Strong Surface Contribution to the Nonlinear Meissner Effect in *d*-Wave Superconductors

A. Zare, T. Dahm, and N. Schopohl

Institut für Theoretische Physik and Center for Collective Quantum Phenomena, Universität Tübingen, Auf der Morgenstelle 14, D-72076 Tübingen, Germany

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We demonstrate that in a d-wave superconductor the bulk nonlinear Meissner effect is dominated by a surface effect due to Andreev bound states at low temperatures. The contribution of this surface effect to the nonlinear response coefficient follows a $1/T^3$ law with the opposite sign compared to the bulk $1/T$ behavior. The crossover from bulk dominated behavior to surface dominated behavior occurs at a temperature of $T/T_c \sim 1/\sqrt{\kappa}$. We present an approximate analytical calculation, which supports our numerical calculations and provides a qualitative understanding of the effect. The effect can be probed by intermodulation distortion experiments.

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In a superconductor with nodes in the gap function, quasiparticles near the gap nodes lead to an intrinsic nonlinear electromagnetic response [1]. In a d-wave superconductor this nonlinear Meissner effect appears as a linear magnetic field dependence of the magnetic penetration depth at low temperatures [1,2], but can more sensitively be probed by temperature dependent intermodulation distortion or harmonic generation experiments [3]. The nonlinear response coefficient shows an upturn at low temperatures following a $1/T$ law in a clean system down to temperatures of the order of $1/\kappa$, where κ is the Ginzburg-Landau parameter of the superconductor. This behavior has been confirmed by intermodulation distortion experiments on high-T_c cuprate superconductors [4–6]. At even lower temperatures nonlocal effects [7], as impurity effects [8], lead to a saturation of this low temperature upturn.

At a surface that has a finite angle with the (100) direction of the crystal, Andreev bound states appear within a coherence length from the surface [9–12]. These states split in the presence of a screening current [13–15] and they carry an anomalous counterflowing paramagnetic surface current [13,16,17]. In previous work we have shown that the anomalous surface current leads to a strong modification of linear response properties [18,19]. Here, we study its influence on the nonlinear Meissner effect. Earlier work has found that the magnetic field dependence of the penetration depth is affected only weakly by surface Andreev bound states [17]. Here, we will show that the contribution of the surface Andreev bound states to the nonlinear response coefficient follows a $1/T^3$ law, which will ultimately dominate the bulk $1/T$ behavior at sufficiently low temperatures. We show that the crossover from bulk dominated behavior to surface dominated behavior occurs at a comparatively high temperature of $T/T_c \sim 1/\sqrt{\kappa}$. This means that even for a high $\kappa \sim 100$ as is realized in the cuprates the effect will become dominant at temperatures below about $0.1T_c$.

In order to calculate the nonlinear response coefficient we solve Eilenberger's equations [20,21] with full momentum and energy dependence. The gap equation and the equation for the current density

$$\mathbf{j}(\mathbf{r}) = 4\pi e N_0 k_B T \sum_{\varepsilon_n>0}^{\omega_c} \langle \mathbf{v}_F(\hat{\mathbf{k}}) g(\mathbf{r}, \hat{\mathbf{k}}, \varepsilon_n)\rangle_{\mathrm{FS}} \tag{1}$$

are solved self-consistently together with the Maxwell equation

$$\nabla \times \nabla \times \mathbf{A}(\mathbf{r}) = \mu_0 \mathbf{j}(\mathbf{r}). \tag{2}$$

Here, $\mathbf{A}$ is the vector potential, $\mathbf{v}_F$ is the Fermi velocity, N_0 the single spin density of states, and $g(\mathbf{r}, \hat{\mathbf{k}}, \varepsilon_n)$ the Eilenberger propagator on Matsubara frequencies ε_n. The full set of equations and a description of the numerical solution procedure based on the Riccati technique [22] can be found in Ref. [19].

We consider a homogeneous superconducting half-space in the region $x \geq 0$ with an external magnetic field $\mathbf{B}_0$ parallel to the z axis, which shall be aligned with the c axis of the crystal structure. In this geometry the current flows along the y direction in the superconductor. The gap function is assumed to have a rotated d-wave form $\Delta(x, \theta) = \Delta_0(x)\cos 2(\theta - \alpha)$, where α is the angle of rotation with respect to the surface and the angle θ denotes the direction of momentum within the ab plane. As this problem is translationally invariant in y and z direction, all quantities only depend on the spatial variable x. The self-consistent solution of Eilenberger's equations on real frequencies allows us to calculate the local, angular resolved normalized density of states

$$N(E, x, \theta) = -\mathrm{Im} g(x, \theta, i\epsilon_n \to E + i0^+). \tag{3}$$

The equation for the y component of the current density (1) can be transformed by contour integration and analytic continuation to the real axis [2,8]:

$$j(x) = \frac{2}{\pi} e N_0 v_F \int_{-\infty}^{\infty} dE \int_0^{\pi} d\theta \sin\theta \cdot f(E)[N_+(E, x, \theta) - N_-(E, x, \theta)], \quad (4)$$

where $f(E) = \frac{1}{1+e^{E/T}}$ is the Fermi function and $N_\pm$ denotes the normalized density of states for comoving and countermoving quasiparticles relative to the condensate flow, i.e., $N_+(E, x, \theta) = N_-(E, x, \theta - \pi)$. Once the current density distribution $j(x)$ is obtained, the magnetic field distribution $B(x)$ and the vector potential $A(x)$ are found from integration of Eq. (2).

For a high-κ superconductor the length scale of variation of the vector potential, the magnetic penetration length λ, is a factor of κ larger than the variation of the Eilenberger propagator g on the length scale of the coherence length $\xi_0 = \hbar v_F/\pi\Delta_0$. Thus, for temperatures $T/T_c \gtrsim 1/\kappa$ it is a very good approximation to evaluate the angular resolved local density of states by a local Doppler shift of the fully nonlocal Eilenberger propagator in the absence of a vector potential, i.e.,

$$N_\pm(E, x, \theta) = N(E \pm e\mathbf{v}_F \cdot \mathbf{A}(x), x, \theta), \quad (5)$$

where $N(E, x, \theta)$ on the right-hand side is calculated with $\mathbf{A}(x) = 0$ but fully includes the surface Andreev bound states. Here, we have chosen the real gauge in which the vector potential is directly proportional to the superfluid velocity $\mathbf{v}_s(x) = -\frac{e}{m}\mathbf{A}(x)$.

In order to determine the lowest order nonlinear response, Eq. (5) is substituted into Eq. (4) and we make a Taylor series expansion of j in the vector potential $A(x)$:

$$j(x) = -2e^2 v_F^2 N_0 \eta_1(x) A(x) + \frac{2e^4 v_F^4 N_0}{\Delta_0^2} \eta_3(x) A^3(x) + \mathcal{O}(A^5). \quad (6)$$

Here, the even terms in A cancel out due to symmetry. After a partial integration the dimensionless expansion coefficients are given by the expressions

$$\eta_1 = 1 + \frac{2}{\pi} \int_0^{\pi} d\theta \sin^2\theta \int_{-\infty}^{\infty} dE \frac{\partial f}{\partial E} N(E, x, \theta), \quad (7)$$

$$\eta_3 = -\Delta_0^2 \frac{2}{\pi} \int_0^{\pi} d\theta \sin^4\theta \int_{-\infty}^{\infty} dE \frac{\partial^3 f}{\partial E^3} N(E, x, \theta), \quad (8)$$

where Δ_0 is the zero temperature gap value in the bulk. Note that in contrast to the bulk calculation [3,8] the expansion coefficients now depend on the distance from the surface. Within a distance of the order of the coherence length they contain contributions from the Andreev bound states. The coefficient η_1 describes the linear response, and the coefficient η_3 the lowest order nonlinear response. The spatial dependence of η_3 is shown in Fig. 1 for a (110) surface ($\alpha = \pi/4$) at a temperature of $T = 0.1T_c$. Deep in the bulk, η_3 is positive and reaches the low temperature value $\Delta_0/2T$ known from previous work [3]. However, when the surface is approached within a few coherence lengths, η_3 changes sign and reaches extremely large negative values at the surface.

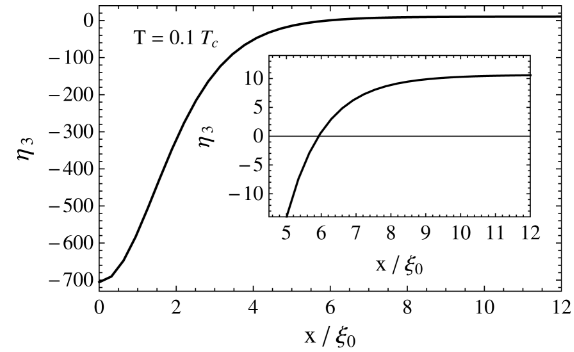

FIG. 1. Spatial dependence of the nonlinear coefficient η_3 at $T = 0.1T_c$ and $\alpha = \pi/4$ as a function of the distance x from the surface in units of the coherence length ξ_0. Inset: larger scale for $x > 4\xi_0$, highlighting the sign change of η_3.

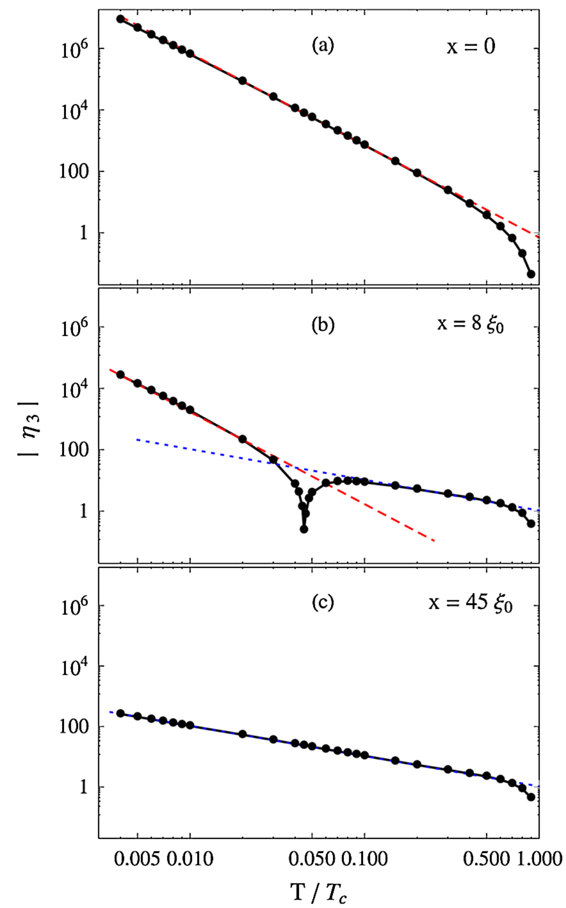

FIG. 2 (color online). Double logarithmic plot of $|\eta_3|$ as a function of temperature T/T_c for three selected positions: (a) $x = 0$, (b) $x = 8\xi_0$, and (c) $x = 45\xi_0$. The red dashed lines show a $1/T^3$ dependence, and the blue dotted lines a $1/T$ dependence.

The temperature dependence of the modulus $|\eta_3|$ is shown in Fig. 2 on a double logarithmic scale for three selected spacial positions. Figure 2(c) shows the temperature dependence at $x = 45\xi_0$ in the bulk. As is well known from previous work, $|\eta_3|$ follows a $1/T$ law at low temperatures (blue dotted line). Right at the surface ($x = 0$), however, Fig. 2(a) demonstrates that $|\eta_3|$ is following a $1/T^3$ behavior (red dashed line). In Fig. 2(b) an intermediate position at $x = 8\xi_0$ is shown. In this case, at higher temperatures a $1/T$ law is followed. At a certain temperature, η_3 changes sign and starts to follow a $1/T^3$ behavior below that temperature. These results clearly show that the nonlinear response coming from the surface area, where the Andreev bound states are present, is much stronger and of opposite sign than the nonlinear response in the bulk.

In a typical intermodulation experiment only the total response of the system is probed. The quantity that is observed is the nonlinear change of the total inductance of the system [3]. The total inductance L can be calculated from the total kinetic and magnetic field energy in the system via the equation

$$\frac{1}{2}LI^2 = \frac{1}{2\mu_0}\int_0^\infty dx(B^2(x) - \mu_0 j(x)A(x)), \tag{9}$$

where $I = \int_0^\infty dx\, j(x)$ is the total current per unit length [3]. Using Eq. (2), $B = dA/dx$, and the fact that the magnetic field vanishes in the bulk, Eq. (9) can be brought by partial integration into the more convenient form

$$L = -\frac{A_0}{I} \tag{10}$$

with $A_0 = A(x = 0)$. To lowest order in A_0 the total current I generally will be of the form

$$I = a_1 A_0 + a_3 A_0^3. \tag{11}$$

The intermodulation response is proportional to the nonlinear coefficient $\frac{\partial^2 L}{\partial I^2}|_{I=0}$ [3]. A straightforward calculation shows that this quantity can be related to the expansion coefficients a_1 and a_3 using Eq. (10):

$$\frac{\partial^2 L}{\partial I^2}\bigg|_{I=0} = \frac{2a_3}{a_1^4}. \tag{12}$$

We have determined a_1 and a_3 from our numerical solution of Eilenberger's equations. The resulting values for $|\frac{\partial^2 L}{\partial I^2}|_{I=0}$ are shown in Fig. 3 as a function of reduced temperature for $\kappa = 63$ (solid black circles) and $\kappa = 1000$ (solid red squares) on a double logarithmic scale. Decreasing the temperature from T_c, for $\alpha = \pi/4$ the nonlinear coefficient initially decreases and changes sign at a temperature near $T/T_c \approx 2.4/\sqrt{\kappa}$. Below that temperature the nonlinear coefficient increases following a $1/T^3$ law and finally diverges at a temperature near $T/T_c \approx 1/\kappa$. For comparison the behavior for $\kappa = 63$ and $\alpha = 0$ is also shown, when the surface states are absent (open circles). In this case there is no sign change and the nonlinear coefficient follows a $1/T$ behavior at low temperatures, as known from the bulk.

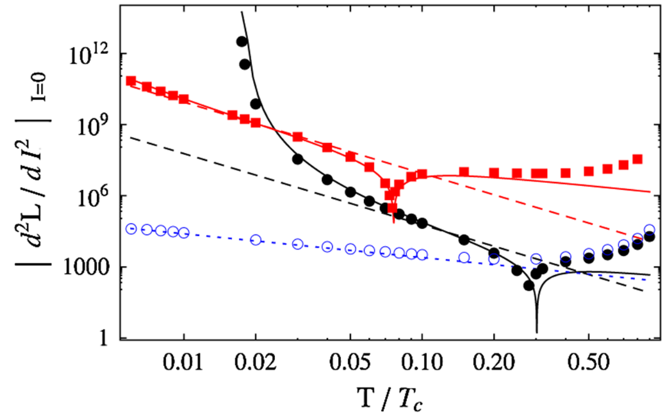

FIG. 3 (color online). Double logarithmic plot of $|\frac{\partial^2 L}{\partial I^2}|_{I=0}$ as a function of temperature T/T_c for $\kappa = 63$ and $\alpha = \pi/4$ (solid black circles), for $\kappa = 1000$ and $\alpha = \pi/4$ (solid red squares), and for $\kappa = 63$ and $\alpha = 0$ (open blue circles). The dashed lines show a $1/T^3$ behavior, and the dotted line a $1/T$ behavior. The solid lines show the approximation Eq. (16) for $\kappa = 63$ (black) and $\kappa = 1000$ (red), respectively.

In order to check the validity of the numerical calculations and obtain a physical understanding of the results, we made an approximate analytical solution of the problem, which we present now. For a piecewise constant gap function, Eilenberger's equations can be solved analytically [22]. As an approximation we assume that the d-wave gap is constant in space. Then the analytical solution of Eilenberger's equations allows us to determine the residue of the zero energy pole of the Eilenberger propagator analytically, which contains the contributions from the zero energy bound states at the surface. As a result, we find the following expression for the bound state contribution to the local, angular resolved density of states for $\alpha = \pi/4$ in the absence of an external field:

$$N_{\rm bs}(E, x, \theta) = \pi\Delta_0|\sin 2\theta|e^{-(4/\pi)|\sin\theta|(x/\xi_0)}\delta(E). \tag{13}$$

The δ function shows that the bound states are only present at zero energy. The exponential factor drops off on a length scale of the coherence length, showing that these states are localized at the surface. Introducing this expression into Eq. (8) the energy integration immediately shows that the bound states lead to a $1/T^3$ scaling, which is of opposite sign than the bulk behavior, because $\frac{\partial^3 f}{\partial E^3}$ is positive at zero energy, but negative at higher energies.

In order to determine the coefficients a_1 and a_3 in Eq. (11), we integrate Eq. (6) using the following approximations. For $\kappa = \lambda/\xi_0 \gg 1$ we can assume that the vector potential varies exponentially on the length scale of the penetration length λ, and make the ansatz

$$A(x) = (A_0 - \epsilon)e^{-x/\lambda} + \epsilon e^{-3x/\lambda}. \tag{14}$$

The functions η_1 and η_3 both vary on the length scale of the coherence length, which is much smaller than λ. Therefore, we can approximate them as

$$\eta_1(x) = c_1\delta(x) + \eta_{1b}, \qquad \eta_3(x) = c_3\delta(x) + \eta_{3b}.$$

Here, η_{1b} and η_{3b} are the bulk values of η_1 and η_3, respectively. The coefficients c_1 and c_3 describe the contributions of the surface bound states. They are obtained by substituting Eq. (13) into Eqs. (7) and (8) and integrating over x from 0 to ∞. This yields $c_1 = -\frac{\pi\Delta_0}{6T}\xi_0$ and $c_3 = -(\pi\Delta_0^3/20T^3)\xi_0$. The parameter ϵ in Eq. (14) is determined from the differential equation Eq. (2) together with Eq. (6) and up to order A_0^3 found to be

$$\epsilon = \frac{1}{8}\frac{e^2 v_F^2 \eta_{3b}}{\Delta_0^2 \eta_{1b}} A_0^3. \tag{15}$$

With these approximations after integrating Eq. (6) we find

$$a_1 = -2e^2 v_F^2 N_0 (c_1 + \lambda\eta_{1b}),$$

$$a_3 = \frac{2e^4 v_F^4 N_0}{\Delta_0^2}\left(c_3 + \frac{\lambda}{4}\eta_{3b}\right).$$

Using the low temperature limiting expressions $\eta_{1b} \sim 1$ and $\eta_{3b} \sim \Delta_0/2T$ finally leads to

$$\frac{\partial^2 L}{\partial I^2}\bigg|_{I=0} = \frac{1}{16e^4 v_F^4 N_0^3 \Delta_0^2 \lambda^3} \frac{\frac{1}{2}\frac{\Delta_0}{T} - \frac{\pi}{5}\frac{1}{\kappa}\frac{\Delta_0^3}{T^3}}{(1 - \frac{\pi}{6}\frac{1}{\kappa}\frac{\Delta_0}{T})^4}. \tag{16}$$

This expression shows that upon lowering the temperature from T_c the total nonlinear response of the system initially follows the $1/T$ increase caused by the bulk nonlinearities (first term in the numerator). At a temperature of the order of $T/T_c \sim 1/\sqrt{\kappa}$ the nonlinearities of the surface states become comparable with the bulk contributions and cancel them (second term in the numerator). Below that temperature the $1/T^3$ increase with the opposite sign dominates due to the surface states. Finally, at a temperature of the order of $T/T_c \sim 1/\kappa$ the nonlinear response diverges (denominator). This divergence signals breakdown of the local, large κ approximation we have used here [17]. The approximate expression Eq. (16) is shown in Fig. 3 together with the numerical results. The agreement is quite good at low temperatures despite the approximations made.

To conclude, we have shown that in a d-wave superconductor surface Andreev bound states lead to a strong contribution to the nonlinear Meissner effect, which follows a $1/T^3$ behavior at low temperatures and is of the opposite sign compared to the bulk nonlinear response. At temperatures below $T/T_c \sim 1/\sqrt{\kappa}$ these contributions dominate the total nonlinear response. Such temperatures are readily available in intermodulation experiments and make them a tool to study surface Andreev bound states. The fingerprint of the Andreev bound states should be a $1/T^3$ temperature dependence and a sign change (180° relative phase change) in the nonlinear part of the inductance. So far, intermodulation experiments have been mostly done on systems with (100) surfaces, where Andreev bound states are absent. In systems with (110) surfaces the effect studied here should become most prominent.

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