Nonlinear microwave response of MgB$_2$

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We calculate the intrinsic nonlinear microwave response of the two gap superconductor MgB$_2$ in the clean and dirty limits. Due to the small value of the $\pi$ band gap, the nonlinear response at low temperatures is larger than for a single gap Bardeen-Cooper-Schrieffer (BCS) $s$-wave superconductor with a transition temperature of 40 K. Comparing this result with the intrinsic nonlinear $d$-wave response of YBa$_2$Cu$_3$O$_7$ (YBCO) we find a comparable response at temperatures around 20 K. Due to its two gap nature, impurity scattering in MgB$_2$ can be used to reduce the nonlinear response if the scattering rate in the $\pi$ band is made larger than the one in the $\sigma$ band.

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High-$T_c$ cuprate thin films are being used for constructing microstrip resonators and filters in the microwave regime. One of the limiting factors is their nonlinear response leading to undesirable harmonic generation and intermodulation. While this nonlinear response is often associated with weak links, there is an intrinsic nonlinearity which sets a lower limit on what can be achieved. This has previously been discussed for the cuprates where the $d$-wave nature of the gap leads to an increase in the intrinsic nonlinear response at low temperatures [1, 2]. The recent discovery of $s$-wave superconductivity in MgB$_2$ with a comparatively high critical temperature of $T_c=40$ K and progress in thin film preparation has led to the possibility of making high Q MgB$_2$ microstrip structures operating at 20 to 30 K. This raises the question of how the nonlinearity of MgB$_2$ compares with that of the cuprate superconductors [3, 4].

Here, we study the intrinsic nonlinear microwave response of MgB$_2$. By now it is well established that MgB$_2$ is a superconductor with two different superconducting gaps associated with different parts of the Fermi surface: a small gap ($\sim 2$ meV) on the $\pi$ band and a large gap ($\sim 7$ meV) on the $\sigma$ band [5, 6]. In a superconductor the intrinsic nonlinear response arises from the backflow of excited quasiparticles at finite temperatures. The total current density $\vec{j}$ can be written as $\vec{j} = ne\vec{v}_s - \vec{j}_{qp}$ where $\vec{v}_s$ is the superfluid velocity and $\vec{j}_{qp}$ the quasiparticle backflow. For a two band system like MgB$_2$ the quasiparticle backflow consists of two contributions, one from each band with $\vec{j}_{qp} = \vec{j}_{qp,\alpha} + \vec{j}_{qp,\pi}$. In the clean limit these are given by

$$\vec{j}_{qp,\alpha} = -2eN_\alpha(0)\int_{-\infty}^{\infty} d\epsilon \left\langle \vec{v}_{F,\alpha} f (\sqrt{\epsilon^2 + \Delta^2_\alpha(T)} \right\rangle_{FS,\alpha}$$

$$+ m \vec{v}_{F,\alpha} \cdot \vec{v}_s$$

For currents flowing in the Boron plane, we expand Eq. (1) up to third order in the current density. This gives the leading $j^2$ nonlinear change of the superfluid density [7, 8].

$$n_s(T,j) = n_s(0) \left[ 1 - \frac{j^2}{j_{c,\pi}^2} \left( b_\pi(T) + \frac{j_{c,\pi}^2}{j_{c,\sigma}^2} b_\sigma(T) \right) \right]$$

Here, the pair-breaking current densities of the two bands are given by $j_{c,\alpha} = eN_\alpha(0)v_{F,\alpha}\Delta_\alpha(0)$. As discussed in [7, 8] the nonlinear coefficients $b_\alpha(T)$ determine the strength of the nonlinear response as a function of temperature and are given by

$$b_\alpha(T) = -\frac{g_\alpha}{4} \Delta_\alpha^2(0) \left( \frac{\eta_\alpha}{n_\alpha(T)} \right)^3 \int_0^{\infty} \frac{dE}{dE^3} \left( \sqrt{\epsilon^2 + \Delta_\alpha^2(T)} \right)$$

Here, $g_\alpha$ is a geometrical Fermi surface factor with $g_\pi=3.36$ and $g_\sigma=1$. The linear part of the superfluid
The nonlinear coefficient in MgB$_2$ (solid line) and the σ band density $n_{\sigma}(T)$ is given by

$$n_{\sigma}(T) / n = \frac{1}{\hbar} \sum_{\alpha=\pi,\sigma} \int_{0}^{\infty} \frac{d\omega_{\alpha,\sigma}}{dE} \left( \sqrt{\omega_{\alpha,\sigma}^2 + \Delta_{\alpha}^2(T)} \right)$$

(4)

where $n_{\alpha}$ is the electron density of the $\alpha$ band. Using the known Fermi velocities and densities of states in MgB$_2$, we find for the relative electron densities $n_{\pi}/n = 0.692$ and $n_{\sigma}/n = 0.308$ and the pair-breaking current densities $j_{c,\pi} = 3.32 \cdot 10^8 \text{A/cm}^2$ and $j_{c,\sigma} = 4.87 \cdot 10^8 \text{A/cm}^2$. Interestingly, these values turn out to be close to the estimate of the pair-breaking current density of about $3 \cdot 10^8 \text{A/cm}^2$ in YBCO, consistent with recent experiments [4]. In Fig. 1 we show the temperature dependence of the total nonlinear coefficient $b(T) = b_{\pi}(T) + b_{\sigma}(T)$ (solid line) along with the contributions from the π band (dashed) and the σ band (dashed-dotted). Due to its smaller gap, the π band contribution dominates at low temperatures and leads to structure around 0.3$T_c$. It is only at temperatures above about 0.75$T_c$ that the contribution from the σ band becomes significant. The total nonlinear coefficient possesses a plateau-like region between 0.3 and 0.7$T_c$ in which a reduction of the temperature does not improve the nonlinear response.

In Fig. 2 we compare the nonlinear coefficient for MgB$_2$ (solid line) with the intrinsic response for a $d$-wave superconductor with $T_c = 93$ K (YBCO, dashed line) and a hypothetical BCS single gap superconductor with $T_c = 40$ K (dashed-dotted line) assuming for simplicity that the pair-breaking current densities are the same. For a $d$-wave superconductor $b(T)$ increases at low temperature because of the gap nodes [1, 2]. For this reason the nonlinear coefficient in MgB$_2$ becomes smaller than the one for YBCO at about 27 K. However, due to the presence of the small gap the nonlinear response in MgB$_2$ is not as small as one would have expected for a single gap $s$-wave superconductor (dashed-dotted line).

The foregoing analysis has been made in the clean limit without any impurity scattering. However, in most current MgB$_2$ films, the scattering rate as judged from the residual resistivity is larger than the two gaps [3]. For this reason, in the following we also want to discuss the dirty limit. In a two band superconductor there are in principle three different scattering rates: the two intraband scattering rates $\Gamma_{\pi}$ and $\Gamma_{\sigma}$ and an interband scattering rate $\Gamma_{\pi\sigma}$. It has been shown that because of the different parity of the local orbitals making up the π and σ bands, the interband scattering rate is much smaller than the intraband scattering rates. Thus, in the following we will neglect $\Gamma_{\pi\sigma}$ and keep only the intraband scattering rates. In the dirty limit the current densities $j_{\alpha}$ in the two bands are then given by [1]

$$\tilde{j}_{\alpha} = -ieN_{\alpha}(0)\pi T \sum_{n=-\infty}^{\infty} \left\langle \tilde{v}_{F,\alpha} \frac{\tilde{\omega}_{n,\alpha} - im\tilde{v}_{F,\alpha} \cdot \tilde{v}_s}{\sqrt{(\tilde{\omega}_{n,\alpha} - im\tilde{v}_{F,\alpha} \cdot \tilde{v}_s)^2 + \Delta_{\alpha}^2(\tilde{T}_c)}} \right\rangle_{FS,\alpha} \label{5}$$

where the renormalized Matsubara frequencies $\tilde{\omega}_{n,\alpha}$ and gaps $\Delta_{\alpha}$ are given by

$$\tilde{\omega}_{n,\alpha} = \Gamma_{\alpha} \frac{\omega_n}{\sqrt{\omega_n^2 + \Delta_{\alpha}^2}} \quad \text{and} \quad \Delta_{\alpha} = \Gamma_{\alpha} \frac{\Delta_{\alpha}}{\sqrt{\omega_n^2 + \Delta_{\alpha}^2}} \label{6}$$

Expanding this expression up to third order in $\tilde{v}_s$ the sums over Matsubara frequencies can be done analyti-
FIG. 3: Temperature dependence of $b(T)$ in the clean (solid line) and dirty limit. In the dirty limit $b(T)$ depends on the relative scattering rates in the two bands of MgB$_2$. Results are shown for $\Gamma_\pi/\Gamma_\sigma = 0.7$ (dotted), 1 (dashed-dotted), and 2 (dashed).

FIG. 4: Dependence of $b$ on ratio $\Gamma_\pi/\Gamma_\sigma$ at a fixed temperature of $T = 0.5 T_c$. For $\Gamma_\pi \gg \Gamma_\sigma$ the nonlinear response is dominated by the $\pi$ band, while for $\Gamma_\pi \ll \Gamma_\sigma$ the $\pi$ band dominates.

In order to have more insight into this unexpected behavior, in Fig. 4 we plot $b$ at a fixed temperature, $T = 0.5 T_c$, as a function of the ratio $\Gamma_\pi/\Gamma_\sigma$ on a double logarithmic scale. We find that $b$ can vary by a factor of order 100 at this temperature. Qualitatively we can understand this behavior as follows: the current density is dominated by the band with the smaller scattering rate, because this band provides the highest conducting channel. If the $\pi$ band scattering rate is smaller, the total response is dominated by the small gap leading to a larger nonlinear response at finite temperature. If, however, the $\sigma$ band scattering rate is smaller, the nonlinear response is dominated by the large gap giving a smaller nonlinear response.

This analysis tells us that optimization of material properties in MgB$_2$ should aim at a higher scattering rate in the $\pi$ band in order to suppress the contribution of the small gap relative to that of the large gap in the $\sigma$ band. This could be achieved by substitutional doping at the Mg site, for example with Aluminum [10]. Our analysis also shows that clean MgB$_2$ does not necessarily provide the lowest nonlinear response.

As has been shown in [2] the intermodulation power emitted by a microstrip resonator also depends on the penetration depth of the material. A shorter penetration depth leads to an increased current density at the edges of the resonator, which increases the intermodulation power. According to Refs. [2] and [8] the intermodulation power $P_{\text{IMD}}$ scales like

$$P_{\text{IMD}} \propto (\Delta \lambda)^2 b^2(T)$$

where $\Delta \lambda$ is a nonlinear coefficient depending on both the geometry of the resonator and the penetration depth. According to band structure calculations, the clean limit zero temperature (London) penetration depth in MgB$_2$ is expected to be near $\lambda_L(0) = 40$ nm [11]. Actual values vary between 60 and 200 nm depending on film quality [9, 11]. Comparing MgB$_2$ with the intrinsic $d$-wave response of YBCO at a temperature of 20 K, we take $\lambda(T = 20 K) \approx 100$ nm for MgB$_2$ and $\lambda(T = 20 K) \approx 160$ nm for YBCO. Assuming a typical film thickness of $t = 400$ nm we find for the microstrip geometry considered in Ref. [2] $\Delta \lambda/t = 4 = 0.173$ (MgB$_2$) and $\Delta \lambda/t = 2.5 = 0.124$ (YBCO). Taking $b(T = 20 K) = 0.563$ for MgB$_2$ and $b(T = 20 K) = 0.855$ for YBCO from Fig. 2 and using Eq. (9) this means that the intermodulation power in YBCO at this temperature would be larger by only a factor of 1.2, i.e. a comparable nonlinear response for both materials. However, due to their ceramic nature, weak links play a much larger role in the high-$T_c$ cuprates than in MgB$_2$. For this reason we expect that the intrinsic nonlinear response will be much easier to
achieve in MgB$_2$ films compared with cuprate films.

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