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LETTER TO THE EDITOR

Longitudinal and transverse parts of the correction term in the Callaway model for phonon conductivity

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Abstract. The correction term in the Callaway model for phonon conductivity is separated into its longitudinal and transverse parts in the presence of phonon dispersion. This will provide, for the first time, a realistic opportunity to speak about the total individual contributions of the phonons, of different polarizations, to the total phonon conductivity.

Due to the complicated form of Parrott's [1] expression for the Callaway [2] correction term, K^{C}, in the generalized two-mode heat conduction model [3], it is usually misinterpreted [4] as indicating that K^{C} is not separable into its longitudinal and transverse parts. A long list of references [5] shows that in all the attempts to estimate the individual contributions of longitudinal and transverse phonons in the total phonon conductivity K, the correction term is always neglected. Recently [6], we have shown that this approximation does not have a sound footing and so, in the following, we give the explicit expressions for the longitudinal and transverse parts of K^{C}.

The phonon distribution $N_\lambda(q)$, in the steady state, is written as

$$N_\lambda(q) = N^0(q) + n_\lambda(q)N^0(q)\{N^0(q)+1\} \tag{1}$$

where the second term is the deviation of the phonon distribution $N^0(q)$ from the equilibrium for the polarization λ. In the presence of the momentum-conserving normal processes, one may write [1]

$$n_\lambda(q) = n_\lambda^0(q) + n_\lambda^1(q). \tag{2}$$

While $n_\lambda^0(q)$ gives rise to the Debye term in the phonon conductivity, $n_\lambda^1(q)$ is responsible for the correction term K_λ^{C}. From Parrott [1], $n_\lambda^1(q)$ can be written as

$$n_\lambda^1(q) = \frac{\hbar q|\nabla T|\mu}{k_{\mathrm{B}}T}\frac{\tau_{\mathrm{n}\lambda}^{-1}}{\tau_{\mathrm{c}\lambda}^{-1}}\left(\sum_\lambda \int q v_{\mathrm{g}\lambda}(q)\omega_\lambda(q)\mu^2\tau_{\mathrm{c}\lambda}\tau_{\mathrm{n}\lambda}^{-1}N^0(q)\{N^0(q)+1\}\,\mathrm{d}^3q\right) \times \left(\sum_\lambda \int q^2\mu^2 N_q^0(N_q^0+1)\tau_{\mathrm{c}\lambda}\tau_{\mathrm{n}\lambda}^{-1}\tau_{\mathrm{r}\lambda}^{-1}\,\mathrm{d}^3q\right)^{-1} \tag{3}$$

where μ is the cosine of the angle between $\boldsymbol{q}$ and the constant vector $\boldsymbol{u}$ (∥ to ∇T) which defines the displaced Planck distribution to which the system will tend due to normal processes. $\tau_{\mathrm{n}\lambda}^{-1}$ and $\tau_{\mathrm{r}\lambda}^{-1}$ are the relaxation rates, respectively, for the normal processes and

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the momentum non-conserving processes. $\tau_c^{-1} = \tau_n^{-1} + \tau_r^{-1}$, and the remaining quantities can be seen in [1].

The expression

$$K_\lambda^C = \sum_q n_\lambda^1(q)\mu v_{g\lambda}\hbar\omega_{q\lambda}N_q^0(N_q^0+1)$$

can be simplified by putting $N_q^0 = [\exp(\hbar\omega/k_BT)-1]^{-1}$, $x=\hbar\omega/k_BT$ and using

$$\int d^3q = 4\pi \int \frac{\omega_{q\lambda}^2}{v_{p\lambda}^2}\frac{1}{v_{g\lambda}}d\omega$$

which means that $|v_{g\lambda}|$ and $|v_{p\lambda}|$ are distinguishable even though the $\omega(q\lambda)$ surfaces are spherical. This ultimately leads to

$$K_\lambda^C = \frac{k_B}{2\pi^2}\left(\frac{k_BT}{\hbar}\right)^3 b_\lambda\beta\int_0^{\theta_\lambda/T} v_{p\lambda}^{-3}(x)\tau_{n\lambda}^{-1}(x)\tau_{c\lambda}(x)J_4(x)\,dx \tag{4}$$

where $b_l = \frac{1}{3}$ and $b_t = \frac{2}{3}$, $J_4x = x^4e^x/(e^x-1)^2$, and

$$\beta = \sum_{\lambda=l,t} b_\lambda \int_0^{\theta_\lambda/T} v_{p\lambda}^{-3}(x)\tau_{n\lambda}^{-1}(x)\tau_{c\lambda}(x)J_4(x)\,dx \times\left(\sum_{\lambda=l,t} b_\lambda\int_0^{\theta_\lambda/T} v_{p\lambda}^{-4}(x)v_{g\lambda}^{-1}(x)\tau_{n\lambda}^{-1}(x)\left(1-\tau_{n\lambda}^{-1}(x)\tau_{c\lambda}(x)\right)J_4(x)\,dx\right)^{-1}.$$

Although β depends upon all the phonon modes, K_λ^C gives the explicit expressions for the longitudinal and transverse parts of K^C. The presence of β in both parts can be justified as follows: since $|\boldsymbol{u}|$ is related to the normal processes which ultimately originate the correction term, a function of $|\boldsymbol{u}|$ must appear in both the parts of K^C. Moreover, with the help of equations (2) and (3) in Parrott's paper [1], it can be shown that $|\boldsymbol{u}| = \beta\hbar|\Delta T|/k_BT^2$. Hence β appears in both parts of K^C.

Using (4), one can calculate the total individual contributions of the longitudinal and transverse parts of the phonon conductivity.

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