RF conductivity and surface impedance of a superconductor taking into account the complex superconducting gap energy

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Abstract
The Mattis-Bardeen theory for the anomalous skin effect in the superconductors has been extended taking the complex gap energy into account and the surface impedance of superconductors has been calculated using the extended Mattis-Bardeen theory. It is found that the surface resistance of the superconductor increases with increasing magnitude of the imaginary part of the gap energy. It is demonstrated that the calculated surface resistance for a NbN film quantitatively agrees with the measured one. It is also found that temperature dependence of Q values of superconducting resonators is well described by those calculated by the extended Mattis-Bardeen equation.

1. Introduction
It has been recently pointed out that a formula for the quasiparticle density of states, in which the superconducting gap energy has a small imaginary part, predicts the presence of the quasiparticle states inside the energy gap (intragap states) [1] and gives good fit for quasiparticle tunnel current in the subgap regime of superconducting tunnel junctions [1, 2, 3]. It is natural to expect that a part of the RF current may be carried by the quasiparticles in the intragap states in addition to those generated by thermal excitations and interaction of electromagnetic field and the Cooper pairs. Then, in order to describe the contribution of the quasiparticles in the intragap states to the RF conductivity or surface impedance of the superconductor, we have tried to extend the Mattis-Bardeen theory [4], which is widely used for the calculation of the RF conductivity or surface impedance of superconductors, taking the complex superconducting gap energy into account.

In this paper, an extension of the Mattis-Bardeen theory taking the imaginary part of the gap energy into account is described at first. Then the surface impedance of a superconductor are calculated using the extended Mattis-Bardeen theory and compared to those reported. Finally it is demonstrated that saturation of the Q value of a superconducting resonator at low temperature can be quantitatively predicted by the extended Mattis-Bardeen theory.
2. Extension of the Mattis-Bardeen theory

2.1. Complex gap energy

Single-particle Green’s function of a superconductor, \( G_{11}(k, E) \), is expressed as

\[
G_{11}(k, E) = \frac{Z(E) E + \epsilon_k}{Z^2(E) E^2 - \phi^2(E) - \epsilon_k^2},
\]

and the poles of the Greens function (1) are given by

\[
Z^2(E) E^2 - \phi^2(E) - \epsilon_k^2 = 0,
\]

where \( Z(E) \) and \( \phi(E) \) are the renormalization parameter and the paring self-energy, respectively \([5, 6]\). Equation (2) may be rewritten as

\[
E = \sqrt{\epsilon_k^2 + \Delta^2},
\]

where \( \epsilon = \epsilon_k/Z_0 \). Setting \( Z = Z_1 + i Z_2, \phi = \phi_1 + i \phi_2 \) and \( \Delta = \Delta_1 + i \Delta_2 \) and substituting them into (2), we get

\[
\Delta_2(E) = \frac{\phi_2(E) - \Delta_1(E) Z_2(E)}{Z_1(E)},
\]

where it is assumed that their imaginary parts are small enough compared to their real parts. Since the energy considering here is much smaller than the phonon specific frequency, the energy dependence of \( Z \) and \( \phi \) can be neglected and represented by the values at the gap edge \( Z_0 = Z(\Delta_0) \) and \( \phi_0 = \phi(\Delta_0) \), where \( \Delta_0 \) is a gap energy. Then (4) can be simplified as

\[
\Delta_2 = \frac{\phi_0 - \Delta_0 Z_0}{Z_0}.
\]

It is noted here that the gap energy \( \Delta \) can have an small imaginary part which is identical to the decay parameter of quasiparticles, \( \Gamma \), derived by Kaplan et al. \([7]\).

The quasiparticle density of states are determined by the equation,

\[
N(E) = -\frac{1}{\pi} \text{Im} \sum_k G_{11}(k, E).
\]

Substituting (1) into (6), we get

\[
N(E) = N(0) \text{Re} \left\{ \frac{E}{\sqrt{E^2 - \Delta^2}} \right\}.
\]
Examples of the density of states of Al and Nb calculated by (7) for a complex number of $\Delta$ are plotted by broken lines in Fig. 1. It is clearly shown that a significant number of quasiparticle states appear inside the energy gap unlike the expectation of the BCS theory. Here we call those quasiparticle states inside the energy gap "intrigap states". Since quasiparticles in the intrigap states may also contribute to the RF conductivity of the superconductor, it is necessary to take the contribution of those quasiparticles into consideration in the calculation of the RF conductivity of the superconductor.

Since the Mattis-Bardeen theory, which is now widely used for the calculation of the RF conductivity or surface resistance of the superconductor, takes only the contribution of thermally-excited quasiparticles into consideration, it is necessary to develop a theory that includes the contribution of the quasiparticles in the intrigap states. Then we try to extend the Mattis-Bardeen theory taking into account the complex gap energy which determines the density of the intragap quasiparticle states.

2.2. Surface resistance

According to the linear response theory, the current density of a superconductor is given by [5]

$$ j(r, t) = \sum_{\omega} \frac{e^2 N(0) v_F}{2\pi^2 \hbar} \int \frac{\mathbf{R}[\mathbf{A}_\omega(r')] I(\omega, R, T) e^{-R/|r|}}{R^4} dr', $$

(8)

where

$$ I(\omega, R, T) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left\{ L(\omega, \epsilon, \epsilon') - \frac{f(\epsilon) - f(\epsilon')}{\epsilon' - \epsilon} \right\} \cos[\alpha(\epsilon - \epsilon')] d\epsilon d\epsilon', $$

(9)

and $\mathbf{R} = r - r'$. $\alpha = R/\hbar v_F$, $v_F$ being the Fermi velocity, $N(0)$ is the electron density of states of one spin at the Fermi surface and $f(E)$ is the usual Fermi function. The spectral function $L(\omega, \epsilon, \epsilon')$ is given by

$$ L(\omega, \epsilon, \epsilon') = \frac{1}{4} \left( \frac{\epsilon \epsilon' + \Delta^2}{\epsilon \epsilon'} \right) \times \frac{f(E') - f(E)}{E' - E - i\hbar \omega - is} + \frac{f(E') - f(E)}{E' - E + i\hbar \omega + is} + \frac{1}{4} \left( \frac{\epsilon \epsilon' + \Delta^2}{\epsilon \epsilon'} \right) \times \frac{1 - f(E) - f(E')}{E + E' - i\hbar \omega - is} + \frac{1 - f(E) - f(E')}{E + E' + i\hbar \omega + is}. $$

(10)

The quasiparticle excitation energy, $E$, is defined by (3). Here we assume that the gap energy, $\Delta$, is represented as a complex number $\Delta = \Delta_1 + i\Delta_2$, where $\Delta_1$ and $\Delta_2$ are real.

In the extreme anomalous limit, we can set $\alpha = R/\hbar v_F = 0$. Here we introduce a complex conductivity $\sigma = \sigma_1 - i\sigma_2$. Then the ratio of the superconducting to normal conductivity is given as,

$$ \frac{\sigma_1 - i\sigma_2}{\sigma_N} = \frac{I(\omega, 0, T)}{-\pi \hbar \omega}, $$

(11)

where the real and the imaginary components, $\sigma_1$ and $\sigma_2$, represent the quasiparticle and Cooper-pair currents in a superconductor, respectively. The integration of (9) over $\epsilon'$ can be easily performed with contour techniques and we get expressions for the complex conductivity $\sigma$ as

$$ \frac{\sigma_1 - \sigma_2}{\sigma_N} = \frac{1}{\hbar \omega} \int_C \left\{ 1 - 2f(E) \right\} \mathcal{D}(E) \left( \frac{1}{E} \right) \left\{ \frac{E(E - \hbar \omega + \Delta^2)}{\sqrt{(E - \hbar \omega)^2 + \Delta^2}} - \frac{E(E + \hbar \omega + \Delta^2)}{\sqrt{(E + \hbar \omega)^2 + \Delta^2}} \right\} dE, $$

(12)

$$ \mathcal{D}(E) = \frac{E}{\sqrt{E^2 - \Delta^2}}, $$

(13)

where the integration is performed along the path $C$: $E = \sqrt{\epsilon^2 + \Delta^2}$ as shown in Fig. 2. We may here change the integration path from the line segment $C_1$ to the path consisting of the two line segments, $C_1$ in parallel to the imaginary axis and $C_2$ on the real axis and the integral equation of right-hand side of (12) can be modified as

$$ \int_C \left[ \cdots \right] dE = \int_{C_1} \left[ \cdots \right] dE + \int_{C_2} \left[ \cdots \right] dE. $$

(14)
The first term of the right-hand side of (14) is appeared by the presence of the imaginary part of the gap energy $\Delta_2$ and represents conduction of quasiparticles in the intra-gap states, while the second term corresponds to conduction of thermally-excited quasiparticles [4]. The specific surface impedance $Z_s$ per unit area of a superconducting film with a thickness $d$ is given by

$$Z_s(\omega) = \sqrt{\frac{i\omega \mu_0}{\sigma}} \coth \left( \sqrt{\frac{i\omega \mu_0}{\sigma}} d \right) = R_s + iX_s$$

(15)

where $\mu_0$ is the permeability of vacuum.

In Fig. 3, calculated surface resistance and reactance for a superconductor with a gap energy of $\Delta_1 = 1.5$ mV and transition temperature of $T_C = 9.0$ K, keeping Nb in mind, at $T = 1.0$ K ($T/T_C = 0.11$). The calculated surface resistance shows remarkable increases as the magnitude of $\Delta_2$ increase and serious deviation from that expected by the Mattis-Bardeen theory is found for $\delta \equiv \Delta_2/\Delta_1 = 10^{-4}$, which is a typical magnitude of the imaginary part of the energy gap measured in the actual Nb film [3]. This is because the number of the thermally-excited quasiparticles at the gap edge get to be so small that surface resistance at $T = 1.0$ K is mainly determined by the numbers of the quasiparticles in the intragap states, which increases with increasing $\delta$. It is also noted here that the surface reactance is not strongly dependent on the magnitude of $\delta$, because the number of Cooper pairs, which determine the magnitude of the surface reactance, at the temperature below $\sim T_C/2$ are approximately constant as long as $\delta \ll 1$.

3. Comparison to experiments

3.1. Surface resistance of a NbN film

Since NbN films have a transition temperature of $\sim 16$ K and their surface resistance have been measured at 4.2 K, which corresponds to the reduced temperature of $T/T_C \approx 0.26$, NbN is selected for the superconductor to compare the present theory with experiment. In Fig. 4, a measured dc I-V curve of NbN/MgO/NbN tunnel junction [8], in which all the NbN and MgO films are epitaxially grown, is shown by circles. We calculated the tunnel current as function of bias voltage using the density of states given by (7). In the calculation of the tunnel current, not only the proximity effect at the interfaces between the MgO barrier and Nb but also the complex number of energy gap are taken into account. Detailed procedure of the calculation of the tunnel current is described in [2]. The calculated tunnel current as a function of voltage for the NbN tunnel junction is plotted by the solid line in the main figure of Fig. 4. Note here that the Ohmic component assumed to be leakage current, which is shown by the broken line in the main figure of Fig. 4, is subtracted from the measured data in the fitting procedure. It is found that the calculated dc I-V curve agrees very well with the measured one. The imaginary part of the gap energy, $\Delta_2$, of the NbN film is determined from $\delta$ that gives the best fit to the rounded structure of the dc I-V curve near the gap voltage. Calculated tunnel

![Fig. 3. Calculated surface impedances at 1.0 K.](image)

![Fig. 4. Measured (circles) and calculated (solid line) dc I-V curves of a NbN/MgO/NbN tunnel junction. The inset shows the magnified dc I-V curves near the gap voltage.](image)
current near the gap voltage are shown by dotted, solid, and broken lines for $\delta = 1, 0 \times 10^{-3}, 8.1 \times 10^{-3}$ and $\delta = 1.0 \times 10^{-2}$ in the inset of Fig. 4, respectively. Thus, $\delta$ for the NbN film is determined to be $8.1 \times 10^{-3}$, which gives the best fit to both the rounded structure near the gap voltage and whole dc I-V curve.

In Fig. 5, the surface resistance of NbN [9] with the same quality as that used in the tunnel junction whose dc I-V curve is shown in Fig. 4 is plotted as a function of frequency by open and filled circles. The solid line represents the calculated surface resistance using (12) and (13), assuming that $\delta = 8.1 \times 10^{-3}$, which is determined by the fitting of the dc I-V curve as previously described. It should be noted here that the calculated surface resistance agrees fairly well with the measured ones. This indicates that the extended Mattis-Bardeen theory taking into account the complex gap energy is useful for the prediction of the surface resistance of a superconductor.

3.2. Q values of superconducting resonators

Temperature dependence of surface impedance can be calculated using equations (12), (13) and (15). In Fig. 6, calculated surface resistance and reactance for the superconductor with a gap energy of $\Delta_1 = 1.5$ mV and transition temperature of $T_C = 9.0$ K, keeping Nb in mind, are plotted as a function of temperature for several magnitudes of $\delta$. It is clearly shown that the calculated surface resistance deviates from the prediction of Mattis-Bardeen theory at low temperature and shows saturation of decrease at low temperature irrespective of the magnitude of $\delta$. On the other hand, the surface reactance is independent of temperature and approximately constant. From these results it can be expected that the quality factor (Q value) of a superconducting resonator may be saturated at low temperature, because the Q value of a superconducting resonator is defined by $Q \equiv X_s/R_s$, where $R_s$ and $X_s$ are the surface resistance and reactance of the superconductor, respectively. It has been well known that the Q value of a superconducting resonator usually shows a saturation of increase at a very low temperature. In Fig. 7, a typical example of the temperature dependence of a Nb superconducting cavity [10] is shown by filled circles, while the simulated Q value using the extended Mattis-Bardeen equations (12), (13) and $Q = X_s/R_s$ by the solid line. The simulated temperature dependence of Q value using the extended Mattis-Bardeen equations taking into account the complex gap energy agrees very well with the measured one. Note that $\delta$ is determined so as to give the best fit to the measured data.

It has been recently shown that the quasiparticle density in a thin film superconducting Al resonator saturates in decrease at low temperature [11]. Since the extended Mattis-Bardeen equation (12) gives the numbers of quasiparticles which contribute to the normal conductivity in a superconductor, it may be possible to simulate the temperature dependence of the quasiparticle density in the superconductor. In Fig. 8 the quasiparticle density as a function of temperature reported by Visser et al. is shown by triangles and squares, while the solid line represents the simulated one using the extended Mattis-Bardeen equation (12). Calculated quasiparticle density is scaled at 0.3 K to the experimental data and $\delta$ is determined so as to give the best fit to the saturated quasiparticle density. It is demonstrated that the experimentally obtained temperature dependence of the quasiparticle density is well predicted by the extended Mattis-Bardeen equation.
taking into account the complex gap energy. From this result we think that such residual quasiparticle at low temperatures can be attributed to those in the intragap states which are appeared by the presence of the imaginary part of the gap energy.

4. Conclusion

The Mattis-Bardeen theory for the superconductors has been extended, taking the complex gap energy into account. It is found the surface resistance of the superconductor increases with increasing magnitude of the imaginary part of the gap energy. The calculated surface resistance for a NbN film using the extended Mattis-Bardeen equation gives a good agreement with that experimentally obtained. Temperature dependence of Q values of superconducting resonators are also well described by the surface reactance and resistance calculated by the extended Mattis-Bardeen equation. Thus, it is important to consider the contribution of quasiparticles in the intragap states, which are appeared by the presence of the imaginary part of the gap energy, to physical quantities of superconductors related to the numbers of quasiparticles at low temperature.

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References