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The Variational Principle and the Phonon Boltzmann Equation

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ABSTRACT. The thermal transport in a solid happens when the material is subjected to a thermal gradient. If free electrons are absent, the thermal transport is due to the phonons, the quasiparticles corresponding to the vibrations of the atoms of the crystal. The equation that describes this transport is the phonon Boltzmann equation. Here we show how to solve it by means of the variational principle.

Introduction. As discussed in [1], the equation that is today known as the phonon Boltzmann equation was first derived by Rudolf Peierls in 1929 [2]. Peierls actually studied the zones of the reciprocal lattices before Léon Brillouin, applying his approach to evaluate the thermal transport by phonons. In this manner he introduced, besides the Boltzmann equation for phonons, also the notion of three-phonon Normal and Umklapp processes [3]. According to Peierls [1], the thermal transport equation can be written as $\dot{n}_{drift}(\vec{q},p)+\dot{n}_{scatt}(\vec{q},p)=0$, where $\dot{n}_{drift}$ is the rate of change of the number of phonons due to the presence of a temperature gradient and $\dot{n}_{scatt}$ is the rate of change due to the scattering of phonons against other phonons, the boundaries of the sample, and electrons, impurities, dislocations and other defects present in the material. $\vec{q},p$ are indicating the wave-vector and the polarization of the considered phonons.

We discussed the solution of the Boltzmann equation in the case of the presence of isotope impurities and electrons in some previous articles [4-8]. In these papers, we approached the solution by means of the relaxation time approximation and by a more specific analysis, containing the true Brillouin zone of the crystal and the three-phonon scattering matrices. In this last case, the solution was achieved through an iterative method [9-10]. From the solution of the Boltzmann equation, we determined the thermal conductivity of the crystals considered in the abovementioned studies. Other methods for determining the lattice thermal conductivity are based on ab-initio and first-principle calculations, and on molecular dynamics simulations [11-23].

Here we will consider another method for solving the phonon Boltzmann equation, based on the variational principle. The exposition of the related theory is aimed to introduce researchers and students of solid-state physics to a different approach to the determination of the thermal transport in crystals. Before discussing the variation method for the Boltzmann equation, let us see the problem in a more general context.

Variational method. Actually, the Boltzmann equation is, in its standard form, an integral-differential equation [24]:

$$X(k)=\int\{\Phi(k)-\Phi(k')\}P(k,k')\,\mathrm{d}k' \qquad (1)$$

In (1), $X(k)$ is a known function that can be dependent on external fields. The integration is on a vector space, which is here simply represented by the single variable k. Function $P(k,k')$ is positive because it is representing a measure of probability. Moreover, $P(k,k')=P(k',k)$.

The problem is to find the function $\Phi(k)$.

Let us define the internal product of two functions Φ and Ψ in the following manner:

$$(\Phi,\Psi)=\int \Phi(k)\,\Psi(k)\,\mathrm{d}k \tag{2}$$

Let us introduce the scattering operator P, so that:

$$X=\mathrm{P}\,\Phi \tag{3}$$

This operator changes the function Φ in another function by an integration.

Properties of the operator P are the following. It is linear and symmetric. Therefore, for any Φ and Ψ, we can write:

$$(\Phi,\mathrm{P}\Psi)=(\Psi,\mathrm{P}\Phi) \tag{4}$$

This property is coming from the abovementioned symmetry of $\mathrm{P}(k,k')$, that is, from:

$$\mathrm{P}(k,k')=\mathrm{P}(k',k) \tag{5}$$

Moreover, P is positive, so that:

$$(\Phi,\mathrm{P}\Phi)\geq 0 \quad \forall\Phi \tag{6}$$

From (3), we deduce the relation:

$$(\Phi,\mathrm{P}\Phi)=(\Phi,X) \tag{7}$$

According to the variational principle, among all the functions satisfying equation (7), the solution of the integral equation is that giving the maximum value of the product $(\Phi,\mathrm{P}\Phi)$.

This fact is easy to demonstrate. If Ψ is any solution of (7), but not of (3), we have (using (6) and (4)):

$$\begin{aligned} 0 &\le (\Phi-\Psi, \mathrm{P}(\Phi-\Psi)) = (\Phi,\mathrm{P}\Phi)+(\Psi,\mathrm{P}\Psi)-(\Phi,\mathrm{P}\Psi)-(\Psi,\mathrm{P}\Phi) \\ &= (\Phi,\mathrm{P}\Phi)+(\Psi,\mathrm{P}\Psi)-2\,(\Psi,X)=(\Phi,\mathrm{P}\Phi)-(\Psi,\mathrm{P}\Psi) \end{aligned} \tag{8}$$

Then:

$$(\Phi,\mathrm{P}\Phi) \ge (\Psi,\mathrm{P}\Psi) \tag{9}$$

To apply this property to the solution of the Boltzmann equation, we use a trial function, made by known functions, which are containing some parameters the value of which we can change. Then, these parameters are varied until the function $(\Phi,\mathrm{P}\Phi)$ attains its maximum value. Let us stress that, in this manner, we do not find the true solution. However, in the case that we have made a good choice of the trial function, the solution is a good approximation of the true result.

Usually, the trial function is of the following type:

$$\Phi(k)=\sum_i \eta_i\ \phi_i(k) \tag{10}$$

In (10), η_i are the parameters we can change, and $\phi_i(k)$ are the known functions. Then, we can write the elements of the matrix and vector corresponding to operator P and function X, that is P_{ij} and X_i according to the set of functions ϕ_i:

$$\mathrm{P}_{ij}=(\phi_i,\mathrm{P}\phi_j) \tag{11}$$

$$X_i=(X,\phi_i) \tag{12}$$

Therefore, we have:

$$(\Phi,\mathrm{P}\Phi)=\sum_{ij}(\eta_i\phi_i,\mathrm{P}\eta_j\phi_j)=\sum_{ij}\eta_i\eta_j(\phi_i,\mathrm{P}\phi_j)=\sum_{ij}\mathrm{P}_{ij}\ \eta_i\ \eta_j \tag{13}$$

$$(\Phi,X)=\sum_i(\eta_i\phi_i,X)=\sum_i\eta_i(X,\phi_i)=\sum_i X_i\ \eta_i \tag{14}$$

According to the variational principle, parameters η_i must satisfy the equation:

$$X_i=\sum_j \mathrm{P}_{ij}\ \eta_j \tag{15}$$

Equation (15) can be solved by means of an algebraic or numerical approach. However, let us stress once more that the choice of functions ϕ_i is quite important, because from it we have a solution which is close to the true solution or not. However, we have also to choose the functions ϕ_i in order to have the products (11), (12) that can be easily calculated. Therefore, these two constraints have to be matched opportunely.

The method outlined here is also known as the Rayleigh–Ritz method, after Walther Ritz and Lord Rayleigh. It is widely used to approximate eigenvalues and eigenvectors.

Phonon Boltzmann equation. Let us express the phonon distribution $n(\vec{q}, p)$ in term of the deviation function $\psi_{\mathbf{q}p}$:

$$n(\vec{q}, p) = n_{\mathbf{q}p} = n_{\mathbf{q}p}^{o} + \psi_{\mathbf{q}p} n_{\mathbf{q}p}^{o} (1 + n_{\mathbf{q}p}^{o}) , \tag{16}$$

where $n_{\mathbf{q}p}^{o}$ is the equilibrium Bose-Einstein distribution. In (16), the phonon distribution in the material is supposed being disturbed by the presence of a thermal gradient.

Writing the Boltzmann equation in the form given in the previous section, we have that it is like:

$$X_{\mathbf{q}}^{p} = \sum_{\mathbf{q}'p'} P_{\mathbf{q}\mathbf{q}'}^{pp'} \psi_{\mathbf{q}'p'} , \quad X_{\mathbf{q}}^{p} = -\mathbf{v}_{\mathbf{q}p} \frac{\partial n_{\mathbf{q}p}^{o}}{\partial T} \cdot \nabla T \tag{17}$$

In (17), we have the phonon group velocity $\mathbf{v}_{\mathbf{q}p}$ and the gradient of the temperature, which is perturbing the equilibrium of phonons.

We can deduce the deviation function $\psi_{\mathbf{q}p}$ applying the Rayleigh-Ritz variational procedure to the trial function:

$$\Phi(\mathbf{q}, p) = \sum_{r} a_r^p \phi_r (\mathbf{q}, p) \tag{18}$$

In (18), $\{\phi_r\}$ is a set of functions that need to be suitably chosen.

According to Srivastava in [25], we can obtain the thermal conductivity κ as:

$$\kappa = \frac{k_B T^2}{\Omega \, |\nabla T|^2} \sum_{r\,p} a_r^p X_r^p , \quad X_r^p = \sum_{\mathbf{q}} X_{\mathbf{q}}^{p} \phi_r (\mathbf{q}, p) \tag{19}$$

We have here the volume of the crystal Ω and the Boltzmann constant k_B. The coefficients a_r^p are obtained by solving the system:

$$X_{\mathbf{q}}^{p} = \sum_{r'} a_{r'}^{p'} \Pi_{rr'}^{pp'}, \quad \Pi_{rr'}^{pp'} = \sum_{\mathbf{qq}'} \phi_r(\mathbf{q}, p) P_{\mathbf{qq}'}^{pp'} \phi_{r'}(\mathbf{q}', p') \tag{20}$$

As we have discussed in [9] and [10] for instance, the phonons are scattered through three-phonon processes and therefore the matrix elements $\Pi_{rr'}^{pp'}$ can be written as:

$$\frac{1}{2}\sum_{\mathbf{q}p}\sum_{\mathbf{q}'p'}\sum_{\mathbf{q}''p''} Q_{\mathbf{q}p,\mathbf{q}'p'}^{\mathbf{q}''p''}[\Phi(\mathbf{q}, p) + \Phi(\mathbf{q}', p') - \Phi(\mathbf{q}'', p'')]^2 = \sum_{rr'}\sum_{pp'} \Pi_{rr'}^{pp'} a_r^p a_{r'}^{p'} \tag{21}$$

In (21), we find the intrinsic transition probability rate for the three-phonon scattering processes:

$$Q_{\mathbf{q}p,\mathbf{q}'p'}^{\mathbf{q}''p''} = \frac{2\pi}{\hbar}\left|\langle \mathbf{q}''p''| H | \mathbf{q}p, \mathbf{q}'p'\rangle\right|^2 n_{\mathbf{q}p}^o n_{\mathbf{q}'p'}^o (1 + n_{\mathbf{q}''p''}^o)\ \delta(\hbar\omega_{\mathbf{q}p} + \hbar\omega_{\mathbf{q}'p'} - \hbar\omega_{\mathbf{q}''p''}) \tag{22}$$

We have, in (22), the phonon angular frequency for given wave-vector and polarization. $\hbar$ is the reduced Planck constant or Dirac constant. δ represents the function delta of Dirac. In (22) we find also the Hamiltonian H, used to describe the set of interacting phonons.

Actually, the explicit form of (17) is:

$$X_{\mathbf{q}}^{p} = \sum_{\mathbf{q}'p'}\sum_{\mathbf{q}''p''} Q_{\mathbf{q}p,\mathbf{q}'p'}^{\mathbf{q}''p''}\left(\psi_{\mathbf{q}p} + \psi_{\mathbf{q}'p'} - \psi_{\mathbf{q}''p''}\right) + \frac{1}{2}\sum_{\mathbf{q}'p'}\sum_{\mathbf{q}''p''} Q_{\mathbf{q}p}^{\mathbf{q}'p',\mathbf{q}''p''}\left(\psi_{\mathbf{q}p} - \psi_{\mathbf{q}'p'} - \psi_{\mathbf{q}''p''}\right) \tag{23}$$

Calculating the thermal conductivity. From what we have previously told, it is clear that the evaluation of the thermal transport by means of the variational approach is a non-trivial task. We have solved it in a previous paper [26], where we considered the variational approach to determine the thermal conductivity of the rare gas crystals. To account for the crystal lattice, we used an isotropic model made of successive shells surrounding the atoms of the crystal. The potential describing the interaction among atoms was a Lennard-Jones potential.

In the framework of the model, we can calculate the dispersions of the longitudinal and transversal angular frequency of phonons by means of the eigenvalue equation:

$$\sum_{(\mathbf{h}\neq 0)} [1 - \cos(\mathbf{q}\cdot\mathbf{h})][(O_h U) + \beta(h)\mathbf{hh}]\boldsymbol{\varepsilon}_{\mathbf{q}p} = M\omega_{\mathbf{q}p}^2 \boldsymbol{\varepsilon}_{\mathbf{q}p} \tag{24}$$

In the equation (24) we find the mass M of each reticular center, $\mathbf{h}$ runs over all the neighbors of the central atom considered as origin (h is the modulus), U is the Lennard-Jones potential, $O_h = h^{-1} d/dh$ and $\beta(h) = O_h^2 U$. $\boldsymbol{\varepsilon}_{\mathbf{q}p}$ are the unit vectors of polarizations.

Let us remember that the Lennard-Jones potential is:

$$U(h) = U_o\left[\left(\frac{r_o}{h}\right)^{12} - \left(\frac{r_o}{h}\right)^{6}\right] \tag{25}$$

In (25), we have two parameters U_o, r_o, which are specific of the material.

The Hamiltonian necessary for giving the intrinsic transition probability (22) is:

$$H = \frac{1}{12}\sum_{\mathbf{l}}\sum_{(\mathbf{h}\neq 0)}\alpha(h)\left[\mathbf{h}\cdot(\boldsymbol{\xi}_{\mathbf{l+h}} - \boldsymbol{\xi}_{\mathbf{l}})\right]^3 + \frac{1}{4}\sum_{\mathbf{l}}\sum_{(\mathbf{h}\neq 0)}\beta(h)\left[\mathbf{h}\cdot(\boldsymbol{\xi}_{\mathbf{l+h}} - \boldsymbol{\xi}_{\mathbf{l}})\right]\left|\boldsymbol{\xi}_{\mathbf{l+h}} - \boldsymbol{\xi}_{\mathbf{l}}\right|^2 \tag{26}$$

Vector $\mathbf{l}$ gives the atomic positions and $\alpha(h) = O_h^3 U$. $\boldsymbol{\xi}_{\mathbf{l}}$ is the displacement of the atom from its average position given by vector $\mathbf{l}$ (the same for $\mathbf{l}+\mathbf{h}$).

Let us define the dimensionless quantities $\mathbf{y} = \mathbf{q}/Q_D$, $\mathbf{y}' = \mathbf{q}'/Q_D$, $\mathbf{y}'' = \mathbf{q}''/Q_D$, in which Q_D is the radius of the Debye sphere, and $\Phi(\mathbf{q}, p) = f_p(y)(\mathbf{u_q}\cdot\mathbf{u})$, where $\mathbf{u_q} = \mathbf{q}/q$ and $\mathbf{u} = \nabla T/|\nabla T|$. In the framework of the isotropic model, the result does not depend on $\mathbf{u}$ [26]. Then, equation (21) becomes:

$$\frac{1}{6}\sum_{\mathbf{q}p}\sum_{\mathbf{q}'p'}\sum_{\mathbf{q}''p''} Q_{\mathbf{q}p,\mathbf{q}'p'}^{\mathbf{q}''p''}\,\Theta = \sum_{rr'}\sum_{pp'}\Pi_{rr'}^{pp'} a_r^p a_{r'}^{p'}$$

$$\Theta = f_p^2(y) + f_{p'}^2(y') + f_{p''}^2(y'') + 2a\, f_p(y) f_{p'}(y') - 2b\, f_p(y) f_{p''}(y'') - 2c\, f_{p'}(y') f_{p''}(y'') \tag{27}$$

In (27), *a*, *b* and *c* are the cosines $\mathbf{u_q}\cdot\mathbf{u_{q'}}$, $\mathbf{u_q}\cdot\mathbf{u_{q''}}$ and $\mathbf{u_{q'}}\cdot\mathbf{u_{q''}}$, respectively.

Functions $f_p(y)$ are those that we must describe by the trial functions:

$$f_p(y) = -\frac{\partial\varpi_p(y)}{\partial y}\left\{\frac{1}{y}\sum_{r=0}^{R} a_r^p y^r\right\} \tag{28}$$

In (28), we have R the maximum value of the exponent involved. We have also the reduced angular frequency:

$$\varpi_p(y) = h_1\left(\frac{2M}{U_o}\right)^{1/2}\omega_{\mathbf{q}p} \tag{29}$$

In it, we find h_1 which is the nearest-neighbor distance and U_o, the parameter of the Lennard-Jones potential (25).

The choice of the trial function of the form given in (28) was made in agreement to the behaviour of the Boltzmann equation in the long wavelength limit.

For $\mathbf{q} \to 0$, we have that [26]:

$$\psi_{\mathbf{q}p} \propto -\frac{(\mathbf{v}_{qp} \cdot \nabla T)}{q} \tag{30}$$

That is:

$$f_p(y) \propto -\frac{1}{y}\frac{\partial \overline{\omega}_p}{\partial y} \tag{31}$$

According to Srivastava, using (19) we have the thermal conductivity [26]:

$$\kappa = \frac{16}{27}\frac{U_o^2 \hbar N}{\Omega\, M\, l_1^2 k_B T^2}\sum_{r\,p} b_r^p \lambda_r^p \tag{32}$$

In (32), we have N the number of atoms in the crystal and parameter $l_1 = 4.37511$ for a F.C.C. lattice. We have also used:

$$a_r^p = \Gamma b_r^b \;;\quad \Gamma = \frac{64}{9}\pi^2 \frac{|\nabla T|}{k_B T^2}\frac{N U_o}{\Omega Q_D^4} \tag{33}$$

$$\lambda_r^p = \int_0^1 y^{r+1}\left(\frac{\partial \overline{\omega}_p}{\partial y}\right)^2 \overline{\omega}_p(y)\, n_p^o(y)\left[1 + n_p^o(y)\right] dy \tag{34}$$

In dimensional terms, (32) means:

$$\begin{aligned}[\kappa] &= \frac{energy^3 \cdot time}{volume \cdot mass \cdot energy \cdot temperature} \\ &= \frac{energy^2 \cdot time^2}{length^3 \cdot mass \cdot temperature \cdot time} \\ &= \frac{energy^2}{length \cdot energy \cdot temperature \cdot time} = \frac{power}{length \cdot temperature}\end{aligned} \tag{32}$$

In [26], we have calculated the matrix elements in (27) and numerically found coefficients b_r^b to use in (32). The result for the thermal conductivity in solid argon is shown in the Figure 1.

For solid argon, the parameters of the interatomic potential and the nearest-neighbor distance at 10 K and 80 K, as deduced from [27] are in the following data: $U_o = 0.58356\times10^{-13} erg$, $r_o = 3.4447\times10^{-8} cm$, $h_1 = 3.7559\times10^{-8} cm$ at 10 K, and $h_1 = 3.8571\times10^{-8} cm$ at 80 K.

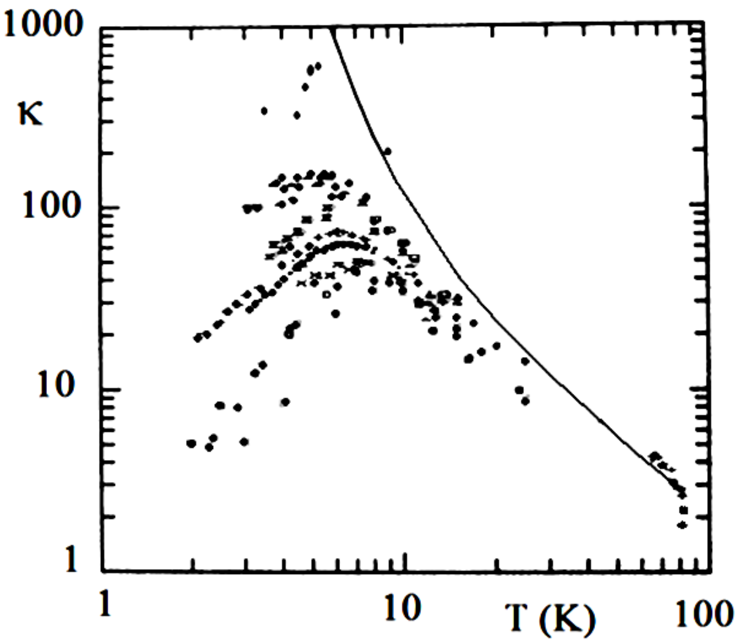

Fig. 1. Thermal conductivity of solid argon (in mW/(cm·°C)) as a function of temperature. The result of the variational calculation is given by the line. The experimental points are from [28-33].

In the calculation of the thermal conductivity we applied the variational procedure in the temperature range between 7 K and 80 K. We have not considered the temperature below 7 K in order to avoid the boundary scattering, which is responsible for the peaks at low temperature that we see in the experimental data.

Summary. In this paper we have shown how a variational method can be used to solve the phonon Boltzmann equation for the determination of the thermal conductivity of a crystal, such as a crystal of solid argon, where only the phonons are transporting the heat. The exposition of the theory is maintained to an introductory level, aiming to show to researchers and students a different approach to the problem of the thermal transport by phonons, different from those previously exposed in [4] and [5]. The variational method is based on the use of a set of trial functions, that need to be chosen in order to have a solution which is quite close to the true solution. Here we have used, to solve the phonon Boltzmann equation, a set of trial functions which have the same behaviour of the deviation function in the long wavelength limit. The fact that the choice was a good one is also given, a posteriori, by a good agreement with the experimental data.

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