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Simulation of the surface temperature profile of a heated slab-shaped sample in the Casimir conduction regime

A G Every†, N P Hewett§, L J Challis and J Cooper‡
† Department of Physics, University of the Witwatersrand, Johannesburg, PO Wits 2050, South Africa
‡ Department of Physics, University of Nottingham, Nottingham NG7 2RD, UK

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Abstract. The integral equation approach of Klitsner and co-workers for boundary limited thermal conductance is adapted for calculating the surface temperature profile of wide slab-shaped samples in which the temperature is independent of the large dimension transverse to the direction of heat flow. It is used to model the surface temperature of a silicon water in which a hot 2DEG is embedded. Noteworthy features emerging from this simulation are temperature discontinuities at the edges of the heat source and sink with the temperature gradient nearby being non-uniform, marked differences between the temperature profiles of the opposite faces, and the existence of a finite thermal gradient in regions where there is no net heat flux.

1. Introduction

The theory of thermal conduction by phonons in the boundary scattering regime, first proposed by Casimir (1938), is now well established and has found abundant experimental support (Berman *et al* 1953, 1955, Klitsner and Pohl 1987). A central assumption of the theory is that in the steady state each element of the surface of a sample is in thermal equilibrium, absorbing all incident radiation and re-emitting as a black body at the same rate. Experimental evidence for this thermalisation has been found at many surfaces (see, e.g., Trumpp and Eisenmenger 1977, Kenmuir *et al* 1987), but its origin is not well understood. It seems clear that intrinsic processes are too weak to produce this thermalisation. The defects that are responsible, and that are also likely to be the cause of the anomalous Kapitza conductance between solids and liquid helium, have been the subject of considerable speculation. We note that the good agreement between the Casimir theory and thermal conductivity experiments on samples with rough surfaces is in itself not evidence for thermalisation, since strong elastic scattering at the surfaces would lead to essentially the same heat flow.

§ Now at British Telecom Research Laboratories, Martlesham Heath, Ipswich, UK.

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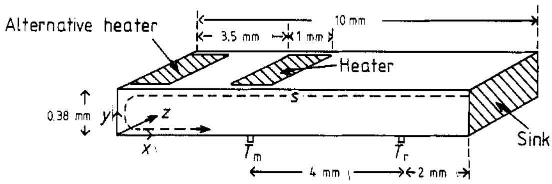

Figure 1. The sample geometry. The thermometer measuring T_m is directly opposite the heater, and T_r is downstream where the thermal gradient is uniform.

The conventional approach to Casimir's theory is as follows: a uniform thermal gradient is assumed to exist along the axis of a rod-shaped sample. Simple angular integrals are then evaluated to obtain the net phonon flux passing through a section normal to the sample's axis. From this the thermal conductivity K and phonon mean free path l are deduced, both of which are sample size dependent quantities rather than bulk properties of the medium. Extensions to the theory have been carried out by a number of investogators, to allow for a proportion of specular reflection at the surfaces and finite sample lengths (Berman *et al* 1953, 1955), various shapes of cross section (Wybourne *et al* 1984, Eddison and Wybourne 1985), and phonon focusing (McCurdy *et al* 1970).

There are, however, situations where a uniform thermal gradient is not assured, and the temperature profile of the sample itself has to be treated as unknown apart from certain boundary constraints. In a recent paper Klitsner *et al* (1988) have taken a more general approach to the Casimir theory by establishing an integral equation for the surface temperature profile of a sample based on the condition of local radiative equilibrium. By means of this equation they are able to explain a pronounced dependence of their measured thermal conductivities of long, polished silicon rods on the placement of heater and thermometers.

In order to gain a more quantitative understanding of our recent measurements of the directional dependence of the phonon emission from two-dimensional electron gases (2DEGs) in the inversion layer of silicon MOSFETs (Hewett *et al* 1989), we have had recourse to an approach that is similar to that of Klitsner *et al* (1988). A typical sample in our experiments has the form of a rectangular wafer 0.38 mm thick, 5 mm wide and of effective length 10 mm as shown in figure 1. The 2DEG is a narrow strip (1 mm wide) located inside the upper face and extending across much of the width (3 mm). The sample sits in a vacuum, heat is generated by passing an electrical current through the 2DEG, and one end of the sample acts as a heat sink with the temperature fixed at around 1 K. Since silicon of this thickness is transparent to phonons of frequency less than 1500 GHz, we can obtain information about the directional dependence of the phonon emission from the 2DEG by investigating the temperature distribution on the opposite face of the sample. We are concerned with how this distribution is affected by the angular distribution of the phonons emitted by the 2DEG under steady state conditions.

In this paper we consider various models for phonon emission by the 2DEG. An integral equation similar to that of Klitsner *et al* (1988) is established for the surface temperature of our sample, and is solved by a finite element method. We find that in the region midway between the heat source and sink there is an approximately uniform thermal gradient as expected. Elsewhere, however, there are significant deviations from this simple behaviour. The temperature profiles of the opposite faces are not in general identical, there are temperature discontinuities, and a thermal gradient exists in a region where there is no net heat flux.

2. Analysis and model 1

To simplify the analysis we assume that power is injected uniformly along the length of the 2DEG heater (this is not necessarily true for a 2DEG in the presence of an applied magnetic field), and that because of the large width to thickness ratio of the sample, the edges play a negligible role in determining the temperature profile, and that the surface temperature is therefore independent of z (see figure 1). The problem thereby becomes one-dimensional, that of determining the temperature dependence $T(s)$, where s is the distance measured around the sample as shown in figure 1. Since heat enters only at one face, the temperature profiles for the two faces are not necessarily the same, i.e. T cannot be regarded as a function of x rather than of s.

In our first model we assume the 2DEG coincides with the upper face and that the heat is generated within this surface. We take the entire heater area to be at a fixed temperature T_h and the heat sink area of the sample to be at a slightly lower temperature T_c. These are the only regions where heat can enter or leave the sample, and we assume there is no significant heat flow within the surface. It follows that under steady state conditions the temperature profile $T(s)$ of the remainder of the surface is such that each surface element, radiating as a black body, emits the same total energy flux as it receives from all other surface elements, including the heat source and sink. No account is taken of specular reflections, which are not expected to be important under the operating conditions we are concerned with.

The energy flux emitted by a surface element $\mathrm{d}A$ at a temperature T towards another surface element located at an angle φ to the surface normal at $\mathrm{d}A$, and subtending solid angle $\mathrm{d}\Omega$ is given by (Berman *et al* 1953)

$$\mathrm{d}F = QT^4 \cos\varphi \, \mathrm{d}A \, \mathrm{d}\Omega \tag{1}$$

and Q is a constant for the system. Integration with respect to z yields the total flux emitted by $\mathrm{d}A$ at position s towards an infinitely long strip of width $\mathrm{d}s'$ at s', which is at an angle $\theta(s')$ to the normal at $\mathrm{d}A$ and which is of angular width $\mathrm{d}\theta = (\mathrm{d}\theta/\mathrm{d}s')\,\mathrm{d}s'$,

$$\mathrm{d}H = (\pi/2)Q(T(s))^4 \, \mathrm{d}A \cos\theta \, \mathrm{d}\theta. \tag{2}$$

The principle of detailed balance requires that the radiation received by $\mathrm{d}A$ from that strip is given by a similar expression, but with $T(s)$ replaced by $T(s')$. Integrating these expressions with respect to s', equating, and eliminating terms quadratic and of higher order in $\delta T = T - T_c$, leads to the integral equation

$$\delta T(s) = \tfrac{1}{2} \int_{\mathrm{all}\,s'} \delta T(s') \cos\theta(s') \frac{\mathrm{d}\theta}{\mathrm{d}s'} \, \mathrm{d}s' \tag{3}$$

which determines the temperature $\delta T(s)$ at all points s where the temperature is not fixed.

For computational purposes we have converted this integral equation into a set of linear equations by partitioning the surface into $N = 208$ parallel strips of approximately

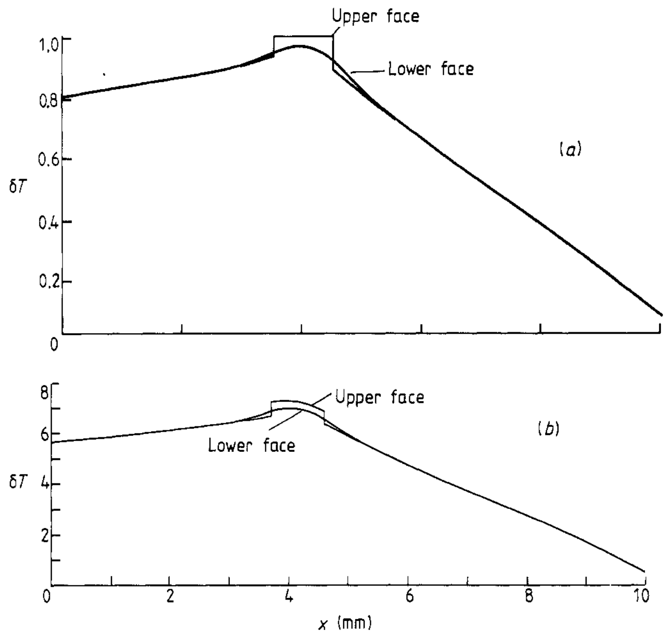

Figure 2. Relative temperature δT versus distance x for: (a) model 1, all heater elements at same temperature; (b) model 2, equal power dissipation in all heater elements.

equal width. (We have done calculations with other numbers of strips, obtaining results substantially in agreement with those reported below). The heat sink comprises four of these strips for which $\delta T = 0$ and the heated surface region another 10 for which $\delta T = 1$ in units of $T_h - T_c$. The temperatures of the remaining $M = 194$ strips are determined by the equations

$$\delta T_s = \sum_{s'=1}^{N} W_{ss'} \delta T_{s'} \qquad s = 1, \ldots, M \tag{4}$$

where

$$W_{ss'} = \begin{cases} G_s \cos\theta_{ss'}\, \delta\theta_{ss'} & s \neq s' \\ 0 & s = s'. \end{cases} \tag{5}$$

and $G_s \simeq \frac{1}{2}$ is a normalisation constant ensuring that

$$\sum_{s'} W_{ss'} = 1.$$

We employ an iterative procedure to solve these equations, starting with assumed values of δT_s, updating δT_s using equation (4), and repeating the cycle until convergence is obtained, which takes a few hundred iterations.

The results of the calculation are shown in figure 2(a). They reveal that in the region midway between heat source and sink the two faces of the sample are at the same temperature, and there is a uniform thermal gradient along the surface, as expected. The magnitude of this thermal gradient agrees, to within a few per cent, with the average gradient obtained by dividing the temperature difference between source and sink by the distance, Δs, between their midpoints. Some other features of the temperature profile are, however, more surprising. Sizable temperature discontinuities occur at the edges of the heat source and sink, and nearby the surface temperature gradients are non-uniform. Neat to the heat source the temperatures of the opposite faces differ appreciably. In the region of the slab remote from the heat sink, there is a finite surface temperature gradient, even though the net heat flux in the x direction there is zero.

These latter features require some explanation as they appear to be in conflict with elementary thermal conduction ideas. The crux of the matter is that under the low temperature conditions to which our model is applicable, there is no significant bulk scattering of phonons, and hence no mechanism by which local thermal equilibrium can be established in the bulk. In contrast, the defective nature of the surface is assumed to bring about sufficient scattering for thermal equilibrium to be established in the surface (or more precisely, in a thin layer, comparable in thickness to the heights of the surface asperities, at the surface). So, while it makes sense to talk of a surface temperature profile, bulk temperature has no meaning, in the strict sense, in this situation. Certainly there are fluxes of phonons passing in all directions through any point in the bulk, but each of these fluxes originates at some point on the surface, and has a Planck spectral composition corresponding to the temperature of that surface point. A unique temperature cannot be ascribed to any point in the bulk, and it follows that the formalism of bulk thermal conduction does not apply. True, some investigators of Casimir conduction do define a sample conductivity in terms of the integrated heat flux along the axis and the temperature difference between the ends of the sample, but this is a sample size dependent quantity and cannot righly be considered a bulk property of the medium.

Our model concerns radiation in an enclosure, and it is on this basis that the results are to be understood. One region of the surface of this enclosure is constrained to be at a temperature $\delta T = 1$ and another region at $\delta T = 0$. Heat balance ensures that all other points on the surface, no matter where they are located, come to equilibrium at temperatures intermediate between these two extremes. The relative influence of the two constrained regions on the temperature at a particular point depends to a large extent on the solid angles subtended by those regions at that point. This explains why the surface temperature falls steadily from the heater towards the sink and also why it decreases in the region beyond the heater remote from the sink. Directly opposite the heater, the solid angle subtended by the heater is by far the larger, but towards the end the two solid angles become comparable. In this remote region the integrated heat flux through any cross section is zero, but this does not imply that the flux is zero at all points on such a section.

Consider now two adjacent surface elements, one on either side of a boundary of the heater. They both, because of their geometrical situation, receive almost identical amounts of radiant heat from all other surface elements. The heater element in addition draws heat from its external source. These quantities all scale with the areas of the elements. Both elements must dispose of their net heat input by radiation, and so there is necessarily a finite temperature difference between the two elements, which persists even when the two elements are reduced in size to zero. This explains the temperature discontinuities that are evident in figure 2(a). Of course, if one were to reformulate the problem and treat the surface as a very thin layer in which thermal equilibrium is established, then the temperature drop would not be discontinuous, but would extend over a distance comparable to the thickness of the layer. Existing measuring techniques would not, however, be able to distinguish between such a narrow transitional region and a true discontinuity. Because of the low effective thermal conductivity and thinness of the surface layer, a negligible amount of heat is conducted along this layer in spite of the high thermal gradient in the transitional region.

3. Model 2

In this second model we assume that the heater power is distributed uniformly over the heater area. This relaxes the constraint that the heater area is at a fixed temperature (the sink though it still taken to be at a fixed temperature T_c). The temperature of each surface element is now determined by the condition that the power emitted from it equals the power absorbed from the other elements plus (for the heater surface elements) the external power dissipation P. The linear equations determining the temperature profile now take the form

$$\delta T_s = \sum_{s'} W_{ss'}\, \delta T_{s'} + K_s \tag{6}$$

where K_s ($=G_s P$ in this case) is a source term.

The results obtained using this model are shown in figure 2(b). There is, as expected, a uniform temperature gradient in the region midway between the heater and the sink, but the temperature profile in the vicinity of the heater is qualitatively different from that of the isothermal heater. The discontinuities in the temperature of the upper face are reduced, and the temperatures of the two faces are now much closer, indeed almost identical, at the centre of the heater. This is evidently the result of the very high aspect ratio which causes the temperature of an element to be largely determined by the temperatures of those directly opposite to it.

We have also calculated the surface temperature distribution for a heater at $x = 0$ and, as expected, find that the linear region now extends to around $x = 1$ mm and that the temperature at $x = 1.5$ mm has the value obtained by extrapolating the linear regions in figures 2(b).

4. Model 3

We next consider the phonon emission from a hot 2DEG treated as a separate radiating surface. This radiation is known to be largely restricted to a cone of directions close to the normal by the need to conserve momentum in the plane of the 2DEG (Rothenfusser *et al* 1986, Challis *et al* 1987). We have investigated the effect of this by introducing a cut-off to the energy flux from the 2DEG for $\theta > \theta_c$ while keeping the total heat output fixed. The 2DEG lies just below the upper surface, so the only upper surface elements directly illuminated by the 2DEG are those immediately above it. The illumination of the end and lower surface elements depends on the value of θ_c. The model assumes that phonons that are subsequently emitted by all surface elements (including those of the Si/SiO_2 interface above the 2DEG) are able to pass through the 2DEG. Phonon attenuation does take place in a 2DEG, but it is only of the order of a few per cent (see, e.g., Hensel *et al* 1984, Kent *et al* 1988). The temperature distributions on the two faces for $\theta_c = 1°$

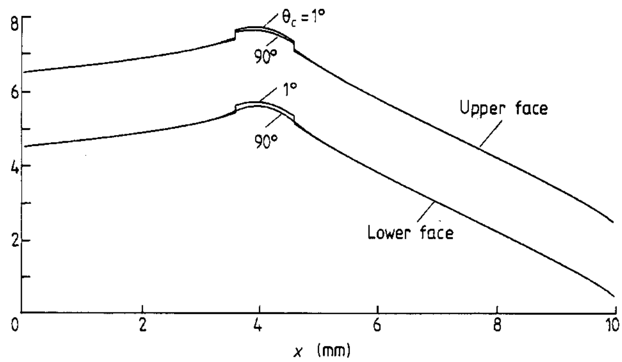

Figure 3. δT versus x for the sample heated by a 2DEG for two different cone angles: $\theta_c = 90°$ (isotropic case) and $\theta_c = 1°$. Curves for upper face have been displaced vertically by two units for clarity.

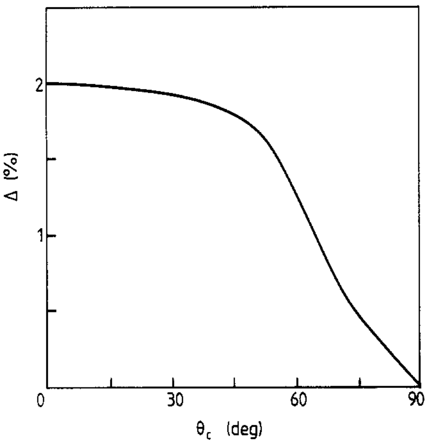

Figure 4. The fractional increase $\Delta = (\delta T_m(\theta_c) - \delta T_m(90°))/\delta T_m(90°)$ in per cent as a function of cone angle θ_c.

are shown in figure 3 and compared with the isotropic case ($\theta_c = 90°$). The temperatures at $x > 5$ mm (>1 mm from the centre of the 2DEG heater) are virtually independent of θ_c as expected, while the maximum temperature on the lower face opposite the heater at $x = 4$ mm increases with decreasing θ_c as a result of the increasingly concentrated intensity in the forward direction. Figure 4 shows the fractional change in the temperature δT_m at $x = 4$ mm as a function of θ_c.

We may compare the 2% change in δT_m with that seen experimentally. The cone angle θ_c within which the phonons are largely emitted can be varied over a wide range by adjusting the gate potential on the Si MOSFET. The maximum change in temperature observed (relative to the end of the sample) was ~2% (Hewett *et al* 1989), so there is quite good agreement. We plan in a later paper to examine the effect of phonon focusing, which we expect to modify the effect.

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