the “wave” function $\phi$ by solving the Andreev equation Eq.(2.8) on the pieces of the trajectory between the knots and then uses Eq.(5.1) to connect the pieces. The scheme allows one to consider the usual and Andreev reflections on equal footing, simultaneously with scattering processes included via the self-energy $\Sigma^R$.

In order to illustrate the method, we calculate the density of states and the super-fluid density for 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 $0 < x < d_R$. The order parameter is $\Delta_L$ and $\Delta_R$.

Consider the periodic zig-zag trajectory in the right layer, formed by the reflections from the boundary at $z = d_R$ and at the interface $z = 0$. Knots are the points where the zig-zag touches the interface. Because of the periodicity, each of the regular solutions $\phi_{\pm}$ is proportional to one of the eigenvectors of the evolution matrix $\hat{U}_x$, defined as $\phi(x + a) = \hat{U}_x \phi(x)$. Here $a$ is the length of the trajectory between two corresponding points $a = d_R / \cos \theta$ and $\theta$ is the angle of the trajectory. As is shown in the article the quasiclassical Green’s function can be calculated as

$$\hat{g}^R(x) = \frac{\hat{U}_x'}{\sqrt{\left(\hat{U}_x\right)'}} , \tag{5.2}$$
FIG. 18: Angle resolved local density of states (DOS) at the interface in a sandwich $\Delta_L = -\Delta_R$, $d_L/\cos\theta = d_R/\cos\theta = v_F/\Delta$. The transparency of the interface $T = 0.90$. Inset: Transparency $T = 0.98$. Observe the finite value of DOS at energy $\varepsilon = 0$.

where $\hat{U}'$ stands for the traceless part of the evolution operator.

Given the interface values of the Green’s function in the left layer one can find the transfer matrix and the Green’s function in the right layer. Then one proceeds with the same calculations in the left layer. Numerical iterations are performed until the self-consistency is reached.

We consider the case when $\Delta_L = -\Delta_R$ (question of the self-consistency of the order parameter is left aside in this case). The angular resolved density of states (DOS) for almost transparent interface $T = 0.9$ is presented in Fig.18. Note the zero value of DOS at small energies.

DOS is extremely sensitive to reflections which leads to the splitting of the zero energy Andreev levels. Accordingly the super-fluid density is also sensitive to the reflection. As seen from Fig.19, the low temperature paramagnetic effect (i.e. $\rho_s < 0$) being strong for the ideal interface ($T = 1$), disappear when the transmission probability is around $T = 0.96$. These findings confirm the theoretical possibility of the paramagnetic effect, and at the same time indicate that the effect
B. Paper II: Superconductivity in Multiple Interface Geometry

In this article the applicability of the quasiclassical theory of superconductivity in restricted geometries is analyzed. The work was motivated by Ref.12, where the validity of quasiclassical theory has been questioned. Namely, the quasiclassical Green’s function has been constructed from the exact solutions to BdG equation in case of double layer sandwich. It turned out that the normalization condition, vital part of the quasiclassical theory, is violated in this case.

The quasiclassical theory of superconductivity, in the formulation from [17], is based on the idea of classical trajectories. In short the quasiparticles propagate along classical trajectories, the interfaces and surfaces are included as a scattering events and described by a scattering matrix. The important point is that the loop like structures are excluded from the scheme. In quasiclassical description the particle propagates only along tree-like trajectories. Even if the branches of the tree can coincide in the real-space, they cannot interfere with each other. The situation is different when the exact theory is consid-

FIG. 19: Space averaged super-fluid density vs. temperature for three different transmission probabilities $T = 1, 0.99, 0.96$. is very sensitive to the interface reflection inevitable in the experiment.
ered. In symmetric set-ups the loops can appear and do significantly contribute to the Green’s function. The analysis of the discrepancies between exact and quasiclassical theories is the main content of the Paper II.

The simplest system where the discrepancy between quasiclassical and exact approach has been reported is the double layer sandwich with a transparent interface sketched on Fig.2. The quasiclassical treatment has been presented in Sec.II.F. Although the set of non-linear equations for the Andreev amplitudes $a_{1,2}$ and $b_{1,2}'$ can be written, it is practically simpler to use an iteration procedure to find numerical values of $a$’s and $b$’s. The exact approach to the problem can be done by solving the Gor’kov equation as presented in Sec.III.D. The closed expression for the Gor’kov Green’s function has been derived earlier in the thesis and the final result is in Eq.(3.23).

Having the expressions for the exact and quasiclassical Green’s function we can compare both theories. For definiteness we consider the trajectory resolved density of states. It is clear from very beginning, that the agreement may be present only on a low resolution level. Strong microscopical variations of the exact density of states must be averaged out in a small region of the phase space. Even then the disagreement due to loops is expected.

First we present the numerical comparison of the density of state in a general case where there is no obvious symmetry, see Fig.10. In this case one encounters a perfect agreement between exact and quasiclassical techniques. The reason is that the loop-like structures are not typically significant.

The situation is quite different in the symmetric sandwich depicted on Fig.(11). Indeed the disagreement is obvious. For the energies above $\Delta$ the peaks in the exact LDOS correspond to the dips in the quasi-classical LDOS. The value of the transmission probability has been chosen so that the first order loops have the maximum possible amplitude.

If the explanation of the effect based on the loops is correct then the agreement should improve if the symmetry of the sandwich is lifted. This is indeed seen from Fig.(12), where the thicknesses of the layers have been altered a just a little ($\Delta a/a \approx 2\%$). One encounters tremendous improvement in the agreement between both quasi-classical and
exact LDOS, fully in accordance with the expectations. Note that while quasi-classical result changed only slightly the exact curve has been drastically affected by the removal of the symmetry. This follows from the fact that the symmetric system is artificial and should be discarded when calculating the measurable quantities, as it is done in quasi-classical theory [14].

In conclusion, the validity of the quasi-classical theory of superconductivity in multiple interface structures [14] has been examined. The Green’s function for the double layer sandwich with a partially transparent interface has been derived using both exact and quasi-classical approaches. Employing expansion of the Green’s function into trajectories the discrepancies has been pointed out. The influence of the loop-like trajectories on the observable - local density of state - has been numerically studied.

It has been shown that the difficulties with the quasi-classical theory originate from the contribution of the higher order loops. The quasi-classical theory of superconductivity is applicable for the description of a typical real sample where some roughness of the interfaces and surfaces is inevitably present. However for the exactly symmetric samples one should use the Gor’kov equations.

C. Paper III: Quasiclassical Theory of Superconductivity: Interfering Paths

In Paper II the difficulties of applicability of quasiclassical theory in certain restricted geometries has been numerically studied. The main point of this Paper III is to give the analytical analysis of the problem and to suggest a technique how to include the loops into the quasiclassical theory.

First a novel derivation of the quasiclassical Green’s function on classical trajectories is presented. We start from Gor’kov equation and split the $\delta$-function source on the r.h.s into two pieces. One which is responsible for a wave propagation to the right direction and the second to the opposite direction. The total Green’s function is then rewritten as a sum of two parts each of them corresponding to the
propagation in opposite direction

\[ iv_F G(x_1, x_2) = g^+(x_1, x_2)e^{ip_F(x_1-x_2)} + g^-(x_1, x_2)e^{-ip_F(x_1-x_2)} \]. \hspace{1cm} (5.3)

From \( g^\pm(x_1, x_2) \) the one-point quasiclassical Green’s function are built. As it has been discussed in the previous paper the quasiclassical theory is well established on tree-like trajectories. In order to pinpoint the difficulties a quasiclassical Green’s function on a single loops is considered. Starting from Gor’kov equation and using the boundary conditions connecting the point \( x \) and \( x + \mathcal{L} \), where \( \mathcal{L} \) is the length of the loop, the expression for the one point quasiclassical Green’s function has been derived

\[ \hat{g}(x) = \frac{1 + U_x}{1 - U_x}, \hspace{1cm} (5.4) \]

where \( U_x \) is a total quasiclassical propagator along the entire loop from the point \( x \) to \( x + \mathcal{L} \). The result has been then used to find the quasiclassical Green’s function on a loop in a homogeneous superconductor. It has been shown that the normalization condition is violated even in this simplest case. However after coarse-graining of the Green’s function, that is averaging with respect to the phase \( p_F \mathcal{L} \) the normalization condition has been restored. This conclusion is valid even in the case of an inhomogeneous superconductor.

The situation is more complicated in the case of double-loop trajectory. The particle not only interferes with itself after passing across the loop but also interacts with the second loop. The interaction is described by a scattering matrix which relates amplitudes in all 4 legs which cross together. The expression for the one point Green’s function at the points at the interface has been derived. Then the normalization condition has been checked. The result significantly differs from the case of a single loop. The normalization condition is violated not only before but also after the coarse-grain averaging. The processes responsible for the violation has been pointed out. The loops of \( \infty \)-like shape have had the main contribution.

The violation of the normalization condition in the case of double layer sandwich, where the \( \infty \)-like shape loops are always present has been already numerically studied in Paper II. The main contribution of this paper has been to analytically support the numerical arguments.
In conclusions, the quasiclassical theory of superconductivity developed in [14] can be used even in restricted geometries provided the set-up excludes the loop-like structures. In a special and highly symmetric cases the exact approach based on Gor’kov equation has to be used instead.

D. Paper IV: Quasiclassical versus Bogolubov - de Gennes Theory of Multi-Layer Systems

Paper IV is concerned with the charge transport in mesoscopic multi-layer systems built of superconductors, normal metals and insulators. The extended version of BdG equation is used in solving the scattering problem and finding the electric current in planar multi-layer structures.

The applicability of the quasiclassical theory in restricted geometries, namely the validity of the quasiclassical normalization condition has been doubted in Ref.12. The situation has been analyzed in Refs.15, 16. However all the effort has been focused only to the simplest possible structures, where the loop-like trajectories, which are the reason for the problems with quasiclassics, appear. Only single or double layer structures has been discussed in literature so far. It is clear that in multi-layer superconducting structures the effect has to be also present. The main goal of paper IV is to carry out the comparison between exact and quasiclassical theories in the case of multi-layer planar superconducting structures.

Consider a multi-layer system which consists of $N$ superconducting planar slabs surrounded by two half-infinite superconductors. The system is depicted on Fig.4. The interfaces can be modeled by the $\delta$ function potentials with the strength $\lambda$. The extended theory based on Bogolubov - de Gennes equation has been proposed. It is based on 4-component wave function which consists of two parts, the original BdG wave function and its derivative. The advantage of the approach being the simplicity in connecting the solutions to BdG equation on the interfaces. The boundary conditions and the general expression for the transfer matrix has been derived (see also Sec.III G). Using the extended BdG theory the expression for the current passing across a multi-layer structure has been presented.
The second part of the article deals with the comparison between the exact results and the quasiclassical theory. As it has been expected both theories give exactly the same result when examining a single layer structure, where no loop-like trajectories are present. But in the case of two or more layers the discrepancies between the electric current calculated using both techniques prevail even when the first order loops are discarded by changing the thicknesses of the layers. It is concluded that the higher order loops also contribute to the result. However, if one considered also symmetry disturbances due to roughness of the wall even the higher order loops would disconnect, leading to the tree-like graph of the trajectories, considered in quasiclassical technique.

It is concluded that the quasiclassical theory is applicable even in the multi-layer geometries if the loop-like graphs, due to symmetry of the system, do not significantly contribute. In the symmetric situations exact theory based on the extended BdG wave function can be used instead.

E. Paper V: Squeezed States of a Particle in Magnetic Field

The problem of a quantum charged particle in homogeneous magnetic field is almost as old as the quantum mechanics itself [40, 41]. The Hamiltonian reads

$$\hat{H} = \frac{1}{2m} \left( \hat{p} - \frac{e}{c} A \right)^2,$$

(5.5)

where $A$ is the vector potential. The Hamiltonian can be formally transformed into a form resembling the Hamiltonian of the linear harmonic oscillator. The oscillator has discrete energy levels and therefore also the charged particle in homogeneous magnetic field has discrete spectrum.

Since the homogeneous field is translation invariant, the generator of translations, generalized momentum $\hat{P}$, commutes with the Hamiltonian. That is why each of the energy level is multiply degenerate. It is not enough to describe a state by just the energy. However, each state can be uniquely identified by two quantum numbers - energy and the eigenvalue of $\hat{P}_i$. This has been done by Landau [40]. He used
one of the Cartesian coordinates of the center of the Larmor circle operator which is directly connected to the generalized momentum $\hat{P}$:

$$\hat{R} = \frac{c}{eB^2} \hat{P} \times \hat{B} \ .$$  \hspace{1cm} (5.6)

One cannot find the common eigenstates of both of the Cartesian coordinates because they do not commute with each other. The Landau states are infinitely extended “strips” with definite energy and one of the Cartesian component of the center of the Larmor circle.

The coherent states of a particle in magnetic field introduced by Malkin and Man’ko [42] are defined as the common eigenfunctions of $\hat{H}$ and $\hat{X} - i\hat{Y}$. These states are well localized and cylindrically symmetric.

The generalization of all the above states take a general linear combination of $\hat{X}$ and $\hat{Y}$. Such states, we call them squeezed states. We construct the stationary squeezed state, $|R, N\rangle$ as a simultaneous eigenfunction of the Hamiltonian and the operator $\hat{X}_\Phi$:

$$\hat{X}_\Phi = \hat{X} \cos \Phi + \hat{Y} \sin \Phi \ ,$$  \hspace{1cm} (5.7)

where $\Phi$ is a complex parameter. $\hat{X}$ and $\hat{Y}$ are the Cartesian coordinates of the operator of the center of Larmor circle $\hat{R}$. The state $|R, N\rangle$ is found from the following system of equations

$$\hat{H}|R, N\rangle = \hbar \omega_c (N + \frac{1}{2})|R, N\rangle \ ,$$  \hspace{1cm} (5.8)

$$\hat{X}_\Phi|R, N\rangle = (X \cos \Phi + Y \sin \Phi)|R, N\rangle \ .$$  \hspace{1cm} (5.9)

The quantum numbers of a state are the Landau level number $N$, and the expectation value of the guiding center position, $R(X, Y)$. $\omega_c = |eB|/mc$ is the cyclotron frequency.

The operators $\hat{X}$ and $\hat{Y}$ do not commute with each other. The Heisenberg uncertainty relation places a condition on the product of their variances $\Delta X \cdot \Delta Y \geq \hbar^2/2$. The actual value of the product depends on the state of the particle. E.g. for the coherent states $\Delta X = \Delta Y = l/\sqrt{2}$, so the Heisenberg relation holds with the equality sign. The squeezed states defined in the paper have one of the variances even smaller then the coherent states, still keeping the product $\Delta X \cdot \Delta Y$
minimum possible. That is why they are called squeezed, stressing that they can be obtained by “squeezing” the minimum uncertainty coherent states.

Solving the set of equations (5.8 - 5.9) in the symmetric gauge we get the following wave function

$$\Psi(r|N, R) = C_\Phi \frac{(ie^{-i\Phi})^N}{\sqrt{2^{N}N!}} \exp\left(\frac{ie}{2\hbar}B \cdot (R \times r) - \frac{\tilde{x}_\Phi}{2l^2} (\tilde{x}_\Phi + i\tilde{y}_\Phi)\right) H_N\left(\frac{\tilde{x}_\Phi}{l}\right)$$

where $H_N(\xi)$ is the Hermite polynomial, $H_N(\xi) = (-1)^N e^{\xi^2} \frac{d^N e^{-\xi^2}}{d\xi^N}$. In the coordinate representation, this expression gives the wave function of the squeezed state $|R, N\rangle$ centered at $R$ and belonging to the $N$-th Landau level; the “rotation angle” $\Phi$ is a complex parameter, $\text{Im} \Phi < 0$.

The squeezed states, eigenfunctions of a non-Hermitian operator $\hat{X}_\Phi$, are generally non-orthogonal. Nevertheless the states from different Landau levels are orthogonal. The overlap integral between any two states from the same Landau level does not depend on the energy level but rather on the distance between the centers of the states. If the distance increases, the overlap integral goes exponentially to zero (on the length-scale of the magnetic length $l$).

The squeezed states, as well as the coherent, are over-complete. One can show that the subset of states with $R$'s on the sites of a periodic lattice is over-complete if the lattice is too dense (the unit cell area $s_0 < 2\pi l^2$) and is not complete for a too dilute lattice ($s_0 > 2\pi l^2$). When $s_0 = 2\pi l^2$ (i.e. the flux through the unit cell equals to the flux quantum $\frac{hc}{e}$), the system of the functions is complete and it remains complete even if a single state is removed; it becomes incomplete, however, if any two states are removed.
VI. CONCLUSIONS

We have analyzed the applicability of the quasiclassical theory of superconductivity in mesoscopic structures. The quasiclassical theory on classical trajectories has been discussed. The generalization of the theory to the cases where the trajectories are mixed by the presence of interfaces has been considered. Since the interfaces violate the condition of applicability of the quasiclassical approximation, the reflection and transmission processes must be included via boundary conditions. The boundary conditions for Andreev “wave” functions, factoring the quasiclassical Green’s function, has been proposed. It has been pointed out that only the tree-like trajectories enter the quasiclassical theory. The Andreev decomposition of the rapidly oscillating and slowly varying parts cannot be unambiguously performed if the loop-like structures would be considered. This exclusion of the loop-like trajectories leads to incorrect results from the quasiclassical theory in certain situations. The simplest structures where the problems with the quasiclassical theory has been reported, double layer sandwich and multi-layer planar systems, have been analyzed in details. The exact calculations based on solutions to Gor’kov and Bogolubov - de Gennes equations have been compared with the quasiclassical results. Since the results found from the exact theories exhibit strong microscopical variations on the scale of $\lambda_F$ they cannot be directly compared with the quasiclassical calculations. The coarse-grain averaged exact quantities have been used for such comparison instead. The main result of the Thesis has been to analyze the terms in exact theory which are missing in the quasiclassical technique. The loop-like structures in the classical trajectory have been clearly identified to be the source of the discrepancies between both theories. It has been concluded that the quasiclassical theory is applicable for the description of a typical real sample where roughness of the interfaces and surfaces is inevitably present. Since most of the real typical samples are non-integrable, the trajectories are tree-like, and the quasiclassical scheme is fully valid. However, for samples, where the conventional quasiclassical theory is inapplicable due to contribution of the interfering path, one can use the modification of the quasiclassical technique which allows for the closed particle orbits.
VI CONCLUSIONS

[18] A.L. Shelankov, Thesis (Ioffe Physicotechnical Institute, Leningrad,
1980).


[43] For example the reflection amplitude on an interface can be written as $r = \sum_n r_n e^{i\alpha_n p_x}$. 

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