# **Thermal conductivity and interference effects in the dynamics of crystals with heavy impurities**

I. Ya. Polischuk, A. P. Zhernov, and L. A. Maksimov

*Znsitute ofHigh Temperatures, Academy ofsciences of the USSR, Moscow*  (Submitted *17* February 1988) Zh. Eksp. Teor. Fiz. 94,259-266 (September 1988)

It is shown that, in the temperature region between the frequency of quasilocal oscillations of heavy isotopic defects of a harmonic crystal and the Debye frequency, the main concentration correction to the thermal conductivity is due to interference processes in phonon scattering by defects and is analogous to the weak localization of electrons in disordered media.

### **1. INTRODUCTION**

The problem of the anomalous behavior of the density of states, of the heat capacity, and of the thermal conductivity of disordered dielectric systems has recently been discussed intensely in the literature.<sup>1-6</sup> The concept of fractons was proposed<sup>3,4</sup> to explain these anomalies; these are localized vibrations on fractals (structures with fractional dimensionality).

The existence of such vibrations was shown<sup>5,6</sup> in a model of a harmonic lattice with random broken bonds which have the properties of a fractal at intermediate distances. It is natural then to use the assumption of the existence of broken, and not weak, but limited bonds.

In our view, the occurrence of localized vibrations in disordered harmonic systems is due in the first place to interference processes in the scattering of phonons by defects and not by a possible fractal structure of these systems. We emphasize that, unlike the localized and quasilocalized modes first discussed,<sup>7,8</sup> associated with isolated impurities, the question is now about normal vibrations encompassing a cluster with a large number of defects.

We study below, using as an example the model of a harmonic lattice with heavy isotopic impurities, ${}^{8}$  the influence of interference effects on the thermal conductivity of crystals, which is analogous to weak localization of electrons in disordered systems.<sup>9</sup> We note that the frequency region  $\omega \leq \omega_0$  ( $\omega_0$  is the quasilocalized frequency) was considered in detail by Kagan.<sup>8</sup> We will be interested in the frequency region  $\omega_0 \ll \omega \ll \omega_D$  ( $\omega_D$  is the Debye frequency), where the corrections associated with coherent scattering of phonons by defects becomes considerable. It turns out that for such frequencies the defect mass can be considered infinite when evaluating the Green's function of the phonons. In percolation theory this corresponds to the problem of broken sites, the properties of which are close to the problem of broken bonds.<sup>10</sup> In this way the results obtained in the present work can be taken over for the model of a harmonic lattice with random broken bonds.

General expressions for the thermal conductivity of a crystal with isotopic defects are obtained in \$2. The Green's function for phonons is evaluated in \$3 in the frequency region  $\omega_0 \ll \omega \ll \omega_D$ , taking account of interference corrections. The self-energy is then determined in an approximation quadratic in the concentration. The two-phonon Green's function is evaluated in \$4. In the last section the thermal conductivity of a crystal is evaluated in the temperature region  $\omega_0 \ll T \ll \omega_D$ .

We use a system of units in which Planck's constant and the main parameters of the unperturbed matrix (lattice constant, atomic mass, and velocity of sound) are equal to unity. For simplicity a scalar model of the vibration is taken.'

## **2. GENERAL EXPRESSIONS FOR THE THERMAL CONDUCTIVITY OF A CRYSTAL WITH ISOTOPIC DEFECTS**

The Hamiltonian of a harmonic lattice with isotopic defects has, in the scalar model, the form

$$
H = H_0 + H_{int}, \qquad H_0 = \frac{1}{2} \sum_i p_i^2 + \frac{1}{2} \sum_{ij} A_{ij} u_i u_j,
$$

$$
H_{int} = \frac{1}{2} (M^{-1} - 1) \sum_i c_i p_i^2.
$$
 (1)

Here *i* is the number of the site of a simple cubic lattice,  $u_i$ and  $p_i$  are the one-component coordinate and momentum operators,  $A_{ij}$  are the force constants, M is the mass of a defect,  $c_i = 1$  if the corresponding site is occupied by a defect and  $c_i = 0$  in the opposite case.

In order to determine the thermal conductivity we start from the expression<sup>12</sup>

$$
\kappa = \lim_{z \to 0} \beta V^{-1} \int_{0}^{\beta} d\tau \int_{0}^{\infty} dt \, e^{-zt} \langle \mathbf{j}_{H}(0) \mathbf{j}_{H}(t+i\tau) \rangle, \quad \text{Im } z > 0;
$$

here  $\beta$ <sup>-1</sup> and *V* are the temperature and volume of system,  $\mathbf{j}_H(t)$  is the energy current operator in the Heisenberg representation. This expression can be written in the form

$$
\kappa = \lim_{z \to 0} \beta V^{-1} \frac{1}{i} \frac{\partial}{\partial z} \langle \mathbf{j}_H | \mathbf{j}_H \rangle_z, \tag{2}
$$

where  $( \langle .|. . \rangle )$ , is the retarded Green's function.

The energy current operator  $\mathbf{j}_H$  has, in model (1), the  $form<sup>13</sup>$ 

$$
\mathbf{j}_H = \frac{1}{2} \sum_{ij} A_{ij} \mathbf{R}_{ji} u_j p_i m_i^{-1}, \tag{3}
$$

where  $m_i^{-1} = 1 + C_i (M^{-1} - 1)$ ,  $\mathbf{R}_{ii}$  is the radius vector between the corresponding sites. For an ideal lattice  $(c_i \equiv 0)$ Eq. (3) goes over into the well-known expression for the phonon energy current. **l4** 

Substituting Eq.  $(3)$  into Eq.  $(2)$ , we find

$$
\kappa = \frac{\beta V^{-1}}{4i} \sum_{i i' j'} A_{ji} R_{ji} A_{j'i'} R_{j'i'} m_i^{-1} m_i^{-1} \lim_{z \to 0} \frac{\partial K(z)}{\partial z}, \qquad (4)
$$

with  $K(z) = \langle \langle u_i | p_i | u_i | p_i \rangle \rangle_z$ . In a way similar to what one

does in the theory of electrical conductivity (see, for example, Ref. 15), the function  $K(z)$  can be written in the form

$$
K(z) = -(2\pi i)^{-1} \oint d\omega f(\omega)
$$
  
\n
$$
\times \{ [\langle u_i | u_j, \rangle_{\omega+i0} - \langle u_i | u_j, \rangle_{\omega-i0}] \langle p_{i'} | p_{i} \rangle_{\omega-z} + [\langle p_{i'} | p_{i} \rangle_{\omega+i0} - \langle p_{i'} | p_{i} \rangle_{\omega-i0}] \langle u_i | u_j, \rangle_{\omega+z} + [\langle u_i | p_{i'} \rangle_{\omega+i0} - \langle u_i | p_{i'} \rangle_{\omega-i0}] \langle u_j, | p_{i} \rangle_{\omega-z} + [\langle u_j | p_{i} \rangle_{\omega+i0} - \langle u_j, | p_{i} \rangle_{\omega-i0}] \langle u_j | p_{i'} \rangle_{\omega+i} \},
$$
\n(5)

where  $f(\omega) = [\exp(\beta \omega) - 1]^{-1}$  is the Planck function. The Green's functions which appear in Eq. (5 ) are related to one another by the exact relations

$$
\langle p_i | p_j \rangle = -m_i \delta_{ij} + m_i m_j \omega^2 \langle u_i | u_j \rangle, \n\langle p_i | u_j \rangle = im_i \omega \langle u_i | u_j \rangle.
$$
\n(6)

Substituting Eqs. (6) and (5) into Eq. (4) we obtain

$$
\kappa = \frac{1}{4} \frac{\beta}{\pi V} \sum_{i \in \mathcal{Y}'} A_{ji} \mathbf{R}_{ji} A_{j'i'} \mathbf{R}_{j'i'} \int_0^{\infty} d\omega \frac{\partial f(\omega)}{\partial \omega} \omega^2
$$
  
 
$$
\times \left[ G_{jj'}(\omega + i0) G_{i'i}(\omega - i0) - \frac{1}{2} G_{jj'}(\omega + i0) G_{i'i}(\omega + i0) - \frac{1}{2} G_{jj'}(\omega - i0) G_{i'i}(\omega - i0) \right], \qquad (7)
$$

where  $G_{ii}(\omega \pm i0) = \langle \langle u_i | u_j \rangle \rangle_{\omega + i0}$ . We shall proceed to the momentum representation in Eq. (7), expressing then the force constants in terms of the unperturbed frequencies  $\omega$ , which in the Debye model are determined by the relation  $\omega_p = |p|$  ( p is the quasimomentum). In addition, averaging over the position of the defects must be carried out in Eq. **(7).** We obtain as a result

$$
\begin{split}\n\mathbf{x} &= \frac{2\beta}{8\pi^4} \int_0^1 d\omega \, \frac{\partial f(\omega)}{\partial \omega} \, \omega^2 \\
&\times \int d^3 p \left( K_p^{+-}(\omega) - \frac{1}{2} \, K_p^{++}(\omega) - \frac{1}{2} \, K_p^{--}(\omega) \right), \qquad (8) \\
\text{where} \\
K_p^{+\pm}(\omega) &= \frac{V}{(2\pi)^3} \int d^3 q \, \mathbf{p} \mathbf{q} \langle G_{\mathbf{p} \mathbf{q}}(\omega \pm i0) \, G_{-\mathbf{q} - \mathbf{p}}(\omega \pm i0) \rangle, \qquad (9)\n\end{split}
$$

where

$$
K_{p}^{\pm\pm}(\omega) = \frac{V}{(2\pi)^{3}} \int d^{3}q \, \mathbf{p} \mathbf{q} \langle G_{\mathbf{p} \mathbf{q}}(\omega \pm i0) \, G_{-\mathbf{q} - \mathbf{p}}(\omega \pm i0) \, \rangle, \quad (9)
$$

while brackets  $\langle \ldots \rangle$  denote the operation of averaging over the position of the defects.

An approximate expression similar to Eq. (7) was obtained by Flicker and Leath<sup>16</sup> with the help of the decoupling of the Green's function  $K(z)$ . The form of expression (8) for the thermal conductivity allows results from the theory of the residual resistance of a normal metal with impurities to be used. It is therefore convenient to describe below the diagram technique with symbols similar to Abrikosov *et* a/."

#### **3. ONE-PHONON GREEN'S FUNCTION**

The following graphical breakdown can be obtained by using standard quantum field theory methods for the Green's function  $G_{ij}(\omega)$  in the coordinate representation,<br>using the Hamiltonian of Eq. (1):<br> $\Rightarrow$  =  $\leftrightarrow$  +  $\leftrightarrow$   $\sim$   $\rightarrow$   $\rightarrow$  +  $\leftrightarrow$   $\sim$   $\rightarrow$   $\rightarrow$   $\rightarrow$   $\rightarrow$   $\rightarrow$  + using the Hamiltonian of Eq. (1):



$$
+\frac{1}{i}+\frac{
$$

where

$$
\mathcal{T}_a = \mathop{\bigcirc}\limits_{a} = \omega^2 \Big( \mathop{\times}\limits_{a} + \mathop{\overbrace{\bigcirc}\limits_{a} \bullet \mathop{\longrightarrow}\limits_{a} + \cdots \Big)} (11)
$$

is the exact single-site  $T$  operator and the thick and thin continuous lines correspond, representively, to the total  $G_{ij}(\omega)$  and free  $G_{ij}^{0}(\omega)$  Green's functions; expression  $\langle \langle p_a | p_a \rangle \rangle_{\omega} = (-1 + \omega^2 G_{aa}^0(\omega))$  corresponds to the dotdash lines; the corresponding constant  $(M^{-1} - 1)$  is set at each cross; the dashed line connects corresponding to one and the same defect. We note that in obtaining Eqs. ( 10) and  $(11)$  we have used Eq.  $(6)$ .

In this section we will be interested in the averaging of the Green's function over the position of the defects

$$
\langle G_{pq}(\omega + i0) \rangle = \delta_{p-q} G_p(\omega + i0),
$$
  
\n
$$
G_p(\omega + i0) = (\omega^2 - p^2 - \Sigma_p(\omega + i0))^{-1};
$$
\n(12)

here  $\Sigma_{\rho}$  ( $\omega + i 0$ ) =  $\Delta_{\rho}(\omega) - i \Gamma_{\rho}(\omega)$  is the self energy. It can be shown that in the coordinate representation the Green's function of Eq. ( 12) takes on the form

$$
G_R(\omega + i0) = -\frac{1}{4\pi^2 R} [2Si(k_D R) - \pi + \pi e^{ikR}] + o(k^2)
$$
  
= 
$$
\begin{cases} -\frac{1}{4\pi^2} \left[ 2 \frac{Si(k_D R)}{R} + i\pi k \right], & kR \ll 1 \\ -\frac{1}{4\pi^2 R} \exp(ikR), & k_D R \gg 1 \end{cases}
$$
; (13)

here  $k_D = (6\pi^2)^{1/2}$ ,  $k = (\omega^2 - \Sigma(\omega + i\,0))^{1/2}$ . To first order, when evaluating  $\Sigma(\omega + i 0)$ , we shall omit in Eq. (10) diagrams with intersecting dashed lines and we shall ignore correlations in the position of defects. It then turns out that the self energy is independent of momentum and satisfies the self-consistent equation

$$
\Sigma(\omega+i0) = \frac{n\omega^2 (M^{-1}-1)}{M^{-1} - (M^{-1}-1)\omega^2 G_{R=0}(\omega+i0)},
$$
\n(14)

when  $n$  is the defect concentration. The quasilocalized frequency corresponds to the pole of Eq. (14)  $\omega_0 \sim M^{-1/2}$ . For  $\omega \leq \omega_0$  the Green's function (12) describes acoustic vibrations while Eq. ( 14) describes the renormalized velocity of sound and the Rayleigh attenuation of phonons  $(\tau^{-1} \sim \omega^4)$ . In the case which interests us,  $\omega \gg \omega_0$ , we have from Eq. (14).

$$
\Sigma(\omega + i0) = n \left[ \frac{k_D}{2\pi^2} + i \frac{k}{4\pi} \right]^{-1}.
$$
 (15)

Equation (15) is independent of the mass  $M$  and corresponds formally to the model of an infinitely heavy defect.

In its form (if one abstracts the factor  $n$ ), Eq. (15) corresponds to the expression for the T-operator for the scattering of particles by a potential of zero radius. This is explained by the fact that an infinitely heavy defect represents a center of force for phonon scattering.

For small values of n and k the self-consistent Eq. (15) has a solution

$$
\Sigma(\omega + i0) = \omega^2 \left[ 1 + \frac{\pi^2}{24} n - \frac{\pi^2}{4} \left( \frac{k'}{k_D} \right)^2 \right] - i \frac{\pi^3 n k'}{k_D^2} \left[ 1 + \frac{n}{8} - \frac{\pi^2}{4} \left( \frac{k'}{k_D} \right)^2 \right],
$$
 (16)

where  $k' = (\omega^2 - \omega_{\star}^2)^{1/2}, \omega_{\star}^2 = 2\pi^2 n/k_D$ . Equation (16) is obtained by ignoring the fact that no pair of defects can occupy one and the same site. Correlation corrections of this type have been considered by many authors (see, for example, Refs. 19 and 20). In our case in the approximation of being quadratic in concentration these corrections to the self energy are determined by the diagrams

$$
\frac{1}{a} + \frac{1}{b} + \frac{1}{c} \qquad (17)
$$

Here the shaded circles correspond to the factor  $T(\omega+i0) = \Sigma(\omega+i0)/n$  [see Eq. (16)], the double line is the Green's function ( 13) with the self energy of Eq. ( 16) and the wavy line is the factor  $(-\delta_{ab})$ . On calculating these diagrams to the same accuracy as in Eq. ( 16) we obtain

$$
\Sigma^{\rm c}(\omega+i0) = \omega^2 \frac{n}{3\pi^2} - i \frac{\pi^3 n k'}{k_B^2} \frac{n}{2\pi^2}.
$$
 (18)

Like expression (16)  $\Sigma^{c}$  ( $\omega + i$  0) is independent of momentum.

We now go over to the evaluation of the interference corrections to the self energy, quadratic in concentration, determined by the diagrams

$$
+\frac{1}{2}
$$

[the symbols are the same as in the diagrams  $(17)$ ]. In degenerate electron systems these diagrams are small" because of the existence of the Fermi surface. The necessity of taking account of diagrams of the type of (19) in the lowdensity electron gas (Boltzmann statistics) has been pointed out by Iakubov and Polischuk.<sup>21</sup>

Summing separately in ( 19) the diagrams with an even and odd number of vertices, we obtain

$$
\Sigma_{p}{}^{i}(\omega+i0) := n^{2} \sum_{m=0}^{\infty} T^{i+2,n}(\omega+i0) \sum_{\mathbf{R}\neq 0} G_{R}^{3+2m}(\omega+i0) e^{i\mathbf{p}\mathbf{R}}
$$

$$
+ n^{2} \sum_{m=0}^{\infty} T^{5+2m}(\omega+i0) \sum_{\mathbf{R}\neq 0} G_{R}^{i+2m}(\omega+i0). \quad (20)
$$

We will evaluate the corrections of Eq. (20) bearing in mind that the value of  $\Sigma_p^i(\omega + i\,0)$  for  $p = k' \gg n$  enters into the thermal conductivity. It is convenient to carry out the summation in Eq.  $(20)$  separately for small and large **R** [in the sense of the inequality of Eq.  $(13)$ , where for large **R** it is convenient to use the following expression from Eqs. ( 13) and (16) ion in Eq. (20) separately for small and large **R** [in the <br> *e* of the inequality of Eq. (13)], where for large **R** it is<br>
venient to use the following expression from Eqs. (13)<br>
(16)<br>  $G_R(\omega+i0) = -\frac{1}{4\pi^2 R} e^{ik'R} e^{-R/2l}$ 

$$
G_R(\omega + i0) = -\frac{1}{4\pi^2 R} e^{ik'R} e^{-R/2l}.
$$
 (21)

We note that in Eq. (21) the phonon mean free path  $l = k_D^2 / \pi^3 n$  is independent of frequency. We give the final expression, corresponding to diagrams (19) for  $k'l \ge 1$ :

$$
\Sigma^{t}(\omega + i0) = \omega^{2} \left[ n\Delta' + \frac{1}{2} \pi^{4} n k_{D}^{3} \ln(k'R^{4}) + \ln 8 + C - 1 - \ln\left( 1 + \frac{\pi}{2k_{D}R^{4}} \right) \right] - i \frac{\pi^{3} n k'}{k_{D}^{2}} \left( n\Gamma' + \frac{\pi^{4}}{2k_{D}^{2}} \frac{n}{k'} \right);
$$
 (22)

here  $R^*$  is a parameter satisfying the condition  $k_D^{-1}$  $\ll R^* \ll (k')^{-1}$  [for  $R \approx R^*$  the Green's function  $G_R$  ( $\omega + i$  0) is equally well described by any of the representations  $(13)$ ];

$$
\Delta' = \sum_{n \leq R^*} \gamma_n (1 - \gamma_n)^{-1} k_D^{-3},
$$
  

$$
\Gamma' = \sum_{n \leq R^*} \gamma_n^2 (3 - 3\gamma_n^2 - 2\gamma_n) (1 + \gamma_n)^{-1} k_D^{-3}, \quad \gamma_n = \text{Si}(k_D R) / R,
$$

Cis the Euler constant.

For such concentration *n* that  $|nln(k'R^*)| \le 1$  and  $(k')^3 \le n \le k'$ , the nonlinear terms in the real part of expressions (16), (18) and (22) can be neglected. Taking account of these inequalities, which contain the main nonlinear correction to the total imaginary part of the self energy, we obtain

$$
\Gamma_{k} \cdot (\omega + i0) = \frac{\pi^3 n k'}{k_B^2} \left( 1 + \frac{\pi^4}{2k_B^2} \frac{n}{k'} \right).
$$
 (23)

The following expression is thus obtained for the Green's function  $(12)$ :

$$
G_p(\omega + i0) = [k'^2 - p^2 + i\Gamma_p(\omega + i0)]^{-1},
$$
\n(24)

and for  $p = k'$ ,  $\Gamma_p(\omega + i 0)$  is given by Eq. (23).

With the help of Eq. (13) we obtain an expression for the density of states:

$$
g(\omega) = -\frac{2}{\pi} \omega \operatorname{Im} G_{R=0}(\omega + i0) = \frac{\omega}{2\pi} \operatorname{Re}[\omega^2 - \Sigma(\omega + i0)]^{n}.
$$
\n(25)

It follows from Eq. (25), in accord with Shklovskii and Efros,<sup>11</sup> that a range  $\omega < \omega_*$  exists within which the density of states goes to zero if  $\omega_0 < \omega_*$ . As regards the heat capacity, taking the acoustic part of the spectrum ( $\omega < \omega_0$ ) into account, it increases with increase in temperature according to a  $T^3$  law ( $T < \omega_0$ ), later reaches a plateau ( $\omega_0 < T < \omega_*$ ) and then again increases as  $T^3$  ( $T > \omega_*$ ). It can be shown that the corrections to the density of states and to the heat capacity associated with the non-linear terms in the self energy, Eqs. (16), (18) and (22) are small ( $\sim n^2$ ) and in the sense the defects behave as isolated defects.

# **4. TWO-PHONON GREEN'S FUNCTION**

The diagram technique described above is genealized directly for evaluating the functions of Eq. (9). It can be shown (in a way similar to that used, for example, by Neal<sup>22</sup>) that these functions satisfy the integral equations

$$
K_p^{\pm \pm} (\omega) = G_p(\omega \pm i0) G_p(\omega \pm i0)
$$
  
\n
$$
\times \left[ -p^2 + p \int dq \, w_{pq}^{\pm \pm} (\omega) q K_{qq}^{\pm \pm} (\omega) \right],
$$
\n(26)

 $\mathsf{x}\left(-p^2+p\int\limits_{0}^{p^2}dq\,w^{\frac{1}{pq}}_{pq}(\omega)qK^{\frac{1}{pq}}_{qq}(\omega)\right],$  (26)<br>and the function  $w^{\pm}_{pq}(\omega)$  is expressed through the irreduand the function  $w_{pq}^{\pm} = (\omega)$  is expressed through the irredu-<br>cible vertex  $W^{\pm} = (\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3, \mathbf{p}_4, \omega)$  with the help of the rela*tion* 

$$
w_{pq}^{\pm\pm}(\omega) = \int W^{\pm\pm}(-\mathbf{p}, \mathbf{q}, -\mathbf{q}, \mathbf{p}, \omega) \cos p\hat{\mathbf{q}} \, d\Omega_{\hat{\mathbf{p}}\hat{\mathbf{q}}}.
$$
 (27)

The method of solving Eq. (24) for  $K_p^+$ <sup>-</sup> ( $\omega$ ) is well known *(see, for example, Refs. 22-24). We give below, omitting the details of the calculation, the final result:* 

$$
K_p^{+-}(\omega)
$$
  
=  $G_p(\omega + i0) G_p(\omega - i0) \left[ -p^2 - pk' \frac{\Gamma_p'(\omega)}{\Gamma_{k'}(\omega) - \Gamma_{k'}(\omega)} \right],$   
(28)  
with  

$$
\Gamma_p'(\omega) = \frac{\Gamma_{k'}(\omega)}{k'} \int_0^{k_p} dq q^3 w_{pq}^{+-} (\omega) G_q(\omega + i0) G_q(\omega - i0).
$$
 (29)

*with* 

$$
\Gamma_p'(\omega) = \frac{\Gamma_{k'}(\omega)}{k'} \int_0^{k_p} dq \, q^3 w_{pq}^{+-}(\omega) G_q(\omega + i0) G_q(\omega - i0). \quad (29)
$$

*To the same accuracy with which the solution (28) and (29)*  was obtained, the integral term in Eq. (26) for  $K^{++}$  and  $K^{--}$ , small in the parameter *n*, can be omitted.

*In this way the problem reduces to the determination of*   $\omega_{pq}^{+}$  <sup>-</sup> ( $\omega$ ).

In the approximation quadratic in concentration the *vertex in which we are interested is determined by the diagrams* 

$$
W^{+-}(-p, q, -q, p, \omega)
$$
\n
$$
= \int_{\rho-\frac{c}{2}}^{\rho-\rho} + \sum_{\substack{-(\alpha-\frac{1}{2})^2 + \cdots + (-\alpha-\frac{1}{2})^2 + \cdots + (-\alpha-\frac{1}{2
$$

*In a similar way to diagram* ( *19), when evaluating (30)*  the leading contribution comes from the region  $R \ge (k')^{-1}$ *and then the two latter diagrams in the case which interests us,*  $p = q = k'$ *, exactly cancel one another, while the first gives zero after carrying out the integration in Eq. (25). Evaluating the fan-shaped diagram in (30), we obtain* 

$$
W^{+-}(-\mathbf{p}, \mathbf{q}, -\mathbf{q}, \mathbf{p}, \omega) = \frac{2n^2 \pi^8}{k_b} \frac{1}{|\mathbf{p} + \mathbf{q}|}.
$$
 (31)

We note that Eq. (31) indicates a large value for the back*scattering probability. Substituting Eq. (31) into Eq. (27) we obtain* 

$$
w_{pq}^{+-}(\omega) = -n^2 \pi^6 / 3k' k_p^4. \tag{32}
$$

*From Eqs. (23), (29) and (32) we obtain the following*  expressions for the magnitude of  $\Gamma'_p(\omega)$  and the "transport" *damping*  $\Gamma^{\text{tr}}(\omega) = \Gamma_{k}(\omega) - \Gamma'_{k}(\omega)$ :

$$
\Gamma_{k'}(\omega) = -\frac{n^2 \pi^7}{6 k_b^3}, \qquad \Gamma^{tr}(\omega) = \frac{\pi^3 n k'}{k_b^2} \left( 1 + \frac{2}{3} \frac{\pi^4}{k_b^2} \frac{n}{k'} \right).
$$
\n(33)

*It can be seen that in order of magnitude the contribution* 

*from the vertex to the correction is the same as from taking account of interference effects in the Green's function (24).* 

## **5. DISCUSSION OFTHE RESULTS**

*The results obtained allow us to carry out an exact inte*gration over momentum inEq. (18). Since for  $p \rightarrow \infty$ ,  $\omega_{pq}^{\pm}$  <sup> $\pm$ </sup> ( $\omega$ )  $\rightarrow$  0,  $\Gamma_{p}(\omega)$   $\rightarrow$  const while the quantity

$$
K_p{}^{+ -}(\omega) - \frac{1}{2}K_p{}^{+ +}(\omega) - \frac{1}{2}K_p{}^{ -}(\omega) \rightarrow 2\Gamma_p{}^2(\omega) p^{-6},
$$

*integration over p can then tend to infinity. As a result, we obtain for the thermal conductivity in the case when phonon scattering by impurities is dominant,* 

$$
\varkappa = \frac{\beta}{2\pi^5} \int\limits_{0}^{\omega_D} d\omega \bigg( -\frac{\partial f(\omega)}{\partial \omega} \bigg) \omega^2 (\omega^2 - \omega^2)^{\frac{n}{2}} [\Gamma^{\text{tr}}(\omega)]^{-1}, \quad (34)
$$

where  $\Gamma^{\text{tr}}(\omega)$  is determined by Eq. (33).

Since for  $\omega < \omega_*$  the Green's function  $K^{+-}$ ,  $K^{++}$  and  $K^{--}$  are real and coincide, the integration in Eq. (34) starts from  $\omega_*$  (this is indirectly connected with the density of states going to zero for  $\omega < \omega_*$ ).

It follows from Eq. (34) that for  $T \gtrsim \omega_D$ ,  $\chi$  is indepen*dent of T. However, in this temperature region scattering of phonons by one another becomes appreciable and the total*  conductivity  $x^{-1} \sim T$ . In the temperature region  $\omega_*$  $\langle T \langle \omega_D, \rangle$  in the absence of interference effects, the thermal conductivity of Eq. (34)  $x \sim T^3$ . We note that such a tem*perature dependence holds when the scattering of phonons by the boundaries of the specimen is dominant. This is con*nected with the fact that for  $T \gg \omega_0$  phonons are scattered by *defects as by immobile centers*  $(M \to \infty)$ *. If*  $\omega_0 < T < \omega_*$  *the thermal conductivity, determined by phonons with*  $\omega > \omega_*$ *, falls exponentially as*  $exp(-\omega_x/T)$  *and becomes an essentially constant contribution to the thermal conductivity associated with heat transport by acoustic phonons with*   $\omega < \omega_0$ . For  $T < \omega_0$  Eq. (34) is unjustified. In this region heat *is transported by acoustic phonons which undergo Rayleigh scattering* ( $\tau^{-1} \sim \omega^4$ ) and correspondingly <sup>14</sup>  $\chi \sim T^{-1}$ .

*We now pass to a consideration of the interference correction. It follows from Eqs. (33) and (34) that the relative contribution of this correction to the thermal conductivity*  for  $\omega_* \ll T \ll \omega_D$  is equal to

$$
\Delta \mathbf{x}/\mathbf{x} \approx -0.5(\lambda_{\mathbf{r}}/l),\tag{35}
$$

where  $\lambda_T = (\hbar/T)$  is the thermal phonon wavelength and *l is the phonon mean free path (see §3).* We note that the *correction in Eq. (35) is the main one and is due to inteference effects (the others, associated for example, with correlations in the position of the defects, are small in the parameter*  $T/\omega_D$ *).* We also point out the quantum nature of this *correction [the explicit dependence of Eq.* ( *35* ) *on fi]* . *As for electrical conductivity, the interference scattering of phonons by defects leads to a reduction in thermal conductivity, associated with the increase in the probability of back scattering."* 

*We note that in the limit of very low temperatures (unlike electrons) the interference correction to the thermal conductivity is insignificant, since heat is transported by phonons which undergo weak Rayleigh scattering for which the probability of back scattering is vanishing small.* 

*The authors thank* **A.** *Ya. Polishchuk for many valuable discussions.* 

- <sup>1</sup>S. Kelham and H. M. Rosenberg, J. Phys. C 14, 1737 (1982).
- $^{2}D$ . E. Farrell, J. E. de Oliveira, and H. M. Rosenberg, Phonon Scattering in Condensed Matter (W. Eisenmenger, K. Lassmann and S. Dottinger eds.), Springer, Berlin (1984), p. 422.
- 'S. Alexander and R. Orbach, J. Phys. (Paris) Lett. **43,** L625 (1982).
- 'S. Alexander, C. Laermans, R. Orbach, and H. M. Rosenberg, Phys. Rev. B28,4615 (1983).
- 50. Entin-Wohlman, S. Alexander, R. Orbach, and Kin-Wah Yu, Phys. Rev. B29,4588 (1984).
- <sup>6</sup>B. Derrida, R. Orbach, and Kin-Wah Yu, Phys. Rev. B29, 6645 (1984).
- 'I. M. Lifshitz, Nuovo Cimento Suppl. **3,** 719 ( 1956).
- <sup>8</sup>Yu. M. Kagan, Materials of the school on the theory of defects in crystals, Institute of Physics of the Georgian SSR Press, Tbilisi 1969, p. 93. "B. L. Altshuler, A. G. Aronov, D. E. Khmelnitskii, and A. I. Larkin,
- Quantum Theory of Solids (I. M. Lifshitz, ed.), Mir, M., 1983, p. 130.
- <sup>10</sup>A. M. Kosevich, Physical Mechanics of Real Crystals, [in Russian] Naukova dumka, Kiev 1981.
- <sup>11</sup>B. I. Shklovshii and A. L. Éfros, Electronic Properties of Doped Semiconductors [in Russian] Nauka, M., 1979.
- <sup>12</sup>D. N. Zubarev, Nonequilibrium Statistical Thermodynamics, Consultants Bureau, New York (1974).
- 'C. P. Enz, Ann. Phys. (Leipzig) **46,** 114 (1966)
- <sup>14</sup>E. M. Lifshitz and L. P. Pitaevskii, Physical Kinetics, Pergamon Press, Oxford (1981).
- <sup>15</sup>v. I. Perel' and G. M. Eliashberg, Zh. Eksp. Teor. Fiz. 41, 886 (1962) [Sov. Phys. JETP **14**, 633 (1962)].
- <sup>16</sup>J. K. Flicker and P. L. Leath, Phys. Rev. B7, 2296 (1973).
- <sup>17</sup>A. A. Abrikosov, L. P. Gor'kov, and I. E. Dzyaloshinskii, Quantum Field-Theoretical in Statistical Physic\, Prentice-Hall Englewood Cliffs, N. J. (1963).
- <sup>18</sup>A. I. Baz, Ya. B. Zel'dovich, and A. M. Perelomov, Scattering, Reactions, and Decay in Nonrelativistic Quantum Mechanics, Wiley, New York ( 1969).
- "R. J. Elliot and D. W. Taylor, Proc. R. Soc. London **A296.** 161 ( 1967).
- <sup>20</sup>F. Yonezawa, Prog. Theor. Phys. **40**, 734 (1968).
- <sup>21</sup>I. T. Iakubov and A. Ya. Polischuk, J. Phys. **B15**, 4029 (1982).
- <sup>22</sup>T. Neal, Phys. Rev. 169, 508 (1968).
- <sup>23</sup>A. A. Abrikosov and L. P. Gor'kov, Zh. Eksp. Teor. 35, 1588 (1958) [Sov. Phys. JETP 8, 1090 (1959)].
- <sup>24</sup>T. S. Langer, Phys. Rev. 120, 714 (1960).

Translated by R. Berman