# Derivation of the modification heating conduction equation of a kind of laser thermal effect by quantum mechanics

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The Fourier equation of heat conduction predicts a paradox that the effect of a thermal impulse (e.g. the thermal effect in pulse laser) in an infinite medium; i.e., a thermal impulse is propagated in an infinite velocity. In order to solve the thermal transport paradox, C. W. Ulbrich and M. Chester have proposed the modification heat conduction equation respectively from different macroscopic viewpoint. This paper derived the modification heat conduction equation according to phonon model and quantum mechanics from microscopic viewpoint.

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It is well known that the Fourier equation of heat conduction predicts infinite velocity of propagation of thermal impulses[1]. Obviously, this result is an absurd on physics (i.e. famous paradox of heat transport). In order to solve the heat transportation paradox, C. W. Ulbrich and M. Chester have proposed the modification heat conduction equation respectively from different macroscopic viewpoint[1,2]. This equation (i.e. Chester modification heat conduction equation) is

$$\frac{\partial^2 T}{\partial t^2} + \frac{1}{\tau}\frac{\partial T}{\partial t} - \frac{K}{\tau c}\nabla^2 T = 0, \tag{1}$$

where $\tau$ is a relaxation time, $c$ is the heat capacity per unit volume, $K$ is the thermal conductivity (the Fourier equation is $\frac{c}{K}\frac{\partial T}{\partial t} - \nabla^2 T = 0$). It is clear that the Eq. (1) resolves the dilemma of infinite propagation velocity for a thermal signal. In fact, Eq. (1) predicts a finite velocity for the propagation of thermal signal. The finite velocity $v_m$ is given by

$$v_m^2 = \frac{K}{\tau c}. \tag{2}$$

The corresponding diffusion equation of Eq. (1) is

$$\tau\frac{\partial \mathbf{J}}{\partial t} + \mathbf{J} = -K\nabla T, \tag{3}$$

where $\mathbf{J}$ is the heat current density. The physical meaning of Eq. (3) is simple. It states that there is a finite buildup time for the onset of thermal currenncy after a temperature gradient is clamped onto a specimen. The heat flow does not start instantaneously but rather grows gradually with a relaxation time $\tau$. Conversely, if a thermal gradient is suddenly removed, there is a lag in the disappearance of the heat current and Eq. (3) exhibits just such a relaxation, whereas Fourier heat diffusion equation $\mathbf{J} = -K\nabla T$ does not. The relaxation time $\tau$ is associated with the communication "time" between phonons (phonon-phonon collisions) for the beginning of resistive flow.

As mentioned above, we knew that Eq. (1) is more reasonable compare with Fourier heat conduction equation.

For the problem of conduction of thermal impulses we should apply Eq. (1), rather than Fourier equation. For heat effects of impulse laser, Eq. (1) is still suitable. In order to apply Eq. (1) to laser heat effect more efficiently, it is necessary to derive Eq. (1) from microscopic mechanism. M. Chester and C. W. Ulbrich obtained Eq. (1) from macroscopic view. We can obtain Eq. (1) from microscopic viewpoint. In following paragraphs we will derive Eq. (1) by means of quantum theory of solids from microscopic viewpoint.

Although the Eq. (1) is more reasonable compare with Fourier heat conduction equation, people always do not like to use it, because it is very difficult to be solved. So, in other paper, we will explain how to solve the Eq. (1) in detail. It will be useful for people to apply Chester modification heat conduction equation.

According to the quantum theory of solid and quantum electrodynamics, when laser photons are cast on a crystal, laser photon comes into non-elastic collision with "public electron in the crystal". After the collision, the photon is absorbed by an electron. The energy of the electron that had absorbed a photon raises and the electron transits to higher energy level from original low energy level[4]. Where vector potential of incident light $\mathbf{A} = A_0\exp[i(\mathbf{K}_p \cdot r - \omega t)]\mathbf{e} + c.c.$. We have

$$H' = \frac{e}{m}\mathbf{P}\cdot\mathbf{A} + \frac{1}{2m}e^2 A^2 \approx \frac{e}{m}\frac{\hbar}{i}\mathbf{A}\cdot\nabla, \tag{4}$$

$H_0 = \frac{P^2}{2m} + V(\mathbf{r})$ and $H = H_0 + H'$ corresponding Schrödinger equation is $H\psi = i\hbar\psi_t$. According to Dirac perturbation theory, the transition probability of the electron from original state $\langle i|$ to final state $\langle f|$ in crystal is

$$P(i,f) = \frac{2\pi}{\hbar}|\langle f|H'|i\rangle|^2\delta(E_f - E_i),$$

but

$$\langle f|H'|i\rangle = \frac{\hbar}{i}\frac{e}{m}\langle f|\mathbf{A}\cdot\nabla|i\rangle = \frac{\hbar}{i}\frac{e}{m}A_0$$

$$\times e^{-i\omega t}[\langle f|(e^{i\mathbf{K}_p\cdot\mathbf{r}} + e^{-i\mathbf{K}_p\cdot\mathbf{r}})\mathbf{e}\cdot\nabla|i\rangle]. \tag{5}$$

   

For absorbing transition, we have

$$\langle f|H'|i\rangle = \frac{\hbar}{i}\frac{e}{m}\langle f|\mathbf{A}\cdot\nabla|i\rangle = \frac{\hbar}{i}\frac{e}{m}A_0$$

$$\times e^{-i\omega t}[\langle f|e^{i\mathbf{K}_p\cdot\mathbf{r}}\mathbf{e}\cdot\nabla|i\rangle]. \qquad (6)$$

In absorbing process, the energy of $i$-state and $f$-state are $E_i = \varepsilon_i + \hbar\omega$ and $E_f = \varepsilon_f$, respectively. So, the transition probability of the electron from $i$-state to $f$-state is

$$P(i,f,\omega) = 2\pi\hbar\frac{e^2}{m^2}A_0^2[\langle f|e^{i\mathbf{K}_p\cdot\mathbf{r}}\mathbf{e}\cdot\nabla|i\rangle]^2$$

$$\times\delta(\varepsilon_f - \varepsilon_i - \hbar\omega). \qquad (7)$$

In Ref. [5], the absorption coefficient of bio-tissue $\eta(\omega) \propto (\hbar\omega - E_g)^{1/2}/\hbar\omega$ have been derived, where $\hbar\omega$ is photon energy and $E_g$ is least energy gap between valence band and conduction band[5]. These electrons that transited higher energy levels will interact with crystal lattices. These interactions of the lattices-electron will produce many higher energy phonons. This process can be explained more clearly with the aid of a Feynman diagram 1. In Fig. 1 we represent the incoming electron in a straight line with an arrow pointing to the left; the interaction with the lattice vibrations is indicated by a vertex; the emerging electron after interaction will be shown again by a straight line with arrow; the emerging phonon by a curly line with an arrow (see Fig. 1)[6]. According to the quantum theory of solids, the phonons can be taken heat energy-carriers, and the heat conduction in the crystal can be regarded as transportation process of the phonons. In the phonons transportation process, the thermal energy current density can be represented as[7]

$$\mathbf{J} = \frac{1}{V}\sum_{j\mathbf{q}} h_j(\mathbf{q})\hbar\omega_{j\mathbf{q}}v_{j\mathbf{q}} = \frac{1}{V}\sum_{j\mathbf{q}} N_j(\mathbf{q})\hbar\omega_{j\mathbf{q}}, \qquad (8)$$

where $n_j(\mathbf{q}), v_{j\mathbf{q}}$ and $\omega_{j\mathbf{q}}$ are respectively the phonon number, the phonon group velocity and the phonon frequency of $j$-group and wave vector=$\mathbf{q}$ in crystal, and the phonon flux density $N = \frac{1}{V}\sum_{j\mathbf{q}} n_j(\mathbf{q})v_{j\mathbf{q}}$.

According to the phonon theory, the phonon flux density is related to the temperature gradient and the phonon-phonon collision in crystal. There are three phonons process in the phonon-phonon collision (see Fig. 2). In three phonons process, the vary rate of $j\mathbf{q}$ phonons can be represented as[8]

$$\left[\frac{\partial n_j(\mathbf{q})}{\partial t}\right]_c = \frac{\hbar\Omega}{64\pi^2 M^3}\sum_{j'j''}\int d\mathbf{q}'$$

$$\times\frac{|\Phi[j\mathbf{q},j'\mathbf{q}',j''(\mathbf{q}-\mathbf{q}')]|^2}{\omega\omega'\omega''}$$

$$\times\{\delta(\omega - \omega' - \omega'')[(n+1)n'n'' - n(n'+1)(n''+1)]$$

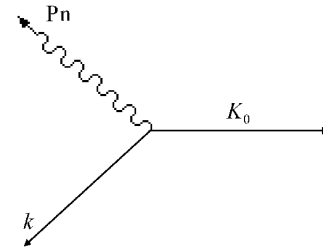$$+2\delta(\omega + \omega' - \omega'')[(n+1)(n'+1)n'' - nn'(n''+1)]\}. \qquad (9)$$


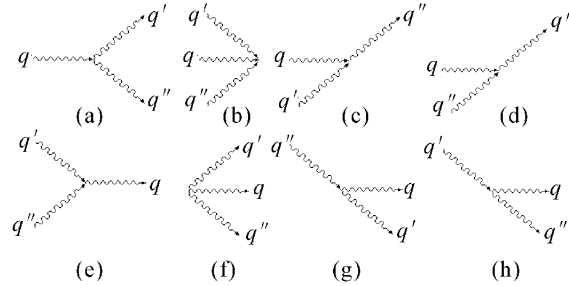
Fig. 1. Feynman diagram spontaneous emission of a phonon.



Fig. 2. The processes or phonon-phonon interactions.

For disequilibrium state $\left[\frac{\partial n_j(\mathbf{q})}{\partial t}\right]_c \neq 0$, but in general case the increment of phonon $\ll$ total phonon number. So we can represent the total phonon number $n = n_0 + \Delta n$, where $n_0$ is even phonon number in heat balance (temperature is $T$), $\Delta n$ is the increment of phonon (owing to phonon-phonon collision)[9,10]. For the increment $\Delta n$, we can use a representation by perturbation theory. The average number of phonon $n_{0j}(\mathbf{q})$ under Bose distribution can be represented as

$$n_{0j}(\mathbf{q}) = \frac{1}{\exp\left(\frac{\hbar\omega_{j\mathbf{q}}}{K_B T}\right) - 1}. \qquad (10)$$

Because $\frac{\partial n_{0j}(\mathbf{q})}{\partial t} = 0(n_{0j}(\mathbf{q})$ is not an explicit function of $t$), and according to the relaxation time approximate method of phonon theory and perturbation theory, we can obtain[10]

$$\left[\frac{\partial n_j(\mathbf{q})}{\partial t}\right]_c = \frac{[n_{0j} - n_j]}{\tau_j(\mathbf{q})} = -\Delta n_j/\tau_j(\mathbf{q}), \qquad (11)$$

where $\tau_j(\mathbf{q})$ is the relaxation time. According to principle of conservation of energy, the total thermal energy currency density

$$\mathbf{J} = \mathbf{J}_0 + \frac{1}{V}\sum_{j'\mathbf{q}'} \Delta n_{j'}\hbar\omega_{j'}(\mathbf{q}')v_{j'\mathbf{q}'}$$

$$= \frac{1}{V}\sum_{j\mathbf{q}} n_{0j}V_j(\mathbf{q})\hbar\omega_{j'\mathbf{q}} + \frac{1}{V}\sum_{j'\mathbf{q}'} \Delta n_{j'}\hbar\omega_{j'}(\mathbf{q}')v_{j'\mathbf{q}'}, \qquad (12)$$

where second term represents thermal energy currency density of "increased phonon" $\sum \Delta n_j$. According to the

heat conduction theory for heat balance, the thermal energy currency density $\mathbf{J}_0$ can be represented as[11]

$$J_{0\alpha} = -\sum_{\beta} K_{\alpha\beta} \frac{\partial T}{\partial x_\beta}, \tag{13}$$

where $J_{0\alpha}$ is $\alpha$ component of $\mathbf{J}_0$, $K_{\alpha\beta}$ is a component of thermal conductivity tensor of anisotropic medium. For isotropic medium we have

$$\mathbf{J}_0 = -K_0 \nabla T, \tag{14}$$

where $\nabla T$ is temperature gradient, $K_0$ is thermal conductivity. According to Eq. (11), the second term in Eq. (12) can be expressed as

$$\Delta \mathbf{J} = -\frac{1}{V} \sum_{j'\mathbf{q}'} \hbar \omega_{j'}(\mathbf{q}') \left[ \frac{\partial n_{j'}}{\partial t} \right]_c \tau_{j'} v_{j'\mathbf{q}'}. \tag{15}$$

It is known that the thermal currency density has statistic property. So we can use the expectation value $\langle \tau_j \rangle$ instead of relaxation time $\tau_j$, we obtain

$$\Delta \mathbf{J} = -\left\{ \frac{1}{V} \sum_{j'\mathbf{q}'} \hbar \omega_{j'}(\mathbf{q}') \left[ \frac{\partial n_{j'}}{\partial t} \right]_c v_{j'\mathbf{q}'} \right\} \langle \tau \rangle$$

$$= \frac{\partial}{\partial t} \left\{ \frac{1}{V} \sum_{j'\mathbf{q}'} \hbar \omega_{j'}(\mathbf{q}') n_{j'} v_{j'\mathbf{q}'} \right\} \langle \tau \rangle$$

$$= \left( \frac{\partial}{\partial t} \mathbf{J} \right) \langle \tau \rangle. \tag{16}$$

From Eqs. (12), (14), (15) and (16) we obtain

$$\mathbf{J} = -K_0 \nabla T - \left( \frac{\partial}{\partial t} \mathbf{J} \right) \tau. \tag{17}$$

It is well known that the continuity equation for heat transportation with density or pressure gradients is

$$C \frac{\partial T}{\partial t} + \nabla \cdot \mathbf{J} = 0, \tag{18}$$

where $C$ is the heat capacity per unit volume. Combined (3) (or (17)) with (18) we can obtain the modification heat conduction Eq. (1). We derived modification heat conduction Eq. (1) from microscopic viewpoint.

From the derivation process mentioned above, we can see that the modification heat conduction equation is an approximation result from microscopic derivation. We have also derived the nonlinear heat conduction equation from rough analysis (this equation is $CT_1 - 2T\nabla T - \partial_n \nabla T + \tau C T_{tt} - K \nabla^2 T = 0$)[12], but that nonlinear heat conduction equation is very difficult for real application. Other necessary illustration is the value of $\tau$. This is a crucial parameter. According to the quantum theory of solid, the relaxation time $\tau$ is related to "thermal wave" and temperature $T$ etc. Hence the solution of Eq. (1) are related to the relaxation time $\tau$. Solving Eq. (1) is very complex. About the solutions of the modification heat conduction equation, we will explain in detail in other paper.

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