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THERMAL CONDUCTIVITY IN SUPERCONDUCTING BOROCARBIDES $\text{LuNi}_2\text{B}_2\text{C}$ AND $\text{YNi}_2\text{B}_2\text{C}$ *

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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 $\text{LuNi}_2\text{B}_2\text{C}$ and $\text{YNi}_2\text{B}_2\text{C}$ is of great interest [1,2]. We have proposed recently the superconducting order parameter [3,4]

$$\Delta(\mathbf{k}) = \frac{1}{2}\Delta(1 + \sin^4 \vartheta \cos(4\varphi)), \quad (1)$$

where ϑ and φ are polar and azimuthal angle of \mathbf{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 (\mathbf{H}) orientation given by the polar angle θ with respect to the c -axis and the azimuthal angle ϕ . First in the absence of \mathbf{H} the specific heat and the electronic thermal conductivity for $\Gamma \ll T \ll \Delta$ are given by

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

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 $\Delta(\mathbf{k})$ given in Eq. (1). Also this leads to a $H^{\frac{3}{2}} \ln(\frac{\Delta}{\tilde{v}\sqrt{eH}})$ 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]

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

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

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

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 $d_{x^2-y^2}$

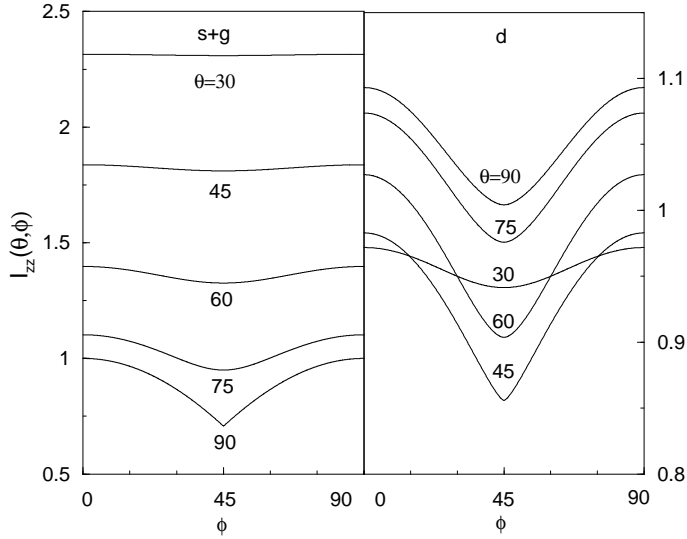


Fig. 1. Angular dependence of $I_{zz}(\theta, \phi)$ which determines $\kappa_{zz}(\theta, \phi)$ in the superclean limit for $s + g$ -wave and d -wave case (up to log-terms in Eq. (3)). Note the different scale in the two cases.

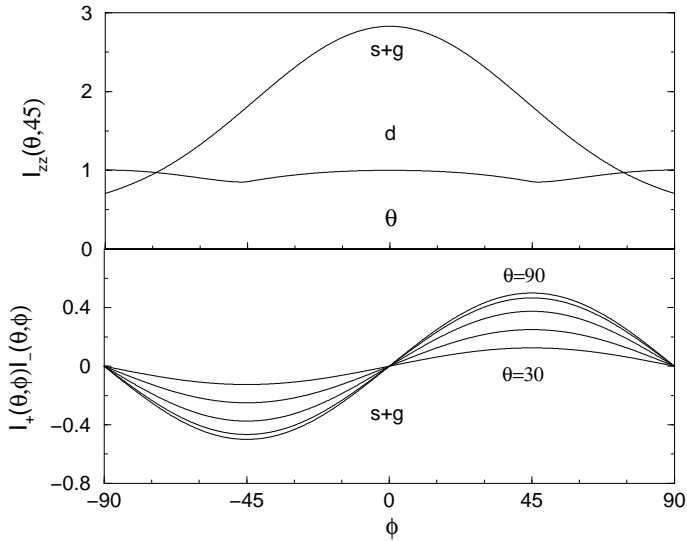


Fig. 2. Upper panel: polar angle variation of $I_{zz}(\theta, 45)$ for $s + g$ - and d -wave case. Lower panel: Angular dependence of the product $I_-(\theta, \phi) \cdot I_+(\theta, \phi)$ for $s + g$ -case which determines the thermal Hall coefficient $\kappa_{xy}(\theta, \phi)$. It vanishes for field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

state with $\Delta(\mathbf{k}) = \Delta \cos(2\phi)$ as in high T_c cuprates [10], CeCoIn₅ [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

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

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 $\theta=90^\circ$ and $\phi = \pm 45^\circ$ 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 $\theta_m \simeq 47^\circ$ which is due to a maximum Doppler shift for $\theta=45^\circ$ 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 whereas for $\theta = 90^\circ$ the minimum is flat. Experimentally however the κ_{zz} thermal conductivity shows very strong cusps at $\theta=90^\circ$ (and $\phi = 0$ due to rotated order parameter) in YNi₂B₂C [5]. This is a strong point for the $s + g$ -wave case being the appropriate one for YNi₂B₂C and LuNi₂B₂C. 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 $\Delta(\mathbf{k})$ in unconventional superconductors.

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