

ously reported.

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the  $\text{CaF}_2:\text{Gd}^{3+}$  crystal used in this work. A more complete account of this work will be published elsewhere.

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## Heat Conductivity in Cylindrical Samples

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In a previous paper,<sup>1</sup> the authors gave the first exact solution of the nonlinearized Boltzmann transport equation for particles with a linear dispersion law (e. g., phonons) subject to point scattering in an infinite slab. The two faces of the slab were in contact with two heat reservoirs at different temperatures, and from the knowledge of the phonon distribution function, the temperature distribution in the slab and the thermal conductivity were derived as a function of all pertinent parameters. These were the temperature, the scattering cross section, the impurity concentration, the slab thickness, and the sound velocity. Hence, one had a model of heat transport in insulators at low temperatures. The results were compared with experimental data obtained on specimens of prismoidal and cylindrical shapes, and good agreement was found despite the fact that an infinite slab is geometrically very different from either a prism or a cylinder.

It is the purpose of the present comment to show that the solution given in the cited paper is valid not only for the infinite slab, but also for a straight prism or cylinder of any cross section and of finite length, provided that the phonons are specularly reflected at the side walls.

First, a heuristic argument: Suppose that people with identical features are milling around in a room of infinite extension on all four sides. Among them is the reader as an observer. Now mirror walls perpendicular to the floor are erected around the observer, making him a member of a sufficiently large crowd enclosed in the prismatic room so created. Can the observer tell by looking around, whether he is in the finite room or in the infinite room? It is intuitively clear that he cannot tell the difference as long as the dimensions of the en-

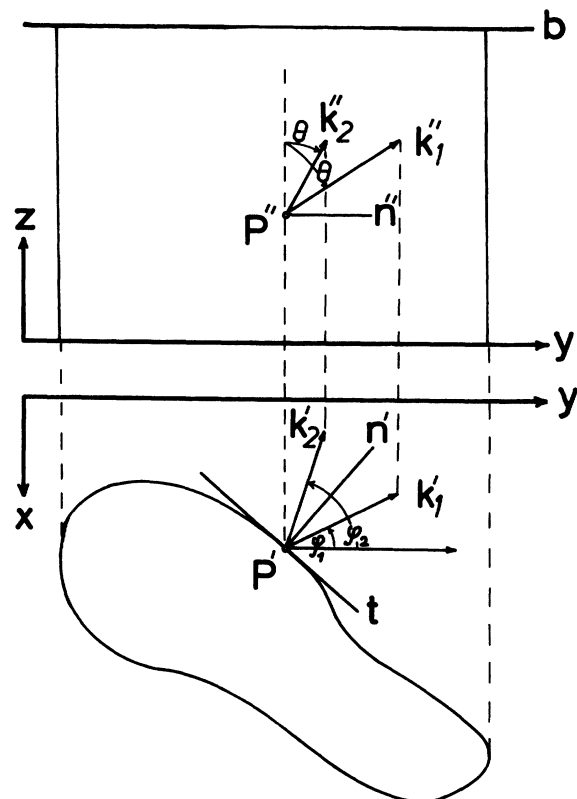


FIG. 1. Projections of a cylinder of arbitrary cross section inscribed into the infinite slab. Bottom: Projection on the  $x$ - $y$  plane. Top: Projection on the  $y$ - $z$  plane. The slab rests on the  $x$ - $y$  plane, and is topped by the plane  $b$ . One and two primes denote the  $x$ - $y$  and  $y$ - $z$  projections of the labeled quantities, respectively. The incident phonon wave vector is  $\vec{k}_1$ , the reflected wave vector is  $\vec{k}_2$  at the point  $P$ . The tangential plane at  $P$  is  $t$ , the normal vector is  $\vec{n}$ . The figure shows that only the azimuthal angle  $\varphi$ , and not the polar angle  $\theta$ , is changed in the reflection.

closure are large compared with his own dimensions. The phonons are in an analogous situation.

To obtain a formal proof, consider a cylinder inscribed into the slab as shown from the side and from the top in Fig. 1. The vectors  $\vec{k}_1$  and  $\vec{k}_2$  represent the quasi-momenta of a phonon incident and specularly reflected from the wall. As shown in Ref. 1, the phonon distribution function  $f(\vec{k}, \vec{x})$  of the stationary, but because of the heat flow, non-equilibrium system has axial symmetry with respect to any line perpendicular to the slab faces. This means that at the point "A" we have

$$f(\vec{k}_1, \vec{x}) = f(k, \theta, \vec{x}) = f(\vec{k}_2, \vec{x})$$

because  $f$  is independent of  $\varphi$ , and  $k$  and  $\theta$  do not change in specular reflection.

Consequently, the distribution function found for

the infinite slab fulfills the boundary conditions of specular reflection on the walls of the cylinder or prism, as well as the Boltzmann equation. Hence, it is the solution of the problem in question. It is further evident that the distribution function is invariant with respect to the introduction of any kind of specularly reflecting walls as long as they are perpendicular to the slab boundaries.

It should be noted that the distribution function, and therefore the conductivity, is independent of the cross-sectional dimensions of the sample. This is not true if the reflection is diffuse rather than specular, or if there is radiative or conductive loss of heat through the walls. We expect therefore, the theory to hold best for highly polished samples.

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### Comment on Generalized Forces in Solids

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A simple model for the application of the Hellmann-Feynman theorem to the equilibrium condition for a solid is discussed.

Some concern over the accuracy of charge densities of solids calculated from Bloch functions has been raised by an article of Wannier *et al.*<sup>1</sup> Using the Hellmann-Feynman theorem, they found a relationship between the charge distribution in a unit cell of a periodic crystal and the equilibrium condition for the crystal, which had explosive consequences for "nearly free-electron" metals. However, Kleinman<sup>2</sup> has considered in detail the electrostatics involved in determining the force acting on a nucleus in a large finite crystal and has concluded that one must take into account the electronic charge density and the nuclei near the surface. The plausibility of Kleinman's conclusion has been questioned on the grounds that it is unusual to expect surface effects to play an important role in the determination of a bulk quantity such as the equilibrium lattice constant.<sup>3</sup> The purpose of this paper is to show explicitly for a simple model that the equilibrium condition is determined by a surface effect.

Let us consider a classical system of  $N + 1$  bodies at positions  $x_n = an$ ,  $n = 0, 1, 2, \dots, N$ , each joined

to its nearest neighbors by springs with spring constant  $K$  and rest length  $a_0$ . The potential energy of the system is then  $U(a) = \frac{1}{2}NK(a - a_0)^2$ , so that  $dU/da = NK(a - a_0)$ . The analog of the Hellmann-Feynman theorem for this system is  $dU = -\sum_n F_n dx_n$  where  $F_n$  is the force on the  $n$ th body produced by the rest of the system. Considering the case of uniform strain,  $dx_n = nda$ , we see that  $dx_0 = 0$  and  $F_n = 0$  for  $1 \leq n \leq N - 1$  since these bodies experience equal and opposite forces from the identically strained springs on either side. Therefore, we have from the Hellmann-Feynman theorem (D'Alembert's principle<sup>4</sup>)  $dU = -F_N dx_N = k(a - a_0) \times Nda$  so that  $dU/da$  is obtained exactly in this case from the force on the body at the end of the chain. This argument is easily generalized to three dimensions, establishing the role of the surface in the equilibrium condition.

By introducing springs joining second neighbors in the chain, we can easily produce a model for the variation of the lattice constant close to the surface, analogous to that described in Kleinman's paper.<sup>2</sup>