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Effective temperature in nonequilibrium state with heat flux using discrete variable model

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A B S T R A C T

The effective temperature, which acts as a criterion for thermalization in systems with heat flux, has been introduced on the bases of a relatively simple discrete variable model (DVM). The DVM is inherently nonlocal and can be used to describe multi-length and -time scale heat conduction including low-dimensional and sub-continuum regimes. Under far from equilibrium conditions when the heat flux tends to its maximum possible value, the effective temperature and the corresponding nonequilibrium entropy go to zero, which points to a possible generalization of the third law in nonequilibrium situations.

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1. Introduction

The conceptual problems of the definition and measurement of temperature in nonequilibrium states, particularly in sub-continuum regimes, attract great attention due to the increasing interest in thermodynamic theories beyond local equilibrium [1–10], in glassy systems [11], in molecular dynamic simulations [8,12–14], in active matter and biological systems [15,16], in the context of the issue of global warming [17], and in technological applications of nanoscale systems and material sciences [8,12, 18–21]. Several approaches have been used to model the temperature evolution under local nonequilibrium conditions starting from both thermodynamic and microscopic bases [1–24], but still a satisfactory definition of the nonequilibrium temperature is an open problem [1,2,12–15,18–21]. Moreover, most of the approaches are usually cumbersome and numerical methods are needed to obtain their solutions. Thus, looking for simpler phenomenological equations leading to reasonable predictions may be useful from the practical point of view as they offer a preliminary approach, which may be refined later by means of cumbersome but more precise methods. One of such approaches is the discrete variable model (DVM) [9,10,22–27], which discretizes the space and time by defining lattice sites of a characteristic size h where the heat carrier temperature (or energy density) is calculated in discrete intervals of time τ. The idea to describe the heat conduction with

space–time discrete variables is closely related to the concept of random walks and lattice Boltzmann method (see [28–31] and references therein). The characteristic length h is the minimum size of the lattice, to which the local temperature $T(x,t)$ can still be assigned. The idea of the minimum space scales employed by the DVM corresponds to the conclusion of Majumdar [18] that "since temperature at a point can be defined only under local thermodynamic equilibrium, a meaningful temperature can be defined only at points separated on an average by the phonon mean free path". It is also consistent with the concept of minimum heat-affected region suggested by Chen [19,20], which assumes that during phonon transport from a nanoscale heat source the minimum size of the heat affected region is of the order of the phonon mean free path. The DVM successfully describes the nano-scale heat conduction in thin films introducing two types of the effective (size-dependent) thermal conductivity [27]. In this paper the DVM is used to introduce and discuss the effective temperature and corresponding entropy for far from equilibrium situation.

2. Discrete variable model

In a one-dimensional description (1D), the discrete approach gives the heat conduction equation as follows [9,10,22–27]

$$U(t+\tau,x) = \frac{1}{2}\big[U(t,x+h) + U(t,x-h)\big] + Q(t+\tau/2,x) \quad (1)$$

where $U(t,x)$ is the energy of the heat carriers at a lattice site $(x-h/2, x+h/2)$ at a time moment t, Q is the external energy

source. The discrete formalism implies that the energy exchange between the lattice occurs on the border between the neighboring lattice, which for the lattices x and $x - h$ is situated at $x - h/2$. Making a coordinate shift $x \rightarrow x + h/2$, we can present the heat flux q through the plane x, which is the border between lattice sites with coordinates $x - h/2$ and $x + h/2$, as follows [9,10,22–27]

$$q(t + \tau/2, x) = \frac{v}{2}[U(t, x - h/2) - U(t, x + h/2)] \qquad (2)$$

where $v = h/\tau$ is the heat-carrier (phonon) velocity, which assumed to be frequency-independent (so-called gray approximation [30,31]). Strictly speaking, this assumption is valid in the Debye approximation, while in a general case there are dispersive effects that make v itself depends on the phonon frequency.

Thus, the DVM, Eqs. (1) and (2), reflects the inherent nonlocality of transfer processes taking into account both time τ and space h scales of energy carriers.

3. Effective temperature θ

Let us consider a heat flux q through a plane with coordinate x. According to Eq. (2) the heat flux can be expressed as [27]

$$q(t + \tau/2) = \frac{v}{2}(U_1 - U_2) \qquad (3)$$

where $U_1 = U(t, x - h/2)$ is the energy of the heat carriers, which move through the plane x from the left to the right, and $U_2 = U(t, x + h/2)$ is the energy of the heat carriers, which move through the plane x from the right to the left. Now let us reformulate Eq. (3) in terms of temperature. Usually the temperature under nonequilibrium condition is defined on the basis of the kinetic energy of the particles and is sometimes referred to as the kinetic temperature [1,2,12,28]. The kinetic temperatures of the heat careers moving in the opposite directions can be defined as $T_1 = U_1/C$ and $T_2 = U_2/C$, respectively, where C is the heat capacity. The corresponding total temperature of the system T is an average of the two temperatures T_1 and T_2: $T = (T_1 + T_2)/2$ [28,30,31]. Note that the kinetic temperature of the nonequilibrium state T is equal to the equilibrium temperature of the system with the same internal energy [28], which is reached by the system after equilibration under adiabatic conditions. Using these definitions of the temperatures and assuming $\tau \ll t$, Eq. (3) gives

$$T_1 = T + q/Cv \qquad (4)$$

$$T_2 = T - q/Cv \qquad (5)$$

Analogous equations for the temperatures of the heat carriers moving in the opposite directions arise in the continuum approaches based on the random walk model [28,29], the Bose–Einstein distribution [3], and the Boltzmann transport equation [30,31]. If the two groups of the heat carriers with T_1 and T_2 equilibrates reversibly, i.e. while producing work, their common final temperature will be [17,32]:

$$\theta = (T_1 T_2)^{1/2} \qquad$$

Indeed, before equilibration the total entropy of the two groups is equal to $S_{neq} = k_B \ln T_1 + k_B \ln T_2 = k_B \ln T_1 T_2$ (k_B is the Boltzmann constant), whereas after equilibration $S_{eq} = 2k_B \ln \theta$, where θ is the common temperature of the groups after equilibration. The entropy change during equilibration is $\Delta S = S_{neq} - S_{eq} = k_B \ln T_1 T_2/\theta^2$. When the system equilibrates reversibly, the entropy does not change, i.e. $\Delta S = 0$, which gives that θ is equal to the geometric mean of the two temperatures T_1 and T_2 [32].

Multiplying Eq. (4) by Eq. (5), we obtain

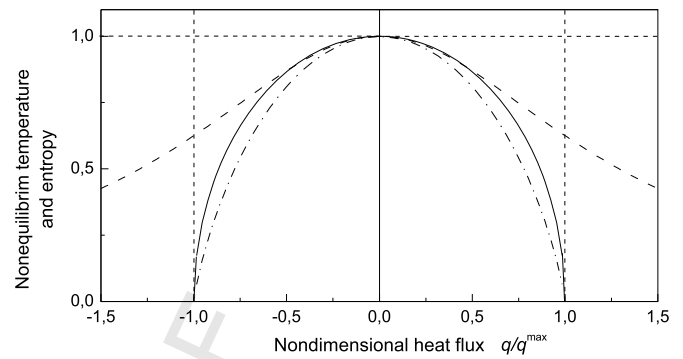$$\theta = T(1 - \hat{q}^2)^{1/2} \qquad (6)$$

Fig. 1. Nondimensional effective temperature θ/T (solid line), Eq. (6), and nondimensional entropy S/S_{eq} (dash-dotted line), Eq. (10), as functions of the nondimensional heat flux $q/q^{\max}$. Nondimensional effective temperature from EIT [1,2] θ_{EIT}/T (dashed line), Eq. (7a), is shown for comparison.

where $\hat{q} = q/CvT$ is the nondimensional heat flux. Fig. 1 shows the effective nondimensional temperature θ/T as a function of the nondimensional heat flux $\hat{q}$ (solid line). In equilibrium $q = 0$ and the effective temperature θ takes its maximum value $\theta^{\max} = T$. As the absolute value of the heat flux $|q|$ increases, θ decreases and reaches zero at the maximum possible value of the heat flux $\hat{q}_{\max} = 1$ (see Fig. 1). The maximum heat flux $q^{\max}$ is reached when all the heat carriers move in the same direction. The result that $\theta \rightarrow 0$ at $|q| \rightarrow q^{\max}$ is confirmed by heat conduction in harmonic chains [1] and in 1D crystal under quantum limit [3]. Thus, θ in Eq. (6) depicts deviation from equilibrium and imposes a physically reasonable upper bound on the heat flux $|q| \leq q^{\max}$ [1,3,8].

For small deviation from equilibrium when $|\hat{q}| \ll 1$, a Taylor series expansion of Eq. (6) gives

$$\theta = T(1 - \hat{q}^2/2) \qquad$$

which corresponds to the effective temperature obtained by Camacho [3] using a maximum entropy formalism in the classical limit and by Dong et al. [7] on the basis of the thermomass theory. This expression can be represented in a slightly different form as

$$\frac{1}{\theta} = \frac{1}{T} + \frac{\hat{q}^2}{2\theta} \qquad (7)$$

Taking into account that for the small deviation from equilibrium $\theta \approx T$, T in the last term of Eq. (7) can substitute for θ, which gives

$$\frac{1}{\theta} = \frac{1}{T} + \frac{\hat{q}^2}{2T} \qquad (7a)$$

Eq. (7a) corresponds to the effective temperature introduced by Extended irreversible thermodynamics (EIT) of Jou et al. [1,2]. The EIT goes beyond the local equilibrium assumption and obtains generalized heat conduction theory by introducing additional state variables, such as heat flux, into the expression of nonequilibrium entropy [1,2]. As a result the nonequilibrium temperature θ_{EIT} is introduced as $\theta_{EIT} = (\partial S/\partial e)^{-1}$, where e is the local energy density [1,2].

Fig. 1 shows the effective temperatures given by the present model, Eq. (6), and by EIT, Eq. (7a), as functions of the heat flux. As it is expected, the two temperatures coincide at a relatively small deviation from equilibrium when $|\hat{q}| \ll 1$, while at a high deviation from equilibrium when $|\hat{q}| \leq 1$, the two temperatures differ substantially (compare solid and dashed curves in Fig. 1).