Elliptic Equations of Heat Transfer and Diffusion in Solids

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Abstract

We propose a modified phenomenological equation for heat and impurity fluxes in solids by analogy with the Cattaneo-Vernotte concept. It leads to the second-order elliptical equations describing the evolution of temperature and impurity profiles with finite rate of propagation. The comparison of transfer peculiarities in the framework of parabolic and elliptic equations is discussed.

1 Introduction

In classical consideration the process of heat transfer in solid is described by a phenomenological parabolic equation based on two assumptions. The first is the continuity of heat propagation

$$\frac{\partial q}{\partial t} + (\nabla \cdot \mathbf{q}) = 0, \tag{1}$$

where q is the volume density of heat, $\mathbf{q}$ is the volume density of heat flux. The second assumption is Fourier's law, which we write as the relationship between heat flux and gradient of heat density

$$\mathbf{q} = -\beta_q \nabla q, \tag{2}$$

where β_q is the coefficient of thermal diffusivity. Substituting (2) into equation (1), we obtain the classical Fourier heat equation [1] in the following form:

$$\frac{\partial q}{\partial t} - \beta_q \Delta q = 0. \tag{3}$$

On the other hand, for the systems that do not perform mechanical work we have

$$dq = c\rho d\theta, \tag{4}$$

where c is specific heat capacity of material, ρ is the mass density, θ is a temperature. Using (4) the equation (3) is transformed to the parabolic equation for temperature

$$\frac{\partial \theta}{\partial t} - \beta_q \Delta\theta = 0. \tag{5}$$

A similar situation occurs in the phenomenological description of impurity diffusion in solids [2]. The continuity condition

$$\frac{\partial n}{\partial t} + (\nabla \cdot \mathbf{n}) = 0, \tag{6}$$

(here n is the impurity concentration, $\mathbf{n}$ is the diffusive flux) combined with Fick's law

$$\mathbf{n} = -\beta_n \ \nabla n, \tag{7}$$

(here β_n is diffusion coefficient) leads us to the parabolic equation for the diffusion flow

$$\frac{\partial n}{\partial t} - \beta_n \Delta n = 0. \tag{8}$$

The disadvantage of the Fourier law of thermal conductivity (2) and Fick law of diffusion (7) is that they lead us to the equations of parabolic type (5) and (8), which describe the instantaneous propagation of heat and impurity [3, 4]. However, this contradicts the physical nature of the heat and mass transfer processes.

To overcome the drawback in heat conduction, a modified Fourier law was proposed, taking into account "inertia" of the heat transfer process [5]-[8]

$$\tau_q \frac{\partial \mathbf{q}}{\partial t} + \mathbf{q} + \beta_q \nabla q = 0, \tag{9}$$

where τ_q is relaxation time depending on material properties. Relation (9) in combination with continuity condition leads us to the wave equation of hyperbolic type

$$\tau_q \frac{\partial^2 \theta}{\partial t^2} + \frac{\partial \theta}{\partial t} - \beta_q \Delta\theta = 0, \tag{10}$$

which is widely discussed as "Cattaneo-Vernotte equation" in a literature [9]-[20]. The equation (9) introduces a very important parameter τ_q that describes the time scale of heat relaxation and allows one to determine the rate of heat propagation as

$$s_q^2 = \frac{\beta_q}{\tau_q}. \tag{11}$$

Besides the spatial scale of heat diffusion is defined as

$$l_q = \sqrt{\beta_q \tau_q} = s_q \tau_q. \tag{12}$$

When $\tau_q = 0$ the Cattaneo-Vernotte equation is transformed to the Fourier equation. The parabolic equation (5) and hyperbolic equation (10) describe the same stationary states, which are determined by Laplace operator, but the dynamics of relaxation to these stationary states is different.

However, eliminating the paradox of instantaneous heat propagation [2, 3, 9], the hyperbolic heat equation leads to other paradoxical results associated with interference of temperature waves, their reflection from the boundaries of the body and the formation of shock heat waves [10]-[20]. Therefore, discussions about the applicability of the Fourier and Cattaneo-Vernotte equations continue [21, 22]. We also note that despite the fact that the phenomenological equations of diffusion and heat transfer are the same, the hyperbolic diffusion equation and diffusion waves are not discussed in a literature. In this paper, we propose an alternative approach to the description of heat and mass transfer, which leads to an elliptic second order equation and describes a different dynamics of heat and impurity propagation.

2 Elliptical equations of heat and mass transfer

Evidently, that the hyperbolic heat equation is a consequence of the concept of "inertia" for heat flow. However this concept raises doubts, since the macroscopic transfer of heat and impurity is associated not with their directed motion, but with chaotic vibrations of atoms of a solid and with the wandering of impurity atoms along the sites and interstices of crystal lattice. Here we try to modify the Cattaneo-Vernotte condition and obtain elliptic equation describing different dynamics of heat and impurity propagation.

Let us define new values

$$\begin{aligned} \mathrm{g}_q &= q, \\ \mathbf{g}_q &= \mathbf{q}, \\ \mathrm{g}_n &= n, \\ \mathbf{g}_n &= \mathbf{n}. \end{aligned} \tag{13}$$

Then we can describe both heat and diffusion processes in general by generalized values g_α and $\mathbf{g}_\alpha$, where index takes the meanings $\alpha \in \{q, n\}$ for heat (q) or for diffusion (n) transfer. We suppose that Cattaneo-Vernotte condition can be changed as follows

$$-\tau_\alpha \frac{\partial \mathbf{g}_\alpha}{\partial t} + \mathbf{g}_\alpha + \beta_\alpha \nabla \mathrm{g}_\alpha = 0, \tag{14}$$

which differs from condition (9) by the sign in front of the time derivative. In addition, we take into account that the circulation of the heat and diffusion flux in a closed loop should be equal to zero. Then the complete system of equations describing the heat and mass transfer processes can be written in the following form:

$$\frac{\partial \mathrm{g}_\alpha}{\partial t} + (\nabla \cdot \mathbf{g}_\alpha) = 0, \tag{15}$$

$$-\tau_\alpha \frac{\partial \mathbf{g}_\alpha}{\partial t} + \mathbf{g}_\alpha + \beta_\alpha \nabla \mathrm{g}_\alpha = 0, \tag{16}$$

$$[\nabla \times \mathbf{g}_\alpha] = 0. \tag{17}$$

The equation (15), as before, the continuity condition. Equation (16) describes the process of the fluxes relaxation. Equation (17) shows that the heat and diffusion mass flows are the vortex free. The system (16) - (17) is equivalent to the following elliptic equations

$$\frac{\partial^2 \mathrm{g}_\alpha}{\partial t^2} - \frac{1}{\tau_\alpha}\frac{\partial \mathrm{g}_\alpha}{\partial t} + s_\alpha^2 \Delta \mathrm{g}_\alpha = 0, \tag{18}$$

$$\frac{\partial^2 \mathbf{g}_\alpha}{\partial t^2} - \frac{1}{\tau_\alpha}\frac{\partial \mathbf{g}_\alpha}{\partial t} + s_\alpha^2 \Delta \mathbf{g}_\alpha = 0. \tag{19}$$

In particular, assuming (4) from the equation (18) we have the following elliptical equations for the temperature field $\theta(\mathbf{r}, t)$ and profile of impurity concentration $n(\mathbf{r}, t)$:

$$\frac{\partial^2 \theta}{\partial t^2} - \frac{1}{\tau_q}\frac{\partial \theta}{\partial t} + s_q^2 \Delta \theta = 0, \tag{20}$$

$$\frac{\partial^2 n}{\partial t^2} - \frac{1}{\tau_n}\frac{\partial n}{\partial t} + s_n^2 \Delta n = 0. \tag{21}$$

Note, that the stationary states of elliptic equations (20) and (21) are the same as for parabolic equations but the time evolution of temperature and concentration is different.

3 Comparison of parabolic and elliptic equations

Let us compare parabolic and elliptic equations considering for example the heat propagation in detail. We write these equations in the similar form

$$\frac{1}{\tau_q}\frac{\partial \theta}{\partial t} - s_q^2 \Delta \theta = 0, \tag{22}$$

$$-\frac{\partial^2 \theta}{\partial t^2} + \frac{1}{\tau_q}\frac{\partial \theta}{\partial t} - s_q^2 \Delta \theta = 0. \tag{23}$$

The equations (22) and (23) admit the solutions in the form of plane waves

$$\theta = A \, \exp\left(i\omega t + i\left(\mathbf{k} \cdot \mathbf{r}\right)\right), \tag{24}$$

where ω is the frequency, $\mathbf{k}$ is the wave vector ($k = |\mathbf{k}|$). The dispersion relation for parabolic equation (22) is

$$i\omega \; = -\tau_q s_q^2 \, k^2. \tag{25}$$

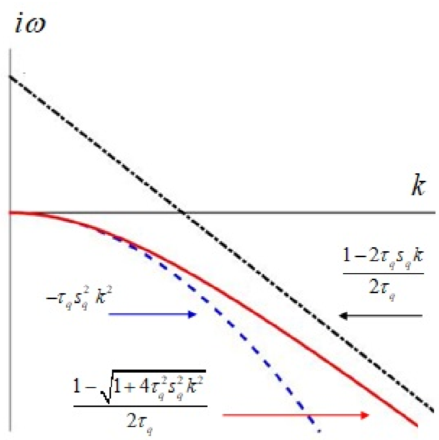

Figure 1: The schematic plot of dispersion curves for parabolic (dashed blue line) and elliptic (solid red line) equations. The asymptote (28) is shown by dot-dashed black line.

The dispersion relation for elliptic equation (23) is

$$\omega^2 + i\frac{1}{\tau_q}\omega + s_q^2 k^2 = 0. \tag{26}$$

From (26) we have the physically meaningful root

$$i\omega = \frac{1 - \sqrt{1 + 4\tau_q^2 s_q^2 k^2}}{2\tau_q}. \tag{27}$$

The schematic plots of (25) and (27) are represented in Fig. 1.

In the region of small k the dependence (27) coincides with dependence (25), while at $k \to \infty$ it tends to the asymptote

$$i\omega = \frac{1 - 2\tau_q s_q k}{2\tau_q}. \tag{28}$$

The relations (25) and (27) show that solutions (24) are the damping functions. The analog of group speed of these waves is imaginary value. For parabolic equation (22) we have

$$i\, v_p = i\frac{d\omega}{dk} = -2\tau_q s_q^2\, k. \tag{29}$$

This value tends to infinity when $k \to \infty$. On the other hand for elliptic equation (23) we have

$$i\, v_e = i\frac{d\omega}{dk} = -\frac{2\tau_q s_q^2 k}{\sqrt{1 + 4\tau_q^2 s_q^2 k^2}}. \tag{30}$$

This quantity tends to be constant $-s_q$ at $k \to \infty$.

The plate cooling

As an example, let us consider one-dimensional problem of cooling a plate with thickness $2l$ uniformly heated to a temperature θ_0 and with zero temperature at the boundaries $x = \pm l$. In this case we have natural spatial scale l and we introduce new dimensionless variables $\tilde{t} = t/\tau_q$ and $\tilde{x} = x/l$. Then the parabolic equation is represented as

$$\frac{\partial \theta}{\partial \tilde{t}} - \lambda^2 \frac{\partial^2 \theta}{\partial \tilde{x}^2} = 0, \tag{31}$$

while elliptic equation is

$$\frac{\partial^2 \theta}{\partial \tilde{t}^2} - \frac{\partial \theta}{\partial \tilde{t}} + \lambda^2 \frac{\partial^2 \theta}{\partial \tilde{x}^2} = 0, \tag{32}$$

where $\lambda = l_q/l$ is the ratio of the diffusion length to half of the plate thickness. Corresponding dispersion relations are

$$i\omega \; = -\lambda^2 k^2 \tag{33}$$

and

$$i\omega = \frac{1 - \sqrt{1 + 4\lambda^2 k^2}}{2}. \tag{34}$$

The solution to this problem in the frame of parabolic equation (31) is expressed by the following Fourier series [1]:

$$\theta_p = \frac{4\theta_0}{\pi} \sum_{m=0}^{\infty} \frac{(-1)^m}{(2m+1)} \cos\left[\frac{(2m+1)\,\pi}{2}\tilde{x}\right] \exp\left[d_{mp}\tilde{t}\right] \tag{35}$$

with decrement of temperature damping

$$d_{mp} = -\frac{\lambda^2\,(2m+1)^2\,\pi^2}{4}. \tag{36}$$

On the other hand, the solution to this problem in the case of elliptical equation (32) is expressed by the following series:

$$\theta_p = \frac{4\theta_0}{\pi} \sum_{m=0}^{\infty} \frac{(-1)^m}{(2m+1)} \cos\left[\frac{(2m+1)\,\pi}{2}\tilde{x}\right] \exp\left[d_{me}\tilde{t}\right] \tag{37}$$

with damping parameter

$$d_{me} = \frac{1 - \sqrt{1 + \lambda^2\,(2m+1)^2\,\pi^2}}{2}. \tag{38}$$

Thus, comparing damping parameters in (36) and (38) one can see that in case of elliptical equation the higher harmonics decay more slowly than in case of parabolic equation in accordance with dispersion dependences (25) and (27).

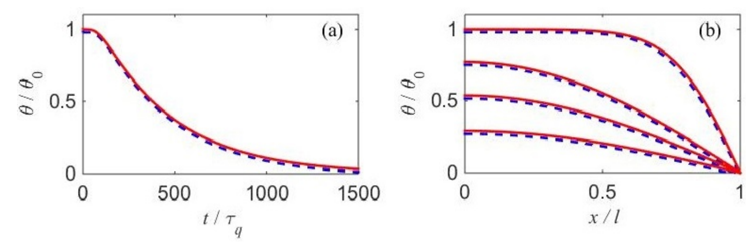

Figure 2: Cooling down the thick plate with $l > l_q$ ($\lambda^2 = 0.001$). Initial temperature $\theta = \theta_0$. (a) Time dependence of temperature at the point $x = 0$. (b) Temperature distributions at different time ($t/\tau_q = 20, 200, 350, 600$). The solutions of parabolic equation are indicated by dashed blue lines. Solutions of elliptic equation are shown by solid red lines.

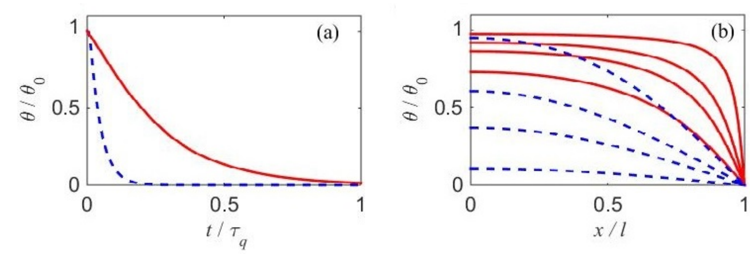

Figure 3: Cooling down the thin plate with $l < l_q$ ($\lambda^2 = 10$). Initial temperature $\theta = \theta_0$. (a) Time dependence of temperature at the point $x = 0$. (b) Temperature distributions at different time ($t/\tau_q = 0.01, 0.03, 0.05, 0.1$). The solutions of parabolic equation are indicated by dashed blue lines. Solutions of elliptic equation are shown by solid red lines.

The results of numerical calculations for the plates with different thicknesses are represented in Fig. 2 and Fig. 3. It is seen that in the case of thick plates ($l > l_q$) the solution of the elliptic equation (red solid curves in Fig. 2a,b) coincides with the solution of the parabolic equation (blue dashed curves in Fig. 2a,b). However, for thin plates ($l < l_q$) the solution to the parabolic equation demonstrates a rapid decrease in temperature gradients and faster cooling of the plate (blue dashed curves in Fig. 3a,b) than in the case of the solution described by the elliptic equation (red solid curves in Fig. 3a,b).

To clarify the time evolution of parabolic and elliptic solutions, we analyze the behavior of zero harmonics. Let us consider the cooling a plate (thickness $2l$) with initial temperature $\theta = \theta_0 \cos(\pi x/2l)$ and with zero temperature at the boundaries $x = \pm l$. In this case

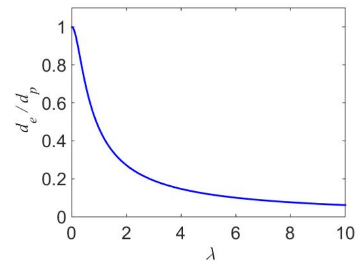

Figure 4: The dependence of the ratio of decrements d_e/d_p on the parameter λ.

$$\theta_p = \theta_0 \cos\left(\frac{\pi\tilde{x}}{2}\right) \exp\left(-\frac{\lambda^2\pi^2}{4}\,\tilde{t}\right) \tag{39}$$

with decrement of temperature damping

$$d_p = -\frac{\lambda^2\pi^2}{4}, \tag{40}$$

and

$$\theta_e = \theta_0 \cos\left(\frac{\pi\tilde{x}}{2}\right) \exp\left(\frac{1-\sqrt{1+\lambda^2\pi^2}}{2}\,\tilde{t}\right) \tag{41}$$

with decrement

$$d_e = \frac{1-\sqrt{1+\lambda^2\pi^2}}{2}. \tag{42}$$

The dependence of the ratio of damping parameters d_e/d_p as the function of λ is represented in Fig. 4. For thick plates when $\lambda^2\pi^2 \ll 1$ we have

$$d_e \approx -\frac{\lambda^2\pi^2}{4} = d_p \tag{43}$$

and time behavior of elliptic and parabolic solutions is practically the same. The temperature profiles at different time and the dependence of temperature at the central point of plate on time are shown in Fig. 5.

In opposite case of thin plate when $\lambda^2\pi^2 \gg 1$ we have

$$d_e \approx -\frac{\lambda\pi}{2} < d_p \tag{44}$$

and elliptical solution predicts slower cooling than parabolic solution. The corresponding profiles and time dependences are shown in Fig.6.

Thus it is seen that the differences between solutions of parabolic and elliptic equations are noticeable only at small spatial scales, when the plate thickness is on the order of or less than the diffusion length.

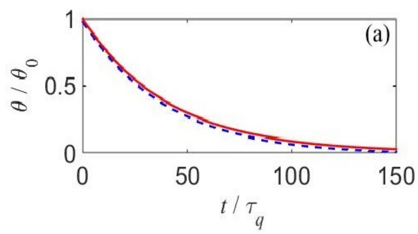

Figure 5: Cooling down the thick plate with $l > l_q$ ($\lambda^2 = 0.01$). Initial temperature $\theta = \theta_0 \cos(\pi x/2l)$. (a) Time dependence of temperature at the point $x = 0$. (b) Temperature distributions at different time ($t/\tau_q = 1, 15, 30, 60$). The solutions of parabolic equation are indicated by dashed blue lines. Solutions of elliptic equation are shown by solid red lines.

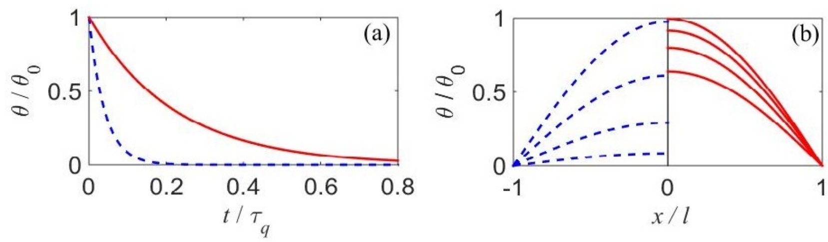

Figure 6: Cooling down the thin plate with $l < l_q$ ($\lambda^2 = 10$). Initial temperature $\theta = \theta_0 \cos(\pi x/2l)$. (a) Time dependence of temperature at the point $x = 0$. (b) Temperature distributions at different time ($t/\tau_q = 0.001, 0.02, 0.05, 0.1$). The solutions of parabolic equation are indicated by dashed blue lines. Solutions of elliptic equation are shown by solid red lines.

4 Conclusion

The generalized equation (14) is an alternative law of changes in heat and diffusion fluxes, which leads to a second-order differential equation of elliptical type (18) describing the evolution of temperature and impurity concentration profiles with finite rate. Solutions of elliptic equation have the same stationary spatial distributions as in the case of parabolic equation, but describe a different dynamics of heat and mass transfer processes. Using simple problem of cooling a plate, it is shown that on large spatial scales, when the plate thickness is greater than the thermal diffusion length, the differences between the solutions of parabolic and elliptical equations are insignificant. However, in the case when the plate thickness is less than the diffusion length, the elliptical-type equation predicts a slower cooling in accordance with finite heat transfer rate. Thus, it has been shown that an elliptic equation provides a finite rate of transfer processes, but it does not have the disadvantages of a hyperbolic equation, which predicts many paradoxical results associated with the possible propagation of heat in the form of real harmonic waves.

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