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***A new first-principles calculation of field-dependent
RF surface impedance of BCS superconductor***

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A NEW FIRST-PRINCIPLES CALCULATION OF FIELD-DEPENDENT RF SURFACE IMPEDANCE OF BCS SUPERCONDUCTOR*

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Abstract

There is a need to understand the intrinsic limit of radiofrequency (RF) surface impedance that determines the performance of superconducting RF cavities in particle accelerators. Here we present a field-dependent derivation of Mattis-Bardeen theory of the RF surface impedance of BCS superconductors based on the shifted density of states resulting from coherently moving Cooper pairs. Our theoretical prediction of the effective BCS RF surface resistance (R_s) of niobium as a function of peak surface magnetic field amplitude agrees well with recently reported record low loss resonant cavity measurements from JLab and FNAL with carefully, yet differently, prepared niobium material. The surprising reduction in resistance with increasing field is explained to be an intrinsic effect.

INTRODUCTION

Superconducting radiofrequency (SRF) accelerating cavities for particle accelerators made from bulk niobium (Nb) materials are the state-of-art facilities for exploring frontier physics. Remarkable results have been achieved: for a single-cell re-entrant shape cavity in Cornell University, the maximum accelerating gradient has been pushed to 52 MV/m with quality factor (Q) higher than 10^{10} at 1.3 GHz and 2 K temperature [1]; and for a single-cell CEBAF shape cavity in JLab, the Q has been pushed to 5×10^{10} with 80 mT magnetic field at 1.47 GHz and 2K temperature [2]. Theories are needed to explain the limitations on the magnetic field, as well as the Q we can achieve for Nb cavities [3], and to be extended to the alternative materials for possible SRF applications. In this paper, the authors are trying to address the intrinsic limit of RF surface impedance that determines the performance of SRF cavities in particle accelerators based on an extension [4] of Mattis-Bardeen theory [5].

EXISTING THEORIES

In Figure 1, we show several cavity performance results (Q vs magnetic field, or R_s vs magnetic field) of several Nb cavities measured in JLab. From the figure one can see that for the 7-cell cavity, an additional electropolishing (EP) after buffer chemical polishing (BCP) extended the peak magnetic field the cavity can achieve, at the same time degraded the quality factor [6]. The single cell cavity

with 3 h 1400°C baking has a quality factor of 5×10^{10} with 80 mT magnetic field, with a quench effect at ~ 100 mT [2].

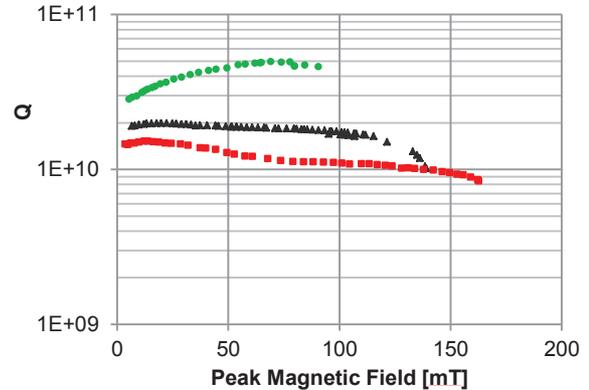


Figure 1: Cavity performance at 2 K for: \blacktriangle 1.5 GHz 7-cell CEBAF cavity with 230 μm BCP \blacksquare 230 μm BCP + 34 μm EP \bullet 1.5 GHz single cell CEBAF cavity with 3 h 1400 $^{\circ}\text{C}$ baking.

The RF surface impedance of a superconductor may be considered a consequence of the inertia of the Cooper pairs in the superconductor. The resulting incomplete shielding of RF field allows the superconductor to store RF energy inside its surface, which may be represented by surface reactance. The RF field that enters the superconductor will interact with quasi-particles, causing RF power dissipation, represented by R_s . Mattis-Bardeen theory was developed to calculate the surface impedance of conventional superconductors at high frequency, low temperature and low field limit [5]. It started from the BCS theory [7], by using the electron states distribution at 0 K and probability of occupation at $T < T_c$, the single-particle scattering operator was calculated and applied into the anomalous skin effect theory to get the surface impedance.

Theories have been developed trying to address the behavior of the cavity performance, and a summary can be found in [8]. These theories, however, did not give a theoretical limit for the quality factor while changing the magnetic field.

In this paper, surface impedance is calculated based on a statement in the BCS theory: States with a net current flow can be obtained by taking a pairing ($k_1\uparrow, k_2\downarrow$) with $k_1+k_2 = 2q$, and $2q$ the same for all virtual pairs [7]. By applying this change into the Mattis-Bardeen theory, a new form of RF field dependence of the surface impedance has been obtained and compared to the experimental results.

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EXTENSION OF MATTIS-BARDEEN THEORY

In BCS theory, paired particles in the ground state, with total mass $2m$ and zero total momentum that occupy state $(\mathbf{k}\uparrow, -\mathbf{k}\downarrow)$, with velocity V_k in random direction, and energy relative to the Fermi sea ε_F (with Fermi velocity at V_F and Fermi momentum P_F) of ε_k , have been considered to give minimum free energy for superconductors. States with a net flow in a certain direction can be obtained by taking a pairing $(\mathbf{k}+\mathbf{q}\uparrow, -\mathbf{k}+\mathbf{q}\downarrow)$, with total momentum $2\mathbf{q}$ the same for all Cooper pairs, corresponding to net velocity $V_s = \hbar\mathbf{q}/m$. This change could be represented in the Fermi sphere, depicted in Figure 2.

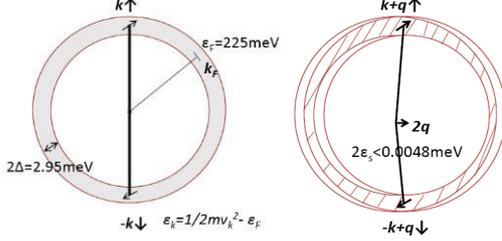


Figure 2. Fermi sphere of the superconductor: in the low field limit (left), and with net momentum $2q$ the same for all Cooper pairs (right). Numbers labeled are based on typical Nb parameters shown in [4].

With this extension, the Bloch energies for the electrons in a Cooper pair no longer remain the same; they split into two different Bloch energies, shown as equations (4) and (5) in [4], following with an angle dependent on each of them: even though the absolute value of V_s is much smaller than that of V_F , the angle α between these two velocities significantly affects the Bloch energies for the electrons. The modified density of state and probability of occupation at $T < T_c$, with their angle integrations shown as equations (21) and (20) in [4], are both angle dependent. The modified density of state, as well as the probability of occupation at $T < T_c$, as a function of the Bloch energy that were shown in Figure 1 in [9] in the low-field limit and Cooper pairs' net momentum to be 0, are plotted in Figure 3 integrated in angle, and in Figure 4 with angle dependence, under a certain Cooper pairs' net momentum.

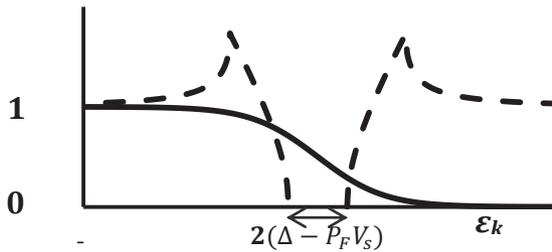


Figure 3: Density of states (dotted curve) and distribution function (solid curve) with moving cooper pairs, angle averaged, plotted with $P_F V_s = \Delta/2$ and $T/T_c = 0.97$.

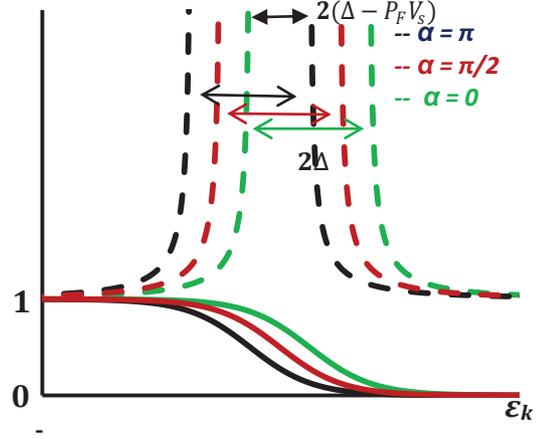


Figure 4: Density of states (dotted curve) and distribution function (solid curve) with moving cooper pairs, angle-dependent.

From the Figures above one can see that even in the average effect, the gap is reduced by a value of $P_F V_s$, the energy that is needed to separate the electrons in a Cooper pair will not change while α changes, with its value constant at 2Δ . If the tunnelling effect is used to measure the gap, which is actually measuring the gap in quasi-particle distribution, this would show a value of $2(\Delta - P_F V_s)$; whereas if infrared spectrum were used to measure the energy to break the Cooper pairs, the value would be 2Δ .

The changes in the modified density of states and probability of occupation cause a significant change in the single particle scattering operator [4, 7], which leads to a field dependence of R_s , with the detailed calculations shown in [4].

CALCULATION RESULTS AND EXPLANATION

Using the following characteristic parameters: $\Delta_0/kT_c(0) = 1.85$, $T_c(0) = 9.25$ K, $T = 2.0$ K, coherence length $\xi_0 = 40$ nm, London penetration depth $\lambda_L(0) = 32$ nm, and mean free path $\iota = 50$ nm, the BCS surface resistances under different field level at 1.5 GHz are calculated. The result is plotted in Figure 5, together with the recently reported R_s measurement between H_{pk} of 5 mT and 90 mT on a CEBAF shape single cell cavity made from ingot niobium with 3 hours 1400°C high temperature baking by Dhakal *et al* [2], after subtracting a 1.7 nΩ temperature independent residual resistance. Similar procedure has been applied to FNAL fine grain Tesla shaped cavity at 1.3 GHz using the same parameters as above, and compared with the experimental data [10] after subtracting 3.0 nΩ residual resistance.

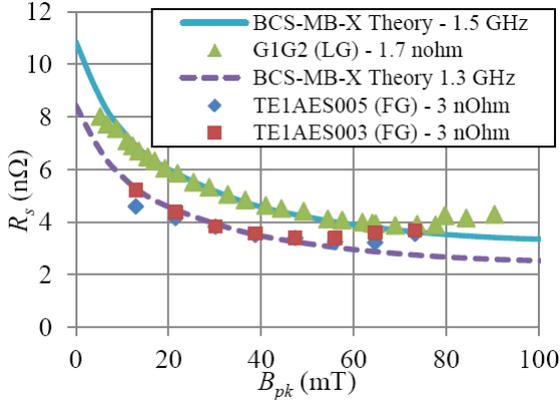


Figure 5: Field-dependent BCS surface resistance at 2.0 K, calculated by Xiao’s code and recent very low loss cavity test data from JLab at 1.5 GHz [2] and FNAL at 1.3 GHz [10] prepared by different methods.

The calculations and the experimental results for three cavities shown above, exhibit a corresponding increasing in Q with field well beyond the range of the familiar “low-field Q slope” at <20 mT, to a value of ~ 80 mT.

From the “golden rule” [9] with $R_s \propto \int_{\Delta}^{\infty} [f(E) - f(E + \hbar\omega)]g(E)dE$, with $\hbar\omega$ the photon energy, the quasi-particles, after absorbing photons, are tending to jump back to their original state after the so-called relaxation time, and at the same time, release energy and cause power dissipation, as shown in the top of Figure 6.

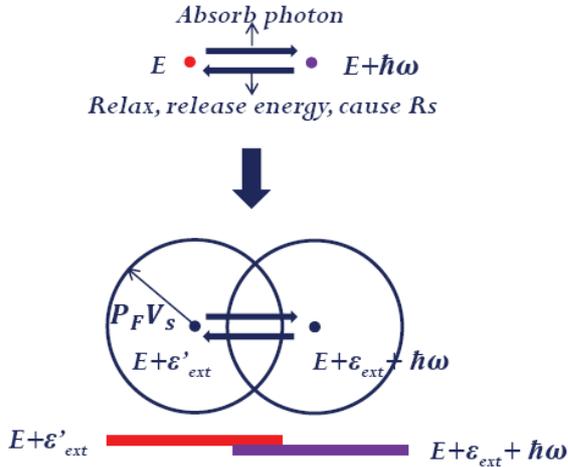


Figure 6: Energy relaxation procedure of quasi-particles: in low field limit (top), and with net momentum $2q$ the same for all Cooper pairs (bottom).

With an angle between \mathbf{V}_F (which could be in any random direction) and \mathbf{V}_s , the Bloch energy for two electrons in a Cooper pair, get split and an angle dependence appears, the energy relaxation which happens between two fixed modified energy states $E + \hbar\omega$ and E in the low field limit changes to between $E + \varepsilon_{\text{ext}} + \hbar\omega$ and $E + \varepsilon'_{\text{ext}}$, with $\varepsilon_{\text{ext}} = P_F V_s \cos\alpha$ being the addition energy from the energy split, and $\varepsilon'_{\text{ext}}$ that for another electron state with different angle α' .

The golden rule in this extension theory changes to $R_s \propto \int_{\Delta}^{\infty} [f(E + \varepsilon_{\text{ext}} + \hbar\omega) - f(E + \varepsilon'_{\text{ext}})] [f(\varepsilon_{\text{ext}}) + f(-\varepsilon_{\text{ext}})] g(E, \alpha) dE$. A consequence appears to be attractive: While the energy relaxation happens from high energy (purple dot in the top chart of Figure 6) to low energy (red dot in the top chart of Figure 6) in Mattis-Bardeen theory, it is possible this procedure happens from low energy (red bar in the bottom chart of Figure 6) to high energy (purple bar in the bottom chart of Figure 6), and the overlap between these two energy ranges could be significant since that $P_F V_s \gg \hbar\omega$ could happen. Although this process “borrows” energy from those scatterings from high energy to low energy, the net effect still obeys the 2nd law of thermodynamics and gives a net power dissipation effect, thus a positive yet decreasing R_s appears with field increasing up to a certain level.

SUMMARY

A field-dependent derivation of Mattis-Bardeen theory of the RF surface impedance of BCS superconductors has been introduced. Calculation results show a good correspondence to the recent high- Q experimental results. The attractive Q -increase with field increase up to 80 mT is explained based on the quasi-particle relaxation procedure that may happen from a lower energy level to higher one.

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