

Beyond the Fourier equation: Quantum hyperbolic heat transport

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Abstract

In this paper the quantum limit of heat transport induced by ultrashort laser pulses is discussed. The new quantum heat transport equation is derived. The relaxation time $\tau = \hbar/mv_h^2$ (v_h = thermal wave velocity) and diffusion coefficient $D^e = \hbar/m$ are calculated.

Key words: Hyperbolic heat transfer; Ultra-short laser pulses; Quantum heat transport.

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1 Introduction

The correlated random walk, whose diffusive analog is described by hyperbolic diffusion equation, is possibly the simplest mathematical model allowing one to incorporate a form of momentum in addition to random or diffusive motion. The correlated random walk differs from the ordinary random walk in that the probabilistic element used at each step is the probability of continuing to move in a given direction rather than the probability of moving in a given direction independent of the direction of the immediately preceding step. Thus the process remains a Markov process.

The solution to a variety of forms of the hyperbolic diffusion equation has been given by Goldstein [1].

There is considerable literature [2, 3, 4] on physical processes in the field of thermophysics leading to a mathematical formulation in terms of a hyperbolic heat conduction equation. The physics behind such application implies that the signal propagation speed is finite rather than infinite as in the case of ordinary diffusion.

Until recently the thermal phenomena studied with the help of hyperbolic heat transfer equation do not consider the quantum aspects of heat transfer [2, 3, 4]. All the results are obtained in classical approximations.

In this paper the quantum limit of heat transfer will be considered and quantum heat transport equation will be developed. The study was motivated by the advent of the ultra – short duration laser pulses, particularly those in attosecond (10^{-18}) [5] and zeptosecond [6] domains. Considering that time in which electron orbits the atomic nucleus is of the order of femtoseconds — with attosecond pulses it is possible penetrate the quantum structure of the path of electrons.

2 Overview of research

In present day materials sciences laser technology is a fundamental tool in such processes as surface deformation, materials hardening, welding, etc. Recently it has been shown possible to study accompanying phenomena on an atomic level. It is well recognized that on deposition of the laser pulse, electromagnetic energy is absorbed by a photon – electron interaction, the magnitude of which is described by the fine structure constant $\alpha = 1/137$. The response of material to the thermal perturbation is governed by the

relaxation time τ . These two parameters fully describe the dynamics of energy transfer of the ultra – short (femtosecond and shorter) laser pulses on a nanometer scale. Conditions in the processes induced by ultra – short laser pulses are in stark contrast with those of longer laser pulse duration, the distinction being that at longer pulse duration (~ 1 ps) excited particles and their surroundings have had sufficient time to approach thermal equilibrium. On the other hand at temporal resolution ~ 1 fs it is possible to resolve the dynamics of nonstationary transport phenomena.

For the transport phenomena of the nonrelativistic electrons there is a stochastic process that is ultimately connected with its propagation, namely the Brownian motion. As is well known Nelson [7] succeed in deriving the Schrödinger equation from the assumption that quantum particles follow continuous trajectories in a chaotic background. The derivation of the usual Schrödinger equation follows only if the diffusion coefficient D associated with quantum Brownian motion takes the value $D = \hbar/2m$ as assumed by Nelson.

In this paper the diffusion process of the quantum particles in context of the thermal energy will be studied. In the paper [8] the heat transport in a thin metal film (Au) was investigated with the help of the hyperbolic heat conduction equation (HHC). It was shown that when the memory of the hot electron gas is taken into account then the HHC is the dominant equation for heat transfer. The hyperbolic heat conduction equation for heat transfer in an electron gas can be written in the form [8]:

$$\frac{1}{c^2} \frac{\partial^2 T}{\partial t^2} + \frac{1}{c^2 \tau} \frac{\partial T}{\partial t} = \frac{\alpha^2}{3} \nabla^2 T. \quad (1)$$

In equation (1) c is the light velocity in vacuum, $\alpha = e^2 \hbar^{-1} c^{-1} = 1/137$ is the fine structure constant and τ is the relaxation time.

In the present paper the quantum limit of the equation (1) will be obtained. When a high energy laser pulse hits the thin metal film it is possible that very short relaxation time are obtained. Since the relaxation time τ strongly depends on the temperature the relaxation times are of the order of 1 fs for $T > 10^3$ K. In this case the mean free path of the hot electron is the same order as the thermal de Broglie wavelength. The temperature region for which mean free path λ is of the order of λ_B (de Broglie wavelength) we will define as the quantum limit of the heat transport and the master equation — the quantum heat transport equation (QHT).

3 Quantum limit of the heat transport

The classical notion of the field was born from a description of material media: the propagation of certain perturbations in such a medium led to the motion of a wave. A field, or a wave, gave initially, therefore, a picture of the collective motions of the medium and their propagation. For example the fluctuations of the electronic density in a solid state plasma are described by “plasma” waves. The classical formalism of the theory of fields is the same whether it is applied to “true” fields, which are thought of as existing in themselves, even in the absence of any material substratum, such as the electromagnetic field, or to a “phenomenological field” produced by the collective motions of a propagating medium. The concept of a frequency, for example, plays the same fundamental role in the analysis of these fields. The quantum synthesis of the concepts of frequency and energy is thus universal, i. e. they do not depend upon the specific nature of the phenomenon being considered and characterize the quantum theory in all its generality. The Planck – Einstein relation

$$E = \hbar\omega$$

holds equally well, therefore, in quantum description of “phenomenological” fields. In other words, one must have a discretization of the energy into packets or quanta, $E = \hbar\omega$, for any waves: acoustic or thermal, with a vibration frequency ω , exactly as for an electromagnetic wave.

In [9] we developed the new hyperbolic heat transport equation which generalizes the Fourier heat transport equation for the rapid thermal processes. The hyperbolic heat conduction equation for the fermionic system can be written in the form:

$$\frac{1}{\left(\frac{1}{3}v_F^2\right)} \frac{\partial^2 T}{\partial t^2} + \frac{1}{\tau \left(\frac{1}{3}v_F^2\right)} \frac{\partial T}{\partial t} = \nabla^2 T, \quad (2)$$

where T — denotes the temperature, τ — the relaxation time for the thermal disturbance of the fermionic system and v_F is the Fermi velocity.

In the subsequent we develop the new formulation of the HHC considering the details of the fermionic system.

To start with we recapitulate the well known results from the simplest fermionic model of the matter: the Fermi gas of electrons in metals.

For the electron gas in metals the Fermi energy has the form [10]:

$$E_F^e = (3\pi^2)^{2/3} \frac{n^{2/3} \hbar^2}{2m_e}, \quad (3)$$

where n — density and m_e — electron mass. Considering that

$$n^{-1/3} \sim a_B \sim \frac{\hbar^2}{m_e e^2} \quad (4)$$

and $a_B =$ Bohr radius, one obtains

$$E_F^e \sim \frac{n^{2/3} \hbar^2}{m_e} \sim \frac{\hbar^2}{m a^2} \sim \alpha^2 m_e c^2, \quad (5)$$

where $c =$ light velocity and $\alpha = 1/137$ is the fine structure constant. For the Fermi momentum p_F , we have

$$p_F^e \sim \frac{\hbar}{a_B} \sim \alpha m_e c \quad (6)$$

and for Fermi velocity v_F ,

$$v_F^e \sim \frac{p_F}{m_e} \sim \alpha c. \quad (7)$$

Considering formula (7), equation (2) can be written as

$$\frac{1}{c^2} \frac{\partial^2 T}{\partial t^2} + \frac{1}{c^2 \tau} \frac{\partial T}{\partial t} = \frac{\alpha^2}{3} \nabla^2 T. \quad (8)$$

As it is seen from (8) the HHC equation is the relativistic equation as it takes into account the finite velocity of light. In order to derive the Fourier law from equation (8) we are forced to break the special theory of relativity and put in equation (8) $c \rightarrow \infty$, $\tau \rightarrow 0$. In addition it was demonstrated from HHC in a natural way, that in electron gas the heat propagation velocity $v_h \sim v_F$ in the accordance with the results of the laser pump probe experiments.

In the following the procedure for the discretization of temperature $T(\vec{r}, t)$ in hot fermion gas will be developed. First of all we introduce the reduced de Broglie wavelength

$$\lambda_B^e = \frac{\hbar}{m_e v_h^e} \quad v_h^e = \frac{1}{\sqrt{3}} \alpha c \quad (9)$$

and mean free path λ^e ,

$$\lambda^e = v_h^e \tau^e. \quad (10)$$

Considering formulae (9), (10) we obtain HHC for electron

$$\frac{\lambda_B^e}{v_h^e} \frac{\partial^2 T^e}{\partial t^2} + \frac{\lambda_B^e}{\lambda^e} \frac{\partial T^e}{\partial t} = \frac{\hbar}{m_e} \nabla^2 T^e. \quad (11)$$

Equation (11) is the hyperbolic partial differential equation which is the master equation for heat propagation in Fermi electron gas. In the following we will study the quantum limit of heat transport in the fermionic systems. We define the quantum heat transport limit as follows:

$$\lambda^e = \lambda_B^e. \quad (12)$$

In that case equation (11) has the form:

$$\tau^e \frac{\partial^2 T^e}{\partial t^2} + \frac{\partial T^e}{\partial t} = \frac{\hbar}{m_e} \nabla^2 T^e, \quad (13)$$

where

$$\tau^e = \frac{\hbar}{m_e (v_h^e)^2}. \quad (14)$$

Equation (13) defines the master equation for quantum heat transport (QHT). Having the relaxation time τ^e one can define the ‘‘pulsations’’ ω_h^e :

$$\omega_h^e = (\tau^e)^{-1} \quad (15)$$

or

$$\omega_h^e = \frac{m_e (v_h^e)^2}{\hbar}$$

, i.e.

$$\omega_h^e \hbar = m_e (v_h^e)^2 = \frac{m_e \alpha^2}{3} c^2. \quad (16)$$

Formula (16) defines the Planck-Einstein relation for heat quanta E_h^e

$$E_h^e = \omega_h^e \hbar = m_e (v_h^e)^2. \quad (17)$$

The heat quantum with energy $E_h = \hbar\omega$ can be named as the *heaton* in complete analogy to the *phonon*, *magnon*, *roton* and etc. For $\tau^e \rightarrow 0$ equations (13), (16) are the quantum Fourier transport equations (QFT) with quantum diffusion coefficients D^e :

$$\frac{\partial T^e}{\partial t} = D^e \nabla^2 T^e, \quad D^e = \frac{\hbar}{m_e}. \quad (18)$$

For finite τ^e for $\Delta t < \tau^e$ equation (13) can be written as follows:

$$\frac{1}{(v_h^e)^2} \frac{\partial^2 T^e}{\partial t^2} = \nabla^2 T^e. \quad (19)$$

Equation (19) is the wave equation for quantum heat transport (QHT).

It is interesting to observe that equation (19) is the wave equation which describes the propagation of the de Broglie thermal wave. For the wave length λ of the wave which is the solution of equation (19) one obtains:

$$\lambda = \frac{v_h}{\omega} = \frac{v_h \hbar}{\omega \hbar} = \frac{\hbar}{p_e}, \quad p_e = m_e v_h, \quad (20)$$

i.e. λ is equal the reduced de Broglie wave length (9).

On the other hand the quantum Fourier equation (18) resembles the free Schrödinger equation. The replacement $t \rightarrow it/2$ turns the quantum diffusion equation into the Schrödinger equation. Both are parabolic and require the same boundary and initial conditions in order to be “well posed”.

The *heaton* energies for electron gas can be calculated from formula (17). For electron gas we obtain from formulae (9), (17) for $m_e = 0.51 \text{ MeV}/c^2$, $v_h = (1/\sqrt{3})\alpha c$

$$E_h^e = 9 \text{ eV}, \quad (21)$$

which is of the order of the Rydberg energy. The numerical values of the relaxation time τ and the quantum diffusion coefficient D can be calculated from formulae (14) and (18).

$$\tau = 10^{-17} \text{ s}, \quad D = 1.2 \cdot 10^{-4} \text{ m}^2\text{s}^{-1}.$$

Concluding, one can say that for the temporal resolution Δt of the order or shorter of the relaxation time $\tau \sim 10^{-17} \text{ s}$ the heat transport phenomena are adequately described by the quantum heat transport equation (QHT), formula (13). It seems that the advent of lasers with attosecond laser pulses open quite new possibility for the study these discrete thermal phenomena [10].

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