Computation of radiative heat transport across a nanoscale vacuum gap

Bair V. Budaev[a] and David B. Bogy[b]
University of California, Etcheverry Hall, MC 1740, Berkeley, California 94720-1740, USA

(Received 27 September 2013; accepted 30 January 2014; published online 11 February 2014)

Radiation heat transport across a vacuum gap between two half-spaces is studied. By consistently applying only the fundamental laws of physics, we obtain an algebraic equation that connects the temperatures of the half-spaces and the heat flux between them. The heat transport coefficient generated by this equation for such structures matches available experimental data for nanoscale and larger gaps without appealing to any additional specific mechanisms of energy transfer. © *2014 AIP Publishing LLC*. [http://dx.doi.org/10.1063/1.4865404]

Let a vacuum layer $0 < x < H$ separate two half spaces A and B that are filled by identical materials and maintained at the temperatures T_A and T_B, respectively. If $T_A \neq T_B$, then there is a non-vanishing net heat flux $\vec{Q} = Q(H, T_A, T_B)\vec{e}_x$, where $\vec{e}_x$ is a unit vector along the x-axis, as shown in Fig. 1. The value of $Q(H, T_A, T_B)$ is determined by the temperatures T_A and T_B, by the width H, and by the material of the half-spaces. If $T_A = T_B$, then $Q(H, T_B, T_B) \equiv 0$. The heat transport coefficient of the gap can be defined as

$$K(H; T_B) = \left.\frac{\partial Q(H, T_A, T_B)}{\partial T_A}\right|_{T_A = T_B} \approx \frac{Q(H, T_A, T_B)}{T_A - T_B}. \qquad (1)$$

This problem has attracted attention since the discovery of the laws of thermal radiation. For a long time, it was accepted that $Q(H, T_A, T_B) = \gamma\sigma\left(T_A^4 - T_B^4\right)$, where σ is a universal constant and $\gamma \leq 1$ is a constant, characterizing the materials. In the late 1960s, it was demonstrated that as H decreases below the dominant wavelength of thermal radiation, the heat transport coefficient increases towards infinity.[1] The first studies of this phenomenon[2,3] were followed by the development of a rather general method that became the foundation for the modern conventional approach to nanoscale radiative heat transport.[4]

The method presented in Ref. 4 adopts the assumption that the thermal radiation is caused by extraneous electric and magnetic random currents whose statistical properties are described by the Fluctuation-Dissipation theorem.[5,6] This method has been applied to a number of problems, but it inherits a controversy of using the equilibrium distributions to the analysis of heat transport, which does not exist in equilibrium systems. This controversy is well-recognized,[7,8] but the methods of handling it are not yet established. Also, this method relies on a "manual" treatment of evanescent waves, the number of which drastically increases in configurations where the vacuum gap is replaced by a multi-layered structure.

The above comments justify the quest for an approach to radiative heat transport that does not rely on assumptions about the mechanisms of heat radiation, but relies only on fundamental laws of physics. Here, we propose an approach that does not require any more principles than are needed to derive Planck's law or the Stefan-Boltzmann law.

To calculate the heat transfer coefficient, we employ the following three-step procedure: (1) Assume that the temperature T_A and the net flux Q are known and compute the heat flux $Q_{A\to B}(T_A, Q)$ from A to B; (2) assume that T_B and Q are known and compute the heat flux $Q_{B\to A}(T_B, Q)$ from B to A; and (3) write the equation

$$Q = Q_{A\to B}(T_A, Q) - Q_{B\to A}(T_B, Q), \qquad (2)$$

and solve it for Q under the assumption that T_A and T_B are known.

It is shown in Ref. 9 that if there is a non-vanishing net heat flux $Q \neq 0$ then the heat radiations inside A and B are not isotropic, but depend on the (incidence) angle between the direction of radiation and the vector $\vec{e}_x$. More precisely, the results of Ref. 9 imply that if $Q \ll 1$, then inside A the thermally excited electromagnetic waves of a single polarization with the incident angle θ has the power spectrum

$$\mathcal{E}(\omega, T_A, Q, \theta) = \frac{1}{2} P\left(\frac{\omega}{1 + q_A\cos\theta}, T_A\right) D(\omega)\sin\theta, \qquad (3)$$

where $q_A = Q/cE_A$, $c(\omega)$ is the phase velocity of electromagnetic waves in the half-spaces, $P(\omega, T)$ is the average thermal energy of a harmonic oscillator at frequency ω in an equilibrium ensemble at temperature T,

$$D(\omega) = \frac{4\pi}{3}\frac{\mathrm{d}}{\mathrm{d}\omega}\left(\frac{\omega}{2\pi c(\omega)}\right)^3 = \frac{\omega^2}{2\pi^2 c^2(\omega) v(\omega)} \qquad (4)$$

is the density of states of electromagnetic fields of one polarization in an infinite half-space represented in terms of the group velocity

$$v(\omega) = c^2(\omega)/[c(\omega) - \omega c'(\omega)], \qquad (5)$$

and

$$E_A = 2\int_0^\infty \mathrm{d}\omega \int_0^\pi \mathcal{E}(\omega, T_A, Q, \theta)\mathrm{d}\theta \qquad (6)$$

is the energy density of thermally excited electromagnetic waves of both polarizations (accounted for by the factor

[a]Electronic mail: bair@berkeley.edu
[b]Electronic mail: dbogy@berkeley.edu

0003-6951/2014/104(6)/061109/4/$30.00

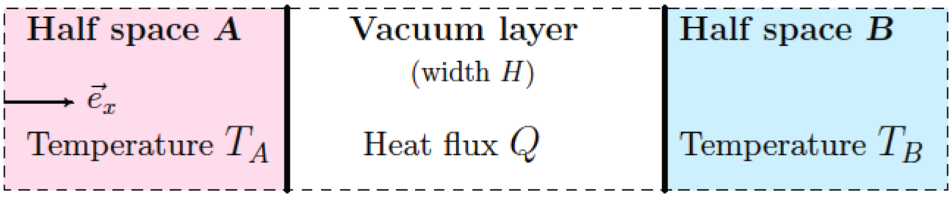

FIG. 1. The problem.

"2"), of all frequencies (accounted for by the integration over ω) and radiated in all directions (accounted for by the integration over θ). A small heat flux $Q \ll 1$ affects the energy density (6) only in the second order, so that in the first order approximation E_A is determined solely by the temperature of the medium.

In order to study the heat exchange between A and B, it is necessary to keep in mind that not all of the electromagnetic waves excited inside one domain carry energy to the other domain. Thus, although in A waves are radiated in all directions, only the waves with $0 \le \theta < \frac{\pi}{2}$ propagate towards B. Moreover, even a wave with $0 \le \theta < \frac{\pi}{2}$ does not deliver all of its energy to B because part of it is reflected back.

Let $R_\nu(\omega H, \theta)$ be the Fresnel reflection coefficient of a plane electromagnetic wave of frequency ω that has the incidence angle θ and a ν-polarization, where $\nu = \perp$ or $\nu = \|$. Then, only the $(1 - |R_\nu(\omega H, \theta)|^2)$-th part of the energy of this wave is transmitted to the domain B. Therefore, since the flux along $\vec{e}_x$ carried by a wave with the incidence angle θ and the energy density $\mathcal{E}$ has the value $\mathcal{Q} = \mathcal{E} v \cos\theta$, the total flux carried from A to B by waves of all polarizations, frequencies, and incidence angles can be represented as

$$Q_{A\to B}(T_A, Q) = \sum_{\nu=\perp,\|} \int_0^\infty \int_0^{\pi/2} v(\omega)\cos\theta \times \mathcal{E}(\omega, \theta, T_A, Q)\left(1 - |R_\nu(\omega H, \theta)|^2\right) \mathrm{d}\theta \mathrm{d}\omega. \tag{7}$$

Similarly, the heat flux $Q_{B\to A}(T_B, Q)$ radiated from B toward A is given by the expression

$$Q_{B\to A}(T_B, Q) = \sum_{\nu=\perp,\|} \int_0^\infty \int_0^{\pi/2} v(\omega)\cos\theta \times \mathcal{E}(\omega, \theta, T_B, -Q)\left(1 - |R_\nu(\omega H, \theta)|^2\right) \mathrm{d}\theta \mathrm{d}\omega, \tag{8}$$

which is obtained from (7) by the replacements of T_A and Q by T_B and $-Q$, respectively. Finally, inserting (7) and (8) into (2) and taking into account (3) with (4), we get the equation

$$Q = \int_0^\infty \int_0^{\pi/2} v(\omega)\sin 2\theta(1 - R^2(\omega H, \theta)) \times \left\{ P\left(\frac{\omega}{1 + Q\cos\theta/c(\omega)E_A}, T_A\right) - P\left(\frac{\omega}{1 - Q\cos\theta/c(\omega)E_B}, T_B\right)\right\} D(\omega) \mathrm{d}\theta \mathrm{d}\omega, \tag{9}$$

where

$$R^2(\omega H, \theta) = \frac{1}{2}\left\{ |R_\perp(\omega H, \theta)|^2 + |R_\|(\omega H, \theta)|^2 \right\} \tag{10}$$

appears as the sole characteristic of the considered structure.

Equation (9) connects the temperatures T_A and T_B with the heat flux Q. If Q and $\Delta T = T_A - T_B$ are small then Eq. (9) reduces to a linear equation,

$$Q = (T_A - T_B)F_0(H; T_B) - Q F_1(H; T_B) + o(Q), \tag{11}$$

with the explicitly defined coefficients

$$F_0 = \int_0^\infty \int_0^{\pi/2} \frac{G(\omega H, \theta) P'_T(\omega, T_B)}{2\pi^2 c^2(\omega)} \omega^2 \mathrm{d}\theta \mathrm{d}\omega, \tag{12}$$

$$F_1 = \int_0^\infty \int_0^{\pi/2} \frac{G(\omega H, \theta) P'_\omega(\omega, T_B)}{2\pi^2 c^3(\omega) E_B} \omega^2 \cos\theta \mathrm{d}\theta \mathrm{d}\omega, \tag{13}$$

where

$$G(\omega H, \theta) = \left\{1 - R^2(\omega H, \theta)\right\} \sin 2\theta. \tag{14}$$

Therefore, assuming that T_B and $\Delta T = T_A - T_B$ are known, we get the expression

$$K(H; T_B) = \frac{F_0(H; T_B)}{1 + F_1(H; T_B)}, \tag{15}$$

which explicitly defines the heat transport coefficient.

To use (12)–(15), it is necessary to know the phase velocity $c(\omega)$ and the reflection coefficients $R_\perp(\omega H, \theta)$, $R_\|(\omega H, \theta)$ of the vacuum gap of width H.

Let ϵ_0 and μ_0 be the permittivity and the permeability of vacuum. Similarly, let ϵ and μ be the corresponding parameters of the half-spaces. Then the phase speeds of electromagnetic waves in vacuum and the medium have the values $c_0 = 1/\sqrt{\epsilon_0 \mu_0}$, $c = 1/\sqrt{\epsilon\mu}$, and the reflection coefficients $R_\perp(\omega H, \theta)$ and $R_\|(\omega H, \theta)$ of the plane waves propagating in the half-spaces with the incident angles θ can be computed by the formulas[10]

$$|R_\nu(\xi, \theta)| = \frac{|(Y_\nu^2 - Z_\nu^2)\sin(\gamma\xi)|}{|(Y_\nu^2 + Z_\nu^2)\sin(\gamma\xi) + 2\mathrm{i} Z_\nu Y_\nu \cos(\gamma\xi)|}, \tag{16}$$

where $\xi \equiv \omega H$,

$$Z_\nu = \begin{cases} c\mu/\cos\theta, \\ c\mu\cos\theta, \end{cases} \quad Y_\nu = \begin{cases} c_0\mu_0/\cos\theta_0, & \text{if } \nu = \perp, \\ c_0\mu_0\cos\theta_0, & \text{if } \nu = \|, \end{cases} \tag{17}$$

and

$$\gamma = \frac{\cos\theta_0}{c_0}, \quad \cos\theta_0 = \sqrt{1 - \frac{c_0^2}{c^2}\cos^2\theta}. \tag{18}$$

In general, the dielectric parameters ϵ and μ have complex values and depend on the frequency ω, so that the complex refractive index $m(\omega) = c_0/c(\omega)$ can be represented as $m(\omega) = n(\omega) + ik(\omega)$, where $n(\omega)$ and $k(\omega)$ are usually referred to as the refractive and absorption indices, respectively. It is well known that $n(\omega)$ and $k(\omega)$ are related by the Kramers-Krönig relations, which, in particular, imply that the refractive index is constant if and only if the absorption index vanishes.[6]

The refractive and absorption indices of common materials are well studied, tabulated, and interpolated. For example, in Ref. 11, the indices of silica are interpolated for the frequencies from the extreme ultraviolet to far infrared. However, it is easy to see that the published data about the refraction and absorption indices describes propagation through a medium of electromagnetic waves generated by some external sources, but it does not adequately describe thermally excited electromagnetic fields inside bodies maintained at constant temperature.

Indeed, when an electromagnetic wave at frequency ω, such as a laser beam or a signal from a radar, propagates in a medium with the absorption index $k(\omega)$, the energy of the wave decays as $e^{-k(\omega)\omega L/c_0}$, where L is the travelled distance. The lost energy does not disappear but is transformed to heat, so that an external electromagnetic wave passing through a medium decays and heats the medium. On the other hand, the thermal radiation in a body maintained at fixed temperature neither gains nor looses energy. The electrons and protons inside the body move and radiate electromagnetic waves. While these waves propagate, part of their energy is absorbed by the matter, which means that it is converted to the energy of other charged particles, which then radiate other electromagnetic waves, etc.

In the steady state at constant temperature, the rate of absorption of thermally excited electromagnetic waves equals the rate of generation of such waves, so that these waves do not decay. Therefore, the absorption index of such waves vanishes and their refraction index becomes a frequency-independent constant.[6] The last statement implies that the phase velocity of thermally excited electromagnetic waves in half-spaces has a constant value which may be considered as a material parameter.

To verify the developed approach, we compare its outcome with the experimental data from Ref. 12 about radiative heat transfer between two closely separated bodies from silica. Since it is extremely difficult to maintain a nanoscale distance between two parallel plates, in these experiments the heat transport was measured between a plate and microspheres of 50 μm and 100 μm in diameter.

The bold dots in Fig. 2 show the results of the measurements from Ref. 12 of the heat transport coefficient between a plate and the sphere separated by $H = 30$ nm, 80 nm, and 200 nm. The thick line in Fig. 2 shows the heat transport coefficient computed by the formulas (12)–(15) for the case when the phase velocity of light in the half-spaces is set as $c = 0.45c_0$. Since our computations and the measurements from Ref. 12 correspond to different structures, the results cannot be directly compared to each other. However, as explained in Refs. 12 and 13, the heat transport coefficient between two plates separated by a nanoscale gap of the width H is about two times higher that the heat transport coefficient between a plate separated by the similar distance from a sphere used in the experiments reported in Ref. 12. Correspondingly, the dotted line in Fig. 2 is obtained by the reduction of the bold line by a factor of two, and it is seen that this line is in good agreement with the experimental data.

The developed method of computation of radiative heat transport across a vacuum gap can also be used for a qualitative analysis of the heat transport coefficient. In particular, it naturally explains the asymptotic behavior of $K(H)$ at both limits $H \to 0$ and $H \to \infty$.

Consider first, the limiting case of a vacuum layer of thickness $H = 0$. In this case, since the materials are the same, $R_\perp = R_\parallel = 0$, and Eq. (9) reduces to the form

$$Q = \frac{1}{\pi^2 c^2}\int_0^\infty [C_A(Q)P(\omega, T_A) - C_B(Q)P(\omega, T_B)]\omega^2 d\omega, \tag{19}$$

where, with the errors of the order $o(Q)$,

$$C_A(Q) \approx \frac{1}{2} + \frac{Q}{2cE_A}, \quad C_B(Q) \approx \frac{1}{2} - \frac{Q}{2cE_B}. \tag{20}$$

Then, incorporating (20) into (19) we get the equation $Q = Q + C_*(T_A^4 - T_B^4) + o(Q)$, which shows that to first-order accuracy, the temperatures must coincide $T_A = T_B$ while the heat flux Q may take any value. This means that the vacuum layer of zero thickness has an infinite heat transport coefficient, which agrees with common sense and with the observation that in a homogeneous space a finite heat flux may exist without any temperature differential.[14]

In a case of a narrow vacuum gap with $H \ll 1$, the reflection coefficient admits the estimate $R(\omega H, \theta) \sim H$, which makes it possible to reduce Eq. (19) to the form

$$\begin{aligned} C_*(T_A^4 - T_B^4) + H^2[f(T_A, Q, E_A) \\ - f(T_B, -Q, E_B)] + o(Q) = 0, \end{aligned} \tag{21}$$

where

$$f(T, Q, E) = \frac{1}{2\pi^2 c^2}\int_0^\infty \int_0^{\pi/2} \frac{R^2(\omega H, \theta)}{H^2} \times P\left(\frac{\omega}{1 + Q\cos\theta/cE}, T\right)\omega^2 \sin 2\theta \, d\theta d\omega, \tag{22}$$

remains finite as $H \to 0$. In this case, (21) implies that if $T_A = T_B$ then $Q = 0$, and if $T_A \neq T_B$ then $Q \sim (T_A - T_B)/H^2$, so that the heat transport coefficient of the narrow gap is proportional to $\sim 1/H^2$, which agrees with the experiments from Ref. 12.

As H increases to infinity, $R^2(\omega H, \theta)$ becomes a highly oscillating periodic function of ω, which implies that if $f(\omega)$ is continuous, then, as $H \to \infty$,

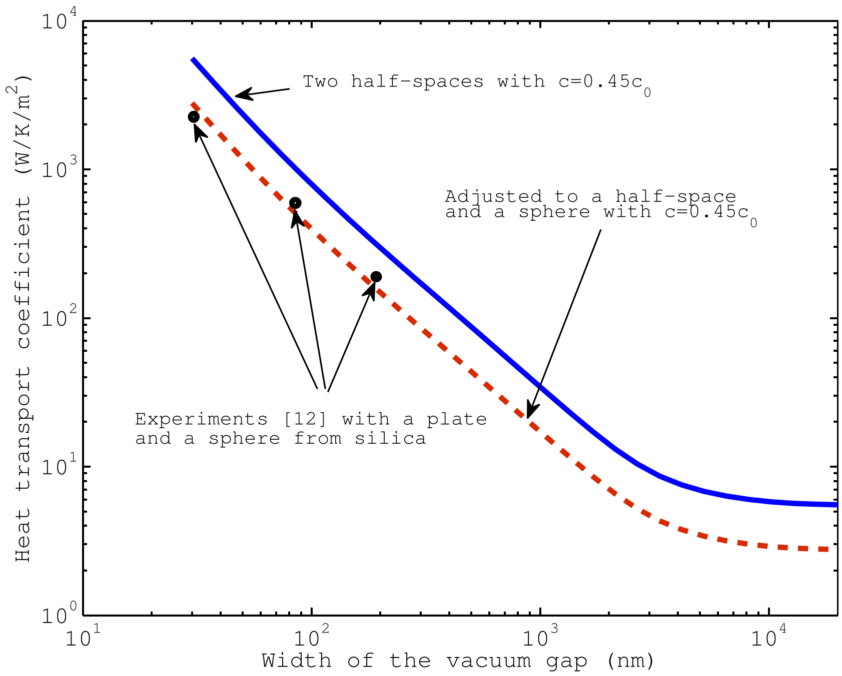

FIG. 2. Heat transport coefficient $K(H)$ of the vacuum gap of the width H. In Ref. 12, it is reported that $K(H)$ at $H = 30$ nm and at $H \to \infty$ has the values $K = 2230\ \mathrm{W/m^2}/K$ and $K = 3.8\ \mathrm{W/m^2}/K$, respectively. The values of $K(H)$ at $H = 80$ nm and $H = 200$ nm are read from Ref. 12, Fig. 4.

$$\int_0^\infty R^2(\omega H, \theta) f(\omega) \mathrm{d}\omega \to r^2(\theta) \int_0^\infty f(\omega) \mathrm{d}\omega, \qquad (23)$$

where $r^2(\theta)$ is the mean value of $R^2(\omega, \theta)$ over all ω. This shows that as H increases, the heat transport coefficient $K(H)$ becomes independent on H.

Despite the simplicity of the proposed method of computation of the heat transport coefficient $K(H)$, the results presented in Fig. 2 not only agree with results from [Ref. 12, Fig. 1(c)] and [Ref. 2, Fig. 4] but also naturally explain the asymptotes of $K(H)$ at two limits $H \to 0$ and $H \to \infty$ without appealing to any specific mechanisms of energy transfer.

The proposed method is based on the extension of the Planck's laws of thermal radiation to systems with a steady heat flux and on the observation that the thermally excited electromagnetic field in the matter should be described in terms of the dielectric functions with a vanishing imaginary part. The proposed method is versatile and admits applications to other similar problems, such as the radiative heat transport across a layered structure between half-spaces of different materials,[15] interface "Kapitsa" thermal resistance,[16] and phonon heat conductance across a sub-10 nm vacuum gap, just to mention a few. The short format of this initial report does not allow our consideration of all of these important applications, but we expect that the demonstrated result will encourage widespread applications of the developed method to such systems.

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

[1] C. M. Hargreaves, Phys. Lett. A **30**(9), 491–492 (1969).
[2] E. G. Cravalho, C. L. Tien, and R. P. Caren, J. Heat Transfer **89**(3), 351–358 (1967).
[3] R. F. Boehm and C. L. Tien, J. Heat Transfer **92**(3), 405–411 (1970).
[4] D. Polder and N. van Hove, Phys. Rev. B **4**(10), 3303–3314 (1971).
[5] S. M. Rytov, *Theory of electric fluctuations and thermal radiation* (Air Force Cambridge Research Center, Bedford, MA, 1959).
[6] L. D. Landau and E. M. Lifshitz, *Electrodynamics of Continuous Media*, Course of Theoretical Physics Vol. 8 (Pergamon Press, 1960).
[7] S. M. Rytov, Yu. A. Kravtsov, and V. I. Tatatarskii, *Principles of Statistical Radiophysics. 3. Elements of Random Fields* (Springer-Verlag, Berlin-Heidelberg-New York, 1987).
[8] M. Messina and R. Antezza, Europhys. Lett. **95**(6), 61002 (2011).
[9] B. V. Budaev and D. B. Bogy, Ann. Phys. **523**(10), 791–804 (2011).
[10] L. M. Brekhovskikh, *Waves in Layered Media*, Applied Mathematics and Mechanics Vol. 16 (Academic Press, New York, 1980).
[11] R. Kitamura, L. Pilon, and M. Jonasz, Appl. Opt. **46**(33), 8118–8133 (2007).
[12] S. Shen, A. Narayanaswamy, and G. Chen, Nano Lett. **9**(8), 2909–2913 (2009).
[13] S. Shen, private communication (2013).
[14] M. Born, *Atomic Physics*, 8th ed. (Dover, 1989).
[15] S. I. Maslovski, C. R. Simovski, and S. A. Tretyakov, Phys. Rev. B **87**, 155124 (2013).
[16] P. L. Kapitsa, J. Phys. (USSR) **4**, 181–210 (1941).