Heat transport by phonon tunneling across layered structures used in heat assisted magnetic recording (HAMR)

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Abstract

In this paper we analyze heat transport by acoustic waves in arbitrary layered structures that may include several vacuum layers. The analysis is based on our prior description of the spectrum of thermally excited waves in systems with a heat flux, and on the new approach to the coupling between acoustic fields in separated bodies and the description of the interference of thermally excited waves. The developed method predicts correct results for all known special cases for both large and closing gaps, agrees with available experiments, explains the phenomena of interface thermal resistance and of thermal rectification (asymmetry of thermal transport). Numerical examples demonstrate the applicability of the approach to the calculation of the heat transport coefficient across nanoscale gaps due to acoustic waves.

1 Introduction

The data density of hard drives is rapidly approaching a limit after which further increase cannot be achieved without radical modifications of the design that has been essentially evolutionary since 1956, when IBM unveiled its first HDD.

A significant change occurred recently by moving from the traditional parallel recording to perpendicular recording. However, this change alone is not sufficient for reaching the projected new data density levels of 10 Tb per square inch. It is expected that further increase in the data density of hard drives will require that a bit of recorded information occupy a spot on the disk smaller than 25 nm, and that this spot will get some form of energy assistance to lower the medium's coercivity to allow the write transducer to record the bit. In Heat Assistance Magnetic Recording (HAMR) systems such assistance is provided by local heating of the magnetic medium to its Curie temperature of about 400°C. Therefore, any HAMR system inevitably includes closely separated disks and read/write heads with different temperatures, and, consequently, the design of such systems must include the analysis of heat exchange between bodies separated by a few nanometers.

There are several mechanism of heat transport between bodies separated by a narrow air-gap: heat can be carried by electromagnetic radiation, by "phonon tunneling" caused by intermolecular interactions across the gap, and by heat conduction through the air. The first two of these mechanisms are related with the processes of electromagnetic and acoustic wave propagation, respectively.

Heat radiation across nanoscale gaps was studied in [1] by a novel method based on the extension of Planck's law from equilibrium systems to systems with a steady heat flux [2].

In [3, 4] this method was adapted to the analysis of heat transport across narrow gaps by acoustic waves, which was made possible by modeling the coupling of lattice vibrations in separated bodies through van der Waals/Casimir forces. This approach was further developed in [5], where the intermolecular forces causing phonon coupling were studied in more detail and the rates of heat transport by acoustic and electromagnetic waves between separated half-spaces of identical materials were compared.

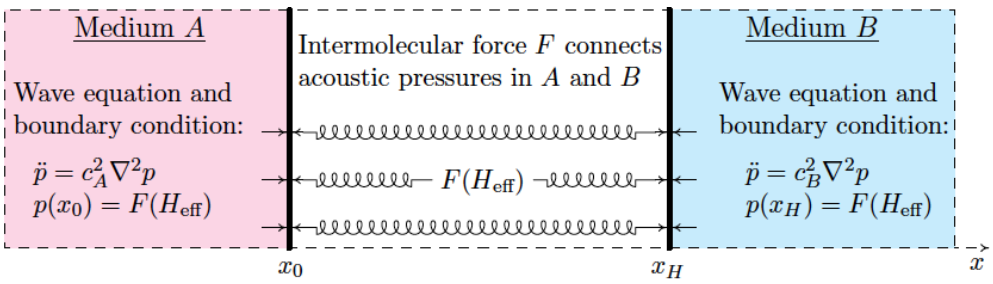
Here we expand the developments of [3, 4, 5] in several new directions. First, instead of a vacuum layer between two indentical half-spaces we consider arbitrary layered structures that may include several vacuum layers and have no restrictions on the materials in the different layers. In particular, the technique developed here is applicable to the analysis of interface thermal resistance between two contacting half-spaces. Another distinctive feature of this study is the formulation of the boundary value problem for acoustic fields in separated half-spaces that takes into account local variations of the width of the gap between them. Finally, unlike in previous studies, here we take into account the interference of thermally excited waves coming from different bodies. It is shown that such interference may significantly increase the heat transport and cause such effects as "thermal rectification", which is the asymmetry of heat transport in different directions.

The paper has three distinctively different parts. The first part develops a model that describes how the van der Waals forces between the molecules from different bodies separated by a narrow vacuum gap connect the acoustic field in these bodies. Then we compute the reflection coefficient of a plane acoustic wave from an arbitrary layered structure, which may include several vacuum gaps. Finally, we calculate the heat transport coefficient of some layered structures, that emulate those which appear in actual structures found in HAMR systems and in other nanoscale devices used for efficient thermal management.

2 A model of acoustic waves tunneling across a nanoscale gap

It is well recognized that heat conduction in solid dielectrics is mostly due to waves of molecular vibrations. These vibrations are supported by intermolecular forces that keep molecules near their equilibrium positions inside a material body. However, such forces are not restricted to be within a material, indeed they can also act across vacuum gaps, implying that they can carry heat across such gaps.

To illustrate how acoustic waves can carry heat across a gap, it suffices to consider the model shown in Fig. 1 where two material half-spaces $x < 0$ and $x > H$ are separated by a vacuum gap $0 < x < H$, whose faces are maintained near the equilibrium positions $x = 0$ and $x = H$ by some external force. Due to thermally excited lattice vibrations in the half-spaces, their faces experience small displacements making the separation between the faces not exactly the constant value H. On the other hand, since intermolecular forces have a rather long range (tens of nanometers), the motion of the atoms near the surface in a body may exert noticeable forces on molecules at distances as far as several microns outside the body [6, 7]. Therefore, lattice vibrations in slightly separated bodies interact and can transfer energy between bodies without their direct contact.



Since the displacements caused by acoustic waves are small compared to the width of the gap, the surfaces of the half spaces may be considered as flat, and the intermolecular force between half-spaces may be considered to be orthogonal to their faces. This force couples acoustic fields in separated media and thus provide heat transport.

Figure 1: A model of interaction of two acoustic media through a narrow gap

To develop the outlined concept of thermal interaction between separated bodies it is necessary to adopt some simplifying assumptions about the lattice vibrations. First, we assume that the materials are isotropic, homogeneous and can be described by a linear theory of elasticity that considers the averaged characteristics of atomic motion computed over microscopic domains containing sufficiently large numbers of atoms. This theory implies the existence of three types of elastic waves: longitudinal waves propagating with the speed c_p and two kinds of transverse waves with the lower speed c_s. Waves of different polarizations propagate inside the media independently of each other, but they strongly interact at the boundaries causing significant complications of the total picture of wave propagation. To eliminate difficulties caused by the boundary interactions of the different kinds of elastic waves, we follow a common practice and describe the thermal properties of solids in terms of the simpler Debye model, which assumes that all three types of thermally excited waves are entirely independent of each other, have their frequencies in the band

$$0 < \omega < \omega_{\text{D}} \equiv \frac{\kappa T_D}{\hbar}, \tag{2.1}$$

where T_D is the Debye temperature, considered as a material parameter, and they propagate in a similar way as acoustic waves in a gas with the single wave speed c_{D} determined by the equation

$$\frac{1}{c_D^3} = \frac{1}{3}\left(\frac{1}{c_p^3} + \frac{2}{c_s^3}\right), \tag{2.2}$$

which presents $1/c_D^3$ as a weighted average of $1/c_p^3$ and $1/c_s^3$.

Acoustic waves with the speed c_{D} can be described in terms of a pressure p that satisfies the wave equation $\ddot{p} = c_D^2 \nabla^2 p$, and defines the acoustic displacement $\boldsymbol{\xi}$ by the formula $\ddot{\boldsymbol{\xi}} = -\boldsymbol{\nabla} p/\rho$, where ρ is the density of the medium in the unperturbed state [8].

In order to describe the oscillations of the surface layers of the half-spaces $x < 0$ and $x > H$ it is necessary to take into account the pressure on the open surfaces of these bodies caused by the van der Waals interatomic forces that originate from the across-gap body.

It is well known that the wavelengths of thermally excited elastic waves in common materials at room temperature are in the range 1–3nm. When such waves approach a plane surface $x = \text{const}$

with incidence angle θ then the surface displacements have wavelengths in the range from 1nm to infinity. Therefore, if the gap is narrower than 5nm then we can assume that it is narrower or comparable with the characteristic wavelength on the surfaces.

Let $\boldsymbol{x}_0$ and $\boldsymbol{x}_H = \boldsymbol{x}_0 + H\boldsymbol{e}_x$ be two points on the surfaces $x = 0$ and $x = H$ located directly across from each other. If H is comparable to or smaller than the characteristic wavelength on the surfaces, the force of interaction between unit areas of the surfaces around $\boldsymbol{x}_0$ and $\boldsymbol{x}_H$ may be approximated by the van der Waals force between the half-spaces separated by the effective distance

$$H_{\text{eff}} = H + \big\langle \xi(\boldsymbol{x}_H + \Delta\boldsymbol{x}) \big\rangle - \big\langle \xi(\boldsymbol{x}_0 + \Delta\boldsymbol{x}) \big\rangle, \qquad \Delta\boldsymbol{x} \perp \boldsymbol{e}_x \tag{2.3}$$

where $\xi(\boldsymbol{x})$ is the displacements along the x-axis of a point $\boldsymbol{x}$ located on one of the open surfaces, $\Delta\boldsymbol{x}$ is a an arbitrary vector parallel to $x = 0$, and $\big\langle \cdot \big\rangle$ denotes the averaging over $\Delta\boldsymbol{x}$ from an area with a radius of the order of H.

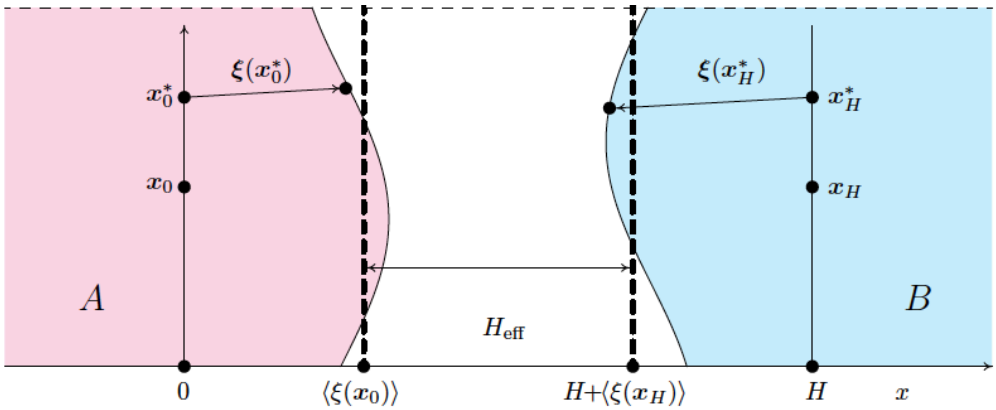
Since H is small in comparison with the wavelength on the surface, the averages in (2.3) and, subsequently, the effective distance (2.3) can be estimated as

$$\big\langle \xi(\boldsymbol{x}_H + \Delta\boldsymbol{x}) \big\rangle \approx \xi(\boldsymbol{x}_H) + \nu H^2 \nabla_\perp^2 \xi(\boldsymbol{x}_H), \quad \big\langle \xi(\boldsymbol{x}_0 + \Delta\boldsymbol{x}) \big\rangle \approx \xi(\boldsymbol{x}_0) + \nu H^2 \nabla_\perp^2 \xi(\boldsymbol{x}_0), \tag{2.4}$$

and

$$H_{\text{eff}} = H + \xi(\boldsymbol{x}_H) - \xi(\boldsymbol{x}_0) + \nu H^2 \left[\nabla_\perp^2 \xi(\boldsymbol{x}_H) - \nabla_\perp^2 \xi(\boldsymbol{x}_0) \right], \tag{2.5}$$

where $\nabla_\perp^2$ is the Laplacian in the plane perpendicular to the x-axis, and ν is a constant that is determined by the averaging procedure. For separation distances smaller than the surface wavelength, this constant is of the order of $\nu \sim \frac{1}{2}$, and its value decreases as the separation increases.



In equilibrium domains A and B are bounded by flat surfaces $x = 0$ and $x = H$. Due to oscillations points $\boldsymbol{x}_0^*$ located near $\boldsymbol{x}_0$ on the surface $x = 0$ are displaced by the vectors $\boldsymbol{\xi}(\boldsymbol{x}_0^*)$ and form a non-flat surface. Points $\boldsymbol{x}_H^*$ located near $\boldsymbol{x}_H$ on the surface $x = H$ are displaced by the vectors $\boldsymbol{\xi}(\boldsymbol{x}_H^*)$ and form another non-flat surface. The interaction between these non-flat surfaces is approximated by the van der Waals force between the average planes $x = \langle \xi(\boldsymbol{x}_0) \rangle$ and $x = H + \langle \xi(\boldsymbol{x}_H) \rangle$.

Figure 2: Computation of van der Waals forces

It is well known that two material half-spaces separated by the distance H are attracted to each other by the van der Waals force per unit area

$$f(H) = \frac{A}{6\pi H^3}, \qquad A \sim 10^{-19}\text{J}, \tag{2.6}$$

where A is the Hamaker constant with a typical value of about 10^{-19}J for interactions across vacuum, [7, Sec 11.1]. Therefore, setting $H = H_{\text{eft}}$ and assuming that the displacements $\boldsymbol{\xi}_0$ and $\boldsymbol{\xi}_H$ are comparable to or smaller than the dominant wavelength of elastic waves and to interatomic distances, we find, using (2.5) that the half-space $x < 0$ is attracted to the half-space $x > H$ by a force per unit area (pressure) that is parallel to the x-axis and has the value

$$F\left(H, [\xi]\right) = f\left(H + \xi(\boldsymbol{x}_H) - \xi(\boldsymbol{x}_0) + \nu H^2\left[\nabla_\perp^2 \xi(\boldsymbol{x}_H) - \nabla_\perp^2 \xi(\boldsymbol{x}_0)\right]\right). \tag{2.7}$$

Then, applying the Taylor expansion about H we approximate (2.7) by

$$F(H, [\xi]) = f(H) + \gamma(H)\left(\nu\big[\nabla_\perp^2 \xi(\boldsymbol{x}_H) - \nabla_\perp^2 \xi(\boldsymbol{x}_0)\big] + \frac{\xi(\boldsymbol{x}_H) - \xi(\boldsymbol{x}_0)}{H^2}\right), \tag{2.8}$$

where

$$\gamma(H) \equiv H^2 |f'(H)| = \frac{A}{2\pi H^2}. \tag{2.9}$$

and $f(H)$ is a static force which helps to keep the body in its equilibrium position and, thus does not contribute to acoustic wave propagation, so that it is ignored hereafter.

From the above we see that the balance of forces on the open surfaces $x = 0$ and $x = H$ can be written in the form

$$p(\boldsymbol{x}_0) = F(H, [\xi]) = p(\boldsymbol{x}_H), \tag{2.10}$$

which may be treated as interface conditions on the faces of the domains $x < 0$ and $x > H$.

3 Reflection coefficient of a vacuum layer between two half-spaces

Let the thermal oscillations depend on time by the exponential factor $\mathrm{e}^{\mathrm{i}\omega t}$. Then the oscillations in the half spaces are described by the Helmholtz equations

$$\nabla^2 p + \frac{\omega^2}{c^2} p = 0, \qquad c = \begin{cases} c_A, & x < 0, \\ c_B, & x > H, \end{cases} \tag{3.1}$$

where c_A and c_B are the sound speeds (Debye) in the half-spaces and $p(x, y, z)$ is the acoustic pressure p connected with the displacement $\xi(x, y, z)$ along the x-axis by the formula $\xi = p'_x/\rho\omega^2$, where ρ is the mass density of the acoustic medium, $\rho = \rho_A$ for $x < 0$ and $\rho = \rho_B$ for $x > H$.

Since the van der Waals force between the faces of the bodies $x < 0$ and $x > H$ depends on the displacements of these faces, the Helmholtz equations (3.1) must be supplemented by the interface conditions (2.10) which reduce to the form

$$p(0) = p(H) = \nu\gamma(H)\big[\nabla_\perp^2 \xi(0) - \nabla_\perp^2 \xi(H)\big] + \frac{\gamma(H)}{H^2}\big[\xi(0) - \xi(H)\big], \tag{3.2}$$

where the coordinates y and z are suppressed, so that $p(x) \equiv p(x, y, z)$ and $\xi(x) \equiv \xi(x, y, z)$.

Let an incident plane wave $\mathrm{e}^{\mathrm{i}\omega(x\cos\theta+y\cos\theta_y+z\cos\theta_z)/c_A}$ propagate in the domain $x<0$. Due to its interaction with the boundaries $x=0$ and $x=H$ this wave generates the reflected wave $R_A\mathrm{e}^{\mathrm{i}\omega(-x\cos\theta_A+e_y y+e_z z)/c_A}$, where $e_y^2+e_z^2=\sin^2\theta_A$, propagating in the domain $x<0$, and the transmitted wave $W_A\mathrm{e}^{\mathrm{i}\omega((x-H)\cos\theta_B+d_y y+e_z z)/c_B}$, where $d_y^2+d_z^2=\sin^2\theta_B$, propagating in $x>H$. These waves form the wave field

$$p(x,y,z)=\begin{cases}\mathrm{e}^{\mathrm{i}\omega(x\cos\theta_A+y\cos\theta_y+z\cos\theta_z)/c_A}+R_A\mathrm{e}^{\mathrm{i}\omega(-x\cos\theta_A+e_y y+e_z z)/c_A}, & x\le 0,\\ W_A\mathrm{e}^{\mathrm{i}\omega((x-H)\cos\theta_B+d_y y+d_z)/c_B}, & x\ge H,\end{cases} \tag{3.3}$$

where θ_A and θ_B are connected by the Snell Law

$$\frac{\sin\theta_A}{c_A}=\frac{\sin\theta_B}{c_B}. \tag{3.4}$$

Then, straightforward calculations produce

$$\begin{aligned} &p(0)\ =1+R_A, \quad \xi(0)\ =\frac{\mathrm{i}\cos\theta_A}{\omega\rho_A c_A}(1-R_A), \quad \nabla_\perp^2\xi(0)\ =\frac{-\omega^2\sin^2\theta_A}{c_A^2}\xi(0),\\ &p(H)=W_A, \qquad \xi(H)=\frac{\mathrm{i}\cos\theta_B}{\omega\rho_B c_B}W_A, \qquad \nabla_\perp^2\xi(H)=\frac{-\omega^2\sin^2\theta_B}{c_B^2}\xi(H), \end{aligned} \tag{3.5}$$

and they reduce (3.2) to algebraic equations for R_A and W_A:

$$\begin{aligned} &1+R_A=W_A,\\ &1+R_A=\frac{\mathrm{i}C}{\omega H^4}\left(\frac{\cos\theta_A}{\rho_A c_A}(1-R_A)-\frac{\cos\theta_B}{\rho_B c_B}W_A\right), \end{aligned} \tag{3.6}$$

where

$$C\equiv C(\omega,H)=\frac{A}{2\pi}\left(1-\nu\omega^2H^2\,\frac{\sin^2\theta_A}{c_A^2}\right), \tag{3.7}$$

From these equations we get the reflection coefficient

$$R_A=\frac{C(\mu_B\cos\theta_A-\mu_A\cos\theta_B)+\mathrm{i}\omega H^4\mu_A\mu_B}{C(\mu_B\cos\theta_A+\mu_A\cos\theta_B)-\mathrm{i}\omega H^4\mu_A\mu_B}. \tag{3.8}$$

represented in terms of the specific acoustic impedances of the media

$$\mu_A=\rho_A c_A, \qquad \mu_B=\rho_B c_B. \tag{3.9}$$

Obviously, if $H\to\infty$ then $R\to -1$, which agrees with the expectation that an infinitely wide gap has total reflection. In the opposite limit $H\to 0$ we have

$$R_A\to\frac{\mu_B\cos\theta_A-\mu_A\cos\theta_B}{\mu_B\cos\theta_A+\mu_A\cos\theta_B}, \tag{3.10}$$

which agrees with the reflection coefficient of a wave with incidence angle θ_A from an interface between materials with acoustic impedances μ_A and μ_B.

The expression (3.8) for the reflection coefficient R_A of a wave arriving from A allows computations of all other reflection and transmission characteristics of the gap. Thus, to compute the

reflection coefficient R_B of the wave arriving from B it suffices to interchange in (3.8) indices A and B. Remarkably, due to (3.4), this interchange does not alter $C(\omega, H)$ from (3.6). Then, the first line of (3.6) implies that the transmission coefficients from A and from B can be computed as $W_A = 1 + R_A$ and $W_B = 1 + R_B$, respectively.

The reflection and transmission coefficients R_A and W_A are convenient for describing wave fields of the type (3.3), which are generated by an incident wave arriving from A. Similarly, R_B and W_B are convenient in cases when the field is generated by an incident wave arriving from B. However, to analyze thermally excited waves in a system of two half-spaces A and B it is more convenient to consider general fields

$$p = \begin{cases} U^- \mathrm{e}^{\mathrm{i}\omega(x\cos\theta_A + y\cos\theta_y + z\cos\theta_z)/c_A} + V^- \mathrm{e}^{\mathrm{i}\omega(-x\cos\theta + e_y y + e_z z)/c_A}, & x < 0, \\ U^+ \mathrm{e}^{\mathrm{i}\omega((x-H)\cos\theta_B + y\cos\theta_y + z\cos\theta_z)/c_B} + V^+ \mathrm{e}^{\mathrm{i}\omega(-(x-H)\cos\theta_B + d_y y + d_z z)/c_B}, & x > H, \end{cases} \tag{3.11}$$

where θ_A and θ_B satisfy the Snell law (3.4), while $U_\pm$, and $V_\pm$ are indefinite coefficients restrained by the linear conditions

$$\mathbb{T} \begin{pmatrix} U^- \\ V_- \end{pmatrix} = \begin{pmatrix} U^+ \\ V_+ \end{pmatrix}, \qquad \mathbb{T} = \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix}, \tag{3.12}$$

where the elements T_{mn} guarantee that the fields in (3.11) obey the interface conditions (3.2).

In order to compute the four matrix elements T_{mn} in terms of the four coefficients R_A, R_B, W_A and W_B, we observe that (3.3) is a particular case of (3.11) with $U^- = 1$, $V^- = R_A$, $U^+ = W_A$, $V^+ = 0$, which means that these $U_\pm$ and $V_\pm$ must obey (3.12). Similarly, we find that (3.12) must be satisfied when $U^- = 0$, $V^- = W_B$, $U^+ = R_B$, $V^+ = 1$. These observations lead to the equations

$$\begin{aligned} &T_{11} + T_{12} \cdot R_A = W_A, && T_{11} \cdot 0 + T_{12} \cdot W_B = R_B, \\ &T_{21} + T_{22} \cdot R_A = 0, && T_{21} \cdot 0 + T_{22} \cdot W_B = 1, \end{aligned} \tag{3.13}$$

and, then, to the representation

$$\mathbb{T} = \frac{1}{1 + R_B} \begin{pmatrix} 1 + R_A + R_B, & R_B \\ -R_A, & 1 \end{pmatrix}, \tag{3.14}$$

It is worth mentioning that as the gap collapses, the reflection coefficient R_B and transmission matrix approach the limits

$$R_B \to -R_A, \qquad \mathbb{T} \to \frac{1}{1 - R_A} \begin{pmatrix} 1, & -R_A \\ -R_A, & 1 \end{pmatrix}, \tag{3.15}$$

the first of which follows from (3.10). These identities connect the transmission matrix and the reflection coefficients of the system of two contacting half-spaces, which may be considered as two half-spaces separated by a vanishing gap.

4 Reflection coefficient of a stack of acoustic and vacuum layers

The reflection coefficient of an arbitrary stack of acoustic layers admits an explicit representation in terms of the layers' thicknesses and of the reflection coefficients of the interfaces between them [9]. Here we extend this representation to the case when the stack includes vacuum layers.

Let G_j with $j = 1, 2, \dots, (m-1)$, be the layers $x_j < x < x_{j+1}$, squeezed between two half-spaces $x < x_0$ and $x > x_m$, which will be referred to as G_0 and G_m, respectively. We assume that some of the domains G_j are occupied my acoustic media, while others are empty, as shown in Fig. 3. Let c_j and μ_j be the sound speed and the specific acoustic impedance of the material layer G_j. If G_j is vacuum gap then we leave its parameters undefined.

For every material layer G_j we introduce two alternative representations of the wave field p_j:

$$\begin{aligned} p_j &= U_j^- \mathrm{e}^{\mathrm{i}\omega[(x-x_j)\cos\theta_j + e_y y + e_z z]/c_j} + V_j^- \mathrm{e}^{\mathrm{i}\omega[-(x-x_j)\cos\theta_j + e_y y + e_z z]/c_j}, \\ &= U_j^+ \mathrm{e}^{\mathrm{i}\omega[(x-x_{j+1})\cos\theta_j + e_y y + e_z z]/c_j} + V_j^+ \mathrm{e}^{\mathrm{i}\omega[-(x-x_{j+1})\cos\theta_j + e_y y + e_z z]/c_j}, \end{aligned} \tag{4.1}$$

where the first representation will be used to describe the interaction of the domain G_j with its left neighbor G_{j-1}, while the other representation will be used to describe interactions of G_j with G_{j+1}. Since both formulas (4.1) represent the same field, it is obvious that their coefficients are related by the linear expressions

$$U_j^+ = U_j^- \mathrm{e}^{\mathrm{i}\omega(x_{j+1}-x_j)\cos\theta_j/c_j}, \qquad V_j^+ = V_j^- \mathrm{e}^{\mathrm{i}\omega(x_j-x_{j+1})\cos\theta_j/c_j}, \tag{4.2}$$

which can be written in the form

$$\begin{pmatrix} U_j^+ \\ V_j^+ \end{pmatrix} = \mathbb{D}_j \begin{pmatrix} U_j^- \\ V_j^- \end{pmatrix}, \tag{4.3}$$

where

$$\mathbb{D}_j = \begin{pmatrix} \mathrm{e}^{\mathrm{i}\omega h_j \cos\theta_j/c_j} & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}\omega h_j \cos\theta_j/c_j} \end{pmatrix}, \qquad h_j = x_{j+1} - x_j, \tag{4.4}$$

may be treated as a "transmission matrix of the layer G_j".

Since G_0 is a half-space unbounded from the left, for the field p_0 in this domain we use only the first representation (4.1) in terms of the pair (U_0^+, V_0^+). Similarly, for the field p_m in the half-space G_m we use only the second representation from (4.1) in terms of the pair (U_0^-, V_0^-). Then, the transmission matrix $\mathbb{T}$ of the entire structure is defined by the relationship (3.12) with $U^\pm$ and $V^\pm$ replaced by $U_0^\pm$ and $V_m^\pm$, respectively.

In order to compute the transmission matrix of the stack of layers G_j, $0 \le j \le m$, we consider first the case when the stack has no gaps, i.e. the case with only material layers. Then $\mathbb{T}$ can computed step-by-step as the product

$$\mathbb{T} = \mathbb{T}_m \mathbb{D}_m \mathbb{T}_{m-1} \mathbb{D}_{m-1} \dots \mathbb{T}_2 \mathbb{D}_1 \mathbb{T}_1. \tag{4.5}$$

where $\mathbb{D}_{j-1}$ is the transmission matrix (4.4) of the layer G_j, and $\mathbb{T}_j$ is the transmission matrix of the interface between G_{j-1} and G_j, which can be computed by the formulas (3.10), (3.15) with G_{i-1} and G_j considered as media A and B, respectively.

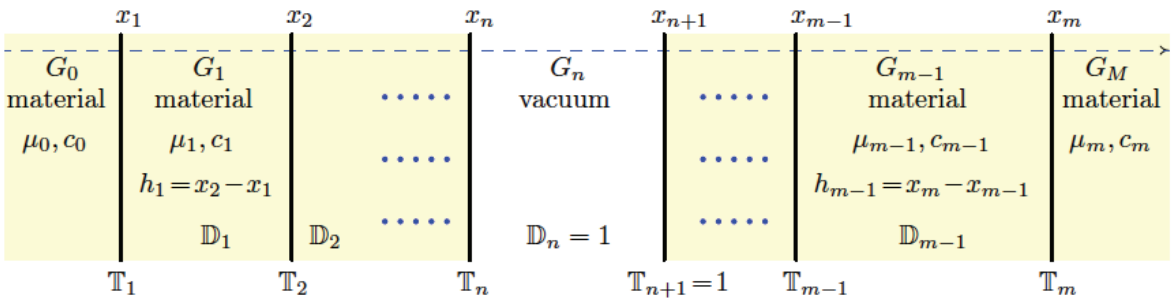


Figure 3: To computation of the reflection coefficient of layered structure

Next, we consider the structure where G_n is a vacuum layer, as shown in Fig. 3. In this case, the transmission matrices T_n and T_{n+1} are not defined, and, (4.5) becomes meaningless. However, in this case the results of the previous section imply that the pair (U^+_{n+1}, V^+_{n+1}) can be computed in terms of the pair (U^+_{n-1}, V^+_{n-1}) multiplied by the transmission matrix of the vacuum gap G_n defined by (3.14) and (3.8). For convenience we agree to denote this matrix by $\mathbb{T}_n$ and set $\mathbb{T}_{n+1} = \mathbb{D}_n \equiv 1$. Then we get the relationship

$$\begin{pmatrix} U^+_{n+1} \\ V^+_{n+1} \end{pmatrix} = \mathbb{T}_{n+1}\mathbb{D}_n\mathbb{T}_n \begin{pmatrix} U^-_{n-1} \\ V^-_{n-1} \end{pmatrix}, \tag{4.6}$$

which looks identical to the corresponding relationship in the case when G_n is a material layer. This coincidence shows that the transmission matrix of an arbitrary stack of material and vacuum layers can be represented by the product (4.5), where for every vacuum layer G_n we set $\mathbb{D}_n \equiv \mathbb{T}_{n+1} \equiv 1$, and define $\mathbb{T}_n$ as a transmission matrix of G_n.

Finally, using the first column of the second line of (3.12) we conclude that the reflection coefficient R_A of the entire stack of layers can be computed as

$$R_A = -\frac{T_{21}}{T_{22}}, \tag{4.7}$$

where T_{12} and T_{22} are the elements of the matrix $\mathbb{T}$ from (4.5).

5 Thermally excited acoustic waves in the half-spaces

Let A and B be two half-spaces $x < 0$ and $x > H$ occupied by acoustic media that are maintained at temperatures T_A and T_B, respectively. We adopt the Debye model and assume that each of these media supports acoustic waves of $N = 3$ different polarization, which do not interact with each other. As in the previous section we assume that c_A and ρ_A are the Debye sound speed and mass density in A, while c_B and ρ_B are the similar parameters in B.

Thermally excited acoustic waves have random amplitudes, directions and phase shifts. All available information about such waves is reduced to the energy spectrum, which is described by the classical Planck's law in the case of thermal equilibrium, or by its generalization for systems with a steady heat flux [2]. The latter states that in the presence of a small heat flux $Q \ll 1$ the

thermally excited acoustic waves of a single polarization in A with frequencies from the interval $(\omega, \omega + \mathrm{d}\omega)$ and with incidence angles from the interval $(\theta_A, \theta_A + \mathrm{d}\theta_A)$ have the energy density

$$\mathrm{d}E_A(\omega, \theta_A; Q) = P\left(\frac{\omega}{1 + q_A \cos\theta_A}, T_A\right) \frac{\omega^2 \sin\theta_A}{4\pi^2 c_A^3}\, \mathrm{d}\theta_A \mathrm{d}\omega, \qquad q_A = \frac{Q}{Q_A}, \tag{5.1}$$

where

$$P(\omega, T) = \frac{\hbar\omega}{\mathrm{e}^{\hbar\omega/\kappa T} - 1}, \tag{5.2}$$

and

$$Q_A = 2N \int_0^{\omega_\mathrm{D}} \int_0^{\theta_A^*} c_A \mathrm{d}E_A = \frac{N\,(1 - \cos\theta_A^*)}{2\pi^2 c_A^2} \int_0^{\omega_\mathrm{D}} P(\omega, T_A)\omega^2 \mathrm{d}\omega \tag{5.3}$$

is the energy flux density of all thermally excited acoustic waves in A that contribute to heat exchange between A and B. The flux (5.3) includes waves of all polarizations (accounted for by the factor "N"), of all frequencies (accounted for by the integration over ω through the cut-off frequency ω_D) and with all incident angles (accounted for by the integration over θ_A) from the intervals $0 \le \theta_A \le \theta_A^*$ and $\pi - \theta_A^* \le \theta_A \le \pi$, limited by the critical angle θ_A^*.

It is known that an acoustic field in a medium with the density ρ and the sound speed c has the energy density $E = p^2/2c^2\rho$, where p is the acoustic pressure [9, Sec. 2.3]. This implies that any plane pressure wave

$$p_A(\omega, \theta_A) = \sqrt{2c_A^2 \rho_A \mathrm{d}E_A(\omega, \theta_A)}\, \mathrm{e}^{\mathrm{i}\alpha}\, \mathrm{e}^{\mathrm{i}\omega(x\cos\theta_A + e_y y + e_z z)/c_A}, \tag{5.4}$$

with arbitrary α, e_y, and e_z constrained by the condition $e_y^2 + e_z^2 = 1 - \cos^2\theta_A$, has the energy density $\mathrm{d}E_A(\omega, \theta_A; Q)$ from (5.1). Therefore, the set of waves (5.4) with random α, θ_A, e_y and e_z may be considered as a statistical ensemble of thermally excited wave fields with a small heat flux Q along the x-axis in the medium A at temperature T_A. Similarly, an ensemble of waves with a heat flux $Q \ll 1$ in the domain B at temperature T_B may be modeled as a set of plane waves

$$p_B(\omega, \theta_B) = \sqrt{2c_B^2 \rho_B \mathrm{d}E_B(\omega, \theta_B)}\, \mathrm{e}^{\mathrm{i}\beta}\, \mathrm{e}^{\mathrm{i}\omega(x\cos\theta_B + d_y y + d_z z)/c_B}, \tag{5.5}$$

where β, θ_B, d_y and d_z take random values constrained by the condition $d_y^2 + d_z^2 = 1 - \cos^2\theta_B$, and $\mathrm{d}E_B(\omega, \theta_B; Q)$ is defined by (5.1) with the index A replaced by B.

If the molecules of the media A and B interact, then acoustic waves in these domains are not independent of each other. This implies that such statistical characteristics of the ensembles of thermally generated waves in A and B as the temperatures T_A, T_B and the heat flux Q are connected, so that if both temperatures are known then the heat flux is defined.

To compute the heat flux Q between half spaces A and B maintained at known temperatures we employ the following plan: a) compute the flux $Q_+(Q)$ carried in A by the waves propagating towards B; b) compute the flux $Q_-(Q)$ carried in A by the waves propagating outwards of B; c) find Q as the solution of the equation

$$Q = Q_+(Q) - Q_-(Q). \tag{5.6}$$

In order to compute $Q_+(Q)$ we observe that the flux along the x-axis carried by the waves (5.4) with frequencies from the interval $(\omega, \omega + \mathrm{d}\omega)$ and incidence angles from the interval $(\theta_A, \theta_A + \mathrm{d}\theta_A)$ has the value $\mathrm{d}Q_+(\omega, \theta_A) = c_A \cos\theta_A \mathrm{d}E_A(\omega, \theta_A)$. Then, combining this formula with (5.1) we find that the total flux in A towards B carried by the waves (5.4) with N polarizations, all frequencies and all incidence angles from the range $0 < \theta_A < \theta_A^*$ can be represented as

$$Q_+(Q) = N \int_0^{\omega_{\mathrm{D}}} \int_0^{\theta_A^*} \mathrm{d}Q_+(\omega, \theta_A) \equiv N \int_0^{\omega_{\mathrm{D}}} \int_0^{\theta_A^*} P(\omega, T_A; \theta_A, q_A) \mathrm{d}\Omega_A, \tag{5.7}$$

where

$$P(\omega, T; \theta, q) = P\left(\frac{\omega}{1 + q\cos\theta}, T\right) \tag{5.8}$$

and

$$\mathrm{d}\Omega_A \equiv \mathrm{d}\Omega_A(\omega, \theta) = \frac{\omega^2 \mathrm{d}\omega \mathrm{d}\sin^2\theta_A}{8\pi^2 c_A^2}. \tag{5.9}$$

The flux $Q_-(Q)$ carried in A outwards from B can be computed by two different ways. It can be computed by (5.7) with the incident angle θ_A replaced by $\pi - \theta_A$. However, since this representation does not involve any parameters of the domain B, its substitution into (5.6) turns the latter into a correct but useless identity, which does not connect Q with the temperature T_B. In order to represent $Q_-(Q)$ in terms of both domains we observe that there are two kinds of waves in A propagating outward of B: the waves (5.4) originating in A and reflected back to A and the waves (5.5) originating in B but transmitted to A. The waves of the first kind appear as the products $R_A(\omega, \theta_A) p_A(\omega, \pi - \theta_A)$, where $R_A(\omega, \theta_A)$ is the reflection coefficient of the wave $p_A(\omega, \pi - \theta_A)$. The waves originating in B appear as the products $W_A(\omega, \theta_B) p_B(\omega, \pi - \theta_B)$, where $W_A(\omega, \theta_B)$ is the transmission coefficient of the plane wave (5.5).

The above implies that the ensemble of waves propagating in A outwards from B consists of plane pressure waves $U\mathrm{e}^{\mathrm{i}\omega(-x\cos\theta_A + e_y y + e_z z)/c_A}$ with the amplitude

$$U = R_A(\omega, \theta_A)\mathrm{e}^{\mathrm{i}\alpha}\sqrt{2c_A^2 \rho_A \mathrm{d}E_A(\omega, \theta_A)} + W_A(\omega, \theta_B)\mathrm{e}^{\mathrm{i}\beta}\sqrt{2c_B^2 \rho_B \mathrm{d}E_B(\omega, \theta_B)}, \tag{5.10}$$

where α, β are random phase shifts, and θ_A, θ_B are incidence angles connected by the Snell law (3.4). Then, the flux along the x-axis carried by the waves (5.10) with frequencies and incidence angles from the intervals $(\omega, \omega + \mathrm{d}\omega)$ and $(\theta_A, \theta_A + \mathrm{d}\theta_A)$, respectively, can be represented as

$$\mathrm{d}Q_-(\omega, \theta_A; Q) = \mathrm{d}Q_-^A + \mathrm{d}Q_-^B + \mathrm{d}Q_-^{AB} \tag{5.11}$$

where

$$\mathrm{d}Q_-^A = c_A \cos\theta_A |R_A(\omega, \theta_A)|^2 \, \mathrm{d}E_A(\omega, \theta_A) \tag{5.12}$$

is the flux carried by the waves originated in A and reflected back to A,

$$\mathrm{d}Q_-^B = \cos\theta_A \, \frac{c_B^2 \rho_B}{c_A \rho_A} \, |W_A(\omega, \theta_B)|^2 \, \mathrm{d}E_B(\omega, \pi - \theta_B) \tag{5.13}$$

is the flux carried by the waves originated in B and transmitted into A, and

$$\mathrm{d}Q_{-}^{AB} = 2c_B \cos\theta_A \sqrt{\frac{\rho_B}{\rho_A}} \left| R_A(\omega,\theta_A) W_A(\omega,\theta_A) \right| \sqrt{\mathrm{d}E_A(\omega,\theta_A)\mathrm{d}E_B(\omega,\pi-\theta_B)} \cos\chi, \tag{5.14}$$

where $\chi = \alpha - \beta + \arg(R_A) - \arg(W_A)$ is a random number, is the contribution of the interference of waves originated in A and in B. If the waves radiated from A and B are not correlated, as happens when these bodies are separated by a large distance, then the average of this term vanishes, and since the heat transport is determined by statistical averages, the term (5.14) may be ignored. However, if the radiations from A and B are correlated, which is the case when the gap between them is smaller than a characteristic wave length of heat carriers, then the average of (5.14) may be comparable to or even exceed (5.12) and (5.13), so that the contribution of (5.14) becomes important for the analysis of heat transport.

The first term (5.12) can be computed using (5.1) and (5.8), (5.9), which immediately gives

$$\mathrm{d}Q_{-}^{A} = |R_A(\omega,\theta_A)|^2 \, P(\omega, T_A; q_A, \theta_A)\mathrm{d}\Omega_A. \tag{5.15}$$

Similarly, for the term (5.13) we get the expression

$$\mathrm{d}Q_{-}^{B} = |W_A(\omega,\theta_B)|^2 P(\omega, T_B; \theta_B, -q_B) \frac{c_A \rho_B \cos\theta_A \sin\theta_B \omega^2 \, \mathrm{d}\omega \mathrm{d}\theta_B}{4\pi^2 c_B^3 \rho_A}, \tag{5.16}$$

but, since it is to be substituted into (5.11) it is convenient to modify it by representing $\sin\theta_B$ and $\mathrm{d}\theta_B$ in terms of θ_A. To proceed, we derive from (3.4) that

$$\sin\theta_B = \frac{c_B}{c_A}\sin\theta_A, \qquad \mathrm{d}\theta_B = \frac{c_B\cos\theta_A}{c_A\cos\theta_B}\,\mathrm{d}\theta_A, \tag{5.17}$$

and take into account the well-known identity

$$\left(1 - |R_A|^2\right) \frac{\cos\theta_B}{c_B\rho_B} = |W_A|^2 \frac{\cos\theta_A}{c_A\rho_A}, \tag{5.18}$$

which connects the transmission coefficient $W_A(\omega,\theta_B)$ from B to A with the reflection coefficient R_A from A to A. Then, the substitution of (5.17) and (5.18) into (5.16) leads to the representation

$$\mathrm{d}Q_{-}^{B} = \left(1 - |R_A(\omega,\theta_A)|^2\right) P(\omega, T_B; \theta_B, -q_B)\mathrm{d}\Omega_A, \tag{5.19}$$

which has a close similarity with (5.15).

In order to compute the last term of (5.11) we first find that

$$\sqrt{\mathrm{d}E_A(\omega,\theta_A)\mathrm{d}E_B(\omega,\theta_B)} = P_{AB}(\omega,\theta_A,Q,T_A,T_B) \sqrt{\frac{\sin\theta_A\sin\theta_B \mathrm{d}\theta_A\mathrm{d}\theta_B}{c_A^3 c_B^3}} \, \frac{\omega^2\mathrm{d}\omega}{4\pi^2}, \tag{5.20}$$

where

$$P_{AB}(\omega,\theta_A,Q,T_A,T_B) = \sqrt{P\left(\frac{\omega}{1+q_A\cos\theta_A}, T_A\right) P\left(\frac{\omega}{1-q_B\cos\theta_B}, T_B\right)}. \tag{5.21}$$

Then, from (5.17), we get the identities

$$\mathrm{d}\theta_A \mathrm{d}\theta_B = \frac{c_B \cos\theta_A}{c_A \cos\theta_B}\,(\mathrm{d}\theta_A)^2, \qquad \sin\theta_A \sin\theta_B = \frac{c_B}{c_A}\sin^2\theta_A \tag{5.22}$$

and reduce (5.20) to the form

$$\sqrt{\mathrm{d}E_A(\omega,\theta_A)\mathrm{d}E_B(\omega,\theta_B)} = P_{AB}(\omega,\theta_A,Q,T_A,T_B)\sqrt{\frac{\cos\theta_A}{c_A c_B\cos\theta_B}}\,\frac{\sin\theta_A\omega^2\mathrm{d}\omega\mathrm{d}\theta_A}{4\pi^2 c_A^2}. \tag{5.23}$$

which leads, in view of (5.18), to the interference contribution to the heat flux in the form

$$\mathrm{d}Q_-^{AB} = 2|R_A(\omega,\theta_A)|\sqrt{1-|R_A(\omega,\theta_A)|^2}P_{AB}(\omega,\theta_A,Q,T_A,T_B)\cos\chi(\omega,\theta_A)\mathrm{d}\Omega_A. \tag{5.24}$$

Finally, incorporating (5.15), (5.19) and (5.24) into (5.11), and integrating $\mathrm{d}Q_-(\omega,\theta_A;Q)$ over the frequencies and incidence angles we arrive at the equation for Q

$$\begin{aligned} Q = N\int_0^{\omega_\mathrm{D}}\int_0^{\theta_A^*}\Big\{ &\left(1-|R_A(\omega,\theta_A)|^2\right)\left[P(\omega,T_A;\theta_A,Q/Q_A)-P(\omega,T_B;\theta_B,-Q/Q_B)\right] \\ &-2|R_A(\omega,\theta_A)|\sqrt{1-|R_A(\omega,\theta_A)|^2}\,P_{AB}(\omega,\theta_A,Q,T_A,T_B)\cos\chi(\omega,\theta_A)\Big\}\mathrm{d}\Omega_A, \end{aligned} \tag{5.25}$$

which involves an yet indefinite random phase function $\chi(\omega,\theta_A)$.

6 Applications

The general equation (5.25) admits considerable simplifications in special cases.

In the case when the reflection coefficient is small $R_A \ll 1$, the last term in (5.25) can be neglected so that (5.25) reduces to the form

$$Q = N\int_0^{\omega_\mathrm{D}}\int_0^{\theta_A^*}\left(1-|R_A(\omega,\theta_A)|^2\right)\left\{P(\omega,T_A;\theta_A,Q/Q_A)-P(\omega,T_B;\theta_B,-Q/Q_B)\right\}\mathrm{d}\Omega_A, \tag{6.1}$$

similar to that used in [1] for the analysis of heat radiation across a narrow, nanoscale vacuum gap. In order to compute the heat transport coefficient $K(T_B) = \lim Q/(T_A - T_B)$, as $T_A \to T_B$, we assume that $|Q| \ll 1$ and $T_A \approx T_B$, and applying the Taylor expansion

$$P(\omega,T+\Delta T;\theta,q) = P(\omega,T) - q\omega\cos\theta P'_\omega(\omega,T) + P'_T(\omega,T)\Delta T + o(q+\Delta T), \tag{6.2}$$

reduce (6.1) to the linear equation

$$(1+\Lambda)Q = \Gamma\Delta T, \tag{6.3}$$

where $\Delta T = T_A - T_B$,

$$\Lambda = N\int_0^{\omega_\mathrm{D}}\int_0^{\theta_A^*}\left(1-|R_A(\omega,\theta_A)|^2\right)\omega P'_\omega(\omega,T_B)F_+(\theta_A,\theta_B)\mathrm{d}\Omega_A, \tag{6.4}$$

$$\Gamma = N\int_0^{\omega_\mathrm{D}}\int_0^{\theta_A^*}\left(1-|R_A(\omega,\theta_A)|^2\right)P'_T(\omega,T_B)\mathrm{d}\Omega_A, \tag{6.5}$$

and $F_+(\theta_A, \theta_B)$ is defined by the formula

$$F_\pm(\theta_A, \theta_B) = \frac{\cos\theta_A}{Q_A} \pm \frac{\cos\theta_B}{Q_B}, \tag{6.6}$$

whose second option (with "−" sign) will be used below.

It is shown in [1] that as the gap's width H between identical materials decreases towards zero then $(1 + \Lambda) \to 0$ at the rate $(1 + \Lambda) \sim O(H^2)$, so that the heat transport coefficient diverges as $O(1/H^2)$, in agreement with experimental data [10]. The analysis of [1] also shows that this asymptote of the heat transport coefficient of a vanishing gap between identical materials, which is provided by the term Λ, is due to the extension of Planck's law to systems with a heat flux. Without this term (6.3) reduces to the formula $Q = \Gamma\Delta T$ arising in the so-called "acoustic mismatch" method [11, 12] based on the assumption that the domains A and B radiate as if they are in thermal equilibrium. This assumption leads to an obviously incorrect prediction that an imaginary interface between identical materials has a finite thermal transport coefficient rather than an infinite one, so that (6.3) appears as an improvement of the acoustic mismatch method. However, it is obvious from (6.4) that $\Lambda \ll 1$ only when $|R_A| \sim 1$, which contradicts the condition $|R_A| \ll 1$, needed to reduce the general equation (5.25) to (6.1). Therefore, the above mentioned incorrect prediction of the acoustic mismatch theory may not be surprising because it arrises in cases with a small reflection coefficient when the strong reflection approximation of Λ is not justified.

Next we consider the opposite extreme case of almost total reflection, i.e. when $|R_A| \approx 1$, which arises in the analysis of heat transport by phonon tunneling across a gap wider than a few nanometers, as well as in the analysis of heat transport by acoustic or electromagnetic waves between bodies with sharply different wave speeds.

In this case we get the estimate $(1 - |R_A|^2) \ll \sqrt{1 - |R_A|^2}$, which makes it possible to ignore the first term in equation (5.25) so that it reduces to the form

$$Q = -2N \int_0^{\omega_{\rm D}} \int_0^{\theta_A^*} r(\omega, \theta_A)\, P_{AB}(\omega, \theta_A, Q, T_A, T_B) \cos\chi(\omega, \theta_A) \mathrm{d}\Omega_A, \tag{6.7}$$

where

$$r(\omega, \theta_A) = |R_A(\omega, \theta_A)| \sqrt{1 - |R_A(\omega, \theta_A)|^2}\,. \tag{6.8}$$

Then, assuming that $|Q| \ll 1$ and $|\Delta T| \ll 1$ we use the Taylor expansion

$$P_{AB}(\omega, \theta_A, Q, T_A, T_B) = P(\omega, T_B) + \frac{1}{2} P'_T(\omega, T_B)\Delta T - \frac{\omega}{2} P'_\omega(\omega, T_B) F_-(\theta_A, \theta_B) Q, \tag{6.9}$$

and reduce (6.7) to the linear equation

$$Q = \Gamma_\chi \Delta T + \Upsilon_\chi, \tag{6.10}$$

whose terms

$$\Gamma_\chi = -N \int_0^{\omega_{\rm D}} \int_0^{\theta_A^*} r(\omega, \theta_A) P'_T(\omega, T_B) \cos\chi(\omega, \theta_A) \mathrm{d}\Omega_A, \tag{6.11}$$

$$\Upsilon_\chi = -2N \int_0^{\omega_{\rm D}} \int_0^{\theta_A^*} r(\omega, \theta_A) P(\omega, T_B)\, \cos\chi(\omega, \theta_A) \mathrm{d}\Omega_A, \tag{6.12}$$

involve random phase shifts $\chi(\omega,\theta_A)$ between radiations from different domains.

If $\chi(\omega,\theta)$ is fixed, then (6.10) appears as an equation for Q with given T_A and T_B. However, when $\chi(\omega,\theta)$ changes the equation (6.10) also changes and defines another Q for the same T_A and T_B. Therefore, since $\chi(\omega,\theta)$ is a random function, the solution Q of equation (6.10) depends on a distribution of χ which cannot be specified without additional physical assumptions.

To specify $\chi(\omega,\theta_A)$ we adopt the principle of maximal entropy production [13] which requires that in the presence of the temperature differential the heat flux takes the maximal possible value in order to reach equilibrium as fast as possible. Based on this principle, the heat flux between half-spaces at given temperatures T_A and T_B should be calculated as the maximal Q which can satisfy (6.10) for arbitrary $\chi(\omega,\theta)$ constrained by the identity

$$\int_0^{\omega_{\rm D}}\int_0^{\theta_A^*} r(\omega,\theta_A)P(\omega,T_B)\,\cos\chi(\omega,\theta_A){\rm d}\Omega_A=0, \tag{6.13}$$

which guarantees that the heat flux does not vanish unless the temperature differential also vanishes.

The above implies that the heat transport coefficient can be represented as

$$K=\max_{\chi}\left\{\Gamma_\chi\right\}, \tag{6.14}$$

where the maximum is computed over all possible distributions of $\chi(\omega,\theta_A)$ constrained by the condition (6.13). This is a standard linear optimization problem and it can be addressed by well-developed algorithms [14, 15]. However, in this particular case, it admits an explicit solution

$$K=\frac{N}{8\pi^2c_A^2}\int_0^{\omega_{\rm D}}\left(\int_0^{\theta_A^*} r(\omega,\theta_A)\sin 2\theta_A{\rm d}\theta_A\right){\rm sign}(\omega-\omega_*)\omega^2P_T'(\omega,T_B){\rm d}\omega, \tag{6.15}$$

where ω_* is selected from the condition

$$\int_0^{\omega_{\rm D}}\left(\int_0^{\theta_A^*} r(\omega,\theta_A)\sin 2\theta_A{\rm d}\theta_A\right){\rm sign}(\omega-\omega_*)\omega^2P(\omega,T_B){\rm d}\omega=0, \tag{6.16}$$

which is equivalent to the constraint (6.13) with $\cos\chi(\omega,\theta_A)={\rm sign}(\omega-\omega_*)$.

To obtain (6.15) we first set $\cos\chi(\omega,\theta_A)\equiv-1$. This selection provides the absolute maximums for K from (6.14) and for the left-hand side of the constraint (6.13), so that any change of the preset values of $\cos\chi(\omega,\theta_A)$ reduces K and pushes the left side of (6.13) closer to zero. Therefore, to get the maximum of K under the constraint (6.13) it suffices to change $\cos\chi(\omega,\theta_A)$ in such way that affects (6.14) as slowly as possible, while changing (6.13) as fast as possible. Observing that the ratio $P(\omega,T)/P_T'(\omega,T)$ monotonically decreases as ω increases we conclude that the best way is to start changing $\cos\chi(\omega,\theta_A)$ at $\omega=0$ and continue until (6.16) is satisfied.

In the general case, when the reflection is neither small nor almost total, we must consider the general equation (5.25) retaining all its terms. However, assuming that $|\Delta T|\ll 1$ and $|Q|\ll 1$ we still can apply Taylor expansions (6.2), (6.9) and reduce (5.25) to the linear equation

$$(1+\Lambda-\Lambda_\chi)Q=(\Gamma+\Gamma_\chi)\Delta T+\Upsilon_\chi, \tag{6.17}$$

where

$$\Lambda_\chi = N \int_0^{\omega_{\rm D}} \int_0^{\theta_A^*} r(\omega,\theta_A)\, \omega P'_\omega(\omega,T_B) F_-(\theta_A,\theta_B)\, \cos\chi(\omega,\theta_A) {\rm d}\Omega_A, \tag{6.18}$$

while the other coefficients are defined by (6.4), (6.5) and (6.11), (6.12). Then, the heat transport coefficient can be represented as a product

$$K = \frac{Q}{\Delta T} = K_0\,(1+K_1), \tag{6.19}$$

where

$$K_0 = \frac{\Gamma}{1+\Lambda} \tag{6.20}$$

coincides with the solution of (6.1), which ignores the contribution of wave interference, while

$$K_1 = \max_\chi \left\{ \frac{\Gamma_\chi/\Gamma + \Lambda_\chi/(1+\Lambda)}{1-\Lambda_\chi/(1+\Lambda)} \right\} \tag{6.21}$$

represents the additional factor that takes into account the wave interference.

Remarkably, the last formula shows that the interference can only increase the heat transport coefficient. Indeed, if all random parameters $\chi(\omega,\theta_A)$ have values such that $\cos\chi(\omega,\theta_A)=0$, then $\Lambda_\chi = \Gamma_\chi = K_1 = 0$, and (6.19), (6.21) imply that $K > K_0$.

Another interesting peculiarity of the expression (6.21) is its asymmetry with respect to the interchange of the domains A and B. Indeed, observing that $F_-(\theta_A,\theta_B)$ defined by (6.6) obeys the identity $F_-(\theta_A,\theta_B) = -F_-(\theta_B,\theta_A)$ we see that Λ_χ from (6.18) changes sign when θ_A and θ_B are interchanged. At the same time, taking into account the last identity in (5.9) we see that the interchange of A and B does not affect any of the other parameters Λ, Λ_χ and Γ that appear in (6.21). Therefore, while the ratio (6.20) is unchanged when A and B are interchanged, the ratio (6.21) is different for the heat transport from A to B and from B to A.

The asymmetry of the heat transport is a well-known phenomenon usually referred to as "thermal rectification". It was first observed in 1936 [16], then its studies intensified in the 1960 – 1970s and exploded in the 2000s, as described in the review [17]. Nevertheless, the phenomenon of thermal rectification is not yet properly explained. Strikingly, in our analysis the thermal rectification appears naturally, as a result of the interference of heat carrying waves.

7 Examples

To test the feasibility of the developed theory we apply it to layered structures resembling those used in read/write heads in Heat Assistant Magnetic Recording systems (HAMR).

A typical structure used in HAMR consists of two "thick" multi-layered parts, one of those is located on a read/write head and another is on a magnetic disk, which is separated from the read/write head-disk interface by a few nanometers wide air gap. The part located on the head includes a silicon substrate, an about 20 nm thick layer of gold, and an about 2 nm thin layer of carbon overcoat. The part located on the disk includes a permalloy substrate, an about 20 nm thick layer of ferromagnetic, and an about 2 nm thin layer of different type of carbon overcoat. Taking into account that the dimensions of both parts considerably exceed the distance between

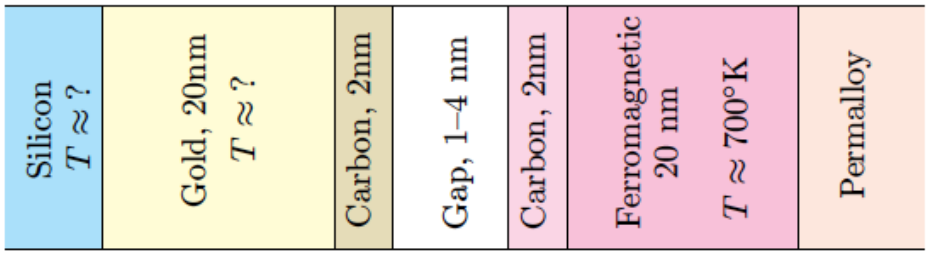


Figure 4: A typical layered structure used in HAMR

them, it seems reasonable to consider a simplified structure which consists of two layered half-spaces separated by a vacuum gap, as shown in Fig. 4.

It is shown above that the rate of heat transport by acoustic waves across a layered structure is determined by its reflectivity: if it is weak then the heat transport coefficient can be computed as $K = \Gamma/(1 + \Lambda)$ with Γ and Λ from (6.4) and (6.5); if the reflectivity is strong then K can be computed by (6.15), (6.16); and, in the general case K is represented by (6.19) – (6.21). Since we are interested in structures with a non-vanishing gap that have strong reflectivity, here we limit ourselves to computations of the heat transport coefficient by (6.15), (6.16).

In order to demonstrate how the parameters of the layered structure affect its thermal conductance we consider two basic structures with variable parameters. The first structure consists of a vacuum gap of variable width between iron and gold half spaces coated by diamond-like carbon layers of variable thickness. In the second basic structure the iron and gold half-spaces are replaced by 20 nm layers of iron and gold backed by the silicon and nickel half-space, respectively.

The results of the computations are shown in Fig. 5 which has six graphs forming three distinctive pairs. The top pair corresponds to structures without carbon overcoats, i.e. with overcoats of zero thickness. The middle and the bottom pairs correspond to the structures with 0.25 nm and 2 nm carbon layers, respectively. In all pairs, the solid lines correspond to the structures with iron and gold half-spaces, while the dashed lines correspond to the structures with iron and gold layers on silicon and nickel substrates.

Fig. 5 shows that the heat transport coefficient is very sensitive to the thickness of the carbon overcoats. This, however, is easily explained in terms of the reflection coefficient of acoustic waves. Indeed, formulas (6.15), (6.16) imply that the heat transport coefficient is determined by the function $r(\omega, \theta) = |R(\omega, \theta)|\sqrt{1 - |R(\omega, \theta)|^2}$, where $R(\omega, \theta)$ is the reflection coefficient of the wave with frequency ω and incidence angle θ. This quantity, averaged with the Planck's function used as a weight, is plotted in Fig. 6, where the two left subplots correspond to the structure with the iron and gold half-spaces, while the right subplots correspond to the structures with iron and gold layers on the silicon and nickel substrates. We see that the carbon overcoats drastically reduce the average value of $r(\omega, \theta)$, especially for the waves with other than normal incidence, which is not surprising because the interfaces between carbon and the other used materials have high reflectivity due to the sharp contrast between the sound speeds on the two sides of such interfaces.

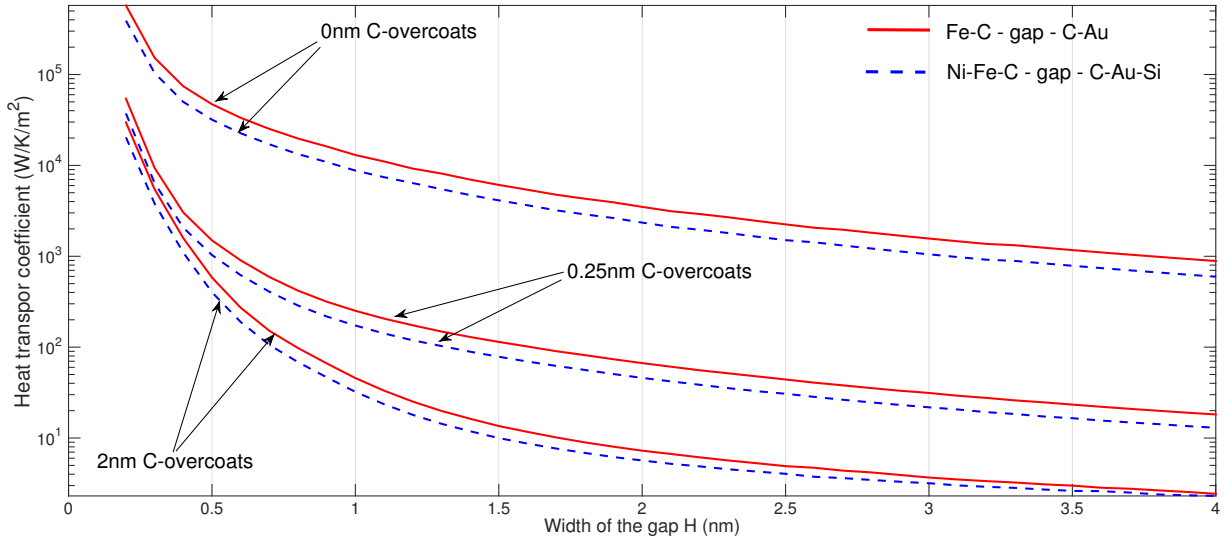


Figure 5: The heat transport coefficient

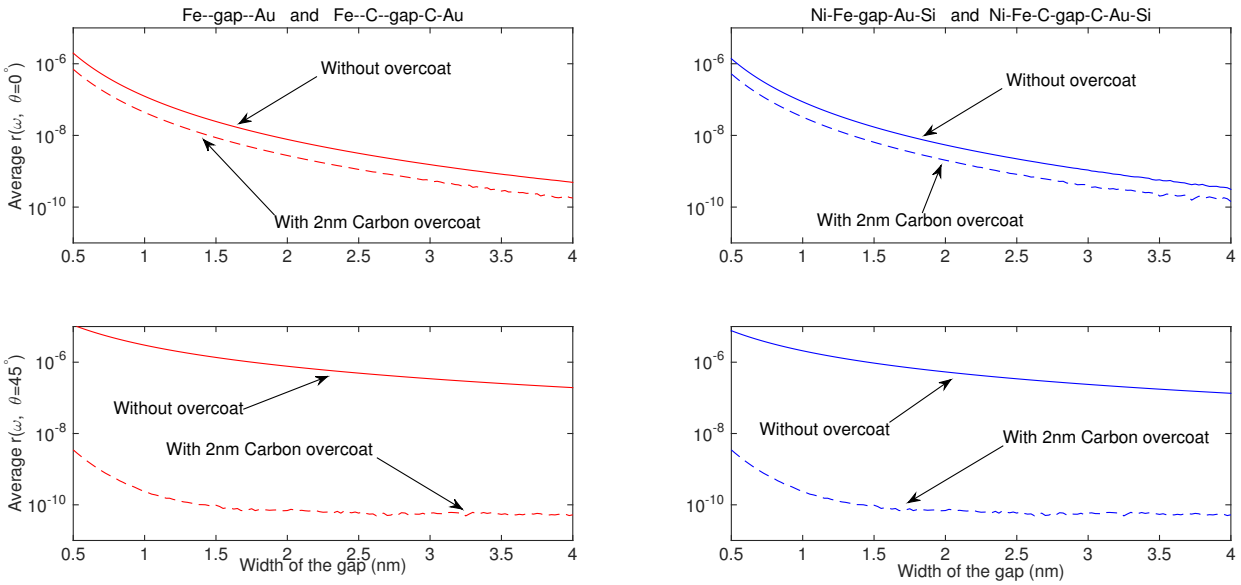


Figure 6: Reflection coefficients of layered structures with and without carbon overcoats

8 Conclusion

The proposed approach to nanoscale heat transport is applicable to the analysis of heat transport by acoustic waves in a virtually arbitrary nanoscale layered structure which may or may not include vacuum gaps. When this method is applied to special cases of large and closing gaps between identical materials, it reproduces analytically correct results. When this method is applied to a

system of two contacting half-spaces from different materials, it describes the interface thermal resistance, widely referred to as Kapitsa resistance. When applied to structures with a vacuum gap, it describes the phenomenon of heat transport by "phonon tunneling", which has attracted significant attention in recent years.

The developed method admits straightforward adaptation to the analysis of radiative heat transport carried by electromagnetic waves, and in this case its predictions agree with exact solutions for limiting cases, as well as with experiments [10]. Independently of whether heat is carried by acoustic or electromagnetic waves, the proposed method naturally explains the asymmetry of heat transport known as "thermal rectification", which currently attracts considerable attention because of the prospects of improving thermal management by the use of "thermal diodes".

The developed approach to heat transport by waves is applicable to a broad range of problems because it strictly follows the fundamental laws of physics and mathematics and avoids the use of unjustified simplifications. Thus, since the transport phenomena *a priori* deal with non equilibrium systems, this method describes spectra of thermal radiation by the generalization of the Planck law to systems with a heat flux. The tunneling of acoustic waves through a narrow gap is described in terms of the boundary value problem which takes into account van der Waals interactions of the separated bodies. Such tunneling has been discussed in the literature for a long time [18], but the possibility of its contribution to heat transport was proposed quite recently [3, 4] and then further developed in [5]. However, previous studies did not take into account the phases of thermally excited waves, which, as shown above, lead to the asymmetry of thermal transport interference of thermally excited waves arriving from different bodies.

The proposed method can be further developed into a practical tool, which may be applied to actual structures found in HAMR systems and in other nanoscale devices used for efficient thermal management.

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