Supplementary material for "Evidence for multiple superconducting gaps in optimally doped BaFe_{1.87}Co_{0.13}As₂ from infrared spectroscopy"

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The characteristic features of a BCS-type superconductor with scattering rate γ much larger than the superconducting energy gap (so-called dirty-limit) 2Δ has been described with the Matthis-Bardeen formalism [1]. Zimmermann *et al.* published a code to calculate the optical response of a BCS superfluid with an isotropic gap for an arbitrary scattering rate [2]. In the dirty limit it yields the same results as the Matthis-Bardeen formalism. We have utilized this code to simulate our experimental data where the gap magnitude is of comparable magnitude as the scattering rate. The code developed by Zimmermann *et al.* contains as input parameters the scattering rate γ , the superconducting gap 2Δ at zero temperature, and the transition temperature T_c . The squared plasma frequency ω_p^2 acts as a scaling parameter which does not affect the spectral shape of the response function.

I. CHARACTERISTIC RESPONSE OF BCS-TYPE SUPERCONDUCTORS WITH A SINGLE GAP

Figure 1 shows the calculated optical conductivity and the reflectivity ratio for the case of a single gap in the extreme dirty limit ($\gamma = 10000 \text{ cm}^{-1}$, $2\Delta = 100 \text{ cm}^{-1}$, and $T_c = 24.5 \text{ K}$) and for the more relevant case that the scattering rate is comparable to the gap magnitude ($\gamma = 200 \text{ cm}^{-1}$, $2\Delta = 100 \text{ cm}^{-1}$, and $T_c = 24.5 \text{ K}$). The plasma frequencies have been scaled as to obtain the same value of the dc conductivity of $\sigma(0) = 10000 \Omega^{-1} \text{ cm}^{-1}$ and thus similar values of the reflectivity ratio. For the former case, $\sigma(\omega)$ follows the behavior of the Mattis-Bardeen formalism in the dirty limit. At 5 K, the conductivity remains almost zero below 2Δ , it has a sharp onset at the so-called gap-edge near 2Δ , and it gradually approaches the normal state values at higher frequency. The reflectivity ratio $R(T < T_c)/R(T \approx T_c)$ also exhibits a pronounced maximum around 2Δ . Above the gap edge, while it deviates from unity up to significantly higher energies, the reflectivity ratio evolves smoothly and does not exhibits any additional anomaly.

Our simulations show that a very similar behavior is obtained for the case of $\sigma(0) = 200 \ \Omega^{-1} \text{cm}^{-1}$ which is intermediate between the clean- and the dirty limit cases. It can be noted that the smaller scattering rate results in steeper changes above the gap edge.



FIG. 1: Optical response of an isotropic BCS gap obtained from the code given in Ref. [2]. The gap-induced features are marked with arrows in conductivity $\sigma(\omega)$ and reflectivity ratio spectra $R(5K)/R_N$. $T_c = 24.5$ K, $2\Delta = 100$ cm⁻¹, $\sigma(0) = 10000$ Ω^{-1} cm⁻¹ are used and $\gamma = 10000$ cm⁻¹ and 200 cm⁻¹ are assumed for the dirty limit and a moderate case respectively.

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FIG. 2: Trial fits with low energy modes in the FIR region. (a) and (b) show the case 1 with one mode at 300 cm⁻¹ and (c) and (d) show the case 2 with two modes at 180 cm⁻¹ and 450 cm⁻¹ respectively, which are compared to two gaps fits without a low energy mode. Parameters of each case are given in Table I.

FITS WITH TWO-GAP MODELS INCLUDING LOCALIZED MODES IN THE FAR-INFRARED II. REGION

The normal state data at 30K have been fitted with a Drude-Lorentz model. Our experimental spectra do not yield any clear evidence for a localized mode in the FIR region. Accordingly, in the paper we did not consider such low-energy modes. Nevertheless, since such low-energy modes have been reported in some recent related publications [3, 4], we still test here whether they could help to improve our two-gap model fits.

In Fig. 2 we show the best attempts to improve the various two-gap models by adding one or two additional

low-frequency Lorentzian oscillators. The fit parameters are summarized in Table I. In case 1 we add one Lorentzian oscillator at 300 cm⁻¹ that has a weight of $\omega_p^2 = 8 \times 10^6$ cm⁻¹. The broad Drude term has less weight and a smaller scattering rate since its tail is partly replaced by the Lorentzian oscillator. For the corresponding conductivity spectra in the superconducting state this results in a reduced quality of the fits for the two-gap models A and B, and only a minor improvement for the two-gap model C. Nevertheless, the fits to the reflectivity ratio remain very poor, i.e. they do not reproduce the overall shape of the spectrum. Note that we cannot increase much further the spectral weight of the Lorentzian oscillator and still obtain a reasonable fit to the normal state spectrum at 30K.

Accordingly, in case 2 we have added another Lorentzian mode in an attempt to improve the two-gap C model. While this can yield a better description of the conductivity spectrum for the two-gap case C, it still yields a poor representation of the reflectivity ratio spectrum in the range of $100 - 200 \text{ cm}^{-1}$ where it does not reproduce the weak kink around 157 $\rm cm^{-1}$. Any further increase in the spectral weight of the Lorentzian modes, while it may help to improve the agreement with reflectivity ratio near 157 $\rm cm^{-1}$, would significantly decrease the quality of the fit to the conductivity spectrum (and also cause problems in fitting the 30K spectrum). These attempts lead us to conclude that the inclusion of additional Lorentzian oscillators does not allow us to simultaneously describe the spectra of the optical conductivity and to reproduce the shape and the kink features of the reflectivity ratio.

	without FIR mode				Case 1				Case 2			
					$\omega_0=300, \ \gamma=500, \ \omega_p^2=0.8$				$\omega_{0,1}=180, \gamma_1=200, \omega_{p,1}^2=0.6$			
									$\omega_{0,2}=450, \gamma_2=560, \omega_{p,2}^2=0.8$			
	Drude 1	$(\gamma = 90)$	Drude 2	$(\gamma = 300)$	Drude 1	$(\gamma = 92)$	Drude 2	$(\gamma = 280)$	Drude 1	$(\gamma = 94)$	Drude 2	$(\gamma = 230)$
	2Δ	ω_p^2	2Δ	ω_p^2	2Δ	ω_p^2	2Δ	ω_p^2	2Δ	ω_p^2	2Δ	ω_p^2
30 K	0	4.45	0	4.3	0	4.85	0	3.1	0	5.0	0	2.35
$2~{\rm gaps}{\text{-}}{\rm B}$	53	4.45	80	4.3	53	4.85	80	3.1	53	5.0	80	2.35
2 gaps-C	53	4.45	157	4.3	53	4.85	157	3.1	53	5.0	157	2.35

TABLE I: Parameters for the various simulations with two isotropic gaps shown in Fig. 2. γ , 2Δ , ω_0 are in cm⁻¹ and ω_p^2 is in 10^7 cm⁻²

[1] Martin Dressel and George Grüner, Electrodynamics of Solids: Optical properties of Electrons in Matter (Cambridge University Press, United Kingdom, 2002).

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[3] E. van Heumen et al., arXiv:0912.0636 (2009).

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