Implications of Reflectance Measurements on the Mechanism for Superconductivity in MgB_2

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(Received 24 July 2001; published 19 November 2001)

Recent optical studies in c-axis oriented superconducting MgB_2 films indicate that the electron-phonon coupling is weak. We reinforce this conclusion by examining the raw reflectance data; its frequency dependence is incompatible with strong electron-phonon scattering. This is further strengthened by analysis of the real part of the conductivity, and by the temperature dependence of the effective Drude scattering rate. Using a realistic electron-phonon spectral shape, we find $\lambda_{tr} \approx 0.15$. To the extent that $\lambda_{tr} \approx \lambda$, this disagrees sharply with model calculations, and is far too low to provide the means for $T_c = 39$ K. A simple model is constructed with coupling to a high frequency excitation, which is consistent with both the low frequency optical data and the high T_c.

DOI: 10.1103/PhysRevLett.87.247001 PACS numbers: 74.25.Gz, 74.20.–z, 74.25.Kc

The discovery of superconductivity in MgB_2 at 39 K [1] has naturally prompted questions about mechanism. Thus far calculations of the electron-phonon coupling strength [2–5] suggest that the conventional electron-phonon mechanism may be responsible for $T_c = 39$ K. Nonetheless, there remains some concern that a significant modification of the theory is required to explain the high T_c, due to anharmonic [6] or nonadiabatic [7,8] effects. In addition, non-electron-phonon mechanisms have been proposed [9,10].

All of these deliberations have been essentially theoretical in nature. On the experimental side, the isotope effect measurements [11,12] can be understood within the electron-phonon framework, but only with very high frequency phonons, and a very large Coulomb repulsion [12,13]. Very recently reflectance measurements on c-axis oriented thin films have been analyzed within the conventional electron-phonon framework [14]. These authors conclude that the electron-phonon coupling in MgB_2 is very weak, $\lambda_{tr} = 0.13 \pm 0.02$. The purpose of this paper is to further analyze their data, with the goal of exploring possible ways in which the reflectance data can be interpreted with a more sizable electron-phonon interaction. We find, in agreement with Tu *et al.* [14] that the reflectance data are not consistent with an electron-phonon interaction sufficiently strong to produce $T_c = 39$ K. Consistency can be achieved if another excitation is assumed to exist at much higher frequency.

Through Kramers-Kronig (KK) analysis of the reflectance data, Tu *et al.* [14] obtain a very Drude-like response at low frequencies. As noted previously for $Ba_{1-x}K_xBiO_3$ [15–17] this will be the case even if the electron-phonon interaction is sizable. In fact, the low frequency Drude result for the real part of the conductivity is given by [see Eq. (13) in [16]]

$$\sigma_{\rm Drude} \equiv \frac{\omega_{\rm Peff}^2}{4\pi}\left(\frac{1/\tau_{\rm eff}}{\nu^2 + (1/\tau_{\rm eff})^2}\right), \qquad (1)$$

where, at low temperature, $1/\tau_{\rm eff} = 1/\tau_{\rm imp}/(1 + \lambda_{tr})$, where $1/\tau_{\rm imp}$ is the elastic scattering rate due to impurities and λ_{tr} is the mass enhancement parameter defined specifically for transport [18,19]. Similarly, $\omega_{\rm Peff} = \omega_{\rm P}/\sqrt{1 + \lambda_{tr}}$ is the effective plasma frequency, with $\omega_{\rm P}$ the bare plasma frequency. This expression properly reduces to the correct zero frequency limit, where renormalization effects are known to cancel [20]. In what follows we make no distinction between the conventional mass enhancement factor λ and the transport version, λ_{tr}, although the latter is to be used in the conductivity while the former enters the single electron self-energy [18,19]. We will return to this point later. The experimentally derived parameters are determined in the normal state at $T = 45$ K [14]: $\omega_{\rm Peff} = 13\,600$ cm^{-1}, and $1/\tau_{\rm eff} = 75$ cm^{-1}. Any model with higher energy excitations that interact with the electrons (such as phonons) must correctly reproduce this low frequency behavior.

To attempt to model these data within the conventional electron-phonon framework we compute the normal state self-energy [21] and compute the optical conductivity effectively in the bubble approximation [19,22], since vertex corrections are implicitly contained in the use of λ_{tr} rather than λ. Calculation of the complex conductivity allows one to compute all the optical functions and, in particular, the reflectance [23].

In Fig. 1 we show the reflectance as a function of frequency, for a variety of model calculations with different overall electron-phonon coupling strengths. For this purpose we have used the model electron-phonon spectrum of Kong *et al.* [2] for the spectral function, $\alpha^2F(\omega)$. As calculated, it has $\lambda = 0.85$, but we have scaled it by a constant to achieve any desired coupling strength. It is characterized by one dominant peak at $\omega = 74$ meV (600 cm^{-1}), which manifests itself in the reflectance as a relatively sharp downward trend, the magnitude of which depends on the coupling strength. Even without the KK analysis, then one can see directly from the reflectance data that the electron-phonon coupling in MgB_2 must be weak. This statement is independent of the precise form of the spectral function used, as we have verified with other

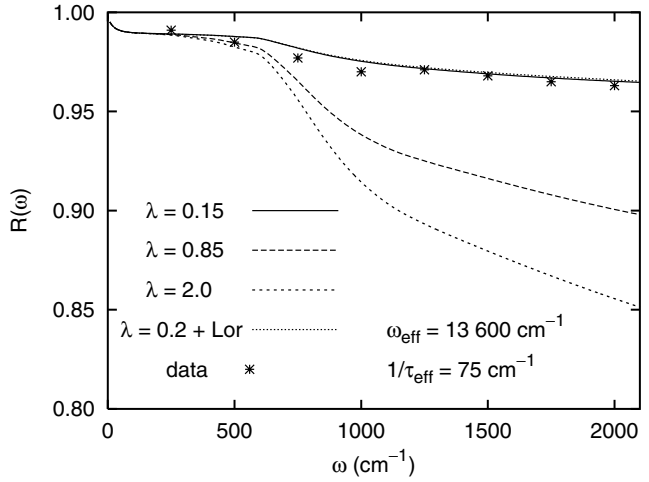

FIG. 1. Reflectance vs frequency; experimental results are shown with symbols, and curves indicate calculations, taking into account different amounts of electron-phonon scattering. The plasma frequency and the impurity scattering rate are determined for each coupling strength to yield the effective plasma frequency and the effective scattering rate indicated. The data are in clear agreement with very weak electron-phonon coupling, including the case where a higher frequency excitation also couples to the electrons.

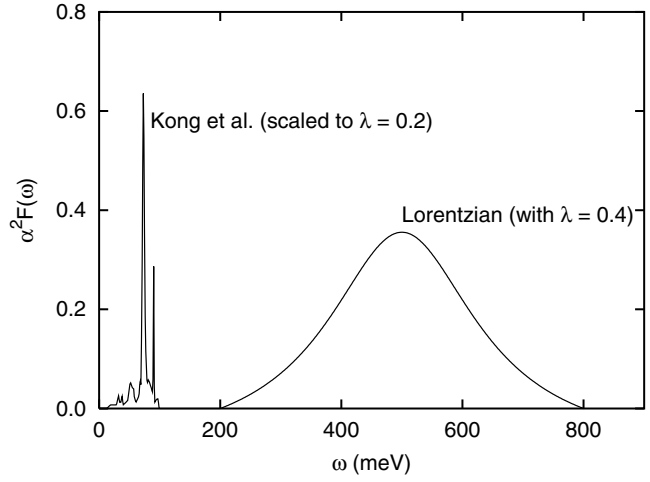

FIG. 2. The model spectral function, consisting of two pieces: the electron-phonon part, taken from Kong *et al.* [2] and scaled to give $\lambda = 0.2$, and a Lorentzian shaped contribution peaked at 0.5 eV, and of unknown origin.

model spectra. The key point is that over the frequency range of the phonons (and a little beyond) the frequency-dependent scattering rate increases in proportion to the coupling strength [15,24], and this results in a reduced reflectance in this frequency range. In this respect we should mention that the model calculation with $\lambda = 0.15$ fits the data shown in Fig. 1 very well, but nonetheless fails at higher frequency. Specifically the reflectance data [14] is significantly lower than the computed result, and shows that at higher frequencies other aspects of the problem are required [25].

Nonetheless, a model which both fits the low frequency reflectance and is capable of producing $T_c = 39$ K consists of a weak electron-phonon spectrum, along with a high frequency excitation (of unknown origin) [26,27], as shown in Fig. 2. For simplicity we have adopted a broad Lorentzian spectrum centered at 0.5 eV. The coupling strength to this additional peak is weak ($\lambda \approx 0.4$), but, because it is at high frequency, the spectrum shown in Fig. 2 results in $T_c = 39$ K [with $\mu^*(\omega_c = 5\ \text{eV}) = 0.17$]. With this spectrum the optical reflectance is calculated and shown as the dotted curve in Fig. 1; it is barely distinguishable from the previous result with $\lambda = 0.15$. Note, however, that we have used $\lambda = 0.2$ for the scaled Kong spectrum, because the high frequency Lorentzian contribution essentially renormalizes the low frequency part: $\alpha^2_{\text{eff}}F(\omega) \sim \alpha^2F(\omega)/(1 + \lambda_{\text{Lor}})$ [26]. Such a spectrum also improves the agreement with the higher frequency reflectance data, but we do not attach a great deal of significance to this fact since other factors also contribute [25]. We therefore have not made any attempts to optimize this agreement.

Note that the calculations shown in Fig. 1 all utilize different values of the plasma frequency and the impurity scattering rate. For example, for the curve calculated with $\lambda_{\text{tr}} = 0.85$, we used $\omega_P = 13\,600\sqrt{1 + \lambda_{\text{tr}}} = 18\,470\ \text{cm}^{-1}$ and $1/\tau_{\text{imp}} = 75(1 + \lambda_{\text{tr}}) = 138\ \text{cm}^{-1}$.

In Fig. 3 we illustrate the same point through the real part of the optical conductivity. In Fig. 3(a) we show the various models already discussed in association with Fig. 1. In Fig. 3(b) we focus on the "Holstein" sideband near and above the characteristic phonon energies. It is clear that a strong electron-phonon coupling (i.e., of order unity or more) disagrees with the data. Moreover, a two-band model would not immediately remedy this problem since this would lead to extra absorption, which would contradict the data. Also shown (dot-dashed curve) is the calculation with the spectrum of Fig. 2. Because of the renormalization of the low frequency spectrum discussed above, the result agrees very closely with the weak coupling calculation.

Another way in which one can analyze the data is through the temperature dependence of some of the optical functions. For this purpose we focus on the temperature dependent scattering rate [16,28], as defined by Eq. (14) of the latter reference. This scattering rate was used to fit the low frequency optical conductivity with a Drude model at various temperatures [14]. Two points determined experimentally are indicated in Fig. 4. In addition, we have plotted the results expected for various electron-phonon coupling strengths, again using the Kong *et al.* [2] spectrum as a model for the spectral function. The data indicate that the effective scattering rate more than doubles between 45 and 295 K; this shows that some inelastic scattering must be present. However, the required coupling strength to reproduce this temperature dependence is $\lambda_{\text{tr}} \approx 0.15$. This is in agreement with our analysis of the frequency-dependent reflectance, and

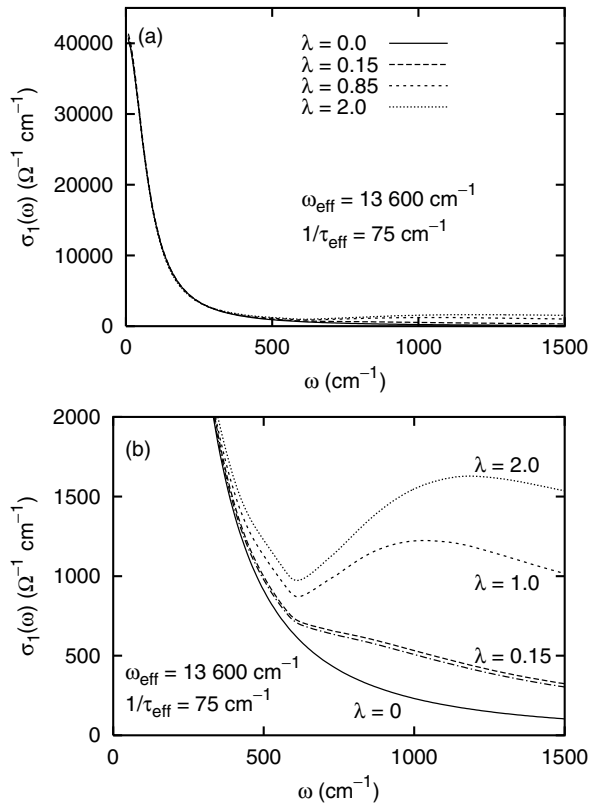

FIG. 3. Real part of the optical conductivity vs frequency, (a) showing the Drude-like peak that has been measured in thin film samples, and (b) on a finer scale, emphasizing the Holstein absorption due to the electron-phonon coupling. As in Fig. 1, the plasma frequency and impurity scattering rate were determined separately for each coupling strength to yield the observed low frequency Drude-like peak. The data (not shown) are in much better agreement with the weak electron-phonon coupling scenario.

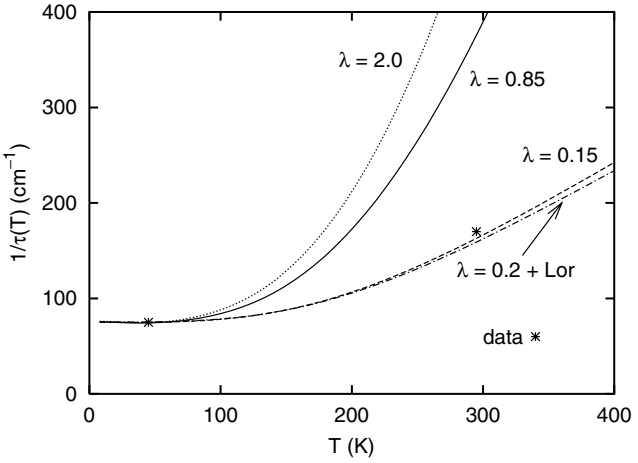

FIG. 4. The temperature dependent effective scattering rate, determined by the amount of electron-phonon coupling. The two data points reported are indicated with symbols. They also indicate that the electron-phonon coupling is weak.

agrees with the estimates of Tu *et al.* based on the optical sum rule and the temperature dependent dc resistivity. This coupling strength is much too small to account for electron-phonon driven superconductivity in this material. Our *ad hoc* model of Fig. 2 again reproduces the correct behavior (dot-dashed curve), indicating that some unknown high frequency excitation may be responsible for superconductivity.

In summary, we have further analyzed the frequency and temperature dependence of the optical reflectance and conductivity in c-axis oriented superconducting MgB_2 films. We have found very strong support for the conclusion of Ref. [14]—namely, the electron-phonon coupling strength as derived from optical measurements is much too small to account for superconductivity in MgB_2. In all, five different (but not independent) analyses have produced this conclusion: (1) the discrepancy between the plasma frequency as determined by the low frequency Drude fit to the conductivity and that determined by the sum rule [14], (2) the fit to the temperature dependence of the dc resistivity data [14], (3) the low frequency dependence of the reflectance, (4) the magnitude of the Holstein sideband in the real part of the conductivity, and (5) the temperature dependence of the Drude width of the low frequency conductivity. These conclusions have been obtained through calculation with a realistic electron-phonon spectral shape, obtained through calculation [2]. Nonetheless, they are quite general, and depend only on the fact that the phonons in this material extend up to a maximum of 100 meV. The data of Tu *et al.* [14] show very convincingly that the coupling to excitations up to these energies must be weak.

In our opinion the most compelling test is the frequency dependence of the reflectance, since this property emerges essentially as raw data, and does not require any KK analysis. If we accept the possibility of a high frequency excitation coupling to electrons to produce superconductivity, as is modeled in Fig. 2, then other consequences would immediately follow. For example, all superconducting properties ought to be very BCS-like.

However, a possibility for reconciling these results with electron-phonon driven superconductivity is that $\lambda_{\rm tr}$ and λ differ significantly. This would be the case, if, for example, the electron-phonon scattering was dominated by forward scattering [29]. Alternatively, Liu *et al.* [5] have suggested that two-phonon scattering may play a significant role in the electron-phonon interaction. Very little is known about the impact of such a nonlinear pairing on either T_c or the conductivity. It may well be, for example, that a much smaller electron-ion coupling is required for T_c, particularly if anharmonicity plays a significant role [5]. In either case one should expect other unusual normal and superconducting state properties; these possibilities should be further explored, both experimentally and theoretically.

I thank Jorge Hirsch for bringing these experimental results to my attention, and for subsequent discussions. This work was supported by the Natural Sciences and Engineering Research Council (NSERC) of Canada and the Canadian Institute for Advanced Research.

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