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THERMAL CONDUCTIVITY IN SUPERCONDUCTING BOROCARBIDES $LuNi_2B_2C$ AND YNi_2B_2C*

P. Thalmeier

Max-Planck-Institute for the Chemical Physics of Solids
Nöthnitzer Str. 40, 01187 Dresden, Germany

and K. Maki

Max-Planck-Institute for the Physics of Complex Systems
Nöthnitzer Str. 38, 01187 Dresden, Germany
Department of Physics and Astronomy, University of Southern California
Los Angeles, CA 90089-0484, USA

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We have recently proposed the $s+g$-wave model for superconducting borocarbides. In spite of a substantial s-wave component, this order parameter exhibits the $\sqrt{H}$ dependent specific heat and a thermal conductivity linear in H in the vortex state. This is characteristic for nodal superconductors when $T, \Gamma \ll \Delta$ where Γ is the quasiparticle scattering rate and Δ the maximum superconducting gap. Here we investigate the thermal conductivity parallel to the c- and a-axis in a magnetic field tilted by θ from the c-axis and rotating within the a–b plane.

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The superconductivity in the rare earth borocarbides $LuNi_2B_2C$ and YNi_2B_2C is of great interest [1,2]. We have proposed recently the superconducting order parameter [3,4]

$$\Delta(\boldsymbol{k}) = \tfrac{1}{2}\Delta(1+\sin^4\vartheta\cos(4\varphi))\,, \tag{1}$$

where ϑ and φ are polar and azimuthal angle of $\boldsymbol{k}$, respectively. Recent thermal conductivity experiments [5] suggest that crystallographic [100] and

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[010] are the nodal directions, *i.e.* the order parameter of Eq. (1) is rotated by $\frac{\pi}{4}$ in the a–b plane. This gap function accounts for the $\sqrt{H}$ dependence of the specific heat and the H-linear term in the thermal conductivity observed recently [6–8]. The aim of this paper is to generalize an earlier result [3] for κ_{zz}, κ_{xx} and κ_{xy} for general magnetic field ($\boldsymbol{H}$) orientation given by the polar angle θ with respect to the c-axis and the azimuthal angle ϕ. First in the absence of $\boldsymbol{H}$ the specific heat and the electronic thermal conductivity for $\Gamma \ll T \ll \Delta$ are given by

$$\frac{C_s}{\gamma_N T} = \frac{27}{4\pi}\zeta(3)\left(\frac{T}{\Delta}\right) + \ldots; \quad \frac{\kappa_{xx}}{T} = \frac{\pi^2}{8}\frac{n}{m\Delta}; \quad \frac{\kappa_{zz}}{T} = \frac{\pi^2}{8}\frac{nC_0}{m\Delta}, \qquad (2)$$

where $C_0 = (\frac{2\Gamma}{\Delta})^{\frac{1}{2}}[\ln(2\sqrt{\frac{\Delta}{\Gamma}})]^{-\frac{1}{2}}$. Note that κ_{xx} obeys the universal behaviour while κ_{zz} does not. This is because the heat current operator j_z^h vanishes on the four second order nodal points $(\vartheta, \varphi) = (\frac{\pi}{2}, \pm\frac{\pi}{4})$ and $(\frac{\pi}{2}, \pm\frac{3\pi}{4})$ for $\Delta(\boldsymbol{k})$ given in Eq. (1). Also this leads to a $H^{\frac{3}{2}} \ln\left(\frac{\Delta}{\tilde{v}\sqrt{eH}}\right)$ dependence of κ_{zz} as discussed below.

In the presence of a magnetic field with general orientation defined by (θ, ϕ) the specific heat and thermal conductivities in the vortex phase are given by [3, 10]

$$\begin{aligned}
\frac{C_s}{\gamma_N T} &= \frac{\tilde{v}\sqrt{eH}}{\sqrt{2}\Delta} I_+(\theta, \phi)\,, \\
\frac{\kappa_{zz}}{\kappa_n} &= \frac{1}{32\sqrt{2}} \ln\left[\frac{2\Delta}{\tilde{v}\sqrt{eH}}\sqrt{\frac{2}{1+\cos^2\theta}}\right] \frac{\tilde{v}^3 (eH)^{\frac{3}{2}}}{\Delta^3} I_{zz}(\theta, \phi)\,, \\
\frac{\kappa_{xx}}{\kappa_n} &= \frac{3}{32}\frac{\tilde{v}^2 (eH)}{\Delta^2} I_+^2(\theta, \phi); \quad \frac{\kappa_{xy}}{\kappa_n} = -\frac{3}{32}\frac{\tilde{v}^2 (eH)}{\Delta^2} I_-(\theta, \phi) I_+(\theta, \phi)\,, \qquad (3)
\end{aligned}$$

where we have the identity $I_{zz}(\theta, \phi) = (1+\cos^2\theta) I_+(\theta, \phi)$ and

$$\begin{aligned}
I_\pm(\theta, \phi) &= \frac{1}{2}\left\{[1 + \cos^2\theta + \sin^2\theta \sin(2\phi)]^{\frac{1}{2}}\right\} \\
&\pm \left\{[1 + \cos^2\theta - \sin^2\theta \sin(2\phi)]^{\frac{1}{2}}\right\}. \qquad (4)
\end{aligned}$$

Here we have assumed the superclean limit defined by $\sqrt{\Delta\Gamma} \ll \tilde{v}\sqrt{eH}$ with $\tilde{v} = \sqrt{v_a v_c}$ where $v_{a,c}$ denote the anisotropic Fermi velocities. The angular dependences of κ_{zz} and κ_{xy} according to Eqs. (3), (4) for the $s+g$-wave case are shown in the left panel of Fig. 1 and in Fig. 2. For comparison, we also present the corresponding angular dependence of κ_{zz} for the $d_{x^2-y^2}$

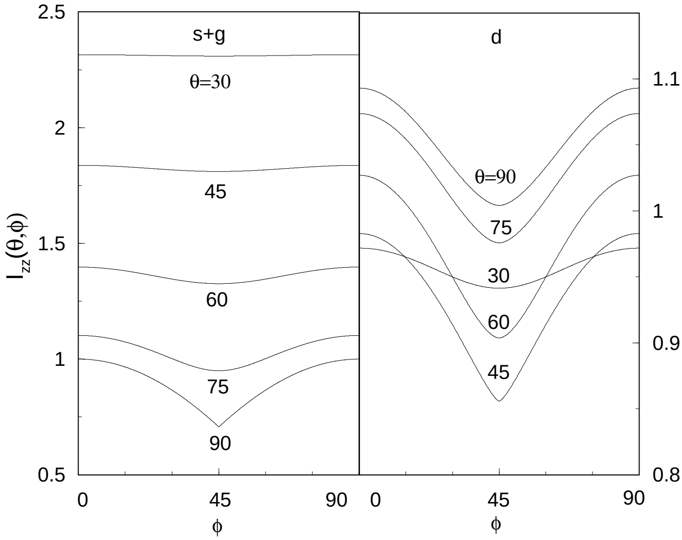

Fig. 1. Angular dependence of $I_{zz}(\theta,\phi)$ which determines $\kappa_{zz}(\theta,\phi)$ in the superclean limit for $s+g$-wave and d-wave case (up to log-terms in Eq. (3)). Note the different scale in the two cases.

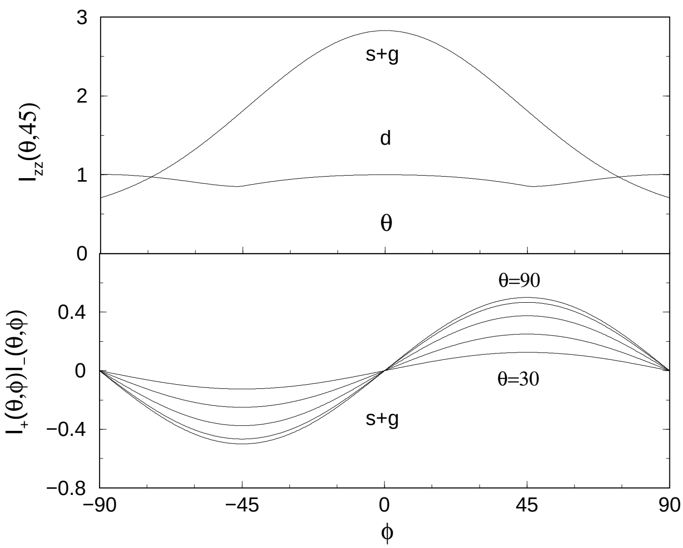

Fig. 2. Upper panel: polar angle variation of $I_{zz}(\theta,45)$ for $s+g$- and d-wave case. Lower panel: Angular dependence of the product $I_-(\theta,\phi)\cdot\, I_+(\theta,\phi)$ for $s+g$-case which determines the thermal Hall coefficient $\kappa_{xy}(\theta,\phi)$. It vanishes for field halfway between the nodal directions due to current compensation.

state with $\Delta(\boldsymbol{k}) = \Delta\cos(2\phi)$ as in high T_c cuprates [10], $CeCoIn_5$ [11] and κ-$(ET)_2Cu(NCS)_2$ [12,13]. Of course, for d-wave superconductors the universal zero-field behaviour is valid both for κ_{xx} and for κ_{zz}, and both exhibit a similar angular dependence in the vortex phase [10]. In this case the dependence on field angles θ, ϕ is given by

$$\begin{aligned} I_\pm(\theta,\phi) &= \frac{1}{2\pi}\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} d\psi J_\pm(\psi); \quad \tilde{I}_+(\theta,\phi) = \frac{1}{2\pi}\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} d\psi(1-\cos(2\psi))J_+(\psi)\,, \\ J_\pm(\psi) &= \Big[1+\frac{1}{2}\sin^2\theta(\sin(2\phi)-\cos(2\psi)) \\ &\quad +\frac{1}{\sqrt{2}}\sin(2\theta)\sin\psi\sqrt{1-\sin(2\phi)}\Big]^{\frac{1}{2}} \\ &\quad \pm\Big[1-\frac{1}{2}\sin^2\theta(\sin(2\phi)+\cos(2\psi)) \\ &\quad +\frac{1}{\sqrt{2}}\sin(2\theta)\sin\psi\sqrt{1+\sin(2\phi)}\Big]^{\frac{1}{2}}. \end{aligned} \tag{5}$$

Then κ_{xx} and κ_{xy} are obtained from $I_\pm(\theta,\phi)$ as in Eq. (3) but now for d-wave:

$$\frac{\kappa_{zz}}{\kappa_n} = \frac{1}{\pi}\frac{\tilde{v}^2(eH)}{\Delta^2}I_{zz}(\theta,\phi); \quad I_{zz}(\theta,\phi) = I_+(\theta,\phi)\tilde{I}_+(\theta,\phi)\,. \tag{6}$$

The ϕ- dependence of κ_{zz} for various θ is shown in comparison to the $s+g$-wave case in Fig. 1. As is readily seen from Fig. 1 in the $s+g$-wave case a pronounced cusp like feature develops for θ=90° and $\phi = \pm 45°$ due to the (second order) point node, while in the $d_{x^2-y^2}$ wave case with an extended line node along c no cusps appear and also the absolute value of angular variation is much smaller. This is clearly visible from the upper panel of Fig. 2 which also shows monotonic θ- dependence for $s+g$-wave and nonmonotonic behaviour for d-wave. The latter has a minimum at $\theta_m \simeq 47°$ which is due to a maximum Doppler shift for θ=45° resulting in a dominating term $I_{zz}(\theta,\phi) \simeq 1-(5/64)\sin^2(2\theta)+\dots$. Note that $I_{zz}(\theta,\phi)$ in Fig. 1 exhibits a rather sharp minimum as function of ϕ at θ_m wheras for $\theta = 90°$ the minimum is flat. Experimentally however the κ_{zz} thermal conductivity shows very strong cusps at θ=90° (and $\phi = 0$ due to rotated order parameter) in YNi_2B_2C [5]. This is a strong point for the $s+g$-wave case being the appropriate one for YNi_2B_2C and $LuNi_2B_2C$. Therefore the thermal conductivity in the superclean limit can discriminate $s+g$-wave against d-wave superconductivity.

The angular dependence of the thermal Hall coefficient κ_{xy} in the $s+g$-wave case is shown in the lower panel of Fig. 2. It exhibits a sign change as function of ϕ and varies smoothly with θ. In the d-wave case κ_{xy} looks rather similar. As we have already discussed elsewhere [14] the thermal conductivity provides a unique window to look at the nodal structure of $\Delta(\boldsymbol{k})$ in unconventional superconductors.

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