On the mechanisms of heat transport across vacuum gaps

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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 does not follow the Stefan-Boltzmann law, which is based on a conventional theory developed for sufficiently wide gaps. This paper describes the structure of thermally excited electromagnetic fields in arbitrarily narrow gaps, and it also shows that heat can be carried across narrow vacuum gaps by acoustic waves. The structure of the acoustic wave fields is also described, and it is shown that they become the dominant heat carriers in gaps narrower than a certain critical width, which is estimated to be a few nanometers.

For example, consider a vacuum gap between silicon half-spaces. When the gap's width is below a critical value, which is about 7.5nm, the contribution of acoustic waves must be taken into account. Assuming that the wavelength of thermally excited acoustic waves is of order 1nm, it may be possible to estimate the contribution of acoustic waves to heat transport across gaps with 4nm $< h <$ 7.5nm by the kinetic theory, but for narrower gaps with $h <$ 4nm this approximation is not valid, and then the full wave theory must be used. Also for gaps narrower than about 2.5nm there is no need to take into account electromagnetic radiation because its contribution is negligible compared to that of acoustic waves.

1 Introduction

The fact that material bodies can exchange heat even when they are separated by vacuum was discovered long ago, and a well-established theory of radiative heat transport convincingly explained this phenomenon and provided methods of computation of heat transport between separated bodies.

However, it has recently become apparent that the theory that makes it possible to estimate the heat flow from the Sun to Earth, separated by millions of kilometers, does not correctly describe heat transport across a narrow, sub-micrometer gap [8,9]. But, the conventional theory of radiative heat transport implies that the heat flux between two half-spaces separated by a vacuum gap does not depend on the gap's width and is described by the Stefan-Boltzmann law:

$$Q = \frac{\pi^2 \kappa_B^4}{60\hbar^3 c_0^2}(T_+^4 - T_-^4), \tag{1.1}$$

where κ_B is the Boltzmann constant, c_0 is the speed of light in a vacuum, and $T_\pm$ are the temperatures of the half-spaces. At the time when this formula was derived the gap was considered narrow when its width was a few millimeters and this formula was convincingly verified for virtually arbitrary gap widths, including narrow ones. However, in the 1960s it was demonstrated that the heat transport between metallic surfaces separated by a gap in the micrometer range significantly exceeded predictions of the Stefan-Boltzmann law [18]. Later experiments confirmed that the heat transport across gaps in the nanometer range may exceed conventional predictions by orders of magnitude [8]. More recent experiments have shown that metals are not exceptions, and that the heat transport between closely spaced dielectric plates of the same materials has order $O(1/h^2)$ when the separation h decreases [22, 24].

After this deficiency of the conventional theory of heat transport between separated bodies was revealed, it has attracted considerable attention, partially because of academic interests but also because of its importance for several areas of technology dominated by the miniaturization trend. 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 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 radiation between the disk and the head to a level that can either corrupt the data or, inversely, be utilized by a heat assisted recording system designed to increase the density of recording.

There is nothing surprising in the observation that heat transport across a narrow gap does not follow the Stefan-Boltzmann formula (1.1). Since this formula involves no gap width dependence it should hold in the case when $h \to 0$ for half-spaces of the same material separated by a gap. However, in this limit the gap appears as an imaginary plane in a homogeneous medium and its conductance must be infinite, which disagrees with (1.1). Despite its transparency this contradiction has not attracted much attention, possibly because of the illusion that it can be explained by reasoning that while heat transport across a vacuum gap is provided exclusively by electromagnetic radiation, when there is no gap it can be carried by additional and more efficient mechanisms that abruptly activate when the gap collapses and thus provide infinite conductivity of the imaginary gap. Although such arguments sound appealing, they are nevertheless misleading, first because the radiative conductance of an infinitesimally narrow gap is itself unbounded 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 transport between slightly separated half-spaces occupied by dielectric solids. In the next section we review the basic mechanisms of heat transport through continuous solids and explain that heat can be carried across a narrow vacuum gap not only by electromagnetic waves but also by acoustic waves. In Section 3 we describe the structure of electromagnetic fields that propagate in a sandwich-like structure with two material half-spaces separated by a vacuum gap, and the following Section 4 describes the acoustic waves propagating in the considered structure. It is shown that both kinds of waves are described by similar formulas which implies that their contributions to heat transport can be studied by a unified method. Finally, in Section 5 we discuss applications of the proposed model and its relationships to other studies.

2 Overview

It is generally accepted that any material body can be considered as a large system of smaller components and that the energy of such a system can be subdivided into its external and internal energies. The external energy includes the kinetic energy of the motion of the system considered as a whole and the potential energy of interactions of the entire system with the exterior world. The internal energy includes the kinetic energy of the individual components, the energy of interactions between the components, and the internal energies of the components, which may be further subdivided into smaller components with their own internal energies.

The energy can be converted from one form to another, and it can pass from one body to another. In particular, the external energy of a body can be converted to its internal energy and *vice versa*. When different bodies interact they may exchange parts of their external or internal energies, or a part of the external energy of one body may be exchanged to a part of the internal energy of another body. If the internal energy of a body increases or decreases by the amount Q then this body is said to receive or to lose the amount Q of heat. Correspondingly, heat transport is a process of changing the internal energy of a body, and heat can be considered as the measure of the internal energy of the body.

Different materials store their internal energies in different forms which implies that there are different mechanisms of heat transport.

It is well known that a material is composed of particles with a somewhat complicated pattern of electric charges performing perpetual thermal motions. It is also known that accelerating electric charges radiate electromagnetic waves that pick up some of the energy of the emitting charge and transport it until it is absorbed by another charge. Since electromagnetic waves can propagate long distances, have high speeds of propagation, and can propagate in vacuum, they appear as versatile heat carriers providing the only means of heat transport across substantially wide vacuum gaps.

In materials heat can be transported not only by electromagnetic radiation but also by mechanical processes. Thus, the internal energy of a gas with single atom molecules consists of the kinetic energy of the moving molecules. During inevitable collisions the faster particles of warmer areas slow down and pass some of their energy to slower particles of cooler areas. This mechanism of heat transport is described by the kinetic theory [12], which implies that heat conduction in gases can be described by the Fourier law

$$\dot{\vec{Q}} = -k_T \vec{\nabla} T, \tag{2.1}$$

where $\dot{\vec{Q}}$ is the heat flux, $\vec{\nabla} T$ is the temperature gradient, and

$$k_T = \frac{1}{3} C \langle v \rangle \Lambda, \tag{2.2}$$

is the thermal conductivity defined in terms of the specific heat C of the average speed $\langle v \rangle$ of the flying molecules, and of the mean-free path Λ that is the average distance traveled by a molecule between consecutive collisions. In a more complex gas of multi-atom molecules the internal energy is determined by the kinetic energies of the translational and rotational motions of the whole molecules and by the vibrational energies of the molecules, which include the kinetic energy and the potential energy of the fields that keep atoms within a molecule. All of these forms of energy are transformed to each other during collisions, which remain the primary mechanism of heat transport in gases of multi-atom molecules, and this is also described by the kinetic theory.

In solid dielectrics there are no flying and colliding particles. Instead, molecules form a lattice and vibrate around their stable positions at the nodes. Correspondingly, the internal energy of such structures is determined by the energy of lattice vibrations which is carried by acoustic waves propagating through the lattice. It is well known that acoustic waves propagate in a perfect lattice without any decay and that for this reason perfect crystals have infinite thermal conductance [1]. However, since real solids are never perfect they have finite thermal conductance, which, despite the fact that the heat is carried by acoustic waves, can often be described by the kinetic theory devised for gases of flying and colliding particles.

The validity of using kinetic theory to describe heat transport in solids is based on the possibility of decomposing an arbitrary wave into wave packets, which are "almost monochromatic" and "almost localized" waves similar to a modulated one-dimensional wave

$$\phi(x,t) = \mathrm{e}^{-(x-ct)^2/2l^2 - \mathrm{i}\omega(x-ct)/c} \tag{2.3}$$

illustrate in Fig. 1. This wave-packet has an "effective" size of the order $\Delta x \approx l$ and at the same time it has the spectrum

$$\widehat{\phi}(x,\xi) = \frac{1}{c\sqrt{2\pi}} \mathrm{e}^{-l^2(\xi-\omega)^2/2c^2 - \mathrm{i}\xi x/c}, \tag{2.4}$$

localized in the frequency band of width $\Delta\omega \approx c/l$ around the dominant frequency ω. It is easy to see that the effective size of the wave-packet is estimated as $\Delta x \approx \lambda\omega/\Delta\omega$, where λ is the dominant wavelength. Therefore, if a packet has a 5% frequency spread and its dominant wavelength is about 2nm, which is typical for silicon at room temperature, then the size of this packet is on the order of 40nm, which is substantially larger than many currently studied nanostructures. If the frequency of vibrations is not restricted, then wave-packets may be as narrow as Dirac's δ-function. However, in real materials the wavelength of lattice vibrations is bounded from below, which implies that wave-packets cannot be arbitrarily small. In particular, as discussed above, wave-packets in silicon at room temperature cannot be smaller than a few tens of nanometers.

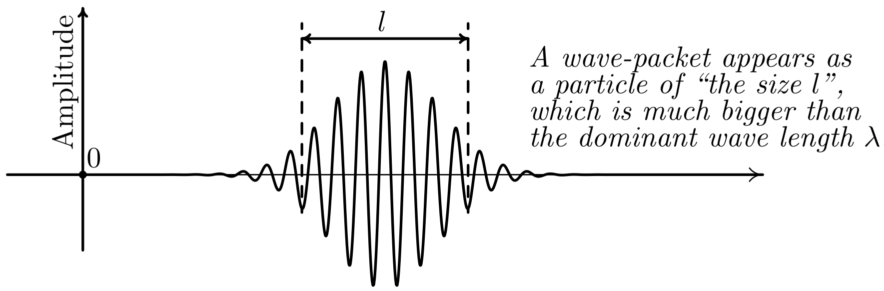


Figure 1: A particle-like wave-packet.

In cases when it is permissible to represent lattice vibrations in terms of wave-packets it is possible to study heat transport in dielectric solids by methods of the kinetic theory devised for gases. Thus, a detailed analysis [14] shows that wave-packets can be treated as isolated objects which move and collide similarly to material particles in gases. Correspondingly, the heat transport in solids can *under these conditions* be described by the Fourier law (2.1) and the heat conductivity can then be determined by the expression (2.2) where the mean-free path Λ is defined as the average distance traveled by a wave-packet between non-linear interactions with other wave-packets. However, the applicability of the kinetic theory to the analysis of heat transport by lattice vibrations is restricted by the requirements that the characteristic sizes of the medium be considerably larger than the wave-packets, which, in turn, are considerably larger than their dominant wavelength. These restrictions alone demonstrate that the kinetic theory, Fourier law and the heat equation, which follows from the Fourier law, cannot be reliably applied to the analysis of heat transport in nanostructured devices.

It is worth noting that such "mechanical" mechanisms of heat transport as collisions of flying particles and acoustic waves are in fact the result of electromagnetic phenomena because lattice vibrations and the repulsion between colliding molecules are caused by the van der Waals intermolecular forces, which are essentially electrostatic forces between electrically neutral molecules with non-vanishing dipole moments [15]. Although this observation suggests that all types of heat transport are associated with electromagnetism, it is nevertheless useful and common to distinguish thermal radiation as the process where the energy is carried directly by electromagnetic waves from other mechanisms where the energy is carried by moving particles which interact with the assistance of electromagnetic forces.

3 Electromagnetic energy carriers

To study heat transport by means of electromagnetic waves it is convenient to adopt the point of view that electrical charges do not directly interact with each other, but instead interact with the electromagnetic field. Thus, the radiation of energy by a particle may be considered as the process whereby an oscillator passes some of its energy to the electromagnetic field, and the absorbtion of energy may be considered as the process by which an oscillator takes energy from the electromagnetic field. From this point of view the energy concentrated in a spatial domain G consists of two forms: the energy of the particles located in G, and the energy of the electromagnetic field in this domain. As a result, the analysis of radiative heat transport can be reduced to the analysis of ensembles of electromagnetic fields in the considered domain, which can be considered without regards to the sources of these fields.

It is well known [13, 17, 21] that electromagnetic energy is evenly divided between two fields with different polarizations, and that each of these fields can be described by the equation

$$\frac{1}{c^2}\frac{\partial^2\Phi}{\partial t^2} = \nabla^2\Phi, \qquad c = \frac{1}{\sqrt{\epsilon\mu}}, \tag{3.1}$$

where c is the speed of light in the material with permittivity ϵ and permeability μ. If the electromagnetic field is localized in some domain G then the theory of partial differential equations implies [7] that any solution of equation (3.1), accompanied by appropriate boundary conditions, can be represented as a superposition

$$\Phi(\vec{r}, t) = \sum_{m,j} u_{mj}(\vec{r})\mathrm{e}^{-\mathrm{i}\omega_m t} \tag{3.2}$$

where $\vec{r} = (x, y, z)$ is the position vector of the observer, ω_m is the spectral frequency which takes one of the values determined by the shape of the domain G and by the boundary conditions, and $u_{mj}(\vec{r})$, where $j = 1, 2, \ldots$, are independent solutions of the Helmholtz equation $\nabla^2 u + (\omega/c)^2\, u = 0$, with the spectral frequency $\omega = \omega_m$. The set of all spectral frequencies is referred to as the spectrum, and the fields $u_{mj}(\vec{r})$, where $j = 1, 2, \ldots$, are referred to as eigenfields, or normal modes, corresponding to ω_m. The number of eigenfields corresponding to a spectral frequency ω_m depends on the frequency, and it may be infinite. If the domain G is unbounded then it may have a continuous spectrum and each spectral frequency may correspond to a continuum of eigenfields, so that the summations in (3.2) may be replaced by integrations.

In general, it may be extremely difficult to describe the spectrum of an arbitrary domain and to compute the corresponding eigenfields. However, in the idealized case when G consists of two half-spaces $x < 0$ and $x > h$ separated by a vacuum layer $0 < x < h$, both of these problems have tractable solutions, which admit many different representations. For example, the wave equation (3.1) can be satisfied by a field

$$\Phi(\vec{r},t;\omega,\vec{e}) = \begin{cases} u_-(\vec{r},\omega,\vec{e})\mathrm{e}^{-\mathrm{i}\omega t}, & \text{if} \quad x<0, \\ u_+(\vec{r},\omega,\vec{e})\mathrm{e}^{-\mathrm{i}\omega t}, & \text{if} \quad x>h, \\ u_0\,(\vec{r},\omega,\vec{e})\mathrm{e}^{-\mathrm{i}\omega t}, & \text{if} \quad 0<x<h, \end{cases} \tag{3.3}$$

where the frequency $\omega \geq 0$ may take any non-negative value, and

$$\begin{aligned} u_-(\vec{r},\omega,\vec{e}) &= A_-(\omega,\vec{e})\mathrm{e}^{\mathrm{i}(d_x x+d_y y+d_z z)\omega/c_-} + B_-(\omega,\vec{e})\mathrm{e}^{\mathrm{i}(-d_x x+d_y y+d_z z)\omega/c_-}, \\ u_+(\vec{r},\omega,\vec{e}) &= A_+(\omega,\vec{e})\mathrm{e}^{\mathrm{i}(e_x x+e_y y+e_z z)\omega/c_+} + B_+(\omega,\vec{e})\mathrm{e}^{\mathrm{i}(-e_x x+e_y y+e_z z)\omega/c_+}, \end{aligned} \tag{3.4}$$

are superpositions of plane waves propagating along the directions determined by the unit vectors $\vec{e} = (e_x, e_y, e_z)$ and $\vec{d} = (d_x, d_y, d_z)$ with the components

$$\begin{aligned} d_x &= \cos\theta_-, \quad d_y = \sin\theta_-\cos\phi_-, \quad d_z = \sin\theta_-\sin\phi_-, \\ e_x &= \cos\theta_+, \quad e_y = \sin\theta_+\cos\phi_+, \quad e_z = \sin\theta_+\sin\phi_+, \end{aligned} \tag{3.5}$$

defined in terms of the spherical angles $\theta_\pm$ and $\phi_\pm$ connected by the Snell's law

$$c_+\sin\theta_- = c_-\sin\theta_+, \qquad \phi_+ = \phi_-. \tag{3.6}$$

As for the field $u_0(\vec{r},\omega,\vec{e})$ inside the gap, it has a structure similar to that of $u_\pm(\vec{r},\omega,\vec{e})$, but it is not specified here because it does not play any role in the subsequent analysis.

In the formulas (3.4) the frequency ω, the direction $\vec{e}_+$ and the pair of coefficients (A_+, B_+) can take arbitrary values, and the other pair (A_-, B_-) is determined by the formula

$$\begin{pmatrix} A_- \\ B_- \end{pmatrix} = \mathbb{T}\begin{pmatrix} A_+ \\ B_+ \end{pmatrix}, \tag{3.7}$$

where

$$\mathbb{T} = \begin{pmatrix} 1 & \bar{R} \\ R & 1 \end{pmatrix}\begin{pmatrix} K & 0 \\ 0 & \bar{K} \end{pmatrix}^{-1} \equiv \begin{pmatrix} 1/K & \bar{R}/\bar{K} \\ R/K & 1/\bar{K} \end{pmatrix} \tag{3.8}$$

is the transmission matrix determined in terms of the reflection and transmission coefficients R and K of the gap, which may be viewed as the "cumulative" characteristics of the gap determining all of its influence on wave propagation in the entire structure.

The reflection and transmission coefficients of the vacuum gap can easily be computed by the method of multiple reflections from the theory of wave propagation in layered media, which is so thoroughly described in the literature [2,10], that for our purposes it suffices to reduce the discussion to a brief summary of the results which are necessary for understanding our further developments.

Consider first the interface between two materials "a" and "b" with the speeds of wave propagation c_a and c_b, respectively. Let R_{ab} and K_{ab} be the reflection and transmission coefficients of an incident wave that arrives at the interface from the side "a" with the incidence angle θ_a and is transmitted to the wave propagating in the domain "b" with the angle θ_b determined by the Snell's law $c_b \sin\theta_a = c_a \sin\theta_b$. Then, using Fresnel formulas [23, Eqs: (7-7-13),(7-7-15)] we find that

$$R_{ab} = \begin{cases} \dfrac{c_a \cos\theta_a - c_b \cos\theta_b}{c_b \cos\theta_b + c_a \cos\theta_a}, & (\|\text{-polarization}), \\ \dfrac{c_b \cos\theta_a - c_a \cos\theta_b}{c_b \cos\theta_a + c_a \cos\theta_b}, & (\perp\text{-polarization}), \end{cases} \tag{3.9}$$

and

$$K_{ab} = \begin{cases} \dfrac{2c_b \cos\theta_a}{c_b \cos\theta_b + c_a \cos\theta_a}, & (\|\text{-polarization}), \\ \dfrac{2c_b \cos\theta_a}{c_b \cos\theta_a + c_a \cos\theta_b}, & (\perp\text{-polarization}), \end{cases} \tag{3.10}$$

where the electromagnetic field is said to have a parallel, or "$\|$", polarization if its electric component is parallel to the plane of incidence, and it has a perpendicular, or "$\perp$", polarization if its electric component is perpendicular to the plane of incidence.

To consider a system of two half-spaces $x < 0$ and $x > h$ occupied by different materials and separated by a vacuum gap $0 < x < h$ we assume that R_- and K_- are the reflection and transmission coefficients of the interface between the left material and the vacuum, which are represented by the formulas (3.9) and (3.10) where the indices "a" and "b" are replaced by "$-$" and "0", respectively. Similarly, R_+ denotes the reflection coefficient of a wave arriving from the right material at the interface between it and the vacuum, and K'_+ denotes the transmission coefficient from the vacuum to the material in $x > h$. Then, the method of multiple reflections [2, 10] implies that the reflection and transmission coefficients from the domain $x < 0$ to the domain $x > h$ are delivered by the expressions

$$R = R_- - \frac{R_+(1 - R_-^2)\mathrm{e}^{2\mathrm{i}\chi_h}}{1 - R_- R_+ \mathrm{e}^{2\mathrm{i}\chi_h}}, \qquad K = \frac{K_- K'_+ \mathrm{e}^{\mathrm{i}\delta_h}}{1 - R_- R_+ \mathrm{e}^{2\mathrm{i}\chi_h}}, \tag{3.11}$$

where

$$\chi_h = h\omega \frac{\cos\theta_0}{c_0}, \qquad \delta_h = h\omega \left(\frac{\cos\theta_0}{c_0} - \frac{\cos\theta_+}{c_+} \right), \tag{3.12}$$

are the phase shifts caused by wave propagation inside the gap.

It is useful to observe that the expressions (3.11) provide meaningful asymptotes of the reflection coefficient of the vacuum gap between identical materials. Thus, assuming that $c_- = c_+ \equiv c$ we can derive from (3.9) and (3.10) the identities

$$\theta_- = \theta_+ \equiv \theta, \qquad R_- = R_+, \qquad K_- K'_- = 1 - (R_-)^2, \tag{3.13}$$

which leads to the simplified expressions

$$R = \frac{R_-\big(1 - \mathrm{e}^{2\mathrm{i}h\cos\theta\omega/c_0}\big)}{1 - R_-^2 \mathrm{e}^{2\mathrm{i}h\cos\theta\omega/c_0}}, \qquad K = \frac{\big(1 - R_-^2\big)\mathrm{e}^{\mathrm{i}h(\cos\theta_0 - \cos\theta)\omega/c_0}}{1 - R_-^2 \mathrm{e}^{2\mathrm{i}h\cos\theta\omega/c_0}}. \tag{3.14}$$

Then, letting $h \to 0$, we see that the first formula in (3.11) reduces to the asymptote

$$R \approx 2\mathrm{i}r_- h \cos\theta\omega/c_0, \tag{3.15}$$

which shows that the reflection coefficient of a narrow gap between identical materials vanishes proportionally to the width h.

4 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. 2 where equal masses m are connected by identical springs with the elastic modulus γ and equilibrium spacing $a > 0$.

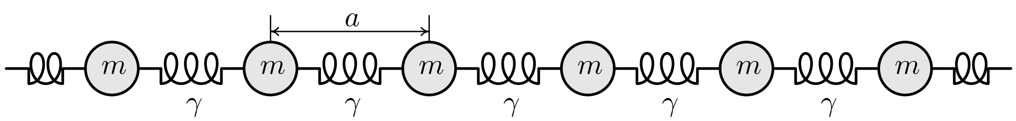


Figure 2: Simple chain.

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

$$m\gamma \frac{\mathrm{d}^2\xi(t,x_n)}{\mathrm{d}t^2} = \frac{\gamma}{a}\big[\xi(t,x_{n+1}) + \xi(t,x_{n-1}) - 2\xi(t,x_n)\big], \qquad x_n = an. \tag{4.1}$$

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

$$\frac{1}{c^2}\frac{\mathrm{d}^2\xi(t,x)}{\mathrm{d}t^2} = \nabla^2\xi(t,x), \tag{4.2}$$

where x is a continuous coordinate, and

$$c = \sqrt{\frac{a\gamma}{m}} = \sqrt{\frac{\gamma}{\rho}}, \tag{4.3}$$

is the sound speed determined by the elastic modulus γ and the mass density ρ 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 with different mass densities and elastic moduli separated by a narrow, but non-vanishing gap.

Next consider the chain shown in Fig. 3 where the masses m_- are located at the nodes $x_n = an$ with $n < 0$ and the masses m_+ are located at the nodes $x_n = h + an$, where $n \geq 0$, and $h > 0$ is an additional parameter that may be viewed as 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

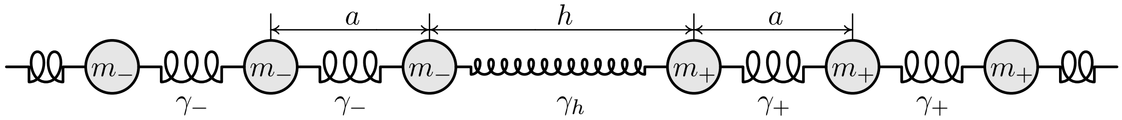


Figure 3: Two separated chains

$x > h$ have the elastic moduli γ_- and γ_+, respectively, and that the spring connecting the nodes x_{-1} and x_0 has the elastic modulus γ_h.

The motion of this chain is described by (4.1), which controls the motion of all particles with $n \neq -1$ and $n \neq 0$, and by the additional equations

$$\begin{aligned} n = 1: \qquad & m_- \frac{\mathrm{d}^2\xi(t,0)}{\mathrm{d}t^2} = \frac{\gamma_h}{h}\big[\xi(t,h) - \xi(t,0)\big] + \frac{\gamma_-}{a}\big[\xi(t,-a) - \xi(t,0)\big], \\ n = 0: \qquad & m_+ \frac{\mathrm{d}^2\xi(t,h)}{\mathrm{d}t^2} = \frac{\gamma_h}{h}\big[\xi(t,0) - \xi(t,h)\big] + \frac{\gamma_+}{a}\big[\xi(t,h+a) - \xi(t,h)\big], \end{aligned} \tag{4.4}$$

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 $a \to 0$, while the distance h between the half-chains remains finite. Then, representing the masses $m_\pm$ as $m_\pm = \rho_\pm a$, where $\rho_\pm$ are the mass-densities of the continuous half-chains, and passing to the limit $a \to 0$ we observe that equations (4.4) reduce to the interface conditions

$$\gamma_- \frac{\partial \xi(t,x)}{\partial x}\bigg|_{x=0} = \gamma_+ \frac{\partial \xi(t,x)}{\partial x}\bigg|_{x=h} = \gamma_h\, \frac{\xi(t,h) - \xi(t,0)}{h}, \tag{4.5}$$

which compliment equation (4.2) describing the motions in the domains $x < 0$ and $x > h$.

It is obvious from (4.5) that if the interconnection $0 < x < h$ is very strong in the sense that $\gamma_h/h \to \infty$ then the two interface conditions (4.5) reduce to the single condition

$$\xi(t,h) = \xi(t,0), \tag{4.6}$$

which implies that the boundary surfaces $x = 0$ and $x = h$ are firmly attached to each other so that the motion of one of them exactly reproduces the motion of another.

In the opposite limiting case of a very weak interconnection when $\gamma_h/h \to 0$, the interface conditions (4.5) reduce to two Neumann boundary conditions

$$\frac{\partial \xi}{\partial x}\bigg|_{x=0} = 0, \qquad \frac{\partial \xi}{\partial x}\bigg|_{x=h} = 0, \tag{4.7}$$

which effectively disconnect the motions in the domains $x < 0$ and $x > h$ so that the motion in each of them is described by the wave equation (4.2) with the Neumann boundary condition.

The one-dimensional mass-spring models discussed above admit generalizations to arbitrary three-dimensional lattices converging, in the continuum limit, to any feasible anisotropic elastic medium which supports the propagation of three different elastic waves with different wave speeds. However, in many common situations it suffices to use Debye's approximation [11, 18], which treats any heat-conducting solid medium as an isotropic continuum supporting propagation of three similar acoustic waves described by the scalar wave equation (4.2) with the wave speed v determined by the mechanical properties of the solid material.

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

$$\rho \frac{\partial^2 \vec{\xi}}{\partial t^2} = -\vec{\nabla} p, \tag{4.8}$$

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 $x > h$ illustrated in Fig. 4 must obey the interface conditions

$$\gamma \left.\frac{\partial^2 p}{\partial x^2}\right|_{x=0} = \gamma \left.\frac{\partial^2 p}{\partial x^2}\right|_{x=h} = \frac{\gamma_h}{h} \left(\left.\frac{\partial p}{\partial x}\right|_{x=h} - \left.\frac{\partial p}{\partial x}\right|_{x=0} \right) \tag{4.9}$$

which generalizes (4.5) and takes into account (4.8).

To use these interface conditions it is necessary to compute the elastic modulus γ_h of the vacuum gap of width h.

Let h be so large compared to the distance between atoms that the interaction between the half-spaces can be treated macroscopically, as an interaction between two continuum media. Then, γ_h can be estimated by the formula

$$\gamma_h = h \left| \frac{\mathrm{d}F}{\mathrm{d}h} \right|, \tag{4.10}$$

were $F(h)$ is the force of interaction between the half-spaces separated by the distance h. This force is computed in [16, §90] by a rather complex method which generates simple asymptotes in two opposite limiting cases $h \gg \lambda_0$ and $h \ll \lambda_0$, where λ_0 is the dominant wavelength of the thermal electromagnetic radiation. As shown in [16, §90], in the first case $F(h)$ has the asymptote

$$F(h) \approx \frac{C_\infty}{h^4}, \qquad C = \frac{\hbar c \pi^2}{240} D_\infty, \qquad h \gg \lambda_0, \tag{4.11}$$

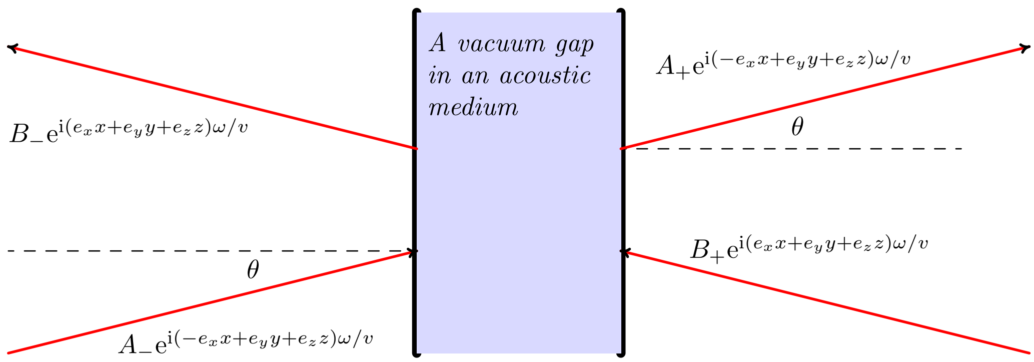
where D_∞ depends on the materials: if both half-spaces are metals then $D_\infty = 1$ and (4.11) coincides with the Casimir force between separated half-spaces [6, 16, 19, 20]. In the case when both half spaces are identical dielectrics, D can be approximated by the formulas [16, Eqs. (90.7), (90.9)]. In the second case of $h \ll \lambda_0$, the force does not depend on the material and has the asymptote

$$F \approx \frac{C_0}{h^3}, \qquad C_0 = \frac{\hbar}{16\pi^2} D_0, \qquad h \ll \lambda_0, \tag{4.12}$$

where D_0 is a constant determined by [16, Eq. (90.4)]. Correspondingly, the modulus γ_h is estimated by the formulas

$$\gamma_h = \begin{cases} \dfrac{4C_\infty}{h^4}, & h \gg \lambda_0 \approx 500 \text{ nm}, \\ \dfrac{3C_0}{h^3}, & h \ll \lambda_0 \approx 500 \text{ nm}, \end{cases} \tag{4.13}$$

where the estimate $\lambda_0 \approx 500\,\text{nm}$ shows the range of applicability of these formulas. If the width of the gap is comparable to the dominant wavelength of the acoustic waves λ_0, then the Casimir force between the half-spaces can be computed by more complex expressions discussed in detail in [6, 16, 19, 20], but the results obtained below show that such expressions are not needed because the contribution of acoustic waves to heat transport is noticeable only when the gap is significantly narrower that λ_0.



Acoustic waves do not propagate in a vacuum gap but a narrow gap provides coupling between waves propagating on its different sides. In particular, it determines the transmission matrix $\mathbb{T}(\vec{e})$ connecting the amplitudes (A_-, B_-) and (A_+, B_+) of coupled pairs of plane waves propagating on different sides of the gap along the direction $\vec{e}$.

Figure 4: Coupling of waves propagating on the different sides of a gap

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

$$p(t, \vec{r}; \omega, \vec{e}) = \begin{cases} A_- e^{i(d_x x + d_y y + d_z z)\omega/c_- - i\omega t} + B_- e^{i(-d_x x + d_y y + d_z z)\omega/c_- - i\omega t}, & \text{if} \quad x < 0, \\ A_+ e^{i(e_x x + e_y y + e_z z)\omega/c_+ - i\omega t} + B_+ e^{i(-e_x x + e_y y + e_z z)\omega/c_+ - i\omega t}, & \text{if} \quad x > h, \end{cases} \tag{4.14}$$

which have the same mathematical structure as the electromagnetic fields (3.4). The fields (4.14) always satisfy equation (4.2), but to satisfy the interface conditions (4.5) the amplitudes $A_\pm$ and $B_\pm$ must satisfy the following conditions

$$\begin{aligned} \gamma_+ \left(\frac{ie_x\omega}{c_+}\right)^2 \left(A_+^h + B_+^h\right) &= \gamma_- \left(\frac{id_x\omega}{c_-}\right)^2 \left(A_- + B_-\right), \\ \gamma_+ \left(\frac{ie_x\omega}{c_+}\right)^2 \left(A_+^h + B_+^h\right) &= \frac{\gamma_h}{h} \left\{ \frac{ie_x\omega}{c_+} \left(A_+^h - B_+^h\right) - \frac{id_x\omega}{c_-} \left(A_- - B_-\right) \right\}, \end{aligned} \tag{4.15}$$

where

$$A_+^h = A_+ e^{ie_x h\omega/c_+}, \qquad B_+^h = B_+ e^{-ie_x h\omega/c_+}. \tag{4.16}$$

It is obvious that if $\gamma_h = 0$, which means that the half-spaces $x < 0$ and $x > h$ are disconnected, then the last equations imply that

$$A_- = -B_-, \qquad A_+ \mathrm{e}^{\mathrm{i}e_x h\omega/c} = -B_+ \mathrm{e}^{-\mathrm{i}e_x h\omega/c}, \tag{4.17}$$

and that the pairs (A_-, B_-) and (A_+, B_+) are independent of each other. However, if $\gamma_h \neq 0$ then equations (4.15) can be reduced to the form

$$\begin{pmatrix} A_- \\ B_- \end{pmatrix} = \mathbb{T}_h \begin{pmatrix} A_+^h \\ B_+^h \end{pmatrix}. \tag{4.18}$$

where $\mathbb{T}_h$ is a matrix that can be computed as follows. First, we write (4.15) as

$$\begin{aligned} A_- + B_- &= \hat{\gamma}\hat{c}^2 A_+ + \hat{\gamma}\hat{c}^2 B_+, \\ A_- - B_- &= \hat{c}\,(1 - \mathrm{i}s)\, A_+^h - \hat{c}\,(1 + \mathrm{i}s)\, B_+^h \end{aligned} \tag{4.19}$$

where

$$\hat{\gamma} = \frac{\gamma_+}{\gamma_-}, \qquad \hat{c} = \frac{c_- \cos\theta_+}{c_+ \cos\theta_-}, \qquad s = \pi \frac{h}{\lambda_+} \frac{\gamma_+}{\gamma_h} \cos\theta_+, \tag{4.20}$$

are three dimensionless parameters, and

$$\lambda = \frac{2\pi c_+}{\omega}, \tag{4.21}$$

is the wavelength in the right half-space $x > h$. Then we obtain the expressions

$$\begin{aligned} 2A_- &= \hat{c}\,\{\hat{\gamma}\hat{c} + 1 - \mathrm{i}s\ \}\, A_+^h + \hat{c}\,\{\hat{\gamma}\hat{c} - 1 - \mathrm{i}s\ \}\, B_+^h, \\ 2B_- &= \hat{c}\,\{\hat{\gamma}\hat{c} - 1 + \mathrm{i}hs\}\, A_+^h + \hat{c}\,\{\hat{\gamma}\hat{c} + 1 + \mathrm{i}hs\}\, B_+^h, \end{aligned} \tag{4.22}$$

from which it follows that

$$\mathbb{T}_h = \frac{\hat{c}}{2} \begin{pmatrix} 1 + \hat{\gamma}\hat{c} - \mathrm{i}s & 1 - \hat{\gamma}\hat{c} - \mathrm{i}s \\ 1 - \hat{\gamma}\hat{c} + \mathrm{i}s & 1 + \hat{\gamma}\hat{c} + \mathrm{i}s \end{pmatrix}. \tag{4.23}$$

After the equations (4.18) are established, they can be converted to the form

$$\begin{pmatrix} A_- \\ B_- \end{pmatrix} = \mathbb{T} \begin{pmatrix} A_+ \\ B_+ \end{pmatrix}. \tag{4.24}$$

where

$$\mathbb{T} = \begin{pmatrix} 1 + \hat{\gamma}\hat{c} - \mathrm{i}s & 1 - \hat{\gamma}\hat{c} - \mathrm{i}s \\ 1 - \hat{\gamma}\hat{c} + \mathrm{i}s & 1 + \hat{\gamma}\hat{c} + \mathrm{i}s \end{pmatrix} \cdot \begin{pmatrix} \mathrm{e}^{2\pi\mathrm{i}h\cos\theta/\lambda} & 0 \\ 0 & \mathrm{e}^{-2\pi\mathrm{i}h\cos\theta/\lambda} \end{pmatrix}, \tag{4.25}$$

is the matrix which directly connects the coefficients (A_-, B_-) and (A_+, B_+).

It is easy to see that $\mathbb{T}$ admits representation in the form

$$\mathbb{T} = \begin{pmatrix} 1/K & \bar{R}/\bar{K} \\ R/K & 1/\bar{K} \end{pmatrix}, \tag{4.26}$$

which coincides with (3.8), where the coefficients K and R here take the values

$$K = \frac{2\mathrm{e}^{-2\pi\mathrm{i}h\cos\theta/\lambda}}{\hat{c}(1 + \hat{\gamma}\hat{c} - \mathrm{i}s)}, \qquad R = \frac{1 - \hat{\gamma}\hat{c} + \mathrm{i}s}{1 + \hat{\gamma}\hat{c} - \mathrm{i}s}. \tag{4.27}$$

This shows that K and R from (4.28) have the meanings of the transmission and reflection coefficients of the considered system of two separated half-spaces which exert on each other a mechanical force with the elastic modulus γ_h.

It is worth mentioning that in certain special case the last formulas can be reduced to transparent asymptotes. Thus, if the half-spaces $x < 0$ and $x > h$ are occupied by identical materials, then these formulas reduce to the form

$$K = \frac{\lambda\gamma_h \mathrm{e}^{-2\pi \mathrm{i} h \cos\theta_+/\lambda}}{\lambda\gamma_h - \mathrm{i}\pi\gamma_+ h \cos\theta_+}, \qquad R = \frac{\mathrm{i}\pi\gamma_h \cos\theta_+}{\lambda\gamma_h - \mathrm{i}\pi\gamma_+ h \cos\theta_+}. \tag{4.28}$$

Then, assuming that the gap is so narrow compared to the wavelength that

$$\frac{\gamma}{\gamma_h}\frac{h}{\lambda}\cos\theta \ll 1, \tag{4.29}$$

we obtain the estimates

$$|K|^2 \approx 1, \qquad |R|^2 \approx \left(\frac{\pi\gamma h \cos\theta}{\gamma_h \lambda}\right)^2, \tag{4.30}$$

which not only agree with the expectation that a vanishing width gap between identical media has full transmission and no reflection, but also show that as the gap narrows the amount of reflected energy decreases proportionally to the square of its width. In the opposite case of a wide gap

$$\frac{\gamma}{\gamma_h}\frac{h}{\lambda}\cos\theta \gg 1, \tag{4.31}$$

we get the estimates

$$|K|^2 \approx \left(\frac{\gamma_h \lambda}{\pi\gamma h \cos\theta}\right)^2, \qquad |R|^2 \approx 1, \tag{4.32}$$

which confirm that a wide gap has full reflection and zero transmission.

5 Discussion and conclusion

The developments in the previous sections imply that although heat in a system of dielectric half-spaces separated by a vacuum gap can be carried by both acoustic and electromagnetic waves, the relative importance of these two types of waves is determined by the gaps's width.

Thus, since electromagnetic waves can freely propagate in a vacuum, the electromagnetic fields in both half-spaces are not independent of each other regardless of the gap's width, and they should be considered as parts of a field distributed in the entire composite space. Mechanical waves can not propagate across gaps unless they are only a few nanometers wide, but on the other hand, when they do propagate they are capable of carrying much more energy than electromagnetic waves. This suggests that heat transport across a vacuum gap strongly depends on the gap's width. In particular, when the gap is wider than tens of nanometers then electromagnetic radiation remains the sole heat carrier, but when the gap is sufficiently narrow acoustic waves become the dominant hear carriers.

Since the transmission matrices of the electromagnetic and acoustic waves depend on the gap's width h, the transport properties of each of these waves also depend on h. However, before discussing the properties of each individual type of carrier, it is worth clarifying under which circumstances the heat is carried mostly by acoustic waves, by electromagnetic waves, or by both.

First we obtain an order-of-magnitude estimate of the the maximal heat flux that can be carried by electromagnetic radiation.

According to [18, Eqn.(63.14)] the average energy density of an ensemble of electromagnetic fields in equilibrium with a material at absolute temperature T has the value

$$E_{EM} \approx \frac{4\sigma}{c_0} T^4 \tag{5.1}$$

where c_0 is the speed of light, and

$$\sigma = \frac{\pi^2 \kappa_B^4}{60 \hbar^3 c_0^2} = 5.67 \cdot 10^{-8} \left(\frac{\mathrm{W}}{\mathrm{m}^2 \mathrm{K}^4} \right) \tag{5.2}$$

is the Stephan-Boltzmann constant. Correspondingly, the maximal heat flux that can be carried by electromagnetic radiation is estimated as

$$Q_{EM} \approx 4\sigma T^4 \approx 1.84 \cdot 10^3 \left(\frac{\mathrm{W}}{\mathrm{m}^2} \right). \tag{5.3}$$

Next we estimate the maximal energy flux that can be carried by acoustic waves.

Using [18, §66] we find that the energy density of a solid can be estimated as

$$E_{Ac} \approx 3 N_{atoms} \kappa_B T D(\Theta/T), \tag{5.4}$$

where $\kappa_B = 1.38 \cdot 10^{-23}\,(\mathrm{W} \cdot \mathrm{s/K})$ is the Boltzmann constant, T is the temperature, Θ is the Debye temperature of the material, and

$$D(x) = \frac{3}{x^3} \int_0^x \frac{\xi^3 \mathrm{d}\xi}{\mathrm{e}^\xi - 1} \tag{5.5}$$

is the Debye function. N_{atoms} is the number of atoms per unit volume, which can be computed as

$$N_{atoms} = \frac{\rho}{A_r \cdot u_a}, \qquad u_a = 1.66 \cdot 10^{-27}\,(\mathrm{kg}), \tag{5.6}$$

where ρ is the mass density of the material, A_r is its atomic weight and u_a is the unified atomic mass unit, which is essentially the weight of a single proton.

Assuming that the mass density, atomic weight and Debye temperature of silicon have the values $\rho = 2.57 \cdot 10^3 \mathrm{kg/m^3}$, $A_r = 28$, and $\Theta = 645\,\mathrm{K}$, we find that at room temperature $T = 300\,\mathrm{K}$

$$N_{atoms} \approx 5.53 \cdot 10^{28}, \qquad D(\Theta/T) \approx 1.96, \tag{5.7}$$

which imply that the energy density of thermally excited acoustic waves in silicon at $T = 300\,\mathrm{K}$ is of the order

$$E_{Ac} \approx 1.34 \cdot 10^9 \left(\frac{\mathrm{W} \cdot \mathrm{s}}{\mathrm{m}^3} \right). \tag{5.8}$$

Then, multiplying this number by the speed of sound in silicon $c = 2200\,\mathrm{m/s}$, we find that the maximal possible heat flux carried by acoustic waves in silicon at room temperature is of the order

$$Q_{Ac} \approx 2.96 \cdot 10^{12} \ \left(\frac{\mathrm{W}}{\mathrm{m}^2}\right). \tag{5.9}$$

The last number is much higher than the maximal heat flux carried by electromagnetic waves (5.3) but it characterizes the heat carrying ability of acoustic waves in a continuous medium. To estimate the contribution of acoustic waves to heat transport across a gap we need to multiply Q_{Ac} by the square of the transmission coefficient $|K|^2$ of the vacuum gap represented by (4.28).

If the characteristic wavelength λ of the acoustic waves is smaller than the gaps's width h, then $|K|^2$ has the order

$$|K|^2 \approx \frac{\gamma_h^2}{\gamma^2} \frac{\lambda^2}{h^2}, \tag{5.10}$$

which depends on the ratio γ_h/γ of the elastic constants of the gap and the continuum and on 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

$$\gamma_h = \gamma \left(\frac{h_0}{h}\right)^3, \tag{5.11}$$

which agrees with the second line of (4.13). Combining the last two formulas we estimate $|K|^2$ as

$$|K|^2 \approx \left(\frac{h_0}{h}\right)^6 \left(\frac{\lambda}{h}\right)^2 = \left(\frac{h_0}{h}\right)^8 \left(\frac{\lambda}{h_0}\right)^2, \tag{5.12}$$

and multiplying this by Q_{Ac} we find that the maximum flux that can be carried by acoustic waves across a gap of width h between silicon half-spaces has the order of

$$Q_{Ac}^h \approx Q_{Ac} \left(\frac{h_0}{h}\right)^8 \left(\frac{\lambda}{h_0}\right)^2, \tag{5.13}$$

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

Now we can estimate the critical 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

$$Q_{Ac} \left(\frac{h_0}{h_*}\right)^8 \left(\frac{\lambda}{h_0}\right)^2 = Q_{EM}, \tag{5.14}$$

which leads to the estimate

$$h_* \approx h_0 \left(\frac{Q_{Ac}}{Q_{EM}}\right)^{1/8} \left(\frac{\lambda}{h_0}\right)^{1/4} \approx 14.2\, h_0 \left(\frac{\lambda}{h_0}\right)^{1/4}. \tag{5.15}$$

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

$$h_* \approx 4.78\,\text{nm}. \tag{5.16}$$

The above estimates show that although heat can be carried across a gap by electromagnetic and acoustic waves, in most cases one of these two heat carriers contributes significantly less that the other and therefore can be neglected. 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 unless the width of the gap h belongs to the band between $0.5h_* < h < 1.5h_*$, which is narrower than a 5nm band in the considered case (5.16), then most of the heat is transported across the gap by only one type of waves.

Since acoustic and electromagnetic waves are described by similar mathematical equations, the analysis of heat transport across narrower and wider gaps can be performed by similar methods, based on the explicit representation of the corresponding wave fields in the considered sandwich-like structure with two half-spaces separated by a gap of width h.

However, due to the considerable difference between the typical wavelengths of thermally excited electromagnetic and acoustic waves, it is possible that other techniques may sometimes be invoked.

Consider first a wide gap of width considerably exceeding the wavelength $\lambda \approx 400$–800 nm of thermally radiated electromagnetic waves at room temperature. In this case, corresponding in Fig. 5 to the domain on the right of the waved line, acoustic waves can be ignored and electromagnetic fields can be represented in terms of wave packets which can be treated as particles [14], so that the radiative heat transport can legitimately be analyzed by the kinetic theory. This approach was well developed in times when several microns were considered a short distance, and it resulted in the Stefan-Boltzmann formula (1.1).

But, when the width of the gap is less than a few wavelengths of thermally excited electromagnetic waves, which is about $\lambda_* \approx 1500$nm at room temperature, the electromagnetic fields can not be represented in terms of wave packets that are small enough compared to the gap's width, and as a result, the Stefan-Boltzmann formula can not be used to describe the thermal flux across the gap. In this case, corresponding in Fig. 5 to the domain on the left side of the wavey line, to estimate the contribution of electromagnetic radiation to thermal transport it is necessary to take into account interference of the waves with their own reflections from the surfaces of the half-spaces, which may be done by use of the full wave theory similar to that developed in [3–5]. If the gap's width is below $1.5h_*$, which is about 7.5nm in the considered example, the contribution of acoustic waves must be taken into account. Assuming that the wavelength of acoustic waves is of order 1nm, it may be possible to estimate the contribution of the acoustic waves to heat transport across gaps with width in the range 4nm $\lesssim h \lesssim$ 7.5nm by the kinetic theory, but for narrower gaps with $h \lesssim$ 4nm this approximation is not legitimate, and the full wave theory, such as that developed in [3–5], must be used.

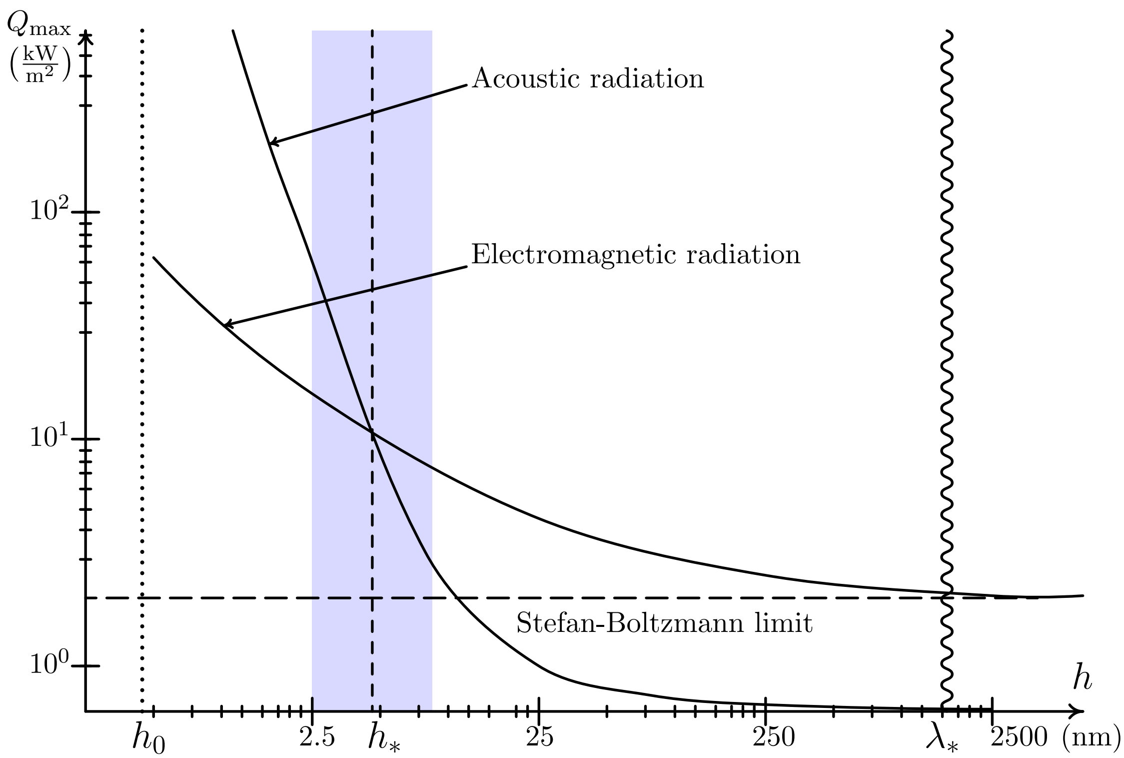


Figure 5: Maximal heat fluxes which may be carried by acoustic and electromagnetic fields

Finally, it should be mentioned, that both electromagnetic and acoustic heat carriers must be taken into account only for gaps having widths in the range between $0.5h_*$ ($\approx$ 2.5nm) and $1.5h_*$ ($\approx$ 7.5nm), which is the shaded strip in Fig. 5. For wider gaps acoustic waves can be neglected, and for narrower gaps there is no need to take into account electromagnetic radiation.

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