Space-time nonlocal model for heat conduction

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We consider a space-time nonlocal heat conduction model with balance laws in the form of integral equations (so-called strong nonlocality). The model identifies two internal parameters—the time τ and the space h scales of nonlocality. In going from the strong nonlocal model to its approximations of various accuracy in the form of partial differential equations, which correspond to weak nonlocality, we introduce two limiting relations between τ and h as $\tau, h \to 0$. In the diffusion limit, which preserves the thermal diffusivity $a = h^2/\tau = \text{const}$ as $\tau, h \to 0$, the strong nonlocal model gives a hierarchy of parabolic equations with an infinite speed of heat waves. In the wave limit, which preserves the ratio $v = h/\tau = \text{const}$ as $\tau, h \to 0$, a hierarchy of hyperbolic equations has been obtained. The hyperbolic equations imply a finite speed of heat waves. These results suggest that for diffusion (low-k) and propagative (high-k) regimes distinct models are responsible for the space-time evolution of the temperature and heat flux. The connection with phonon hydrodynamic theory and applications to other problems are discussed.

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I. INTRODUCTION

Classical thermodynamics leads to a heat conduction equation of parabolic type, which is local, both in time and space. A local theory is adequate when the mean free path and the mean free time are relatively short. Such a theory is based on the local balance equation of energy, the Gibbs equation, and the local balance equation of entropy, which for a rigid isotropic solid take the form

$$\rho \frac{dU(\mathbf{x},t)}{dt} = -\nabla \mathbf{q}(\mathbf{x},t) , \qquad (1)$$

$$dS(\mathbf{x},t) = T^{-1}dU(\mathbf{x},t) , \qquad (2)$$

$$\rho \frac{d\mathbf{S}(\mathbf{x},t)}{dt} + \nabla \mathbf{J}(\mathbf{x},t) = \sigma(\mathbf{x},t) , \qquad (3)$$

where U is the specific internal energy per unit mass, ρ is the mass density, \mathbf{q} is the heat flux, S is the specific entropy per unit mass, T is the temperature, \mathbf{J} is the entropy flux, and σ is the entropy production per unit volume and time. Undoubtedly the local theory has worked well in many applications. However, the local theory is unable to explain some sufficiently rapid (high-frequency) phenomena [1-20]. When one is interested in high-frequency phonon hydrodynamics at low temperatures [8-12], second sound in liquid helium and in certain dielectric crystals [9], high-frequency perturbations in polymeric fluids [13], laser annealing of silicon and germanium [14], shock waves [15], the glass transition of high viscosity liquids [16], heat conduction in gases of molecules with internal degrees of freedom [3,17], ultrafast

heat transport in thin gold films under femstosecond laser irradiation [18], or high-speed traveling waves in excitable media [5,19], the space-time nonlocal effects should be taken into account. In these situations the mean free path and/or the mean free time of excitations, i.e., internal scales, are comparable with the characteristic spacetime scales of the process. The purpose of this paper is to formulate space-time nonlocal balance laws in the integral form and then, working in a way similar to that of the classical theory, obtain heat transfer equations. We also discuss the connection with phonon hydrodynamic theory and applications to other problems.

II. SPACE-TIME NONLOCAL MODEL

Equations (1)-(3) can be cast in the space-time nonlocal form

$$\rho[U(\mathbf{x},t+\tau)-U(\mathbf{x},t)] = \frac{1}{V} \int_{1}^{t+\tau} \mathbf{\Phi} \mathbf{q}(\mathbf{x},t) d\mathbf{w} dt , \qquad (4)$$

$$S(\mathbf{x},t+\tau)-S(\mathbf{x},t)=T^{-1}[U(\mathbf{x},t+\tau)-U(\mathbf{x},t)], \qquad (5)$$

$$\rho[S(\mathbf{x},t+\tau)-S(\mathbf{x},t)] + \frac{1}{V} \int_{t}^{t+\tau} \oint_{\omega} \mathbf{J}(\mathbf{x},t) d\mathbf{w} dt$$

$$= \int_{t}^{t+\tau} \int_{V} \sigma(\mathbf{x},t) dv dt , \quad (6)$$

where τ is the time scale of nonlocality, and $V \sim h^3$ and $\omega \sim h^2$ are the volume and surface, corresponding to the space scale of nonlocality, h. To avoid undue mathematical complications let us consider the one-dimensional case. Then Eq. (4) reduces to

$$\rho[U(x,t+\tau)-U(x,t)]$$

$$=-\frac{\tau}{2h}[q(x+h,t+\gamma\tau)-q(x-h,t+\gamma\tau)];$$

here the coefficient $0<\gamma<1$ appeared due to the integration over time. Introduction of this equation into (5) yields

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$$\rho[S(x,t+\tau)-S(x,t)] = -\frac{\tau}{2h} \left[\frac{q(x+h,t+\gamma\tau)}{T(x+h,t)} - \frac{q(x-h,t+\gamma\tau)}{T(x-h,t)} \right]$$

$$-\frac{1}{2T^{2}h} \left[\left[q(x+h,t+\gamma\tau) + q(x-h,t+\gamma\tau) \right] \left| h \frac{\partial T}{\partial x} + \frac{h^{3}}{3!} \frac{\partial^{3}T}{\partial x^{3}} + \cdots \right|$$

$$+ \left[q(x+h,t+\gamma\tau) - q(x-h,t+\gamma\tau) \right] \left| \frac{h^{2}}{2} \frac{\partial^{2}T}{\partial x^{2}} + \frac{h^{4}}{4!} \frac{\partial^{4}T}{\partial x^{4}} + \cdots \right| \right].$$

$$(7)$$

Here the first large square bracket on the right hand side of Eq. (7) is the entropy flux and the second large square bracket is the nonlocal entropy production, which according to the second law is positive definite. To ensure the positive character of the entropy production in the balance equation (7) one should assume

$$\frac{\tau}{h} [q(x+h,t+\gamma\tau) + q(x-h,t+\gamma\tau)]$$

$$= -\frac{\mu_0}{T^2} \left[h \frac{\partial T}{\partial x} + \frac{h^3}{3!} \frac{\partial^3 T}{\partial x^3} + \cdots \right], \quad (8)$$

$$\frac{\tau}{h} [q(x+h,t+\gamma\tau) - q(x-h,t+\gamma\tau)]$$

$$= -\frac{\mu_1}{T^2} \left[\frac{h^2}{2} \frac{\partial^2 T}{\partial x^2} + \frac{h^4}{4!} \frac{\partial^4 T}{\partial x^4} + \cdots \right]; \quad (9)$$

here $\mu_0 > 0$, and $\mu_1 > 0$.

Introduction of (9) into (4) yields the nonlocal heat conduction equation,

$$c\rho \left[\tau \frac{\partial T}{\partial t} + \frac{\tau^2}{2} \frac{\partial^2 T}{\partial t^2} + \cdots \right]$$

$$= \frac{\mu_1}{2T^2} \left[\frac{h^2}{2} \frac{\partial^2 T}{\partial x^2} + \frac{h^4}{4!} \frac{\partial^4 T}{\partial x^4} + \cdots \right]. \quad (10)$$

Here we take into account that u=cT, with c the specific heat per unit mass. Expansion of the left hand side of eq. (8) into a Taylor series gives the evolution equation for heat flux,

$$q + \gamma \tau \frac{\partial q}{\partial t} + \frac{h^2}{2} \frac{\partial^2 q}{\partial x^2} + \cdots$$

$$= -\frac{\mu_0 h}{2\tau T^2} \left[h \frac{\partial T}{\partial x} + \frac{h^3}{3!} \frac{\partial^3 T}{\partial x^3} + \cdots \right]. \quad (11)$$

Both the nonlocal heat conduction equation (10) and nonlocal heat flux equation (11) contain an infinite number of terms with two small parameters τ and h. To obtain equations with a finite number of terms one must specify the relation between τ and h as $\tau, h \to 0$ [5-7].

A. Diffusion law

For diffusionlike processes we introduce the finite value of the thermal diffusivity $a = h^2/\tau$:

$$\lim_{\tau,h\to 0} h^2/\tau = a = \text{const} . \tag{12}$$

In such a case in the first-order approximation Eqs. (10) and (11) reduce to the (classical) parabolic heat conduction equation and Fourier law, respectively:

$$c\rho \frac{\partial T}{\partial t} = \lambda \frac{\partial^2 T}{\partial x^2} , \qquad (13)$$

$$q = -\lambda \frac{\partial T}{\partial x} , \qquad (14)$$

where $\lambda = \mu_0 a / 2T^2 = \mu_1 a / 4T^2$ is the thermal conductivity. Equations (13) and (14) are local ones, in both time and space.

The second-order approximations to Eqs. (10) and (11) are

$$c\rho \left| \frac{\partial T}{\partial t} + \frac{\tau}{2} \frac{\partial^2 T}{\partial t^2} \right| = \lambda \left| \frac{\partial^2 T}{\partial x^2} + \frac{h^2}{12} \frac{\partial^4 T}{\partial x^4} \right|,$$
 (15)

$$q + \gamma \tau \frac{\partial q}{\partial t} + \frac{h^2}{2} \frac{\partial^2 q}{\partial x^2} = -\lambda \left[\frac{\partial T}{\partial x} + \frac{h^2}{6} \frac{\partial^3 T}{\partial x^3} \right]. \quad (16)$$

These equations are nonlocal in both time [the second terms on the left hand side of (15) and (16)] and space [the last term on the left hand side of (16) and the last terms on the right hand side of (15) and (16)]. Note that classical local equations (13) and (14), nonlocal equations (15) and (16), and the higher order approximations imply the infinite speed for thermal signals (thermal waves). This fact is in accordance with the diffusion relation between τ and h (12). Equation (15) is like the equation deduced by Chester [8] in his analysis of high-frequency phonon hydrodynamics at low temperature. Comparison between (15) and the results of [8] clearly demonstrates that at low temperatures in solids the scales of time-space nonlocality τ and h are symbols for combinations of relaxation time averages and speed average values [8],

$$\tau = \langle R^2 \rangle \langle R / \tau_R \rangle^{-1} ,$$

$$h^2 = 60 \langle S_0^2 \rangle (\langle S_0^{-2} \rangle \langle R / \tau_R \rangle D)^{-1}$$

$$\times (\langle R \rangle \langle R \tau_c^2 \rangle - \langle R^2 \tau_c \rangle \langle \tau_c \rangle) ,$$
(17)

where τ_R is a relaxation time for momentum-nonconserving process (the umklapp processes in which momentum is lost from the phonon system), τ_N is a relaxation time for normal processes that preserve phonon momentum, $R = \tau_R (\tau_R + \tau_N)^{-1}$, $\tau_c^{-1} = \tau_N^{-1} + \tau_R^{-1}$, $D = \lambda/c\rho$ is the thermal diffusivity, s_0 is the speed average over the propagation of transverse and longitudinal modes [8]. Using (13) one can rearrange (15) to the next form,

$$c\rho \left[\frac{\partial T}{\partial t} + \frac{\tau}{2} \frac{\partial^2 T}{\partial t^2} - \frac{h^2}{12} \frac{\partial^3 T}{\partial t \partial x^2} \right] = \lambda \frac{\partial^2 T}{\partial x^2} , \qquad (18)$$

which is just an equation of the Jeffrey's type [9]. The mixed derivative $\partial^3 T/\partial t \partial x^2$ arises also in the two-temperature model [7,17] and in the random walk theory with a "swaying" behavior of a random walker [20]. Moreover, Eq. (18) can be obtained from a heat flux equation of the Guyer-Krumhansl type [10], which was derived from the linearized Boltzmann equation for the pure phonon field at low temperatures. Comparison between (18) and the results of [10] leads to the following identifications:

$$\tau/2 = \tau_R, \quad h^2 = 7\tau_N \tau_R C_0^2$$
 (19)

where C_0 is the average (sound) speed of the phonons. Thus, according to (17) and (19) the time scale of nonlocality τ may be identified at low temperatures in solids as the characteristic time of the resistive collisions τ_R . The square of the space scale of nonlocality, h^2 , is of the order of $h_N h_R$, where $h_R = C_0 \tau_R$ and $h_N = C_0 \tau_N$ are the mean free paths of phonons. It should be noted that this procedure, i.e., rearranging Eq. (15) into the Jeffrey's form (18), can only be used for nonsteady processes. At the steady state the Jeffrey's equation reduces to the classical local heat conduction equation $\partial^2 T/\partial x^2 = 0$, but Eq. (15) gives the nonlocal steady-state equation

$$\frac{\partial^2 T}{\partial x^2} + \frac{h^2}{12} \frac{\partial^4 T}{\partial x^4} = 0 . {(20)}$$

This equation, adapted to cylindrical coordinates, can be used to study Poiseuille flow of phonons. But we consider here another example of using Eq. (20). Our purpose is to describe the temperature field in a very pure crystal [11]. In this case the only scattering mechanisms are normal (momentum-conserving) phonon-phonon processes in the bulk of the crystal and interaction of phonons with external surfaces. Consider a one-dimensional thin slab of thickness $2L \gg h_n$ with heat flowing along the x direction. The solution of (20) is

$$T(x) - T_0 = -\delta T \sinh(x/h_0) \sinh(L/h_0)$$

where $h_0 = h/2\sqrt{3}$, $T_0 = \text{const}$, and $2\delta T$ is the temperature difference between the walls so $T(-L) = T_0 + \delta T$ and $T(+L) = T_0 - \delta T$. This solution coincides with the results obtained by Sussman and Thellung [11] using a mean free time approximation for the phonon distribution function. It describes a situation where the temperature remains practically constant $[T(x) \approx T_0]$ in the bulk of the crystal and changes abruptly in the vicinity of the

surfaces $x = \pm L$ within a distance of the order of the mean free path h_0 . In the bulk of the crystal, heat flow may proceed by drift motion of phonons with no temperature gradient. At the surface no drift motion is possible because of the nonconservation of momentum and thus the heat flux is due to the heat conduction process with a temperature gradient. This example clearly demonstrates the importance of the nonlocal effects when the characteristic scale of the process under consideration is of the order of the internal scale h_0 . In the local limit $L \gg h$ one has the temperature jumps $\pm \delta T$ at the surfaces $x = \pm L$. The nonlocal effects smooth these discontinuities and lead to continuous change of temperature within a distance $x \sim h_0$. Similar phenomena which can also exhibit space nonlocal effects in the vicinity of the walls are the thermal conduction in polished single crystals of pure silicon in the low-temperature boundary-scattering regime [12] and the viscosity of polymeric fluids squeezed in a microscopic size channel [13]. Other examples where space nonlocality becomes prominent are laserannealing experiments on surface layers of silicon [14], shock waves [15], high viscosity liquids near the glass transition [16], and gases of molecules with internal degrees of freedom [17].

B. Wave law

For propagative (high-k) regimes, when one should take into account the finite speed of thermal signals, we introduce the "wave" relation between τ and h [5-7]. It means that the ratio $v = h/\tau$ remains finite when τ and h tend to zero;

$$\lim_{t,h\to 0} h/\tau = v = \text{const} . \tag{21}$$

For the "wave" limiting relation (21) the first-order approximation to Eqs. (10) and (11) are

$$\frac{1}{\tau_R} \frac{\partial T}{\partial t} + \frac{\partial^2 T}{\partial t^2} = C_T^2 \frac{\partial^2 T}{\partial x^2} , \qquad (22)$$

$$\frac{1}{\tau_R}q + 2\gamma \frac{\partial q}{\partial t} = -C\rho C_T^2 \frac{\partial T}{\partial x} ; \qquad (23)$$

here $C_T = (\mu_0 v^2 / C \rho T^2)^{1/2}$ is the speed of thermal signals (Thermal waves [5,9]). Equations (22) and (23) are the well known telegraph equation and Maxwell-Cattaneo equation, respectively [3-7,9]. They transmit waves of temperature with finite speed C_T . Experiments showing heat waves (second sound) have been successfully carried out at low temperatures in liquid helium and in certain dielectric crystals [9]. Ultrafast heat transport, consistent with wave propagation, has also been observed in thin gold films under femtosecond laser irradiation [18].

In accordance with the wave relation (21), not only the telegraph equation (22) but also the higher order approximations imply finite speed of heat waves.

III. CONCLUDING REMARKS

The results presented show the significance of nonlocal effects in transport processes. They can be described by

balance laws in the integral form, which correspond to so-called strong nonlocality. These balance laws lead, unlike in the classical local theory, to appearance of a natural internal characteristic length (space scale of nonlocality) and a characteristic time (relaxation time or time scale of nonlocality). Strictly speaking, all physical phenomena depend, to some extent, on these internal scales because of the discrete (phonon, atomic, molecule, etc.) structure and inertia properties of the matter. In order to obtain evolution equations for the temperature and heat flux in the form of partial differential equations, which correspond to weak nonlocality, we introduce two distinct limiting relations between the internal space-time scales hand τ . For diffusionlike processes with a small characteristic speed $v_0 < C_T$, we preserve thermal diffusivity $a=h^2/\tau=$ const as $\tau,h\to 0$. In such a case the strong nonlocal model gives a set of partial differential equations of parabolic type with an infinite speed of heat waves. If the characteristic speed of the process v_0 is of the order of C_T (so-called propagative regimes), then we must

preserve $v = h/\tau = \text{const}$ as $t, h \to 0$. In this case the strong nonlocal model leads to a set of partial differential equations of hyperbolic type. A number of terms in these sets depend on the order of approximation, but the type (hyperbolic or parabolic) of evolution equations does not depend on it. The type of these equations is determined by the limiting relation between the internal space-time scales.

These results suggest that for diffusion(low-k) and propagative (high-k) regimes distinct models are responsible for the space-time evolution of the temperature and heat flux. The implications of this idea may apply to other problems. In fact, all iteration schemes of the kinetic theory, including the Navier-Stokes theory, the Chapman-Enskog method, and the Grad method, make use of expansions in powers of small parameters—the mean free time or the mean free path of a molecule. The limiting relation, i.e., the basic invariant of the process, balances the time and space nonlocal effects in accordance with the main properties of the process.

- [1] R. E. Nettleton, Phys. Fluids 3, 216 (1960).
- [2] I. Muller, Z. Phys. 198, 329 (1967).
- [3] D. Jou, J. Casas-Vazquez, and G. Lebon, Rep. Prog. Phys. 51, 1105 (1988); J. Non-Equilib. Thermodyn. 17, 383 (1992).
- [4] L. S. Garcia-Colin and F. J. Uribe, J. Non-Equilib. Thermodyn. 16, 89 (1991).
- [5] S. L. Sobolev, Usp. Fiz. Nauk 161, 5 (1991) [Sov. Phys. Usp. 34, 217 (1991)].
- [6] S. L. Sobolev, Phys. Lett. A163, 101 (1992).
- [7] S. L. Sobolev, J. Phys. III 3, 12 (1993).
- [8] M. Chester, Phys. Rev. 145, 76 (1964).
- [9] D. D. Joseph and L. Preziosi, Rev. Mod. Phys. 61, 41 (1989).
- [10] R. A. Guyer and J. A. Krumhansl, Phys. Rev. 148, 778

(1966).

- [11] J. A. Sussman and A. Thellung, Proc. Phys. Soc. London 81, 1122 (1963).
- [12] T. Klitsner, J. E. Van Cleve, H. E. Fisher, and R. O. Johl, Phys. Rev. B 38, 7576 (1988).
- [13] A. C. Eringen, Int. J. Eng. Sci. 29, 1515 (1991).
- [14] G. D. Mahan and F. Claro, Phys. Rev. B 38, 1963 (1988).
- [15] D. Jou and D. Pavon, Phys. Rev. A 44, 6496 (1991).
- [16] J. Jäckle, Physica A 162, 377 (1990).
- [17] S. L. Sobolev and G. B. Manelis, Sov. J. Chem. Phys. (to be published).
- [18] S. Brorson, J. Fujimoto, and E. Ippen, Phys. Rev. Lett. 59, 1962 (1987).
- [19] S. L. Sobolev, J. Low Temp. Phys. 83, 307 (1991).
- [20] S. L. Sobolev (unpublished).