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Frequency Dependence of Optical Conductivity in MgB_2 Superconductor

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Abstract

Using Green's function method, the frequency dependence of optical conductivities of high-quality MgB_2 film is calculated in the framework of the single- and two-band model. By comparing the numerical and experimental results, it is shown that the single-gap isotropic model is insufficient to understand consistently optical behaviors. Also, it is concluded that the two-band model consistently describes the optical behaviors. In the two-gap model, we consider that the both components of optical conductivity are a weighted sum of the contribution from σ and π bonds and hybridization between them is negligible.

Keywords

MgB_2, Optical Conductivity, Two Gap Model, BCS Theory, Green Function Theory

1. Introduction

The discovery of MgB_2 superconductor [1] at relatively high temperature $T_C = 39\ \text{K}$ has appealed much attention in theoretical and applied condensed matter physics. This material has been known as the first superconductor which has two energy gaps at the Fermi surface: 1) in the two dimensional band (σ) and 2) three dimensional band (π) [2] [3]. The inter-band scattering between them is negligible. To explore the mechanism of superconductivity in this material, it is crucial to determine the symmetry of the superconducting order parameter which governs the behavior of quasiparticle excitations below T_C.

There have been several studies to detect the MgB_2 gaps. The isotope effect of boron has suggested that MgB_2 is a BCS-type superconductor [4] and the high T_C is realized through strong electron-phonon coupling with

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light boron mass. Several studies have shown two different superconducting gaps [5] [6]: a gap much smaller than the expected BCS value and another is comparable to the BCS value given by $2\Delta = 3.53 k_B T_C$. Their ratio is estimated to be $\Delta_{\min}/\Delta_{\max} \approx 0.3 - 0.4$ using several experiments. The two-gap model is shown to consistently describe the optical conductivity and thermodynamic properties of MgB_2 [7]-[9]. However, there is no general agreement whether MgB_2 is an s-wave BCS type superconductor or not. In conventional s-wave superconductors, there is no quasiparticle excitation at low energies and the thermodynamic and transport coefficients decay exponentially at low temperatures. In this superconductors, the deviation of penetration depth $\Delta\lambda(T)$ from its zero temperature value $\lambda(0)$ exhibits activated behavior [10] *i.e.* $\Delta\lambda(T) \propto \mathrm{e}^{-\Delta/T}$ (we set $k_B = \hbar = 1$ through the paper), reflecting the isotropic BCS energy gap at the Fermi surface. In contrast, in unconventional superconductors with gap nodes, such as in high-T_C oxides, power law behaviors are expected in thermodynamic and transport coefficients at low temperatures [11].

Pronin *et al*. measurements [12] show that the low temperature dependence of penetration depth of MgB_2 film has a T^2 behavior. This disagreement with BCS calculations could be caused by an additional absorption. Also, theoretical calculations of A. A. Golubov *et al*. [13] and A. Brinkman *et al*. [14] show that the penetration depth is well described by two band model.

Kaindl *et al*. [15] measured both components of complex conductivity of MgB_2 film as a function of frequency for different temperatures. They compared their results with conventional superconductors and concluded that their results were inconsistent with BCS calculations. This disagreement with BCS calculations could be caused by an additional absorption.

In this paper we introduce the new view of the frequency dependence of optical properties of MgB_2. Numerical calculations of frequency dependence of optical conductivities are carried out by proposing different kinds of energy gaps. We show that the optical conductivities are well described by a two-band superconductor model with different anisotropies in *k*-space. First, we conclude that the single-gap model is insufficient to understand consistently the optical behaviors. Then, it will be shown that the two-gap model with different symmetries in *k*-space is sufficient to understand optical properties. In this model the larger gap $\Delta\sigma$ approximately follows of ordinary usual BCS-like curve and the smaller gap $\Delta\pi$ deviates from the usual BCS-like behavior and is similar to a d-wave energy gap. Both gaps are expected to close at the same transition temperature.

2. Formulation of the Problem

Our model of MgB_2 by a Hamiltonian has two bands, labeled σ and π, which hybridize through an inter-site hopping term, then the Hamiltonian reads

$$H = H_c + H_d + H_{cd} \tag{1}$$

where

$$H_c = \sum_{p\sigma} \varepsilon_p c^+_{p\sigma} c_{p\sigma} + \frac{1}{2} \sum_{pp'q\sigma\sigma'} V_{cc}(q) c^+_{p+q,\sigma} c^+_{p'-q,\sigma} c_{p',\sigma} c_{p,\sigma} \tag{2}$$

$$H_d = \sum_{p\sigma} \varepsilon_p d^+_{p\sigma} d_{p\sigma} + \frac{1}{2} \sum_{pp'q\sigma\sigma'} V_{dd}(q) d^+_{p+q,\sigma} d^+_{p'-q,\sigma} d_{p',\sigma} d_{p,\sigma} \tag{3}$$

$$H_{cd} = \frac{1}{2} \sum_{pp'q\sigma\sigma'} V_{cd}(q) \left(c^+_{p+q,\sigma} c^+_{p'-q,\sigma} d_{p',\sigma} d_{p,\sigma} + d^+_{p+q,\sigma} d^+_{p'-q,\sigma} c_{p',\sigma} c_{p,\sigma} \right). \tag{4}$$

Here, *c* and *d* are referred to σ and π bands with creation and annihilation operators c^+, *c*, d^+, *d*, respectively, and ε_p is the quasi-particle energy with respect to Fermi energy. The pairing potentials V_{cc} and V_{dd} act intra-band and V_{cd} is the inter-band interaction dominated by multi-phonon processes. We define the green function for the σ-band as [16]

$$G_c(p, \tau - \tau') = -\left\langle T_\tau c_{p,\sigma}(\tau) c^+_{p,\sigma}(\tau') \right\rangle \tag{5}$$

$$F_c(p, \tau - \tau') = \left\langle T_\tau c_{-p,\downarrow}(\tau) c^+_{p,\uparrow}(\tau') \right\rangle \tag{6}$$

$$F^+_c(p, \tau - \tau') = \left\langle T_\tau c^+_{p,\uparrow}(\tau) c_{-p,\downarrow}(\tau') \right\rangle. \tag{7}$$

We can write the similar equations for π band. By using the Gorkov equations in superconducting state:

$$\left(-\frac{\partial}{\partial\tau}-\varepsilon_p\right)G_c\left(p,\tau-\tau'\right)+\Delta_c\left(p\right)F_c^+\left(p,\tau-\tau'\right)=\delta\left(\tau-\tau'\right) \tag{8}$$

$$\left(-\frac{\partial}{\partial\tau}+\varepsilon_p\right)G_c\left(p,\tau-\tau'\right)+\Delta_c\left(p\right)G_c\left(p,\tau-\tau'\right)=0 \tag{9}$$

where $\Delta_c\left(p\right)$ is the gap energy in σ band and is determined by

$$\Delta_c\left(p\right)=-\sum_q V_{cc}\left(q\right)F_c\left(p-q,0\right)-\sum_q V_{cd}\left(q\right)F_d\left(p-q,0\right). \tag{10}$$

We assume that the hybridization between σ and π bands is negligible, and then the last term in Equations (1) and (10) can be ignored. In this case two parts of the Hamiltonian (H_c and H_d) are independent. Therefore, the σ and π bands has the similar relations and we omit the indexes *c* and *d*.

Optical conductivity describes the linear response of a material, which is exposed to an electromagnetic field. This field induces shielding currents

$$J_i\left(q,\omega\right)=-\sum_j K_{ij}\left(q,\omega\right)A_j\left(q,\omega\right) \tag{11}$$

where $i,j=x,y,z$, ω is the phonon energy, $A_j\left(q,\omega\right)$ is the Fourier transform of the covariant vector potential and $K_{ij}\left(q,\omega\right)$ is the response kernel which depends only on the properties of the material. It can be expressed in terms of quasiparticle propagators $G\left(q,\omega\right)$ and once this is known, the optical conductivity follows

$$\sigma\left(q,\omega\right)=\frac{i}{\omega}K\left(q,i\omega\right). \tag{12}$$

The real and imaginary parts of the optical conductivity are given by

$$\sigma_{1s}=\operatorname{Re}\sigma\left(\omega\right)=-\frac{1}{\omega}\operatorname{Im}\left[K\left(q,\omega+i\delta\right)\right] \tag{13}$$

$$\sigma_{2s}=\operatorname{Im}\sigma\left(\omega\right)=-\frac{1}{\omega}\operatorname{Re}\left[K\left(q,\omega+i\delta\right)\right] \tag{14}$$

where δ is a positive infinitesimal. The response kernel is given by the current-current correlation function as [16]

$$K\left(q,i\omega\right)=-\frac{1}{3V}\int_0^\beta \mathrm{d}\tau\left\langle J\left(q,\tau\right)\cdot J\left(-q,0\right)\right\rangle \tag{15}$$

where *V* is the volume of the system and the current expression in the case of noninteracting particle is given by

$$J\left(q\right)=\frac{e}{m}\sum_q\left(\vec{P}+\frac{\vec{q}}{2}\right)c^+_{p+q,\sigma}c_{p,\sigma}. \tag{16}$$

By using Equation (16), Equation (15) can be written as

$$\begin{aligned}K_{ij}\left(q,i\omega\right)=\frac{2e^2}{3Vm^2}\sum_p p_ip_j\Bigg\{&\frac{1}{2}\left(f\left(E_{p+}\right)-f\left(E_{p-}\right)\right)\left[1+\frac{\varepsilon_{p+}\varepsilon_{p-}}{E_{p+}E_{p-}}+\frac{\Delta_{p+}\Delta_{p-}}{E_{p+}E_{p-}}\right]\frac{1}{i\omega+E_{p+}-E_{p-}}\\&+\frac{1}{4}\left(1-f\left(E_{p+}\right)-f\left(E_{p-}\right)\right)\left[\left(1-\frac{\varepsilon_{p+}}{E_{p+}}\right)\left(1+\frac{\varepsilon_{p-}}{E_{p-}}\right)-\frac{\Delta_{p+}\Delta_{p-}}{E_{p+}E_{p-}}\right]\frac{1}{i\omega-E_{p+}-E_{p-}}\\&+\frac{1}{4}\left(1-f\left(E_{p+}\right)-f\left(E_{p-}\right)\right)\times\left[\frac{\Delta_{p+}\Delta_{p-}}{E_{p+}E_{p-}}-\left(1+\frac{\varepsilon_{p+}}{E_{p+}}\right)\left(1-\frac{\varepsilon_{p-}}{E_{p+}}\right)\right]\times\frac{1}{i\omega+E_{p+}+E_{p-}}\Bigg\}\end{aligned} \tag{17}$$

where $p+=p+q/2$ and $p-=p-q/2$.

Here, we consider thin film satisfying $d\ll\xi\approx\upsilon_F/\Delta$ for the film thickness *d* and the coherence length ξ. In these cases we can regard $p+$ and $p-$ as independent variables. Since $q\upsilon_F\gg\Delta\approx\omega$ we can do Abrikosov's replacement [17]

$$\sum_q \to N(0)\frac{1}{4q\upsilon_F}\int \mathrm{d}\varepsilon_{p+}\mathrm{d}\varepsilon_{p-}. \tag{18}$$

Then in the isotropic case we obtain the Mattis-Bardeen formula from Equations (13) and (14):

$$\begin{aligned}\frac{\sigma_{1s}}{\sigma_n}(\omega) &= \frac{1}{\omega}\int_\Delta^{\omega-\Delta}\mathrm{d}EN(E)N(\omega-E)\big(1-2f(\omega+E)\big)\left(1-\frac{\Delta^2}{E(\omega-E)}\right)\Theta(\omega-2\Delta)\\ &+2\frac{1}{\omega}\int_\Delta^{\infty}\mathrm{d}EN(E)N(\omega+E)\big(f(E)-f(\omega+E)\big)\left(1+\frac{\Delta^2}{E(\omega+E)}\right)\end{aligned} \tag{19}$$

$$\frac{\sigma_{2s}}{\sigma_n}(\omega) = \frac{1}{\omega}\int_{\max(-\Delta,\Delta-\omega)}^{\Delta}\mathrm{d}E\big(1-2f(\omega+E)\big)\frac{E(E+\omega)+\Delta^2}{\sqrt{\Delta^2-E^2}\sqrt{(E+\omega)^2-\Delta^2}} \tag{20}$$

where σ_n is the real part of the conductivity for normal state and $N(E)=E\big/\sqrt{E^2-\Delta^2}$ is the density of states that generalized to $N(E)=\left\langle \operatorname{Re} E\big/\sqrt{E^2-\Delta_k^2}\right\rangle_k$, where the bracket indicates the average over the Fermi surface.

3. Numerical Results

Now, we present the numerical solutions of complex conductivity of MgB_2 film in the frequency range $0<k<16\ \mathrm{cm}^{-1}$ for different temperatures. We use the temperature dependence of energy gaps as [18]

$$\Delta_{\sigma,\pi}(T)=\Delta_{\sigma,\pi}(T_0)\times\left\{1-(T/T_C)^{p_{\sigma,\pi}}\right\}^{1/2}. \tag{21}$$

The anisotropy of d-wave gap considered in this paper is

$$\Delta_\pi(T,k)=\Delta_\pi(T)(1+a\cos 2\theta). \tag{22}$$

Here, θ is the angular deviation of $\hat{k}$ from the given node direction in the basal plan. The parameter a determines the anisotropy. We have chosen $\Delta_\sigma(T_0)=3.71\ \mathrm{meV}$, $\Delta_\pi(T_0)=1.18\ \mathrm{meV}$, $p_\sigma=2.98$ and $p_\pi=1.78$ so that the theoretical curves for two-band model at lowest frequency $(\omega=2\ \mathrm{meV})$ match the experimental values of σ_2 (solid squares curve of Figure 3 in Ref. [15]). For $\Delta_\pi(T,k)$, the average over the Fermi surface in Equation (19) for $0<a<1$ is given by:

$$\left\langle \operatorname{Re}\frac{\omega}{\sqrt{\omega^2-\Delta_\pi^2(T,k)}}\right\rangle=\frac{1}{2}\sqrt{\frac{\omega}{a\omega}}F\left(\frac{\pi}{2},k\right),\ (1-a)\Delta<\omega<(1+a)\Delta \tag{23}$$

$$=\frac{1}{2}\sqrt{\frac{\omega}{a\omega}}F(\gamma,k),\quad (1+a)\Delta<\omega \tag{24}$$

where $k^2=\big(\omega-(1-a)\Delta\big)\big/2\omega$, $\gamma=\sin^{-1}\sqrt{4a\Delta\omega\big/\big[\big(\omega-(1-a)\Delta\big)\big(\omega+(1+a)\Delta\big)\big]}$ and $F(\gamma,k)$ is the elliptic integral of the first kind.

In **Figure 1** and **Figure 2** we show our numerical results for the real and imaginary parts of optical conductivity as a function of frequency for $T=6\ \mathrm{K}$ and $a=0.5$. The solid and dotted curves represent the real and imaginary parts of optical conductivity for s-wave and d-wave gaps separately. These curves do not fit the experimental results of Kaindl *et al.* [15], which is shown in the Figure 3 of their paper. The d-wave curve of real part of conductivity is bigger than s-wave curve at same temperature. Thus the main contribution to the optical absorption comes from π band. However, within the single-gap model, it is difficult to understand the optical behaviors measured by experimental method of Kaindl *et al.* [15].

Here, a two-band model with different anisotropies is investigated. We assume that the hybridization between σ and π bands is negligible so that the optical conductivities are given by

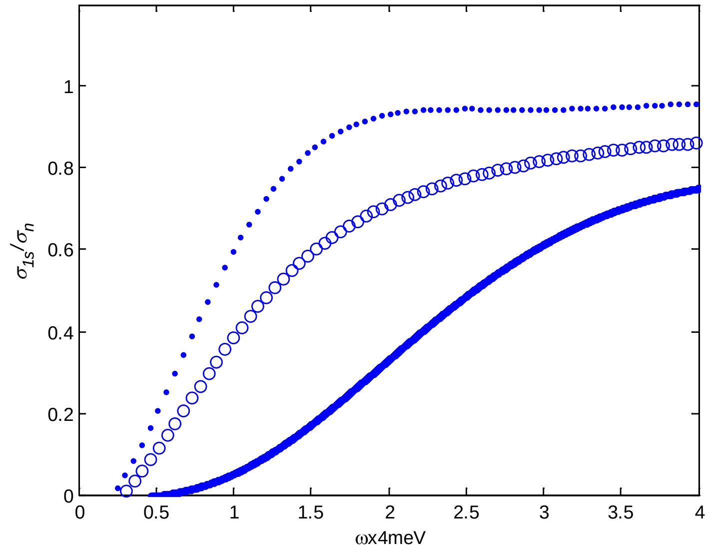

Figure 1. Frequency dependence of the real part of optical conductivity $\sigma_1(\omega)$ normalized to its normal state value $\sigma_{1N}(40\text{ K})$ for $T = 6\text{ K}$. The solid and dotted curves represent the real part of optical conductivity for s-wave and d-wave gaps separately. The open circle curve indicates $\sigma_1(\omega)$ using the two-band model.

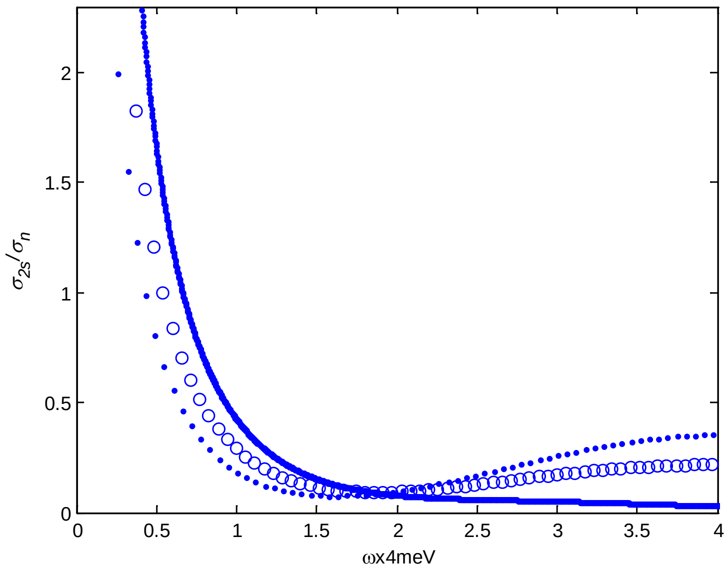

Figure 2. Frequency dependence of the imaginary part of optical conductivity $\sigma_2(\omega)$ normalized to its normal state value $\sigma_{1N}(40\text{ K})$ for $T = 6\text{ K}$. The solid and dotted curves represent the imaginary part of optical conductivity for s-wave and d-wave gaps separately. The open circle curve indicates $\sigma_2(\omega)$ using the two-band model.

$$\sigma_1 = w_{1\sigma}\sigma_{1\sigma} + w_{1\pi}\sigma_{1\pi} \tag{25}$$

$$\sigma_2 = w_{2\sigma}\sigma_{2\sigma} + w_{2\pi}\sigma_{2\pi} \tag{26}$$

$w_{1\sigma}$, $w_{1\pi}$, $w_{2\sigma}$ and $w_{2\pi}$ are the weighting factors with $w_{1\sigma} + w_{1\pi} = 1$ and $w_{2\sigma} + w_{2\pi} = 1$, which determines the contributions from σ and π bands. The open circle curves in **Figure 1** and **Figure 2** indicate optical conductivities using the present two-band anisotropic model. For $\omega > 1$, these curves are in good agreement with experimental result of Kaindl *et al*.

In this curves, the best fit to the experimental data are obtained if we assign the ratio of the weights of the σ band to that of the π-band as $w_{1\sigma}/w_{1\pi} = 0.35/0.65$ and $w_{2\sigma}/w_{2\pi} = 0.4/0.6$, which approximately agrees with band structure [19] and complex conductivity [20] calculations, respectively. These weights show that the main contribution to the optical conductivities comes from the three dimensional band. The open circle, solid and dotted curves in **Figure 3** and **Figure 4** are calculated for $T = 6\ \text{K}$, $T = 17.5\ \text{K}$ and $T = 24\ \text{K}$ respectively. These curves are in good agreement with Kaindl *et al*. [15] measurements.

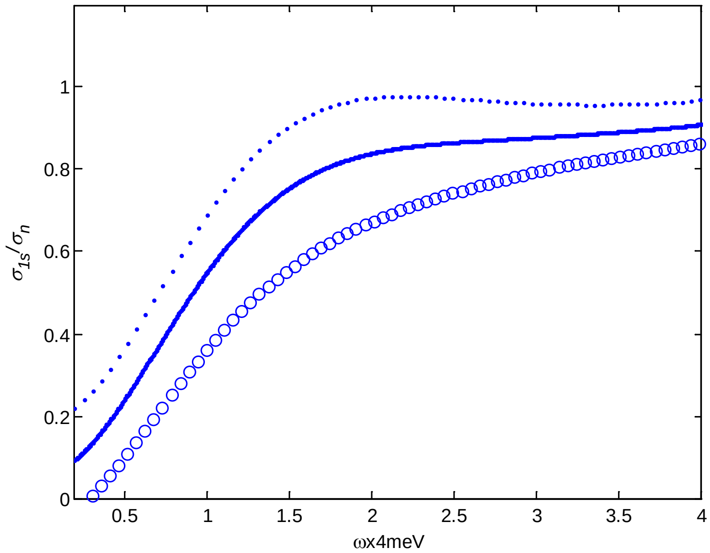

Figure 3. Frequency dependence of Real part of conductivity for different temperatures. The open circle, solid and dotted curves are calculated for $T = 6\ \text{K}$, $T = 17.5\ \text{K}$ and $T = 24\ \text{K}$ respectively.

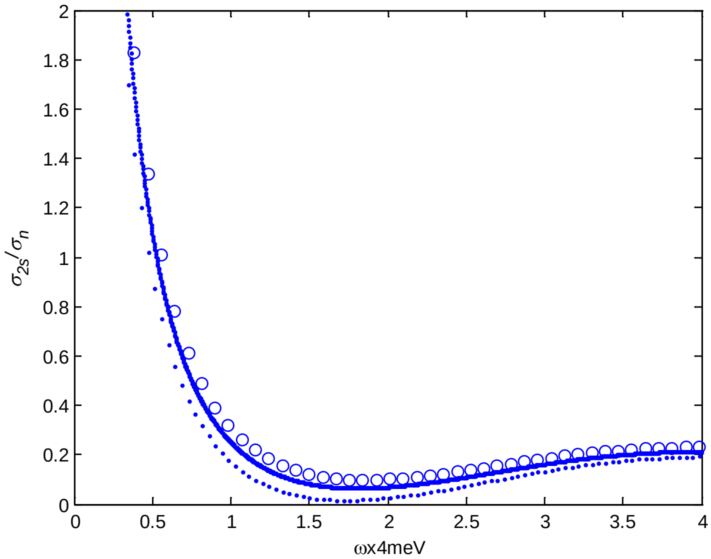

Figure 4. Frequency dependence of imaginary part of conductivity for different temperatures. The open circle, solid and dotted curves are calculated for $T = 6\ \text{K}$, $T = 17.5\ \text{K}$ and $T = 24\ \text{K}$ respectively.

4. Conclusion

By using Green's function method and linear response theory we have calculated the frequency dependence of the real and imaginary parts of optical conductivity of MgB_2 film in the framework of two-band theory. We have shown that a single-gap model is insufficient to describe the optical behaviors, but the two-band model with different symmetries can explain the experimental results consistently. Also, we have shown that the electrons in π band have greater contribution in the optical and transport behaviors than do electrons in the σ band. We have considered that the optical conductivities are a weighted sum of the continuation from each band and the interaction between them is negligible.

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