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Boundary-limited thermal conduction of crystalline rods oriented near phonon-focusing caustics

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ABSTRACT

We apply the Casimir model for boundary-limited heat conduction to single-crystal rods oriented near phonon-focusing caustics. We show that rods with axes close to the direction of an external conical refraction caustic, a highly degenerate caustic that exists for certain hexagonal crystals, exhibit a thermal conductivity that diverges logarithmically on approaching the caustic. For rods with axes close to the directions of the more generic fold and cusp caustics, the conductivity remains finite, but displays singular behavior with a 1/2- or 1/3-power law falloff with angular deviation from the caustic. Moreover, in the direction of a fold caustic, the Casimir conduction is not necessarily a maximum. Numerical results are presented for zinc, with the quasi-transverse branch providing examples of the external conical refraction and fold caustics, and in a certain sense, also the cusp caustic.

1. Introduction

The Casimir model [1] for boundary-limited thermal conduction has enjoyed considerable success over the years in accounting for the thermal conductivities of dielectric rods at low temperatures, when boundary scattering of thermal phonons dominates over bulk scattering, and the effective phonon mean free path $\bar{l}$ is controlled by the lateral dimensions of the rod. The model leads to an expression for the conductivity of a rod similar to the familiar kinetic theory result for bulk thermal conductivity

$$\kappa = \frac{1}{3} C_V \bar{v} \bar{l}, \tag{1}$$

where $\bar{v}$ is a suitably averaged phonon velocity, and C_V is the specific heat at constant volume. Well below the Debye temperature, since $\kappa \propto C_V$, the conductivity falls off as the cube of the absolute temperature T, a result that has been confirmed in numerous measurements, see e.g. Refs. [2–4]. In recent years the main focus of attention has shifted to the burgeoning field of nanoscale thermal transport [5–7], where even at room temperature the boundary scattering of phonons can play a significant role. Studies of thermal conduction in nanowires and other nanostructures [5–13] have stimulated renewed interest in boundary-limited thermal conductivity at low temperatures [14–16].

The important influence of elastic anisotropy on thermal conduction in the Casimir regime was first recognized in the seminal paper by McCurdy, Maris and Elbaum [17]. In an elastically anisotropic medium the acoustic slowness surface, $S(\mathbf{s}) = 0$, i.e. the surface representing the directional dependence of the phonon slowness $\mathbf{s} = \mathbf{k}(\omega)/\omega$, where $\mathbf{k}$ is the wave vector and ω the angular frequency, is non-spherical. As a consequence, the phonon group or ray velocity $\mathbf{V} = \nabla_{\mathbf{k}}\omega(\mathbf{k})$, which is normal to the slowness surface, is not in general parallel to the wave vector. This gives rise to the phenomenon of phonon focusing, whereby the ray vectors associated with a uniform distribution of phonon slownesses are strongly concentrated in directions normal to regions of the slowness surface where the curvature is small. The resulting phonon flux intensity from a point source is proportional to the Maris phonon enhancement factor [18–20]

$$M = 1/\big(s^3 V |K|\big), \tag{2}$$

where $K = 4\alpha\beta$ is the Gaussian curvature and 2α and 2β are the principal curvatures of the slowness surface. A point on the slowness surface where one of the principal curvatures passes through zero on changing sign maps onto a caustic where $M = \infty$. Phonon-focusing caustics—sharp maxima in intensity for certain directions corresponding to zero Gaussian curvature of the slowness surface—are indeed observed in many measured phonon images [21,22].

It might seem plausible that for a rod oriented in such a focusing direction, the Casimir conductivity should be higher than elsewhere, but this is not invariably the case, as we show below.

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The study [17] and subsequent works [23–29] reported numerical calculations of directionally dependent conductivities in a number of crystals of various symmetries and shapes of cross section, and experimental work [30–32] has provided evidence in support of the predictions. However, a clear physical understanding of the role of phonon-focusing caustics in Casimir conduction has hitherto been missing. What happens if the rod axis lies exactly in, or very close to the direction of a caustic? Will the thermal conductivity of an infinite rod oriented in a caustic direction remain finite? Will we observe different behavior for different types of caustics? Addressing these questions constitutes the substance of this paper.

We give attention to the three most common phonon-focusing caustics: (a) the line or fold caustic, which is to be found in the direction of a sharp fold in the acoustic wave surface, i.e. the surface representing the directional dependence of the group velocity, (b) the cusp caustic where two line caustics meet to form a cusp, with the cusp separating an inner region where locally the wave surface is triplicated, from the outer region where it is comprised of a single sheet, and (c) the external conical refraction caustic, which is displayed by certain hexagonal crystals, for which there is a cone of slowness vectors, all of which map onto the same group velocity vector pointing along the principal axis, and being the apex of a cone in the wave surface.

We establish that the conductivity of a long rod exhibits singular behavior when oriented in the vicinity of a phonon caustic, and identify the specific types of singular behavior for the three caustic types mentioned above. This singular behavior is determined by the local geometry of the slowness surface associated with the caustic. Superimposed on this singular component of κ, is a smoothly varying background which all phonons with a component of group velocity parallel to the rod axis contribute to, and which can therefore be regarded as a property of the global geometry of the slowness surface. For illustrative purposes we present the calculated directionally dependent effective phonon mean free path of a hexagonal zinc crystal rod, which provides examples of the three types of singularities. As expected, these singular features are less pronounced than in ballistic transport from a point source in a bulk solid. We find that the Casimir conductivity of an infinite rod oriented in the direction of a fold or cusp caustic remains finite. Surprisingly, the Casimir conduction is not necessarily even a maximum in the direction of a fold caustic. On the other hand, the thermal conductivity of an infinite rod oriented near the external refraction caustic diverges logarithmically on approach to the caustic direction. Exactly in the direction of the external conical refraction caustic, the Casimir conductivity becomes infinite, implying that in practice the conductivity will be limited either by a finite length of the rod or by remnant bulk scattering.

2. Evaluation of Casimir model for anisotropic media

We follow a procedure established by McCurdy et al. [17] (their Eqs. (5), (11) and (12)) for calculating the thermal conductivity κ of an infinitely long anisotropic solid cylinder of radius R much larger than the dominant phonon wavelength, i.e., the Casimir conductivity. It assumes the absence of bulk scattering, perfectly diffuse scattering at the surface, and cross section isotherms. At temperatures much lower than the Debye temperature it renders the formula

$$\kappa = \frac{4Rk_B}{45}\left(\frac{k_B T}{\hbar}\right)^3 \sum_{j=1}^{3} \Lambda_j; \qquad \Lambda_j = \int_{4\pi} \frac{s_j^3 V_{j\parallel}^2 d\Omega}{|V_{j\perp}|}, \tag{3}$$

where the sum is over the three acoustic branches, k_B is Boltzmann's constant and $\hbar$ is Planck's constant, $V_{j\parallel}$ is the phonon group velocity component parallel to the axis of the rod and $V_{j\perp}$ the component perpendicular to the axis. The integral is over all directions of the slowness $\mathbf{s}_j$, $d\Omega$ being the solid angle element in which the slowness vector lies. Representing the thermal conductivity by Eq. (1), the effective phonon mean free path, normalized to the diameter of the rod, is in turn given by [17]

$$\ell = \bar{\ell}/2R = \frac{1}{3\pi^2 \langle s^2\rangle} \sum_{j=1}^{3} \Lambda_j, \tag{4}$$

with $\bar{v}$ interpreted as $\langle s^2\rangle/\langle s^3\rangle$, where the averages are taken over all directions and for the three acoustic branches. ℓ is unity in the case of an isotropic solid, but varies with direction for an anisotropic solid. In highlighting the effects of phonon focusing on Casimir conduction, there can be advantage in displaying the variation in direction of ℓ rather than κ.

The issue of partial specularity has been examined both from a theoretical [17] and experimental [4] point of view, and evidence points to an increase in specularity and hence reduction in diffuse scattering as the temperature is lowered and the dominant phonon wavelength increases. There is also evidence for an increase in specularity for phonons incident on the surface at grazing angles. Detailed models have been proposed for the influence of surface roughness on scattering [13]. The influence of the shape of the cross section of the rod has also been examined by various authors, and attention has also been given to finite length to lateral dimension aspect ratio. While recognizing the validity of all these concerns, the aim of the present paper is to specifically highlight the influence of elastic anisotropy, through phonon focusing, on boundary-limited thermal conduction. It serves our purposes under the circumstances to treat all other factors in as simple a manner as possible, i.e. by adopting the assumptions enunciated in the previous paragraph.

Inspection of Eq. (3) reveals that important contributions to the boundary-limited thermal conductivity in an infinitely long rod oriented in a particular direction in an anisotropic medium come from phonons of each branch for which $|V_{j\perp}| \ll |V_{j\parallel}|$, i.e. phonons whose group velocities lie close to the axis of the rod. These are associated with portions of the slowness surface oriented normal to the axis of the rod. We proceed to calculate what this contribution is for a small angular cone of phonon slowness vectors of a particular branch (the branch index j is henceforth suppressed) for which locally the slowness surface equation can be approximated by a low order polynomial expression of the form [33]

$$\begin{aligned} S(\mathbf{s}) &= (s_3 - s_{30}) + \left\{\alpha(s_1 - s_{10})^2 + \beta(s_2 - s_{20})^2 + \cdots\right\} \\ &= \hat{s}_3 + \left\{\alpha\hat{s}_1^2 + \beta\hat{s}_2^2 + \cdots\right\} = 0, \end{aligned} \tag{5}$$

where $\mathbf{s}_0 = (s_{10}, s_{20}, s_{30})$ is the point on the slowness surface where the normal points exactly along the rod axis. We will label this the s_3 direction, and take s_1 and s_2 to be located along the directions of the principal curvatures 2α and 2β of the slowness surface at $\mathbf{s}_0$. For elliptic points on the slowness surface (α and β of the same sign) and hyperbolic points (α and β opposite in sign) it is sufficient to truncate the expansion in (5) after quadratic terms. The coefficients α and β have dimensions of inverse slowness and it will be convenient to express results below in terms of the dimensionless quantities $\tilde{\alpha} = \alpha s_0$ and $\tilde{\beta} = \beta s_0$, and likewise we will employ the dimensionless slownesses $\tilde{s}_1 = \hat{s}_1/s_0$, and $\tilde{s}_2 = \hat{s}_2/s_0$. For parabolic points, where one of the principal curvatures is zero, the expansion (5) needs to be extended to higher order, as we show later.

For any given neighboring point on the slowness surface $\mathbf{s} = \mathbf{s}_0 + \hat{\mathbf{s}}$, the associated group velocity is given by [34]

$$\mathbf{V} = \nabla_{\mathbf{k}}\omega(\mathbf{k}) = \frac{\nabla_{\mathbf{s}} S(\mathbf{s})}{\mathbf{s}\cdot\nabla_{\mathbf{s}} S(\mathbf{s})}, \tag{6}$$