сообщения
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исследований
дубна

E17-86-632

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PHONON RELAXATION ON ISOTOPIC IMPURITIES: A SOLVABLE MODEL

1986

The Boltzmann equation is an integro-differential equation and, usually, does not allow an exact treatment [1]. A number of solvable models is very limited and most interesting of them are based on rather drastic assumptions about the form of the collision operator (as, for example, the Claro and Wannier model [2]).

On the other hand, transport phenomena are usually described by the Boltzmann equation. As a rule, the so-called relaxation time approximation is used. However, this approximation, while intuitively a very useful concept, has to be handled with care [1]. From this point of view the solvable cases of the Boltzmann equation will play a role of guideposts when a detailed study of a more complex phenomenon is performed.

The purpose of this paper is to pay attention to the relaxation of phonons scattered by isotopic impurities (or by vacancies) in a crystal of cubic symmetry that can serve as an example of the exactly solvable case of the Boltzmann phonon equation.

The object under consideration is a phonon gas in an elastic continuum of cubic symmetry. Consequently, the phonons are equivalent to sound wave quanta of frequency $\omega(\vec{k}, j) = |\vec{k}| \cdot c(\hat{\vec{k}}, j)$, with sound velocity, $c(\hat{\vec{k}}, j)$, depending, in general, on the wave-vector direction given by the versor (unit vector) $\hat{\vec{k}} = \vec{k}/|\vec{k}|$. Three acoustic phonon branches appear, so $j = 1,2,3$.

In a very pure (chemically and structurally) and large sample at helium temperature the isotope impurities can play the role of main scatterers. Samples fulfilling the above conditions have recently been used in experiments on ballistic propagation of phonons [3]. It seems then quite reasonable to consider the model in which phonons in their relaxation process are scattered only by isotopic impurities (by differences in mass only) [4,5].

Let us disturb the phonon system so that both homogeneity and cubic symmetries remain unchanged. The phonon distribution functions, $N(\vec{k}, j; t)$, will relax according to the Boltzmann phonon equation [4,5]

$$\frac{\partial}{\partial t} N(\vec{k}, j; t) = \frac{1}{N} \sum_{\vec{k}', j'} w(\vec{k}, j; \vec{k}', j') \cdot [N(\vec{k}', j'; t) - N(\vec{k}, j; t)] \cdot \delta(\omega(\vec{k}', j') - \omega(\vec{k}, j)), \tag{1}$$

w is the transition probability, and for a sample with randomly distributed isotopic atoms it can be written as [6]

$$w(\vec{k}, j; \vec{k}', j') = \frac{\pi}{4} g\omega(\vec{k}, j)\omega(\vec{k}', j') \cdot |\hat{e}(\vec{k}, j) \cdot \hat{e}(\vec{k}', j')|^2, \quad (2)$$

where $\hat{e}$ is the polarization vector. Here
$g = \sum_i f_i (1 - M_i/M)$,
where f_i is a fraction of unit cells with the mass M_i and M is the averaged mass of unit cell, $M = \Sigma_i f_i M_i$.

Since energy is conserved in the scattering process (1), then $\omega(\vec{k}, j) = \omega(\vec{k}', j') = \omega$ and thus the long-wave phonon can be labelled by its frequency ω, wave direction $\hat{k}$ and branch j to which it belongs, i.e., $\{\vec{k}, j\} = \{\hat{k}, \omega, j\}$.

The coefficient of $N(\vec{k}, j; t)$ in the right-hand side of equation (1) is traditionally called the reciprocal of the relaxation time:

$$\tau^{-1}(\vec{k}, j) = \frac{1}{N}\sum_{\vec{k}'j'} w(\vec{k}, j; \vec{k}', j')\delta(\omega(\vec{k}', j') - \omega(\vec{k}, j)) =$$
$$= \frac{v_0 g}{8\pi} \cdot \omega^4 \sum_{j'} \frac{1}{4\pi}\int d\Omega(\hat{k}') \cdot c^{-3}(\hat{k}', j')|\hat{e}(\hat{k}, j) \cdot \hat{e}(\hat{k}', j')|^2. \quad (3)$$

Here $v_0 = V/N$ is the volume of a unit cell, and the integral should be performed over the solid angle $\Omega(\hat{k})$ in the wave-vector space under the constraint $\omega(\vec{k}, j) = \omega$.

At this stage, usually the anisotropy in (3) is neglected by taking for the product $|\hat{e}(\hat{k}, j) \cdot \hat{e}(\hat{k}', j')|$ its approximate value equal to $1/\sqrt{3}$, i.e., to the cosine of the angle between random directions [4].

However, for elastic continuum of cubic symmetry no such approximation is needed because using only the symmetry argument one can show that the relaxation time is both direction- and branch-independent [6]. Indeed, the right-hand side of equation (3) contains the matrix expression

$$F_{\alpha\beta} = \sum_{j'} \frac{1}{4\pi}\int d\Omega(\hat{k}')c^{-3}(\hat{k}', j')\hat{e}^{\alpha}(\hat{k}', j')\hat{e}^{\beta}(\hat{k}', j'),$$

which for the case of cubic symmetry is simply proportional to the unit matrix $F_{\alpha\beta} = \delta_{\alpha\beta} c_D^{-3}$, where c_D is the Debye velocity defined by

$$c_D^{-3} = \frac{1}{3}\sum_{\alpha} F_{\alpha\alpha} = \frac{1}{3}\sum_j \frac{1}{4\pi}\int d\Omega(\hat{k})c^{-3}(\hat{k}, j).$$

Here the normalization condition of the polarization vector is taken into account in the form $|\hat{e}(\hat{k}, j)| = 1$. As a result, we have got one relaxation time common for all directions and branches j, given by

$$\tau^{-1}(\vec{k}, j) = \frac{v_0}{4} g\omega^4 c_D^{-3} \equiv \tau_c^{-1}(\omega). \quad (4)$$

Using the same symmetry argument one can get that the remaining part of the collision operator in (1) is nothing but an averaged value of the phonon distribution function:

$$\langle N(\omega; t)\rangle \equiv \frac{1}{3}\sum_j \frac{1}{4\pi}\int d\Omega(\hat{k})\left(\frac{c_D}{c(\hat{k}, j)}\right)^3 N(\omega, \hat{k}, j; t). \quad (5)$$

So, the cubic symmetry allows us to rewrite the Boltzmann equation (1) in the following simple form

$$\left(\frac{\partial}{\partial t} + \tau_c^{-1}(\omega)\right)N(\omega, \hat{k}, j; t) = \tau_c^{-1}(\omega)\langle N(\omega; t)\rangle. \quad (6)$$

The same result can be found for an isotropic elastic medium. We should also stress here the analogy between the Boltzmann phonon equation (6) and the Lorentz model describing a gas of low density [7].

Averaging equation (6) according to the definition (5) one immediately can see that $\langle N(\omega; t)\rangle$ is constant in time

$$\langle N(\omega; t)\rangle = \langle N(\omega; t = 0)\rangle \equiv \bar{N}(\omega). \quad (7)$$

The fact that the averaged number of phonons with frequency ω is conserved simplifies the Boltzmann phonon equation essentially. Instead of the integro-differential equation (1) we have got a simple integral eqaution of the first order the solution of which has the form

$$N(\omega, \hat{k}, j; t) = [N(\omega, \hat{k}, j; t = 0) - \bar{N}(\omega)]e^{-t/\tau_c(\omega)} + \bar{N}(\omega). \quad (8)$$

This result justifies the traditional approximation [4,5] ignoring the direction and branch-dependence in equation (2).

The conclusion is that the disturbed phonon distribution function relaxes towards its average value $\bar{N}$ with the relaxation time exactly the same as in the so-called relaxation-time approximation. In other words, the relaxation-time approximation serves as an exact solution of the Boltzmann phonon equation (1) for elastic continuum of cubic symmetry. All the above results are, of course, also valid for an isotropic elastic medium.

We should emphasize, however, that for the systems of lower symmetry (hexagonal, tetragonal, etc.) the relaxation time, contrary to (3), is direction- and branch-dependent [8], which preserves an integro-differential character of equation (1) and therefore the phonon relaxation will be more complex.

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Received by Publishing Department
on September 23, 1986.

Петру З.К. E17-86-632

Релаксация фононов на изотопических примесях: точнорешаемая модель

Найдено точное решение уравнения Больцмана, описывающего релаксацию акустических фононов на изотопических примесях /или на вакансиях/, для случая упругой среды кубической симметрии.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Сообщение Объединенного института ядерных исследований. Дубна 1986

Petru Z.K. E17-86-632

Phonon Relaxation on Isotopic Impurities: A Solvable Model

The exact solution of the Boltzmann equation describing relaxation of acoustic phonons on isotopic impurities (or on vacancies) is presented for the case of elastic continuum of cubic symmetry.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

Communication of the Joint Institute for Nuclear Research. Dubna 1986