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Surface impedance of superconductors with magnetic impurities

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Motivated by the problem of the residual surface resistance of the superconducting radio-frequency (SRF) cavities, we develop a microscopic theory of the surface impedance of s-wave superconductors with magnetic impurities. We analytically calculate the current response function and surface impedance for a sample with spatially uniform distribution of impurities, treating magnetic impurities in the framework of the Shiba theory. The obtained general expressions hold in a wide range of parameter values, such as temperature, frequency, mean free path, and exchange coupling strength. This generality, on the one hand, allows for direct numerical implementation of our results to describe experimental systems (SRF cavities, superconducting qubits) under various practically relevant conditions. On the other hand, explicit analytical expressions can be obtained in a number of limiting cases, which makes possible further theoretical investigation of certain regimes. As a feature of key relevance to SRF cavities, we show that in the regime of “gapless superconductivity” the surface resistance exhibits saturation at zero temperature. Our theory thus explicitly demonstrates that magnetic impurities, presumably contained in the oxide surface layer of the SRF cavities, provide a microscopic mechanism for the residual resistance.

PACS numbers:

I. INTRODUCTION

Magnetic impurities in s-wave superconductors have been a subject of interest for a long time. Shortly after the development of the Bardeen-Cooper-Schrieffer (BCS) theory of superconductivity¹, Abrikosov and Gor’kov (AG) demonstrated² that magnetic impurities introduced into the sample in moderate concentrations lead to the suppression of superconductivity. If the magnetic scattering rate $1/\tau_s > 1/\tau_s^*$ exceeds the critical value $1/\tau_s^* \approx 0.88 T_{c0}$, where T_{c0} is the transition temperature of a sample without magnetic impurities (we set $\hbar = 1$ throughout the paper), the superconductivity is completely suppressed at all temperatures. In contrast, much stronger nonmagnetic disorder is required to suppress superconductivity: the scattering rate $1/\tau \sim \epsilon_F$ must be on the order of the Fermi energy $\epsilon_F \sim 10^3 T_{c0}$.

According to the AG and subsequent^{3–10} theories, even below the critical value, $1/\tau_s < 1/\tau_s^*$, the presence of magnetic impurities can result in the regime of “gapless superconductivity” (GSC), where the superconducting order parameter Δ is nonzero, yet the single-particle density of states (DOS) $\nu(\epsilon)$ does not vanish down to the Fermi level $\epsilon = 0$, Fig. 1. The GSC regime is predicted to occur quite generically, although the magnitude of the “subgap” DOS is parameter-dependent. Even for low scattering rate $1/\tau_s \ll 1/\tau_s^*$ and weak exchange coupling J , $\nu_F J \ll 1$ (ν_F is the normal state DOS at the Fermi level per one spin projection), optimal fluctuations in the impurity distribution produce “tails” in the DOS^{8–10} below the “hard gap” predicted by the AG theory, Fig. 1(a). The GSC regime becomes much more pronounced with increasing the exchange coupling and/or scattering rate, Fig. 1(b), as the Shiba theory^{4,7} demonstrates. This is also supported by a recent numerical study¹¹ of a different, but mathematically equivalent model.

In the GSC regime, gapless quasiparticle excitations give rise to dissipation even at zero temperature¹². Although this dissipation mechanism (caused either by the natural presence of magnetic impurities or unintentional/unavoidable contamination of the sample with them) may be negligible for most practical applications of superconductors, it could play an important role in devices that require high quality performance. One example of such systems are the superconducting radio-frequency (SRF) cavities, widely used in particle accelerators (see Ref. 13 for a review and references therein; another notable system is superconducting qubits). The SRF cavities are characterized by exceptional quality factors, which are, however, limited to a finite residual value $\sim 10^{10}$ at temperatures $T \ll T_c$ much smaller than the superconducting transition temperature T_c , where the contribution from thermally excited quasiparticles vanishes.

Despite the high practical relevance of problem, there is no commonly accepted theoretical explanation of the origin of the residual Ohmic losses in SRF cavities. Given the above properties, it was recently argued in Ref. 16 that they could indeed be attributed to the presence of magnetic impurities in the system. Although the bulk of Nb samples used for SRF cavities is typically very clean, a disordered oxide surface layer forms due to exposure to atmosphere¹⁴, Fig. 2. Most importantly, magnetic moments can develop¹⁵ in the oxygen vacancies of the sub-stoichiometric Nb_2O_5 layer of thickness $\sim 5 - 10\text{nm}$. Since the typical penetration depth of the electro-magnetic field is $\sim 45\text{nm}$, this means that superconductivity could be partially suppressed in a considerable fraction of the operating region. Scanning tunneling spectroscopy measurements of the SRF cavity samples performed in Ref. 16 revealed the surface tunneling DOS with appreciable “subgap” contribution, consider-

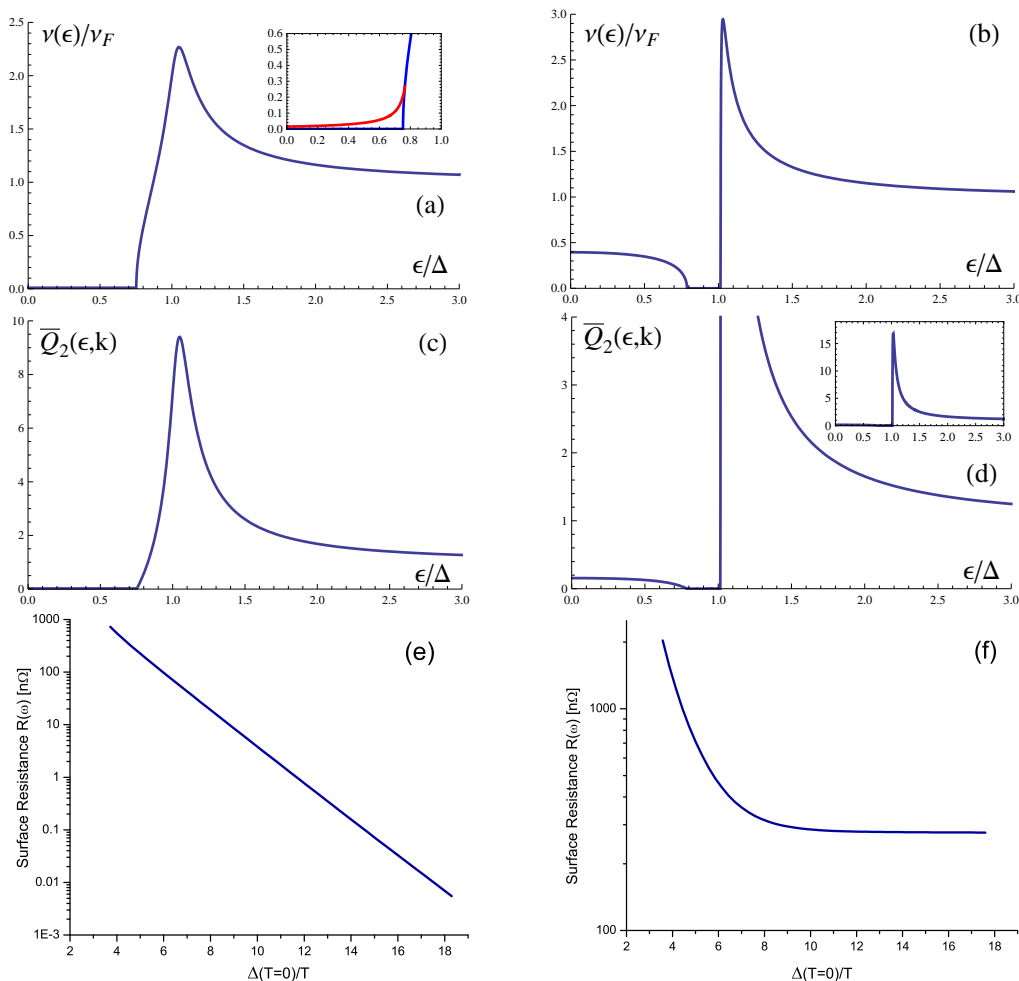


FIG. 1: Regimes of “gapped” [(a), (c), (e), weaker exchange coupling $\nu_F J$ and lower scattering rate $1/\tau_s$; parameters of the Shiba theory used: $1/(\tau_s \Delta) = 0.04$, $\gamma = 0.95$] and “gapless” [(b), (d), (f), stronger exchange coupling and/or higher scattering rate; parameters used: $1/(\tau_s \Delta) = 0.17$, $\gamma = 0$] superconductivity. (a) and (b): The single-particle density of states (DOS) $\nu(\epsilon)$, obtained from the Shiba theory Eqs. (4.8)-(4.12), and (6.1). The inset in (a) schematically shows (in red) the “tail” of the DOS produced by optimal fluctuations of impurity distribution – exponentially small nonperturbative effect, not captured by the AG-Shiba theory and not considered in the present paper. (c) and (d): The function $\bar{Q}_2(\epsilon, k)$ [Eq. (5.3)] describing the dissipative contribution to the current response from a given energy ϵ , see Secs. V and VI for details. The plots are presented for $k = 0$; the inset in (d) shows the full range of $\bar{Q}_2(\epsilon, k)$. The function $\bar{Q}_2(\epsilon, k)$ is nonzero if and only if $\nu(\epsilon)$ is nonzero. (e) and (f): The temperature dependence of the surface resistance $R(\omega)$, obtained from the main Eqs. (3.1), (3.3), (4.1), (4.15), (4.16), and (4.17) of the paper by numerically calculating the integrals over ϵ and k . In the gapped regime (e), $R(\omega) \propto \exp(-\Delta^*/T)$ is exponential at lower temperatures and vanishes at $T = 0$. In the gapless regime (f), for moderate “subgap” DOS, the surface resistance $R(\omega)$ is exponential at lower but finite temperatures and saturates to a nonzero value at $T = 0$. The latter case reproduces the commonly observed experimental behavior²².

ably greater than one would expect from a high-purity Nb material. Combined with good fits to the Shiba theory, these data suggested magnetic impurities in the oxide surface layer as an important contributing factor to the dissipation in SRF cavities.

To support this idea, in the present work, we develop a microscopic theory of the surface impedance of s-wave superconductors with magnetic impurities. According to the surface chemistry of the air-exposed Nb samples¹⁴, Fig. 2, the real SRF cavity material is most appropriately described by a model of disordered surface layer that con-

tains both magnetic and nonmagnetic impurities, while the rest of the sample is weakly disordered or pure. In principle, such model can be studied in the framework of the quasiclassical approach to superconductivity based on the Eilenberger equation^{17,18}. However, this involves solving a self-consistency problem for a system of differential equations, which, for realistic parameter values, is challenging even using numerical methods.

Instead, here we consider a simpler model of a superconducting sample with uniform in space distribution of magnetic and nonmagnetic impurities, Fig. 3. The main

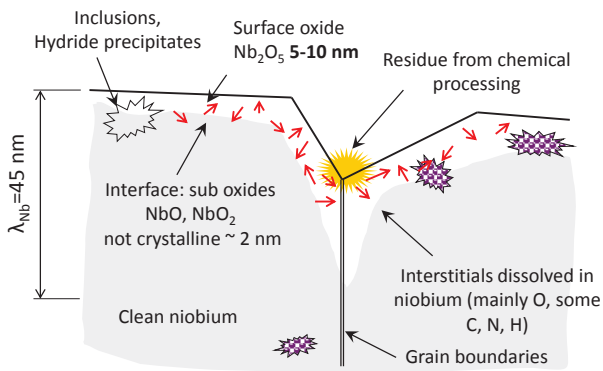


FIG. 2: Typical structure of the surface layer of the air-exposed Nb samples used for SRF cavities. Localized magnetic moments can form¹⁵ in oxygen vacancies of the Nb_2O_5 layer of thickness $\sim 5\text{-}10\text{nm}$. Typical penetration depth of the RF electromagnetic field is $\sim 45\text{nm}$.

practical advantage is that for this model we are able to analytically obtain the general expressions for the current response function and surface impedance. The expressions are valid, within the approximations of the theory, in a wide range of parameter values and, in the general case, only the resulting integrals need to be calculated numerically. This generality allows for the application of our theory to the description of experimental systems, such as SRF cavities and superconducting qubits, in various practically relevant regimes. On the other hand, if necessary, explicit analytical expressions can be obtained in numerous limiting cases.

The current response function and surface impedance of superconductors without magnetic impurities are provided by the Mattis-Bardeen¹⁹ and Abrikosov-Gor'kov-Khalatnikov²⁰ theories (see also Ref. 21,22), in the presence and absence of nonmagnetic disorder, respectively. The surface impedance of superconductors with magnetic impurities was previously studied in Refs. 23,24 in the limit $\nu_F J \ll 1$ of weak exchange coupling of the AG theory. In the present work, we consider the case of arbitrary exchange coupling strength $\nu_F J$, treating the interactions of conduction electrons with magnetic impurities within the framework of the Shiba theory. This

sufficiently widens the range of impurity concentrations, where the GSC regime (of particular interest to us) with appreciable DOS at the Fermi level occurs.

As the feature of key relevance to SRF cavities, we demonstrate that the presence of magnetic impurities does lead to the saturation of the surface resistance at zero temperature in the GSC regime.

Our theory employs the linear response formalism and is therefore valid as long as the superconducting state is not appreciably suppressed by the magnetic field H . For type-II superconductors in thermal equilibrium, the upper bound for this is set by the first critical field H_{c1} , above which the system becomes unstable towards creation of vortices. Real SRF cavities, however, are known to operate in a metastable vortex-free state that persists up to a higher “superheating” field $H_{sh} > H_{c1}$ ^{25–28}. Thus, our theory should be applicable in the range $H \lesssim H_{sh}$.

At higher fields $H \sim H_{sh}$ one could, in fact, expect a cooperative effect of the two dissipation mechanisms: magnetic disorder could create “hot spot” regions²⁹ of locally suppressed superconductivity at the surface and thus trigger proliferation of vortices. Such regime deserves a separate study.

The rest of the paper is organized as follows. In Sec. II, the studied system is presented and the main approximations are formulated. In Sec. III, the surface impedance and current response function are introduced. In Sec. IV, the current response function is calculated. In Sec. V, the low-frequency expansion is performed. In Sec. VI, the key result pertaining to the presence of magnetic impurities – finite residual surface resistance in the GSC regime – is demonstrated. Concluding remarks are presented in Sec. VII.

II. MODEL

We assume the superconducting sample occupies the half-space $z > 0$ and contains both nonmagnetic and magnetic impurities, which are distributed uniformly in space with densities n and n_s , respectively, Fig. 3. Within the framework of the BCS theory^{1,30}, the Hamiltonian of the system can be written as

$$\hat{H} = \int_{z>0} d^3\mathbf{r} \left\{ \hat{\psi}_\sigma^\dagger \left[E \left(|\hat{\mathbf{p}} - \frac{e}{c} \mathbf{A} \right) - \epsilon_F + \sum_a u \delta(\mathbf{r} - \mathbf{r}_a) \right] \hat{\psi}_\sigma + \sum_b J \mathbf{s}_b \left(\hat{\psi}_\sigma^\dagger \boldsymbol{\sigma}_{\sigma\sigma'} \hat{\psi}_{\sigma'} \right) \delta(\mathbf{r} - \mathbf{r}_b) + \Delta \left[\hat{\psi}_\uparrow \hat{\psi}_\downarrow + \hat{\psi}_\downarrow^\dagger \hat{\psi}_\uparrow^\dagger \right] \right\}$$

Here, $\hat{\psi}_\sigma = \hat{\psi}_\sigma(\mathbf{r})$ is the electron field operator, $\sigma, \sigma' = \uparrow, \downarrow$ are the spin indices, $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is the vector of Pauli matrices, and summation over repeated spin indices is implied; $E(p)$ is the electron spectrum, which we assume isotropic in momentum \mathbf{p} , $p = |\mathbf{p}|$, $\hat{\mathbf{p}} = -i\nabla$; $\mathbf{A} = \mathbf{A}(t, \mathbf{r})$

is the vector potential of the electromagnetic field penetrating the sample; Δ is the superconducting order parameter, which has to be found self-consistently in the presence of magnetic impurities.

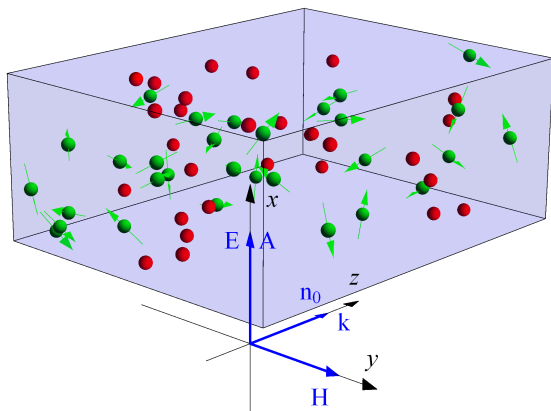


FIG. 3: Studied system: a half-infinite ($z > 0$) superconducting sample with magnetic (green) and nonmagnetic (red) impurities uniformly distributed over its volume. Relation between the wave-vector \mathbf{k} , electric \mathbf{E} and magnetic \mathbf{H} fields, and the vector potential \mathbf{A} is shown.

Next, \mathbf{r}_a and \mathbf{r}_b are random positions of nonmagnetic and magnetic impurities, respectively. We use the conventional disorder averaging technique³⁰ (“noncrossing” approximation) and, to keep calculations simpler, assume contact interaction potential of impurities (“point disorder”). We (i) treat magnetic impurities as classical spins described by the unit vectors \mathbf{s}_b and assume them unpolarized, (ii) consider arbitrary exchange coupling strength $\nu_F J$, summing the full perturbation series for a single impurity. These are the approximations of the Shiba theory⁴.

Note that the exponentially small subgap contribution (“tail”) to the DOS arising from the optimal fluctuations of magnetic disorder^{8–10} is not captured within the noncrossing approximation. This nonperturbative effect is dominant only in the limit of weak exchange coupling $\nu_F J \ll 1$ and small impurity concentration, such that $1/(\tau_s T_{c0}) \ll 1$. In this work, we concentrate on more significant contributions to the DOS that arise at larger impurity concentration and/or stronger exchange coupling.

III. SURFACE IMPEDANCE

The complex surface impedance

$$Z(\omega) = R(\omega) + iX(\omega) \quad (3.1)$$

(see, e.g., Refs. 22,31) relates the electric $\mathbf{E}(z)e^{-i\omega t}$ and magnetic $\mathbf{H}(z)e^{-i\omega t}$ fields at frequency ω at the interface $z = 0$ between the vacuum and sample as

$$\mathbf{E}(0) = \frac{c}{4\pi} Z(\omega) [\mathbf{H}(0) \times \mathbf{n}_0], \quad (3.2)$$

where $\mathbf{n}_0 = (0, 0, 1)$ is the unit vector normal to the surface pointing into the sample, Fig. 3. The real part $R(\omega)$ of the impedance (3.1) determines the energy flux (averaged over the oscillation period)

$$W = \frac{1}{2} \left(\frac{c}{4\pi} \right)^2 R(\omega) |\mathbf{H}(0)|^2$$

of the electro-magnetic field per unit area from the vacuum into the sample and is referred to as the “surface resistance”.

The general³² expression for the surface impedance of a uniformly disordered system reads

$$Z(\omega) = -i \frac{4\pi\omega \lambda(\omega)}{c^2}, \quad \lambda(\omega) = \frac{2}{\pi} \int_0^{+\infty} \frac{dk}{k^2 + 4\pi Q(\omega, k)/c^2}. \quad (3.3)$$

Here, $Q(\omega, k)$ is the linear current response function of an infinite sample in Fourier representation, dependent on the frequency ω and the absolute value $k = |\mathbf{k}|$ of the wave-vector \mathbf{k} . In Eq. (3.3), we also introduce the complex penetration depth $\lambda(\omega)$: its real part $\text{Re}\lambda(\omega)$ is the actual penetration depth that determines the decay scale of the electromagnetic field into the bulk. The Ohmic dissipation is determined by the imaginary part $Q_2(\omega, k)$ of the current response function

$$Q(\omega, k) = Q_1(\omega, k) - iQ_2(\omega, k). \quad (3.4)$$

According to Eq. (3.3), the surface resistance $R(\omega)$ is finite, only if $Q_2(\omega, k)$ is nonzero.

The response function $Q(\omega, k)$ defines the relation

$$\mathbf{j}(\omega, \mathbf{k}) = -\frac{1}{c} Q(\omega, k) \mathbf{A}(\omega, \mathbf{k}) \quad (3.5)$$

in the Fourier representation between the electric current $\mathbf{j}(\omega, \mathbf{k})$ and the electro-magnetic field, described by the vector potential $\mathbf{A}(\omega, \mathbf{k})$. The trivial tensor structure of Eq. (3.5) holds for cubic crystal symmetry and, in particular, for the isotropic electron spectrum $E(|\mathbf{p}|)$ assumed here. It is convenient to work in the gauge of absent scalar potential $\varphi(\omega, \mathbf{k}) = 0$. Additionally, the vector potential $\mathbf{A}(\omega, \mathbf{k})$ may be assumed to satisfy the constraint

$$\mathbf{A}(\omega, \mathbf{k}) \mathbf{k} = 0, \quad (3.6)$$

which significantly simplifies the calculations. This is equivalent to the local electroneutrality condition, which is a very good approximation for superconductors. The geometric relation between the wave-vector \mathbf{k} , vector potential $\mathbf{A}(\omega, \mathbf{k})$, and electric $\mathbf{E}(\omega, \mathbf{k}) = \frac{i\omega}{c} \mathbf{A}(\omega, \mathbf{k})$ and magnetic $\mathbf{H}(\omega, \mathbf{k}) = [i\mathbf{k} \times \mathbf{A}(\omega, \mathbf{k})]$ fields is shown in Fig. 3.

In the next section, we calculate the current response function $Q(\omega, k)$, which fully determines the surface impedance (3.3).

IV. CURRENT RESPONSE FUNCTION

According to the general Kubo formalism^{30,31}, the expression for the linear current response function [Eq. (3.5)] can be written down as

$$Q(\omega, k) = Q_0 \frac{-3i}{2} \int_{-\infty}^{+\infty} d\epsilon \left[\left(\tanh \frac{\epsilon_+}{2T} - \tanh \frac{\epsilon_-}{2T} \right) \langle jj \rangle^{RA}(\epsilon, \omega, k) + \tanh \frac{\epsilon_-}{2T} \langle jj \rangle^{RR}(\epsilon, \omega, k) - \tanh \frac{\epsilon_+}{2T} \langle jj \rangle^{AA}(\epsilon, \omega, k) \right], \quad (4.1)$$

$$\langle jj \rangle^{ab}(\epsilon, \omega, k) = \left\langle n_\alpha^2 \int \frac{d\xi}{2\pi} [G^a(\epsilon_+, \mathbf{p}_+) G^b(\epsilon_-, \mathbf{p}_-) + F^a(\epsilon_+, \mathbf{p}_+) F^b(\epsilon_-, \mathbf{p}_-)] \right\rangle_{\mathbf{n}}, \quad a, b = R, A. \quad (4.2)$$

In Eq. (4.1), we introduced

$$Q_0 = 2(ev_F)^2 \nu_F / 3, \quad (4.3)$$

where $v_F = (dE/dp)_{p=p_F}$ is the Fermi velocity, p_F is the Fermi momentum, $E(p_F) = \epsilon_F$, and $\nu_F = p_F^2 / (2\pi^2 v_F)$. The quantity $Q_0 = Q(0, 0)|_{T=0, \text{clean}}$ is the value of the current response function for a clean system at $\omega = 0$, $k = 0$, and $T = 0$; it can be related to the formal London penetration depth λ_{L0} (which can be introduced as a characterization parameter, regardless whether the London limit actually applies) as

$$1/\lambda_{L0}^2 = 4\pi Q_0 / c^2. \quad (4.4)$$

The quantities Q_0 and λ_{L0} describe the corresponding clean system and are determined only by the band structure parameters.

In Eq. (4.2),

$$G^R(\epsilon, \mathbf{p}) = \frac{\tilde{\epsilon} + \xi}{\tilde{\epsilon}^2 - \xi^2 - \tilde{\Delta}^2}, \quad F^R(\epsilon, \mathbf{p}) = \frac{\tilde{\Delta}}{\tilde{\epsilon}^2 - \xi^2 - \tilde{\Delta}^2}, \quad (4.5)$$

$$G^A(\epsilon, \mathbf{p}) = [G^R(\epsilon, \mathbf{p})]^*, \quad F^A(\epsilon, \mathbf{p}) = [F^R(\epsilon, \mathbf{p})]^*,$$

are the retarded (R) and advanced (A) “normal” (G) and “anomalous” (F) Green’s functions, averaged over disorder, where the conventionally introduced^{2,4} functions $\tilde{\epsilon}$ and $\tilde{\Delta}$ are defined below. For point disorder and due to the property (3.6), the “ladder” contribution³⁰ vanishes, and the current-current correlation functions (4.2) are determined by the products of disorder-averaged Green’s functions.

Further, in Eqs. (4.1), (4.2), and (4.5), ϵ is the energy relative to the Fermi level ϵ_F , and $\epsilon_\pm = \epsilon \pm \omega/2$, $\mathbf{p}_\pm = \mathbf{p} \pm \mathbf{k}/2$. We split the integration over momentum

$$\int \frac{d^3 \mathbf{p}}{(2\pi)^3} \dots = \nu_F \left\langle \int d\xi \dots \right\rangle_{\mathbf{n}}, \quad \langle \dots \rangle_{\mathbf{n}} = \int_{|\mathbf{n}|=1} \frac{d\mathbf{n}}{4\pi} \dots,$$

in a standard way into the integration over its absolute value $p = |\mathbf{p}|$, expressed in terms of $\xi = E(p) - \epsilon_F$, and averaging over its direction, expressed in terms of the unit vector $\mathbf{n} = \mathbf{p}/p$.

Equation (4.2) defines the correlation functions of the current components perpendicular to \mathbf{k} , see Eq. (3.6), and so, n_α are the components of $\mathbf{n} = (n_x, n_y, n_z)$ perpendicular to \mathbf{k} : if $\mathbf{k} = (0, 0, k)$, as in Fig. 3, then

$\alpha = x, y$. Since the spectrum is isotropic, the integral $I(\mathbf{nk}) = \int \frac{d\xi}{2\pi} \dots$ in Eq. (4.2) depends just on $\mathbf{nk} = n_z k$ and angular averaging is reduced to calculating the integral

$$\langle n_\alpha^2 I(\mathbf{nk}) \rangle_{\mathbf{n}} = \frac{1}{4} \int_{-1}^1 dn_z (1 - n_z^2) I(n_z k). \quad (4.6)$$

Note that for the integration order as in Eqs. (4.1) and (4.2) – first over ξ and then over ϵ – the contribution to $Q(\omega, k)$ arising from the dependence of the current operator on the vector potential is already compensated for.

It is convenient to introduce the (retarded) quasiclassical Green’s functions^{17,18}

$$\{g, f\}(\epsilon) = \frac{i}{\pi} \int d\xi \{G^R, F^R\}(\epsilon, \mathbf{p}), \quad (4.7)$$

which, according to Eq. (4.5), equal

$$g(\epsilon) = \frac{\tilde{\epsilon}}{\sqrt{\tilde{\epsilon}^2 - \tilde{\Delta}^2}} = \frac{v}{\sqrt{v^2 - 1}}, \quad (4.8)$$

$$f(\epsilon) = \frac{\tilde{\Delta}}{\sqrt{\tilde{\epsilon}^2 - \tilde{\Delta}^2}} = \frac{1}{\sqrt{v^2 - 1}}. \quad (4.9)$$

Within the Shiba theory⁴, the function

$$v = v(\epsilon) \equiv \frac{\tilde{\epsilon}}{\tilde{\Delta}} = \frac{g(\epsilon)}{f(\epsilon)} \quad (4.10)$$

satisfies the equation

$$v\Delta = \epsilon + \frac{1}{\tau_s} \frac{\sqrt{1 - v^2}}{\gamma^2 - v^2} v. \quad (4.11)$$

Here,

$$\gamma = \frac{1 - (\pi\nu_F J)^2}{1 + (\pi\nu_F J)^2} \quad (4.12)$$

is the parameter of the Shiba theory characterizing exchange coupling strength and τ_s is the scattering time on magnetic impurities,

$$\frac{1}{\tau_s} = \frac{n_s}{2\pi\nu_F} (1 - \gamma^2) = 2\pi\nu_F n_s \frac{J^2}{[1 + (\pi\nu_F J)^2]^2}.$$

In the weak coupling limit $\nu_F J \ll 1$ of the AG theory², $\gamma^2 = 1$.

We also introduce the function $h(\epsilon)$ as

$$\sqrt{\tilde{\epsilon}^2 - \tilde{\Delta}^2} = h(\epsilon) + \frac{i}{2\tau}, \quad (4.13)$$

which is related to $g(\epsilon)$ and $f(\epsilon)$ as

$$h(\epsilon) = \frac{1}{2} \left(\frac{\epsilon}{g(\epsilon)} + \frac{\Delta}{f(\epsilon)} \right). \quad (4.14)$$

In Eq. (4.13), τ is the scattering time on nonmagnetic impurities,

$$\frac{1}{\tau} = 2\pi\nu_F n u^2.$$

Solving Eq. (4.11) for v (in the general case – numerically), one obtains $g(\epsilon)$, $f(\epsilon)$, and $h(\epsilon)$. Integration over ξ in Eq. (4.2) is straightforward and we obtain

$$\langle jj \rangle^{RA}(\epsilon, \omega, k) = \frac{1}{2} [g(\epsilon_+)g^*(\epsilon_-) + f(\epsilon_+)f^*(\epsilon_-) + 1] \langle \bar{j}\bar{j} \rangle^{RA}(\epsilon, \omega, k), \quad \langle \bar{j}\bar{j} \rangle^{RA}(\epsilon, \omega, k) = \left\langle \frac{in_\alpha^2}{h(\epsilon_+) - h^*(\epsilon_-) + i/\tau - v_F \mathbf{n}k} \right\rangle_{\mathbf{n}}, \quad (4.15)$$

$$\langle jj \rangle^{RR}(\epsilon, \omega, k) = \frac{1}{2} [1 - g(\epsilon_+)g(\epsilon_-) - f(\epsilon_+)f(\epsilon_-)] \langle \bar{j}\bar{j} \rangle^{RR}(\epsilon, \omega, k), \quad \langle \bar{j}\bar{j} \rangle^{RR}(\epsilon, \omega, k) = \left\langle \frac{in_\alpha^2}{h(\epsilon_+) + h(\epsilon_-) + i/\tau - v_F \mathbf{n}k} \right\rangle_{\mathbf{n}}, \quad (4.16)$$

and $\langle jj \rangle^{AA}(\epsilon, \omega, k) = [\langle jj \rangle^{RR}(\epsilon, \omega, k)]^*$, $\langle \bar{j}\bar{j} \rangle^{AA}(\epsilon, \omega, k) = [\langle \bar{j}\bar{j} \rangle^{RR}(\epsilon, \omega, k)]^*$. Angular averaging in Eq. (4.15) and (4.16) can also be performed explicitly according to Eq. (4.6),

$$\begin{aligned} & \langle \bar{j}\bar{j} \rangle^{RR,RA}(\epsilon, \omega, k) = \\ & = \frac{-i}{4v_F k} \left[\left(1 - \frac{l_0^2}{(v_F k)^2} \right) \ln \frac{l_0 - v_F k}{l_0 + v_F k} - 2 \frac{l_0}{v_F k} \right], \quad (4.17) \end{aligned}$$

where

$$l_0 = \begin{cases} h(\epsilon_+) - h^*(\epsilon_-) + i/\tau, & \text{for } RA, \\ h(\epsilon_+) + h(\epsilon_-) + i/\tau, & \text{for } RR. \end{cases}$$

Equations (4.1), (4.15), (4.16), and (4.17), combined with Eqs. (4.8)-(4.14) of the Shiba theory, provide the answer for the current response function $Q(\omega, k)$ and constitute the main result of our work. Within the approximations of the theory, these equations are valid at arbitrary values of frequency ω , temperature T , and six microscopic parameters characterizing the system. Three standard parameters^{19,20} describe the clean system:

- the superconducting transition temperature T_{c0} or, equivalently, the superconducting order parameter Δ_0 at $T = 0$ for a system without magnetic impurities;
- the current response Q_0 [Eq. (4.3)] or, equivalently, the formally introduced London penetration depth λ_{L0} [Eq. (4.4)] for a clean system at $T = 0$;
- the Fermi velocity v_F .

The other three parameters describe disorder:

- the nonmagnetic scattering time τ ;

- the magnetic scattering time τ_s ;
- the exchange coupling strength $\nu_F J$ or, equivalently, the Shiba parameter γ [Eq. (4.12)].

In the general case, Eqs. (4.1), (4.15), (4.16), and (4.17) provide the most explicit analytical form of the current response function $Q(\omega, k)$ possible. The function is given by the integral over energy ϵ in Eq. (4.1), where the dependence of the integrand on the absolute value of momentum k is explicit in Eqs. (4.17), while the dependence on ϵ is obtained from the well-known Shiba equation (4.11), the solution to which determines the functions $g(\epsilon)$, $f(\epsilon)$, and $h(\epsilon)$.

For arbitrary values of parameters, the solution to the Shiba equation and the integrations over ϵ for the current response $Q(\omega, k)$ and over k for the surface impedance $Z(\omega)$ [Eq. (3.3)] need to be carried out numerically. The generality of the obtained results, however, should make them applicable to a variety of realistic experimental regimes.

On the other hand, in a number of limiting cases, the general formulas can be further simplified and in many cases explicit analytical expressions for the current response function and surface impedance can be obtained. Analysis of such limiting cases is straightforward and we do not present it here.

In the weak coupling limit $\nu_F J \ll 1$ of the AG theory² ($\gamma = 1$), the results of Refs. 23,24 are (presumably) recovered, and in the complete absence of magnetic impurities [$1/\tau_s = 0$, $h(\epsilon) = \sqrt{\epsilon^2 - \Delta^2}$, $g(\epsilon) = \epsilon/h(\epsilon)$, $f(\epsilon) = \Delta/h(\epsilon)$] the Mattis-Bardeen theory¹⁹ is reproduced.

In the next two sections, we consider the low-frequency limit $\omega \ll \Delta$, most relevant for practical applications to SRF cavities, and concentrate on the key property

pertaining to the presence of magnetic impurities – finite residual surface resistance in the GSC regime.

V. LOW FREQUENCY EXPANSION

The typical operating frequencies of the SFR cavities are $\omega \sim c/L \sim 10^{-2} \text{meV} \ll \Delta \sim 1 \text{meV}$, where $L \sim 10 \text{cm}$

is the typical size of the cavity. Thus for practical applications to SRF cavities, one may perform the low-frequency expansion in $\omega \ll \Delta$. Separating the real (“nondissipative”) and imaginary (“dissipative”) parts [Eq. (3.4)] of $Q(\omega, k)$ [Eq. (4.1)], in the leading order in ω for each, we obtain,

$$Q_1(k) = Q_0 \frac{3i}{2} \int_{-\infty}^{+\infty} d\epsilon \tanh \frac{\epsilon}{2T} \{ [f(\epsilon)]^2 \langle \bar{j}j \rangle^{RR}(\epsilon, 0, k) - [f^*(\epsilon)]^2 \langle \bar{j}j \rangle^{AA}(\epsilon, 0, k) \}, \quad (5.1)$$

$$Q_2(\omega, k) = Q_0 \omega \int_{-\infty}^{+\infty} d\epsilon \left(-\frac{dn_0(\epsilon)}{d\epsilon} \right) \bar{Q}_2(\epsilon, k), \quad (5.2)$$

$$\bar{Q}_2(\epsilon, k) = \frac{3}{2} \{ [f(\epsilon)]^2 \langle \bar{j}j \rangle^{RR}(\epsilon, 0, k) + [f^*(\epsilon)]^2 \langle \bar{j}j \rangle^{AA}(\epsilon, 0, k) + [1 + |g(\epsilon)|^2 + |f(\epsilon)|^2] \langle \bar{j}j \rangle^{RA}(\epsilon, 0, k) \}. \quad (5.3)$$

Here, $n_0(\epsilon) = 1/[\exp(\epsilon/T) + 1]$ is the Fermi distribution function.

The real part $Q_1(k)$ [Eq. (5.1)] is finite at $\omega = 0$ and determines the penetration depth $\lambda(\omega = 0)$ [Eq. (3.3)] of the quasistatic magnetic field (Meissner effect). On the other hand, the imaginary part $Q_2(\omega, k) \propto \omega$ [Eqs. (5.2) and (5.3)], which determines the dissipation, is nonzero only at finite frequency and is linear in it³⁵ at $1/\tau_s \gg \omega$. Since $Q_2(\omega, k)$ is smaller than $Q_1(k)$ at least in ω/Δ , one may also expand Eq. (3.3) in $Q_2(\omega, k)$ to obtain

$$Z(\omega) = \frac{32\pi\omega}{c^4} \int_0^{+\infty} dk \frac{Q_2(\omega, k)}{[k^2 + 4\pi Q_1(k)/c^2]^2}. \quad (5.4)$$

Thus the surface resistance $R(\omega) \propto \omega^2$ is quadratic in frequency, which is the most common dependence observed experimentally in SRF cavities¹³.

VI. RESIDUAL SURFACE RESISTANCE

We now turn to the key finding of our work. The function $\bar{Q}_2(\epsilon, k)$ [Eqs. (5.3)] describes the contribution to the dissipative part $Q_2(\omega, k)$ [Eq. (5.2)] of the current response function from quasiparticles with a given energy ϵ , while the derivative $-dn_0(\epsilon)/d\epsilon$ constrains their distribution to the range $|\epsilon| \lesssim T$ around the Fermi level. As is well known^{18,30}, the real part $g_1(\epsilon)$ of the normal Green’s function $g(\epsilon) = g_1(\epsilon) - ig_2(\epsilon)$ [Eq. (4.8)] determines the DOS

$$\nu(\epsilon) = \nu_F g_1(\epsilon). \quad (6.1)$$

Inspecting Eqs. (5.2) and (5.3), we notice that

$$\bar{Q}_2(\epsilon, k) = 0 \Leftrightarrow \nu(\epsilon) = 0. \quad (6.2)$$

Indeed, if $g_1(\epsilon) = 0$, i.e., $g(\epsilon) = -ig_2(\epsilon)$ is imaginary, then, according to Eqs. (4.8), (4.9), and (4.14), so are $f(\epsilon) = -if_2(\epsilon) = -i\sqrt{1 + g_2^2(\epsilon)}$ and $h(\epsilon)$. In this case, $\langle \bar{j}j \rangle^{RA}(\epsilon, 0, k) = \langle \bar{j}j \rangle^{RR}(\epsilon, 0, k) = \langle \bar{j}j \rangle^{AA}(\epsilon, 0, k)$ and the function (5.3) does vanish,

$$\bar{Q}_2(\epsilon, k) = \frac{3}{2} \langle \bar{j}j \rangle^{RA}(\epsilon, 0, k) [-2f_2^2(\epsilon) + 1 + g_2^2(\epsilon) + f_2^2(\epsilon)] = 0.$$

We do not present a more cumbersome rigorous proof of the converse here. Instead, the property (6.2) is clearly illustrated in Figs. 1(a), (b), (c), (d).

Thus, as one would intuitively expect, only the energies ϵ at which the DOS $\nu(\epsilon)$ is nonzero contribute to dissipation. At $T = 0$ the envelope function $-dn_0(\epsilon)/d\epsilon \rightarrow \delta(\epsilon)$ becomes a delta-function and only the excitations at the Fermi level $\epsilon = 0$ contribute,

$$Q_2(\omega, k)|_{T=0} = Q_0 \omega \bar{Q}_2(\epsilon = 0, k). \quad (6.3)$$

According to (6.2), as the central result, we obtain that the system exhibits finite surface resistance (5.4) at $T = 0$ if and only if the DOS at the Fermi level is nonvanishing, i.e. the system is in the GSC regime.

$$R(\omega)|_{T=0} > 0 \Leftrightarrow \nu(\epsilon = 0) > 0.$$

The result is illustrated in Figs. 1. If the spectrum has a gap $\bar{\Delta}$ (DOS “tails”^{8–10} are not captured by the AG-Shiba theory), Figs. 1(a),(c),(e), the surface resistance obeys an activation law $R(\omega) \propto e^{-\bar{\Delta}/T}$ at temperatures $T \ll \bar{\Delta}$, eventually vanishing at $T = 0$.

On the other hand, in the gapless regime, Figs. 1(b),(d),(f), the surface resistance $R(\omega)$ saturates to a finite value at $T = 0$. We note that in

experiments it is quite typical²² for $R(\omega)$ to exhibit both the saturation at $T = 0$ and an activation behavior $R(\omega) \propto \exp(-\Delta^*/T)$ at finite but low temperatures $T \lesssim \Delta^*$, with Δ^* close to the value of the superconducting order parameter Δ of a clean sample. Such behavior can be realized, if the finite DOS $\nu(\epsilon = 0) \ll \nu_F$ at the Fermi level is much smaller than the DOS $\nu(\epsilon \gtrsim \Delta) \sim \nu_F$ above the “nominal” gap. In the framework of the Shiba theory, this is possible in the limit of low magnetic scattering rate $1/\tau_s \ll \Delta$ and stronger exchange coupling $\nu_F J \sim 1$, the case shown in Figs. 1(b),(d),(f). Thus, our microscopic model can reproduce the typical experimental temperature dependence of the surface resistance.

VII. CONCLUSION

In conclusion, we developed a microscopic analytical theory of the surface impedance of s-wave superconductors with magnetic impurities. The theory can potentially be applied to a variety of superconducting systems and is of direct relevance to the problem of the residual surface resistance of SFR cavities. We explicitly demonstrated that, in the regime of gapless superconductivity, the system exhibits saturation of the surface resistance at zero temperature – a routinely observed, but largely un-

explained experimental feature. This substantiates the recent conjecture¹⁶ that magnetic impurities, formed at the surface of the oxide surface layer, could be the dominant dissipation mechanism limiting the performance of the SFR cavities. Our theory is valid in the wide range of parameter values and can be used for direct comparison with experimental data, as will be presented elsewhere³⁶.

Note added. After a preprint³⁷ of the present work became available, a paper³⁸ came out, in which the same problem was studied in the diffusive limit ($\tau\Delta \ll 1$) and for weak exchange coupling ($\pi\nu_F J \ll 1$), with an emphasis on the quasiparticle contribution from the vicinity of the spectral gap. The approach of Ref. 38 based on the Keldysh formalism and Usadel equation is equivalent to ours in that limit and most of the analytical results of Ref. 38 can be obtained as asymptotic expansions of our general formulas.

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of electrons at the interface with vacuum, this assumption is generally not crucial: since the current is created predominantly by electrons with momenta nearly parallel to the surface, the impedance is only weakly sensitive to the properties of the surface scattering^{33,34}.

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the integral over ϵ in Eq. (5.2) has a logarithmic divergency at $\epsilon = \Delta$, which has to be cut by frequency ω . However, at finite $1/\tau_s$, the integral is convergent.

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