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Violation of the maximum principle and negative solutions for pulse propagation in Guyer–Krumhansl model

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ABSTRACT

Heat transport in Guyer–Krumhansl model is studied and analytical solutions for the proper one-dimensional differential equation are explored by the operational method. Exact analytical solution is demonstrated. With its help sudden heat surge propagation is analytically described and compared with the solution for gradual heat wave propagation. The example of the application of the study to the heat transport in ultra-thin films is given. Influence of the Knudsen number on heat transport for short pulses and for gradual heat waves is demonstrated. The negativity and the maximum principle violation for the obtained solutions are discussed.

1. Introduction

Fourier's law of heat conduction [1], which relates linearly the temperature gradient to the heat flux, is one of the most common laws in continuum physics; it provides excellent agreement between theory and experiment for more than 90% of the cases. It is undoubtedly the best model for heat conduction in undeformable solids. However, due to its shortcomings, noted by Onsager in 1931 [2], the Fourier's model "can be viewed only as an approximation of the heat conduction, which neglects the time needed for acceleration of the heat flow". The most important related phenomenon is the second sound [3]. It was observed also in solid crystals via properly designed experiments [4–7] with the heat pulse technology. To address the second sound phenomenon, Cattaneo [8] proposed the following simple equation: $(\tau\partial_t^2 + \partial_t)T = D_T\nabla^2 T$, in which temperature disturbance propagates like damped waves, D_T is the heat conductivity and τ is the relaxation time. The ratio $v_t = \sqrt{D_T/\tau}$ is a velocity like quantity, representing the speed of the heat wave in the medium, which characterises the thermal wave propagation the same way as the diffusion behaviour is characterised by the diffusivity. The model supposes that the heat flow does not start instantaneously after a temperature gradient was imposed at the boundary of the domain, but is delayed by a relaxation time τ after the application of the temperature gradient. The parameter τ is the intrinsic thermal material property, which gives a lag between the change of the temperature gradient and the respective reaction of the heat flow on it. It is associated with the linkage time of phonon–phonon collision, necessary for the initiation of a heat flow and is a measure of the thermal inertia of the medium. With the additional constant term Cattaneo's equation turns into telegraph equation. Despite relative success of Cattaneo's relation in description of the second sound, predicted finite value for the heat wave velocity $\sqrt{D_T/\tau}$ disagrees with the observed experimental data and it does not describe heat pulse propagation in non-metallic very pure crystals, like Bi or Na F at very low temperature. Some physical contradictions, related to Cattaneo's equation, were described, for example, in [9,10] and mathematical contradictions were evidenced, for example, in [11–13]. Importantly, it was shown that the telegraph equation did not preserve the non-negativity of its solutions and that the maximum principle was not valid even for the one-dimensional hyperbolic heat space.

The most popular and discussed improvement of Cattaneo's relation, is, perhaps, due to Guyer and Krumhansl (GK) [14], who solved the linearised Boltzmann equation for a phonon field in dielectric crystals at low temperature and derived a non-local extension of Cattaneo's equation. In what follows we will explore its analytical solution and check whether it preserves the maximum principle and non-negativity of solutions. In its turn the Guyer–Krumhansl equation can be viewed as particular case of a more general heat conduction equation, derived in [15].

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2. Exact analytical bounded solution of Guyer–Krumhansl equation

Guyer–Krumhansl equation in one dimension is typically written as follows [16]:

$$\left(\frac{\partial^2}{\partial t^2}+\varepsilon\frac{\partial}{\partial t}-\delta\frac{\partial^3}{\partial t\,\partial x^2}\right)F(x,t)=\left(\alpha\frac{\partial^2}{\partial x^2}+\kappa^2\right)F(x,t),$$
$$\alpha,\ \varepsilon,\ \delta,\ \kappa=const \tag{1}$$

with $\kappa = 0$. However, we will keep the constant source term κ^2 for more generality. Its interpretation might be the radiation into the environment with small difference temperature or another kind of heat source; its mathematical role will be explored in what follows. Parameters $\alpha,\ \varepsilon,\ \delta$ must be nonnegative according to the Second Law. When bulk phonon mean free paths l are comparable with the structure scale L, for example, in one-dimensional thin film or wire, which thickness may be of the same order of magnitude as, or even smaller than the mean free path of the phonons [17,18], neither Casimir phonon [19] nor Fourier diffusion [1] theories are accurate and thermal transfer is influenced by both internal and boundary scattering. In this case ballistic transport plays significant role; it was observed in ultra-thin films, nanowires and other quasi one-dimensional structures and it is currently in focus of research [20–29]. However, GK equation is not limited to the description of the above mentioned physical phenomenon. Indeed, it was demonstrated that heat propagation at room temperature also obeys GK relation. Experimental results for such measurements with heat pulse are published in [27]. In this context we would like to note that the ballistic transport, being the free propagation of phonons (when it is applicable), is not the sole phenomenon, related to GK equation. Since GK type heat conduction was measured in room temperature and in porous and composite materials, where the kinetic pictures cannot work, it would be more correct to call the regime, when $\delta > \alpha/\varepsilon$ — over-diffusive transport, following Tang and Araki [28]. If $\delta = \alpha/\varepsilon$, the solution is pure Fourier (see Figs. 2 and 4 in what follows). Eq (1) can be conveniently written in terms of heat conductivities as follows:

$$\left(\tau\frac{\partial^2}{\partial t^2}+\frac{\partial}{\partial t}\right)F(x,t)=\left(k_b\frac{\partial^3}{\partial t\partial x^2}+k_T\frac{\partial^2}{\partial x^2}+\mu\right)F(x,t), \tag{2}$$

where $k_b=\delta/\varepsilon,\ \tau=1/\varepsilon,\ \mu=\kappa^2/\varepsilon,\ k_T=\alpha/\varepsilon$ is the heat diffusivity. Following the request of researchers we derived bounded analytical solution for Eq. (1) with the initial function $f(x)$ [30], employing the operational method [31–34] and Laplace transforms, as follows:

$$F(x,t)=\frac{e^{-\frac{t}{2}\varepsilon}t}{4\pi}\int_0^\infty\frac{d\xi}{\xi\sqrt{\xi}}e^{-\frac{t^2}{16\xi}-\xi(\varepsilon^2+4\kappa^2)}\int_{-\infty}^{\infty}e^{-\zeta^2}\hat{S}f(x)d\zeta, \tag{3}$$

where

$$\hat{S}=e^{v\partial_x^2},\quad v=a+ib\zeta,\quad a=t\delta/2-4\xi\alpha+2\xi\varepsilon\delta,\quad b=2\sqrt{\xi}\delta. \tag{4}$$

The heat operator $\hat{S}$ is the solution of Fourier heat equation:

$$\partial_t F_{\mathrm{Fou}}(x,t)=\alpha\ \partial_x^2 F_{\mathrm{Fou}}(x,t) \tag{5}$$

and its action can be obtained via Gauss transforms [31,35]:

$$F_{\mathrm{Fou}}(x,t)\equiv\exp(\alpha t\partial_x^2)f(x)$$
$$=\frac{1}{2\sqrt{\pi t\alpha}}\int_{-\infty}^{\infty}\exp\left\{-\frac{(x-\xi)^2}{4t\alpha}\right\}f(\xi)d\xi. \tag{6}$$

Analytical solutions for several types of initial functions, such as $f(x)=x^n, f(x)=x^ne^{\gamma x}, f(x)=\delta(x)$ were obtained earlier in [30]. For example, for the initial monomial $F(x,0)=x^n$ in GK equation the following solution arises:

$$F(x,t)|_{f(x)=x^n}=\frac{e^{-\frac{t}{2}\varepsilon}t}{4\pi}\int_0^\infty\frac{d\xi}{\xi\sqrt{\xi}}e^{-\frac{t^2}{16\xi}-\xi(\varepsilon^2+4\kappa^2)}$$
$$\times\int_{-\infty}^{\infty}e^{-\zeta^2}H_n(x,a+2i\delta\zeta\sqrt{\xi})d\zeta, \tag{7}$$

where $H_n(x,y)$ are Hermite polynomials of two variables [36,37]:

$$H_n(x,y)=\exp\left(y\frac{\partial^2}{\partial x^2}\right)x^n=n!\sum_{r=0}^{[n/2]}\frac{x^{n-2r}y^r}{(n-2r)!r!},$$
$$\sum_{n=0}^{\infty}\frac{t^n}{n!}H_n(x,y)=\exp(xt+yt^2). \tag{8}$$

The integration in (7) with account for the sum presentation (8) can be easily accomplished. For instance, for $f(x)=x^2$ it yields the following simple solution:

$$F(x,t)|_{f(x)=x^2}=e^{-\frac{t}{2}(\sqrt{V}+\varepsilon)}\left(x^2+t\delta+\frac{t}{\sqrt{V}}(\delta\varepsilon-2\alpha)\right),\quad V=\varepsilon^2+4\kappa^2. \tag{9}$$

Similarly we can obtain the solution for any given n.

Modelling experimental data by analytical functions frequently employs expansions in Fourier series. On the other hand, it is well-known that Fourier heat diffusion is not always applicable for describing heat transport at short wave lengths. By these reasons we give the analytical solution of GK equation for the initial harmonic function $f(x)=\exp(inx)$. The action of the heat operator $\hat{S}$ transforms it: $\hat{S}e^{inx}=e^{v\,\partial_x^2}e^{inx}=e^{inx-n^2v}=e^{inx-n^2(\delta t/2-4\xi\alpha+2\xi\varepsilon\delta+2i\zeta\sqrt{\xi}\delta)}$, and yields the following bounded solution of the GK equation (1) and (2):

$$F(x,t)=e^{inx}\frac{e^{-\frac{t}{2}(\varepsilon+n^2\delta)}t}{4\pi}\int_0^\infty\frac{d\xi}{\xi\sqrt{\xi}}e^{-\frac{t^2}{16\xi}-\xi(\varepsilon^2+4\kappa^2+2n^2(-2\alpha+\varepsilon\delta))}\int_{-\infty}^{\infty}e^{-\zeta^2}e^{-ic\zeta}d\zeta,$$
$$c=2n^2\delta\sqrt{\xi}. \tag{10}$$

Straightforward integration results in the following solution for $f(x)=\exp(inx)$ (see [30]):

$$F(x,t)|_{f(x)=\exp(inx)}=\exp\left(inx-\frac{t}{2}(\bar{\varepsilon}+\sqrt{U})\right),$$
$$\bar{\varepsilon}=\varepsilon+n^2\delta,\quad U=\bar{\varepsilon}^2+4(\kappa^2-\alpha n^2). \tag{11}$$

Interestingly, the solution (11) of GK type equation (1) with initial harmonic function $f(x)=\exp(inx)$ is also the solution for the telegraph equation:

$$\left(\frac{\partial^2}{\partial t^2}+\bar{\varepsilon}\frac{\partial}{\partial t}\right)F(x,t)=\left(\alpha\frac{\partial^2}{\partial x^2}+\kappa^2\right)F(x,t), \tag{12}$$

where the coefficient of the first order time derivative depends on the harmonic number: $\bar{\varepsilon}=\varepsilon+n^2\delta$. Therefore, for the initial function, expandable in Fourier series $\varphi(x)=\sum_n c_n\exp(inx)$, the solutions of Eqs. (1) and (12) for the same set of $\alpha,\ \varepsilon,\ \kappa,\ \delta$ are identical: $\Phi=\sum_n c_nF(x,t)$, where $F(x,t)$ is given by (11). Then, in certain sense, GK equation for the harmonic initial function can be viewed as Cattaneo's equation with harmonic dependent coefficient of $\partial/\partial t:(\varepsilon+n^2\delta)\partial/\partial t$.

In what follows we shall consider few other examples of initial functions and analyze the behaviour of the respective solutions. Basically, they consist in the integrated weighted action of heat diffusion operator $\hat{S}$ on the initial functions. The heat pulse technique is common for the heat conductivity measurements (see, for example, [38]). Heat pulses may have different shapes and lengths; unfortunately, experimental results not always account for this factor [39]. In what follows we will compare the evolution of the initial function in the form of the instant and point heat pulse,