ISSN: 2692-5397
DOI: 10.33552/MCMS.2024.05.000621
Modern Concepts in Material Science
Iris Publishers

Review article

Heat Transport Equations in Elastic Nanosystems

Angelo Morro*

DIBRIS-Department of informatics, Bioengineering, Robotics and system Engineering University/Organization: university of Genoa, Italy

***Corresponding author:** Angelo Morro, DIBRIS-Department of informatics, Bioengineering, Robotics and system Engineering university/Organization: University of Genoa, Italy

Received Date: February 07, 2024

Published Date: February 20, 2024

Abstract

The paper is devoted to some modelling equations for heat propagation in nanosystems. The purpose is to investigate the thermodynamic consistency so that appropriate constitutive restrictions are established. First a second-order differential equation is considered, with two phase lags, that fits experimental data on heat propagation in graphene. Next a non-local model is examined through a rate-type equation with second-order spatial derivatives of the heat flux. For generality the body is allowed to be elastically deformable. The thermodynamic consistency leads to some simplifications and relates the whole model to free energy function of temperature, strain, and heat flux.

Keywords: Heat propagation in graphene; Relaxation in nanosystems, Thermal wave equations; Non-local equations; Thermodynamic consistency

Introduction

The classical Fourier theory of heat conduction is widely applied in thermal processes also because of its simplicity and reliability in many thermal processes. It is based on Fourier's law for the heat flux q,

$$q = -\kappa \nabla \theta,$$

where θ is the (absolute) temperature, Δ denotes the gradient and κ is the conductivity. Yet there are many contexts where Fourier's theory is inadequate. Conceptually, it is paradoxical that a theory predicts propagation with infinite speed as is the case for Fourier's theory. The Maxwell-Cattaneo (MC) equation [1-3].

$$\tau \partial_t q + q = -\kappa \nabla \theta, \quad (1)$$

where τ is a time constant and ∂_t is the partial time derivative avoids the paradox of infinite speed of propagation. Indeed, a wide literature has been developed as to the proper formulation in that eq. (1) is viewed as a constitutive equation and accordingly it has to satisfy the objectivity principle and to be thermodynamically consistent. Among others, refs [4-8] give exhaustive accounts of these topics and their developments in the literature.

Now, though the MC equation remedies the paradox, there are experiments on heat propagation in graphene [9] whereby an equation more involved than (1) is appropriate to fit the results. Indeed a good fit has been obtained with the equation

$$\frac{1}{\alpha}\partial_t \theta + \frac{\tau_q}{\alpha}\partial_t^2 \theta = \Delta\theta + \tau_\theta \partial_t \Delta\theta, \quad (2)$$

where α is the thermal diffusivity, τ_q, τ_θ two relaxation times or phase lags, and Δ is the Laplacian operator. Indeed, the fact that the fitting indicates comparable values for τ_q and τ_θ, respectively 1.85 and 1.01 ps, makes eq. (2) worthy of attention. Accordingly, though eq. (2) is again plagued by the paradox of infinite speed of propagation, it is of interest to clarify the origin of (2) and to cast it in a context of continuum physics.

Other experiments [10] show a good fit with the solution of the Guyer-Krumhansl equation,

$$\tau\partial_t q + q = -\kappa\nabla\theta + l^2\left[\Delta q + 2\nabla(\nabla . q)\right], \qquad (3)$$

a linear approximation of the nonlinear Guyer-Krumhansl equation [11, 12]

$$\tau\partial_t q + q = -\kappa\nabla\theta + \frac{2\tau}{\theta c}(q.\nabla)q + l^2\left[\Delta q + 2\nabla(\nabla . q)\right], \qquad (4)$$

where c is the specific heat and l a parameter justified by phonon processes. Nanodevices suffer from dissipation of heat at a rate that is not explained by the previous equations. Consistently, the decrease of the thermal conductivity (see, e.g., [10, 13, 14]), which hinders heat exchange, calls for more involved materials models. Furthermore, nanoscale systems with dimensions comparable to the mean-free path of particles (or phonons) non-local effects are required to be inserted in the model. In addition, in microdevices working at high frequencies also relaxation effects occur so that realistic models need to account for the time delay of relaxation processes.

Based on these observations, this paper has a twofold purpose. First to investigate the appropriate continuum framework for equations of the form (2). Secondly, to examine non-local generalizations of (4) and to establish the restrictions placed by the thermodynamic consistency.

Balance equations and entropy principle

The body under consideration occupies a time-dependent region Ω. A point of the body is labelled by the position vector $\mathbf{X}$ in a reference configuration R. Hence we let $X = \chi(\mathbf{X}, t)$ provide the position x in Ω in terms of the position $\mathbf{X} \in R$ and the time t. The body is deformable and we let $\mathbf{F}$, $F_{ik} = \partial_{X_k}\chi_i$, be the deformation gradient. The velocity v is defined by $\mathbf{v} = \partial_t\chi$ while $\nabla = \partial_x$ is the gradient operator. The tensor $\mathbf{L}$ denotes the velocity gradient, $L_{ij} = \partial_{x_j} v_i$. We let ρ be the mass density, $\mathbf{T}$ the Cauchy stress, ε the internal energy density, and η the entropy density (per unit mass). For any pair of vectors $\mathbf{a}, \mathbf{b}$ we let $\mathbf{a}\cdot\mathbf{b}$ denote the inner product; likewise for any pair of tensors $\mathbf{A}, \mathbf{B}$ we let $\mathbf{A}\cdot\mathbf{B} = A_{ij}B_{ij}$. For any function $f(\mathrm{X}, t)$ we denote by a superposed dot the material derivative and we have $\dot{f} = \partial_t f + (v\cdot\nabla)f$. The superscript $\mathbf{T}$ means transpose of a tensor, sym the symmetric part, and skw the skew-symmetric part; 1 denotes the unit second-order tensor and $\otimes$ the dyadic product.

By the conservation of mass, the mass density ρ is subject to the continuity equation

$$\dot{\rho} = -\rho\nabla\cdot\mathbf{v}. \qquad (5)$$

The equation of motion is given the form

$$\rho\dot{v} = \nabla\cdot\mathrm{T} + \rho b, \qquad (6)$$

where b is the body force and $(\nabla\cdot\mathbf{T})_i = \partial_{x_j}T_{ij}$. By the balance of angular momentum it follows $\mathbf{T} = \mathbf{T}^T$. The balance of energy leads to the equation

$$\rho\dot{\varepsilon} = \mathbf{T}\cdot\mathbf{D} - \nabla\cdot\mathrm{q} + \rho r, \qquad (7)$$

where r is the (external) energy supply, q is the heat flux, D = symL is the stretching tensor. The balance of entropy is written in the form

$$\rho\dot{\eta} + \nabla\cdot\left(\frac{q}{\theta} + \mathrm{k}\right) - \frac{\rho r}{\theta} = \rho\gamma \geq 0, \qquad (8)$$

which means that $q/\theta + \mathrm{k}$ is the entropy flux, r/θ the entropy supply and γ the rate of entropy production; the assumption $\gamma \geq 0$ specifies the law of increase of entropy. Equation (8) is referred to as Clausius-Duhem (CD) inequality. We state the entropy principle as follows: physically admissible models are required to satisfy the CD inequality (8) subject to the balance equations (5)-(7).

Substitution of $(\nabla\cdot q - \rho r)/\theta$ from (7) yields

$$\rho\theta\dot{\eta} - \rho\dot{\varepsilon} + \mathbf{T}\cdot\mathbf{D} - \frac{1}{\theta}q\cdot\nabla\theta + \theta\nabla\cdot\mathrm{k} = \rho\theta\gamma \geq 0.$$

Using the Helmholtz free energy

$$\psi = \varepsilon - \theta\eta$$

we can write

$$-\rho\left(\dot{\psi} + \eta\dot{\theta}\right) + T\cdot D - \frac{1}{\theta}q\cdot\nabla\theta + \nabla\cdot\mathrm{k} = \rho\theta\gamma \geq 0. \qquad (9)$$

Heat transport equation with two phase lags

The unusual form of (2) calls for a possible physical model. Let the body be rigid and assume

$$\varepsilon = \varepsilon_0 + c(\theta - \theta_0),$$

the specific heat c being a positive constant. Hence the balance of energy results in

$$\rho c\partial_t\theta = -\nabla\cdot q, \qquad (10)$$

where no heat supply is allowed. The heat conduction consists of two fluxes, $\mathrm{q}_1, \mathrm{q}_2$, , with

$$\mathrm{q} = \mathrm{q}_1 + \mathrm{q}_2.$$

The flux q_1 represents heat conduction due to light particles (electrons) and then modelled by a Fourier law,

$$\mathrm{q}_1 = -\kappa_1\nabla\theta. \qquad (11)$$

The flux q_2 describes heat conduction of heavy particles (ions) and hence is affected by a relaxation property; we model this property by the MC law

$$\tau_q\partial_t\mathrm{q}_2 + \mathrm{q}_2 = -\kappa_2\nabla\theta, \qquad \tau_q > 0. \qquad (12)$$

Both κ_1 and κ_2 are constant, symmetric, non-singular tensors. Time differentiation of (11) gives

$$\partial_t q_1 = -\kappa_1 \nabla \partial_t \theta \quad (13)$$

while (10) leads to

$$\rho c \partial_t^2 \theta = -\nabla \cdot \partial_t q. \quad (14)$$

Hence by (10) plus τ_q times (14) we obtain

$$\rho c \partial_t^2 \theta + \rho c \tau_q \partial_t^2 \theta = -\nabla \cdot q - \tau_q \nabla \cdot \partial_t q = -\nabla \cdot \left[q_1 + \tau_q \nabla \cdot \partial_t q_1 \right] - \nabla \cdot q_2 - \tau_q \nabla \cdot \partial_t q_2$$

and then

$$\rho c \partial_t^2 \theta + \rho c \tau_q \partial_t^2 \theta = \nabla \cdot \left(\kappa_1 + \kappa_2 \right) \nabla \theta + \tau_q \nabla \cdot \kappa_1 \partial_t \theta. \quad (15)$$

In isotropic materials we have

$$\kappa_1 = \kappa_1 1, \qquad \kappa_2 = \kappa_2 1,$$

and hence (16) becomes

$$\rho c \partial_t^2 \theta + \rho c \tau_q \partial_t^2 \theta = \left(\kappa_1 + \kappa_2 \right) \Delta \theta + \tau_q \kappa_1 + \kappa_2 \Delta \partial_t \theta. \quad (16)$$

If, as we prove in a while, $\kappa_1, \kappa_2 > 0$ we can define

$$\kappa = \kappa_1 + \kappa_2, \qquad \tau_\theta = \tau_q \frac{\kappa_1}{\kappa} > 0,$$

and hence eq. (2) follows with $\alpha = \kappa / \rho c$.

We now investigate the thermodynamic consistency of the model (11)-(12). body is undeformable (D = 0) then the CD inequality simplifies to

$$-\rho \left(\dot{\psi} + \eta \dot{\theta} \right) - \frac{1}{\theta} \left(q_1 + q_2 \right) \cdot \nabla \theta = \rho \theta \gamma; \quad (17)$$

the assumption $k = 0$ will be shown to be consistent with the constitutive equations. Owing to eqs. (11)-(12) we let

$$\Gamma = \left(\theta, q_2, \nabla \theta \right)$$

be the set of variables. Time differentiation of $\psi\left(\theta, q_2, \nabla \theta\right)$ and substitution in (17) results in

$$-\rho \left(\partial_\theta \psi + \eta \right) \partial_t \theta - \rho \partial_{\nabla \theta} \psi \cdot \nabla \partial_t \theta - \rho \partial_{q_2} \psi \cdot \partial_t q_2 - \frac{1}{\theta} \left(q_1 + q_2 \right) \nabla \theta = \rho \theta \gamma.$$

Substitution of $\partial_t q_2$ from eq. (12) leads to

$$-\rho \left(\partial_\theta \psi + \eta \right) \partial_t \theta - \rho \partial_{\nabla \theta} \psi \cdot \nabla \partial_t \theta + \frac{\rho}{\tau_q} \partial_{q_2} \psi \cdot q_2 + \left(\frac{\rho}{\tau_q} \partial_{q_2} \psi \kappa_2 - \frac{1}{\theta} q_2 \right) \cdot \nabla \theta - \frac{1}{\theta} q_1 \cdot \nabla \theta = \rho \theta \gamma. \quad (18)$$

The linearity and arbitrariness of $\nabla \partial_t \theta, \partial_t \theta$ imply

$$\partial_{\nabla \theta} \psi = 0, \qquad \eta = -\partial_\theta \psi,$$

and then (18) simplifies to

$$\frac{\rho}{\tau_q} \partial_{q_2} \psi \cdot q_2 + \left(\frac{\rho}{\tau_q} \partial_{q_2} \psi \kappa_2 - \frac{1}{\theta} q_2 \right) \cdot \nabla \theta - \frac{1}{\theta} q_1 \cdot \nabla \theta = \rho \theta \gamma. \quad (19)$$

Assume $q_1 \to 0$ as $\nabla \theta \to 0$ (which is obviously true for (11).

Hence eq. (19) implies that

$$\frac{\rho}{\tau_q} \partial_{q_2} \psi = \kappa_2^{-1} q_2, \qquad \partial_{q_2} \psi \cdot q_2 \geq 0, \qquad q_1 \cdot \nabla \theta \leq 0, \quad (20)$$

and hence

$$\rho \theta \gamma = \frac{\rho}{\tau_q} \partial_{q_2} \psi \cdot q_2 - \frac{1}{\theta} q_1 \cdot \nabla \theta.$$

The obvious integration of the first condition in (20) yields

$$\psi = \Psi\left(\theta\right) + \frac{\tau_q}{2\rho} q_2 \cdot \kappa_2^{-1} q_2$$

and, by the inequalities in (20) we find

$$\kappa_1 > 0, \qquad \kappa_2 > 0,$$

Consequently, the model (10)-(12) with two different fluxes is consistent with thermodynamics provided only that the conductivity tensors κ_1, κ_2 are positive definite.

A simpler derivation of (2) is obtained by considering a formal generalization of the MC equation in the form

$$\tau_q \partial_t q + q = -\lambda \nabla \theta - \lambda \tau_\theta \partial_t \nabla \theta; \quad (21)$$

if $\tau_\theta = 0$ we recover the MC equation. To obtain the differential equation (2) we assume the balance of energy in the form (10) so that

$$\rho c \partial_t \theta = -\nabla \cdot q, \qquad \rho c \partial_t^2 \theta = -\nabla \partial_t q. \quad (22)$$

Computing the divergence of (21) and using (22) we find (2) with $\alpha = \lambda / \rho c$.

Non-local models of heat conduction in elastic nanosystems

The possible large values of spatial gradients, of temperature and heat flux, in nanosystems motivate both non-local terms and the time derivative of the heat flux in the modelling of heat conduction. To fix ideas we observe that quite a general equation has been considered in [1] in the form

$$\hat{o}\partial_t \mathrm{q} + \mathrm{q} = -\kappa\nabla\theta + m_1 \mathrm{q}(\nabla\cdot q) + m_2(q\cdot\nabla)q + m_3\nabla q^2 + m_4\Delta q + m_5\nabla(\nabla\cdot q) + m_6 q(q\cdot\nabla\theta) + m_7 q^2\nabla\theta, \quad (23)$$

where $\mathrm{q}^2 = \mathrm{q}\cdot\mathrm{q}$ and the coefficients $m_1, m_2, \ldots, m_7$ are allowed to depend on temperature.

This indicates that a thermodynamically consistent scheme embodying in some way eq. (23) needs $\theta, \mathrm{q}, \nabla\theta, \nabla\mathrm{q}, \nabla\nabla\mathrm{q}$ among the variables.

As a further generalization we let the nanosystem be deformable and hence we let the material properties be affected by the deformation gradient $\mathbf{F}$. Hence we let

$$\theta, \mathbf{F}, \mathrm{q}, \nabla\theta, \nabla\mathrm{q}, \nabla\nabla\mathrm{q}$$

be the variables describing the nanosystem. Indeed, the scalars ψ and ε should depend on invariants of $\mathbf{F}$; for definiteness we then assume that ψ depends on F through the Green-Lagrange strain

$$\mathrm{E} = \frac{1}{2}\left(\mathbf{F}^T\mathbf{F} - 1\right).$$

By the objectivity principle ([6], ch. 4; [7], § 1.9) the constitutive equations are required to be form-invariant under Euclidean transformations. This means that the constitutive equations involve scalars, vectors, and tensors relative to Euclidean transfor-mations. The time derivative is not form invariant; the transform of the time derivative is different from the time derivative of the transform. That is why objective time deriva-tives are used for rate equations in continuum mechanics. The simplest objective time derivative is the corotational one, namely

$$\overset{\circ}{\mathrm{q}} = \dot{\mathrm{q}} - \mathrm{W}\mathrm{q},$$

where W is the spin tensor, $W_{ij} = \frac{1}{2}\left(\partial_{xj}\upsilon_i - \partial_{xi}\upsilon_j\right)$. Hence we ask for the thermodynamic consistency of the rate equation

$$\tau\overset{\circ}{\mathrm{q}} + \mathrm{q} = -\kappa\nabla\theta + m_1\mathrm{q}(\nabla\cdot q) + m_2(q\cdot\nabla)q + m_3\nabla q^2 + m_4\Delta q + m_5\nabla(\nabla\cdot q) + m_6 q(q\cdot\nabla\theta) + m_7 q^2\nabla\theta, \quad (24)$$

Equation (24) can then be viewed as a constitutive equation for the rate q in terms of the variables $\theta, \mathbf{F}, \mathrm{q}, \nabla\theta, \nabla\mathrm{q}, \nabla\nabla\mathrm{q}$, where $m_1, m_2, \ldots, m_7$ may depend on θ and $\mathbf{F}$, possibly through J = det F. Notice that eq. (24) implies

$$\dot{\mathrm{q}} = \frac{1}{\tau}\left\{\tau\mathrm{W}\mathrm{q} - \mathrm{q} - \kappa\nabla\theta + m_1\mathrm{q}(\nabla\cdot q) + m_2(q\cdot\nabla)q + m_3\nabla q^2 + m_4\Delta q + m_5\nabla(\nabla\cdot q) + m_6 q(q\cdot\nabla\theta) + m_7 q^2\nabla\theta\right\}. \quad (25)$$

We then start with the assumption

$$\psi = \psi\left(\theta, \mathrm{E}, \mathrm{q}, \nabla\theta, \nabla\mathrm{q}, \nabla\nabla\mathrm{q}\right).$$

Compute $\dot{\psi}$, substitute in the CD inequality (9) and divide by θ to obtain

$$\frac{1}{\theta}\left\{-\rho\left(\partial_\theta\psi + \eta\right)\dot{\theta} - \rho\partial_E\psi\cdot\dot{E} - \rho\partial_q\psi\cdot\dot{\mathrm{q}} - \rho\partial_{\nabla\theta}\cdot(\nabla\theta)^{\cdot} - \rho\partial_{\nabla q}\psi\cdot(\nabla q)^{\cdot} - \rho\partial_{\nabla\nabla q}\psi\cdot(\nabla\nabla q)^{\cdot} + \mathbf{T}\cdot\mathbf{D}\right\} - \frac{1}{\theta^2}\mathrm{q}\cdot\nabla\theta + \nabla\cdot\mathrm{k} = \rho\gamma \geq 0.$$

In light of the identity

$$(\nabla q)^{\cdot} = \nabla\dot{q} - \left(\mathrm{L}^T\nabla\right)\mathrm{q}$$

we have

$$-\frac{\rho}{\theta}\partial_{\nabla q}\psi\cdot(\nabla\mathrm{q})^{\cdot} = -\nabla\cdot\left(\frac{\rho}{\theta}\partial_{\nabla q}\psi\,\dot{\mathrm{q}}\right) + \left[\nabla\cdot\left(\frac{\rho}{\theta}\partial_{\nabla q}\psi\right)\right]\cdot\dot{\mathrm{q}} + \frac{\rho}{\theta}\left(\nabla\mathrm{q}\otimes\partial_{\nabla q}\psi\right)\cdot(\mathrm{D}+\mathrm{W}),$$

Where $\left(\nabla\mathrm{q}\otimes\partial_{\nabla q}\psi\right)_{ij} = \partial_{xi}q_k\partial_{\partial xjqk}\psi.$. Hence the CD inequality (9) can be written in the form

$$\frac{1}{\theta}\{-\rho(\partial_\theta\psi+\eta)\dot\theta-\rho\partial_E\psi\cdot\dot{\mathrm{E}}+\left(\mathrm{T}+\rho\left(\nabla \mathrm{q}\otimes\partial_{\nabla q}\psi\right)\right)\cdot\mathrm{D}+\rho\left(\nabla\mathrm{q}\otimes\partial_{\nabla q}\psi\right)\cdot\mathrm{W}$$
$$-\rho\delta_q\psi\cdot\dot{\mathrm{q}}-\rho\partial_{\nabla q}\cdot(\nabla\theta)^{\cdot}-\rho\partial_{\nabla q}\psi\cdot(\nabla\mathrm{q})^{\cdot}-\rho\partial_{\nabla\nabla q}\psi\cdot(\nabla\nabla\mathrm{q})^{\cdot}\}$$
$$-\frac{1}{\theta^2}\mathrm{q}\cdot\nabla\theta+\nabla\cdot\left(\mathrm{k}-\frac{\rho}{\theta}\partial_{\nabla q}\psi\right)=\rho\gamma\geq 0,$$

where $\delta_q\psi$ is the variational derivative,

$$\delta_q\psi=\partial_q\psi-\frac{\theta}{\rho}\nabla\cdot\left(\frac{\rho}{\theta}\partial_{\nabla q}\psi\right)=\partial_q\psi-\frac{\theta}{\rho}\partial_{xi}\left(\frac{\rho}{\theta}\partial_{\partial xjq}\psi\right).$$

The derivative $\dot{\mathrm{q}}$ is not arbitrary in that $\dot{\mathrm{q}}=\overset{\circ}{\mathrm{q}}+\mathrm{Wq}$ is given by eq. (24). Furthermore $\dot{\mathrm{E}}$ and D are related by the identity $\dot{\mathrm{E}}=\mathrm{F}^T\mathrm{DF}$.

Hence upon substitution of $\dot{\mathrm{q}}$ from (24) and multiplication by θ we have

$$-\rho(\partial_\theta\psi+\eta)\dot\theta+\left(\mathrm{T}+\rho\nabla\mathrm{q}\otimes\partial_{\nabla q}\psi-\rho\mathrm{F}\partial_E\psi\mathrm{F}^T\right)\cdot\mathrm{D}+\rho\left(\nabla\mathrm{q}\otimes\partial_{\nabla q}\psi\right)\cdot\mathrm{W}$$
$$-\rho\partial_{\nabla\theta}\psi\cdot(\nabla\theta)^{\cdot}--\rho\partial_{\nabla\nabla q}\psi\cdot(\nabla\nabla\mathrm{q})^{\cdot}-\frac{1}{\theta}\mathrm{q}\cdot\nabla\theta+\theta\nabla\cdot\left(\mathrm{k}-\frac{\rho}{\theta}\partial_{\nabla q}\psi\,\dot{\mathrm{q}}\right)$$
$$-\frac{\rho}{\tau}\delta_q\psi\cdot\{\tau\mathrm{W}q-q-\kappa\nabla\theta+m_1\mathrm{q}(\nabla\cdot q)+m_2(q\cdot\nabla)q+m_3\nabla q^2+m_4\Delta q$$
$$+m_5\nabla(\nabla\cdot q)+m_6q(q\cdot\nabla\theta)+m_7q^2\nabla\theta\}=\rho\theta\gamma\geq 0.$$

This form of the CD inequality allows us to see the possible arbitrariness and hence to find the corresponding consequences. First we notice that $(\nabla\theta)^{\cdot},(\nabla\nabla\mathrm{q})^{\cdot},\theta$ can take arbitrary values and meanwhile without affecting the constitutive functions $\psi,\eta,\mathrm{T},\mathrm{k},\gamma$. Owing to the linearity it follows that

$$\partial_{\nabla\theta}\psi=0,\qquad\partial_{\nabla\nabla q}\psi=0,\qquad\eta=-\partial_\theta\psi.$$

The linearity and arbitrariness of W and D imply that

$$\nabla\mathrm{q}\otimes\partial_{\nabla q}\psi-\delta_q\psi\otimes\mathrm{q}\in\mathrm{Sym},\qquad\mathrm{T}=\rho\mathrm{F}\partial_E\psi\mathrm{F}^T-\rho\nabla\mathrm{q}\otimes\partial_{\nabla q}\psi.\tag{27}$$

Hence we are left with

$$\theta\nabla\cdot\left(\mathrm{k}-\frac{\rho}{\theta}\partial_{\nabla q}\psi\,\dot{\mathrm{q}}\right)+\nabla\theta\left(-\frac{1}{\theta}\mathrm{q}+\frac{\rho\kappa}{\tau}\delta_q\psi-m_6\frac{\rho}{\tau}(\delta_q\psi\cdot\mathrm{q})\mathrm{q}-m_7\frac{\rho\mathrm{q}^2}{\tau}\delta_q\psi\right)$$
$$-\frac{\rho}{\tau}\delta_q\psi\cdot\{-\mathrm{q}+m_1\mathrm{q}(\nabla\cdot q)+m_2(q\cdot\nabla)q+m_3\nabla q^2+m_4\Delta q+m_5\nabla(\nabla\cdot q)\}$$
$$=\rho\theta\gamma\geq 0.\tag{28}$$

Definite consequences of inequality (28) follow in particular cases. Assume $m_1,m_2,m_3=0$. We notice that

$$-\frac{\rho}{\tau}\delta_q\psi\cdot\{m_4\Delta q+m_5\nabla(\nabla\cdot q)\}=-\partial_{xi}\left(\frac{\rho m_4}{\tau\theta}\delta_q\psi\partial_{xi}q\right)+\partial_{xi}q\cdot\left(\partial_{xi}\frac{\rho m_4}{\tau\theta}\delta_q\psi\right)$$
$$-\nabla\cdot\left(\frac{\rho m_5}{\tau\theta}\delta_q\psi\nabla\cdot q\right)+(\nabla\cdot q)\nabla\cdot\left(\frac{\rho m_5}{\tau\theta}\delta_q\psi\right)\tag{29}$$

For any field q we have

$$\partial_{xi}q\cdot\left(\partial_{xi}\frac{\rho m_4}{\tau\theta}\delta_q\psi\right)+(\nabla\cdot q)\nabla\cdot\left(\frac{\rho m_5}{\tau\theta}\right)\geq 0$$

if

$$\frac{\rho m_4}{\tau\theta}\delta_q\psi=\alpha q,\qquad\frac{\rho m_5}{\tau\theta}\delta_q\psi=\beta q,$$

where α, β are positive constants. Assuming it is so we can use (29) and write eq. (28) in the form

$$\theta\nabla\cdot\left\{\mathrm{k}-\frac{\rho}{\theta}\partial_{\nabla q}\psi\,\dot{\mathrm{q}}-\frac{\rho m_4}{\tau\theta}\delta_q\psi\left(\nabla q\right)^T-\frac{\rho m_5}{\tau\theta}\delta_q\psi\nabla\cdot q\right\}$$
$$+\nabla\theta\cdot\left(-\frac{1}{\theta}\mathrm{q}+\frac{\rho\kappa}{\tau}\delta_q\psi-m_6\frac{\rho}{\tau}\left(\delta_q\psi\cdot\mathrm{q}\right)\mathrm{q}-m_7\frac{\rho \mathrm{q}^2}{\tau}\delta_q\psi\right)+\frac{\rho}{\tau}\delta_q\psi\cdot q=\rho\theta\gamma\geq 0. \tag{30}$$

Inequality (30) holds if

$$\mathrm{k}=\frac{\rho}{\theta}\partial_{\nabla q}\psi\,\dot{\mathrm{q}}-\frac{\rho m_4}{\tau\theta}\delta_q\psi\left(\nabla q\right)^T-\frac{\rho m_5}{\tau\theta}\delta_q\psi\nabla\cdot q, \tag{31}$$

$$-\frac{1}{\theta}\mathrm{q}+\frac{\rho\kappa}{\tau}\delta_q\psi-m_6\frac{\rho}{\tau}\left(\delta_q\psi\cdot\mathrm{q}\right)\mathrm{q}-m_7\frac{\rho\mathrm{q}^2}{\tau}\delta_q\psi=0, \tag{32}$$

$$\delta_q\psi\cdot q=\tau\theta\gamma\geq 0. \tag{33}$$

The reduced inequality (33) implies that

$$\delta_q\psi=\mu q,\qquad \mu\geq 0.$$

This is true if $\partial_{\nabla q}\psi=0$ and then $\delta_q\psi=\partial_q\psi$. Thus we let

$$\psi=\psi\left(\theta,E,\mathrm{q}\right)=\Psi\left(\theta,E\right)+\hat{\psi}\left(\theta,q\right),\qquad q=\left|\mathrm{q}\right|. \tag{34}$$

Equation (32) then simplifies to

$$-\frac{1}{\theta}\mathrm{q}+\frac{\rho\kappa}{\tau}\partial_q\hat{\psi}\frac{\mathrm{q}}{q}-m_6\frac{\rho}{\tau}\partial_q\left(\frac{\mathrm{q}}{q}\cdot\mathrm{q}\right)\mathrm{q}-m_7\frac{\rho}{\tau}q^2\partial_q\hat{\psi}\frac{\mathrm{q}}{q}=0,$$

whence

$$-1+a\partial_q\hat{\psi}\frac{1}{q}-b\partial_q\hat{\psi}q=0,\quad a=\frac{\rho\theta\kappa}{\tau},\quad b=\left(m_6+m_7\right)\frac{\rho\theta}{\tau}.$$

It follows that
$$\partial_q\hat{\psi}=\frac{q}{a-bq^2}.$$

Thus, by (33), $\partial_q\hat{\psi}$ is required to satisfy

$$\partial_q\hat{\psi}q=\frac{q^2}{a-bq^2}\geq 0\qquad\forall q\geq 0.$$

As it follows by letting $q\to 0$ and $q\to\infty$ we find the necessary and sufficient conditions

$$a>0,\qquad b\leq 0.$$

Consequently we find that

$$\kappa>0,\qquad m_6+m_7\leq 0.$$

If $b<0$ then it follows

$$\hat{\psi}=\frac{1}{2\left|b\right|}\ln\left(a+\left|b\right|q^2\right). \tag{35}$$

If, instead, $b=0$ then

$$\hat{\psi}=\frac{1}{2a}q^2=\frac{\tau}{2\rho\theta\kappa}q^2. \tag{36}$$

Since we have assumed $m_1, m_2, m_3=0$ then the non-local model is thermodynamically consistent if it is settled as follows. The heat flux q is governed by the rate equation

$$\tau\overset{\circ}{\mathrm{q}}+\mathrm{q}=\left[\left(m_7\mathrm{q}^2-\kappa\right)1+m_6\mathrm{q}\otimes\mathrm{q}\right]\nabla\theta+m_4\Delta\mathrm{q}+m_5\nabla\left(\nabla\cdot\mathrm{q}\right), \tag{37}$$

where m_4, m_5, m_6, m_7 are allowed to depend on temperature. The entropy principle ulti-mately requires that

$$\psi=\psi\left(\theta,E,q\right),$$

where $q=\left|\mathrm{q}\right|$. For definiteness we assume ψ in the form (34) and then we find that if

$$\frac{\rho m_4}{\tau\theta q}\partial_q\hat{\psi}\ \text{and}\ \frac{\rho m_5}{\tau\theta q}\partial_q\psi$$

are constants then

$$\mathrm{k}=-\frac{\rho m_4}{\tau\theta q}\partial_q\hat{\psi}\mathrm{q}\left(\nabla\mathrm{q}\right)^T-\frac{\rho m_5}{\tau\theta q}\partial_q\psi\mathrm{q}\left(\nabla\cdot\mathrm{q}\right)$$

is the extra-entropy flux and

$$\psi=\Psi\left(\theta,E\right)+\hat{\psi}\left(\theta,q\right)$$

is the free energy where ψ is given by (35) or (36) according as $m_6+m_7<0$ or $m_6+m_7=0$.

Conclusions

This paper deals with two model equations for heat propagation in nanosystems. The equation with two phase lags (2) is shown to arise from a physical model with two heat fluxes, one for the Fourier-type for light particles (possibly electrons) and one for heavy particles (possibly ions) which involve a relaxation term. The whole physical scheme is found to be thermodynamically consistent.

The second equation is non-local in character in that involves higher-order spatial derivatives of the heat flux thus generalizing the linear Guyer-Krumhansl equation (3). For generality the body is allowed to be elastically deformable. The thermodynamical consistency is then proved for the non-linear objective rate equation (37) subject to

$$a = \frac{\rho\theta\kappa}{\tau} > 0, \quad b = (m_6 + m_7)\frac{\rho\theta}{\tau} \leq 0,$$

with free energy

$$\psi(\theta, E, q) = \Psi(\theta, E) + \frac{1}{2|b|}\ln\left(a + |b| q^2\right),$$

with $q = |\mathrm{q}|$. The dependence on b generalizes previous models by allowing for the non-linear terms parameterized by m_6 and m_7. If $b = 0$ then $\widehat{\psi}$ is given by (36).

As to the stress tensor, it follows that heat conduction effects on the stress emerge through the formal dependence of the free energy on $\nabla\mathrm{q}$. Hence the stress behaviour is not affected by letting the objective derivative be the corotational one and the free energy be independent of $\nabla\mathrm{q}$. This indicates the guideline for a simple model accounting for heat conduction with non-local and non-linear properties.

Acknowledgment

The research leading to this work has been developed under the auspices of INDAM-GNFM.

Conflict of Interest

None.

References

1. Y Guo, D Jou, M Wang (2017) Macroscopic heat transport equations and heat waves in nonequilibrium states. Physica D: Nonlinear Phenomena 342: 24-31.
2. JC Maxwell (1965) On the dynamic theory of gases. in The Scientific Papers of JC Maxwell 2: 26-78.
3. C Cattaneo (1948) Sulla conduzione del calore. Atti Sem Mat Fis Univ Modena 3: 3-21.
4. R Kovacs (2024) Heat equations beyond Fourier: From heat waves to thermal metamaterials, Physics Reports 1048: 1-75.
5. B Straughan (2011) Heat Waves, Springer, New York, USA.
6. C Truesdell (1977) A First Course in Rational Continuum Mechanics. vol. 1, Academic Press, New York, USA.
7. A Morro, C Giorgi (2023) Mathematical Modelling of Continuum Physics. Birkhauser, Cham.
8. DD Joseph, L Preziosi (1989) Heat Waves. Rev Modern Phys 61: 41-73.
9. J Zhang, X Huang, Y Yue, J Wang, X Wang (2011) Dynamic response of graphene to thermal impulse. Phys Rev B 84: 235416
10. Hennessy MG, Myers TG (2020) Guyer-Krumhansl heat conduction in thermoreflectance experiments, in Multidisciplinary Mathematical Modelling. Applications of Mathematics to the Real World, F. Font and T.G. Myers eds pp. 21-34.
11. VA Cimmelli, A Sellitto, D Jou (2010) Nonequilibrium temperatures, heat waves, and nonlinear heat transport equations. Phys Rev B 81: 054301
12. A Morro (2023) On the modelling of heat conduction in crystals via higher-grade terms. Nanotecnol Adv Mater Sci 6: 1-4.
13. Cahill DG (2014) Nanoscale thermal transport. II Appl Phys Rev 1: 011305
14. Dong Y (2015) Dynamical Analysis of Non-Fourier Heat Conduction and Its Appli-cation in Nanosystems, Springer, New York, USA.