

**Electronic thermal conductivity of multigap superconductors: Application to MgB<sub>2</sub>**

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The remarkable field dependence of the electronic thermal conductivity observed in MgB<sub>2</sub> can be explained as a consequence of multigap superconductivity. A key point is that for moderately clean samples, the mean free path becomes comparable to the coherence length of the smaller gap over its entire Fermi surface. In this case, quasiparticle excitations bound in vortex cores can easily be delocalized, causing a rapid rise in the thermal conductivity at low magnetic fields. This feature is in marked contrast to that for anisotropic or nodal gaps, where delocalization occurs only on part of the Fermi surface.

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**I. INTRODUCTION**

The unexpected discovery of superconductivity in MgB<sub>2</sub> with a relatively high  $T_c = 38$  K (Ref. 1) aroused great interest and was soon followed by experiments which established phonon mediated *s*-wave superconductivity, e.g., a B-isotope effect,<sup>2</sup> a coherence peak in the <sup>11</sup>B nuclear relaxation rate,<sup>3</sup> and an exponential dependence for temperatures  $T \lesssim 10$  K.<sup>4,5</sup> Theoretical studies concluded that the coupling of the holes in the  $2p_\sigma$  bands of the B planes to bond stretching modes was strong and primarily responsible for superconductivity. The electron-phonon coupling on the parts of the Fermi surface associated with  $2p_\pi$  bands is much weaker.<sup>6-10</sup>

Despite its standard origin, superconductivity in MgB<sub>2</sub> has several unusual properties pointing toward a more complex nature. One aspect is the presence of two gaps of different magnitudes. Their ratio is estimated as  $r = \Delta_0^S / \Delta_0^L \sim 0.3-0.4$  based on various experiments.<sup>4,11-15</sup> Evidence of two gaps is also provided by the rapid rise of the specific-heat coefficient,  $\gamma_s(H)$ , at very low magnetic fields.<sup>4,15</sup> Orbital dependent superconductivity was proposed theoretically by several authors with the primary (secondary) gap associated with the  $\sigma$ - ( $\pi$ ) bands.<sup>6,16-18</sup>

Recent studies of the in-plane thermal conductivity in a magnetic field show an unusual field dependence.<sup>19</sup> For fields both parallel and perpendicular to the *c* axis, the electronic thermal conductivity  $\kappa_s(H)$  exhibits a steep increase in the low-field region of the mixed state, suggesting a large release of mobile quasiparticles in the mixed state. This contrasts strongly with the behavior of conventional *s*-wave superconductors, where quasiparticles bound in the vortex cores make very little contribution to  $\kappa_s$  except very close to  $H_{c2}$ .<sup>20,21</sup> At first glance, a small secondary gap  $\Delta_0^S$  in multiband models would provide enough carriers for transport at low fields. However, they would be nonmobile carriers inherent in their *s*-wave character. It is our aim here to reexamine thermal transport for multigap superconductors and show the drastic influence of sample purity on the characteristic behavior of  $\kappa_s(H)$ .

The measured MgB<sub>2</sub> samples are regarded as being in the moderately clean regime: experimental estimates of the mean free path give  $l \sim 500-800$  Å, compared with the inplane coherence length  $\xi_{ab} \sim 120$  Å derived from  $H_{c2}$ , which is

determined by the primary superconducting  $\sigma$  band.<sup>22</sup> The relevant length scale here to be compared with  $l$  is, however,  $\xi_0^S$  of the passive  $\pi$  band. Thus we may consider quasiparticles in the  $\sigma$  band in the moderately clean regime, while those in the  $\pi$  band with  $\xi_0^S \sim \xi_0^L/r$  can be in marginally clean regime. The numerical calculation based on the Bogoliubov-de Gennes framework shows that low-energy states in the smaller gap are loosely bound in vortex cores.<sup>23</sup> Moreover, recent scanning tunneling spectroscopy measurements confirmed a large  $\xi_0^S \approx 500$  Å in MgB<sub>2</sub>.<sup>24</sup> Since the magnitude of the secondary gap is small all over the Fermi surface, we expect a distinctively different behavior of  $\kappa_s(H)$  compared to single-band superconductors with an anisotropic gap or even gap nodes. In the following we will at various points compare the two-gap behaviors with that of anisotropic single-gap superconductors.

In view of these circumstances, we analyze the field dependence of  $\kappa_s$  and the density of states (DOS)  $N_s$ . In the following section, we introduce Pesch's solution<sup>25-27</sup> for the quasiclassical formalism,<sup>28,29</sup> which is known to be valid for the range of purity in question. Next we show that quasiparticle excitations in the small gap bound in the vortex cores can easily be delocalized, causing a rapid rise at low magnetic field. It turns out that the rapid rise originates mainly from a drastic enhancement of the transport lifetime all over the Fermi surface in the marginally clean regime. To confirm the importance of contributions from the whole Fermi surface of the small gap, we show a comparison of two-gap model to anisotropic *s*- and *d*-wave models. The field dependence of the two-gap model is definitely stronger than that obtained for any of the single-band models. Conversely, superclean samples should exhibit a behavior very similar to that of conventional *s*-wave superconductors. Finally, we give brief comment on low-field behaviors, where the existence of the small gap becomes also important.

**II. THERMAL CONDUCTIVITY IN A MAGNETIC FIELD**

We restrict our considerations to the case of the in-plane thermal current with  $H \parallel z$ . Thus in-plane impurity scattering is the most important for the thermal transport. The scattering matrix between  $\sigma$  and  $\pi$  bands is assumed to be small because of the different parity of the two orbitals under the

reflection  $z \rightarrow -z$ .<sup>30</sup> Thus we neglect interband impurity scattering completely and discuss contributions from each bands independently. In order to calculate  $\kappa_s(H)$  and  $N_s(H)$ , we introduce the quasiclassical propagators

$$\hat{g}(\omega_n, \hat{\mathbf{k}}, \mathbf{R}) = \begin{pmatrix} -ig & f \\ -f^\dagger & ig \end{pmatrix} \equiv \int \frac{d\xi}{\pi} \hat{\tau}_3 \hat{G}(\omega_n, \mathbf{k}, \mathbf{R}), \quad (1)$$

where  $\hat{G}$  is the Nambu-Gorkov Green's function matrix with the fermionic Matsubara frequency,  $\omega_n$ , the center of mass coordinate  $\mathbf{R}$ , and the relative momentum  $\mathbf{k}$ .  $\tau_3$  is the  $z$  component of the Pauli matrices acting on the particle-hole space and  $\hat{\mathbf{k}} \equiv \mathbf{k}_F/|\mathbf{k}_F|$  is the unit wave vector at the Fermi surface. They satisfy the normalization condition  $\hat{g}^2 = -\hat{1}$  and obey the Eilenberger equations ( $\hbar = c = k_B = 1$  hereafter),

$$[[i\tilde{\omega}_n + e\mathbf{v}_F \cdot \mathbf{A}(\mathbf{R})] \hat{\tau}_3 - \hat{\Delta}(\hat{\mathbf{k}}, \mathbf{R}), \hat{g}] + i\mathbf{v}_F \cdot \nabla_{\mathbf{R}} \hat{g} = 0, \quad (2)$$

or, explicitly,

$$\mathcal{L}_+ f = 2g \Delta(\hat{\mathbf{k}}, \mathbf{R}), \quad \mathcal{L}_- f^\dagger = 2g \Delta^*(\hat{\mathbf{k}}, \mathbf{R}), \quad (3)$$

$$\mathbf{v}_F \cdot \nabla_{\mathbf{R}} g - \Delta^*(\hat{\mathbf{k}}, \mathbf{R}) f + \Delta(\hat{\mathbf{k}}, \mathbf{R}) f^\dagger = 0, \quad (4)$$

with

$$\mathcal{L}_\pm = 2\tilde{\omega}_n - 2ie\mathbf{v}_F \cdot \mathbf{A}(\mathbf{R}) \pm \mathbf{v}_F \cdot \nabla_{\mathbf{R}}, \quad (5)$$

which are supplemented by the gap and Maxwell equations. Here we have introduced the gap matrix

$$\hat{\Delta}(\hat{\mathbf{k}}, \mathbf{R}) = \begin{pmatrix} 0 & \Delta(\hat{\mathbf{k}}, \mathbf{R}) \\ -\Delta^*(\hat{\mathbf{k}}, \mathbf{R}) & 0 \end{pmatrix} \quad (6)$$

and the renormalized frequency  $\tilde{\omega}_n = \omega_n + \sigma(\omega_n)$ , where  $\sigma$  is the diagonal element of the impurity self-energy, which will be determined by the Born approximation for the two-gap and single-gap anisotropic  $s$ -wave models, while the  $T$ -matrix approximation is used for the single-gap  $d$  wave. We have neglected vertex corrections.

Instead of solving these transportlike equations self-consistently, we adopt the Brandt-Pesch-Tewordt approximation.<sup>25</sup> In this approximation, an Abrikosov solution is used for vortex lattice structures, and the spatial dependence of the magnetic field is replaced by the external uniform field  $H$ . Only the uniform component  $\bar{g}$  is kept, since the higher Fourier  $\mathbf{K}$  components of  $g(\mathbf{R})$  decrease rapidly as  $\exp(-\Lambda^2 K^2)$ ,  $\Lambda = 1/\sqrt{2eH}$  being the magnetic length. On the other hand, the exact spatial dependence of the anomalous propagators is taken into account including the phase variation due to the vortices. Although this theory was designed to work well for  $H \lesssim H_{c2}$ , especially in strongly type-II superconductors like  $\text{MgB}_2$ , a detailed comparison to numerical solutions yields good agreement both for  $s$ - and  $d$ -wave superconductors over almost the whole field range.<sup>31</sup> This numerical study also shows that the frequently applied Volovik-theory,<sup>32</sup> yielding  $\gamma_s \propto H$  for an  $s$ -wave gap and  $\gamma_s \propto \sqrt{H}$  for gaps with lines of zeros, is restricted to the very low-field region. This indicates the im-

portance of quasiparticle transfer between vortices even in the relatively low-field region.<sup>33</sup>

Following Pesch,<sup>26,31,34</sup> the solutions in Eq. (2) can be obtained formally as follows. With use of  $\bar{g}$ , Eq. (3) can be inverted as

$$f = 2\text{sgn}(\omega_n) \bar{g} \int_0^\infty dt \exp[-\mathcal{L}_+ \text{sgn}(\omega_n) t] \Delta(\hat{\mathbf{k}}, \mathbf{R}). \quad (7)$$

Assuming the Abrikosov solution for the vortex lattice ( $p_n = 2\pi n/b$ ,  $b$  being the lattice constant in the  $y$  direction),

$$\Delta(\hat{\mathbf{k}}, \mathbf{R}) = \sum_n C_n e^{ip_n y} \exp[-(x - \Lambda^2 p_n)^2 / 2\Lambda^2], \quad (8)$$

with appropriate normalization constants  $C_n$  for a given structure of the lattice, after straightforward calculation with the help of Eq. (7) we obtain

$$\overline{ff^\dagger} = -i\sqrt{\pi} \bar{g}^2 \left( \frac{2\Lambda \bar{\Delta}(\hat{\mathbf{k}})}{v_{F\perp}(\hat{\mathbf{k}})} \right)^2 W'(iu_n), \quad (9)$$

where  $W(u) = e^{-u^2} \text{erfc}(-iu)$  is the Faddeeva function and  $u_n = \tilde{\omega}_n \text{sgn}(\omega_n) [2\Lambda/v_{F\perp}(\hat{\mathbf{k}})]$ . Here  $\bar{\Delta}(\hat{\mathbf{k}})$  denotes the spatial average of the gap and  $v_{F\perp}(\hat{\mathbf{k}})$  is the component of  $\mathbf{v}_F$  perpendicular to the field. Making use of the normalization condition,  $\bar{g}^2 + \overline{ff^\dagger} = 1$ , (after analytic continuation to the upper half plane,  $i\omega_n \rightarrow \omega + i\delta$ ), we finally obtain

$$\bar{g}_{\hat{\mathbf{k}}}(\omega) = [1 - i\sqrt{\pi} [2\Lambda \bar{\Delta}(\hat{\mathbf{k}})/v_{F\perp}(\hat{\mathbf{k}})]^2 W'(u)]^{-1/2}. \quad (10)$$

The real part of  $\bar{g}_{\hat{\mathbf{k}}}(\omega)$  is nothing but the angle-dependent DOS normalized by the normal state DOS  $N_n$ . In order to get the closed-form solution, we use the Born approximation for the  $s$ -wave scattering self-energy, i.e.,

$$\sigma(\omega) = \langle \bar{g}_{\hat{\mathbf{k}}}(\omega) \rangle / 2\tau_n, \quad (11)$$

where  $\tau_n$  is the lifetime in the normal state and  $\langle \dots \rangle$  represents an angular average over the Fermi surface. Then we can determine the self-consistent  $\sigma(\omega)$  numerically.

From the linear response of the thermal current  $j_{hi}$  to the temperature gradient  $-\nabla_j T$  in an extended version of Eilenberger equations with a time-dependent perturbation, we obtain the thermal conductivity tensor<sup>27-29</sup> as

$$\kappa_s^{ij} = v_F^2 N_n \int_0^\infty d\omega \left( \frac{\omega}{T} \right)^2 \text{sech}^2 \left( \frac{\omega}{2T} \right) \times \langle \hat{k}_i \hat{k}_j \text{Re}[\bar{g}_{\hat{\mathbf{k}}}(\omega)] \text{Re}[\tau_{\hat{\mathbf{k}}}(\omega)] \rangle. \quad (12)$$

By a comparison with the simple kinetic theory, the transport lifetime, which is denoted as  $\text{Re}[\tau_{\hat{\mathbf{k}}}(\omega)]$ , is given by

$$\frac{1}{2\tau_{\hat{\mathbf{k}}}(\omega)} = \sigma(\omega) + \sqrt{\pi} \frac{2\Lambda \bar{\Delta}^2(\hat{\mathbf{k}})}{v_{F\perp}(\hat{\mathbf{k}})} \frac{\text{Re}[W(u) \bar{g}_{\hat{\mathbf{k}}}(\omega)]}{\text{Re}[\bar{g}_{\hat{\mathbf{k}}}(\omega)]}. \quad (13)$$

Here scattering by the vortices appears in addition to quasiparticle broadening due to impurities. Note that Eqs. (10)–

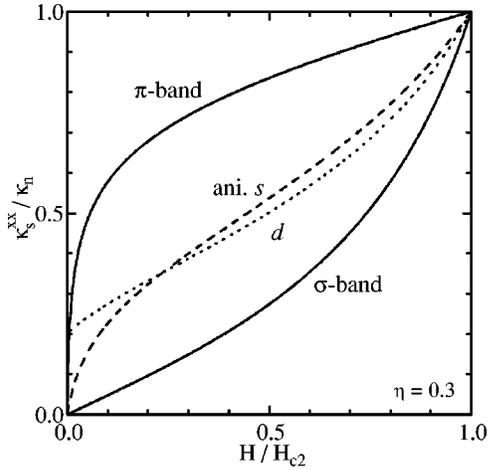


FIG. 1. The field dependence of the in-plane thermal conductivity. For  $\eta=0.3$ , the contribution from the marginally clean passive  $\pi$  band shows a rapid rise at very low field, while that from the active  $\sigma$  band gives a conventional behavior. Anisotropic  $s$ - and  $d_{x^2-y^2}$ -wave cases are given for comparison.

(13) can be reduced to the conventional expressions in the  $H=0$  limit.<sup>35</sup> Moreover one finds  $\bar{g}_{\hat{k}}=1$  and  $\tau_{\hat{k}}=\tau_n$  in the normal state.

We concentrate on the  $T\rightarrow 0$  limit in this paper. The gap function is factorized as

$$\bar{\Delta}(\hat{\mathbf{k}}) = r\Delta_0\varphi_{\hat{k}}\sqrt{1-H/H_{c2}}, \quad (14)$$

where we use  $0 < r < 1$  for the smaller gap and  $r=1$  for the larger gap or the single-band case. The shape of the averaged gap function  $\bar{\Delta}(\hat{\mathbf{k}})$  is given by  $\varphi_{\hat{k}}$ , e.g.,  $\varphi_{\hat{k}}=1$  for an isotropic  $s$ -wave gap. In order to elaborate the difference of the gap structures, later we will make a comparison of the two-gap model to the  $d_{x^2-y^2}$  wave,  $\varphi_{\hat{k}}=\hat{k}_x^2-\hat{k}_y^2$  and the anisotropic  $s$  wave,<sup>36</sup>  $\varphi_{\hat{k}}=1/\sqrt{1+a\hat{k}_z^2}$ . We use the square-root field dependence in Eq. (14) inferred from Ginzburg-Landau theory.

### III. APPLICATION TO MgB<sub>2</sub>

We discuss now  $\kappa_s^{xx}(H)$  for MgB<sub>2</sub> and the other cases based on this theory. For MgB<sub>2</sub> for simplicity we use a spherical (cylindrical) Fermi surface for the  $\pi$ - ( $\sigma$ -) band and the parameters  $n \equiv N_n^\pi/N_n^\sigma = 1.5$ ,  $q \equiv v_F^\pi/v_F^\sigma = 1.5$ , and  $r \equiv \Delta_0^S/\Delta_0^L = \Delta_0^\pi/\Delta_0^\sigma = 0.35$ . The impurity scattering rate for the  $\sigma$  band is moderate,  $\eta \equiv 1/2\tau_n\Delta_0^\sigma = 0.3$ . These parameters are within the range of current estimates.<sup>17,19,22,24</sup> In Fig. 1, the contribution from the  $\pi$  band shows a rapid rise for very low fields, while that from the  $\sigma$  band displays rather conventional behavior. This rapid rise is caused by the drastic enhancement of the quasiparticle lifetime of the smaller gap over the entire Fermi surface as vortices are introduced. In contrast, as we demonstrate for an anisotropic  $s$  wave (ani.  $s$ ) and  $d_{x^2-y^2}$  ( $d$ ) in Fig. 1, the delocalization of quasiparticles occurs only on parts of the Fermi surface. Here the anisotropy parameter  $a=15$  was used. Since the resonant scatter-

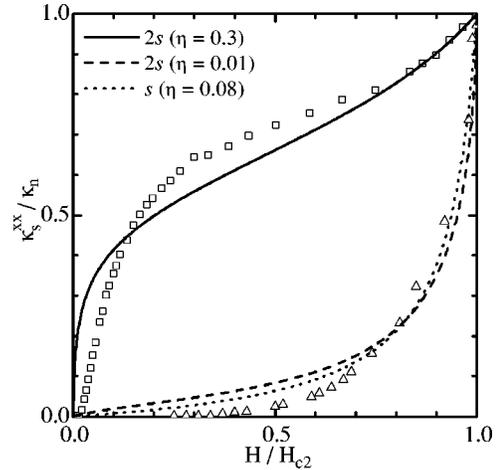


FIG. 2. Comparison with the experimental data of MgB<sub>2</sub> for  $H\parallel z$  (squares) (Ref. 19). The two-gap model ( $2s$ ) with  $\eta=0.3$  (solid line) explains overall features of the experimental data. The results for Nb (triangles) (Ref. 20) are taken from Fig. 2 of Ref. 37. The two-gap model in the superclean limit (dashed line) shows a behavior similar to that of a conventional  $s$ -wave model (dotted line).

ing may become important in the case of a  $d_{x^2-y^2}$  wave, we adopted the  $T$ -matrix approximation,  $\sigma = \langle \bar{g}_{\hat{k}} \rangle / 2\tau_n (\cos^2\delta + \langle \bar{g}_{\hat{k}} \rangle^2 \sin^2\delta)$  with the unitarity limit  $\delta = \pi/2$ .<sup>38</sup>

The sum of both bands gives  $\kappa_s^{xx}(H)$  for MgB<sub>2</sub> in Fig. 2. The overall features reproduce the experimental data (squares) (Ref. 19) well, with the two-band model ( $2s$ ) for  $\eta=0.3$ . Similarly, the single-band isotropic  $s$ -wave model with  $\eta=0.08$  ( $s$ ) gives a reasonable fit for Nb (triangles).<sup>20</sup> The transport properties depend sensitively on the purity of samples, as we can see by considering  $\kappa_s^{xx}(H)$  of the two-band model for the superclean regime,  $\eta=0.01$  (dashed line). This shows a behavior similar to that of a conventional  $s$ -wave superconductor (dotted line). In the limit  $\eta\rightarrow 0$ , putting  $\tilde{\omega}=0$  in Eqs. (10)–(13), we obtain the low-field expression for the  $\pi$  band as

$$\frac{\kappa_s^{xx}}{\kappa_n} = \frac{\pi^{3/2}}{5\sqrt{2}} \frac{q^2 \eta}{r^3} \frac{H}{H_{c2}}. \quad (15)$$

Thus, even in the case of small  $r$ , the low-field dependence of  $\kappa_s$  remains small due to the factor  $\eta$  in the numerator. In other words, in the low-field region the excited quasiparticles are almost localized in the vortex cores even in the case of the smaller gap. On the other hand, the slope of  $N_s(0)$  is considerably enhanced for small  $r$  as

$$\frac{N_s(0)}{N_n} = \frac{\pi^2}{8\sqrt{2}} \frac{q}{r} \sqrt{\frac{H}{H_{c2}}}. \quad (16)$$

It would be interesting to test this predicted change of behavior for  $\kappa_s(H)$  in high-quality samples.

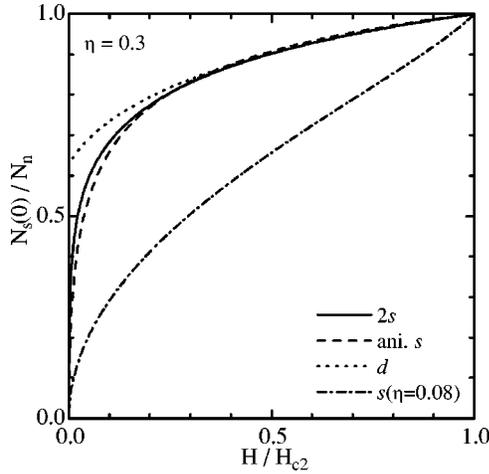


FIG. 3. The  $H$  dependence of the DOS at  $\omega=0$ . All parameters are the same as those in Fig. 1. All curves except for  $s$  waves are similar to each other (apart from the residual DOS in the  $d$ -wave case).

The thermal conductivity  $\kappa_s$  is governed by two characteristic quantities, the DOS  $\text{Re}[\bar{g}_k(\omega)]$  and the transport lifetime  $\text{Re}[\tau_k(\omega)]$  [See Eq. (12)]. We analyze both here to elucidate the origin of the above behavior.

#### A. Density of states

The field dependence of the DOS is shown in Fig. 3, where all parameters are the same as those used in Fig. 1. The sharp rise of the DOS is consistent with experimental observations of  $\gamma_s(H)$  in the polycrystalline samples.<sup>4,15</sup> Even though there is a big difference between the two-band model and the single-gap models in  $\kappa_s^{xx}(H)$ ,  $N_s(H)$  shows no drastic differences apart from the presence of a residual DOS in the  $d$ -wave case as  $H \rightarrow 0$ .

#### B. Transport lifetime

The appropriate measure of quasiparticle delocalization is the transport lifetime in the plane. We discuss the lifetime of quasiparticles in the passive  $\pi$  band, where  $r=0.35$ ,  $v_F^S/v_F^L=1.5$  and  $\hat{k} \perp z$ . The field dependence of  $\text{Re}[\tau_{s\perp}/\tau_n]$  is shown in Fig. 4 for  $\eta=0.01, 0.07$ , and  $0.3$ . As expected, the transport lifetime changes drastically, if the marginally clean regime ( $\eta=0.3$ ) is approached, showing a rapid rise in the low-field region. The enhancement of the quasiparticle lifetime occurs over the entire Fermi surface. In addition, the slope of the DOS is much enhanced as shown in Fig. 3. These effects cooperatively yield the steep rise in the thermal conductivity shown in Fig. 2. The superclean regime ( $\eta=0.01$ ), in contrast, gives only a weak field dependence for low fields due to the quasiparticle localization in this case.

#### IV. LOW-FIELD BEHAVIOR

Finally, we comment on the thermal conductivity for  $H \gtrsim H_{c1}$  which is not covered by our theory. Experimentally, a sudden drop of  $\kappa_s$  is observed as the magnetic field barely

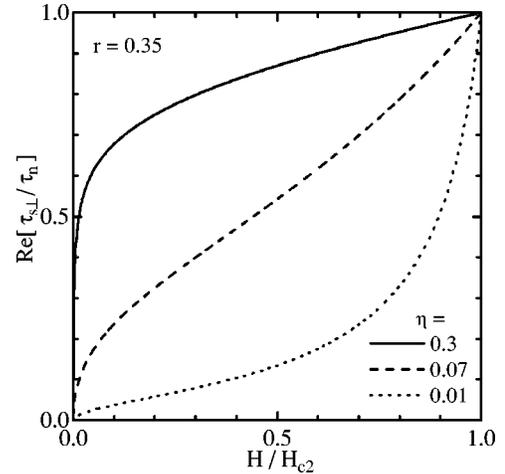


FIG. 4. The  $\eta$  dependence of the in-plane transport lifetime of the smaller gap with  $r=0.35$ . The purity of the samples significantly affects  $\tau_{s\perp}$  in the moderately clean regime.

exceeds  $H_{c1}$ .<sup>19</sup> The reduction of  $\kappa_s$  is usually attributed to the decrease of the phonon contribution, since phonons are scattered by the quasiparticles in the vortex cores. Usually this kind of mechanism leads to a more gentle reduction of  $\kappa_s$ .<sup>20,21</sup>

For  $\text{MgB}_2$  the conditions are more complex. (1) For  $T \ll \Delta_0^S$  all quasiparticle contributions are frozen out in the zero-field limit and they remain localized in the vortex cores for  $H \gtrsim H_{c1}$ . There is a stronger scattering of phonons from core states in multigap models. Since the core DOS is considerably larger for the  $\pi$  band [the DOS is  $\sim E_F/(r\Delta_0^L)^2$ ] than for the  $\sigma$  band.<sup>39</sup> (2) For  $T \sim \Delta_0^S$  the quasiparticles in the  $\pi$  band are sufficiently excited to contribute to the zero-field thermal conductivity. When vortices appear, this quasiparticle contribution is also reduced by scattering at the vortices with localized quasiparticles in the  $\sigma$  band. This effect, in combination with the phonon effect, leads to an even stronger drop of  $\kappa_s$ . These simple considerations of the multigap effect are in good qualitative agreement with the experiment.<sup>19</sup>

#### V. CONCLUSIONS

In summary, we have discussed the inplane thermal conductivity and the DOS in a magnetic field along the  $z$  axis in the multigap superconductor  $\text{MgB}_2$ . The rapid rise of  $\kappa_s(H)$  in the low field region is a special feature of a multigap superconductor in moderately clean samples. Even in the presence of a small gap, we predict a conventional behavior (a shallow increase of  $\kappa_s$  in the low-field region and a rapid increase at fields close to  $H_{c2}$ ) for superclean samples. The sensitivity to sample quality has to be carefully taken into account in the interpretation of thermal transport data in a multigap superconductor. In addition, the field dependence of the two-gap model is definitely stronger than that obtained for any of the single-band models even with line nodes, since the portion of the small gap spreads over its entire Fermi surface. In the low-field region just above  $H_{c1}$ , the phononic

thermal current experiences a definitely stronger scattering by excited quasiparticles in a small gap with a larger DOS. With elevated temperature, delocalized quasiparticles in the small gap are also scattered by localized ones in the large gap. Both effects cause a rather strong drop in the thermal conductivity just above  $H_{c1}$  as vortices enter. All these features will help us to identify multigap superconductors properly.

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