Theoretical description of thermal transient grating experiment: dynamical and kinetic approaches.

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Summary. Thermal grating technique is a promising method for direct measurement of transient anomalous heat conduction. This work analyses approaches for theoretical description of this experiment. Kinetic and dynamical approaches to problem of initial sinusoidal perturbation are found to be handful. Behavior of amplitude decay calculated from these models plays a role of a signature of heat conduction regime. Decay of amplitude is analyzed using analytical, and molecular dynamics approaches. A comparison with available literature is presented.

Experimental studies confirm that in in ultrapure materials heat can propagate ballistically (non-diffusively), which leads to the phenomenon of thermal superconductivity [1, 2, 3, 4] . This fact opens up broad perspectives for the practical applications of ultrapure crystals for design of new materials with unique properties and devices constructed with use of these materials [4].

The difficulty in study of ballistic thermal processes in real materials lies in the fact that it occurs at very high speeds (speed of sound in crystals, e.g., >10 km/s for graphene [5]). Moreover, since the process is fundamentally different from Fourier's law, it lacks the thermal conductivity coefficient as a material parameter. However, even when the Fourier's law does not hold, in an experimental setting and molecular dynamic simulations when a steady non-equilibrium temperature gradient is applied to the specimen, it turns out that it is convenient to use the mathematical formulation of Fourier's law and to observe the size dependence of thermal conductivity as a signature of anomalous regimes [6, 7, 8, 9]. Thus, experimental methods, which have now already become a standard, have been developed to determine the thermal conductivity coefficient from Fourier's law [10]. These methods, however, cannot describe transient processes. A promising alternative of steady methods is the thermal grating technique which is a direct measurement of transient anomalous heat conduction [11].

In this work we focus on the theoretical description of transient thermal grating experiment [11]. In this experiment a sinusoidal periodic temperature excitation is created on a surface of the sample. Thus, a two dimensional heat transport occurs. Since the sinusoidal initial profile is excited along one axis, the heat transport remains quasi one dimensional. Let us consider initial temperature distribution as a periodic harmonic function along the spatial coordinate x.

$$T(x,0)=e^{iqx}, \tag{1}$$

where $q=\frac{2\pi}{L}$ is a wavenumber, L is the period of initial excitation. Let us assume that the evolution of this excitation remains periodic in space and has the form

$$T(x,t)=A_1(t)e^{iqx}, \tag{2}$$

where $A_1(t)$ is the amplitude which depends on time t.

The solution for function $A(t)$ can be found using different approaches and methods. Let us first consider the model where the heat transport is modeled using the particles – heat carriers which are called phonons [12]. Probability density function $f(x,y,t,u,v)$ describing distribution of these particles is goverened by the Boltzmann transport equation

$$\frac{\partial f}{\partial t}+u\frac{\partial f}{\partial x}+v\frac{\partial f}{\partial y}=f^{scat}, \tag{3}$$

where f^{scat} is the function describing scattering between the particles. Let us for simplicity first consider the case when $f^{scat}=0$, i.e., when the particles propagate without scaterring – ballistically. In the one dimensional case the equation then takes the form

$$\frac{\partial f}{\partial t}+u\frac{\partial f}{\partial x}=0, \tag{4}$$

and f is not deendent of y: $f=f(x,t,u,v)$. Let us consider isotropic "grey" medium, i.e., medium where all the particles propagate in all directions with the same absolute velocity. Let us suppose that the distribution function corresponds to Eqs. (1), (2) and has the form

$$f(x,0,u,v)=f^0(u,v)e^{iqx}, \quad f(x,t,u,v)=A_2(t)f^0(u,v)e^{iqx}. \tag{5}$$

Substitution of this anzatz (5) into (4) yeilds a linear diferential equation for A_2

$$\frac{\partial A_2}{\partial t}+iquA_2=0, \tag{6}$$

and solving the this equation yeilds

$$A_2(t)=e^{-iqut}. \tag{7}$$

Thus the solution for f has the form $f(x, u, v, t) = f_0(u, v)e^{i(qx-qut)}$. Initial distribution over velocities for a case of grey medium, i.e., all the particles has constant absolute velocities and uniformly distributed random directions, may be written in the form

$$f_0(u, v) = \frac{1}{\pi}\delta(u^2 + v^2 - c^2), \tag{8}$$

where c is the absolute velocity of particles, and the factor $1/\pi$ arises from normalizing condition $\int\int f_0(u, v)\mathrm{d}u\mathrm{d}v = 1$. Density of particles given in a chosen point of space in time $\rho(x, t)$ is found by integration over all velocities

$$\rho(x, t) = \frac{1}{\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\delta(u^2 + v^2 - c^2)e^{i(qx-qut)}\mathrm{d}u\mathrm{d}v. \tag{9}$$

We are interested in the decay of the amplitude and not in the spatial dependency e^{iqx}. From (9) it is seen that amplitude is described by

$$A_3(t) = \frac{1}{\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\delta(u^2 + v^2 - c^2)e^{-iqut}\mathrm{d}u\mathrm{d}v. \tag{10}$$

Change of variables to the polar coordinates in integration in (10) $u = r\sin\theta$, $v = r\cos\theta$, $\mathrm{d}u\mathrm{d}v = r\mathrm{d}r\mathrm{d}\theta$ yeilds

$$A_3(t) = \frac{1}{\pi}\int_0^{2\pi}\int_0^{\infty}\delta(r^2 - c^2)e^{-iqrt\cos\theta}r\mathrm{d}r\mathrm{d}\theta = \frac{1}{2\pi}\int_0^{2\pi}e^{-iqct\cos\theta}\mathrm{d}\theta = J_0(cqt), \tag{11}$$

where J_0 is a Bessel function of the first kind. Molecular dynamical simulation performed to check analytical prediction, Eq. (11). Simulation results confirm analytical predictions.

We would like to note that Bessel function has a power decay of amplitude $\sim 1/\sqrt{(t)}$, thus, obtained result contradicts with results obtained from the dynamical approach in [13] and solution of BTE from the kinetic approach [14]. The study of this discrepancy is a direction for further research.

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