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ABSTRACT

Nonlocal and nonlinear transport theories at nanoscale: Applications to wave propagation

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Many books and/or papers have been published on linear generalizations of Fourier's equation in order to introduce relaxational and nonlocal effects for the heat flux [1–9]. Describing a heat-pulse propagation with a finite speed [10–15], in agreement with experimental observations, such works are of much conceptual interest both because they may be applied to small systems (the characteristic size of which is comparable to the mean-free path of the heat carriers) [16–23] or to fast processes (as for instance response to short laser pulses) [24–28], and because they have stimulated generalized formulations of non-equilibrium thermodynamics, with generalized expressions of the entropy and of the entropy flux incorporating heat-flux contributions [1–4, 7, 22, 29, 30].

The linear generalizations of Fourier's equation should be only employed to analyze the propagation of small-amplitude waves. When the amplitude of temperature waves (or of heat-flux waves) is not negligible, in fact, nonlinear effects cannot be neglected: this is the case, for example, when short and intense laser pulses are applied to heat a given material. Therefore, there is much interest in generalizing the linear theory of heat waves which has been, up to now, a fruitful stimulus to generalizations of non-equilibrium thermodynamics [1–4, 7, 9, 11, 12, 14, 29, 31–34] to nonlinear situations, namely, for waves with sufficiently high amplitudes [18, 20, 35–39]; indeed, there are many possible nonlinear generalizations and, from a thermodynamic point of view, it is of special interest selecting the forms which fit in a most direct way with the requirements of the second law of thermodynamics.

The present thesis aims at being a contribution to the study of heat waves when nonlinear and/or nonlocal generalizations of the Maxwell-Cattaneo equation in the context of extended thermodynamics [1, 4, 7, 35, 40] are introduced. Whereas nonlocal effects in heat transport have led to fruitful analogies with hydrodynamics, especially in the so-called phonon hydrodynamics, in the present thesis we also show how some particular nonlinear effects lead to fruitful analogies with nonlinear optics. We think that these analogies of heat transport with hydrodynamics and with optics are a nice illustration of the deep unity of physics, where results in some field may also be helpful to other fields, provided that the connection between both fields is found. The present thesis is a contribution in that direction, and the results contained in it may be of interest to current researches aiming to find new ways of control and applications of the heat flux, which is the main goal of the so-called phononics [25, 27]. In particular, the interaction of intense laser pulses with heat-conducting solids has motivated nonlinear phononics [24, 26, 28], requiring a combination of nonlinear optics and nonlinear heat transport.

The plan of this thesis is the following.

In Chapter 1 we recall the basic mathematical definitions and concepts which will be employed in this thesis, and briefly summarize the theoretical thermodynamic background.

In Chapter 2 a theoretical model to describe heat transport in functionally graded nanomaterials is developed in the framework of extended thermodynamics. The heat-transport equation used in the proposed theoretical model is of the Maxwell-Cattaneo type. We study the propagation of acceleration waves in functionally graded materials. In the special case of functionally graded $Si_{1-c}Ge_c$ thin layers, we point out the influence of the composition gradient on the propagation of heat pulses. A possible use of heat pulses as exploring tool to infer the inner composition of functionally graded materials is suggested.

In Chapter 3 we analyze the role played by nonlocal and genuinely nonlinear effects in the wave propagation. The study is performed both in the case of a rigid body (i.e., for heat pulse propagation), and in the case of a non-rigid body (i.e., for thermoelastic pulse propagation). In the framework of Extended Irreversible Thermodynamics the compatibility of our theoretical model with second law is proved.

In Chapter 4, starting from a nonlinear generalization of the Maxwell-Cattaneo equation (derived in a conservation-dissipation formalism in the framework of extended thermodynamics), an analogy with the theory of nonlinear electromagnetic waves is pointed out. This analogy emphasizes several physical aspects of the nonlinear theory and allows a parallelism with nonlinear optics, which may be of interest in nonlinear phononics. The proposed nonlinear equation for heat waves is used to analyze how the amplitude of nonlinear heat wave may influence the speed of propagation.

In Chapter 5 we finally study the influence of nonlocal and nonlinear effects on the heat-wave propagation when a two-temperature model, which allows to describe the different regimes which electrons and phonons can undergo in the heat-transfer phenomenon, is used.

The research presented in this thesis has led to the following published papers:

1. A. Sellitto, M. Di Domenico, "Nonlocal and nonlinear contributions to the thermal and elastic high-frequency wave propagations at nanoscale", *Continuum Mech. Thermodyn.*, vol. 31, pp. 807-821 (2019).

2. B.-Y. Cao, M. Di Domenico, B.-D. Nie, A. Sellitto, "Influence of the composition gradient on the propagation of heat pulses in functionally graded nanomaterials", *Proc. R. Soc. A*, vol. 475, p. 20180499 (15 pages) (2019).

3. M. Di Domenico, D. Jou, A. Sellitto, "Nonlinear heat waves and some analogies with nonlinear optics", *Int. J. Heat Mass Transfer*, vol. 156, pp. 119888 (8 pages) (2020).

4. M. Di Domenico, D. Jou, A. Sellitto, "Heat-flux dependence of the speed of nonlinear heat waves: Analogies with the Kerr effect in nonlinear optics", *Int. J .Therm. Sci.*, vol. 161, pp. 106719 (2021).

5. A. Sellitto, I. Carlomagno, M. Di Domenico, "Nonlocal and nonlinear effects in hyperbolic heat transfer in a two-temperature model", *Z. Angew. Math. Phys.*, vol. 72, pp. 1 (2021).

Contents

Bibliography

[1] I. Müller and T. Ruggeri, *Rational Extended Thermodynamics.* New York: Springer, second ed., 1998.

[2] G. Lebon, D. Jou, and J. Casas-Vázquez, *Understanding non-equilibrium thermodynamics.* Berlin: Springer, 2008.

[3] V. A. Cimmelli, "Different thermodynamic theories and different heat conduction laws," *J. Non-Equilib. Thermodyn.*, vol. 34, pp. 299–333, 2009.

[4] D. Jou, J. Casas-Vázquez, and G. Lebon, *Extended Irreversible Thermodynamics.* Berlin: Springer, fourth revised ed., 2010.

[5] M. Wang, B.-Y. Cao, and Z.-Y. Guo, "General heat conduction equations based on the thermomass theory," *Front. Heat Mass Transf.*, vol. 1, p. 013005, 2010.

[6] D. Y. Tzou, *Macro- to Microscale Heat Transfer: The Lagging Behaviour.* United Kingdom: Wiley, second ed., 2014.

[7] A. Sellitto, V. A. Cimmelli, and D. Jou, *Mesoscopic Theories of Heat Transport in Nanosystems*, vol. 6 of *SEMA-SIMAI Springer Series.* Springer International Publishing, 2016.

[8] M. Mongioví, D. Jou, and M. Sciacca, "Non-equilibrium thermodynamics, heat transport and thermal waves in laminar and turbulent superfluid helium," *Physics Reports*, vol. 726, pp. 1–72, 2018.

[9] P. Rogolino, R. Kovács, P. Ván, and V. A. Cimmelli, "Generalized heat-transport equations: parabolic and hyperbolic models," *Contin. Mech. Thermodyn.*, vol. 30, pp. 1245–1258, 2018.

[10] F. Vázquez, J. del Río, and A. Aguirre, "Nonlinear heat waves in extended irreversible thermodynamics," *J. Non-Equilib. Thermodyn.*, vol. 20, pp. 252–262, 1995.

[11] B. Straughan, *Heat waves.* Berlin: Springer, 2011.

[12] P. Ván and T. Fülöp, "Universality in heat conduction theory: weakly nonlocal thermodynamics," *Ann. Phys.*, vol. 524, pp. 470–478, 2012.

[13] A. H. Akbarzadeh, Y. Cuib, and Z. T. Chen, "Thermal wave: from nonlocal continuum to molecular dynamics," *RSC Adv.*, vol. 7, pp. 13623–13636, 2017.

[14] R. Kovács and P. Ván, "Generalized heat conduction in heat pulse experiments," *Int. J. Heat Mass Transfer*, vol. 83, pp. 613–620, 2015.

[15] L. Zhang, X. Zhang, and S. Peng, "Wave propagation model of heat conduction and group speed," *Continuum Mech. Thermodyn.*, vol. 30, pp. 879–887, 2018.

[16] D. Jou and J. Casas-Vázquez, "Nonequilibrium absolute temperature, thermal waves and phonon hydrodynamics," *Physica A*, vol. 163, pp. 47–58, 1990.

[17] J. Shiomi and S. Maruyama, "Non-Fourier heat conduction in a single-walled carbon nanotube: Classical molecular dynamics simulations," *Phys. Rev. B*, vol. 73, p. 205420 (7 pages), 2006.

[18] D. Jou and A. Sellitto, "Focusing of heat pulses along nonequilibrium nanowires," *Phys. Lett. A*, vol. 374, pp. 313–318, 2009.

[19] D. Jou, A. Sellitto, and F. X. Álvarez, "Heat waves and phonon-wall collisions in nanowires," *Proc. R. Soc. A*, vol. 467, pp. 2520–2533, 2011.

[20] D.-S. Tang, Y.-C. Hua, and B.-Y. Cao, "Thermal wave propagation through nanofilms in ballistic-diffusive regime by Monte Carlo simulations," *Int. J. Therm. Sci.*, vol. 109, pp. 81–89, 2016.

[21] F. Vázquez, A. Figueroa, and I. Rodríguez-Vargas, "Nonlocal and memory effects in nanoscaled thermoelectric layers," *J. Appl. Phys.*, vol. 121, p. 014311 (4 pages), 2017.

[22] A. Sellitto and M. Di Domenico, "Nonlocal and nonlinear contributions to the thermal and elastic high-frequency wave propagations at nanoscale," *Continuum Mech. Thermodyn.*, vol. 31, pp. 807–821, 2019.

[23] F. Vázquez, P. Ván, and R. Kovács, "Ballistic-diffusive model for heat transport in superlattices and the minimum effective heat conductivity," *Entropy*, vol. 22, p. 167 (15 pages), 2020.

[24] M. Först, C. Manzoni, S. Kaiser, Y. Tomioka, Y. Tokura, R. Merlin, and A. Cavalleri, "Nonlinear phononics as an ultrafast route to lattice control," *Nature Phys.*, vol. 7, pp. 854–856, 2011.

[25] N. Li, J. Ren, L. Wang, G. Zhang, P. Hänggi, and B. Li, "Colloquium: Phononics: Manipulating heat flow with electronic analogs and beyond," *Rev. Mod. Phys.*, vol. 84, pp. 1045–1066, 2012.

[26] A. Subedi, A. Cavalleri, and A. Georges, "Theory of nonlinear phononics for coherent light-control of solids," *Phys. Rev. B*, vol. 89, p. 220301, 2013.

[27] G. Wehmeyer, T. Yabuki, C. Monachon, J. Wu, and C. Dames, "Thermal diodes, regulators, and switches: Physical mechanisms and potential applications," *Appl. Phys. Rev.*, vol. 4, p. 041304, 2017.

[28] A. von Hoegen, R. Mankowsky, M. Fechner, M. Först, and A. Cavalleri, "Probing the interatomic potential of solids with strong-field nonlinear phononics," *Nature*, vol. 555, no. 7694, pp. 79–82, 2018.

[29] D. Jou and L. Restuccia, "Mesoscopic transport equations and contemporary thermodynamics: an introduction," *Contemp. Phys.*, vol. 52, pp. 465–474, 2011.

[30] V. A. Cimmelli, D. Jou, T. Ruggeri, and P. Van, "Entropy principle and recent results in non-equilibrium theories," *Electronic Open Journal Entropy*, vol. 16, no. 3, pp. 1756–1807, 2014.

[31] D. D. Joseph and L. Preziosi, "Heat waves," *Rev. Mod. Phys.*, vol. 61, pp. 41–73, 1989.

[32] M. Honner, "Heat waves simulation," *Comput. Math. Appl.*, vol. 38, pp. 233–243, 1999.

[33] Y. Dong, B.-Y. Cao, and Z.-Y. Guo, "Generalized heat conduction laws based on thermomass theory and phonon hydrodynamics," *J. Appl. Phys.*, vol. 110, p. 063504 (6 pages), 2011.

[34] T. Ruggeri and M. Sugiyama, *Rational Extended Thermodynamics beyond the Monatomic Gas*. Berlin: Springer, 2018.

[35] F. X. Álvarez, J. Casas-Vázquez, and D. Jou, "Robustness of the nonequilibrium entropy related to the maxwell-cattaneo heat equation," *Phys. Rev. E*, vol. 77, p. 031110, 2008.

[36] V. A. Cimmelli, A. Sellitto, and D. Jou, "Nonequilibrium temperatures, heat waves, and nonlinear heat transport equations," *Phys. Rev. B*, vol. 81, p. 054301 (9 pages), 2010.

[37] A. Sellitto, V. A. Cimmelli, and D. Jou, "Analysis of three nonlinear effects in a continuum approach to heat transport in nanosystems," *Physica D*, vol. 241, pp. 1344–1350, 2012.

[38] C. de Tomas, A. Cantarero, A. F. Lopeandia, and F. X. Álvarez, "Form kinetic to collective behavior in thermal transport on semiconductors and semiconductor nanostructures," *J. Appl. Phys.*, vol. 115, p. 164314, 2014.

[39] D.-S. Tang, Y.-C. Hua, B.-D. Nie, and B.-Y. Cao, "Phonon wave propagation in ballistic-diffusive regime," *J. Appl. Phys.*, vol. 119, p. 124301, 2016.

[40] P. Ván, "Weakly nonlocal irreversible thermodynamics," *Ann. Phys.*, vol. 12, pp. 146–173, 2003.