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Thermal Networks from Phonon Boltzmann's Transport Equation: Part I – Fundamentals

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Abstract—Thermal networks are introduced from the gray phonon Boltzmann's transport equation. A reference thermal network is then investigated. It is shown that the responses of this thermal network cannot be accurately approximated by the responses of the thermal networks from either the heat diffusion or the heat wave equations.

I. INTRODUCTION

Much efforts are reported in literature for investigating thermal networks [1], [2]. In almost all these works heat transfer is assumed to be modelled by the heat diffusion equation. Heat transfer is due to phonons, at least in dielectrics and semiconductors and the heat diffusion equation is not accurate in predicting the distribution of phonons under the following conditions [3]:

- (a) when the mean free path of the phonons become comparable to or larger than the characteristic length scale of the problem;
- (b) when the time scale of the problem becomes comparable to or smaller than the relaxation time of the phonons.

If only condition (b) holds, the heat wave equation [4] can be used for predicting the distribution of phonons. However if both conditions (a) and (b) hold, as in problems of semiconductor technology, Boltzmann's transport equation has to be used [5], [6], [8], provided the wave nature of the phonons can be neglected.

A few works have been reported in literature for defining thermal networks from the heat wave equation [4]. However, as far as we know, no works have been done for defining thermal networks from the phonon Boltzmann's transport equation. In this paper we tackle this question.

Firstly the gray phonon Boltzmann's transport equation is introduced. Secondly boundary conditions are introduced in such a way the limit equation of the transport equation is the heat wave equation.

The thermal networks from the transport equation are then introduced. These thermal networks are shown to preserve the thermodynamic properties of the transport equation. They can be used also as boundary condition independent models.

A reference thermal network from the transport equation is then considered. Its response is determined in closed form and is compared to the responses of the thermal networks from both the heat diffusion equation and the heat wave equation. In such a way it is shown that the responses of the thermal network from the transport equation cannot be accurately approximated by the responses of the thermal networks from either the heat diffusion or the heat wave equations.

II. TRANSPORT EQUATION

Let Σ be a spatially *homogeneous* region. Let \mathbf{r} be the position vector and $\boldsymbol{\Omega}$ be the direction vector. The energy density rise $e(\mathbf{r}, \boldsymbol{\Omega}, t)$ with respect to a *reference* energy density is assumed to be ruled by the gray phonon Boltzmann's transport equation [3], [5], [6]

$$\frac{\partial e}{\partial t}(\mathbf{r}, \boldsymbol{\Omega}, t) + v\boldsymbol{\Omega} \cdot \nabla e(\mathbf{r}, \boldsymbol{\Omega}, t) + \frac{e(\mathbf{r}, \boldsymbol{\Omega}, t) - \langle e(\mathbf{r}, \boldsymbol{\Omega}, t) \rangle}{\tau} = g(\mathbf{r}, \boldsymbol{\Omega}, t) \quad (1)$$

in which $g(\mathbf{r}, \boldsymbol{\Omega}, t)$ is the source density and

$$\langle e(\mathbf{r}, \boldsymbol{\Omega}, t) \rangle = \frac{1}{4\pi} \int_{4\pi} e(\mathbf{r}, \boldsymbol{\Omega}, t) d\boldsymbol{\Omega}.$$

The material properties are the phonon group velocity v , the relaxation time τ , the phonon mean free path $l = v\tau$, the volumetric heat capacity c and the thermal conductivity $k = cvl/3$. In the following table reference values are reported for silicon:

v	$6.40 \cdot 10^3$ m/s
τ	$6.28 \cdot 10^{-12}$ s
l	$4.02 \cdot 10^{-8}$ m
c	$1.66 \cdot 10^6$ J/m ³ K
k	$1.42 \cdot 10^2$ W/m K

With this equation, all phonons are grouped together in one mode and characterized by a single group velocity and relaxation time. No distinction is made between the different phonon modes.

The temperature rise $x(\mathbf{r}, t)$ with respect to the reference temperature and the heat flux $\mathbf{q}(\mathbf{r}, t)$ are functions of $e(\mathbf{r}, \boldsymbol{\Omega}, t)$, as follows

$$x(\mathbf{r}, t) = \frac{4\pi}{c} \langle e(\mathbf{r}, \boldsymbol{\Omega}, t) \rangle, \\ \mathbf{q}(\mathbf{r}, t) = 4\pi v \langle \boldsymbol{\Omega} e(\mathbf{r}, \boldsymbol{\Omega}, t) \rangle.$$

Hereafter it will turn out to be useful to rewrite Eq. (1) in its *even-parity* formulation [7]

$$\frac{\partial e^+}{\partial t}(\mathbf{r}, \boldsymbol{\Omega}, t) + v\boldsymbol{\Omega} \cdot \nabla e^-(\mathbf{r}, \boldsymbol{\Omega}, t) + \frac{e^+(\mathbf{r}, \boldsymbol{\Omega}, t) - \langle e^+(\mathbf{r}, \boldsymbol{\Omega}, t) \rangle}{\tau} = g^+(\mathbf{r}, \boldsymbol{\Omega}, t) \\ \frac{\partial e^-}{\partial t}(\mathbf{r}, \boldsymbol{\Omega}, t) + v\boldsymbol{\Omega} \cdot \nabla e^+(\mathbf{r}, \boldsymbol{\Omega}, t) + \frac{e^-(\mathbf{r}, \boldsymbol{\Omega}, t) - \langle e^-(\mathbf{r}, \boldsymbol{\Omega}, t) \rangle}{\tau} = g^-(\mathbf{r}, \boldsymbol{\Omega}, t)$$

in which the even (+) and odd (−) operators are defined as follows

$$e^+(\mathbf{r}, \mathbf{\Omega}, t) = \frac{e(\mathbf{r}, \mathbf{\Omega}, t) + e(\mathbf{r}, -\mathbf{\Omega}, t)}{2},$$

$$e^-(\mathbf{r}, \mathbf{\Omega}, t) = \frac{e(\mathbf{r}, \mathbf{\Omega}, t) - e(\mathbf{r}, -\mathbf{\Omega}, t)}{2}.$$

III. BOUNDARY CONDITIONS

Conditions on the boundary $\partial\Sigma$ of the Σ region have to be introduced for the transport equation [8]. Hereafter we show how the boundary conditions for the heat diffusion equation can be extended to the transport equation.

Let \mathbf{n} be a unit vector normal to surface Γ at a point \mathbf{r} . Let

$$\mathbf{\Omega}^n = \mathbf{\Omega} - 2(\mathbf{\Omega} \cdot \mathbf{n})\mathbf{n}$$

be the unit vector symmetric of $\mathbf{\Omega}$ with respect to Γ at \mathbf{r} . The energy density rise $e(\mathbf{r}, \mathbf{\Omega}, t)$ can be written at \mathbf{r} as the sum of two terms

$$e(\mathbf{r}, \mathbf{\Omega}, t) = e^t(\mathbf{r}, \mathbf{\Omega}, t) + e^n(\mathbf{r}, \mathbf{\Omega}, t) \quad (2)$$

in which

$$e^t(\mathbf{r}, \mathbf{\Omega}, t) = \frac{e(\mathbf{r}, \mathbf{\Omega}, t) + e(\mathbf{r}, \mathbf{\Omega}^n, t)}{2}$$

$$e^n(\mathbf{r}, \mathbf{\Omega}, t) = \frac{e(\mathbf{r}, \mathbf{\Omega}, t) - e(\mathbf{r}, \mathbf{\Omega}^n, t)}{2}$$

Using the geometrical relations

$$\mathbf{\Omega}^n \cdot \mathbf{n} = -\mathbf{\Omega} \cdot \mathbf{n},$$

$$(\mathbf{n} \times \mathbf{\Omega}^n) \times \mathbf{n} = (\mathbf{n} \times \mathbf{\Omega}) \times \mathbf{n},$$

it is straightforward to show that

$$x(\mathbf{r}, t) = \frac{4\pi \langle e^t(\mathbf{r}, \mathbf{\Omega}, t) \rangle}{c}$$

$$\mathbf{q}(\mathbf{r}, t) \cdot \mathbf{n} = 4\pi v \langle \mathbf{\Omega} \cdot \mathbf{n} e^n(\mathbf{r}, \mathbf{\Omega}, t) \rangle.$$

Thus $e^t(\mathbf{r}, \mathbf{\Omega}, t)/c$ defines the temperature rise $x(\mathbf{r}, t)$ and $v\mathbf{\Omega} \cdot \mathbf{n} e^n(\mathbf{r}, \mathbf{\Omega}, t)$ defines the component $\mathbf{q}(\mathbf{r}, t) \cdot \mathbf{n}$ of the heat flux normal to Γ .

As a result, boundary conditions for the heat diffusion equation can be transformed into boundary conditions for the transport equation (1), by substituting $x(\mathbf{r}, t)$ into $e^t(\mathbf{r}, \mathbf{\Omega}, t)/c$ and $\mathbf{q}(\mathbf{r}, t) \cdot \mathbf{n}$ into $v\mathbf{\Omega} \cdot \mathbf{n} e^n(\mathbf{r}, \mathbf{\Omega}, t)$.

In this way, for instance, Dirichlet's and Neumann's boundary conditions for the heat diffusion equation are transformed respectively into

$$e^t(\mathbf{r}, \mathbf{\Omega}, t) = f^t(\mathbf{r}, \mathbf{\Omega}, t), \quad (3)$$

$$e^n(\mathbf{r}, \mathbf{\Omega}, t) = f^n(\mathbf{r}, \mathbf{\Omega}, t), \quad (4)$$

$f^t(\mathbf{r}, \mathbf{\Omega}, t)$ and $f^n(\mathbf{r}, \mathbf{\Omega}, t)$ being assigned distributions.

In this way also, if Σ is not spatially homogeneous but composed of spatially homogeneous sub-regions, so that the material properties are *piecewise linear* functions of \mathbf{r} , then the boundary conditions for the heat diffusion equation at the interface of two different materials are transformed into

$$\left[\frac{e^t(\mathbf{r}, \mathbf{\Omega}, t)}{c(\mathbf{r})} \right] = 0, \quad (5)$$

$$[v(\mathbf{r})e^n(\mathbf{r}, \mathbf{\Omega}, t)] = 0, \quad (6)$$

in which the brackets indicate the jump passing from one side of the interface to the other.

IV. THERMODYNAMIC PROPERTIES

Hereafter we assume that the Σ region is composed of spatially homogeneous sub-regions Σ_i . In each of these sub-region, Eq. (1) holds. At each interface separating homogeneous sub-regions, boundary conditions (5), (6) hold. On one part of the boundary $\partial\Sigma$ of Σ , boundary condition (3) is assumed. On the other part of $\partial\Sigma$ boundary condition (4) is assumed.

It is straightforward to show that the non-homogeneous boundary condition (3) is equivalent to the homogeneous boundary condition, after introducing a superficial source distribution $v(\mathbf{r}) \mathbf{\Omega} \cdot \mathbf{n} f^t(\mathbf{r}, \mathbf{\Omega}, t)$. In a similar way, the non-homogeneous boundary condition (4) is equivalent to the homogeneous boundary condition after introducing a superficial source distribution $v(\mathbf{r}) \mathbf{\Omega} \cdot \mathbf{n} f^n(\mathbf{r}, \mathbf{\Omega}, t)$. Thus we can assume that boundary conditions (3), (4) are homogeneous.

The transport equation introduced in this way satisfies the following *thermodynamic* properties.

Property 1 (Passivity): For each time interval $t_1 \leq t \leq t_2$ it results in

$$W(t_2) \leq W(t_1) + \int_{t_1}^{t_2} dt \int_{\Sigma} \frac{4\pi \langle g(\mathbf{r}, \mathbf{\Omega}, t) e(\mathbf{r}, \mathbf{\Omega}, t) \rangle}{c(\mathbf{r})} d\mathbf{r},$$

$W(t)$ being the nonnegative quantity

$$W(t) = \int_{\Sigma} \frac{2\pi \langle e^2(\mathbf{r}, \mathbf{\Omega}, t) \rangle}{c(\mathbf{r})} d\mathbf{r}.$$

Proof: Multiplying Eq. (1) by $e(\mathbf{r}, \mathbf{\Omega}, t)/c(\mathbf{r})$ and by taking the mean with respect to $\mathbf{\Omega}$, it follows

$$\frac{\partial}{\partial t} \frac{\langle e^2(\mathbf{r}, \mathbf{\Omega}, t) \rangle}{2c(\mathbf{r})} + \frac{\langle (e(\mathbf{r}, \mathbf{\Omega}, t) - \langle e(\mathbf{r}, \mathbf{\Omega}, t) \rangle)^2 \rangle}{c(\mathbf{r})\tau(\mathbf{r})} + \nabla \cdot \left(\frac{v(\mathbf{r}) \langle \mathbf{\Omega} e^2(\mathbf{r}, \mathbf{\Omega}, t) \rangle}{2c(\mathbf{r})} \right) = \frac{\langle g(\mathbf{r}, \mathbf{\Omega}, t) e(\mathbf{r}, \mathbf{\Omega}, t) \rangle}{c(\mathbf{r})}$$

By integrating with respect to \mathbf{r} over each homogeneous region Σ_i , it follows

$$\frac{d}{dt} \int_{\Sigma_i} \frac{\langle e^2(\mathbf{r}, \mathbf{\Omega}, t) \rangle}{2c(\mathbf{r})} d\mathbf{r} + \int_{\Sigma_i} \frac{\langle (e(\mathbf{r}, \mathbf{\Omega}, t) - \langle e(\mathbf{r}, \mathbf{\Omega}, t) \rangle)^2 \rangle}{c(\mathbf{r})\tau(\mathbf{r})} d\mathbf{r} + \int_{\partial\Sigma_i} \frac{v(\mathbf{r}) \langle \mathbf{\Omega} \cdot \mathbf{n} e^2(\mathbf{r}, \mathbf{\Omega}, t) \rangle}{2c(\mathbf{r})} d\mathbf{r} = \int_{\Sigma_i} \frac{\langle g(\mathbf{r}, \mathbf{\Omega}, t) e(\mathbf{r}, \mathbf{\Omega}, t) \rangle}{c(\mathbf{r})} d\mathbf{r}.$$

By summing these equations for all the homogeneous regions Σ_i , since

$$\int_{\partial\Sigma_i} \frac{v(\mathbf{r}) \langle \mathbf{\Omega} \cdot \mathbf{n} e^2(\mathbf{r}, \mathbf{\Omega}, t) \rangle}{2c(\mathbf{r})} d\mathbf{r} = \int_{\partial\Sigma_i} \frac{v(\mathbf{r}) \langle \mathbf{\Omega} \cdot \mathbf{n} e^t(\mathbf{r}, \mathbf{\Omega}, t) e^n(\mathbf{r}, \mathbf{\Omega}, t) \rangle}{c(\mathbf{r})} d\mathbf{r},$$

since $v(\mathbf{r})e^n(\mathbf{r}, \mathbf{\Omega}, t)$ and $e^t(\mathbf{r}, \mathbf{\Omega}, t)/c(\mathbf{r})$ are continuous across the interfaces separating homogeneous regions Σ_i and since either $e^t(\mathbf{r}, \mathbf{\Omega}, t)$ or $e^n(\mathbf{r}, \mathbf{\Omega}, t)$ are zeros on the boundary $\partial\Sigma$, it results in

$$\frac{d}{dt} \int_{\Sigma} \frac{\langle e^2(\mathbf{r}, \mathbf{\Omega}, t) \rangle}{2c(\mathbf{r})} d\mathbf{r} + \int_{\Sigma} \frac{\langle (e(\mathbf{r}, \mathbf{\Omega}, t) - \langle e(\mathbf{r}, \mathbf{\Omega}, t) \rangle)^2 \rangle}{c(\mathbf{r})\tau(\mathbf{r})} d\mathbf{r} = \int_{\Sigma} \frac{\langle g(\mathbf{r}, \mathbf{\Omega}, t) e(\mathbf{r}, \mathbf{\Omega}, t) \rangle}{c(\mathbf{r})} d\mathbf{r}.$$

Integrating this equation with respect to time for $t_1 \leq t \leq t_2$ and multiplying by 4π , the thesis follows. ■

Property 2 (Reciprocity): In the Laplace transform domain s , for any couple of situations $\mathbf{g}_1(\mathbf{r}, \boldsymbol{\Omega}, s)$, $\mathbf{e}_1(\mathbf{r}, \boldsymbol{\Omega}, s)$ and $\mathbf{g}_2(\mathbf{r}, \boldsymbol{\Omega}, s)$, $\mathbf{e}_2(\mathbf{r}, \boldsymbol{\Omega}, s)$ it results in

$$\begin{aligned} \int_{\Sigma} \frac{4\pi \langle \mathbf{g}_1(\mathbf{r}, \boldsymbol{\Omega}, s) \mathbf{e}_2(\mathbf{r}, -\boldsymbol{\Omega}, s) \rangle}{c(\mathbf{r})} d\mathbf{r} &= \\ &= \int_{\Sigma} \frac{4\pi \langle \mathbf{g}_2(\mathbf{r}, \boldsymbol{\Omega}, s) \mathbf{e}_1(\mathbf{r}, -\boldsymbol{\Omega}, s) \rangle}{c(\mathbf{r})} d\mathbf{r} \end{aligned}$$

Proof: Multiplying by $\mathbf{e}_2(\mathbf{r}, -\boldsymbol{\Omega}, s)/c(\mathbf{r})$ the Laplace transform of Eq. (1), with source density $\mathbf{g}_1(\mathbf{r}, \boldsymbol{\Omega}, s)$ and energy density $\mathbf{e}_1(\mathbf{r}, \boldsymbol{\Omega}, s)$, by taking the mean with respect to $\boldsymbol{\Omega}$ and by integrating with respect to \mathbf{r} over each sub-region Σ_i it results in

$$\begin{aligned} s \int_{\Sigma_i} \frac{\langle \mathbf{e}_1(\mathbf{r}, \boldsymbol{\Omega}, s) \mathbf{e}_2(\mathbf{r}, -\boldsymbol{\Omega}, s) \rangle}{2c(\mathbf{r})} d\mathbf{r} + \\ + \int_{\Sigma_i} \frac{\langle \mathbf{e}_1(\mathbf{r}, \boldsymbol{\Omega}, s) \mathbf{e}_2(\mathbf{r}, -\boldsymbol{\Omega}, s) \rangle - \langle \mathbf{e}_1(\mathbf{r}, \boldsymbol{\Omega}, s) \rangle \langle \mathbf{e}_2(\mathbf{r}, -\boldsymbol{\Omega}, s) \rangle}{c(\mathbf{r})\tau(\mathbf{r})} d\mathbf{r} + \\ + \int_{\Sigma_i} \frac{v(\mathbf{r}) \langle \boldsymbol{\Omega} \cdot \nabla \mathbf{e}_1(\mathbf{r}, \boldsymbol{\Omega}, s) \mathbf{e}_2(\mathbf{r}, -\boldsymbol{\Omega}, s) \rangle}{c(\mathbf{r})} d\mathbf{r} = \\ = \int_{\Sigma_i} \frac{\langle \mathbf{g}_1(\mathbf{r}, \boldsymbol{\Omega}, s) \mathbf{e}_2(\mathbf{r}, -\boldsymbol{\Omega}, s) \rangle}{c(\mathbf{r})} d\mathbf{r} \end{aligned}$$

By subtracting this equation to the equation obtained by exchanging indices 1 and 2 it results in

$$\begin{aligned} \int_{\Sigma_i} \frac{\langle \mathbf{g}_1(\mathbf{r}, \boldsymbol{\Omega}, s) \mathbf{e}_2(\mathbf{r}, -\boldsymbol{\Omega}, s) - \mathbf{g}_2(\mathbf{r}, \boldsymbol{\Omega}, s) \mathbf{e}_1(\mathbf{r}, -\boldsymbol{\Omega}, s) \rangle}{c(\mathbf{r})} d\mathbf{r} = \\ = \int_{\partial\Sigma_i} \frac{v(\mathbf{r}) \langle \boldsymbol{\Omega} \cdot \mathbf{n} \mathbf{e}_1(\mathbf{r}, \boldsymbol{\Omega}, s) \mathbf{e}_2(\mathbf{r}, -\boldsymbol{\Omega}, s) \rangle}{c(\mathbf{r})} d\mathbf{r} \end{aligned}$$

By summing these equations for all the homogeneous regions Σ_i multiplied by 4π , since

$$\begin{aligned} \int_{\partial\Sigma_i} \frac{v(\mathbf{r}) \langle \boldsymbol{\Omega} \cdot \mathbf{n} \mathbf{e}_1(\mathbf{r}, \boldsymbol{\Omega}, s) \mathbf{e}_2(\mathbf{r}, -\boldsymbol{\Omega}, s) \rangle}{2c(\mathbf{r})} d\mathbf{r} = \\ = \int_{\partial\Sigma_i} \frac{v(\mathbf{r}) \langle \boldsymbol{\Omega} \cdot \mathbf{n} \mathbf{e}_1^t(\mathbf{r}, \boldsymbol{\Omega}, s) \mathbf{e}_2^n(\mathbf{r}, -\boldsymbol{\Omega}, s) \rangle}{4c(\mathbf{r})} d\mathbf{r} + \\ + \int_{\partial\Sigma_i} \frac{v(\mathbf{r}) \langle \boldsymbol{\Omega} \cdot \mathbf{n} \mathbf{e}_2^t(\mathbf{r}, -\boldsymbol{\Omega}, s) \mathbf{e}_1^n(\mathbf{r}, \boldsymbol{\Omega}, s) \rangle}{4c(\mathbf{r})} d\mathbf{r}, \end{aligned}$$

since $v(\mathbf{r})\mathbf{e}_1^n(\mathbf{r}, \boldsymbol{\Omega}, s)$, $v(\mathbf{r})\mathbf{e}_2^n(\mathbf{r}, \boldsymbol{\Omega}, s)$, $\mathbf{e}_1^t(\mathbf{r}, \boldsymbol{\Omega}, s)/c(\mathbf{r})$ and $\mathbf{e}_2^t(\mathbf{r}, \boldsymbol{\Omega}, s)/c(\mathbf{r})$ are continuous across the interfaces separating homogeneous regions Σ_i and since either $\mathbf{e}_1^t(\mathbf{r}, \boldsymbol{\Omega}, s)$ and $\mathbf{e}_2^t(\mathbf{r}, \boldsymbol{\Omega}, s)$ or $\mathbf{e}_1^n(\mathbf{r}, \boldsymbol{\Omega}, s)$ and $\mathbf{e}_2^n(\mathbf{r}, \boldsymbol{\Omega}, s)$ are zeros on the boundary $\partial\Sigma$, the thesis follows. ■

V. LIMIT EQUATION

The linear transport equation reduces to the heat wave equation when the geometric scale of the problem are larger than the phonon mean free path [9]. Precisely from the even-parity formulation of the transport equation, by assuming

$$g^-(\mathbf{r}, \boldsymbol{\Omega}, t) = 0, \quad (7)$$

$$e^+(\mathbf{r}, \boldsymbol{\Omega}, t) = c(\mathbf{r})x(\mathbf{r}, t), \quad (8)$$

$$e^-(\mathbf{r}, \boldsymbol{\Omega}, t) = \frac{3}{v(\mathbf{r})}\boldsymbol{\Omega} \cdot \mathbf{q}(\mathbf{r}, t), \quad (9)$$

it follows within each Σ_i homogeneous sub-region

$$c(\mathbf{r}) \frac{\partial x(\mathbf{r}, t)}{\partial t} + \nabla \cdot \mathbf{q}(\mathbf{r}, t) = g(\mathbf{r}, t) \quad (10)$$

$$\frac{1}{\tau(\mathbf{r})} \frac{\partial \mathbf{q}(\mathbf{r}, t)}{\partial t} + \mathbf{q}(\mathbf{r}, t) = -k(\mathbf{r}) \nabla x(\mathbf{r}, t) \quad (11)$$

in which

$$g(\mathbf{r}, t) = 4\pi \langle g^+(\mathbf{r}, \boldsymbol{\Omega}, t) \rangle.$$

Boundary conditions (5), (6) at the interfaces separating homogeneous regions Σ_i become respectively

$$[x(\mathbf{r}, t)] = 0,$$

$$[\mathbf{q}(\mathbf{r}, t) \cdot \mathbf{n}] = 0.$$

Conditions (3), (4) at the boundary $\partial\Sigma$, assumed homogeneous, become respectively homogeneous Dirichlet's and Neumann's boundary conditions

$$x(\mathbf{r}, t) = 0,$$

$$\mathbf{q}(\mathbf{r}, t) \cdot \mathbf{n} = 0.$$

All these equations define the heat wave equations, which is thus the limit of the transport equation.

Besides the thermodynamic properties for the transport equation reduce to the thermodynamic properties for the heat wave equation. In fact, from Eqs. (7), (8), (9), Properties 1, 2 reduce to the following

Property 3 (Passivity): For each time interval $t_1 \leq t \leq t_2$ it results in

$$W(t_2) \leq W(t_1) + \int_{t_1}^{t_2} dt \int_{\Sigma} g(\mathbf{r}, t) x(\mathbf{r}, t) d\mathbf{r},$$

$W(t)$ being the nonnegative quantity

$$W(t) = \frac{1}{2} \int_{\Sigma} c(\mathbf{r}) x^2(\mathbf{r}, t) + \frac{\tau(\mathbf{r})}{k(\mathbf{r})} \mathbf{q}^2(\mathbf{r}, t) d\mathbf{r}.$$

Property 4 (Reciprocity): In the Laplace transform domain s , for any couple of situations $\mathbf{g}_1(\mathbf{r}, s)$, $\mathbf{x}_1(\mathbf{r}, s)$ and $\mathbf{g}_2(\mathbf{r}, s)$, $\mathbf{x}_2(\mathbf{r}, s)$ it results in

$$\int_{\Sigma} \mathbf{g}_1(\mathbf{r}, s) \mathbf{x}_2(\mathbf{r}, s) d\mathbf{r} = \int_{\Sigma} \mathbf{g}_2(\mathbf{r}, s) \mathbf{x}_1(\mathbf{r}, s) d\mathbf{r}$$

VI. THERMAL NETWORKS

Thermal networks are now introduced from the transport equation by defining its powers and temperature rises. The source term is supposed to be given by

$$g^+(\mathbf{r}, \boldsymbol{\Omega}, t) = \sum_i^{n^+} \mathbf{f}^+(\mathbf{r}, \boldsymbol{\Omega}) \mathbf{P}^+(t) \quad (12)$$

$$\frac{g^-(\mathbf{r}, \boldsymbol{\Omega}, t)}{c(\mathbf{r})} = \sum_i^{n^-} \mathbf{f}^-(\mathbf{r}, \boldsymbol{\Omega}) \mathbf{T}^-(t) \quad (13)$$

Besides we introduce

$$\mathbf{T}^+(t) = \int_{\Sigma} \frac{4\pi \langle \mathbf{f}^+(\mathbf{r}, \boldsymbol{\Omega})^T e^+(\mathbf{r}, \boldsymbol{\Omega}, t) \rangle}{c(\mathbf{r})} d\mathbf{r},$$

$$\mathbf{P}^-(t) = \int_{\Sigma} 4\pi \langle \mathbf{f}^-(\mathbf{r}, \boldsymbol{\Omega})^T e^-(\mathbf{r}, \boldsymbol{\Omega}, t) \rangle d\mathbf{r},$$

being

$$\begin{aligned}\mathbf{f}^+(\mathbf{r}, \boldsymbol{\Omega}) &= [f_1^+(\mathbf{r}, \boldsymbol{\Omega}) \dots, f_{n^+}^+(\mathbf{r}, \boldsymbol{\Omega})], \\ \mathbf{f}^-(\mathbf{r}, \boldsymbol{\Omega}) &= [f_1^-(\mathbf{r}, \boldsymbol{\Omega}) \dots, f_{n^-}^-(\mathbf{r}, \boldsymbol{\Omega})], \\ \mathbf{P}^+(t) &= [P_1^+(t), \dots, P_{n^+}^+(t)]^T, \\ \mathbf{P}^-(t) &= [P_1^-(t), \dots, P_{n^-}^-(t)]^T, \\ \mathbf{T}^+(t) &= [T_1^+(t), \dots, T_{n^+}^+(t)]^T, \\ \mathbf{T}^-(t) &= [T_1^-(t), \dots, T_{n^-}^-(t)]^T.\end{aligned}$$

Functions $P_i^+(t)$ and $T_i^+(t)$ with $i = 1 \dots n^+$ are respectively the powers and temperature rises at n^+ ports of the thermal network. Functions $P_i^-(t)$ and $T_i^-(t)$ with $i = 1 \dots n^-$ are respectively the powers and temperature rises at the other n^- ports of the thermal network. Besides let

$$\begin{aligned}\mathbf{P}(t) &= [\mathbf{P}^+(t)^T, \mathbf{P}^-(t)^T]^T \\ \mathbf{T}(t) &= [\mathbf{T}^+(t)^T, \mathbf{T}^-(t)^T]^T\end{aligned}$$

be the column vectors of the powers and temperature rises at the ports of the thermal network.

With this definition of port variables, the thermal network preserves the thermodynamic properties of the transport equation:

Property 5 (Passivity): For each time interval $t_1 \leq t \leq t_2$ it results in

$$W(t_2) \leq W(t_1) + \int_{t_1}^{t_2} \mathbf{T}^T(t) \mathbf{P}(t) dt$$

Proof: From the definition of port variables it results in

$$\begin{aligned}& \int_{\Sigma} \frac{4\pi \langle g(\mathbf{r}, \boldsymbol{\Omega}, t) e(\mathbf{r}, \boldsymbol{\Omega}, t) \rangle}{c(\mathbf{r})} d\mathbf{r} = \\ &= \int_{\Sigma} \frac{4\pi \langle g^+(\mathbf{r}, \boldsymbol{\Omega}, t) e^+(\mathbf{r}, \boldsymbol{\Omega}, t) \rangle}{c(\mathbf{r})} d\mathbf{r} + \\ &+ \int_{\Sigma} \frac{4\pi \langle g^-(\mathbf{r}, \boldsymbol{\Omega}, t) e^-(\mathbf{r}, \boldsymbol{\Omega}, t) \rangle}{c(\mathbf{r})} d\mathbf{r} = \\ &= \mathbf{P}^+(t)^T \int_{\Sigma} \frac{4\pi \langle \mathbf{f}^+(\mathbf{r}, \boldsymbol{\Omega})^T e^+(\mathbf{r}, \boldsymbol{\Omega}, t) \rangle}{c(\mathbf{r})} d\mathbf{r} + \\ &+ \mathbf{T}^-(t)^T \int_{\Sigma} 4\pi \mathbf{f}^-(\mathbf{r}, \boldsymbol{\Omega})^T e^-(\mathbf{r}, \boldsymbol{\Omega}, t) d\mathbf{r} = \\ &= \mathbf{P}^+(t)^T \mathbf{T}^+(t) + \mathbf{T}^-(t)^T \mathbf{P}^-(t) = \\ &= \mathbf{T}^T(t) \mathbf{P}(t).\end{aligned}$$

Thus the thesis straightforwardly follows from Property 1. ■

Property 6 (Reciprocity): In the Laplace transform domain s , for any couple of situations $\mathbf{P}_1(s)$, $\mathbf{T}_1(s)$, and $\mathbf{P}_2(s)$, $\mathbf{T}_2(s)$, it results in

$$\mathbf{T}_1^T(s) \mathbf{P}_2(s) = \mathbf{T}_2^T(s) \mathbf{P}_1(s)$$

Proof: From the definition of port variables it results in

$$\begin{aligned}& \int_{\Sigma} \frac{4\pi \langle \mathbf{g}_1(\mathbf{r}, \boldsymbol{\Omega}, s) \mathbf{e}_2(\mathbf{r}, -\boldsymbol{\Omega}, s) \rangle}{c(\mathbf{r})} d\mathbf{r} = \\ &= \int_{\Sigma} \frac{4\pi \langle \mathbf{g}_1^+(\mathbf{r}, \boldsymbol{\Omega}, s) \mathbf{e}_2^+(\mathbf{r}, \boldsymbol{\Omega}, s) \rangle}{c(\mathbf{r})} d\mathbf{r} - \\ &- \int_{\Sigma} \frac{4\pi \langle \mathbf{g}_1^-(\mathbf{r}, \boldsymbol{\Omega}, s) \mathbf{e}_2^-(\mathbf{r}, \boldsymbol{\Omega}, s) \rangle}{c(\mathbf{r})} d\mathbf{r} = \\ &= \mathbf{P}_1^+(s)^T \int_{\Sigma} \frac{4\pi \langle \mathbf{f}_1^+(\mathbf{r}, \boldsymbol{\Omega})^T \mathbf{e}_2^+(\mathbf{r}, \boldsymbol{\Omega}, s) \rangle}{c(\mathbf{r})} d\mathbf{r} -\end{aligned}$$

$$\begin{aligned}& - \mathbf{T}_1^-(s)^T \int_{\Sigma} 4\pi \langle \mathbf{f}_1^-(\mathbf{r}, \boldsymbol{\Omega})^T \mathbf{e}_2^-(\mathbf{r}, \boldsymbol{\Omega}, s) \rangle d\mathbf{r} = \\ &= \mathbf{P}_1^+(s)^T \mathbf{T}_2^+(s) - \mathbf{T}_1^-(s)^T \mathbf{P}_2^-(s)\end{aligned}$$

In a similar way it results in

$$\begin{aligned}& \int_{\Sigma} \frac{4\pi \langle \mathbf{g}_2(\mathbf{r}, \boldsymbol{\Omega}, s) \mathbf{e}_1(\mathbf{r}, -\boldsymbol{\Omega}, s) \rangle}{c(\mathbf{r})} d\mathbf{r} = \\ &= \mathbf{P}_2^+(s)^T \mathbf{T}_1^+(s) - \mathbf{T}_2^-(s)^T \mathbf{P}_1^-(s)\end{aligned}$$

Thus from Property 2 it is

$$\begin{aligned}\mathbf{P}_1^+(s)^T \mathbf{T}_2^+(s) - \mathbf{T}_1^-(s)^T \mathbf{P}_2^-(s) &= \\ &= \mathbf{P}_2^+(s)^T \mathbf{T}_1^+(s) - \mathbf{T}_2^-(s)^T \mathbf{P}_1^-(s)\end{aligned}$$

or equivalently

$$\begin{aligned}\mathbf{P}_1^+(s)^T \mathbf{T}_2^+(s) + \mathbf{P}_1^-(s)^T \mathbf{T}_2^-(s) &= \\ &= \mathbf{P}_2^+(s)^T \mathbf{T}_1^+(s) + \mathbf{P}_2^-(s)^T \mathbf{T}_1^-(s)\end{aligned}$$

from which the thesis follows. ■

We notice that these thermal networks can be used also as *boundary condition independent* models [1]. To this aim it is sufficient to include proper superficial source distributions on the boundary $\partial\Sigma$ in the form given by Eqs. (12), (13).

We also notice that if the transport equation reduces to the heat wave equation then the thermal networks here introduced reduce to the thermal network for the heat wave equation [4]. In this case the port variables $P_i^-(t)$, $T_i^-(t)$ with $i = 1 \dots n^-$ vanish. Besides

$$\mathbf{T}^+(t) = \int_{\Sigma} \mathbf{f}(\mathbf{r})^T x(\mathbf{r}, t) d\mathbf{r},$$

being

$$\mathbf{f}(\mathbf{r}) = 4\pi \langle \mathbf{f}^+(\mathbf{r}, \boldsymbol{\Omega}) \rangle.$$

VII. APPLICATION

Let us consider an infinite material of phonon group velocity v , relaxation time τ , phonon mean free path $l = v\tau$, volumetric heat capacity c and thermal conductivity $k = cvl/3$. Let power $\mathbf{P}_1^+(s)$ be uniformly and isotropically generated in a sphere \mathcal{S}_1 of radius L_1 and power $\mathbf{P}_2^+(s)$ be uniformly and isotropically generated in a sphere of radius L_2 . Let the centers of \mathcal{S}_1 , \mathcal{S}_2 be L_{12} apart. By introducing the temperature rises $\mathbf{T}_1^+(s)$, and $\mathbf{T}_2^+(s)$ in \mathcal{S}_1 and \mathcal{S}_2 respectively, as shown in Section VI, a two-port thermal network is defined from the transport equation. Hereafter we derive the impedance matrix of this two-port thermal network.

Let us introduce the normalized variables

$$\rho = \frac{|\mathbf{r}|}{l}, \quad p = \tau s.$$

By proceeding as in [9], [10] it follows that the temperature distribution due to a unit power in the sphere of radius L_1 is

$$x(\mathbf{r}, s) = R F(\rho, p|l_1) (1 + p)$$

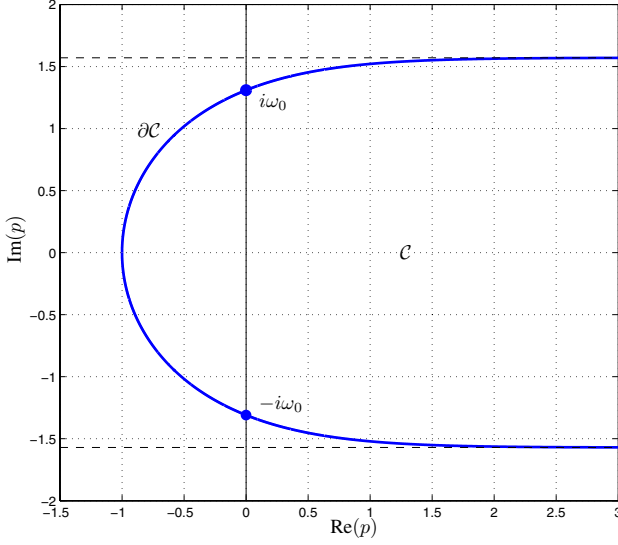


Fig. 1. Region \mathcal{C} . The intersections of $\partial\mathcal{C}$ with the imaginary axis are at $\pm i\omega_0$, with $\omega_0 \approx 1.309$.

in which $R = 3/(kl)$, $l_1 = L_1/l$,

$$F(\rho, p|l_1) = \begin{cases} \frac{\frac{1}{l_1} G\left(\frac{\rho}{l_1}, l_1 \frac{1+p}{\nu_0(p)}\right)}{N_0(p)\nu_0(p)} + \int_0^1 \frac{\frac{1}{l_1} G\left(\frac{\rho}{l_1}, l_1 \frac{1+p}{\nu}\right)}{N(\nu, p)\nu} d\nu & p \in \mathcal{C}, \\ \int_0^1 \frac{\frac{1}{l_1} G\left(\frac{\rho}{l_1}, l_1 \frac{1+p}{\nu}\right)}{N(\nu, p)\nu} d\nu & p \notin \mathcal{C}, \end{cases}$$

and

$$G(\xi, q) = \begin{cases} \frac{3}{8\pi\xi} \frac{2q - \frac{(1+q)}{\xi}(e^{-q(1-\xi)} - e^{-q(1+\xi)})}{q^3} & \xi \leq 1, \\ \frac{3}{8\pi\xi} \frac{(q-1)e^{-q(\xi-1)} + (q+1)e^{-q(\xi+1)}}{q^3} & \xi \geq 1. \end{cases}$$

\mathcal{C} is the convex region of the complex plane, shown in Fig. 1, whose boundary $\partial\mathcal{C}$ is a curve of equations

$$\begin{aligned} \operatorname{Re}(p) &= \xi \log \sqrt{\frac{1+\xi}{1-\xi}} - 1 \\ \operatorname{Im}(p) &= \pm \frac{\pi}{2} \xi \end{aligned}$$

with $0 \leq \xi \leq 1$,

$$N(\nu, p) = \nu \left(1 - \frac{\nu}{1+p} \tanh^{-1} \nu\right)^2 + \nu \left(\frac{\pi}{2} \frac{\nu}{1+p}\right)^2,$$

$\nu_0(p)$ is the root, with positive real part, of equation

$$\frac{\nu_0(p)}{1+p} \tanh^{-1} \frac{1}{\nu_0(p)} = 1,$$

and

$$N_0(p) = \frac{1}{2} \frac{\nu_0^3(p)}{1+p} \left(\frac{1}{1+p} \frac{1}{\nu_0^2(p)} - 1 - \frac{1}{\nu_0^2(p)} \right).$$

The impedance matrix

$$\mathbf{Z}(s) = \begin{bmatrix} Z_{11}(s) & Z_{12}(s) \\ Z_{21}(s) & Z_{22}(s) \end{bmatrix}$$

is then derived using [11]. It results in

$$\begin{aligned} Z_{11}(s) &= R E(p|l_1)(1+p) \\ Z_{22}(s) &= R E(p|l_2)(1+p) \end{aligned}$$

in which $l_2 = L_2/l$,

$$E(p|l_1) = \begin{cases} \frac{\frac{1}{l_1} L\left(l_1 \frac{1+p}{\nu_0(p)}\right)}{N_0(p)\nu_0(p)} + \int_0^1 \frac{\frac{1}{l_1} L\left(l_1 \frac{1+p}{\nu}\right)}{N(\nu, p)\nu} d\nu & p \in \mathcal{C} \\ \int_0^1 \frac{\frac{1}{l_1} L\left(l_1 \frac{1+p}{\nu}\right)}{N(\nu, p)\nu} d\nu & p \notin \mathcal{C} \end{cases}$$

being

$$L(q) = \frac{3}{8\pi} \left(\frac{3 - 3q^2 + 2q^3}{q^5} - 3e^{-2q} \frac{1 + 2q + q^2}{q^5} \right).$$

Besides

$$Z_{12}(s) = Z_{21}(s) = R D(p|l_1, l_2, l_{12})(1+p)$$

in which $l_{12} = L_{12}/l$,

$$D(p|l_1, l_2, l_{12}) = \begin{cases} \frac{\frac{1}{l_{12}} C\left(\frac{1+p}{\nu_0(p)}|l_1, l_2, l_{12}\right)}{N_0(p)\nu_0(p)} + \int_0^1 \frac{\frac{1}{l_{12}} C\left(\frac{1+p}{\nu}|l_1, l_2, l_{12}\right)}{N(\nu, p)\nu} d\nu & p \in \mathcal{C} \\ \int_0^1 \frac{\frac{1}{l_{12}} C\left(\frac{1+p}{\nu}|l_1, l_2, l_{12}\right)}{N(\nu, p)\nu} d\nu & p \notin \mathcal{C} \end{cases}$$

being

$$\begin{aligned} C(q|l_1, l_2, l_{12}) &= \frac{9}{16\pi} J(l_1 q) J(l_2 q) e^{-l_{12} q}, \\ J(u) &= \frac{u-1}{u^3} e^u + \frac{u+1}{u^3} e^{-u}. \end{aligned}$$

Hereafter the case $l_1 = l_2 = 1/2$, $l_{12} = 3/2$ is considered, representative of current scale of semiconductor silicon technology. The Nyquist plot of the impedance matrix is shown in Fig. 2. The power impulse thermal response matrix and the power step thermal response matrix, numerically computed from the impedance matrix as in [12], are shown in Figs. 3, 4. Comparisons with the responses of the thermal networks derived from the heat diffusion equation and from the heat wave equation are also shown.

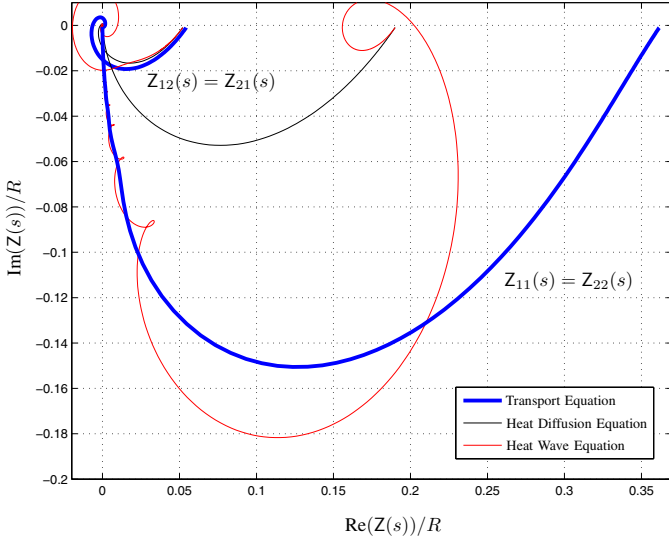


Fig. 2. Nyquist plots of the thermal impedances from both the transport equation, the heat diffusion equation and the heat wave equation.

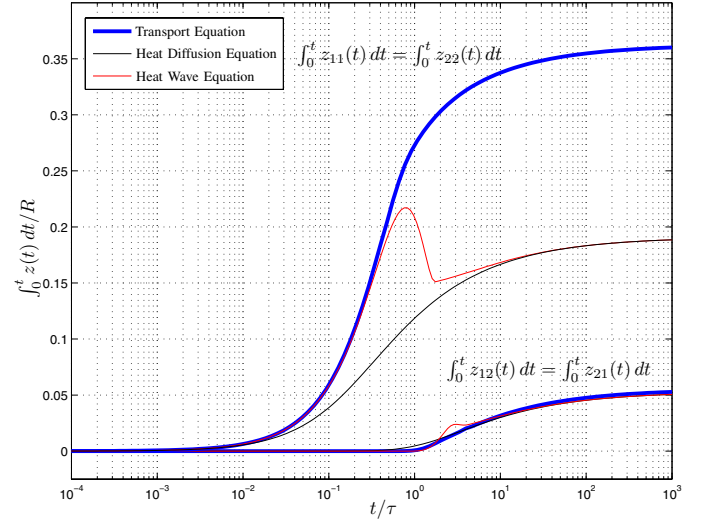


Fig. 4. Plots of the power step thermal responses from both the transport equation, the heat diffusion equation and the heat wave equation.

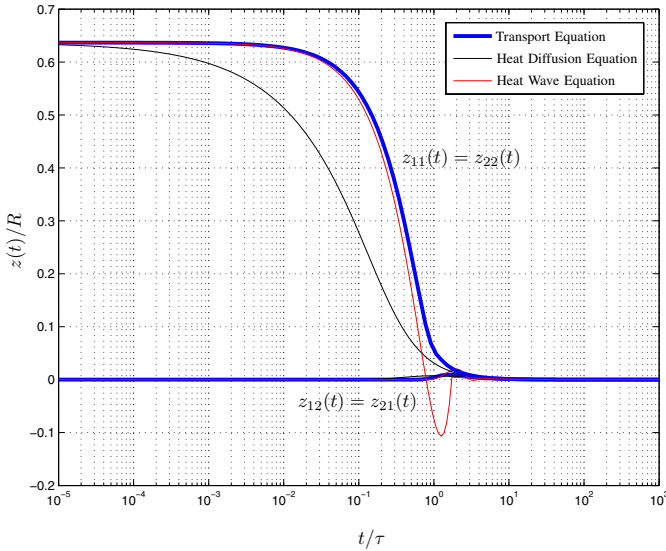


Fig. 3. Plots of the power impulse thermal responses from both the transport equation, the heat diffusion equation and the heat wave equation.

At the current scale of semiconductor silicon technology, the responses of the thermal networks obtained by means of the transport equation are different from the thermal response obtained by means of the heat diffusion equation. The thermal network from the heat wave equation is able to approximate the response of the thermal network from the transport equation only at high frequencies. However at low frequencies it does not approximate the response of the thermal network from the transport equation. Instead it approximates the response of the thermal network from the heat diffusion equation.

VIII. CONCLUSIONS

Thermal networks have been introduced from the gray phonon Boltzmann's transport equation in such a way that its thermodynamic properties are preserved. A reference thermal network has been investigated. It has been shown that the responses of this thermal network cannot be accurately approximated by the responses of the thermal networks from either the heat diffusion or the heat wave equations.

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