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Behavior of the linearized ballistic-conductive model of heat conduction in three-dimensional space

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The heat equation, based on Fourier's law, is commonly used for description of heat conduction. However, Fourier's law is valid under the assumption of local thermodynamic equilibrium, which is violated in very small dimensions and short timescales, and at low temperatures. As a replacement for Fourier's law, many models have been proposed within the framework of various theories. In this paper we study the behavior of solutions to an initial value problem in 3D in the framework of the linearized ballistic-conductive (BC) model. As a result, an unphysical effect is detected when the temperature in the heat wave takes negative values.

Keywords: non-Fourier heat conduction, hyperbolic heat conduction, the ballistic-conductive model, initial value problem.

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Introduction

The heat equation, based on Fourier's law, is commonly used for description of heat conduction. However, Fourier's law is valid under the assumption of local thermodynamic equilibrium, which is violated at the micro- and nanoscale, in ultrafast processes, and also at very low temperatures [1–5]. As a substitute for Fourier's law, many models have been proposed in the framework of various theories [1–13]. However, none of these models can serve as a complete substitute for Fourier's law.

In dielectrics, heat transfer is carried out by phonons, inasmuch as the contribution of electrons to heat transfer is negligibly small [2–4]. The transport of phonons is described by the Boltzmann equation for phonons (the Peierls–Boltzmann equation). However, solving this equation is very difficult. Therefore, approximations to the Peierls–Boltzmann equation are of considerable interest.

In the article [14], a ballistic-conductive (BC) model of heat conduction in the framework of nonequilibrium thermodynamics with internal variables was proposed. In the papers [15,16], the linearized form of this model was tested on experimental data and showed a quantitative description of heat transfer by transversal ballistic phonons, while demonstrating a qualitative description of the second sound. The linearized form of the BC model is described by a hyperbolic system of partial differential equations, which ensures the finiteness of the velocity of thermal energy propagation. The study of the linearized BC model is of considerable interest, inasmuch as it can be considered not only in the framework of nonequilibrium thermodynamics, but also as a hyperbolic approximation to the Peierls-Boltzmann equation, which is a hyperbolic integro-differential partial differential equation. From this point of view, the Cattaneo model (hyperbolic heat equation) is the first hyperbolic approximation to the Peierls–Boltzmann equation, and the linearized BC model is the second one.

In this paper, in the framework of the linearized BC model, the initial value problem in three-dimensional space is studied. An effect has been found where, when thermal energy is added to the system, the temperature in the heat wave takes values lower than the background temperature.

1. Statement of the Initial Value Problem

Let us consider a system of equations in three-dimensional space that describe the BC model of heat conduction [14–17]:

$$\rho c \partial_t T + \nabla \cdot \mathbf{q} = f, \tag{1a}$$

$$-m_1 \partial_t \mathbf{q} + \nabla \frac{1}{T} + l_{21} \nabla \cdot \mathbf{Q} = l\mathbf{q}, \tag{1b}$$

$$-m_2 \partial_t \mathbf{Q} = l_{11}\mathbf{Q} + l_{12} \nabla \mathbf{q}, \tag{1c}$$

where $T(\mathbf{r}, t)$ is temperature, $\mathbf{q}(\mathbf{r}, t)$ is a heat flux vector, $f(\mathbf{r}, t)$ is a thermal energy source, $\mathbf{Q}(\mathbf{r}, t)$ is an internal variable (second-order tensor function), $\mathbf{r} = (x_1, x_2, x_3)$, ρ is density, c is specific heat capacity. Equation (1a) is a standard equation for the balance of thermal energy. Relations (1b) and (1c) are constitutive equations obtained in the framework of nonequilibrium thermodynamics with internal variables After linearization, the system (1) takes the form of

$$\rho c \partial_t T + \nabla \mathbf{q} = f,$$

$$\tau_q \partial_t \mathbf{q} + \mathbf{q} = -\lambda \nabla T + \kappa_{21} \nabla \mathbf{Q},$$

$$\tau_Q \partial_t \mathbf{Q} + \mathbf{Q} = -\kappa_{12} \nabla \mathbf{q}, \quad (2)$$

where $\tau_q = m_1/l$, $\tau_Q = m_2/l_{11}$, $\kappa_{21} = l_{21}/l$, $\kappa_{12} = l_{12}/l_{11}$, $\lambda = 1/lT_0^2$, where T_0 is background temperature relative to which linearization occurs. The parameters τ_q and τ_Q are the characteristic relaxation times of the variables $\mathbf{q}$ and $\mathbf{Q}$.

After bringing to a dimensionless form and redefinition of the quantities, the system (2) takes the form

$$\partial_t T + \nabla \mathbf{q} = f, \quad (3a)$$

$$\tau_q \partial_t \mathbf{q} + \mathbf{q} + \nabla T + \kappa \nabla \mathbf{Q} = \mathbf{0}, \quad (3b)$$

$$\tau_Q \partial_t \mathbf{Q} + \mathbf{Q} + \kappa \nabla \mathbf{q} = \mathbf{0}, \quad (3c)$$

where all quantities and parameters are dimensionless, $\kappa > 0$. At $\kappa = 0$, the equation (3b) takes the form of the Cattaneo equation. At $\tau_Q = 0$, the system (3) leads to the Guyer-Krumhansl heat equation. At $\tau_q = 0$ and $\kappa = 0$, the equation (3b) takes the form of Fourier's law. Thus, the linearized BC model is a generalization of the known models.

By excluding the variables $\mathbf{q}$ and $\mathbf{Q}$ in the system (3), we find that the temperature satisfies the equation

$$\tau_q \tau_Q \partial_t^3 T + (\tau_q + \tau_Q)\partial_t^2 T + \partial_t T - \Delta T - (\tau_Q + \kappa^2)\partial_t \Delta T$$
$$= \tau_q \tau_Q \partial_t^2 f + (\tau_q + \tau_Q)\partial_t f + f - \kappa^2 \Delta f. \quad (4)$$

The equation (4) is hyperbolic, its characteristic numbers are $\lambda_{1,2} = \pm v$, $v = \left[(1 + \kappa^2/\tau_Q)/\tau_q\right]^{1/2}$, $\lambda_3 = 0$. The hyperbolicity of the equation provides a finite velocity of propagation of thermal energy equal to v.

Let us suppose that the medium was at rest until $t = 0$ and the initial temperature was zero. In this case, the initial conditions for the system (3) are $T|_{t=0} = 0$, $\mathbf{q}|_{t=0} = 0$, $\mathbf{Q}|_{t=0} = 0$. By substituting these conditions into the equations (3b) and (3c), the conditions $\partial_t \mathbf{q}|_{t=0} = 0$, $\partial_t \mathbf{Q}|_{t=0} = 0$ are obtained. As a result, we get the initial conditions for the equation (4):

$$T|_{t=0} = 0, \quad \partial_t T|_{t=0} = f|_{t=0}, \quad \partial_t^2 T|_{t=0} = \partial_t f|_{t=0}. \quad (5)$$

2. Solving the Initial Value Problem

From the equation (4) and the initial conditions (5) it follows the Fourier-Laplace transform of the solution of the Cauchy problem is

$$\mathscr{L}\mathscr{F} T(\boldsymbol{\xi}, s) = \frac{[\tau_q \tau_Q s^2 + (\tau_q + \tau_Q)s + 1 + \kappa^2 \xi^2]\mathscr{L}\mathscr{F} f(\boldsymbol{\xi}, s)}{\tau_q \tau_Q s^3 + (\tau_q + \tau_Q)s^2 + [1 + (\tau_Q + \kappa^2)\xi^2]s + \xi^2},$$

where $\mathscr{F}$ is the Fourier transform defined by the formula $\mathscr{F}\Phi(\boldsymbol{\xi}) = \int_{\mathrm{R}^3} \Phi(\mathbf{r}) e^{i\boldsymbol{\xi}\mathbf{r}} d\mathbf{r}$, $\mathscr{L}$ is the Laplace transform expressed by the formula $\mathscr{L}\Phi(s) = \int_0^\infty \Phi(t) e^{-st} dt$.

Below we assume that the source is instantaneous, namely $f = \varphi(\mathbf{r})\delta(t)$, where $\delta(\cdot)$ is the Dirac delta function. In this case, $\mathscr{L}\mathscr{F} f(\boldsymbol{\xi}, s) = \mathscr{F}\varphi(\boldsymbol{\xi})$, and the Fourier-Laplace transform of the solution to the initial value problem is expressed by the formula

$$\mathscr{L}\mathscr{F} T(\boldsymbol{\xi}, s) = \frac{s^2 + as + (\tau_q \tau_Q)^{-1}(1 + \kappa^2 \xi^2)}{s^3 + as^2 + bs + c} \mathscr{F}\varphi(\boldsymbol{\xi})$$
$$= \frac{u^2 + Cu + D}{(u - 2A)[(u + A)^2 + B^2]} \mathscr{F}\varphi(\boldsymbol{\xi})$$
$$= \left[\frac{E}{u - 2A} + \frac{F(u + A) + G}{(u + A)^2 + B^2}\right] \mathscr{F}\varphi(\boldsymbol{\xi}),$$

where

$$a = \tau_q^{-1} + \tau_Q^{-1}, \; b(\xi) = (\tau_q \tau_Q)^{-1} + v^2 \xi^2, \; c(\xi) = (\tau_q \tau_Q)^{-1} \xi^2,$$

v is the speed of propagation of thermal energy.

$$s^3 + as^2 + bs + c = u^3 + \chi u + \psi,$$
$$s = u - a/3, \quad \chi(\xi) = -a^2/3 + b,$$
$$\psi(\xi) = 2(a/3)^3 - ab/3 + c,$$
$$A = (\alpha + \beta)/2, \quad B = \sqrt{3}(\alpha - \beta)/2, \quad C = a/3,$$
$$D = -2a^2/9 + (\tau_q \tau_Q)^{-1}(1 + \kappa^2 \xi^2),$$
$$\alpha = \sqrt[3]{-\psi/2 + \sqrt{\Delta}}, \quad \beta = \sqrt[3]{-\psi/2 - \sqrt{\Delta}},$$
$$\Delta = (\chi/3)^3 + (\psi/2)^2,$$

the roots α and β are chosen so that the equality $\alpha\beta = -\chi/3$ is true and the value A is real,

$$E = \frac{4A^2 + 2AC + D}{9A^2 + B^2}, \quad F = 1 - E,$$

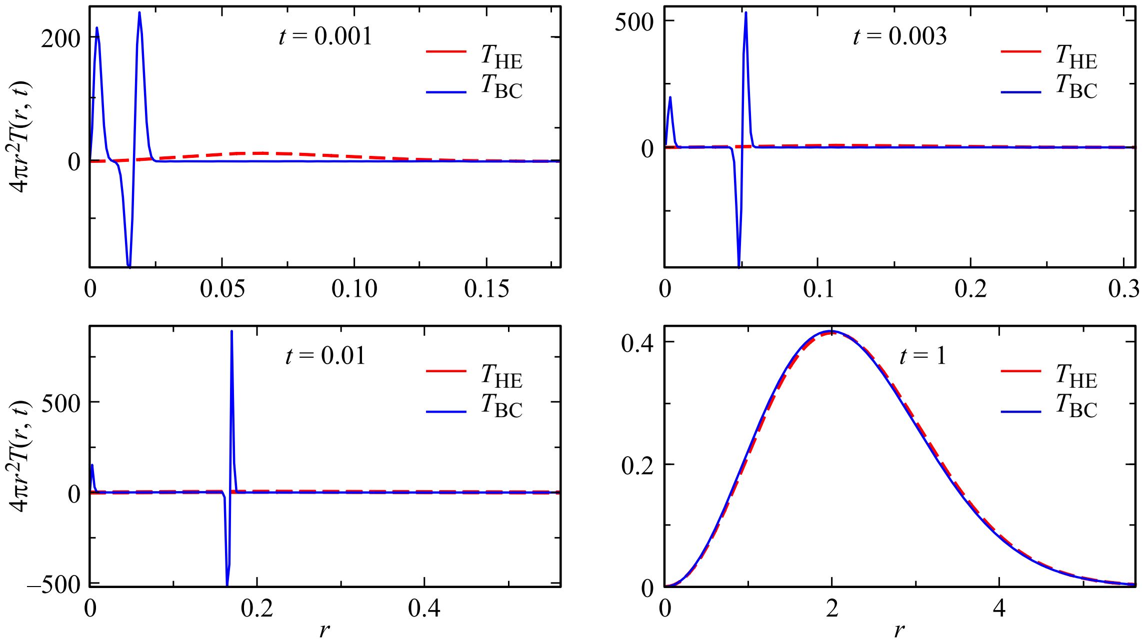
$$G = \frac{-3A^3 + AB^2 + (3A^2 + B^2)C - 3AD}{9A^2 + B^2}.$$

Considering the equation $s = u - a/3$, we get an expression for the inverse Laplace transform

$$\mathscr{L}^{-1}\left[\frac{E}{u - 2A} + \frac{F(u + A) + G}{(u + A)^2 + B^2}\right] = e^{-\mu_1 t} E + e^{-\mu_2 t}$$
$$\times \left[F \cos Bt + G \frac{\sin Bt}{B}\right],$$

where $\mu_1 = -2A + a/3$, $\mu_2 = A + a/3$. As a result, we get that the Fourier transform of the solution of the initial value problem has the form

$$\mathscr{F} T(\boldsymbol{\xi}, t) = \left\{e^{-\mu_1 t} E + e^{-\mu_2 t}\left[F \cos Bt + G B^{-1} \sin Bt\right]\right\}$$
$$\times \mathscr{F}\varphi(\boldsymbol{\xi}).$$



The solution T_{BC} of the initial value problem (4), (5) in comparison with the solution T_{HE} of the initial value problem for the heat equation.

The solution to the problem (4), (5) is found by means of the inverse Fourier transform:

$$T(\mathbf{r},t) = (2\pi)^{-3}\int\limits_{R^3} \mathscr{F}T(\boldsymbol{\xi},t)e^{-i\boldsymbol{\xi}\mathbf{r}}d\boldsymbol{\xi}.$$

We assume that at the initial moment $t = 0$ a unit amount of thermal energy was released at the origin, namely $f(\mathbf{r},t) = \varphi(\mathbf{r})\delta(t)$, where $\varphi(\mathbf{r}) = (\sqrt{2\pi}\sigma)^{-3}\exp(-r^2/2\sigma^2)$, $r = |\mathbf{r}|$, $\sigma \ll 1$. In this case $\mathscr{F}\varphi(\boldsymbol{\xi}) = \exp(-\sigma^2\xi^2/2)$, $\xi = |\boldsymbol{\xi}|$, the temperature distribution is spherically symmetrical and is calculated by formula

$$T(r,t) = \frac{1}{2\pi^2 r}\int\limits_0^\infty \xi\mathscr{F}T(\xi,t)\sin(r\xi)d\xi. \qquad (6)$$

The figure shows the solution (6) to the Cauchy problem (4), (5) with source $f(\mathbf{r},t) = \varphi(\mathbf{r})\delta(t)$. Parameter values are $\tau_q = 0.0156$, $\tau_Q = 0.0058$, $\kappa^2 = 0.0196$, $\sigma = 0.002$. These parameter values correspond to the dimensional parameter values from [16]. The graph shows a heat wave propagating at a speed of v, with the temperature in this wave taking values below the background temperature ($T = 0$ corresponds to an absolute temperature equal to the background temperature T_0). The peak near the origin corresponds to the zero characteristic number of the equation (4). The figure also shows the solution of the Cauchy problem for the heat equation $\partial_t T - \Delta T = f$, $T|_{t=0} = 0$ with the same source f.

Conclusion

An effect has been found where, when thermal energy is added to the system, the temperature in the heat wave takes values below the background temperature.

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Conflict of interest

The author declares that he has no conflict of interest.

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