Green's function in proximity-contact superconducting-normal double layers

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The Green's function in a proximity-contact superconducting-normal (*S-N*) finite double layer with a spatially varying pair function and with finite reflection coefficient R at the interface is discussed in the clean limit. We first obtain a solution of the Gor'kov equation in a form including a quasiclassical evolution operator that can fully describe the spatial variation of the quasiclassical Green's function. Then we perform analytically the averages of the Green's function over rapidly oscillating phase factors due to the quantum interference effects in the finite double layers. The averaged results of the Matsubara Green's function and the density of states are written in terms of elliptic integrals. The effect of finite R is illustrated on the tunneling density of states. The applicability of the present theory to *S-N* superlattice is mentioned. We show that the conventional normalization condition of the quasiclassical Green's function does not hold in the double-layer system with finite R.

I. INTRODUCTION

The proximity-contact superconducting-normal (*S-N*) double-layer system as depicted in Fig. 1 has been intensively studied theoretically and experimentally.[1] Theoretical treatments so far reported[2-4] are, however, mostly based on the ideal model.[5,6] In the ideal *S-N* double-layer model, the pair function $\Delta(z)$ in the *S*-side is assumed to be constant. In the *N* side, the electrons are assumed to have the same Fermi momentum p_F and the same Fermi velocity v_F as in the *S* side but be free from the pairing interaction. Thus the *S-N* interface is assumed to have an electron transmission coefficient of unity. In actual *S-N* double-layer systems, however, the Fermi velocity of the *N* side is not necessarily equal to that of the *S* side. Even if one can assume that the wave functions can be connected smoothly at the interface, the difference in the Fermi velocity yields a finite reflection coefficient

$$R=\left|\frac{v_F^N-v_F^S}{v_F^N+v_F^S}\right|^2 . \tag{1.1}$$

Moreover, the pair function cannot be constant, because it is depressed near the interface due to the proximity effects. In particular, in the $R=0$ ideal model, the order parameter near the interface shows a rapid variation which depends on the cutoff energy of the pairing interaction.[6]

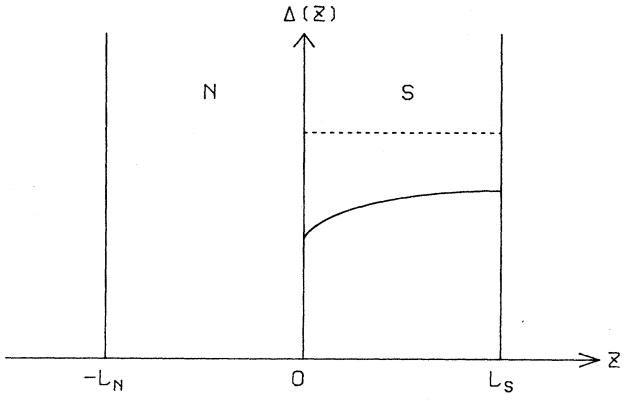

FIG. 1. Typical *S-N* geometry. A self-consistent pair potential in the *S* side is plotted by the solid curve in the case where the *S* side is a pure superconductor with bulk transition temperature T_c with the width $2\pi T_c L_S/v_F^S=1$, the *N* side is a pure metal without pairing interaction with the width $2\pi T_c L_N/v_F^N=1$ and the reflection coefficient at the interface is $R=0.5$. For comparison, the constant pair function of the corresponding bulk superconductor is also plotted by the broken line. See the discussion in Sec. VII of the text.

Recently, some attempts[7,8] to treat more general models have been reported. They are based on the quasiclassical Green's-function method[9,10] which is known to be able to treat the spatial variation of the order parameter even at low temperatures. Zaĭtsev[7] introduced a sufficiently general interface model, though the translational symmetry along the interface is assumed, and obtained boundary conditions at the interface for the quasiclassical Green's function. He showed that the boundary conditions at the interface are characterized by the reflection coefficient R and also showed that at finite R the order parameter is discontinuous at the interface in contrast to the assumption so far made in the treatments within the Ginzburg-Landau equation approach.[11] Millis *et al.*[8] generalized Zaĭtsev's formulation so that a magnetically active interface can be incorporated. The boundary conditions equivalent to Zaĭtsev's have been derived also by Ashauer *et al.*,[12] Kieselmann,[13] and Nagai and Hara[14] by slightly different methods. Kieselmann succeeded in obtaining a self-consistent pair function in a semi-infinite system with finite R where a normal metal film is adsorbed on a semi-infinite superconductor.

In finite double-layer systems, however, the conventional quasiclassical technique cannot be directly applied, because of the presence of the quantum interference

effects due to the finite width of the layers. The conventional quasiclassical formulation consists of the Eilenberger equation for the quasiclassical Green's function $\hat{g}$ and the normalization condition which is given in the present notation as

$$\hat{g}^2=-1 \ . \tag{1.2}$$

In Zaĭtsev's derivation[7,8] of the boundary condition for $\hat{g}$, the conventional normalization condition of Eq. (1.2) is taken for granted. In semi-infinite systems, one can prove that Eq. (1.2) holds.[7,15] Hara and Nagai[16] proved that, in single-layer systems, Eq. (1.2) is also valid for $\hat{g}$ averaged over the rapidly oscillating phase factor that comes from the quantum interference effects. In double-layer systems with finite R, however, the $\hat{g}$ averaged over the two rapidly oscillating phase factors does not satisfy the conventional normalization condition as we shall show below.

In this paper, we present a formulation to solve the Gor'kov equation in the double-layer system with Zaĭtsev's interface[7] under a given general pair function. We follow closely Zaĭtsev's prescription.[7] But we do not try to obtain the boundary conditions for $\hat{g}$, instead we directly solve the boundary problem at the Gor'kov equation level. This is possible if one introduces an evolution operator U which generates the spatial evolution of the quasiclassical Green's function. The evolution operator can fully describe the effects by the spatial variation of the pair function. We obtain a closed expression for the Green's function written in terms of the evolution operator U and the parameters which characterize the boundary conditions. The expression is general enough to incorporate even the magnetic active interface proposed by Millis *et al.*[8] The Green's function thus obtained still contains rapidly oscillating phase factors due to the quantum interference effects. We show that one can explicitly take the averages over the rapidly oscillating phase factors. Once the equation of the evolution operator is solved for a given pair function at the quasiclassical level, our final formulas give the desired averaged Green's function in a closed form. The averaged Green's function includes only the reflection coefficient R and does not depend on the phases of the reflection and transmission amplitudes at the interface. It also does not depend on whether the boundary condition at the layer ends is the fixed end condition or the free end condition.

This paper is organized as follows. In Sec. II we show that the quasiclassical Green's function is intimately related to the Andreev approximation[17] in solving the Bogoliubov–de Gennes equation. We introduce the evolution operator U. In Sec. III boundary conditions at the interface and at the end walls are discussed. Zaĭtsev's interface model[7] is discussed rather in detail. We obtain a formal solution of the Greens' function in the double-layer system. In Sec. IV we consider the Green's function with Matsubara frequency. We show that one can explicitly take the averages over the rapidly oscillating phase factors due to the quantum interference effects. The averaged results can be written in terms of the elliptic integrals. In Sec. V we discuss the density of states. The averaged density of states is also written in terms of the elliptic integrals. In Sec. VI some applications of the present formulation are presented. As limiting cases, the half infinite systems and the finite double-layer systems with a constant pair function are considered and the results are compared with previous work. The applicability of the present theory to the S-N superlattice is discussed. The final section is devoted to summary and discussion. Throughout this paper, we use the units $\hbar=k_B=1$.

II. QUASICLASSICAL GREEN'S FUNCTION

In this section, we show that the quasiclassical Green's function[9,10] can be reconstructed from the solutions of the Bogoliubov–de Gennes equation within the Andreev approximation.[17] For more details, we refer the reader to Refs. 7, 14, and 16. We introduce the evolution operator which generates the spatial evolution of the quasiclassical Green's function. Discussion of the present section can be applied to either side of the double layers and is relevant to singlet as well as to triplet superconductors.

We consider a geometry as shown in Fig. 1. The widths of the layers L_S and L_N are assumed to be still much longer than the Fermi wavelength $1/p_F$, but not necessarily longer than the coherence length ξ. The interface and the boundaries are assumed to have translational symmetry in the x,y plane. The momentum component parallel to the boundary is, therefore, a conserved quantity. For a given parallel momentum $\mathbf{p}$, the Bogoliubov–de Gennes equation for the four-dimensional Nambu amplitude Ψ is written as

$$\int dz' \begin{bmatrix} [\xi_{\parallel}-(1/2m^*)\partial_z^2]\delta(z-z') & \tilde{\Delta}(\mathbf{p},z,z') \\ \tilde{\Delta}^{\dagger}(\mathbf{p},z',z) & -[\xi_{\parallel}-(1/2m^*)\partial_z^2]\delta(z-z') \end{bmatrix} \Psi(z')=E\Psi(z) \ , \tag{2.1}$$

where $\xi_{\parallel}=\mathbf{p}^2/2m^*-\mu$, m^* is the effective mass, and

$$\tilde{\Delta}(\mathbf{p},z,z')=\sum_{p_z>0}\Delta(\mathbf{p}_F^+,z)e^{ip_z(z-z')} + \sum_{p_z<0}\Delta(\mathbf{p}_F^-,z)e^{ip_z(z-z')} \tag{2.2}$$

with $\Delta(\mathbf{p}_F^{\pm},z)$ the position-dependent pair function at the Fermi momentum $\mathbf{p}_F^{\pm}$. In Eq. (2.2), we have defined two Fermi momenta $\mathbf{p}_F^+$ and $\mathbf{p}_F^-$ associated with the parallel momentum $\mathbf{p}$, as depicted in Fig. 2. Throughout this paper $\cos\theta$ and $p_{Fz}\equiv p_F\cos\theta$ are defined to be positive.

When the pair function $\Delta(\mathbf{p}_F^{\pm},z)$ varies smoothly on the scale of the coherence length, one can solve Eq. (2.1)

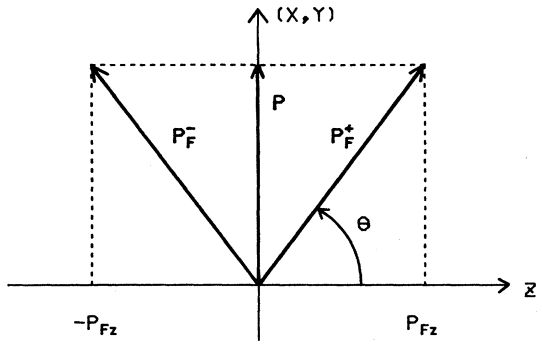

FIG. 2. Fermi momenta $\mathbf{p}_F^+$ and $\mathbf{p}_F^-$ associated with the momentum $\mathbf{p}$ parallel to the interface and to the walls. Note that throughout this paper p_{Fz} and $\cos\theta$ are defined to be positive.

within the Andreev approximation[17] to find

$$\Psi_l(z)=\sum_{\alpha=\pm1}\Phi_{\alpha l}(z)e^{i\alpha p_{Fz}z}\ , \tag{2.3}$$

where $p_{Fz}=p_F\cos\theta$ is the z component of the Fermi momentum $\mathbf{p}_F^+$. The slowly varying amplitudes $\Phi_{\alpha l}$ satisfy the Andreev equation[17]

$$\begin{bmatrix}-\alpha iv_{Fz}\partial_z & \Delta(\mathbf{p}_F^\alpha,z)\\ \Delta^\dagger(\mathbf{p}_F^\alpha,z) & \alpha iv_{Fz}\partial_z\end{bmatrix}\Phi_{\alpha l}=E_l\Phi_{\alpha l}\ , \tag{2.4}$$

where $v_{Fz}=v_F\cos\theta=p_F\cos\theta/m^*$. The slowly varying amplitudes are expected to form a complete set in a sense that

$$\sum_l\Phi_{\alpha l}(z)\Phi_{\alpha l}^\dagger(z')=\tilde{\delta}(z-z')\equiv\int_{-p_{Fz}}^{p_{Fz}}\frac{dp_z}{2\pi}e^{ip_z(z-z')}\ . \tag{2.5}$$

The tilded δ function plays the same role as the δ function on the length scale much longer than $1/p_F$.

The Gor'kov Green's function can be constructed from the Nambu amplitudes as

$$G(z,z',\varepsilon)=\sum_l\frac{\Psi_l(z)\Psi_l^\dagger(z')}{\varepsilon-E_l}\ . \tag{2.6}$$

Substituting Eq. (2.3) into Eq. (2.6), one finds that the Gor'kov Green's function is decomposed as

$$\begin{aligned}G(z,z',\varepsilon)=&G_{++}(z,z')\exp[ip_{Fz}(z-z')]\\&+G_{--}(z,z')\exp[-ip_{Fz}(z-z')]\\&+G_{+-}(z,z')\exp[ip_{Fz}(z+z')]\\&+G_{-+}(z,z')\exp[-ip_{Fz}(z+z')]\ ,\end{aligned} \tag{2.7}$$

where

$$G_{\alpha\beta}(z,z')=\sum_l\frac{\Phi_{\alpha l}(z)\Phi_{\beta l}^\dagger(z')}{\varepsilon-E_l} \tag{2.8}$$

which satisfies the equation

$$\left[\varepsilon-\begin{bmatrix}-\alpha iv_{Fz}\partial_z & \Delta(\mathbf{p}_F^\alpha,z)\\ \Delta^\dagger(\mathbf{p}_F^\alpha,z) & \alpha iv_{Fz}\partial_z\end{bmatrix}\right]G_{\alpha\beta}(z,z')=\delta_{\alpha\beta}\tilde{\delta}(z-z')\ . \tag{2.9}$$

It is useful for later use to introduce the notion of "directional space"[8] which is a two-dimensional space spanned by $\alpha=\pm1$. From Eq. (2.9), one finds that the diagonal (in the directional space) elements G_{++} and G_{--} have a jump at $z=z'$, i.e.,

$$G_{\alpha\alpha}(z+0,z)-G_{\alpha\alpha}(z-0,z)=-i\frac{\alpha}{v_{Fz}}\rho_3 \tag{2.10}$$

but off-diagonal elements have no jump. Here ρ_3 is a Pauli matrix in particle-hole space.

Now we define quasiclassical Green's function $\hat{g}_{\alpha\beta}(z)$ by

$$\hat{g}_{\alpha\beta}(z)\pm i(\gamma_3)_{\alpha\beta}=-2v_{Fz}\rho_3G_{\alpha\beta}(z\pm0,z)\ , \tag{2.11}$$

where γ_3 is a Pauli matrix in the directional space. From Eq. (2.9) it follows that

$$iv_{Fz}\partial_z\hat{g}_{\alpha\beta}=-\alpha(\varepsilon-\hat{\Delta}_\alpha)\rho_3\hat{g}_{\alpha\beta}+\hat{g}_{\alpha\beta}\beta(\varepsilon-\hat{\Delta}_\beta)\rho_3\ , \tag{2.12}$$

where

$$\hat{\Delta}_\alpha=\begin{bmatrix}0 & \Delta(\mathbf{p}_F^\alpha,z)\\ \Delta^\dagger(\mathbf{p}_F^\alpha,z) & 0\end{bmatrix}\ . \tag{2.13}$$

Equation (2.12) for the diagonal elements is nothing but the Eilenberger[9] equation. Usually, the Eilenberger equation is solved under the conventional normalization condition $\hat{g}_{\alpha\alpha}^2=-1$. As was emphasized in Refs. 14 and 16, however, the normalization condition depends on the boundary condition of the problem under consideration. We shall show below that the normalization constant is not always equal to -1 in the present double-layer system.

It is convenient to introduce an evolution operator U_α which satisfies

$$iv_{Fz}\partial_zU_\alpha(z,z')=-\alpha(\varepsilon-\hat{\Delta}_\alpha)\rho_3U_\alpha(z,z')\ , \tag{2.14}$$

and

$$U_\alpha(z,z)=1\ . \tag{2.15}$$

The evolution operator U has an important property

$$\det U_\alpha(z,z')=1\ , \tag{2.16}$$

which can be proved from Eqs. (2.14) and (2.15). We can obtain a formal solution of Eq. (2.12) to be

$$\hat{g}_{\alpha\beta}(z)=U_\alpha(z,z_0)\hat{g}_{\alpha\beta}(z_0)U_\beta^{-1}(z,z_0)\ . \tag{2.17}$$

This is important because solving the Eilenberger equation has been reduced to solving Eq. (2.14) with the initial condition Eq. (2.15).

Physical quantities of interest such as current, order parameter, etc. are obtained from the position diagonal elements of the Gor'kov Green's function

$$\begin{aligned}G(z,z,\varepsilon)=-\frac{1}{2v_{Fz}}\rho_3[&\hat{g}_{++}(z)+\hat{g}_{+-}(z)e^{2ip_{Fz}z}\\&+\hat{g}_{-+}(z)e^{-2ip_{Fz}z}+\hat{g}_{--}(z)]\ .\end{aligned} \tag{2.18}$$

Since the middle two terms have rapidly varying part $\exp(\pm 2ip_{Fz}z)$, they do not contribute as long as the slowly varying quantities are concerned. For instance, the gap equation is written in a form

$$\Delta(\mathbf{p}_F,z)=-\pi T\sum_{\omega_n}\frac{N(0)}{2}\int_0^{\pi/2}\sin\theta' d\theta' \times\sum_{\alpha=\pm 1} v_{\mathbf{p}_F,\mathbf{p}_F'^{\alpha}}(\hat{g}_{\alpha\alpha}(z))_{\mathrm{OD}}\ , \tag{2.19}$$

where $N(0)$ is the density of states at the Fermi surface, $v_{\mathbf{p},\mathbf{p}'}$ is the pairing interaction, and $(\hat{g})_{\mathrm{OD}}$ is the off-diagonal (in particle-hole space) element of the quasiclassical Matsubara Green's function. Thus the diagonal elements $\hat{g}_{++}(z)$ and $\hat{g}_{--}(z)$ are relevant quantities. This is the reason a lot of efforts[7,8,12–14] have been made to find boundary conditions which are closed within the diagonal elements only. In order to treat the boundary problem, however, it is useful to treat all the elements on equal footing.

III. BOUNDARY CONDITIONS

In this section, we consider first the boundary conditions for the Nambu amplitudes in the double-layer geometry as shown in Fig. 1 and then transform them to those for the Green's functions. Formal solutions for the Green's function are obtained. We use a superscript or a subscript N (S) to denote the quantities in the N (S) side. The N side is not necessarily a normal metal but can be another kind of superconductor than the S side.

Let us first consider the N-S interface boundary located at $z=0$. We follow closely the prescription proposed by Zaĭtsev.[7] The proximity interface is assumed to be confined within a narrow range $-\delta<z<\delta$, where δ is of order of $1/p_F$. It follows that the Nambu amplitudes Ψ^N and Ψ^S given in the preceding section should be the asymptotic solution of the interface problem. Since the interface process is a high-energy ($\sim E_F$) and short-range ($\sim 1/p_F$) process, it is governed by the rapidly varying part of the Nambu amplitudes and is consequently common to both the superfluid and the normal phases. The interface process is, therefore, characterized by the two independent asymptotic solutions Ψ_1 and Ψ_2 at the Fermi surface:

$$\Psi_1=\begin{cases}\exp(+ip_{Fz}^N z)+r\exp(-ip_{Fz}^N z) & \text{for } z<-\delta\\ d\exp(+ip_{Fz}^S z) & \text{for } z>\delta\ ,\end{cases} \tag{3.1}$$

$$\Psi_2=\begin{cases}\tilde{d}\exp(-ip_{Fz}^N z) & \text{for } z<-\delta\\ \exp(-ip_{Fz}^S z)+\tilde{r}\exp(+ip_{Fz}^S z) & \text{for } z>\delta\ ,\end{cases} \tag{3.2}$$

where r and d are the reflection and the transmission amplitude, respectively, and $\tilde{d}=dv_{Fz}^N/v_{Fz}^S$, $\tilde{r}=-r^*d/d^*$. Noting that the Nambu amplitudes Ψ^N and Ψ^S are given by appropriate linear combinations of Ψ_1 and Ψ_2, we obtain the boundary conditions of the form

$$\sqrt{v_{Fz}^N}\Phi_\alpha^N(0)=\sum_{\beta=\pm 1}\hat{M}_{\alpha\beta}\sqrt{v_{Fz}^S}\Phi_\beta^S(0)\ , \tag{3.3}$$

where $\hat{M}$ is a 2×2 matrix in the directional space given by

$$\hat{M}=\frac{1}{\sqrt{D}}\begin{bmatrix}\exp(-i\theta_d) & \sqrt{R}\exp[i(\theta_d-\theta_r)]\\ \sqrt{R}\exp[-i(\theta_d-\theta_r)] & \exp(i\theta_d)\end{bmatrix}\ , \tag{3.4}$$

where $D=1-R=1-|r|^2$, $r=|r|\exp(i\theta_r)$, and $d=|d|\exp(i\theta_d)$. The boundary condition does not depend on the low-lying energy states according to the spirit of the Andreev approximation. It is worth noting that the phases θ_r and θ_d are rapidly varying functions of the interface position. As we shall show below, the interface effect on the Green's functions is characterized only by the reflection coefficient R and does not depend on the phases θ_r and θ_d when appropriate averages are taken over rapidly oscillating phase factors.

Recently Millis *et al.*[8] discussed that the magnetically active interface can also be treated by generalizing the matrix $\hat{M}$. For the particle current to be conserved at the interface, the general $\hat{M}$ should satisfy[8]

$$\gamma_3=\hat{M}\gamma_3\hat{M}^\dagger\ , \tag{3.5}$$

where γ_3 is a Pauli matrix in the directional space.

Let us turn to the boundary at the left end $z=-L_N$. From the demand that there is no net current across the boundary, it follows that

$$\Phi_+^N(-L_N)\exp(-ip_{Fz}^N L_N)+\exp(i\eta_N)\Phi_-^N(-L_N)\exp(ip_{Fz}^N L_N)=0\ . \tag{3.6}$$

The phase η_N is arbitrary. When $\exp(i\eta_N)=1$, one has a fixed end condition and when $\exp(i\eta_N)=-1$ one has a free end condition. The averaged Green's function, however, does not depend on η_N (see below). In the same way, we have a boundary condition at the right end $z=L_S$:

$$\exp(i\eta_S)\Phi_+^S(L_S)\exp(ip_{Fz}^S L_S)+\Phi_-^S(L_S)\exp(-ip_{Fz}^S L_S)=0\ . \tag{3.7}$$

Now we discuss how the above boundary conditions are converted to those for the Green's functions. Let us start from the S-N interface. From the definition and the boundary condition Eq. (3.3), we find that

$$(\hat{g}^N(0)+i\gamma_3)_{\alpha\beta}=-2v_{Fz}^N\rho_3 G^N_{\alpha\beta}(0,-0)=-2v_{Fz}^N\rho_3\sum_l\frac{\Phi^N_{\alpha l}(0)\Phi^{N\dagger}_{\beta l}(-0)}{\varepsilon-E_l}$$
$$=-2\sqrt{v_{Fz}^N v_{Fz}^S}\rho_3\sum_l\frac{\hat{M}_{\alpha\gamma}\Phi^S_{\gamma l}(0)\Phi^{N\dagger}_{\beta l}(-0)}{\varepsilon-E_l}$$
$$=-2v_{Fz}^S\rho_3\sum_l\frac{\hat{M}_{\alpha\gamma}\Phi^S_{\gamma l}(0)\Phi^{S\dagger}_{\delta l}(-0)\hat{M}^\dagger_{\delta\beta}}{\varepsilon-E_l}=(\rho_3\hat{M}\rho_3[\hat{g}^S(0)+i\gamma_3]\hat{M}^\dagger)_{\alpha\beta}\ . \tag{3.8}$$

Since $\rho_3\hat{M}\rho_3=\hat{M}$ and $\gamma_3=\hat{M}\gamma_3\hat{M}^\dagger$, we obtain a simple result

$$\hat{g}^N(0)=\hat{M}\hat{g}^S(0)\hat{M}^\dagger\ , \tag{3.9}$$

which has been obtained by Zaĭtsev[7] and Millis *et al.*[8]

At the left end $z=-L_N$, we find from Eq. (3.6) that

$$(\hat{g}^N(-L_N)-i\gamma_3)_{\alpha\beta}=-2v_{Fz}^N\rho_3 G^N_{\alpha\beta}(-L_N,-L_N+0)$$
$$=-2v_{Fz}^N\rho_3\sum_l\frac{\Phi^N_{\alpha l}(-L_N)\Phi^{N\dagger}_{\beta l}(-L_N+0)}{\varepsilon-E_l}$$
$$=2v_{Fz}^N\rho_3\sum_l\frac{\Phi^N_{-\alpha l}(-L_N)\Phi^{N\dagger}_{\beta l}(-L_N+0)}{\varepsilon-E_l}\exp(\alpha i\tilde{\eta}_N)$$
$$=-(\hat{g}^N(-L_N)-i\gamma_3)_{-\alpha\beta}\exp(\alpha i\tilde{\eta}_N)\ , \tag{3.10}$$

where $\tilde{\eta}_N=2p_{Fz}^N L_N+\eta_N$. Thus

$$\hat{g}^N_{++}(-L_N)+i=\hat{g}^N_{--}(-L_N)+i=-e^{-i\tilde{\eta}_N}\hat{g}^N_{+-}(-L_N)\ , \tag{3.11}$$

$$\hat{g}^N_{++}(-L_N)-i=\hat{g}^N_{--}(-L_N)-i=-e^{i\tilde{\eta}_N}\hat{g}^N_{-+}(-L_N)\ . \tag{3.12}$$

In a similar way, we find the boundary condition at the right end of the S side:

$$\hat{g}^S_{++}(L_S)+i=\hat{g}^S_{--}(L_S)+i=-e^{-i\tilde{\eta}_S}\hat{g}^S_{-+}(L_S)\ , \tag{3.13}$$

$$\hat{g}^S_{++}(L_S)-i=\hat{g}^S_{--}(L_S)-i=-e^{i\tilde{\eta}_S}\hat{g}^S_{+-}(L_S)\ , \tag{3.14}$$

where $\tilde{\eta}_S=2p_{Fz}^S L_S+\eta_S$.

For semi-infinite systems ($L_N=\infty$ or $L_S=\infty$), the Green's functions take bulk values at some infinity. In that case, the quasiclassical Green's functions satisfy the conventional normalization condition

$$\hat{g}^2_{++}(z)=\hat{g}^2_{--}(z)=-1 \quad \text{for any } z\ . \tag{3.15}$$

Zaĭtsev[7] and Millis *et al.*[8] obtained a set of boundary conditions at the interface for the diagonal (in the directional space) elements of $\hat{g}$ by eliminating the off-diagonal elements from Eq. (3.9) using the conventional normalization condition.[15] Their results can be applied only to semi-infinite systems. In the case of finite double layers, the normalization constant on the right-hand side (rhs) of Eq. (3.15) is not known at the beginning.

In contrast to previous work, here we directly solve the system of equations for the Green's functions. Let us first put

$$h^N=\hat{g}^N_{++}(-L_N)=\hat{g}^N_{--}(-L_N) \tag{3.16}$$

and

$$h^S=\hat{g}^S_{++}(L_S)=\hat{g}^S_{--}(L_S)\ . \tag{3.17}$$

Then, using Eq. (2.17) and Eqs. (3.11)–(3.14), we find

$$\hat{g}^N(0)=\hat{U}^N\begin{bmatrix}h^N & -(h^N+i)\\ -(h^N-i) & h^N\end{bmatrix}\hat{U}^{N-1} \tag{3.18}$$

and

$$\hat{g}^S(0)=\hat{U}^S\begin{bmatrix}h^S & -(h^S-i)\\ -(h^S+i) & h^S\end{bmatrix}\hat{U}^{S-1}\ , \tag{3.19}$$

where

$$\hat{U}^N=\begin{bmatrix}U^N_+ e^{i\tilde{\eta}_N/2} & \\ & U^N_- e^{-i\tilde{\eta}_N/2}\end{bmatrix}\ ,$$
$$\hat{U}^S=\begin{bmatrix}U^S_+ e^{-i\tilde{\eta}_S/2} & \\ & U^S_- e^{i\tilde{\eta}_S/2}\end{bmatrix} \tag{3.20}$$

with $U^N_\pm=U^N_\pm(0,-L_N)$ and $U^S_\pm=U^S_\pm(0,L_S)$. Combining Eqs. (3.18) and (3.19) with Eq. (3.9), we find

$$[h^N(\gamma_3+i\gamma_2)+i\gamma_1]\mathcal{M}=\mathcal{M}[h^S(\gamma_3+i\gamma_2)-i\gamma_1]\ , \tag{3.21}$$

where

$$\mathcal{M}\equiv\hat{U}^{N-1}\hat{M}\hat{U}^S=\sum_{i=0}^{3}m_i\gamma_i\ . \tag{3.22}$$

Expanding Eq. (3.21) in terms of the Pauli matrices γ_i's

in the directional space, one finds

$$h^N=i(m_0-m_1)(m_3+im_2)^{-1} \tag{3.23}$$

and

$$h^S=i(m_3+im_2)^{-1}(m_0+m_1)\ . \tag{3.24}$$

Although the above results are valid for general interface matrix $\hat{M}$, they can be much simplified in the nonmagnetic interface considered by Zaĭtsev.[7] After some manipulations, we find

$$h^N=(-i)\frac{e^{i\phi_N}+A_N}{e^{i\phi_N}-A_N}\ , \tag{3.25}$$

$$h^S=(-i)\frac{e^{i\phi_S}+A_S}{e^{i\phi_S}-A_S}\ , \tag{3.26}$$

where

$$A_N=(U_+^N)^{-1}\frac{Q_S e^{-i\phi_S}-\sqrt{R}}{1-\sqrt{R}\,Q_S e^{-i\phi_S}}U_-^N\ , \tag{3.27}$$

$$A_S=(U_-^S)^{-1}\frac{e^{-i\phi_N}+\sqrt{R}\,Q_N}{Q_N+\sqrt{R}\,e^{-i\phi_N}}U_+^S\ , \tag{3.28}$$

$$Q_N=U_+^N(U_-^N)^{-1}\ , \tag{3.29}$$

$$Q_S=U_+^S(U_-^S)^{-1}\ , \tag{3.30}$$

$$\phi_N=2p_F^N\cos\theta_N L_N+\eta_N+\theta_r\ , \tag{3.31}$$

and

$$\phi_S=2p_F^S\cos\theta_S L_S+\eta_S-\theta_r+2\theta_d\ . \tag{3.32}$$

The phases ϕ_N and ϕ_S are rapidly varying functions of layer sizes L_S and L_N and also of the polar angles of the Fermi momenta. We are not interested, however, in the size accuracy of order $1/p_F$ and in the accuracy of the polar angle of order $1/p_F L$. Apart from the correction of order $1/p_F L$, therefore, the physical quantities of interest are obtained from the diagonal (in the directional space) elements of the quasiclassical Green's functions averaged over the phases ϕ_N and ϕ_S. Moreover, in actual systems the phases θ_r, θ_d, η_N, and η_S will be random variables reflecting the microscopic irregularities at the interface and at the walls. It follows that the averages over the phases ϕ_N and ϕ_S can be performed independently in spite of the fact that the polar angles of the N and S sides are connected by the parallel momentum conservation condition $p_F^N\sin\theta_N=p_F^S\sin\theta_S$. As a result, the averaged Green's function do not depend on the phases of the interface reflection amplitudes but are determined only by the reflection coefficient R. They do not depend on whether the boundary conditions at the layer ends are fixed end conditions or free end conditions.

Since the evolution operators include no rapidly oscillating phase factors, the averaged quasiclassical Green's functions at arbitrary positions are given by

$$\langle\langle\hat{g}_{\alpha\alpha}^N(z)\rangle\rangle=U_\alpha^N(z,-L_N)\langle\langle h_N\rangle\rangle[U_\alpha^N(z,-L_N)]^{-1}\ , \tag{3.33}$$

$$\langle\langle\hat{g}_{\alpha\alpha}^S(z)\rangle\rangle=U_\alpha^S(z,L_S)\langle\langle h_S\rangle\rangle[U_\alpha^S(z,L_S)]^{-1}\ , \tag{3.34}$$

where $\langle\langle\ \rangle\rangle$ means the double average over ϕ_N and ϕ_S.

IV. MATSUBARA GREEN'S FUNCTION

In the rest of this paper, we confine ourselves to the proximity effects, where the N side is a pure normal metal with no pairing interaction and the S side is a pure singlet superconductor. The pair function in the S side varies spatially due to the proximity effect. In this section, we consider the Matsubara Green's function in which $\varepsilon=i\omega_n$ and show that the Green's functions averaged over the phases ϕ_N and ϕ_S can be expressed in terms of the complete elliptic integrals.

In the case of the singlet superconductor, we have only to treat the 2×2 matrix in particle-hole space. For the Matsubara frequency $\varepsilon=i\omega_n$, the evolution operator in the N side is given by

$$U_\pm^N=\exp\left[\mp\frac{\omega_n L_N}{v_{Fz}^N}\rho_3\right]\equiv\begin{bmatrix}e^{\mp\kappa_N/2} & \\ & e^{\pm\kappa_N/2}\end{bmatrix}\ , \tag{4.1}$$

where $\kappa_N=2\omega_n L_N/v_{Fz}^N$. In the S side, the evolution operator is parametrized by two complex numbers $\alpha=\alpha'+i\alpha''$ and $\beta=\beta'+i\beta''$ with the relation $\alpha'\beta'+\alpha''\beta''=1$:

$$U_+^S=\begin{bmatrix}\alpha' & i\alpha'' \\ i\beta'' & \beta'\end{bmatrix}\ , \tag{4.2}$$

$$(U_-^S)^{-1}=(U_+^S)^\dagger=\begin{bmatrix}\alpha' & -i\beta'' \\ -i\alpha'' & \beta'\end{bmatrix}\ , \tag{4.3}$$

$$Q_S=\begin{bmatrix}|\alpha|^2 & -i(\alpha'\beta''-\alpha''\beta') \\ i(\alpha'\beta''-\alpha''\beta') & |\beta|^2\end{bmatrix}\ , \tag{4.4}$$

where Eqs. (4.2) and (4.3) can be derived from the structure of the evolution equation and the property $\det U_\pm^S=1$. Once the evolution equation with the initial condition Eq. (2.15) is solved, one can obtain an analytic expression for the averaged Green's function as we shall show just below. The present approach is more useful than the conventional quasiclassical approach in which one should solve the Eilenberger equation with complicated nonlinear boundary conditions.[7,8] Moreover, as we shall show below, the conventional approach cannot be generally applied to the double-layer system.

A. *N*-side Green's function

Let us first consider the average of h^N over ϕ_N;

$$\langle h^N\rangle_N=\frac{1}{2\pi}\int d\phi_N(-i)\frac{e^{i\phi_N}+A_N}{e^{i\phi_N}-A_N}$$

$$=\frac{1}{2\pi i}\oint dz(-i)\frac{1}{z}\frac{z+A_N}{z-A_N}\ , \tag{4.5}$$

where the integral over z is along a unit circle in the complex z plane. One can prove that

$$|\det A_N| = 1 \ . \tag{4.6}$$

It follows that one of the eigenvalues of A_N is located inside the unit circle and the other is outside. Now we perform the z integral using the residue theorem. For that purpose, it is convenient to rewrite

$$A_N = \zeta_N \tilde{A}_N \ , \tag{4.7}$$

$$\zeta_N = -\frac{e^{-i\phi_S}}{(1-\sqrt{R}\,q_1 e^{-i\phi_S})(1-\sqrt{R}\,q_2 e^{-i\phi_S})} \ , \tag{4.8}$$

$$\tilde{A}_N = (U_+^N)^{-1}[2\sqrt{R}\,\cos\phi_S - (Q_S + RQ_S^{-1})]U_-^N \ , \tag{4.9}$$

where q_1, q_2 are the eigenvalues of the matrix Q_S with $q_1 q_2 = 1$. Noting that $\tilde{A}_N$ is a Hermite matrix for $\varepsilon = i\omega_n$, we can evaluate the z integral to obtain

$$\langle h^N \rangle_N = -i\frac{\tilde{A}_N - \frac{1}{2}\,\mathrm{tr}\,\tilde{A}_N}{[(\frac{1}{2}\,\mathrm{tr}\,\tilde{A}_N)^2 - \det \tilde{A}_N]^{1/2}} \ , \tag{4.10}$$

where the sign in front is so chosen that it should recover the sign at the normal limit ($\omega_n \gg T_c$). At this stage, we note that $\langle h^N \rangle_N$ satisfies the conventional normalization condition, i.e.,

$$(\langle h^N \rangle_N)^2 = -1 \ . \tag{4.11}$$

This agrees with Hara and Nagai[16] who proved that in a slab geometry the quasiclassical Green's function averaged over rapidly varying phases satisfies the conventional normalization condition. The present double-layer system can be taken as a slab system in which the righ-hand boundary has an internal structure (superconductor). However, $\langle h^N \rangle_N$ still contains another rapidly oscillating phase factor which comes from the quantum interference effects within the S side. When the second average over ϕ_S is taken, the averaged Green's function no longer satisfies the conventional normalization condition. It implies that the conventional quasiclassical formulation invoking the conventional normalization condition cannot be applied to the present double-layer system. Exceptional cases occur when $R=0$ and $R=1$ where $\langle h^N \rangle_N$ no longer depends on ϕ_S. When $R=0$, there is no reflection at the interface; therefore the double-layer system may be regarded as a single-layer system with the walls at $z=-L_N$ and at $z=L_S$. This corresponds to the slab geometry considered by Hara and Nagai.[16] On the other hand, when $R=1$ each layer may be regarded as independent system without any proximity.

Now we evaluate the second average over ϕ_S.

$$\langle\langle h^N \rangle_N \rangle_S = \frac{1}{2\pi}\int_0^{2\pi} d\phi_S \langle h^N \rangle_N (\cos\phi_S) = \frac{1}{\pi}\int_{-1}^{1} dx \frac{1}{(1-x^2)^{1/2}} \langle h^N \rangle_N (x) \ . \tag{4.12}$$

Using Eqs. (4.1) and (4.4), the explicit form of the integrand of Eq. (4.12) is given by

$$\langle h^N \rangle_N (x) = -i\frac{\begin{bmatrix} ax-b & ic \\ -ic & -(ax-b) \end{bmatrix}}{[(ax-b)^2+c^2]^{1/2}} \ , \tag{4.13}$$

where

$$a = 2\sqrt{R}\ \mathrm{sh}(\kappa_N) \ , \tag{4.14}$$

$$b = (1+R)\frac{|\alpha|^2+|\beta|^2}{2}\mathrm{sh}(\kappa_N) + (1-R)\frac{|\alpha|^2-|\beta|^2}{2}\mathrm{ch}(\kappa_N) \ , \tag{4.15}$$

$$c = (1-R)(\alpha'\beta'' - \alpha''\beta') \ . \tag{4.16}$$

The result of the second average is written in terms of the complete elliptic integrals:

$$\langle\langle h^N \rangle_N \rangle_S = -i\frac{2}{\pi\sqrt{D}}\begin{bmatrix} X & icY \\ -icY & -X \end{bmatrix} \ , \tag{4.17}$$

where

$$X = \left[\frac{a^2-b^2+c^2+D}{2b}K(k) - \frac{a^2+b^2+c^2+D}{2b}\Pi(\nu,k)\right] \ , \tag{4.18}$$

$$Y = K(k) \ , \tag{4.19}$$

$$D = [(a^2+b^2+c^2)^2 - 4a^2b^2]^{1/2} \ . \tag{4.20}$$

Here K is the first kind complete elliptic integral and Π is the third kind complete elliptic integral defined by

$$\Pi(\nu,k) = \int_0^1 \frac{dx}{(1+\nu x^2)[(1-x^2)(1-k^2x^2)]^{1/2}} \ , \tag{4.21}$$

where

$$k^2 = \frac{a^2-b^2-c^2+D}{2D} \ , \tag{4.22}$$

$$\nu = \frac{a^2+b^2+c^2-D}{2D} \ . \tag{4.23}$$

Here we consider the two special cases $R=0$ and $R=1$. The $R=0$ system has been considered in the literature. In this case, one finds that $k=\nu=0$, consequently $\Pi = K = \pi/2$. Thus we find from Eq. (4.17) that

$$\langle\langle h^N \rangle_N \rangle_S = -i\frac{\begin{bmatrix} -b & ic \\ -ic & b \end{bmatrix}}{(b^2+c^2)^{1/2}} \tag{4.24}$$

which can be also obtained directly from Eq. (4.13) by putting $R=0$. The $R=1$ case sometimes occurs when the Fermi momenta p_F^S and p_F^N are different, consequently the parallel momentum conservation law $p_F^S \sin\theta_S = p_F^N \sin\theta_N$ does not hold at some polar angles. For $R=1$, the Green's function takes a bulk normal system form, i.e.,

$$\langle\langle h^N \rangle_N \rangle_S = i\,\mathrm{sgn}(\omega_n)\rho_3 \ . \tag{4.25}$$

B. *S*-side Green's function

First we consider the average of h^S over ϕ_S.

$$\langle h^S\rangle_S=\frac{1}{2\pi}\int d\phi_S\,(-i)\frac{e^{i\phi_S}+A_S}{e^{i\phi_S}-A_S}$$
$$=\frac{1}{2\pi i}\oint dz\,(-i)\frac{1}{z}\frac{z+A_S}{z-A_S}\,. \tag{4.26}$$

Noting that $|\det A_S|=1$, we can evaluate the z integral in the same way as for the N-side Green's function to obtain

$$\langle h^S\rangle_S=i\frac{\tilde{A}_S-\frac{1}{2}\mathrm{tr}\,\tilde{A}_S}{[(\frac{1}{2}\mathrm{tr}\,\tilde{A}_S)^2-\det\tilde{A}_S]^{1/2}}\,, \tag{4.27}$$

where

$$A_S=\zeta_S\tilde{A}_S\,, \tag{4.28}$$

$$\zeta_S=\frac{e^{-i\phi_N}}{(1+\sqrt{R}\,e^{\kappa_N}e^{-i\phi_N})(1+\sqrt{R}\,e^{-\kappa_N}e^{-i\phi_N})}\,, \tag{4.29}$$

$$\tilde{A}_S=[2\sqrt{R}\,\cos\phi_N+(1+R)\,\mathrm{ch}(\kappa_N)](U_-^S)^{-1}U_+^S$$
$$+(1-R)\,\mathrm{sh}(\kappa_N)(U_-^S)^{-1}\rho_3U_+^S\,. \tag{4.30}$$

In the rhs of Eqs. (4.27), the sign in front has been chosen in the same spirit as in the N side.

Now we evaluate the average over ϕ_N:

$$\langle\langle h^S\rangle_S\rangle_N=\frac{1}{2\pi}\int_0^{2\pi}d\phi_N\langle h^S\rangle_S(\cos\phi_N)$$
$$=\frac{1}{\pi}\int_{-1}^{1}dx\frac{1}{(1-x^2)^{1/2}}\langle h^S\rangle_S(x)\,, \tag{4.31}$$

where

$$\langle h^S\rangle_S(x)=i\left[\frac{2\sqrt{R}\,x+(1+R)\mathrm{ch}(\kappa_N)}{[(2\sqrt{R}\,x+m)^2+n^2]^{1/2}}\left[\frac{\mathrm{Re}(\alpha^2-\beta^2)}{|\alpha^2-\beta^2|}\rho_3-\frac{\mathrm{Im}(\alpha^2-\beta^2)}{|\alpha^2-\beta^2|}\rho_2\right]\right.$$
$$\left.+\frac{(1-R)\mathrm{sh}(\kappa_N)}{[(2\sqrt{R}\,x+m)^2+n^2]^{1/2}}\left[\frac{\mathrm{Re}(\alpha^2+\beta^2)}{|\alpha^2-\beta^2|}\rho_3-\frac{\mathrm{Im}(\alpha^2+\beta^2)}{|\alpha^2-\beta^2|}\rho_2\right]\right]\,, \tag{4.32}$$

with

$$m=(1+R)\,\mathrm{ch}(\kappa_N)+(1-R)\,\mathrm{sh}(\kappa_N)\frac{|\alpha|^4-|\beta|^4}{|\alpha^2-\beta^2|^2}\,, \tag{4.33}$$

$$n=(1-R)\,\mathrm{sh}(\kappa_N)\frac{2\,\mathrm{Im}(\alpha^2\beta^{*2})}{|\alpha^2-\beta^2|^2}\,. \tag{4.34}$$

The integral over x is again written in terms of the complete elliptic integrals. We finally obtain

$$\langle\langle h^S\rangle_S\rangle_N=i\left[[X+Y(1+R)\,\mathrm{ch}(\kappa_N)]\left[\frac{\mathrm{Re}(\alpha^2-\beta^2)}{|\alpha^2-\beta^2|}\rho_3-\frac{\mathrm{Im}(\alpha^2-\beta^2)}{|\alpha^2-\beta^2|}\rho_2\right]\right.$$
$$\left.+Y(1-R)\,\mathrm{sh}(\kappa_N)\left[\frac{\mathrm{Re}(\alpha^2+\beta^2)}{|\alpha^2-\beta^2|}\rho_3-\frac{\mathrm{Im}(\alpha^2+\beta^2)}{|\alpha^2-\beta^2|}\rho_2\right]\right]\,, \tag{4.35}$$

where

$$X=\frac{2}{\pi\sqrt{D}}\frac{4R+m^2+n^2+D}{2m}[\Pi(\nu,k)-K(k)]\,, \tag{4.36}$$

$$Y=\frac{2}{\pi\sqrt{D}}K(k)\,, \tag{4.37}$$

$$D=[(4R+m^2+n^2)^2-16Rm^2]^{1/2}\,, \tag{4.38}$$

$$k^2=\frac{4R-m^2-n^2+D}{2D}\,, \tag{4.39}$$

$$\nu=\frac{4R+m^2+n^2-D}{2D}\,. \tag{4.40}$$

Finally we consider the two special cases $R=0$ and $R=1$. The $R=0$ result can be directly obtained from Eq. (4.32) by putting $R=0$. When $R=1$, from Eqs. (4.35)–(4.40) we find that

$$\langle\langle h^S\rangle_S\rangle_N=i\left[\frac{\mathrm{Re}(\alpha^2-\beta^2)}{|\alpha^2-\beta^2|}\rho_3-\frac{\mathrm{Im}(\alpha^2-\beta^2)}{|\alpha^2-\beta^2|}\rho_2\right]\,. \tag{4.41}$$

In particular, when the pair function $\Delta(z)$ is spatially constant,

$$\langle\langle h^S\rangle_S\rangle_N=\frac{1}{(\omega_n^2+\Delta^2)^{1/2}}\begin{bmatrix}i\omega_n & \Delta\\ -\Delta & -i\omega_n\end{bmatrix}\,. \tag{4.42}$$

V. DENSITY OF STATES

In this section we consider the Green's functions for real frequency $\varepsilon=\omega$ and discuss the density of states defined by

$$n_\alpha(\omega,z)\equiv\sum_l \delta(\omega-E_l)\Phi_{\alpha l}(z)\Phi^\dagger_{\alpha l}(z)$$
$$=\frac{1}{4\pi i v_{Fz}^N}\rho_3[\hat{g}_{\alpha\alpha}(\omega+i0,z)-\hat{g}_{\alpha\alpha}(\omega-i0,z)] . \quad (5.1)$$

For the real frequency $\varepsilon=\omega$, the evolution operator in the N side is given by

$$U_\pm^N=\exp\left[\pm\frac{i\omega L_N}{v_{Fz}^N}\rho_3\right]\equiv\begin{bmatrix} e^{\pm i\lambda_N/2} & \\ & e^{\mp i\lambda_N/2}\end{bmatrix} , \quad (5.2)$$

where $\lambda_N=2\omega L_N/v_{Fz}^N$. In the S side, the evolution operator is parametrized by two complex numbers γ and δ with the relation $|\gamma|^2-|\delta|^2=1$:

$$U_+^S=\begin{bmatrix}\gamma & \delta\\ \delta^* & \gamma^*\end{bmatrix} , \quad (5.3)$$

$$(U_-^S)^{-1}=[(U_+^S)^*]^{-1}=\begin{bmatrix}\gamma & -\delta^*\\ -\delta & \gamma^*\end{bmatrix} , \quad (5.4)$$

$$Q_S=\begin{bmatrix}\gamma^2-\delta^2 & -\gamma\delta^*+\gamma^*\delta\\ \gamma\delta^*-\gamma^*\delta & \gamma^{*2}-\delta^{*2}\end{bmatrix} . \quad (5.5)$$

The density of states defined above still contains rapidly oscillating phase factors. We take averages over ϕ_N and ϕ_S and show that the averaged density of states can be also expressed in terms of the complete elliptic integrals. We discuss the average in the N side and in the S side separately.

A. N-side Density of states

Let us first consider the average over ϕ_N of the density of states at the left end $z=-L_N$:

$$\langle n(\omega,-L_N)\rangle_N=\langle n_+(\omega,-L_N)\rangle_N=\langle n_-(\omega,-L_N)\rangle_N$$
$$=\frac{\rho_3}{4\pi i v_{Fz}^N}\langle h^N(\omega+i0)-h^N(\omega-i0)\rangle_N$$
$$=\frac{\rho_3}{4\pi i v_{Fz}^N}\oint\frac{dz}{2\pi i}\frac{1}{z}[h^N(\omega+i0)-h^N(\omega-i0)] , \quad (5.6)$$

where

$$h^N(\omega\pm i0)=(-i)\frac{z+A_N(\omega\pm i0)}{z-A_N(\omega\pm i0)} , \quad (5.7)$$

$$A_N=\zeta_N\tilde{A}_N , \quad (5.8)$$

$$\zeta_N=-\frac{e^{-i\phi_S}}{(1-\sqrt{R}\,q_1e^{-i\phi_S})(1-\sqrt{R}\,q_2e^{-i\phi_S})} , \quad (5.9)$$

$$\tilde{A}_N=(U_+^N)^{-1}[2\sqrt{R}\cos\phi_S-(Q_S+RQ_S^{-1})]U_-^N . \quad (5.10)$$

Let the eigenvalues of A_N be A_1 and A_2. Then we find from $|\det A_N|=1$ that

$$|A_1||A_2|=1 , \quad (5.11)$$

and

$$|A_1|=\sqrt{|\tilde{A}_1/\tilde{A}_2|},\quad |A_2|=\sqrt{|\tilde{A}_2/\tilde{A}_1|} , \quad (5.12)$$

where $\tilde{A}_1$ and $\tilde{A}_2$ are the eigenvalues of $\tilde{A}_N$.

The integral over z can be evaluated by use of the residue theorem. The density of states becomes nonzero in the following situation. When $\varepsilon=\omega-i0$, one of the eigenvalues of A_N, say A_1, is located just inside the unit circle peripheral and A_2 is just outside: At the same time, when $\varepsilon=\omega+i0$, A_1 is located just outside the unit circle peripheral and A_2 is just inside. Since A_1 and A_2 are analytic functions of ε, the above situation occurs only when $|A_1|=|A_2|=1$ at $\varepsilon=\omega$. The eigenvalues of $\tilde{A}_N$ are the roots of the second-order equation

$$x^2-\operatorname{tr}\tilde{A}_N x+\det\tilde{A}_N=0 . \quad (5.13)$$

When $\varepsilon=\omega$, one can show that Eq. (5.13) has real coefficients. For the condition $|A_1|=|A_2|=1$ or $|\tilde{A}_1|=|\tilde{A}_2|$ to hold, Eq. (5.13) should have complex conjugate roots, namely, the discriminant of Eq. (5.13) should be negative:

$$D=(\tfrac{1}{2}\operatorname{tr}\tilde{A}_N)^2-\det\tilde{A}_N<0 . \quad (5.14)$$

This is the desired condition for the averaged density of states to be nonzero. By use of the residue theorem, we obtain

$$\langle n(\omega,-L_N)\rangle_N=\pm i\frac{\rho_3}{2\pi v_{Fz}^N}\frac{\tilde{A}_N-\frac{1}{2}\operatorname{tr}\tilde{A}_N}{\sqrt{-D}} , \quad (5.15)$$

where the explicit forms of the rhs are given from Eqs. (5.5) and (5.10) by

$$\rho_3(\tilde{A}_N-\tfrac{1}{2}\operatorname{tr}\tilde{A}_N)=-i[(u\cos\phi_S-v)-w\rho_1] , \quad (5.16)$$

$$D=w^2-(u\cos\phi_S-v)^2 , \quad (5.17)$$

where ρ_1 is a Pauli matrix in particle-hole space and

$$u=2\sqrt{R}\sin\lambda_N , \quad (5.18)$$

$$v=(1+R)\sin\lambda_N\operatorname{Re}(\gamma^2-\delta^2)-(1-R)\cos\lambda_N\operatorname{Im}(\gamma^2-\delta^2) , \quad (5.19)$$

$$w=(1-R)\operatorname{Im}(2\gamma\delta^*) . \quad (5.20)$$

The sign in the rhs of Eq. (5.15) can be fixed by the following observation. From the definition Eq. (5.1), the density of states is a positive definite Hermite matrix. On the other hand, one finds that the rhs of Eq. (5.15) can be diagonalized by the orthogonal matrix

$$T=\frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\ 1 & -1\end{bmatrix} . \quad (5.21)$$

From the requirement that the n diagonalized through the transformation T should be positive definite, we finally obtain

$$\langle m^N\rangle_N \overset{\text{def}}{=} 2\pi v_{Fz}^N\, {}^tT\langle n(\omega,-L_N)\rangle_N T = \frac{\begin{bmatrix} |u\cos\phi_s - v - w| & \\ & |u\cos\phi_S - v + w| \end{bmatrix}}{[(u\cos\phi_S - v)^2 - w^2]^{1/2}} . \tag{5.22}$$

Now we take the second average over ϕ_S. The special cases $R=0$ and $R=1$ are trivial. When $R=0$, we find that

$$\langle\langle m^N\rangle_N\rangle_S = \frac{\begin{bmatrix} |v+w| & \\ & |v-w| \end{bmatrix}}{(v^2-w^2)^{1/2}} \quad \text{for } v^2-w^2>0 \tag{5.23}$$

and when $R=1$, the density of states becomes just the normal bulk form, i.e.,

$$\langle\langle m^N\rangle_N\rangle_S = 1 . \tag{5.24}$$

For general R, we should consider the integral

$$\langle\langle m^N\rangle_N\rangle_S = \frac{1}{\pi}\int_{-1}^{1} dx \frac{\begin{bmatrix} |x-\lambda_+| & \\ & |x-\lambda_-| \end{bmatrix}}{[(1-x^2)(x-\lambda_+)(x-\lambda_-)]^{1/2}} , \tag{5.25}$$

where

$$\lambda_\pm = \frac{v\pm w}{u} . \tag{5.26}$$

The integral over x can be again expressed in terms of the complete elliptic integrals of first kind and third kind, but it depends on the relative positions of $\lambda_\pm$. The details are discussed in Appendix A.

B. *S*-side density of states

Let us first consider the average over ϕ_S of the density of states at the right end $z=L_S$:

$$\langle n(\omega,L_S)\rangle_S = \langle n_+(\omega,L_S)\rangle_S = \langle n_-(\omega,L_S)\rangle_S = \frac{\rho_3}{4\pi i v_{Fz}^S}\langle h^S(\omega+i0)-h^S(\omega-i0)\rangle_S = \frac{\rho_3}{4\pi i v_{Fz}^S}\oint \frac{dz}{2\pi i}\frac{1}{z}[h^S(\omega+i0)-h^S(\omega-i0)] . \tag{5.27}$$

The same argument as in the N side yields

$$\langle m^S\rangle_S \overset{\text{def}}{=} 2\pi v_{Fz}^S\, {}^tT\langle n(\omega,L_s)\rangle_S T = \begin{cases} \dfrac{\begin{bmatrix} |I_+||2\sqrt{R}x-\Lambda_+| & \\ & |I_-||2\sqrt{R}x-\Lambda_-| \end{bmatrix}}{[I_+I_-(2\sqrt{R}x-\Lambda_+)(2\sqrt{R}x-\Lambda_-)]^{1/2}} & \text{for } D<0 , \\ 0 \quad \text{otherwise} , \end{cases} \tag{5.28}$$

where

$$D = -I_+I_-(2\sqrt{R}x-\Lambda_+)(2\sqrt{R}x-\Lambda_-) , \tag{5.29}$$

$$x = \cos\phi_N , \tag{5.30}$$

$$I_\pm = \mathrm{Im}(\gamma\pm\delta)^2 , \tag{5.31}$$

$$R_\pm = \mathrm{Re}(\gamma\pm\delta)^2 \tag{5.32}$$

and

$$\Lambda_\pm = -(1+R)\cos\lambda_N + (1-R)\sin\lambda_N \frac{R_\pm}{I_\pm} . \tag{5.33}$$

When $R=0$ and $R=1$, m no longer depends on $\cos\phi_N$. For general R, we should take the second average over ϕ_N. According to the energy $\varepsilon=\omega$, two cases occur.

Case A. $I_+I_->0$ *propagating regime.* In this case, the energy states of interest are propagating states in the S side. The average over ϕ_N takes a similar form to the second average in the N side, i.e.,

$$\langle\langle m^S\rangle_S\rangle_N = \frac{1}{\pi}\int_{-1}^{1} dx \frac{\begin{bmatrix} (|I_+/I_-|)^{1/2}|x-\lambda_+| & \\ & (|I_-/I_+|)^{1/2}|x-\lambda_-| \end{bmatrix}}{[(1-x^2)(x-\lambda_+)(x-\lambda_-)]^{1/2}} , \tag{5.34}$$

where $\lambda_\pm=\Lambda_\pm/2\sqrt{R}$. This integral can be evaluated in the same way as in the N side second average. For details, see

Appendix A.

Case B. $I_+I_-<0$ *damping regime.* In this case, the energy states of interest are damping states in the S side, but there occurs finite density of states due to the proximity effects. The average over ϕ_N, in this case, takes a form

$$\langle\langle m^S\rangle_S\rangle_N=\frac{1}{\pi}\int_{-1}^{1}dx\frac{\begin{bmatrix}(|-I_+/I_-|)^{1/2}|x-\lambda_+| & \\ & (|-I_-/I_+|)^{1/2}|x-\lambda_-|\end{bmatrix}}{[-(1-x^2)(x-\lambda_+)(x-\lambda_-)]^{1/2}}\ . \tag{5.35}$$

The integral again depends on the relative position of $\lambda_\pm$. The details are given in Appendix B.

VI. SOME APPLICATIONS

In this section, we discuss some applications of the present formulation. First, we consider a half infinite model and show that the conventional quasiclassical approach is valid in half infinite systems. Next, we discuss the R dependence of the density of states which can be observed in tunneling experiments. We discuss finally the application of the present formulation to the S-N superlattice.

A. Half infinite system ($L_S=\infty$)

We consider the Matsubara Green's function in the case where a finite width normal metal film is adsorbed on a sufficiently large width superconductor [$L_S\gg\xi_S=v_F^S/\Delta(T)$]. In this case, the order parameter depression due to the proximity effect will be confined near the interface and the pair function $\Delta(z)$ will tend to the bulk value Δ for $z\gg\xi_S$. We can expect, therefore, that the evolution operator U_+^S can be written as

$$U_+^S(0,L_S)=\begin{bmatrix}\alpha' & i\alpha''\\ i\beta'' & \beta'\end{bmatrix}=W\exp\left[\frac{\omega_n\rho_3+\Delta\rho_2}{v_{Fz}^S}L_S\right]\ , \tag{6.1}$$

where W is a finite matrix and independent of L_S. It follows that α and β will contain a divergent factor $e^{\kappa_S/2}$ [$\kappa_S=2(\omega_n^2+\Delta^2)^{1/2}L_S/v_{Fz}^S$].

Now we consider the $\langle h^N\rangle_N$ given by Eq. (4.13). Since b and c will diverge as e^{κ_S} but a is finite, we find that

$$\langle h^N\rangle_N\underset{L_S\to\infty}{\to}-i\frac{\begin{bmatrix}-b & ic\\ -ic & b\end{bmatrix}}{(b^2+c^2)^{1/2}}\ , \tag{6.2}$$

which is independent of $\cos\phi_S$ and satisfies the conventional normalization condition. We can also show that, when $L_S\to\infty$, the $\langle h^S\rangle_S$ of Eq. (4.32) becomes just the bulk form as is expected. It implies that for half infinite systems the conventional quasiclassical approach can be safely applied. In fact, Eq. (6.2) completely agrees with the result by Kieselmann[13] who treated the model within the conventional quasiclassical formalism.

B. Tunneling density of states

Here we consider the density of states at $z=-L_N$. An ideal tunneling experiment is expected to observe the density of states at the surface of the normal metal film given by

$$N(\omega)=\tfrac{1}{2}\,\mathrm{tr}\langle\langle n(\omega,-L_N)\rangle\rangle \tag{6.3}$$

with $\cos\theta_N\simeq1$ (note that the double average gives the density of states averaged over the Fermi momentum within the range $p_F^N|\cos\theta_N-1|\lesssim2\pi/L_N$). We assume for simplicity $\Delta(z)=\Delta$, though not justified, and discuss the R dependence of the density of states.

When the pair function is spatially constant, the evolution operator is given by

$$U_+^S=\exp\left[-i\frac{\omega\rho_3+i\Delta\rho_2}{v_F^S}L_S\right]$$
$$=C-i\frac{\omega\rho_3+i\Delta\rho_2}{(|\omega^2-\Delta^2|)^{1/2}}S\ , \tag{6.4}$$

where $\lambda_S=2L_S(|\omega^2-\Delta^2|)^{1/2}/v_F^S$ and

$$C=\cos(\lambda_S/2),\quad S=\sin(\lambda_S/2)\quad\text{for }\omega^2>\Delta^2\ , \tag{6.5}$$

$$C=\cosh(\lambda_S/2),\quad S=\sinh(\lambda_S/2)\quad\text{for }\omega^2<\Delta^2\ . \tag{6.6}$$

Substituting Eqs. (6.5) and (6.6) into Eq. (5.3), we obtain explicit expressions for the density of states. In Fig. 3, we plot the $N(\omega)$ for $R=0$ and 0.6. The $R=0$ case has been already discussed by Entin-Wohlman and Bar-Sagi[3] and by Gallagher.[4] We choose the sizes as $2L_N\Delta/v_F^N=5$ and $2L_S\Delta/v_F^S=2$ so that the comparison with Gallagher can be made. As can be seen in Fig. 3, the effect of finite R cannot be neglected in the finite double-layer system. In general, the finite R reduces the proximity effects and makes the density of states have more features of the normal bulk system. For instance, the de Gennes–Saint-James[5] bound state peak becomes considerably broad at finite R. It is interesting to note that as R increases there develop energy ranges in which the density of states is just equal to the normal bulk value (see Appendix A). The details of the R dependence of the compound resonance effects shall be considered elsewhere.

C. S-N superlattice

The S-N superlattice can be formulated in a similar way to that discussed in Sec. III. In particular, the Green's function for an ideal $R=0$ superlattice with lat-

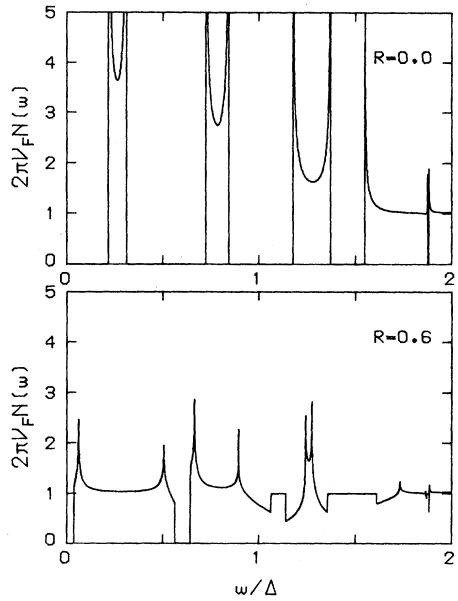

FIG. 3. The tunneling density of states at the surface of the normal layer in the case with the constant pair function Δ in the S side is plotted vs energy at $R=0.0$ and 0.6. The vertical axis is $2\pi v_F^N N(\omega)$ and the horizontal axis is ω/Δ. The layer widths are chosen as $2L_N\Delta/v_F^N=5$ and $2L_S\Delta/v_F^S=2$.

tice constants l_S and l_N is given just by that of the present $R=0$ double-layer system with $L_S=l_S/2$ and $L_N=l_N/2$. Thus the density of states with $R=0$ in Fig. 3 just gives the density of states of the normal layer at the interface of the $R=0$ superlattice with $2l_N\Delta/v_F^N=10$ and $2l_S\Delta/v_F^S=4$.

We briefly discuss this correspondence. In the superlattice, the Nambu amplitude is given by a Bloch wave type

$$\Psi(z)=\Psi_{n,k}(z)e^{ikz}\,, \tag{6.7}$$

where n is the band index and k is the Bloch wave number. When z is incremented by single period (l_S+l_N), the Nambu amplitude acquires a phase factor $\exp[ik(l_S+l_N)]$. The density of states or the quasiclassical Green's function contains a sum over the Bloch wave number k within $0<k(l_S+l_N)<2\pi$. On the other hand, the Green's function of the $R=0$ double-layer system contains a phase factor $\exp[i(\phi_s+\phi_N)]$ as can be seen from Eqs. (3.25)–(3.32). The phase average taken over ϕ_S and ϕ_N corresponds to the sum over the Bloch wave number k.

The superlattice with finite R includes a bit more complicated situations. This shall be discussed in a forthcoming paper.

VII. DISCUSSION

We have obtained a solution of the Gor'kov equation in a double-layer system with Zaĭtsev's interface[7] under a general pair function. The solution is written in terms of the evolution operator at the quasiclassical level and the parameters characterizing the boundary conditions. By decomposing the solution, we can extract the physically relevant quasiclassical Green's function which at this stage still contains the rapidly oscillating phase factors due to the quantum interference effects. We have shown that the averages over the rapidly oscillating phase factors can be explicitly performed. The averaged Green's function is characterized solely by the reflection coefficient R at the interface.

The averages can be regarded as averages over the layer sizes within the range of order $1/p_F$ or as averages over the Fermi momenta within the range of order $1/L_{N,S}$. Thus the initially assumed parallel momentum conservation condition is somehow relaxed by the averages. We expect therefore that the present formulation can be applied to a wide range of proximity-contact systems.

We have shown that the conventional normalization condition does not hold in the finite double-layer system with nonzero R. Our formulation, however, retains the advantages of the quasiclassical theory in that the evolution operator U can carry all the information on the spatial dependence of the pair function. Even in the case where the conventional quasiclassical technique can be applied, it is more easy to solve the evolution equation (2.14) with the simple initial condition Eq. (2.15) than to solve the Eilenberger equation[9] with the complicated nonlinear boundary conditions.[7,8,12–14]

Using the present formulation, we can compute the self-consistent pair function. In Fig. 1, we plot our preliminary results of the numerical calculation of the self-consistent pair potential in the case where the S side is a pure superconductor with bulk transition temperature T_c with the width $2\pi T_c L_S/v_F^S=1$, the N side is a pure metal without pairing interaction with the width $2\pi T_c L_N/v_F^N=1$ and the reflection coefficient $R=0.5$ at the interface. Details of the calculations with various applications shall be reported elsewhere.

APPENDIX A

In this appendix, we discuss the integral of the form

$$J_\pm=\frac{1}{\pi}\int_{-1}^{1}dx\frac{|x-\lambda_\pm|}{[(1-x^2)(x-\lambda_+)(x-\lambda_-)]^{1/2}}\,. \tag{A1}$$

Case I. $\lambda_+>\lambda_-$. (i) When $1<\lambda_-<\lambda_+$,

$$J_+=\frac{2/\pi}{[(\lambda_+-1)(\lambda_-+1)]^{1/2}}(\lambda_++1)\Pi\left[\frac{2}{\lambda_+-1},k\right], \tag{A2}$$

$$J_-=\frac{2/\pi}{[(\lambda_+-1)(\lambda_-+1)]^{1/2}}(\lambda_--1)\Pi\left[\frac{-2}{\lambda_-+1},k\right] \tag{A3}$$

with

$$k^2=\frac{2(\lambda_+-\lambda_-)}{(\lambda_+-1)(\lambda_-+1)}\,. \tag{A4}$$

(ii) When $-1<\lambda_-<1<\lambda_+$,

$$J_+=\frac{2/\pi}{[2(\lambda_+-\lambda_-)]^{1/2}}(\lambda_++1)\Pi\left[\frac{\lambda_-+1}{\lambda_+-\lambda_-},k\right], \quad \text{(A5)}$$

$$J_-=\frac{2/\pi}{[2(\lambda_+-\lambda_-)]^{1/2}}(1-\lambda_-)\left[\Pi\left[\frac{\lambda_-+1}{-2},k\right]-K(k)\right] \quad \text{(A6)}$$

with

$$k^2=\frac{(\lambda_+-1)(\lambda_-+1)}{2(\lambda_+-\lambda_-)}. \quad \text{(A7)}$$

(iii) When $\lambda_-<-1<1<\lambda_+$,

$$J_+=J_-=0. \quad \text{(A8)}$$

(iv) When $-1<\lambda_-<\lambda_+<1$,

$$J_+=J_-=1. \quad \text{(A9)}$$

(v) When $\lambda_-<-1<\lambda_+<1$,

$$J_+=\frac{2/\pi}{[2(\lambda_+-\lambda_-)]^{1/2}}(\lambda_++1)\times\left[\Pi\left[\frac{\lambda_+-1}{2},k\right]-K(k)\right], \quad \text{(A10)}$$

$$J_-=\frac{2/\pi}{[2(\lambda_+-\lambda_-)]^{1/2}}(1-\lambda_-)\Pi\left[\frac{1-\lambda_+}{\lambda_+-\lambda_-},k\right] \quad \text{(A11)}$$

with

$$k^2=\frac{(\lambda_+-1)(\lambda_-+1)}{2(\lambda_+-\lambda_-)}. \quad \text{(A12)}$$

(vi) When $\lambda_-<\lambda_+<-1$,

$$J_+=\frac{-2/\pi}{[(\lambda_+-1)(\lambda_-+1)]^{1/2}}(\lambda_++1)\Pi\left[\frac{2}{\lambda_+-1},k\right], \quad \text{(A13)}$$

$$J_-=\frac{-2/\pi}{[(\lambda_+-1)(\lambda_-+1)]^{1/2}}(\lambda_--1)\Pi\left[\frac{-2}{\lambda_-+1},k\right] \quad \text{(A14)}$$

with

$$k^2=\frac{2(\lambda_+-\lambda_-)}{(\lambda_+-1)(\lambda_-+1)}. \quad \text{(A15)}$$

Case II. $\lambda_+<\lambda_-$. In all the cases, J_+ is equal to the J_- in Case I with λ_+,λ_- interchanged and J_- is equal to the J_+ in Case I with λ_+,λ_- interchanged.

APPENDIX B

In this appendix, we discuss the integral of the form

$$K_\pm=\frac{1}{\pi}\int_{-1}^{1}dx\frac{|x-\lambda_\pm|}{[-(1-x^2)(x-\lambda_+)(x-\lambda_-)]^{1/2}}. \quad \text{(B1)}$$

Case I. $\lambda_+>\lambda_-$. (i) When $1<\lambda_-<\lambda_+$,

$$K_+=K_-=0. \quad \text{(B2)}$$

(ii) When $-1<\lambda_-<1<\lambda_+$,

$$K_+=\frac{2/\pi}{[2(\lambda_+-\lambda_-)]^{1/2}}(\lambda_+-1)\Pi\left[\frac{\lambda_--1}{\lambda_+-\lambda_-},k\right], \quad \text{(B3)}$$

$$K_-=\frac{2/\pi}{[2(\lambda_+-\lambda_-)]^{1/2}}(\lambda_-+1)\left[\Pi\left[\frac{\lambda_--1}{2},k\right]-K(k)\right] \quad \text{(B4)}$$

with

$$k^2=\frac{(\lambda_++1)(1-\lambda_-)}{2(\lambda_+-\lambda_-)}. \quad \text{(B5)}$$

(iii) When $\lambda_-<-1<1<\lambda_+$,

$$K_+=\frac{2/\pi}{[(\lambda_++1)(1-\lambda_-)]^{1/2}}(\lambda_+-1)\Pi\left[\frac{-2}{\lambda_++1},k\right], \quad \text{(B6)}$$

$$K_-=\frac{-2/\pi}{[(\lambda_++1)(1-\lambda_-)]^{1/2}}(\lambda_-+1)\Pi\left[\frac{-2}{1-\lambda_-},k\right] \quad \text{(B7)}$$

with

$$k^2=\frac{2(\lambda_+-\lambda_-)}{(1-\lambda_-)(\lambda_++1)}. \quad \text{(B8)}$$

(iv) When $-1<\lambda_-<\lambda_+<1$,

$$K_+=\frac{2/\pi}{[(\lambda_++1)(1-\lambda_-)]^{1/2}}(1-\lambda_+)\times\left[\Pi\left[\frac{\lambda_+-\lambda_-}{\lambda_--1},k\right]-K(k)\right], \quad \text{(B9)}$$

$$K_-=\frac{2/\pi}{[(\lambda_++1)(1-\lambda_-)]^{1/2}}(\lambda_-+1)\times\left[\Pi\left[\frac{\lambda_--\lambda_+}{\lambda_++1},k\right]-K(k)\right] \quad \text{(B10)}$$

with

$$k^2=\frac{2(\lambda_+-\lambda_-)}{(1-\lambda_-)(\lambda_++1)}. \quad \text{(B11)}$$

(v) When $\lambda_-<-1<\lambda_+<1$,

$$K_+=\frac{2/\pi}{[2(\lambda_+-\lambda_-)]^{1/2}}(1-\lambda_+)\times\left[\Pi\left[\frac{\lambda_++1}{-2},k\right]-K(k)\right], \quad \text{(B12)}$$

$$K_- = \frac{-2/\pi}{[2(\lambda_+ - \lambda_-)]^{1/2}}(\lambda_- + 1)\Pi\left[\frac{\lambda_+ + 1}{\lambda_- - \lambda_+}, k\right] \quad \text{(B13)}$$

with

$$k^2 = \frac{(\lambda_+ + 1)(1 - \lambda_-)}{2(\lambda_+ - \lambda_-)} . \quad \text{(B14)}$$

(vi) When $\lambda_- < \lambda_+ < -1$,

$$K_+ = K_- = 0 . \quad \text{(B15)}$$

Case II. $\lambda_+ < \lambda_-$. In all the cases, K_+ is equal to the K_- in Case I with λ_+, λ_- interchanged and K_- is equal to the K_+ in Case I with λ_+, λ_- interchanged.

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