

On the role of acoustic waves (phonons) in equilibrium heat exchange across a vacuum gap

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April 27, 2011

Abstract

Heat exchange between closely positioned bodies has become an important issue for many areas of modern technology including, but not limited to, integrated circuits, atomic force microscopy and high-density magnetic recording, which deal with bodies separated by gaps as narrow as a few nanometers. It is now recognized that heat transport across a gap of sub-micron width noticeably exceeds the limit set by the conventional theory of radiative heat transfer. This papers shows than if the gap's width is below a certain value, estimated as about 10 nanometers for silicon at room temperature, then, in addition to electromagnetic radiation, significant heat is a also carried by acoustic waves. Moreover, as the width of the gap decreases below about 5 nanometers, acoustic waves rapidly become the dominant heat carrier.

1 Introduction

The common perception that electromagnetic radiation provides the only means of heat exchange between bodies separated by a vacuum gap has both theoretical and experimental justifications. Thus, conventional theory recognizes three mechanisms of heat transfer: conduction, convection and radiation [5]. Conduction is caused by interactions between particles that do not change their average positions, as in solids, convection occurs when the energy is transported by drifting particles, as in fluids and gases, and radiation is the energy transport by electromagnetic waves. According to these definitions, conduction and convection are impossible in a vacuum because there are no particles in a vacuum, but electromagnetic waves, on the other hand, propagate most efficiently in a vacuum. So, radiation is apparently the only heat carrier in a vacuum. This theoretical conclusion is strongly supported by the design of the Dewar flask, which is made from nested vessels separated by an evacuated space. If the walls of the vessels are covered by mirrors that block radiation then, independently of the thickness of the vacuum layer, the flask provides such excellent thermal insulation that it leaves little doubt about the absence of conduction and convection in a vacuum.

The fact that material bodies can exchange heat across a vacuum was discovered long ago, and the theory of radiative heat transport provided methods of computation of heat transfer between separated bodies. However, in the 1960s it was demonstrated that heat transport between metallic surfaces separated by a gap in the micrometer range significantly exceeded predictions of the conventional theory. New experiments confirmed that heat transport across gaps between similar metals in the nanometer range may exceed conventional predictions by orders of magnitude [3]. More recent experiments have shown that metals are not exceptions, and that heat transport between closely spaced dielectric plates of the same materials becomes unbounded as the separation distance decreases [9, 10].

After this deficiency of the conventional theory of heat transport between separated bodies was revealed this phenomenon attracted considerable attention, inspired by its importance for several areas of technology. In particular, modern microelectronic devices are packed so densely that their performance may be affected by heat exchange between the components, so that heat management becomes important not only for energy saving but also to ensure correct functionality. Heat exchange between closely separated objects may also play a critical role in such technologies as high-resolution microscopy and data recording, for example. Indeed, the resolution of a 20nm size detail using a probe of an atomic force microscope or a plasmonic hyper-lens requires that they be placed within a distance of the order of 20nm from the object, which is close enough to cause undesirable thermal disturbance. Similarly, in modern magnetic storage devices the distance between the recording head and the disk's surface may be as small as a few nanometers, which is close enough to increase the thermal conductance between the disk and the head to the level that can either corrupt the data or, alternatively, be utilized by a heat assisted recording system designed to increase the density of recording.

There is nothing surprising in the observations that heat transport across a narrow gap between identical materials diverges as the width of the gap vanishes. Indeed, if the gap's width reduces to the distance between molecular layers, the two separated bodies form a homogeneous medium and then the thermal conductance of such an imaginary interface must be infinite.

Despite the transparency of the last reasoning, it has not attracted much attention, possibly, because of the illusion that although heat transport across a vacuum gap is provided exclusively by electromagnetic radiation, when the gap collapses, some more efficient mechanisms abruptly activate and thus provide infinite conductivity of the imaginary interface. Although such arguments sound appealing, they are nevertheless misleading. First because the radiative conductance of an infinitesimally narrow gap is itself unbounded [2], and also because a sufficiently narrow gap

supports the propagation of acoustic waves which are known to be primary heat carriers in solids, and, therefore, which must also be considered as the gap closes.

This paper discusses the mechanisms of heat conduction between slightly separated solid half-spaces. First we discuss the mechanism of heat transport in a one-dimensional spring-mass model of a uniform crystalline lattice. Then, we modify this model to include a weaker link (across a gap) and formulate a simple three dimensional model of heat conductance by acoustic waves (phonons) across a narrow gap. Finally, we estimate the width of the gap for which heat conductance by means of acoustic waves dominates thermal transfer due to radiation.

2 Mechanical heat carriers

The simplest model of lattice vibrations that carry heat in dielectric solids is a chain of particles connected by springs. Consider, for simplicity, the one-dimensional uniform chain shown in Fig. 1 where equal masses $m = \rho a$ are connected by identical springs with the elastic modulus γ and equilibrium spacing $a > 0$, so that ρ appears as a mass density of the chain.

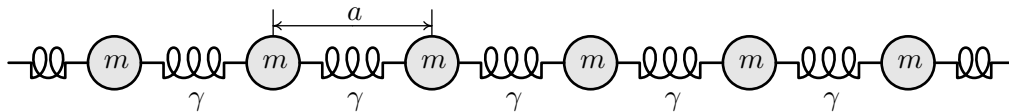


Figure 1: Simple chain.

Let $\xi(t, x_n)$ be the displacement of the n th particle identified by its position of equilibrium $x_n = an$. Then the motion of these particles is described by the equation

$$\rho a \frac{d^2 \xi(t, x_n)}{dt^2} = \frac{\gamma}{a} [\xi(t, x_{n+1}) + \xi(t, x_{n-1}) - 2\xi(t, x_n)], \quad x_n = an. \quad (2.1)$$

When the spacing vanishes as $a \rightarrow 0$ but the density ρ remains constant, the nodes x_n become continuously spread over the real line and the last equations converge to the wave equation

$$\frac{1}{c^2} \frac{d^2 \xi(t, x)}{dt^2} = \nabla^2 \xi(t, x), \quad c = \sqrt{\frac{\gamma}{\rho}}, \quad (2.2)$$

where x is a continuous coordinate, and c is the sound speed determined by the elastic modulus γ and the mass density $\rho = m/a$ of the continuum.

This elementary model can be extended to more complex cases. In particular it can be used to model two continuous half-spaces separated by a narrow, but non-vanishing gap.

Consider the chain shown in Fig. 2 where the masses $m_- = \rho_- a$ are located at the nodes $x_n = an < 0$ and the masses $m_+ = \rho_+ a$ are located at $x_n = h + an$, where $n \geq 0$, and $h > 0$ is the spacing between two uniform half-chains occupying the domains $x < 0$ and $x > h$. Assume that

the springs inside the half-chains $x < 0$ and $x > h$ have the elastic moduli γ_- and γ_+ , respectively, and that the spring connecting x_{-1} and x_0 has the elastic modulus γ_h .

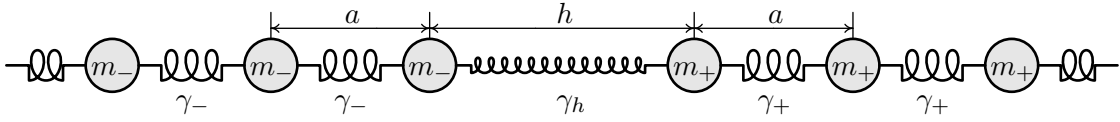


Figure 2: Two separated chains

The motion of this chain is described by the equations (2.1), which controls the motion of all particles with $n \neq -1$ and $n \neq 0$, and by two additional equations

$$\begin{aligned} n = 1 : \quad \rho_- a \frac{d^2 \xi(t, 0)}{dt^2} &= \frac{\gamma_h}{h} [\xi(t, h) - \xi(t, 0)] + \frac{\gamma_-}{a} [\xi(t, -a) - \xi(t, 0)], \\ n = 0 : \quad \rho_+ a \frac{d^2 \xi(t, h)}{dt^2} &= \frac{\gamma_h}{h} [\xi(t, 0) - \xi(t, h)] + \frac{\gamma_+}{a} [\xi(t, h + a) - \xi(t, h)], \end{aligned} \quad (2.3)$$

for the particles located at the boundaries of the homogeneous half-chains.

Let the spacing of the uniform chains $x < 0$ and $x > h$ vanish as $a \rightarrow 0$, while the distance h between them remains finite. Then, passing to the limit $a \rightarrow 0$ we observe that (2.3) reduce to the interface conditions

$$\gamma_- \frac{\partial \xi(t, x)}{\partial x} \Big|_{x=0} = \gamma_+ \frac{\partial \xi(t, x)}{\partial x} \Big|_{x=h} = \gamma_h \frac{\xi(t, h) - \xi(t, 0)}{h}, \quad (2.4)$$

which compliment the wave equation (2.2) describing the motions in $x < 0$ and $x > h$.

If the interconnection $0 < x < h$ is very strong in the sense that $\gamma_h/h \rightarrow \infty$ then (2.4) reduce to the single condition

$$\xi(t, h) = \xi(t, 0), \quad (2.5)$$

which implies that the boundaries $x = 0$ and $x = h$ are firmly connected to each other so that the motion of one of them exactly reproduces the motion of the other. In the opposite limiting case of a very weak interconnection when $\gamma_h/h \rightarrow 0$, conditions (2.4) reduce to Neumann boundary conditions

$$\frac{\partial \xi}{\partial x} \Big|_{x=0} = 0, \quad \frac{\partial \xi}{\partial x} \Big|_{x=h} = 0, \quad (2.6)$$

which imply that the domains $x < 0$ and $x > h$ move independently of each other.

The models discussed above admit generalizations to three-dimensional models of any feasible anisotropic elastic medium. However, in many common situations it suffices to use Debye's approximation [4, 8], which treats any heat-conducting solid as an isotropic continuum supporting propagation of three similar acoustic waves described by the scalar wave equation (2.2) with the wave speed v determined by the mechanical properties of the material.

In Debye's model, heat carriers in a dielectric solid occupying some domain G are represented by an acoustic pressure field $p(\vec{r}, t)$ which is related to the displacement vector field $\vec{\xi}(\vec{r}, t)$ by

$$\rho \frac{\partial^2 \vec{\xi}}{\partial t^2} = -\vec{\nabla} p, \quad (2.7)$$

and satisfies the wave equation $\ddot{p} = c^2 \nabla^2 p$ inside G and appropriate boundary and interface conditions on ∂G . In particular the acoustic pressure $p(\vec{r}, t)$ in a system of two interacting half-spaces $x < 0$ and $x > h$ must obey the interface conditions

$$\gamma \frac{\partial^2 p}{\partial x^2} \Big|_{x=0} = \gamma \frac{\partial^2 p}{\partial x^2} \Big|_{x=h} = \frac{\gamma_h}{h} \left(\frac{\partial p}{\partial x} \Big|_{x=h} - \frac{\partial p}{\partial x} \Big|_{x=0} \right) \quad (2.8)$$

which generalizes (2.4) and takes into account (2.7).

To use these interface conditions it is necessary to know the elastic modulus γ_h of the vacuum gap of width h . If h is large compared to the intermolecular distance then γ_h can be estimated by the formula

$$\gamma_h = h \left| \frac{dF}{dh} \right|, \quad (2.9)$$

where $F(h)$ is the force of interaction between the half-spaces separated by the distance h . This force is computed in [6, 7] by a rather complex method which, however, generates simple asymptotes in some special but still representative cases. In particular, if both half-spaces are identical dielectrics separated by a distance $h \ll \lambda_0$, with $\lambda_0 \approx 500\text{nm}$ at room temperature, then $F \approx C_0/h^3$, where C_0 is a constant determined by [7, Eq. (90.4)]. Correspondingly, the modulus γ_h is estimated as

$$\gamma_h \approx \frac{3C_0}{h^3}, \quad h \ll \lambda_0 \approx 500 \text{ nm}. \quad (2.10)$$

Properties of the wave equations imply that acoustic eigenfields in the system of two interacting half-spaces $x < 0$ and $x > h$ can be decomposed into monochromatic fields

$$p(t, \vec{r}; \omega, \vec{e}) = \begin{cases} A_- e^{i(d_x x + d_y y + d_z z)\omega/c_- - i\omega t} + B_- e^{i(-d_x x + d_y y + d_z z)\omega/c_- - i\omega t}, & \text{if } x < 0, \\ A_+ e^{i(e_x x + e_y y + e_z z)\omega/c_+ - i\omega t} + B_+ e^{i(-e_x x + e_y y + e_z z)\omega/c_+ - i\omega t}, & \text{if } x > h, \end{cases} \quad (2.11)$$

where the coefficients A_{\pm} and B_{\pm} are related by the equations

$$\begin{pmatrix} A_- \\ B_- \end{pmatrix} = \mathbb{T} \begin{pmatrix} A_+ e^{2\pi i h \cos \theta / \lambda} \\ B_+ e^{-2\pi i h \cos \theta / \lambda} \end{pmatrix}, \quad \mathbb{T} = \begin{pmatrix} 1/K & \bar{R}/\bar{K} \\ R/K & 1/\bar{K} \end{pmatrix}, \quad (2.12)$$

where \mathbb{T} is the transmission matrix represented in terms of the transmission and reflection coefficients K and R of the gap, which can be computed by the methods of the theory of wave propagation in layered media [1]. Without going into detail we mention that if the half-spaces $x < 0$ and $x > h$ are occupied by identical materials then these coefficients are described by the formulas

$$K = \frac{\lambda \gamma_h e^{-2\pi i h \cos \theta_+ / \lambda}}{\lambda \gamma_h - i\pi \gamma_+ h \cos \theta_+}, \quad R = \frac{i\pi \gamma_h \cos \theta_+}{\lambda \gamma_h - i\pi \gamma_+ h \cos \theta_+}, \quad (2.13)$$

that generate asymptotes

$$|K| \approx 1, \quad |R| \approx \frac{\pi\gamma h \cos \theta}{\gamma_h \lambda}, \quad \text{if} \quad \frac{\gamma}{\gamma_h} \frac{h}{\lambda} \cos \theta \ll 1, \quad (2.14)$$

$$|K| \approx \frac{\gamma_h \lambda}{\pi\gamma h \cos \theta}, \quad |R| \approx 1, \quad \text{if} \quad \frac{\gamma}{\gamma_h} \frac{h}{\lambda} \cos \theta \gg 1, \quad (2.15)$$

which confirm that a vanishingly narrow gap between identical media has full transmission and no reflection, and that, oppositely, a wide gap has full reflection but no transmission.

3 Heat carrying capability of acoustic waves

It is shown above that acoustic waves can penetrate the vacuum gap separating material half-spaces and that, therefore, these waves can carry heat across a vacuum gap. However, the importance of this channel of heat transfer strongly depends on the gap's width. In particular, for wider gaps electromagnetic radiation remains the sole heat carrier, but for sufficiently narrow gaps acoustic waves become the dominant heat carriers. To justify this statement it suffices to obtain order-of-magnitude estimates of the maximal rates of heat exchange between separated half-spaces which can be provided by electromagnetic radiation and by acoustic waves.

First we estimate the maximal rate of heat exchange that can be carried by acoustic waves. Using [8, §66] we find that the energy density of a solid can be estimated as

$$E_{Ac} \approx 3N\kappa_B T D \left(\frac{\Theta}{T} \right), \quad N = \frac{\rho}{A_r \cdot u_a}, \quad D(x) = \frac{3}{x^3} \int_0^x \frac{\xi^3 d\xi}{e^\xi - 1}, \quad (3.1)$$

where $\kappa_B = 1.38 \cdot 10^{-23}$ (J/K) is the Boltzmann constant, T is the temperature, Θ is the Debye temperature of the material, and N is the number of atoms per unit volume represented in terms of the mass density of the material ρ , of its atomic weight A_r , and the atomic mass unit $u_a = 1.66 \cdot 10^{-27}$ kg, which is essentially the weight of a single proton. For silicon at room temperature ($T = 300$ K) we find that $N \approx 5.53 \cdot 10^{28}$, and $D(\Theta/T) \approx 1.96$, which imply that the energy density of thermally excited acoustic waves is of the order $E_{Ac} \approx 1.34 \cdot 10^9$ J/m³. Then, multiplying this number by the speed of sound we find that the maximal heat flux that can be carried by acoustic waves in silicon at room temperature is of the order

$$Q_{Ac} \approx 2.96 \cdot 10^{12} \text{ (W/m}^2\text{)}. \quad (3.2)$$

Similarly, to estimate the maximal heat flux Q_{EM} that can be carried across a vacuum gap between two half spaces at room temperature, we recall [8, Eqn.(63.14)] that the energy density of the electromagnetic radiation in equilibrium at temperature T has the value $E_{EM} \approx 4\sigma T^4/c_0$, where

c_0 is the speed of light, and $\sigma = 5.67 \cdot 10^{-8} \text{ W/m}^2\text{K}^4$ is a constant. Correspondingly, multiplying Q_{EM} by c_0 we find that

$$Q_{EM} \approx 1.84 \cdot 10^3 \text{ (W/m}^2\text{)}. \quad (3.3)$$

It is obvious from (3.2) and (3.3) that acoustic waves are capable of carrying much more heat than electromagnetic radiation. However, while electromagnetic radiation freely propagates across a vacuum gap, transmission of acoustic waves strongly depends on the gap's width, and to estimate the capability of acoustic waves to carry heat across a gap we need to multiply Q_{Ac} by the square of the transmission coefficient $|K|^2$ from (2.13).

If the characteristic wavelength λ of the acoustic waves is larger than the gaps's width h , then $|K| \approx (\gamma_h/\gamma)(\lambda/h)$, which is determined by the ratio γ_h/γ of the elastic constants of the gap and the continuum and by the ratio λ/h of the wavelength to the width of the gap. To estimate the elastic modulus γ_h of a narrow gap we assume that it coincides with the modulus γ of a continuum medium in the case when the separation h coincides with the intermolecular distance h_0 , which may be considered as the smallest possible distance between the half-spaces. From this assumption we get $\gamma_h = \gamma (h_0/h)^3$, which agrees with (2.10), and then we get the estimate

$$|K| \approx \left(\frac{h_0}{h}\right)^4 \left(\frac{\lambda}{h_0}\right). \quad (3.4)$$

Finally, multiplying Q_{Ac} by $|K|^2$ we find that the maximum flux that can be carried by acoustic waves across a gap of width h between silicon half-spaces is of order

$$Q_{Ac}^h \approx Q_{Ac} \left(\frac{h_0}{h}\right)^8 \left(\frac{\lambda}{h_0}\right)^2, \quad (3.5)$$

where λ is the typical wavelength of heat carrying acoustic waves.

Now we can estimate the separation distance h_* at which the maximal heat flux carried by electromagnetic waves is on par with the maximal heat flux carried by acoustic waves. Thus, equalizing Q_{EM} and Q_{Ac}^h we get the equation which shows that

$$h_* \approx h_0 \left(\frac{Q_{Ac}}{Q_{EM}}\right)^{1/8} \left(\frac{\lambda}{h_0}\right)^{1/4} \approx 14.2 h_0 \left(\frac{\lambda}{h_0}\right)^{1/4}. \quad (3.6)$$

If we set $h_0 = 0.235\text{nm}$ (the value for silicon crystal) and $\lambda = 1\text{nm}$, which is a typical wavelength of acoustic waves in silicon at room temperature, then

$$h_* \approx 4.78 \text{ nm}, \quad (3.7)$$

which is the distance comparable with widths of gaps in many modern devices, such is the gap between the head and the disk in a hard drive, for instance.

4 Conclusion

The obtained results show that heat can be carried across a gap by both electromagnetic and acoustic waves, but in most cases only one of these two heat carriers has to be taken into account because the relative contribution of the other one is negligible. Indeed, if the gap has the critical width $h = h_*$ then acoustic and electromagnetic waves carry equal amounts of heat across the gap. However, if the gap's width is 50% more or less than h_* then the contribution of the acoustic waves is about twenty five times less or more, while the contribution of electromagnetic waves remains practically unchanged. This observation implies that in the considered case (3.7) of silicon at room temperature, both electromagnetic and acoustic heat carriers must be taken into account only for gaps with the width in the range between $0.5h_*$ ($\approx 2.5\text{nm}$), and $1.5h_*$ ($\approx 7.5\text{nm}$), which is the shaded strip in Fig. 3. For wider gaps acoustic waves can be neglected, and for narrower gaps there is no need to take into account electromagnetic radiation.

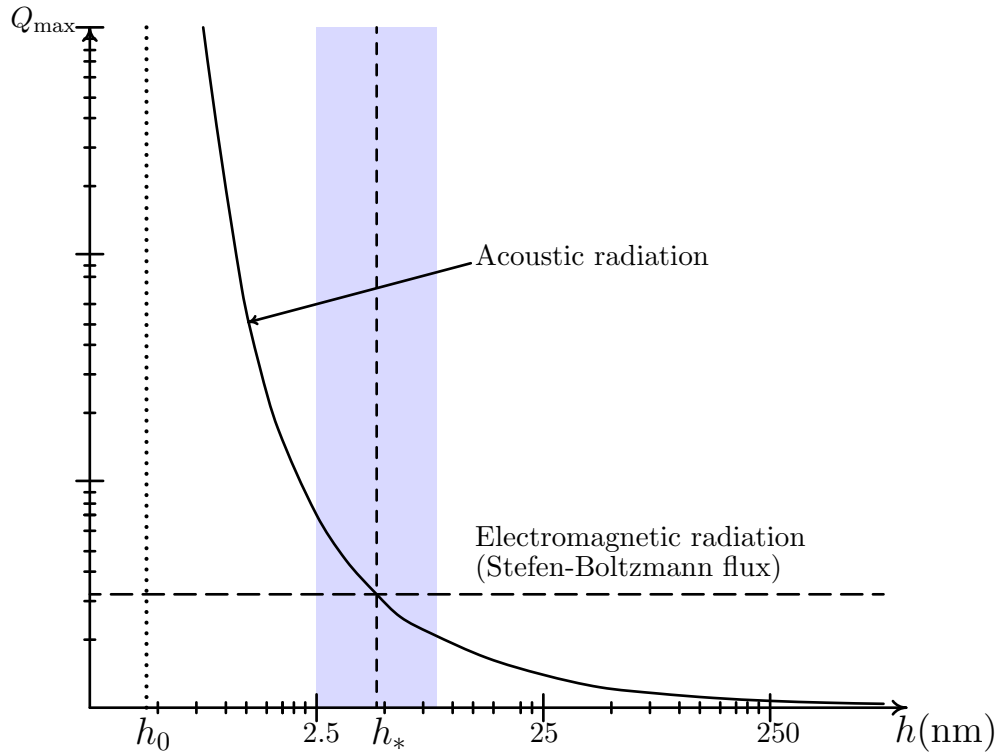


Figure 3: Contributions of acoustic and electromagnetic waves to heat exchange between half-spaces in thermal equilibrium

It should be mentioned that Fig. 3 does not show heat fluxes between separated half-spaces maintained at different temperatures. Instead, this figure illustrates the intensity of heat exchange between half-spaces in thermal equilibrium. It is well known that if two bodies are in thermal

equilibrium this does not mean that they do not exchange heat, it means that the flows of heat in the different directions are equal to each other. In particular, if two half-spaces are in thermal equilibrium then each of them receives from its counterpart an equal amount of electromagnetic energy that is represented by the Stefan-Boltzmann law. For gaps narrower than the typical wavelength of thermal radiation, this amount shows little dependence on the distance between half-spaces, and, correspondingly, it is shown in Fig. 3 by a horizontal dashed line. As shown here, separated half spaces still exchange heat by thermally excited acoustic waves, but since such waves noticeably decay with gap width in a vacuum, the intensity of energy exchange carried by acoustic waves sharply decays as the gap's width increases, which is shown in Fig. 3 by a solid line.

Acknowledgment

This work was supported by the William S. Floyd, Jr., Distinguished Chair, held by D. Bogy.

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