Electronic Thermal Conductivity of Multi-Gap Superconductors with Application to MgB$_2$

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The remarkable field dependence of the electronic thermal conductivity observed in MgB$_2$ can be explained as a consequence of multi-gap superconductivity. A key point is that for moderately clean samples, the mean free path becomes comparable to 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.

The unexpected discovery of superconductivity in MgB$_2$ with a relatively high $T_c = 38$ K[1] aroused great interest and was soon followed by experiments which established phonon mediated $s$-wave superconductivity, e.g., a B-isotope effect[2], a coherence peak in $^{11}$B nuclear relaxation rate[3] and an exponential dependence for temperatures $T \lesssim 10$ K[4]. Theoretical studies concluded that the coupling of the holes in the $2p_z$-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 to $2p_z$-bands is much weaker.

Despite its standard origin, superconductivity in MgB$_2$ has several unusual properties pointing towards a more complex nature. One aspect is the presence of two gaps of different magnitude. Their ratio is estimated as $\Delta_{s}/\Delta_{\pi} \sim 0.3$–0.4 based on various experiments[5,6]. Evidence for two gaps is also provided by the rapid rise of the specific-heat coefficient, $\gamma_s(H)$, at very low magnetic fields[7]. Orbital dependent superconductivity has been proposed theoretically by several authors with the primary (secondary) gap associated with the $\sigma$- ($\pi$)-bands[8,9].

Recent studies of the inplane thermal conductivity in a magnetic field show an unusual field dependence[10]. 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, 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 give very little contribution to $\kappa_s$ except very close to $H_{c2}$[11,12]. At first glance, a small secondary gap $\Delta_{\pi}^s$ 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$_2$ samples are regarded as being in the moderately clean regime: experimental estimates of the mean free path give $\ell \sim 500$–800 $\text{Å}$, compared with the inplane coherence length $\xi_{s0} \sim 120$ $\text{Å}$ derived from $H_{c2}$, which is determined by the primary superconducting $\sigma$-band[13]. The relevant length scale here to be compared with $\ell$ is, however, $\xi_{\pi0}^s$ of the passive $\pi$-band. Thus, we may consider the quasiparticles in the $\sigma$-band in the moderately clean regime, while those in the $\pi$-band with $\Delta_{\pi}^s \sim \xi_{\pi0}^s/\ell$ 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[14]. Moreover, recent scanning tunneling spectroscopy measurements confirmed a large $\xi_{\pi0}^s \sim 500$ $\text{Å}$ in MgB$_2$[15]. 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 view of these circumstances, we analyze the field dependence of $\kappa_s$ and the density of states (DOS) $N_s$. For this purpose we introduce Pesch’s solution[16] for the quasiclassical formalism[17], which is known to be valid for the range of purity in question. We show that the quasiparticle excitations in the small gap bound in the vortex cores can easily be delocalized in the marginally clean regime, causing a rapid rise at low magnetic field. This field dependence is definitely stronger than that obtained for any of the single-band models. On the contrary, superclean samples should exhibit a behavior very similar to that of conventional $s$-wave superconductors.

We restrict our considerations to the case of the inplane thermal current with $H \parallel z$. Thus inplane impurity scattering is the most important for the thermal transport. The scattering matrix between $\sigma$- and $\pi$-bands is assumed to be small[14] because of the different parity of the two orbitals under the reflection $z \rightarrow -z$. 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,

$$\hat{g}(\omega_n, \mathbf{k}, R) = \left( \begin{array}{cc} g & f \\ f^\dagger & -g \end{array} \right) = \frac{i}{\pi} \int d\xi \tau_3 \hat{G}(\omega_n, \mathbf{k}, R), \quad (1)$$

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 \( \tilde{k} \equiv k_F/|k_F| \) is the unit wave vector at the Fermi surface. They satisfy the normalization condition \( \tilde{g}^2 = 1 \) and obey the Eilenberger equations (\( h = c = k_B = 1 \) hereafter),

\[
\left( i\tilde{\omega}_n + e\mathbf{v}_F \cdot \nabla \right) \tilde{\tau}_3 - \Delta(\tilde{k}, \mathbf{R}, \tilde{g}) + i\mathbf{v}_F \cdot \nabla \mathbf{R} \tilde{g} = 0, \tag{2}
\]

supplemented by the gap and Maxwell equations. We introduce the gap matrix

\[
\tilde{\Delta} = \begin{pmatrix}
0 & \Delta(\tilde{k}, \mathbf{R}) \\
-\Delta^*(\tilde{k}, \mathbf{R}) & 0
\end{pmatrix}, \tag{3}
\]

and the renormalized frequency, \( \tilde{\omega}_n = \omega_n + \sigma(\omega_n) \), where \( \sigma \) is the diagonal element of the impurity self-energy determined by the Born or the \( T \)-matrix approximation in this study. We neglect vertex corrections.

Instead of solving these transport-like equations self-consistently, we adopt the Brandt-Pesch-Tewordt (BPT) approximation. 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 \( \tilde{g} \) is kept, since the higher Fourier \( K \)-components of \( g(\mathbf{R}) \) decrease rapidly as \( \exp(-\Lambda^2 K^2) \), \( \Lambda = 1/\sqrt{2\pi H} \) 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 MgB\(_2\), a detailed comparison to numerical solutions yields good agreement both for \( s \)- and \( d \)-wave superconductors over almost the whole field range. This numerical study also shows that the frequently applied Volovik-theory 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 importance of quasiparticle transfer between vortices even in the relatively low-field region.

By means of BPT, the solutions in eq. (3) can be obtained formally (after analytic continuation) as

\[
\tilde{\mathcal{F}}_{\mathbf{k}}(\omega) = \left[ 1 - i\sqrt{\pi} \frac{2\Lambda \tilde{\Delta}(\tilde{k}, \mathbf{R})}{\mathbf{v}_F \perp (\tilde{k})} W'(u) \right]^{-1/2}, \tag{4}
\]

where \( u = \tilde{\omega}[2\Lambda/\mathbf{v}_F \perp (\tilde{k})] \), \( W(u) = e^{-u^2} \text{erfc}(-iu) \) and \( \tilde{\omega} = \omega + i\tau \). Here \( \tilde{\mathcal{F}}_{\mathbf{k}}(\omega) \) denotes the spatial average of the gap and \( \mathbf{v}_F \perp (\tilde{k}) \) is the component of \( \mathbf{v}_F \) perpendicular to the field. The real part of \( \tilde{\mathcal{F}}_{\mathbf{k}}(\omega) \) is nothing but the angle-dependent DOS normalized by the normal-state DOS, \( N_0 \). In order to get the closed-form solution, we use the Born approximation for the \( s \)-wave scattering self-energy, i.e., \( \sigma(\omega) = \langle \tilde{\mathcal{F}}_{\mathbf{k}}(\omega) \rangle/2\tau_\text{n} \), where \( \tau_\text{n} \) is the lifetime in the normal state and \( \langle \cdots \rangle \) represents 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 \( -\nabla_j T \), we obtain the thermal conductivity tensor:

\[
\kappa_{ij} = v_F^2 N_\text{n} \int_0^\infty d\omega \left( \frac{\omega}{T} \right)^2 \text{sech}^2 \left( \frac{\omega}{2T} \right) \times \left\langle k_i k_j \Re \tilde{\mathcal{F}}_{\mathbf{k}}(\omega) | \Re \tilde{\mathcal{F}}_{\mathbf{k}}(\omega) \right\rangle. \tag{5}
\]

The comparison with the simple kinetic theory defines the transport lifetime, \( \Re \tilde{\mathcal{F}}_{\mathbf{k}}(\omega) \):

\[
\frac{1}{2\tau_\text{k}(\omega)} = \sigma(\omega) + \sqrt{\pi} \frac{2\Lambda \tilde{\Delta}(\tilde{k})}{\mathbf{v}_F \perp (\tilde{k})} \frac{\Re \tilde{\mathcal{F}}_{\mathbf{k}}(\omega)}{\Re \tilde{\mathcal{F}}_{\mathbf{k}}(\omega)}. \tag{6}
\]

Here scattering by the vortices appears in addition to quasiparticle broadening due to impurities. Note that eqs. (5) - (6) can be reduced to the conventional expressions in the \( H = 0 \) limit. Moreover one finds \( \tilde{\mathcal{F}}_{\mathbf{k}} = 1 \) and \( \tau_\text{k} = \tau_\text{n} \) in the normal state.

We concentrate on the \( T \to 0 \) limit in this paper. The gap function is factorized as

\[
\tilde{\Delta}(\mathbf{k}) = r \Delta_0 f_k \sqrt{1 - H^2/H_{c2}^2}, \tag{7}
\]

where \( r \) represents the smaller gap, \( 0 < r < 1 \), while \( r = 1 \) is used for the larger gap or the single-band case. The shape of the averaged gap function \( \tilde{\Delta}(\mathbf{k}) \) is given by \( f_k \); e.g., \( f_k = 1 \) for an isotropic \( s \)-wave, \( f_k = \tilde{k}_x^2 - \tilde{k}_y^2 \) for \( d_{x^2-y^2} \)-wave and \( f_k = 1/\sqrt{1 + \alpha k^2} \) for anisotropic \( s \)-wave. We use the square-root field dependence inferred from the Ginzburg-Landau theory.

We discuss now \( \kappa_{\infty}^x(H) \) for MgB\(_2\) and the other cases based on this theory. For MgB\(_2\) we use for simplicity a spherical (cyindrical) Fermi surface for the \( \pi \)- (\( \sigma \))-band and the parameters \( n = N_0^\pi/N_0^\sigma = 1.5, q = v_{F}\perp/v_{F}\parallel = 1.5 \) and \( r = \Delta_0^\pi/\Delta_0^\sigma = \Delta_0^\sigma/\Delta_0^\pi = 0.35 \). The impurity scattering rate for the \( \sigma \)-band is moderate, \( \eta = 1/2\tau_\text{n} \) for anisotropic \( s \)-wave.

These parameters are within the range of current estimates. In Fig. 4, 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 anisotropic \( s \)-wave (ani. \( s \)) and \( d_{x^2-y^2} \)-wave (\( d \)) in Fig. 5, the delocalization of quasiparticles occurs only on parts of the Fermi surface. Here, the anisotropy parameter \( a = 15 \) was used. We adopted the unitarity limit, \( \delta = \pi/2 \) in the \( T \)-matrix self-energy, i.e., \( \sigma = (\tilde{\mathcal{F}}_{\mathbf{k}})/2\tau_\text{n}(\cos^2 \delta + (\tilde{\mathcal{F}}_{\mathbf{k}})^2\sin^2 \delta) \) for \( d_{x^2-y^2} \)-wave.

The sum of both bands gives \( \kappa_{\infty}^z(H) \) for MgB\(_2\) in Fig. 6. The overall features reproduce the experimental data (squares) 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.
FIG. 1: The field dependence of the inplane 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 conventional behavior. Anisotropic \( s \)-wave and \( d_{x^2-y^2} \)-wave cases are given for comparison.

FIG. 2: Comparison with the experimental data of MgB\(_2\) for \( H \parallel z \) (squares).\(^\text{1} \) The two-gap model (2s) with \( \eta = 0.3 \) (solid line) explains overall features of the experimental data. The results for Nb (triangles)\(^\text{2} \) are taken from Fig. 2 of Ref.\(^\text{3} \). The two-gap model in the superclean limit (dashed line) shows a behavior similar to that of a conventional \( s \)-wave model (dotted line).

The proper measure of quasiparticle delocalization is the transport lifetime in the plane. We discuss the lifetime of quasiparticles in the passive \( \pi \)-band, where \( r = 0.35 \), \( v_F^\pi/v_F^s = 1.5 \) and \( k \parallel z \). The field dependence of \( \text{Re}[\tau_{\pi}/\tau_0] \) is shown in Fig. 2 of Ref.\(^\text{4} \) 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 yield cooperatively the steep rise in the thermal conductivity shown

FIG. 3: The \( H \)-dependence of the DOS at \( \omega = 0 \). All parameters are the same as those in Fig. 2. All curves except for \( s \)-wave are similar to each other (apart from the residual DOS in the \( d \)-wave case).

\[^{1}\text{The thermal conductivity } \kappa, \text{ is governed by two characteristic quantities, the DOS and the transport lifetime. We analyze both here in order to elucidate the origin of the above behavior. The field dependence of the DOS is shown in Fig. 3, where all parameters are the same as those used in Fig. 2. The sharp rise of the DOS is consistent with experimental observations of } \gamma_s(H) \text{ in the polycrystalline samples.}^{2}\]

\[^{2}\text{Even though there is a big difference between the two-band model and the single-gap models in } \kappa^{xx}_s(H), \text{ } N_s(H) \text{ shows no drastic differences apart from the presence of a residual DOS in the } d \text{-wave case as } H \rightarrow 0.\]

\[^{3}\text{The appropriate measure of quasiparticle delocalization is the transport lifetime in the plane. We discuss the lifetime of quasiparticles in the passive } \pi \text{-band, where } r = 0.35, \text{ } v_F^\pi/v_F^s = 1.5 \text{ and } k \parallel z. \text{ The field dependence of } \text{Re}[\tau_{\pi}/\tau_0] \text{ is shown in Fig. 2 of Ref.}^{3} \text{ for } \eta = 0.01, 0.07 \text{ and 0.3. As expected, the transport lifetime changes drastically, if the marginally clean regime (} \eta = 0.3 \text{) is approached, showing a rapid rise in the low-field region. The enhancement of the quasiparticle lifetime occurs over the entire Fermi surface. In addition, the slope of the DOS is much enhanced as shown in Fig. 3. These effects yield cooperatively the steep rise in the thermal conductivity shown}\]
FIG. 4: The $\eta$ dependence of the inplane transport lifetime of the smaller gap with $r = 0.35$. The purity of the samples affects significantly on $\tau_{s \perp}$ in the moderately clean regime.

in Fig. 3. 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.

Finally, we comment on the thermal conductivity for $H \approx H_{c1}$ which is not covered by our theory. Experimentally, a sudden drop of $\kappa$ as observed as the magnetic field barely exceeds $H_{c1}$. 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 $\kappa_s$. For MgB$_2$ the conditions are more complex. For $T \ll \Delta_0^2$ all quasiparticle contributions are frozen out in the zero-field limit and they remain localized in the vortex cores for $H \approx H_{c1}$. There is a stronger scattering of phonons from core states in multi-gap models. Since the core DOS is considerably larger for the $\pi$-band (DOS $\sim E_F/(r\Delta_0^1)^2$) than for the $\sigma$-band. For $T \sim \Delta_0^2$ the quasiparticles in $\pi$-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 multi-gap effect are in good qualitative agreement with the experiment.

In summary, we have discussed the inplane thermal conductivity and the DOS in a magnetic field along the $z$-axis in the multi-gap superconductor MgB$_2$. The rapid rise of $\kappa_s(H)$ in the low field region is a special feature of a multi-gap superconductor in moderately clean samples. Even in the presence of a small gap, we predict conventional behavior for superclean samples. This sensitivity to sample quality has to be carefully taken into account in the interpretation of thermal transport data in a multi-gap superconductor.

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