Second-quantization description of Andreev reflection and the relation to quasiparticle wave approaches

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A second-quantization description is given for Andreev reflection. We introduce an effective interaction Hamiltonian for the interface between the superconductor and. the normal metal, which enables us to treat transmission and reflection consistently. The interaction Hamiltonian couples quasiparticles in the normal region (N) and Bogoliubov quasiparticles in the superconducting region (S). It facilitates the description of the elementary excitations of the SN-coupled system, that are generated by Andreev reflections. Moreover, it naturally brings us to the description where the effect of macroscopic quantum fluctuations of the superconducting state on Andreev reflections is considered. This provides a powerful tool for investigating of the mesoscopic aspects of Andreev reflection.

I. INTRODUCTION

In superconductor —normal-metal (SN) coupled systems, Andreev reflection,¹ which occurs at the SN interface, plays the most important role in determining the electronic properties of the system. Analyses of this effect, however, have been done in the wave equation description,²⁻⁴ by using the Bogoliubov-de Genne equation²⁻⁴ and by ignoring the effect of quantum fluctuations of the macroscopic phase of the superconducting state on the quasiparticles. In such a treatment, Andreev reflection is seen as a result of a boundary condition for the waves across the SN interface.

The most interesting aspect of Andreev reflection is the interaction between the microscopic quasiparticles and the macroscopic phase of the superconducting state. For example, Kümmel analyzed the effect of Andreev reflection on the superconducting state and derived the phase-shift of the superconducting order parameter induced by Andreev reflected quasiparticles (see also Refs. 3 and 4).

Ignoring the quantum fluctuation of the macroscopic phase in the solutions of their wave equations was very reasonable because usually the superconducting region is big enough to ignore. However, the quantum fluctuation has become more important in light of mesoscopic physics. Wave equation approaches, which ignore the fluctuation, are becoming inadequate for analyzing some quantum-mechanical phenomena at the SN interface, e.g., the effect of a very small superconducting electrod or the effect of dissipation in our recently proposed quasiparticle interferometer.

In this paper, we formulate Andreev reflection in a second quantization manner. This enables us to treat the phase shift caused by Andreev reflection as an operator that presents quantum fluctuations of the superconducting state. It also shows clearly that Andreev reflection is the manifestation of the virtual transfer of quasiparticles through the interface. The paper is organized into sections. Section II shows our "wave-bundle approximation" used to treat the electron transfer through a barrier as a linear coupler. In Sec. III, we briefly explain macroscopic quantum fluctuations in superconducting states and define operators that express the fluctuations. Section IV is the heart of our paper, where we formulate Andreev reflection in a second quantization manner both for the excitation energy above the superconducting gap and for that within the gap. The results of this formulation are discussed in Sec. V. Section VI is the conclusion and offers some future perspectives for our results.

II.BARRIER AS ^A LINEAR COUPLER

For simplicity, we limit our analysis to a onedimensional, i.e., single-mode, case. Our theory can easily be expanded to higher dimensionality. In conventional transfer-Hamiltonian treatment of the tunneling barrier problem, the whole Hamiltonian is given by

$$
\mathcal{H} = \mathcal{H}_L + \mathcal{H}_R + \mathcal{H}_T , \qquad (1)
$$

where \mathcal{H}_L , \mathcal{H}_R are the unperturbed left and right electrode Hamiltonians, and \mathcal{H}_T is

$$
\sum_{\substack{k,q\\= \uparrow, \downarrow}} (a_{Rk\sigma}^{\dagger} a_{Lg\sigma} + \text{H.c.}) .
$$
 (2)

Since the unperturbed states, created by a_{Lk}^{\dagger} and a_{Rq}^{\dagger} are localized in the left and right electrodes, neither state has momentum. Therefore, the eigenstates of H , obtained as the superposition of the unperturbed states relative to the transfer Hamiltonian, do not propagate either. This means that conventional treatment cannot provide a consistent description of both transmission and reflection.

Here, we propose a Hamiltonian to treat the barrier problem, $H = H_L + H_R + H_{int}$, with

$$
\mathcal{H}_L = \sum_{\substack{k \\ \sigma = \uparrow, \downarrow}} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma}, \quad \mathcal{H}_R = \sum_{\substack{q \\ \sigma = \uparrow, \downarrow}} \varepsilon_q d_{q\sigma}^\dagger d_{q\sigma}, \tag{3}
$$

and

 \boldsymbol{o}

$$
\mathcal{H}_{int} = \sum_{\substack{k,q \ \sigma = \uparrow, \downarrow}} t(c_{k\sigma}^{\dagger} d_{q\sigma} + \text{H.c.})
$$
\n
$$
+ \sum_{\substack{k>0 \ \sigma = \uparrow, \downarrow}} r(c_{-k\sigma}^{\dagger} c_{k\sigma} + \text{H.c.})
$$
\n
$$
+ \sum_{\substack{q>0 \ q>0}} r(d_{-q\sigma}^{\dagger} d_{q\sigma} + \text{H.c.}). \tag{4}
$$

As shown in Fig. 1, the operators $c_{k\sigma}^{\dagger}$ and $d_{q\sigma}^{\dagger}$ create trav-
eling waves with excitation energies $\varepsilon_k = \hbar^2 k^2 / 2m - \mu_I$ and $\varepsilon_q = \hbar^2 q^2 / 2m - \mu_R$ and spin σ , where m is the electron's effective mass, and μ_L and μ_R are the chemical potentials in the left and right electrodes. As pointed out by Bardeen,⁷ the eigenstates of \mathcal{H}_L and \mathcal{H}_R are not exactly orthogonal. However, we ignore this fact because it is not important in the following discussion.

Because the electrode states on both sides extend semiinfinitely, the energy levels are continuous. This makes analysis difficult. Suppose a wave bundle, having an excitation energy around ε_k and energy width $\Delta \varepsilon$, comes from the left-hand side. We identify the operator annihilating this wave bundle as $C_{k,\sigma}$, and similarly the operators $C_{-k\sigma}$, $D_{q\sigma}$, and $D_{-q\sigma}$. This situation is illustrate in Fig. 2. In addition, we take the summation only for $k = q$ in the first term of Eq. (4) when considering the coupling between these wave bundles. This invokes no serious error. The interaction energies between the wave bundles are

$$
t_0 = \Delta \varepsilon N(0)ta, \quad r_0 = \Delta \varepsilon N(0)ra \quad , \tag{5}
$$

where $N(0)$ is the density of states per unit length of the electrode and a is the length of the electrodes. Having this length value is significant because, when only a barrier is given, we cannot determine the absolute value of the coupling energy t or r . For example, consider a barrier sandwiched by two quantum wells each with the length a . We can estimate the coupling energy t by calculating the energy splitting between the bonding and antibonding states. The resulting t value is inversely proportional to a. Namely, the determination of the coupling energy requires information about not only the barrier but also the states on both sides of it. A barrier itself always gives the value of ta. Although the physical meaning of the length a is unclear in cases where the states on both sides extend semi-infinitely, it is natural to think that ta and ra are physical entities rather than t and r .

FIG. 1. Representation of the barrier problem. Forward and backward waves are considered in order to consistently treat transmission and reflection.

FIG. 2. Coupling between four wave-bundle states across the tunneling barrier.

The Heisenberg equation of motion for the operators, $C_{k\sigma}$, $C_{-k\sigma}$, $D_{q\sigma}$, $D_{-q\sigma}$, is given by

$$
i\hbar \begin{bmatrix} \dot{C}_{k\sigma}(\tau) \\ \dot{C}_{-k\sigma}(\tau) \\ \dot{D}_{q\sigma}(\tau) \\ \dot{D}_{-q\sigma}(\tau) \end{bmatrix} = \delta_{kq} \begin{bmatrix} 0 & r_0 & t_0 & 0 \\ r_0 & 0 & 0 & t_0 \\ t_0 & 0 & 0 & r_0 \\ 0 & t_0 & r_0 & 0 \end{bmatrix} \begin{bmatrix} C_{k\sigma}(\tau) \\ C_{-k\sigma}(\tau) \\ D_{q\sigma}(\tau) \\ D_{-q\sigma}(\tau) \end{bmatrix}, \quad (6)
$$

where the overdot means $\partial/\partial \tau$. Equation (6) expresses of the barrier as a linear coupler.

By solving this equation under the initial condition

$$
C_{k\sigma}(0) = 1, \quad C_{-k\sigma}(0) = D_{q\sigma}(0) = D_{-q\sigma}(0) = 0 \tag{7}
$$

we get the time evolution of these operators as follows:

$$
C_{k\sigma}(\tau) = \cos(t_0 \tau/\hbar) \cos(r_0 \tau/\hbar) ,
$$

\n
$$
C_{-k\sigma}(\tau) = \cos(t_0 \tau/\hbar) \sin(r_0 \tau/\hbar) ,
$$

\n
$$
D_{q\sigma}(\tau) = \sin(t_0 \tau/\hbar) \cos(r_0 \tau/\hbar) ,
$$

\n
$$
D_{-q\sigma}(\tau) = \sin(t_0 \tau/\hbar) \sin(r_0 \tau/\hbar) .
$$
\n(8)

The interaction time τ_{int} is estimated as

$$
\tau_{\rm int} = \frac{\pi \hbar}{\Delta \varepsilon} \tag{9}
$$

based on the uncertainty relation. The small argument approximation for Eq. (8) gives the transmission probabil-

ity T and the reflection probability R as
\n
$$
T = (t_0 \tau_{int} / \hbar)^2 = \pi^2 N(0)^2 a^2 t^2,
$$
\n
$$
R = (r_0 \tau_{int} / \hbar)^2 = \pi^2 N(0)^2 a^2 r^2.
$$
\n(10)

The probability conservation law,

$$
T + R = \pi^2 N(0)^2 a^2 (t^2 + r^2) = 1 , \qquad (11)
$$

must be satisfied. These results consistently fall directly between ordinary time-dependent perturbation treatment and Landauer's formula.⁸ In the following sections, we will use this wave-bundle approximation.

III. PSEUDO-SPIN REPRESENTATION OF SUPERCONDUCTING STATES AND MACROSCOPIC QUANTUM FLUCTUATIONS

When the right-side electrode is superconducting, the Hamiltonian of the electrode becomes the so-called reduced Bardeen-Cooper-Schrieffer (BCS) Hamiltonian:⁹

$$
\mathcal{H}_R = \sum_{\substack{q \\ \sigma = \uparrow, \downarrow}} \varepsilon_q d_{q\sigma}^{\dagger} d_{q\sigma} - \frac{1}{2} V \sum_{\substack{q, q', p \\ \sigma, \sigma' = \uparrow, \downarrow}} d_{q+p\sigma}^{\dagger} d_{q'-p\sigma'} d_{q'\sigma'}^{\dagger} d_{q\sigma}.
$$
\n(12)

One of the most convenient ways to treat superconducting states is using pseudospin representation, which also enables us to consider macroscopic quantum fluctuations of superconducting states.

A. Pseudospin for superconducting states

Anderson introduced the pseudo-spin treatment of the superconducting ground state of the BCS-reduced Hamiltonian.¹⁰ Consider pseudospins given by

$$
s_{kz} = \frac{1}{2} (1 - d_k^{\dagger} d_k - d_{-k}^{\dagger} d_{-k}),
$$

\n
$$
s_k^- = d_k^{\dagger} d_{-k}^{\dagger}, \quad s_k^+ = d_{-k} d_k,
$$
\n(13)

where, d_k^{\dagger} (d_k) is the creation (annihilation) operator of a single electron in the state k . k includes the electron spin indices that k has up spin and $-k$ has down spin. This follows the commutation relations

$$
[s_k^+, s_{k'}^-] = 2s_{kz} \delta_{kk'}, \qquad (14a)
$$

$$
[s_{kz}, s_{k'}^{\pm}] = \pm s_k^{\pm} \delta_{kk'}, \qquad (14b)
$$

$$
\{s_k^+, s_k^- \} = 1 \tag{14c}
$$

Using these operators, macroscopic operators for a superconducting state are obtained by

$$
S^{-} = \sum_{k} s_{k}^{+}, \quad S^{+} = \sum_{k} s_{k}^{-}, \quad S_{z} = -\sum_{k} s_{k z} . \quad (15)
$$

These operators satisfy the angular-momentum commutation relations:¹¹

$$
[S_z, S^{\pm}] = \pm S^{\pm} \tag{16a}
$$

$$
[S^+, S^-] = 2S_z \tag{16b}
$$

The square of the total angular-momentum operator

$$
S_{\text{tot}}^2 = \frac{1}{2}(S^+S^- + S^-S^+) + S_z^2 \tag{17}
$$

has the eigenvalue $J(J+1)$. Angular momentum, i.e., a superconducting state, is characterized by this J and the eigenvalue m of S_z , where

$$
-J \leq m \leq J \tag{18}
$$

The total angular momentum J corresponds to the number of the states that Cooper pairs can occupy; therefore,

$$
J \simeq N(0) a \hbar \omega_D , \qquad (19)
$$

where ω_D is the Debye frequency. This value J can be regarded as a constant in the following discussion. The value m means the number of the condensed Cooper pairs, whose "mean" value is determined by the (reduced) BCS Hamiltonian, that is, by the parameters, the electron energy ε_k of the state k, and the attractive interaction V .¹² By introducing the eigenstates $|m \rangle$ of S_z , relations

$$
S_z|m\rangle = m|m\rangle , \qquad (20a)
$$

$$
S^{\pm}|m\rangle = \sqrt{(J\mp m)(J\pm m+1)}|m\pm 1\rangle \qquad (20b)
$$

are obtained. In the case of a superconducting state because $m \ll J$ even at absolute zero temperature, Eq. (20b) becomes

$$
S^{\pm}|m\rangle = J|m\pm 1\rangle . \qquad (21)
$$

Now we have $S^+S^- = S^+S^- = J^2$; therefore, we can define operators

$$
S^{\dagger} = \frac{1}{J} S^{\dagger} = \exp[-i\hat{\phi}], \qquad (22a)
$$

(13)
$$
S = \frac{1}{J}S^{-} = \exp[i\hat{\phi}].
$$
 (22b)

It should be noted that the phase $\hat{\phi}$ is an operator, not a c number. S^{\dagger} adds exactly one Cooper pair to the superconducting electrode, and S annihilates one without causing any change in the quasiparticle occupancies.

B. BCS ground states

As described above, the BCS Hamiltonian determines the mean value of S_z and ϕ , except for the arbitrariness of the origin of the phase ϕ . In the so-called BCS ground state⁹

(15)
$$
\Phi_0 = \Pi_k (u_k + v_k e^{i\hat{\phi}} d_k^{\dagger} d_{-k}^{\dagger}) |0\rangle ,
$$
 (23)

 u_k , v_k , and ϕ are merely the mean values. From the quantum-mechanical viewpoint in the preceding section, they are operators that have quantum fiuctuations. In fact, u_k and v_k can be represented by a pseudospin operator such as

$$
u_k = \cos\frac{1}{2}\hat{\theta}_k \tag{24a}
$$

$$
v_k = \sin\frac{1}{2}\hat{\theta}_k \tag{24b}
$$

where

$$
\cos \theta_k = s_{kz} \tag{24c}
$$

Without the restriction by the BCS Hamiltonian, state Eq. (23) can cover from the phase-definite state to the number-definite state.

The so-called BCS state is the state where u_k , v_k , and ϕ are regarded as c numbers having the mean values given by the Harniltonian. It should be noted that the BCS state is not the phase-definite state.

These kinds of discussions on the macroscopic quantum-mechanical aspects cannot be carried out by conventional wave equation treatments using the Bogoliubov-de Gennes equations because they regard the above operators as c numbers in the light of the mean-field approximation.

C. Phase-number uncertainty

Let us make a real "phase-definite state" and a Let us make a real "phase-definite state" and a
"number-definite state." The number-definite state is the "number-definite state." The number-definite state is the eigenstate of S_z , that is, $|m \rangle$. Under the approximation eigenstate of S_z , that is, $|m \rangle$. Under the approximation $J \gg 1$, a phase-definite state $|\phi \rangle$ is given in terms of $|m \rangle$ as

$$
|\phi\rangle = \frac{1}{A} \sum_{m=-J}^{J} \exp[i\phi m]|m\rangle , \qquad (25)
$$

where

$$
\phi = \frac{n\pi}{2(J+1)} \tag{26}
$$

and Λ is a normalization constant and n is an integer. Because $J \gg 1$, ϕ is effectively a continuous number. From Eq. (25), we obtain

$$
S|\phi\rangle = \exp[i\phi]| \phi\rangle . \tag{27}
$$

Therefore we can express the operator S as

$$
S = \sum_{\phi} |\phi \rangle e^{i\phi} \langle \phi | \ . \tag{28}
$$

Contrarily, the number-definite state is expressed in terms of the phase-definite states $|\phi\rangle$ as

$$
|m\rangle = \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} \exp[-i\phi m] |\phi\rangle d\phi . \qquad (29)
$$

To reproduce the commutation rule expressed by Eq. (16a), we require that

$$
[\hat{\phi}, S_z] = i \tag{30}
$$

This gives an uncertain relation between the phase ϕ and $\cos\hat{\theta}_k =$
the Cooper-pair number N, resulting

$$
\delta \phi \delta N \ge \frac{1}{2} \tag{31}
$$

For the BCS states at the absolute-zero temperature, δN is on the order of $\sqrt{N(0)a\Delta_0\pi}$, where Δ_0 is the mean value of the superconducting order parameter. In the case of a small metal particle (1- μ m radius), $\delta N \sim 10^5$. This value is large enough to ignore the quantum fluctuation of the phase. However, near the superconducting critical temperature, δN becomes so small that the phase fluctuations cannot be neglected. Suppose another case, where superconductivity is induced in a degenerated semiconductor island by the proximity effect. In this case, $\delta N \sim 10^3$ and the phase fluctuations become significant. Moreover, in the case of a superconductor —normal metal —coupled system, because the small capacitance at the interface strongly suppresses the charge transfer through the interface, i.e., the fluctua tions of the number, the phase fluctuation is emphasized.

D. Elementary excitations of quasiparticles

From the preceding preparations, the quasiparticle excitations from the superconducting ground state can easi1y be written down. Electronlike Bogoliubov quasiparticles are given by

$$
\gamma_{k\uparrow} = u_k d_{k\uparrow} - v_k d_{-k\downarrow}^{\dagger} S \tag{32a}
$$

$$
\gamma_{-k\downarrow} = u_k d_{k\downarrow} + v_k d_{-k\uparrow}^{\dagger} S \tag{32b}
$$

where v_k , v_k , and S are the operators defined by Eqs. $(24a)$, $(24b)$, and $(22b)$.¹³ They are operators which act in the Cooper-pair subspace. Therefore, the elementary excitations has not only microscopic operators but also macroscopic operators, and change the quasiparticle state and the superconducting state at the same time.

Because $u_k^2 + v_k^2 = 1$ is always satisfied, the excitation Eqs. (32a) and (32b) annihilate the exact charge e. Therefore, they are gauge invariant.

Similarly to the mean-field approximation, H_R can be diagonalized with these operators of Bogoliubovquasiparticles, but not those of pure electrons or holes. In order to satisfy the charge conservation requirement, we distinguished between an electronlike Bogoliubov quasiparticle and a holelike Bogoliubov quasiparticle. This leads to

$$
\mathcal{H}_R = \sum_q E_q (\gamma_{q\uparrow}^\dagger \gamma_{q\uparrow} + \gamma_{q\downarrow}^\dagger \gamma_{q\downarrow}) + W_0 , \qquad (33)
$$

where W_0 is a constant energy shift.

Here we discuss quantum fluctuations of u_k and v_k for the BCS state. For the BCS state, $\hat{\theta}_k$ in Eqs. (24a) and $(24b)$ is given by¹²

$$
\sin \hat{\theta}_k = \frac{\Delta}{\sqrt{\Delta^2 + \epsilon_k^2}} \tag{34a}
$$

$$
\cos\hat{\theta}_k = \frac{\varepsilon_k}{\sqrt{\Delta^2 + \varepsilon_k^2}} \tag{34b}
$$

where Δ is the superconducting order parameter. Therefore, quantum fluctuations of u_k and v_k come from the quantum fluctuation $\delta\Delta$ of Δ . From Eqs. (34a) and (34b) the quantum fluctuations of u_k and v_k are on the order of

$$
\frac{\varepsilon_k \delta \Delta}{\Delta_0^2} \quad (\varepsilon_k \ll \Delta_0) \tag{35a}
$$

$$
\frac{\delta \Delta}{\Delta_0} \quad (\varepsilon_k \sim \Delta_0) \tag{35b}
$$

$$
\frac{\Delta_0 \delta \Delta}{\epsilon_k^2} \quad (\epsilon_k \gg \Delta_0) \tag{35c}
$$

where Δ_0 is the BCS mean value of Δ . Equations (35a), (35b), and (35c) show that in the cases of $\varepsilon_k < \Delta_0$ and $\varepsilon_k >> \Delta_0$, the quantum fluctuations are negligible, and the fluctuation has its maximum value when $\varepsilon_k \sim \Delta_0$. In the pseudospin treatment, because the superconducting order parameter Δ is given by

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$$
\Delta = \frac{1}{2} V \sum_{k'} \sin \theta_{k'} , \qquad (3)
$$

we obtain

$$
\delta \Delta \sim \text{VN}(0) a \hbar \omega_D \delta \phi \tag{37}
$$

On the other hand, the mean-field theory gives the mean value Δ_0 as

$$
\Delta_0 = \frac{\hbar \omega_D}{\sinh(1/VN(0)a)} \tag{38}
$$

As the result,

$$
\frac{\delta \Delta}{\Delta_0} \sim VN(0)a \sinh\left(\frac{1}{VN(0)a}\right)\delta\phi . \tag{39}
$$

From Eq. (31), $\delta\phi$ is on the order of $1/\sqrt{N(0)a\Delta_0}$, so

 E_q . (39) becomes

$$
V\sqrt{N(0)a/\hbar\omega_D}\sinh^{3/2}\left(\frac{1}{VN(0)a}\right). \tag{40}
$$

This shows the natural fact that when $VN(0)a$ gets small, the quantum fluctuation of the superconductivity becomes large and the superconductivity breaks. However, when $VN(0)a$ becomes large, fluctuations of u_k, v_k become negligible more rapidly than those of the macroscopic phase ϕ .

Therefore, we hereafter regard u_k, v_k as c numbers, and S, S^{\dagger} as operators.

IV. SECOND QUANTIZATION FORMULATION OF ANDREEV REFLECTION

Bogoliubov transformation of Eqs. (32a) and (32b) transforms the interaction Hamiltonian into

$$
\mathcal{H}_{int} = t \sum_{\substack{k,q \\ \sigma = \uparrow, \downarrow}} (a_q c_{k\sigma}^\dagger \gamma_{q\sigma} + \text{H.c.}) + t \sum_{k,q} (v_q^* S^\dagger c_{-k\downarrow} \gamma_{q\uparrow} + \text{H.c.}) - t \sum_{k,q} (v_q^* S^\dagger c_{-k\uparrow} \gamma_{q\downarrow} + \text{H.c.})
$$
\n
$$
+ r \sum_{\substack{k > 0 \\ \sigma = \uparrow, \downarrow}} (c_{-k\sigma}^\dagger c_{k\sigma} + \text{H.c.}) + r \sum_{\substack{q > 0 \\ \sigma = \uparrow, \downarrow}} (|u_q|^2 - |v_q|^2) (\gamma_{-q\sigma}^\dagger \gamma_{q\sigma} + \text{H.c.}) + 2r \sum_{q} (u_q v_q S \gamma_{q\uparrow}^\dagger \gamma_{q\downarrow}^\dagger + \text{H.c.}) \,. \tag{41}
$$

A. Above the superconducting gap

In order to apply our wave-bundle approximation to the superconducting electrode, we must introduce the operator

$$
\Gamma_{q\sigma} = \sum_{\varepsilon_q - \Delta\varepsilon/2 < E_p < \varepsilon_q + \Delta\varepsilon/2} \frac{\gamma_{\rho\sigma}}{\sqrt{\Delta\varepsilon N(0)a}} \tag{42}
$$

For $E_q \gg |\Delta|$, $\Gamma_{q\sigma} \simeq \gamma_{q\sigma}$. However, generally it is given that $\{\Gamma_{q1\sigma1}, \Gamma_{q2\sigma2}^{\dagger}\} = \delta_{q1q2} \delta_{\sigma1\sigma2} N_s (E_q) / N(0)$, where $N_s(E_p)=N(0)/(u_p^2-v_p^2)$. Therefore, $\Gamma_{q\sigma}$ is not a real Fermion operator but a pseudo-Fermion one. In terms of these operators, \mathcal{H}_{int} is expressed as

$$
\mathcal{H}_{int} = t_0 \sum_{\substack{k=q \ p=1,1}} (u_q C_{k\sigma}^{\dagger} \Gamma_{q\sigma} + \text{H.c.}) + t_0 \sum_{k=q} (v_q^* S^{\dagger} C_{-k\downarrow} \Gamma_{q\uparrow} + \text{H.c.}) - t_0 \sum_{k=q} (v_q^* S^{\dagger} C_{-k\uparrow} \Gamma_{q\downarrow} + \text{H.c.})
$$
\n
$$
+ r_0 \sum_{\substack{k>0 \\ \sigma = \uparrow,1}} (C_{-k\sigma}^{\dagger} C_{k\sigma} + \text{H.c.}) + r_0 \sum_{\substack{q>0 \\ \sigma = \uparrow,1}} (|u_q|^2 - |v_q|^2) (\Gamma_{-q\sigma}^{\dagger} \Gamma_{q\sigma} + \text{H.c.}) + 2r_0 \sum_{q} (u_q v_q S \Gamma_{q\uparrow}^{\dagger} \Gamma_{q\downarrow}^{\dagger} + \text{H.c.}), \qquad (43)
$$

where $\sum_{k=q}$ represents the summation of the states in which $\varepsilon_k = E_q$. Consequently, the Heisenberg equation of motion for a set of operators, $C_{k\uparrow}$, $C_{-k\uparrow}$, $C_{k\downarrow}^{\dagger}$, $C_{-k\downarrow}^{\dagger}$, $\Gamma_{q\uparrow}$, $\Gamma_{-q\uparrow}$, $\Gamma_{q\downarrow}^{\dagger}$, $\Gamma_{-q\downarrow}^{\dagger}$, is [see Eq. (44)]

under the approximation that E_q , ε_q , and $|\Delta|$ are negligible compared to μ_R

The elementary excited states are obtained by solving Eq. (44) as an eigenvalue equation. Here we will show some important elementary excited states. First, let us consider a case of perfect transmission (i.e., there is no normal reflection at the interface). When $r = 0$, we can choose a smaller set of the linearly independent operators, $C_{k\uparrow}$, $C_{-k\downarrow}^{\dagger}$, $\Gamma_{q\uparrow}$, $\Gamma_{-q\downarrow}^{\dagger}$. The operators for elementary excitations are given by

$$
\alpha_{k1\pm} = \frac{1}{\sqrt{F}} (u_q C_{k\uparrow} + v_q SC_{-k\downarrow}^{\dagger} \pm \Gamma_{q\uparrow}) , \qquad (45)
$$

$$
\alpha_{k2\pm} = \frac{1}{\sqrt{F}} (v_q^* S^{\dagger} C_{k\uparrow} - u_q^* C^{\dagger}_{-k\downarrow} \pm \Gamma^{\dagger}_{-q\downarrow}) \,, \tag{46}
$$

where $F=1+[\text{Re}(\sqrt{u_a^2-v_a^2})]^2$. Therefore, $F=2$ when where $F = 1 + [Re(\nabla u_q^2 - v_q^2)]^2$. Therefore, $F = 2$ where $\varepsilon_k >> |\Delta|$. α_{k1} corresponds to the processes in which an electron comes in, a hole is Andreev reflected, and the hole goes out. α_{k2} corresponds to those in which a hole comes in and an electron goes out.

As described above, since the operator S is nearly a c number $e^{i\phi}$ for the negligible phase fluctuation of the superconductor, Eqs. (45) and (46) reproduce the phenomenon in which an Andreev-reflected particle is phase-shifted by the macroscopic phase of the superconductor ϕ . If the superconductor is not in a phase-definite state, S causes the side effect of Andreev reflection on the superconductor and changes from a c number into a q number.

When normal reflection occurs at the barrier, the explicit expressions of the solutions for elementary excited states are a little complicated. Here, we restrict ourselves to commenting on the important characters of the obtained elementary excited states. The quantummechanical character is the same as in the previous normal reflection-free case. Every excitation consists of the linear combination of the eight operators in Eq. (21). When the probabilities for transmission and reflection are calculated as described in Sec. II, they are the same as those obtained by conventional calculations.

B. Within the superconducting gap

When the excitation energy ε_k is smaller than the superconducting gap energy $|\Delta|$, the density of states in the superconductor vanishes. This is quite important for Andreev reflection because an incident quasiparticle (electron or hole) must be either normally reflected or Andreev reflected at the interface and is never transferred into the superconducting region. If one extrapolates the above formulation to include the region in which E_q is above formulation to include the region in which E_q is
within the superconducting gap $(E_q < |\Delta|)$, q becomes a complex number. Formally, Γ_q^{\dagger} creates an evanescent wave that exponentially decays into the superconductor. This appears in the conventional approach. In the second-quantization description, however, evanescer waves are not physical entities. Therefore, the wave bundle approximation is no longer applicable to the superconducting electrode.

Here, we show a different approach appropriate in the situation. In the superconducting gap, all Bogoliubovquasiparticle excitations in the superconductor are virtual. These virtual Bogoliubov-quasiparticle excitations are the true character of the evanescent Bogoliubovquasiparticles that appear in the wave equation approach. As shown in Fig. 3, there are two types of processes for taking these virtual excitations into account as intermediate states. One is the process by which an electronlike Bogoliubov quasiparticle is excited and then annihilated. In the other, an electron like Bogoliubov quasiparticle is excited, but a holelike Bogoliubov quasiparticle is annihilated. In the latter case, one Cooper pair is created in the superconducting electrode.

We can renormalize these virtual excitations by unitary transformation. The unitarily transformed whole Hamiltonian is given by

$$
\mathcal{H}' = \mathcal{H}_L + \mathcal{H}_{int} \tag{47}
$$

Here

$$
\mathcal{H}'_{int} = -\frac{1}{4}t^2 \sum_{E_q > \Delta} \sum_{k_1, k_2 > 0, \sigma} \left[\frac{1}{E_q - \varepsilon_{k_1}} + \frac{1}{E_q - \varepsilon_{k_2}} \right] (|u_q|^2 - |v_q|^2) (c_{k_1\sigma}^\dagger c_{k_2\sigma} + c_{k_1\sigma}^\dagger c_{k_2\sigma})
$$
\n
$$
+ \frac{1}{2}t^2 \sum_{E_q > \Delta} \sum_{k_1, k_2 > 0} u_q v_q \left[\frac{1}{E_q - \varepsilon_{k_1}} + \frac{1}{E_q - \varepsilon_{k_2}} \right] [S^\dagger (c_{k_1\uparrow} c_{k_2\downarrow} + c_{k_1\uparrow} c_{k_2\downarrow}) + \text{H.c.}]
$$
\n
$$
+ \sum_{\substack{k > 0 \\ \sigma = 1, \downarrow}} r (c_{-k\sigma}^\dagger c_{k\sigma} + \text{H.c.}) . \tag{48}
$$

The first term in Eq. (48) represents the self-energy correction to the electron energies in the normal region. It results in a change in the electron density of states at the edge of the superconducting gap. Nevertheless, we ignore the infiuence of this term because it is not significant in light of our wave-bundle approximation. The second term in the equation represents Andreev reflection itself.

Applying the wave-bundle approximation in ways similar to the above analysis, we get the interaction Hamiltonian for wave bundles in the normal region:

$$
\mathcal{H}'_{\text{int}} = -\frac{1}{2}t_1^2 \sum_{k,\sigma} X C_{k\sigma}^{\dagger} C_{k\sigma} + t_1^2 \sum_{k>0} Y \left[S^{\dagger} (C_{k\uparrow} C_{-k\downarrow} + C_{-k\uparrow} C_{k\downarrow}) + \text{H.c.} \right] + r_0 \sum_{\substack{k>0 \ \sigma = \uparrow, \downarrow}} (C^{\dagger}_{-k\sigma} C_{k\sigma} + \text{H.c.}), \tag{49}
$$

where

$$
X = \int_{\Delta}^{\infty} \frac{|u_q|^2 - |v_q|^2}{E_q - \varepsilon_k} N_s(E_q) dE_q = -\frac{N(0)}{2} \ln(\Delta - \varepsilon_k) + \text{const.}
$$
\n(50)

and

$$
Y = \int_{\Delta}^{\infty} \frac{u_q v_q^*}{E_q - \varepsilon_k} N_s(E_q) dE_q = \frac{\Delta N(0)}{\sqrt{\Delta^2 - \varepsilon_k^2}} \arccos \left(\frac{\Delta - \varepsilon_k}{2\Delta} \right)^{1/2}, \qquad (51)
$$

and

$$
t_1 = [\Delta \varepsilon N(0)a]^{1/2}t \tag{52}
$$

Guinea and Schön gave a Hamiltonian similar to Eq. (49) by phenomenological intuition.¹⁴ We derived the Hamiltonian microscopically and determined the dependences of the coefficients on the energy.

We can get the elementary excitations by solving the eigenstates for the Heisenberg equation of motion for a set of operators, obtained from Eq. (49}:

$$
i\hbar \begin{bmatrix} \dot{C}_{k\uparrow}(\tau) \\ \dot{C}_{-k\uparrow}(\tau) \\ \dot{C}_{-k\downarrow}^{\dagger}(\tau) \\ \dot{C}_{k\downarrow}^{\dagger}(\tau) \end{bmatrix} = \begin{bmatrix} 0 & r_{0} & -t_{1}^{2}YS & 0 \\ r_{0} & 0 & 0 & -t_{1}^{2}YS \\ -t_{1}^{2}YS^{\dagger} & 0 & 0 & -r_{0} \\ 0 & -t_{1}^{2}YS^{\dagger} & -r_{0} & 0 \end{bmatrix} \begin{bmatrix} C_{k\uparrow}(\tau) \\ C_{-k\uparrow}(\tau) \\ C_{-k\downarrow}^{\dagger}(\tau) \\ C_{k\downarrow}^{\dagger}(\tau) \end{bmatrix} . \tag{53}
$$

For example,

FIG. 3. Two renormalizing processes of Bogoliubovquasiparticle virtual excitation. One gives the renormalization for the one-body electron energies. The other gives the Andreev reflection.

$$
\beta_{k1} = \frac{1}{\sqrt{2}} \left[C_{k\uparrow} - \frac{r}{\sqrt{t^4 Y^2 + r^2}} C_{-k\uparrow} + \frac{t^2 Y}{\sqrt{t^4 Y^2 + r^2}} S C_{-k\downarrow}^{\dagger} \right],
$$

\n
$$
\beta_{k2} = \frac{1}{\sqrt{2}} \left[C_{-k\uparrow} - \frac{r}{\sqrt{t^4 Y^2 + r^2}} C_{k\uparrow} + \frac{t^2 Y}{\sqrt{t^4 Y^2 + r^2}} S C_{k\downarrow}^{\dagger} \right],
$$

\n
$$
\beta_{k3} = \frac{1}{\sqrt{2}} \left[C_{k\downarrow}^{\dagger} + \frac{r}{\sqrt{t^4 Y^2 + r^2}} C_{-k\downarrow}^{\dagger} + \frac{t^2 Y}{\sqrt{t^4 Y^2 + r^2}} S^{\dagger} C_{-k\uparrow} \right],
$$

\n
$$
\beta_{k4} = \frac{1}{\sqrt{2}} \left[C_{-k\downarrow}^{\dagger} + \frac{r}{\sqrt{t^4 Y^2 + r^2}} C_{k\downarrow}^{\dagger} + \frac{t^2 Y}{\sqrt{t^4 Y^2 + r^2}} S^{\dagger} C_{k\uparrow} \right].
$$

\n(54)

The first one corresponds exactly to the process in which an electron comes in, is normally reflected, and Andreev reflected.

V. DISCUSSION

A. Comparison with the conventional approaches

If we compare the results of this unitary transformation to those from the extrapolation of the expression for waves above the gap, we can clarify the relationship between the conventional wave equation approach and our approach. The amplitudes are the same. The phase shift by the macroscopic phase is completely the same when the superconductor is in the phase-definite state. However, a phase shift like the GoosHanchen shift, which appears in the extrapolation, does not exist in the unitary transformation approach. The role of the operator S is the same as in the case above the superconducting gap.

Because the so-called BCS state is not the phase definite state, S always has quantum fluctuations. In cases as discussed in Sec. III, it is not negligible. Although, of course, the phase shift itself by Andreev reflection is not an observable quantity, it becomes observable, for example, in the geometry of our proposed in $terferometer⁶$ and in the superconductor-normalmetal —superconductor (SNS) Josephson junction. In the case of our interferometer, the quantum fluctuation of the phase appears as quantum noise in the current through the wave guide. In the proceeding subsection we discuss more concretely the effect in an SNS junction.

The conventional approach shows the imperfection of the time-reversal characteristic of Andreev reflection, that is, the wave numbers of the incident electron and the Andreev reflected hole are not exactly inverse to each other when the excitation energy ε_k is finite. In our approach, however, the time-reversal characteristic is always perfect. This is a fault in our formulation due to the fact that the operator S does not express the momentum of the Cooper pair. The most important advantage of the unitary-transformation approach is the fact that it clearly shows that Andreev reflection is the manifestation of the virtual transfer of quasiparticles through the interface and that the virtual excitations of Bogoliubov quasiparticles are the true image of evanescent Bogoliubov quasiparticles. It enables us to treat both the macroscopic and microscopic degrees of freedom at the same time.

In this paper, we consider only the transfer of quasiparticles and ignore the transfer of Cooper pairs in getting the Andreev reflection. If the virtual transfer of Cooper pairs is taken into account, it induces the superconducting proximity effect.¹⁵ Namely, Andree conducting proximity effect.¹⁵ Namely, Andreev reflection and the proximity effect are different aspects of the same physical phenomenon. In reality, both occur at the same time at the SN interface. If you concentrate on the quasiparticles, you see the Andreev reflection at the interface. Contrarily, if you pay attention to the superconducting order parameters, you see the proximity effect. An analysis of the proximity effect, considering the virtual transfer of Cooper pairs will appear elsewhere.¹⁶ A new scheme for analyzing the superconducting proximity effect will be given there.

B. One application example of the formulation: Josephson current

One formulation application is presented with the Josephson current in a superconductor —normalmetal —superconductor (SNS) coupled system. A more detailed analysis including the effects of finite temperatures will be published elsewhere.¹⁷

An easy analysis can be done with a Hamiltonian after the wave-bundle approximation, i.e., Eq. (49). However, our present formulation limits the applicable case in which $L < \xi_N$, where L is the length of the normal region and ξ_N is the superconducting coherence length in the normal region.

In the case of a symmetrical SNS system, the Hamiltonian for the normal region is given by

$$
\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{L\text{int}} + \mathcal{H}_{R\text{int}} \,. \tag{55}
$$

where

$$
\mathcal{H}_{0} = \sum_{\substack{k \\ \sigma = \uparrow, \downarrow}} \varepsilon_{k} c_{k\sigma}^{\dagger} c_{k\sigma}
$$
\n
$$
+ r_{0} \sum_{\substack{k > 0 \\ \sigma = \uparrow, \downarrow}} (e^{-ikL} C_{-k\sigma}^{\dagger} C_{k\sigma} + \text{H.c.})
$$
\n
$$
+ r_{0} \sum_{\substack{k > 0 \\ \sigma = \uparrow, \downarrow}} (e^{+ikL} C_{-k\sigma}^{\dagger} C_{k\sigma} + \text{H.c.}), \qquad (56)
$$

$$
\mathcal{H}_{L\text{int}} = t_1^2 \sum_{k>0} Y[S_L^{\dagger} (C_{k\uparrow} C_{-k\downarrow} + C_{-k\uparrow} C_{k\downarrow}) + \text{H.c.}], \tag{57}
$$

$$
\mathcal{H}_{R\text{int}} = t_1^2 \sum_{k>0} Y[S_R^{\dagger} (C_{k\uparrow} C_{-k\downarrow} + C_{-k\uparrow} C_{k\downarrow}) + \text{H.c.}].
$$
 (58)

In order to derive the Josephson current, we follow the method by Kresin.¹⁸ The Josephson current density $\langle j_s \rangle$ _{micro}, by taking the average of the microscopic degrees of freedom, is given by

$$
\langle j_s \rangle_{\text{micro}} = \frac{2ie}{\hbar} \frac{k_B T}{L^2} \sum_{\epsilon_n > 0} \sum_{k} |\Delta(\epsilon_k)|^2 [K(k; \epsilon_n) S_L S_R^{\dagger} - K(k; \epsilon_n) S_R S_L^{\dagger}],
$$
\n(59)

where T is the temperature and $\epsilon_n = 2\pi (n+1)k_B T$ are thermal frequencies, and

$$
K(k; \epsilon_n) = G_a(k; \epsilon_n) G_a(-k; -\epsilon_n)
$$

- G_b(k; \epsilon_n) G_b(-k; -\epsilon_n) (60)

is the two-body Green function that expresses the propagation of the Cooper pairs through the normal region. Moreover,

$$
\Delta(\varepsilon_k) = t_1^2 \frac{\Delta N(0)a}{\sqrt{\Delta^2 - \varepsilon_k^2}} \arccos \left(\frac{\Delta - \varepsilon_k}{2\Delta} \right)^{1/2}.
$$
 (61)

 $G_a(k;\epsilon_n)$ and $G_b(k;\epsilon_n)$ are the Green functions in the normal region derived from the Hamiltonian \mathcal{H}_0 of Eq. (56},by solving the Dyson's equation in Fig. 4. They are given by

$$
G_a(k;\epsilon_n) = \frac{i\epsilon_n - \epsilon_k}{(i\epsilon_n - \epsilon_k)^2 - 4r_0^2 \cos^2 kL},
$$
 (62)

$$
G_b(k;\epsilon_n) = \frac{2r_0 \cos kL}{(i\epsilon_n - \epsilon_k)^2 - 4r_0^2 \cos^2 kL} \tag{63}
$$

FIG. 4. Dyson's equations for Green functions in the normal region from the Hamiltonian Eq. (33), where $g_0 = 1/(i\epsilon_n - \epsilon_k)$.

Note that Σ_k in Eq. (59) means the summation of the wave-bundle states.

We rewrite the operators S_L , S_R as

$$
S_L = e^{i\hat{\phi}L}, \quad S_R = e^{i\hat{\phi}R} \tag{64}
$$

 (5) In the presence of the time-reversal symmetry, Eq. (59) reduces to

$$
\langle j_s \rangle_{\text{micro}} = j_0(T, t_1, r_0, L) \sin(\hat{\phi}_L - \hat{\phi}_R) , \qquad (65)
$$

where $j_0(T,t_1,r_0,L)$ is the c-number coefficient that includes the effects of the transfers and the normal reflections across the superconductor-normal-metal interfaces and the length of the normal region. Note that in our formulation, ϕ_L and ϕ_R are not c numbers, but are operators because S_L and S_R are q numbers. here, the phase-current relation is sinusoidal because we took only the lowest-order contribution of Cooper-pair transfers through the interfaces. This is justified in the case where normal reflections at the interfaces are intense.

There are two quantum-mechanical degrees of freedom in Eq. (65): $\hat{\phi}_{-} = \hat{\phi}_{L} - \hat{\phi}_{R}$ and $\hat{\phi}_{+} = \hat{\phi}_{L} + \hat{\phi}_{R}$. $\hat{\phi}_{-}$ is the canonical conjugate quantity for the difference of the particle number between the left and the right superconducting electrodes, and $\hat{\phi}_+$ is that for the particle number in the normal region. Both $\hat{\phi}_-$ and $\hat{\phi}_+$ are quantum mechanical quantities in a small SNS junction. If the quantum fluctuations of these degrees of freedom are ignored, Eq. (65) is a classical Josephson current. Here, however, the quantum fluctuations of $\hat{\phi}_-$ are closely related to phenomena such as macroscopic quantum tunneling and macroscopic quantum coherence. On the other hand, the quantum fluctuations of $\hat{\phi}_+$ work as a dissipation for the phenomena.

An effect of the fluctuation, which is easy to understand, is the quantum noise in the Josephson current. From Eq. (65), the quantum fluctuation δj_s of the currentis given by
 $\langle \delta j_s \rangle_{\text{macro}}^2 = j_0^2 [\langle \sin^2 \hat{\phi}_- \rangle - \langle \sin \hat{\phi}_- \rangle^2]$ is given by

$$
\langle \delta j_s \rangle_{\text{macro}}^2 = j_0^2 [\langle \sin^2 \hat{\phi}_- \rangle - \langle \sin \hat{\phi}_- \rangle^2]
$$

$$
\sim 2 j_0^2 \sin 2 \phi_-^0 \sin \frac{\delta \phi_-}{2} , \qquad (66)
$$

where ϕ^0 is the mean value of $\hat{\phi}$ and $\delta\phi$ is its fluctuation. This is a kind of quantum shot noise that comes from the particle aspect of Cooper pairs.

VI. CONCLUSION

We formulated the Andreev reflection in a second quantization manner. In this formulation, the Andreev reflection is explained in terms of the elementary excitation of a superconductor —normal-metal (SN} -coupled system. The description of the excitation includes operators for both the quasiparticles and the superconducting state. Operators for the superconducting state enables us to consider the effect of macroscopic fluctuations on Andreev reflection. Therefore, this allows us to treat both the microscopic and macroscopic quantum-mechanical aspects of Andreev reflection. In our formulation, the Andreev reflection involves operators that do not commutate with the operators for the superconducting state, thus affecting the equation of motion for a macroscopic variable in a system with an SN interface. For example,

our formulation is needed to analyze the mesoscopically quantum-mechanical aspects of the quasiparticle interferometer we recently proposed: a Josephson junction with normal metallic branches. Thus, our formulation has opened a door to the mesoscopic physics of Andreev reflection.

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FIG. 1. Representation of the barrier problem. Forward and backward waves are considered in order to consistently treat transmission and reflection.