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# Influence of a magnetic field on the thermal conductivity of d-wave high- $T_c$ superconductors

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**Abstract.** The influence of a magnetic field on the electronic contribution  $\kappa_e$  to the thermal conductivity of a d-wave superconductor is described. We use the kinetic expression for  $\kappa_e$  in terms of a number of carriers deduced from the electronic specific heat of a d-wave superconductor. We calculate the field and temperature dependence of the scattering rate of normal heat-carrying electrons scattered by quasi-particle excitations in the 2D-like vortex cores. Near  $T_c$ , the experimental results on various  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  and  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$  samples are quite well reproduced by this model, as in the s-wave case with a small difference between the deduced physical parameters. However, experimental results on the field dependence of the thermal conductivity at very low temperatures are shown to be incompatible with an s-wave gap parameter but can be explained by considering a d-wave order parameter. More reasonable parameter values are found herein.

## 1. Introduction

The thermal conductivity of high- $T_c$  superconductors remains an interesting and controversial transport coefficient [1]. The influence of a magnetic field on the thermal conductivity is similar in various high- $T_c$  cuprates [2–7]; the magnetothermal conductivity  $\kappa(B)$  is observed to decrease as the magnetic induction  $B$  is increased and this relative decrease is less pronounced when the temperature is raised.

The first phenomenological model of the magnetothermal conductivity of high- $T_c$  superconductors was proposed by Richardson *et al* [2] who assumed that phonons were moving as Bloch waves in a periodic vortex lattice potential, thus supposing that the vortex lattice is quite regular. These workers obtained an unusual stretched exponential  $B \exp(-B^{1/4})$  behaviour for the excess thermal resistivity in the temperature range near  $T_c/2$ . Bougrine *et al* [4] derived the origin of such a theoretical law from a model including bound and free vortices on intragranular and intergranular defects. The exponent 1/4 was shown to be a particular value specific to the  $(B, T)$  regime examined by Richardson *et al*. In fact, characteristic lengths such as the mean free path, the penetration depth and the characteristic defect size control the value of the exponent in the stretched exponential.

However, this phonon model seems implausible since high- $T_c$  compounds present intrinsic and extrinsic defects which act as pinning centres of vortices. This should lead to a rather irregular vortex lattice. Furthermore, at temperatures not far below  $T_c$  such a lattice is rather unstable.

In recent work [8,9], we showed that the temperature dependence of the thermal conductivity of the high- $T_c$  cuprates could be well described by considering an electronic origin of the peak observed below  $T_c$  [1] together with assuming a  $d_{x^2-y^2}$ -wave gap

parameter. In the present work, we calculate the field dependence of the electronic contribution to the thermal conductivity of a d-wave superconductor. We show that experimental results on various high- $T_c$  materials can be well described by this model with a small difference between the deduced physical parameters from the s-wave case. However, the field dependence of  $\kappa$  at very low temperatures is shown to be incompatible with our previous calculations on the magnetothermal conductivity of an s-wave superconductor [7]. The data are much better reproduced with a d-wave gap parameter. More reasonable parameter values are found herein.

The theoretical model is presented in section 2. In section 3, the results are compared with the experimental data on various  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  and  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$  samples. Conclusions are finally drawn in section 4.

## 2. Theoretical model

The expression for the magnetothermal resistivity is given by [10]

$$\kappa^{-1}(B, T) = \kappa^{-1}(0, T) + \kappa_{e-v}^{-1}(B, T) \quad (1)$$

where  $\kappa(0, T)$  is the thermal conductivity in the absence of a field, and  $\kappa_{e-v}^{-1}(B, T)$  the excess thermal resistivity due to the scattering of electrons by the vortex cores. Note that the phonon ‘background’ as well as the electron–phonon, electron–electron and electron–defect scattering contributions are contained in  $\kappa(0, T)$ . The magnetic induction dependence of  $\kappa$  is thus calculated here to arise only from the electron–vortex scattering.

The magnetic induction dependence of the electronic thermal conductivity can be derived using the well known kinetic formula [11]

$$\kappa_{e-v}(B, T) = \frac{1}{3} C_e(B, T) v_F^2 \tau_{e-v}(B, T) \quad (2)$$

where  $C_e(B, T)$  is the electronic specific heat,  $v_F = \sqrt{2\varepsilon_F/m^*}$  is the Fermi velocity, with  $\varepsilon_F$  the Fermi energy and  $m^*$  the effective mass of electrons, and  $\tau_{e-v}^{-1}$  is the electron–vortex scattering rate.

Moler *et al* [12] recently analysed the temperature and magnetic induction dependence of the electronic specific heat of a single crystal of  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ . They extracted the following phenomenological expression when the field is applied along the c axis:

$$C_e(B, T) = (\gamma(0) + AB^{1/2})T \quad (3)$$

with  $\gamma(0) = 3.06 \text{ mJ mol}^{-1} \text{ K}^{-2}$  and  $A = 0.91 \text{ mJ mol}^{-1} \text{ K}^{-2} \text{ T}^{-1/2}$  from data fits. The linear temperature behaviour and the magnetic induction dependence of  $C_e$  are specifically characteristic of a d-wave superconductor. It is well known in contrast that the electronic specific heat of an s-wave superconductor decreases exponentially at low temperatures [13]. Moreover, equation (3) implies that the density  $N(\varepsilon_F, B)$  of states near the Fermi level increases with increasing induction as  $B^{1/2}$ , a dependence which has been theoretically predicted for a superconductor with lines of nodes in the gap, such as in a d-wave superconductor [14].

On the other hand, there is theoretical as well as experimental evidence that the electronic structure of a 2D vortex consists of bound quasi-particles which occupy discrete energy levels of the order of  $\varepsilon_n = n\hbar^2/m^*\xi_{ab}^2(T)$  ( $n = 1, 2, \dots$ ) [15, 16], where we use  $\xi_{ab}(T)$  as the in-plane temperature-dependent coherence length given by

$$\xi_{ab}(T) = \xi_{ab}(0) \sqrt{T_c/(T_c - T)}. \quad (4)$$

The scattering rate  $\tau_{e-v}^{-1}$  of heat-carrying electrons by these bound quasi-particles is calculated by considering the Coulomb scattering (corresponding to the well known potential

$V(r) = e^2/\varepsilon_c r$  where  $\varepsilon_c$  is the dielectric constant of the medium) of electrons by the pinned bound states in a 2D circular well, thus taking into account the usual pancake vortex structure of high- $T_c$  compounds. These bound states are characterized by the following wavefunctions [17]

$$\Psi_{n,l,m} = \frac{\sqrt{2\pi}}{r_0^{3/2}} j_l\left(\frac{n\pi r}{r_0}\right) Y_l^m\left(\frac{\pi}{2}, \varphi\right) \quad (5)$$

where  $r_0 = \hbar v_F / \sqrt{\Delta_{ab}^2(T) - \varepsilon_n^2(T)}$  is the localization radius in the vortex core, with  $\Delta_{ab}(T)$  the temperature-dependent superconducting gap parameter along the  $a$ - $b$  plane,  $j_l(kr)$  is the spherical Bessel function and  $Y_l^m(\frac{\pi}{2}, \varphi)$  are the spherical harmonics projected in the  $(x, y)$  plane.

The field and temperature dependences of the d-wave gap parameter can be approximated by [18, 19]

$$\Delta(\mathbf{k}, B, T) = \Delta(0)[\hat{k}_x^2 - \hat{k}_y^2] \tanh(\alpha \sqrt{(T_c(B) - T)/T}) \sqrt{1 - (B/B_{c2})} \quad (6)$$

where  $\Delta(0)$  is the zero-temperature energy gap,  $\hat{k}_x = k_x a$  and  $\hat{k}_y = k_y b$  with  $a$  and  $b$  the crystal parameters along the  $a$  and  $b$  axes, respectively,  $B_{c2}$  is the upper critical field and  $\alpha \approx 2$  [18].

The electron-vortex scattering rate is usually given by

$$\tau_{e-v}^{-1} = \frac{V}{2\pi^3} \int d\mathbf{k}' C(\mathbf{k}, \mathbf{k}') \quad (7)$$

where  $C(\mathbf{k}, \mathbf{k}')$  is the scattering probability which is in the second-order Born approximation [11]

$$C(\mathbf{k}, \mathbf{k}') = \frac{2\pi}{\hbar} \left| \left\langle \mathbf{k}, \psi \left| \frac{e^2}{\varepsilon_c r} \right| \mathbf{k}', \psi' \right\rangle \right|^2 f^0(E)(1 - f^0(E')) f^0(\varepsilon_n) \delta(E' - E) \quad (8)$$

where  $\mathbf{k}$  and  $\mathbf{k}'$  are the wavevectors of the incoming and outgoing electrons, respectively,  $\psi$  is the wavefunction of the bound states in the vortex cores and  $E = \sqrt{\varepsilon(\mathbf{k})^2 + \Delta(\mathbf{k}, B, T)^2}$  is the quasi-particle energy spectrum. Considering the wavefunctions given in equation (5) and the gap parameter given by equation (6), we then obtain the following expression for  $\tau_{e-v}^{-1}$ :

$$\tau_{e-v}^{-1} = \frac{2m^* \pi^3}{\hbar^3 \varepsilon_F^2} \left(\frac{e^2}{\varepsilon_c}\right)^2 \sum_{n,l} g(n, l) \frac{\Delta_{ab}^2(T) - \varepsilon_n^2(T)}{1 + \exp(2\varepsilon_n(T)/k_B T)} \left(\frac{B}{B_{c2}}\right)^{1/2} \quad (9)$$

where

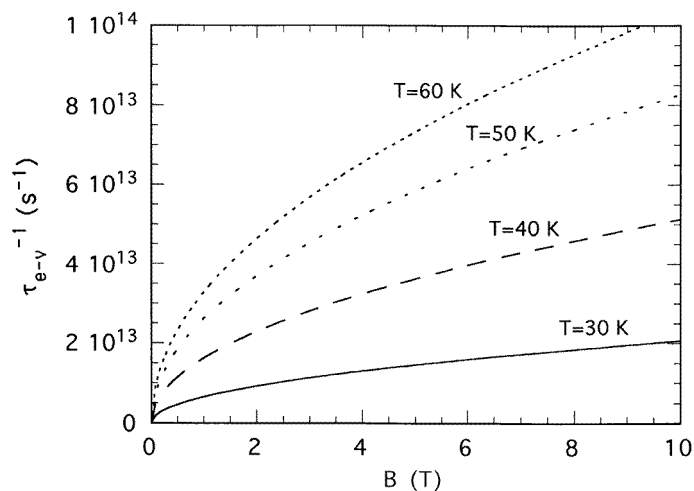
$$g(n, l) = \frac{1}{n} \frac{\Gamma(l + \frac{1}{2})}{\Gamma(l + 1)\Gamma(\frac{1}{2})} F(l + \frac{1}{2}, \frac{1}{2}; l + 1; 1) \quad (10)$$

and  $F(\alpha, \beta; \gamma; z)$  is the hypergeometric function.

It should be emphasized that the term  $(B/B_{c2})^{1/2}$  in equation (9) comes from the fact that the density of quasi-particles in the vortex state of a d-wave superconductor is proportional to the square root of the magnetic induction [14, 19]. It has been shown by Volovik [14] that this quasi-particle density dependence, i.e.  $N(B) \propto \sqrt{B}$ , arises mainly from the electrons located far away from the vortex centre owing to the presence of lines of nodes in the energy gap. These nodes result from the parity of the band structure on the  $k_x = \pm k_y$  lines. They are such that the wavefunction changes sign on both sides of the lines of nodes. The  $\sqrt{B}$  dependence thus reflects such a microscopic feature. Since a d-wave gap parameter

possesses nodes for strict symmetry reasons whereas the zeros are ‘accidental’ [20] (or ‘smooth’) and do not imply at all a change in sign of the wavefunction in an anisotropic s-wave superconductor (and can be in fact smeared out in inhomogeneous materials), it can be understood that the vortex structure of an isotropic and that of an anisotropic s-wave superconductor have rather similar field dependences like  $N(B) \propto B$  [15]. The expression of the electron–vortex scattering rate as given by equation (9) is thus wholly characteristic of a d-wave superconductor. In fact, we shall show in the next section that the expression for the magnetothermal conductivity of an s-wave superconductor does not agree with experimental data at very low temperatures because of that field dependence.

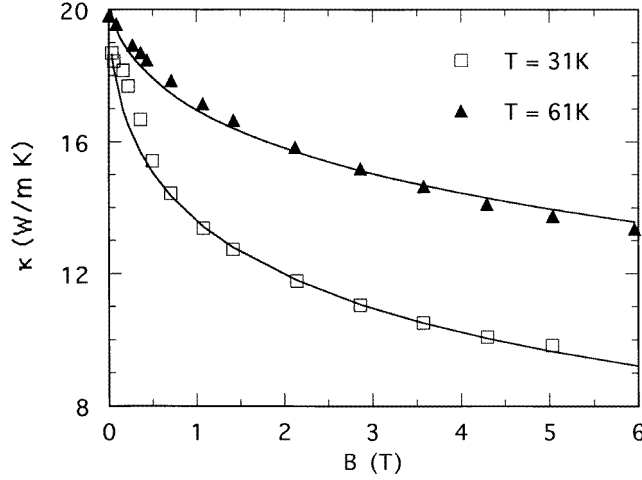
In figure 1 the electron–vortex scattering rate  $\tau_{e-v}^{-1}$  given in equation (9) is shown to increase with increasing temperature and magnetic induction. This result is understood from the fact that the available number of states of thermally excited quasi-particles in the core of vortices increases with increasing temperature. Since the number of vortices is also proportional to the magnetic induction, the electron–vortex scattering rate also increases when the magnetic induction is increased. For comparison with the s-wave case, let us refer the reader to equations (8) and (9) and figure 2 of our previous work on the subject [7]. By mere visual comparison, it can be deduced that the field and temperature dependences of  $\tau_{e-v}^{-1}$  are quite different for both gap parameter symmetries. From the discussion above, it can be pointed out that the expression for the electron–vortex scattering rate of an anisotropic s-wave superconductor (with gap minima in the superconducting order parameter) should also be similar to the isotropic s-wave case discussed in [7]. Therefore  $\tau_{e-v}^{-1}$  in an anisotropic s-wave superconductor has quite a different field dependence from that in d-wave materials.



**Figure 1.** Magnetic induction dependence of the electron–vortex scattering rate  $\tau_{e-v}^{-1}$  at different temperatures.

### 3. Results and discussion

The data on the total magnetothermal conductivity  $\kappa(B)$  of an untwinned single crystal of  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  [2] and of polycrystalline samples of  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  and  $\text{YBa}_2(\text{Cu}_{0.95}\text{Fe}_{0.05})_3\text{O}_{7-\delta}$  [4] are shown in figure 2 and figure 3, respectively. Recent



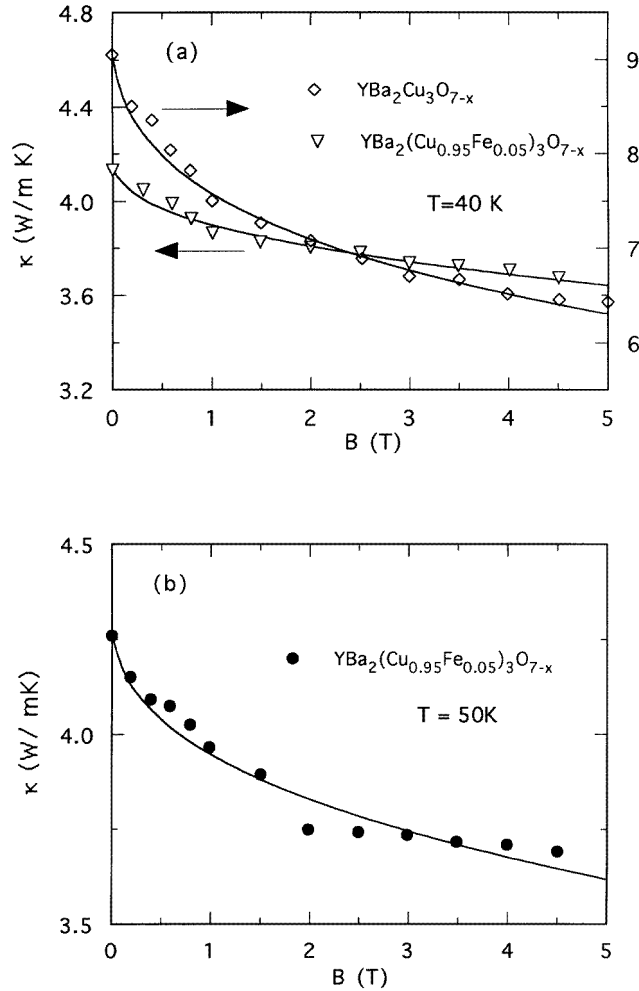
**Figure 2.** Thermal conductivity of an untwinned single crystal of  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  versus the magnetic induction  $B$  at  $T = 31$  K and  $T = 61$  K. (From [2].)

results obtained by Pogorelov *et al* [6] on a single crystal of  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$  are presented in figure 4. Sample preparation and experimental methods to measure the temperature and magnetic induction dependence of the thermal conductivity of these samples were described in [2, 4, 6]. One can see that  $\kappa$  decreases rapidly for  $B < 2$  T and then ‘saturates’ for higher values of the induction. Moreover, the relative decrease in  $\kappa(B)$  is less important when the temperature is increased. Note also that  $\kappa(B)$  decreases less rapidly in the case of  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$  (see figure 4).

For the theoretical fits from equations (1)–(9) shown in figures 2–4, we fix the order of magnitude of the physical parameters to be  $T_c = 90$  K,  $m^* = 4m_0$ ,  $B_{c2} = 100$  T and  $\Delta_{ab}(0) = 25$  meV for  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  [21, 22] and  $T_c = 85$  K,  $m^* = 8m_0$ ,  $B_{c2} = 100$  T and  $\Delta_{ab}(0) = 20$  meV for  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$  [21, 23]. The resulting theoretical curves are in very good agreement with experimental data. The values of the theoretical ‘free parameters’ obtained from the fits (table 1) are quite reasonable.

**Table 1.** Free parameters obtained by the fit of equations (1)–(9) to different sample data [2, 4, 6]. The parameters  $\gamma(0)$  and  $A$  are related to the electronic specific heat in the presence of a magnetic field,  $\varepsilon_F$  is the Fermi energy and  $\xi_{ab}(0)$  is the zero temperature coherence length in the  $a$ – $b$  plane.  $\kappa(0, T)$  is the value of the thermal conductivity in the absence of a field and is directly read from experimental data.

Sample	$\gamma(0)$ ( $\text{J mol}^{-1} \text{K}^{-2}$ )	$A$ ( $\text{J mol}^{-1} \text{K}^{-2} \text{T}^{-1/2}$ )	$\varepsilon_F$ (eV)	$\xi_{ab}(0)$ ( $\text{\AA}$ )	$\kappa(0, T)$ ( $\text{W m}^{-1} \text{K}^{-1}$ )
$\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ (single crystal)	$3.1 \times 10^{-3}$	$6 \times 10^{-4}$	0.25	12.4	18.6 ( $T = 31$ K) 19.8 ( $T = 61$ K)
$\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ (ceramics)	$2.7 \times 10^{-3}$	$5 \times 10^{-4}$	0.27	12.9	9 ( $T = 40$ K)
$\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta} + 5\%$ Fe (ceramics)	$3.6 \times 10^{-3}$	$1.2 \times 10^{-3}$	0.23	12.1	4.1 ( $T = 40$ K) 4.2 ( $T = 50$ K)
$\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ (single crystal)	$1.5 \times 10^{-3}$	$3.2 \times 10^{-3}$	0.18	10.5	2.9 ( $T = 35$ K) 2.5 ( $T = 50$ K)

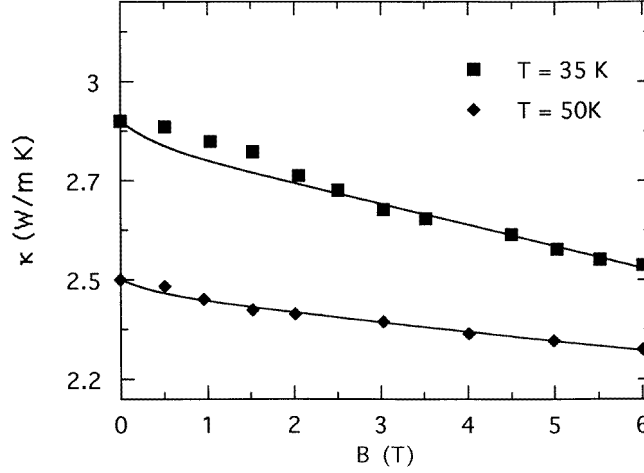


**Figure 3.** (a) Thermal conductivity of  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  ceramics ( $\diamond$ ) as a function of the magnetic induction  $B$  at  $T = 40$  K and of  $\text{YBa}_2(\text{Cu}_{0.95}\text{Fe}_{0.05})_3\text{O}_{7-\delta}$  [4] ceramics ( $\nabla$ ) at the same 40 K temperature. (From [4].) (b) Thermal conductivity of  $\text{YBa}_2(\text{Cu}_{0.95}\text{Fe}_{0.05})_3\text{O}_{7-\delta}$  ceramics ( $\bullet$ ) as a function of the magnetic induction  $B$  at  $T = 50$  K. (From [6].)

Several remarks are in order. We stress that the fit is slightly less precise for the case of polycrystalline systems. This can be understood since ceramic samples contain a high density of defects and data scattering is usually more important. Moreover, some contribution may then also arise from the thermal conductivity  $\kappa_c$  along the  $c$  axis.

The values found for  $\gamma(0)$  and  $A$  are interestingly comparable with those obtained by Moler *et al* [12] for the specific heat (see below equation (3)). This result is an important consistency test based on two different properties for arguing on the symmetry of the order parameter. Also the values of the coherence length  $\xi(0)$  and the Fermi energy  $\varepsilon_F$  are much more realistic in the d-wave model than in the s-wave case [7].

It is furthermore of interest to discuss the parameter  $\gamma(0)$ . From table 1, we see that  $\gamma(0)$  increases when Fe impurities are added to the  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  sample, in agreement



**Figure 4.** Magnetic induction dependence of the thermal conductivity of a single crystal of  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$  at  $T = 35$  K and  $T = 50$  K. (From data in [6].)

with the experimental results of Junod *et al* [24] on the specific heat of polycrystalline samples. In this respect, Sun and Maki [25] have recently calculated the electronic specific heat of a d-wave superconductor and found that  $\gamma(0)$ , which is related to the residual density of states at the Fermi level, increases indeed when the fraction of impurities is increased.

Next, let us note that, even though the fits within a d-wave model are slightly better than for an s-wave gap symmetry [7], the difference is not very drastic and could be argued to arise from the presupposed fixing of the physical parameters. In view of the success found in analysing the low-temperature regime for the field-free case [8], it is of interest to check whether some more definite conclusion can be drawn in the  $\kappa(B)$  case at low temperatures.

The data on the field dependence of the thermal conductivity of  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  and  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$  single crystals at  $T = 6$  K were reported recently [6] and are shown in figure 5. These data can be analysed with our previous s-wave model [7] and with the above d-wave model. The fits are shown in figure 5(a) and 5(b), respectively. One can readily see that the data are much better described by the d-wave model. From the discussion in section 2, it can also be realized that the data should be not well reproduced through analytical work even by considering an anisotropic s-wave gap parameter.

Also, the values of the free parameters obtained within the s-wave model are quite unrealistic since we find that  $\varepsilon_F = 25$  eV and  $\xi(0) = 207$  Å for  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  and  $\varepsilon_F = 46$  eV and  $\xi(0) = 198$  Å for  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ . We remind the reader that the expression for the magnetothermal conductivity of an s-wave superconductor is given by [7]

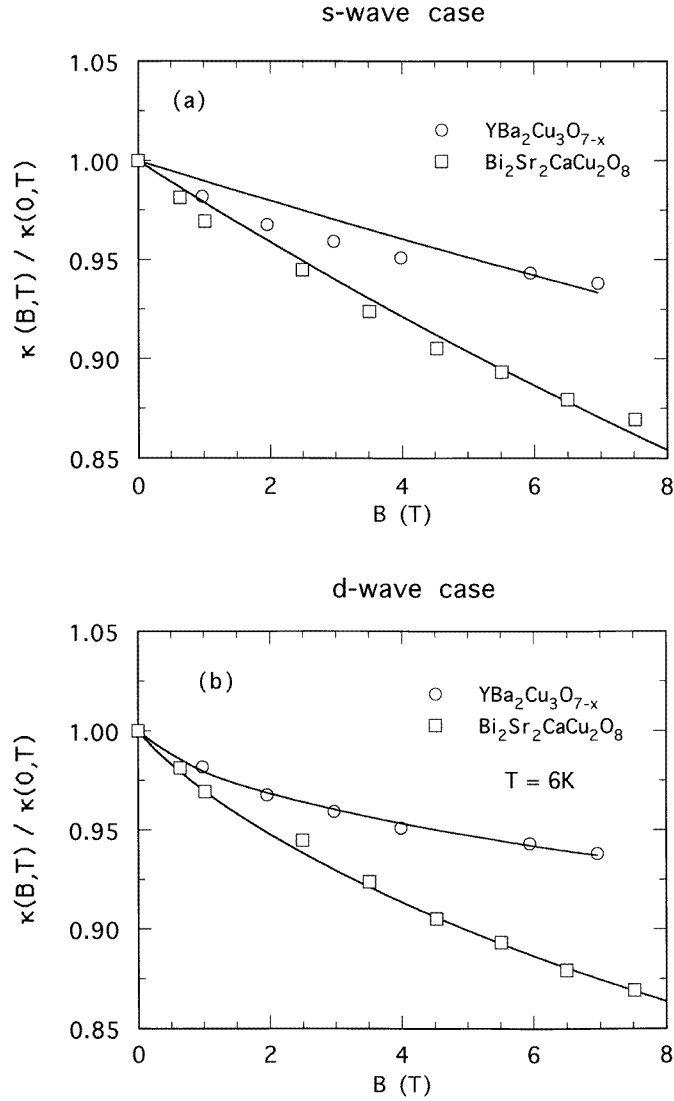
$$\kappa_{e-v}(B, T) = \frac{\pi^2 k_B^2 T}{3 m^*} n_0 \exp\left(-\frac{\Delta(0)}{k_B T} \sqrt{\frac{T_c(B) - T}{T_c(B)}} \sqrt{1 - \left(\frac{B}{B_{c2}}\right)^2}\right) \tau_{e-v}(B, T) \quad (11)$$

where  $\tau_{e-v}^{-1}$  is given by

$$\tau_{e-v}^{-1} = \frac{e^5 B_{c2}}{\hbar^2 c \varepsilon_F^2} \sum_n \frac{\sqrt{\Delta^2(T) - \varepsilon_n(T)^2}}{1 + \exp(2\varepsilon_n/k_B T)} \left(\frac{B}{B_{c2}}\right). \quad (12)$$

Therefore the basic explanation about the difference in behaviour results from the rapidly decreasing exponential term in equation (11) which comes from the quasi-particle density





**Figure 5.** Field dependence of the thermal conductivity of  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  and  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$  single crystals [6] at  $T = 6 \text{ K}$  and fits with (a) the s-wave model and (b) the d-wave model.

in an s-wave superconductor. Hence, the amplitude (pre-factor) of the electron–vortex relaxation time should be quite large in order to reproduce the experimental results. Hence, from equation (12), this implies a quite large (and unrealistic) value of the Fermi energy.

Note, on the other hand, that the values of the physical parameters resulting from the low- $T$  region in the d-wave case are again very realistic:  $\gamma(0) = 2.6 \times 10^{-3} \text{ J mol}^{-1} \text{ K}^{-2}$ ,  $A = 7.6 \times 10^{-4} \text{ J mol}^{-1} \text{ K}^{-2} \text{ T}^{-1/2}$ ,  $\varepsilon_F = 0.26 \text{ eV}$  and  $\xi(0) = 12.7 \text{ \AA}$  for  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  and  $\gamma(0) = 1.2 \times 10^{-3} \text{ J mol}^{-1} \text{ K}^{-2}$ ,  $A = 5.6 \times 10^{-4} \text{ J mol}^{-1} \text{ K}^{-2} \text{ T}^{-1/2}$ ,  $\varepsilon_F = 0.23 \text{ eV}$  and  $\xi(0) = 10.5 \text{ \AA}$  for  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ .

#### 4. Conclusions

In this work, we have calculated the field dependence of the thermal conductivity of a d-wave superconductor, considering that electrons are mainly scattered by the bound states in the vortex cores. Experimental results on various  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  and  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$  samples are quite well reproduced by this model with very realistic values of the free parameters.

The data in the ‘intermediate-temperature’ range ( $T \approx 30\text{--}50$  K) could also be well reproduced by our previous s-wave model [7] but with values of the coherence length  $\xi(0) \approx 20$  Å slightly too large. We have shown here that theoretical fits to the magnetothermal conductivity of high- $T_c$  materials at low temperatures in the s-wave model (either isotropic or anisotropic) are not very good and lead to quite unphysical values of the Fermi energy and the coherence length. On the other hand, this field dependence at low temperatures is very well described by the d-wave model and this is due to the presence of lines of nodes in  $\Delta(\mathbf{k})$  with changes in the wavefunction sign across the lines due to the parity of the band structure on the  $k_x = \pm k_y$  lines.

A more elaborate theory going beyond the second-order Born approximation, thus taking into account multiple-scattering effects, could be envisaged. Dissipation from the flux line lattice motion could then also be considered. This might be helpful in order to reproduce better the data at low fields, namely the small shoulder observed in that  $(B, T)$  region (see figures 2 and 4). It should be noted that such a region is near the vortex glass–vortex liquid transition, a feature nevertheless outside the scope of this paper.

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