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Thermal Conductivity of Superconducting MgB_2

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ABSTRACT

Employing the Geilikman-Kresin (GK) theory, we address the experimental data obtained by Bauer *et al*., and by Schneider *et al*., on the thermal conductivity (κ) of superconducting MgB_2. The two gaps of this compound have *qualitatively* been understood via the well-known Suhl, Matthias, and Walker's (SMW) approach to multi-gap superconductivity. Since this approach is based on *one*-phonon exchange mechanism for the formation of Cooper pairs, it cannot give a *quantitative* account of the values of T_c and the multiple gaps that characterize MgB_2 and other high-T_c superconductors (SCs). Despite this fact and some rather ambiguous features, it has been pointed out in a recent critical review by Malik and Llano (ML) that the SMW approach provides an important clue to deal with an SC the two gaps of which close at the same T_c: consider the possibility of the interaction parameters in the theory to be temperature-dependent. Guided by this clue, ML gave a complete summary of parameters that *quantitatively* account for the T_c and the gaps of MgB_2 via the generalized BCS equations (GBCSEs). GBCSEs which we recall, invoke multi-phonon exchange mechanism for the formation of Cooper pairs and multiple Debye temperatures to deal with composite SCs. The parameter-values given in ML are used here to calculate the temperature-dependent gaps, which are an essential input for the GK theory. Notable features of this work are: 1) κ_{MgB_2} is calculated for both—the scenario in which the two gaps of MgB_2 close/do not close at the same temperature whence it is found that 2) the latter scenario yields results in better agreement with experiment.

KEYWORDS

MgB_2; Thermal Conductivity; Multiple Gaps; Generalized-BCS, Geilikman, and Geilikman-Kresin Equations; Two-Phonon Exchange Mechanism; Cooper Pairs with Different Binding Energies

1. Introduction

Thermal conductivity (κ) of a superconductor (SC) is an important parameter from the point of view of applications; additionally, it helps in the theoretical understanding of the superconducting state [1]. An appreciation of the latter follows by recalling that: 1) in the kinetic theory, κ is proportional to the following properties of the heat carriers: a) number density, b) specific heat and c) mean free path (MFP); this is so regardless of whether the system is in the normal or the superconducting state. A nontrivial statement about MFP in any system at any temperature T is that it has the same value for both the normal and the superconducting states [2]. This, indeed, is not so for the other two properties. 2) The feature that distinguishes the superconducting state from the normal state is that the former is characterized by the existence of a temperature-dependent gap $\Delta(T)$ which is zero for the latter state. 3) The increase in $\Delta(T)$—from zero at $T = T_c$ to its maximum value at $T = 0$—is synonymous with a similar increase in the number of density of Cooper pairs (CPs) and hence with a *decrease* in the number density of heat carriers because CPs have zero entropy.

The existence of a gap in an SC at any T thus profoundly affects (lowers) both, the number density of the heat carriers (the *unpaired* electrons) and their specific heat. If κ of an SC at any T does not have a value as low as one might expect on these grounds, it is so because the lower the T is, the greater the MFP is. There is another feature that affects κ: heat is transported not only by electrons, but also by phonons—the quanta of lattice vibrations. The determination of κ due to any of these carriers requires the solution of a Boltzmann equation taking into account the nature of the dominant scattering processes appropriate for a given sample. If one is dealing with a composite superconductor (CS), there are additional complicating factors. Calculation of $\kappa(T)$ of a CS is thus a rather formidable problem; we refer the reader to the lucid review by Uher [1] for its further elaboration.

The basic equations that yield the thermal conductivity of an SC based on the BCS theory [3] were given by Geilikman (G) [4], and by Geilikman and Kresin (GK) [5]. While the equation given by G determines κ_{es}, the electronic thermal conductivity of a simple superconductor when the scattering of electrons by impurities is the dominant process, the equation given by GK determines κ_{gs}, the thermal conductivity due to phonons when phonon-electron scattering dominates. Not surprisingly, one finds that an application of these equations requires knowledge of $\Delta(T)$ of the SC for all $T \le T_c$. We note that equations similar to the G and the GK equations were also derived by Bardeen, Rickayzen and Tewordt (BRT) [6].

In this paper, we address the experimental data on the thermal conductivity of MgB_2 obtained by Bauer (B) *et al*. [7], and by Schneider (S) *et al*. [8], in an approach that supplements the G [4] and the GK [5] equations by the recently derived generalized BCS equations (GBCSEs) [9]. Indeed, each of the groups [7,8] that obtained the said data also carried out a similar study based on the G and GK/BRT equations. Analyses of the data in these papers, however, were carried out without a detailed knowledge of the T-variation of the two gaps that characterize MgB_2. Employing GBCSEs to calculate the values of these gaps for $0 \le T \le T_c$, we attempt here to shed light on their role, individually and collectively, in determining the total thermal conductivity of the compound. We note that in the earlier work [10-12] in which GBCSEs were used for a variety of high-temperature superconductors (HTSCs), the gap-values were calculated only at $T = 0$.

An experimental feature of MgB_2 as reported by, e.g., Iavarone *et al*. [13] is that its two gaps close at the same temperature (~40 K). This is a situation that was envisaged by Suhl, Matthias, and Walker (SMW) [14] in a seminal paper. Partly for this reason and partly because of a lack of an alternative framework, multi-gap superconductivity has been understood solely via the SMW approach for about five decades now. It is therefore natural to ask: why can't one use it to address the T_c and the gap-values of the high-T_c SC (HTSC) MgB_2? Since the approach was originally given in the context of transition *elements*, it can only be *adapted* for composite SCs such as MgB_2 which has no d-electrons. Such attempts have of course been made. Thus, making out a case for going beyond even the Eliashberg superconductivity, Liu *et al*. [15] were led to attribute the existence of the two gaps in MgB_2 to the multiple band structure of its Fermi surface that brings into play different phonon modes; in particular, based on density-functional calculations invoking *two-phonon exchange mechanism* they arrived at the value of $\lambda_{sc}^{eff} = 1.01$ (clean limit) for the effective electron-phonon coupling constant which, they concluded, "is arguably consistent with the measured T_c of nearly 40 K." In another appeal to the SMW approach in the context of MgB_2, Choi *et al*. [16] invoked a qualitative picture similar to that of [15]. In this paper [16] the multiple gaps and T_c of MgB_2 were attributed to the existence of two separate populations of electrons—nicknamed "red" and "blue," leading them to note: "Stated differently, electrons on different parts of the Fermi surface form pairs with *different binding energies*."

Notwithstanding the above developments, the SMW approach has till now not led to a framework in which the T-dependent gaps and T_c of an HTSC may be *calculated*. However, it seems interesting that it should have led to such concepts as *two-phonon exchange* mechanism [15] and CPs with *different binding energies* [16]. Further, in a recent critical review [17] of the SMW approach, it has been pointed out that it gives yet another clue to deal with an SC the two gaps of which close at the same T_c, the clue being: consider also the possibility of the interaction parameters in the theory to be T-dependent. These are precisely the concepts that are manifestly incorporated in the Bethe-Salpeter equation (BSE)-based approach that led to GBCSEs (Approach 2 hereafter); this approach has already been shown to deal *quantitatively* with the multiple gaps and T_cs of a variety of HTSCs with a measure of success [10-12]. It is worth noting that each interaction parameter in Approach 2 satisfies the Bogoliubov constraint for the BCS theory given by

$$\lambda \le 0.5, \tag{1}$$

as discussed in [18].

The paper is organized as follows. In the next section, we give an account of GBCSEs and the G and the GK equations which form our framework. Since it was reported in [13] that both the gaps of MgB_2 close at about 40 K, we consider in Section 3 the experimental data of both the B [7] and the S [8] groups in this scenario (Scenario 1). Additionally, for reasons spelled out below, we use as input the T-dependent gap values for the G and GK equations when the two gaps of MgB_2 close at *different* temperatures (Scenario 2). Interestingly, it is found that whereas both the scenarios lead to almost indistinguishable results for $0.448 \le t \equiv T/T_c \le 1$, the latter scenario yields results in better agreement with experiment for $t < 0.448$. To avoid repetition, we present here the results of our calculations pertaining to the data of only B's group. Our findings pertaining to the data of the other group are of course summarized. The final section sums up our findings.

2. Framework

Our framework has three constituents. The first of these is concerned with calculating the values of $\Delta_1(T)$ and $\Delta_2(T)$ of MgB_2 for all $0 \le T \le T_c$ via GBCSEs in both the scenarios mentioned above. We first deal with Scenario 2 in which the interaction parameters are T-independent and recall that the BCS equation for $\Delta(T)$ for a simple SC is:

$$1 = \lambda \int_0^{k_B\Theta} \mathrm{d}\xi \frac{\tanh\left[\frac{1}{2k_BT}\left(\xi^2+\Delta^2\right)^{1/2}\right]}{\left(\xi^2+\Delta^2\right)^{1/2}}. \quad (2)$$

The GBCSE equivalent to (2) is [9,19]:

$$1 = \lambda \int_{|W_1|/2}^{k_B\Theta+|W_1|/2} \mathrm{d}x \frac{\tanh\left[\frac{x}{2k_BT}\right]}{x}, \quad (3)$$

or

$$1 = \lambda \int_{\beta|W_1|/4}^{\Theta/2T+\beta|W_1|/4} \mathrm{d}x \frac{\tanh(x)}{x}, \quad (3a)$$

where $\beta = 1/k_BT$, k_B being the Boltzmann constant, Θ the Debye temperature, and $2|W_1|$ is the binding energy of a CP that is bound via one-phonon exchanges (recall that the energy required to break a CP is 2Δ). Note that putting $W_1 = 0$ in (3) *or* $\Delta = 0$ in (2) yields the familiar BCS equation for T_c of the SC. This already suggests a connection between W and Δ. Further, it is readily seen that when $T = 0$ (tanh = 1) and $\lambda \to 0$, both (2) and (3) yield: $\Delta_0 = 2k_B\Theta\exp(-1/\lambda) = |W_0|$.

The generalized version of (3) when CPs in a CS are bound via two-phonon exchanges is [9]:

$$1 = \lambda_1^c \int_{|W_2|/2}^{k_B\Theta_1^c+|W_2|/2} \mathrm{d}x \frac{\tanh\left[\frac{x}{2k_BT}\right]}{x} + \lambda_2^c \int_{|W_2|/2}^{k_B\Theta_2^c+|W_2|/2} \mathrm{d}x \frac{\tanh\left[\frac{x}{2k_BT}\right]}{x}, \quad (4)$$

or

$$1 = \lambda_1^c \int_{\beta|W_2|/4}^{\Theta_1^c/2T+\beta|W_2|/4} \mathrm{d}x \frac{\tanh(x)}{x} + \lambda_2^c \int_{\beta|W_2|/4}^{\Theta_2^c/2T+\beta|W_2|/4} \mathrm{d}x \frac{\tanh(x)}{x}, \quad (4a)$$

where λ_i^c is the interaction parameter due to the i^{th} species of ions in the CS, to be distinguished from λ_i, which denotes the interaction parameter of the same species in its free state; a similar distinction applies to Θ_i^c and Θ_i; $2|W_2|$ is the binding energy of a CP bound via two phonon exchanges. The equation for T_c of the CS in this case follows by putting $W_2 = 0$ in (4a):

$$1 = \lambda_1^c \int_0^{\Theta_1^c/2T_c} \mathrm{d}x \frac{\tanh(x)}{x} + \lambda_2^c \int_0^{\Theta_2^c/2T_c} \mathrm{d}x \frac{\tanh(x)}{x}. \quad (5)$$

The two Debye temperatures in the problem cater to the anisotropy of the CS [9]. The physical significance of CPs bound via one- and two-phonon exchange mechanisms is that there are two kinds of "glues" or "springs" that bind them, leading to two binding energies in the problem.

The framework of GBCSEs [9] has been applied to a variety of CSs [10-12]; the set of parameters thus arrived at for MgB_2 is [10]:

$$\Theta_{\mathrm{B}}^c = 1062\ \mathrm{K},\ \Theta_{\mathrm{Mg}}^c = 322\ \mathrm{K}; \quad \lambda_{\mathrm{B}}^c = 0.2216,\ \lambda_{\mathrm{Mg}}^c = 0.1073. \quad (6)$$

These lead via (4a) and (5) to

$$|W_2(0)| = 6.28\ \mathrm{meV};\ T_c = 39\ \mathrm{K}, \quad (7)$$

The parameters corresponding to B alone in (6) lead via (3a) and the BCS equation for T_c (Equation (5) with $\lambda_2^c = 0$) to

$$|W_1(0)| = 2.03\ \mathrm{meV},\ T_{c1} = 13.2\ \mathrm{K}. \quad (7a)$$

Hence we use $|W_{1,2}|$ and $|\Delta_{1,2}|$ interchangeably from now on; the T-dependent values of these can be calculated via (3a) and (4a). Note that both the λs in (6) satisfy the Bogoliubov constraint given in (1) above.

If experiment dictates that the smaller gap of MgB_2 also closes at about 39 K (and not at about 13 K)—as has been reported in [13], then to address Scenario 1 one must invoke T-dependence of the interaction parameters in the theory. It has recently been shown that [19], even in the BCS theory for elemental superconductors, such dependence has a bearing on the violation of the alleged universality of the relation $2\Delta/k_BT_c = 3.53$. For a detailed discussion of how the SMW approach also implies such dependence of the interaction parameters, we refer the reader to [17], where it is noted that the requirement of closure of both the gaps in MgB_2 is met by replacing λ_1^c and λ_2^c above as follows:

$$\lambda_1^c \to \lambda_1^c(T) = \lambda_1^c + \alpha_1 T,\ \alpha_1 = 1.7923\times10^{-3}\ \mathrm{K}^{-1}$$
$$\lambda_2^c \to \lambda_2^c(T) = \lambda_2^c + \alpha_2 T,\ \alpha_2 = -2.749\times10^{-5}\ \mathrm{K}^{-1}. \quad (8)$$

Figure 1 shows how these replacements in (3a) and (4a) lead to closure of both the gaps at the 39 K.

We now turn to the second constituent of our framework: the G equation for $\kappa_{es}(T)$ when electrons are scattered predominantly by impurities. This equation is [4]:

$$\kappa_{es} = A' F_{es}(T), \tag{9}$$

where A' is independent of T,

$$F_{es}(T) = k_B T \int_{u(T)}^{\infty} \frac{x^2 \mathrm{d}x}{(\mathrm{e}^x + 1)(1 + \mathrm{e}^{-x})} \tag{10}$$

and

$$u(T) = \Delta(T)/k_B T .$$

We note that [4] also gives an alternative expression for the integral in (10) as a sum of three terms (one of which is a sum of an infinite number of terms). Having checked our results obtained directly via (10) with those obtained via the alternative form, we have not reproduced the latter here.

The final constituent of our framework is the GK equation for κ_{gs} when the phonons are scattered predominantly by electrons. This equation is [5]:

$$\kappa_{gs}(T) = B' T^2 F_{gs}(T), \tag{11}$$

where B' is independent of temperature, and

$$F_{gs}(T) = \int_0^{2u(T)} \frac{\mathrm{d}x\, x^4 \mathrm{e}^x}{(\mathrm{e}^x - 1)^2 \left[2x - 2\ln\left\{ \frac{\exp(u(T)+x)+1}{\exp(x-u(T))+1} \right\} \right]} + \int_{2u(T)}^{\infty} \frac{\mathrm{d}x\, x^4 \mathrm{e}^x}{(\mathrm{e}^x - 1)^2 \left[x + 2u(T) - 2\ln\left\{ \frac{\exp(u(T)+x)+1}{\exp(x-u(T))+1} \right\} \right]} \tag{12}$$

As was the case for (11), [5] also gives an alternative expression for the RHS of (12) which now comprises many terms some of which are sums of infinite number of terms. Again, having checked our results obtained directly via (12) with those obtained via the alternative form, we have not quoted the latter here.

3. Total Thermal Conductivity κ_s of MgB_2 in the Superconducting State

We first address the data under consideration in Scenario 1, *i.e.*, when both the gaps close at the same T_c. To this end we solve (3a) and (4a) for $\Delta_1(T)$ and $\Delta_2(T)$ with Θ-values taken from (6) and expressions for $\lambda(T)$ as given in (8); the results are given in Table 1. With $\Delta(T)$s known, we are enabled to calculate, for each of the gap-values, $F_{es}(T, \Delta)$ and $F_{gs}(T, \Delta)$ via (10) and (12), respectively. This exercise is carried out at each of the 38 temperatures below T_c for which the experimental values of the total thermal conductivity κ_s are given in the data of B *et al.*

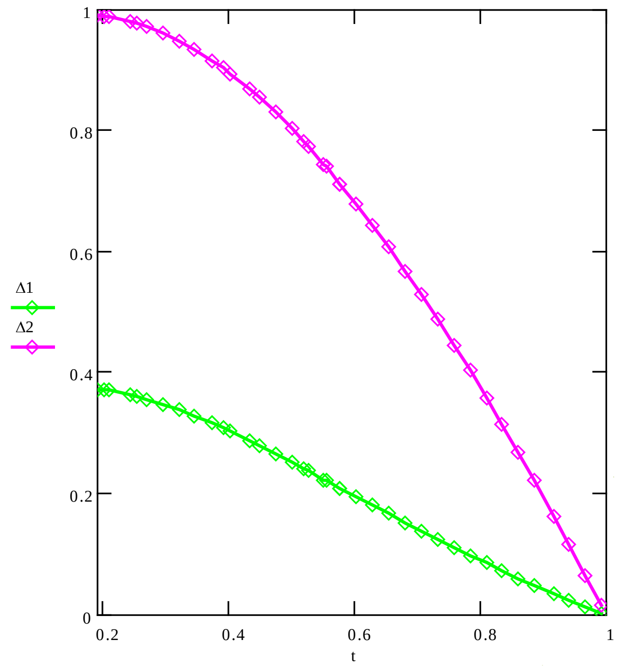

Figure 1. Variation of the reduced gaps of MgB_2 with t for $0.1902 \le t = T/39 \le 1$ obtained via solutions of (3a) and (4a) with inputs from (6) and (8).

[7]. The results of these calculations are also given in Table 1.

Using (9) and (11), we now write

$$\kappa_s(T) = \kappa_{es} + \kappa_{gs} = A' F_{es}(T) + B' T^2 F_{gs}(T) \tag{13}$$

as

$$\begin{aligned} \kappa_s^r(T) &\equiv \frac{\kappa_s(T)}{\kappa_s(T_c)} = \frac{\kappa_{es}(T) + \kappa_{gs}(T)}{\kappa_s(T_c)} \\ &= \left[\frac{A' F_{es}(T_c)}{\kappa_s(T_c)} \right] \frac{F_{es}(T)}{F_{es}(T_c)} + \left[\frac{B' T_c^2 F_{gs}(T_c)}{\kappa_s(T_c)} \right] \frac{F_{gs}(T)}{F_{gs}(T_c)} t^2 \\ &\equiv A f_{es}(t) + B f_{gs}(t) t^2, \end{aligned} \tag{14}$$

where κ_s^r denotes reduced thermal conductivity, $t = T/T_c$, and A, B, f_{es} and f_{gs} are dimensionless.

Equation (14) pertains to the situation when the SC is characterized by one gap; when there are two gaps, we have

$$\begin{aligned} \kappa_s^r(T) &= \kappa_{es1}^r(t, \Delta_1) + \kappa_{gs1}^r(t, \Delta_1) \\ &\quad + \kappa_{es2}^r(t, \Delta_2) + \kappa_{gs2}^r(t, \Delta_2) \\ &= A\left[f_{es1}(t, \Delta_1) + f_{es2}(t, \Delta_2) \right] \\ &\quad + B\left[f_{gs1}(t, \Delta_1) + f_{gs2}(t, \Delta_2) \right] t^2. \end{aligned} \tag{15}$$

We now need to reduce the four F's in Table 1; this is done by using the set of values given in the last row of the table:

Table 1. **Values of $\Delta_1(T)$, $F_{es}(T, \Delta_1)$, $F_{gs}(T, \Delta_1)$ and $\Delta_2(T)$, $F_{es}(T, \Delta_2)$ and $F_{gs}(T, \Delta_2)$ for all $T \le T_c$ in the data of B *et al*. [7] in the scenarios: a) both the gaps close at 39 K and b) Δ_1 closes at 13.2 K while Δ_2 closes at 39 K. Entries corresponding to b) are marked in red. In both the scenarios Θ's are as given in (6). In the former scenario $\Delta_1(T)$ is calculated via (3a) with λ_1^c given by (9), and $\Delta_2(T)$ via (4a) with λs given by (9) and (11). In the latter scenario, $\Delta_1(T)$ and $\Delta_2(T)$ are calculated with λs as in (6). $F_{es}(T)$ and $F_{gs}(T)$ corresponding to each $\Delta(T)$ are calculated via (14a) and (16a), respectively. κ_s(T) is calculated via (19). Entries marked with (*) are used as input to fix A and B.**

T	$t = T/39$	$\Delta_1(T)$ meV	$F_{es}(T, \Delta_1)$ $\times 10^{-3}$	$F_{gs}(T, \Delta_1)$	$\Delta_2(T)$ meV	$F_{es}(T, \Delta_2)$ $\times 10^{-4}$	$F_{gs}(T, \Delta_2)$	$\kappa_{es}(T, \Delta_1)$	$K_{gs}(T, \Delta_1)$ $\times 10^{-3}$	$\kappa_{es}(T, \Delta_2)$	$K_{gs}(T, \Delta_2)$	$\kappa_s(T)\vert_{th}$	$\kappa_s(T)\vert_{exp}$
7.8313	0.2008	2.3368 1.479	0.4322 0.7859	381.53 78.84	6.212 6.2583	0.0713 0.06749	1.363.105 1.460.105	5.836 10.637	0.022 1.728	0.096 0.091	7.983 3.200	13.937 13.937	13.9374*
9.4315	0.2418	2.288 1.1298	0.7261 1.1416	176.36 35.424	6.155 6.2206	0.3112 0.2924	2.664.104 2.889.104	9.805 15.461	0.015 1.126	0.42 0.396	2.263 0.9184	12.503 16.777	19.2367
10.4677	0.2684	2.2423 0.8616	0.9342 1.4264	116.11 15.983	6.101 6.1827	0.6377 0.5961	1.185.104 1.297.104	12.615 19.306	0.012 0.626	0.861 0.807	1.24 0.508	14.728 20.635	24.047
12.4586	0.3195	2.1299 0.2573	1.346 1.7648	59.65 8.404	5.958 6.0763	1.8266 1.6911	3.490.103 3909.9	18.136 23.902	0.0097 0.4661	2.461 2.29	0.567 0.2164	21.174 26.409	33.8843
14.4752	0.3712	1.991 0	1.752 2.0519	35.38 7.212	5.759 5.9202	3.9804 3.6596	1.339.103 1531.6	23.606 27.790	0.0078 0.540	5.363 4.956	0.294 0.1147	29.271 32.862	41.8619
15.6230	0.4006	1.9038 0	1.974 2.2146	27.85 7.212	5.622 5.809	5.6777 5.2084	839.76 973.94	26.598 29.994	0.0071 0.629	7.65 7.054	0.215 0.0849	34.470 37.133	48.5756
17.4586	0.4477	1.7553 0	2.311 2.4748	20.42 7.212	5.368 5.5972	9.0843 8.3292	430.26 510.51	31.138 33.518	0.0065 0.7855	12.24 11.281	0.137 0.0556	43.522 44.855	53.7372
19.4661	0.4991	1.5844 0	2.656 2.7593	15.79 7.212	5.045 5.3175	13.651 12.566	223.19 271.27	35.787 37.371	0.0063 0.9766	18.393 17.019	0.089 0.0367	54.275 54.428	67.0045
20.4718	0.5249	1.4966 0	2.821 2.9019	14.25 7.212	4.865 5.1586	16.19 14.957	164.19 201.71	38.01 39.302	0.0063 1.08	21.814 20.257	0.072 0.0302	59.903 59.591	71.5823
21.5887	0.5536	1.3982 0	3.000 3.0602	12.91 7.212	4.654 4.9675	19.14 17.774	118.48 147.02	40.422 41.446	0.0063 1.201	25.789 24.072	0.058 0.0245	66.275 65.5443	78.5762
22.4880	0.5766	1.3186 0	3.14 3.1877	12.05 7.212	4.474 4.8044	21.577 20.108	92.094 115.28	42.308 43.153	0.0064 1.301	29.073 27.234	0.049 0.0208	71.436 70.408	80.5136
24.4904	0.628	1.1412 0	3.445 3.4715	10.62 7.212	4.045 4.3966	27.037 25.55	54.487 68.33	46.418 47.017	0.0067 1.546	36.43 34.604	0.034 0.0146	82.888 81.637	91.0589
26.5235	0.6801	0.9629 0	3.746 3.7597	9.62 7.212	3.573 3.9404	32.379 31.0313	33.86 41.99	50.474 50.92	0.0071 1.813	43.627 42.027	0.025 0.0106	94.133 92.9595	98.2931
28.5546	0.7322	0.7884 0	4.041 4.0476	8.9 7.212	3.066 3.4314	37.289 36.228	22.494 30.04	54.448 54.819	0.0076 2.101	50.243 49.066	0.019 0.009	104.72 103.896	107.6549
30.5499	0.7833	0.622 0	4.328 4.3304	8.38 7.212	2.536 2.8822	41.589 40.878	16.125 18.74	58.315 58.649	0.0082 2.405	56.037 55.364	0.016 0.00624	114.38 114.022	115.6430
32.5361	0.8343	0.462 0	4.611 4.612	7.99 7.212	1.98 2.2868	45.36 44.969	12.353 13.77	62.129 62.463	0.0089 2.728	62.118 60.904	0.014 0.0052	123.27 123.375	120.3485
33.5426	0.8601	0.384 0	4.754 4.7547	7.82 7.212	1.688 1.9664	47.09 46.807	11.033 12.05	64.055 64.396	0.0092 2.9	63.449 63.394	0.013 0.0048	127.799 127.799	127.799*
34.5088	0.8848	0.310 0	4.891 4.8916	7.68 7.212	1.402 1.6468	48.67 48.514	10.019 10.74	65.901 66.25	0.0096 3.0689	65.578 65.705	0.012 0.0046	131.50 131.963	131.9507
36.6796	0.9405	0.151 0	5.199 5.1993	7.42 7.212	0.759 0.8854	51.96 51.936	8.369 8.65	70.051 70.419	0.010 3.467	70.011 70.342	0.012 0.00403	140.53 137.130	140.2963
38.7056	0.9925	0.0115 0	5.487 5.4865	7.23 7.212	0.096 0.1195	54.86 54.865	7.335 7.37	73.932 74.309	0.011 3.861	73.918 74.309	0.012 0.00395	147.94 148.625	145.2463
39	1	0	5.528	7.212	0	55.28	7.212	74.484	0.011	74.7484	0.011	148.99	146.5531

$$\kappa_s\left(T_c\right) = 146.5531\ \text{meV}\cdot\text{cm}^{-1}\cdot\text{deg}^{-1},$$

$$F_{es}\left(39\right) = 5.528\times10^{-3},\ \text{and}\ F_{gs}\left(39\right) = 7.212.$$

To proceed further we need to fix A and B. We do so by appealing to the experimental values of κ_s at two temperatures. This enables us to calculate κ_s at the remaining 36 temperatures.

The above calculations are repeated for Scenario 2. Given below are the values for A and B found at different combinations of temperatures in the two scenarios (the values in the parentheses correspond to Scenario 2):

$$T_1 = 7.8313,\ T_2 = 33.5426:$$
$$A = 0.50935\left(0.50637\right),$$
$$B = 7.14796\times10^{-5}\left(2.65104\times10^{-5}\right)$$

$$T_1 = 7.8313,\ T_2 = 36.6796:$$
$$A = 0.50903\left(0.50468\right),$$
$$B = 7.15124\times10^{-5}\left(2.68075\times10^{-5}\right)$$

$$T_1 = 7.8313,\ T_2 = 38.7056:$$
$$A = 0.49924\left(0.49487\right),$$
$$B = 7.25321\times10^{-5}\left(2.85307\times10^{-5}\right)$$

$$T_1 = 8.0886,\ T_2 = 37.7058:$$
$$A = 0.51533\left(0.51086\right),$$
$$B = 9.80056\times10^{-5}\left(3.6537\times10^{-5}\right)$$

In each scenario, the results for $\kappa_s(T)$ yielded by all of the above pairs of A, B values are similar. The values adopted by us are those given in the top set. While we have thus calculated $\kappa_s(T)$s at each of the remaining 36 temperatures in the data under consideration, we have given in **Table 1**—for both the scenarios—the results at 20 temperatures to save space. Also given in this table are, separately, the contributions of the electronic and the lattice parts of the thermal conductivity due to each gap. **Figure 2** gives plots of $\kappa_s(T)\big|_{\text{theory}}$ (and its constituents) in the two scenarios—together with the plot of $\kappa_s(T)\big|_{\text{exp}}$—plotted against the reduced temperature.

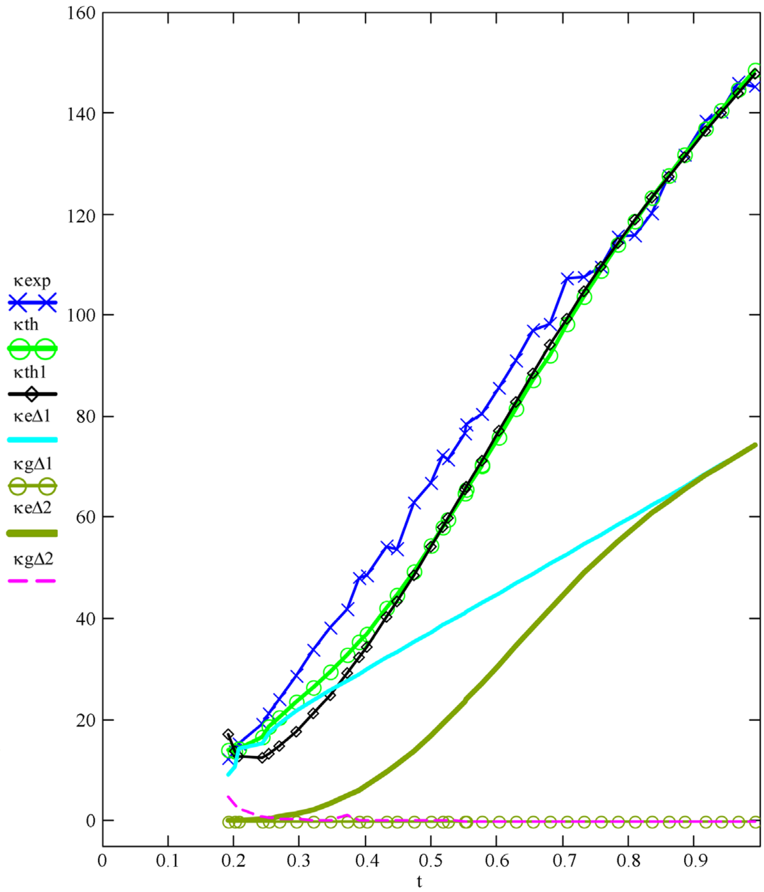

Figure 2. **Clockwise, plots of: a) the experimental values of the total thermal conductivity κ_t (meV·cm^{-1}·deg^{-1}) against $t = T/T_c$ (blue) for all $T \le T_c$ in the data of B *et al.* [7]; b) the theoretical values of κ_s in Scenario 2 (green); c) the theoretical values of κ_s in Scenario 1 (black). The remaining four plots correspond to Scenario 2: uppermost of these is for the electronic part of κ_t due to the smaller gap, followed by the similar part due to the larger gap. The two coincident plots at the bottom of the figure are the lattice parts of the total thermal conductivity due to the two gaps.**

We have also analyzed the data of S *et al*. [8] by following the same approach. Typically, both A and B now have somewhat lower values than was the case for the data of B *et al*. An example: with T_1 = 0.452423 K and T_2 = 25.84772 K, we obtain:

$A = 0.48412, B = 1.01782 \times 10^{-6}$. **Figure 3** gives plots of $\kappa_s(T)\big|_{\text{exp}}$ and $\kappa_s(T)\big|_{\text{theory}}$ against some selected reduced temperatures for this case.

4. Discussion

1) While it has been reported [13] that the two gaps of MgB_2 close at the same T_c (Scenario 1), *this result does not pertain to the conditions under which thermal conductivity is determined*. For this reason we chose here to also address the experimental data in the additional scenario in which the gaps close at different T_cs (Scenario 2). In both cases, as can be seen from **Table 1**, the total thermal conductivity is constituted predominantly by the electronic part. While both $\kappa_{es}(T, \Delta_1)$ and $\kappa_{es}(T, \Delta_2)$ decrease with T, near T_c, $R \equiv \kappa_{es}(T, \Delta_1)/\kappa_{es}(T, \Delta_2) \approx 1$. Further, at the lowest temperature in the table, $R \approx 60$ (Scenario 1) and $R \approx 115$ (Scenario 2). Thus: a) in the entire range of temperature to which the experimental data of B *et al*. [7] pertain, *i.e.*, $0.2008 \le t \le 1$, $\kappa_{gs}(t)$ makes negligible contribution to $\kappa_s(t)$ in both the scenarios, b) in the range $0.4477 \le t \le 1$, the results in the two scenarios differ by no more than 3%, and c) for $t < 0.4477$, $\kappa_s(t)$-values in Scenario 1 are lower than in Scenario 2—by about 40% at $t = 0.2684$, for example. Overall, the latter scenario is thus found to be in better agreement with experiment

2) In order to shed light on the above findings, we draw attention to the following relations obtained via the Gorter-Casimir two-fluid theory of superconductivity, as in, e.g., [20]:

$$n_s(t) \equiv N_s(t)/N_s(0) = 1 - t^4, \quad 1 \ge n_s(t) \ge 0 \quad (0 \le t \le 1) \tag{16}$$

where N_s is the density of superconducting electrons. So far as the temperature dependence in (16) is concerned, it has been noted that "some authors report other exponent values or related expressions" [20], but that does not concern us here.

The second relation in (16) is strikingly similar to

$$1 \ge \delta(t) \equiv \Delta(t)/\Delta(0) \ge 0. \tag{17}$$

We thus infer that *greater* the value of $\delta(t)$ greater is the fraction of superconducting electrons (or CPs) and therefore *smaller* the fraction of available electrons as heat-carriers. It is only under this circumstance that heat is predominantly carried by phonons, *i.e.*, when t is close to 0 K. This explains the result in para 1 (a) in this section: the contribution of $\kappa_{gs}(t)$ to $\kappa_s(t)$ is negligible because bulk of the data under consideration pertains to values of t not close enough to 0 K. Note that in both the scenarios the Sp. Ht. and the MFP of electrons have the same values at any T. The result in para 1 (c) is explicable if the sum of the gap-values at any t is naively regarded as proportional to the number of superconducting electrons (or CPs) at that t. An example: at $t = 0.3195$ the sum of the two gap values is 8.0879 in Scenario 1 and 6.3336 meV in Scenario 2. This implies that there are *fewer* CPs in the latter scenario (and therefore *more* left over electrons as carriers of heat) than in the former. This is reflected in the κ_s values: 21.174 (Scenario 1), 26.409 $W \cdot cm^{-1} \cdot deg^{-1}$ (Scenario 2).

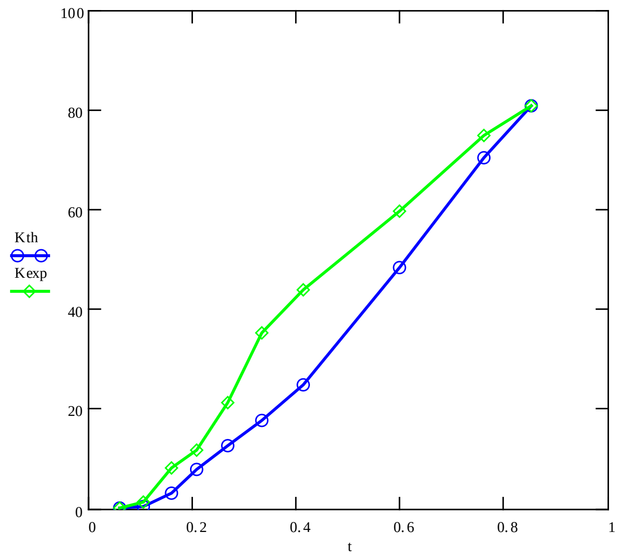

Figure 3. Plots of the experimental values (green) of total thermal conductivity ($meV \cdot cm^{-1} \cdot deg^{-1}$) in the data of S *et al*. [8] against $t = T/T_c$ at some selected temperatures below T_c and their theoretical counterparts (blue) in Scenario 2.

3) The result in para 1 (b) implies that number of carriers in the stated range is more or less the same in both the scenarios; this however is not seen as convincingly as in the preceding case.

4) A feature of our approach is that we have not relied upon the Wiedemann-Franz law to separate out the lattice part of the total thermal conductivity. There is a difference of opinion about the utility of this law for the problem addressed here: while B *et al*. [7] have found it useful for the analysis of their data, Sologubenko *et al*. [21] have questioned its applicability for MgB_2 at low temperatures.

5) We now report our findings about the data of S *et al*. [8], the values of A and B for which were given above. We note that at around the same temperatures below 39 K, the values of $\kappa_s(T)$ reported by S *et al*. are lower than the values reported by B *et al*. [7]. At the highest temperature below 39 K, for example, they quote κ (38.86986 K) = 80.4 $mW \cdot cm^{-1} deg^{-1}$ as against κ (38.7056) = 145.2463

$mWcm^{-1}deg^{-1}$ quoted by B *et al*. We also note that B *et al*. have reported their data up to $T = 7.4187$ K, whereas S *et al*. have done so up to $T = 1.8752$ K. The differences in the values of $\kappa_s(T)$ of the two groups can be ascribed to the compositional differences of the samples and the manners of their preparation since these can cause the scattering mechanism in the two samples to differ. This is an observation about which S has remarked [22]: "Concerning the MgB_2 sample quality, I fully agree with you. It was the early time of superconducting MgB_2. Thus, sample composition, granularity etc. may differ significantly from group to group. This assumption is also supported by varying reported values of, e.g., the thermoelectric power."

6) It seems interesting to point out that the approach followed in this paper is remarkably similar to the qualitative approach of Sologubenko *et al*. [21], who have noted: "Thus, we consider two subsystems of quasiparticles with gaps Δ_1 and Δ_2, different parameters E_1 and E_2 of phonon-electron scattering, and separate contributions κ_{e1} and κ_{e2} to the heat transport." In this manner—in the early days of MgB_2—they were able to give good estimates of the zero-temperature values of the two gaps.

5. Conclusions

1) We have presented here a detailed study of the thermal conductivity of MgB_2 in the superconducting state via GBCSEs that were derived from a BSE by appealing to the twin concepts of a superpropagator and multiple Debye temperatures. This approach manifestly gives the ideas of Liu *et al*. [15], Choi *et al*. [16], and Sologubenko *et al*. [21] a concrete form.

2) A remarkable result of this paper is: while over a substantial range of temperatures below T_c the results in Scenario 1 are indistinguishable from those of Scenario 2, the latter scenario yields results in progressively better agreement with experiment when $T \leq 15$ K. As is well known, thermal conductivity is a non-equilibrium phenomenon; it is measured under conditions of no electric current. Since a thermal current tends to drag a small electric current with it, this current must be balanced by an equal and opposite current. In an SC, it is balanced by a supercurrent. For these reasons, measurement of thermal conductivity requires a rather elaborate experimental setting up. It is not inconceivable therefore that cumulative effect of the stresses caused by this setting up lifts the "degeneracy" of the two gaps closing at the same T.

3) We finally note that the approach followed here may also shed light on whether or not the Tl- and the Bi-based HTSCs are characterized by three gaps—the possibility of which was suggested in [11].

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