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Lattice Thermal Resistivity due to the Phonon Scattering by Imperfection in Two-Dimensions
−Effect of the Localization of Phonons−

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同位元素のように質量の異なるイオンを不純物として含んだ2次元格子系において，フォノンの固有関数の局在性について理論的に調べ，その前駆現象の熱伝導度への影響を計算した。

用いた方法は次のようである：2粒子グリーン関数の充たす方程式を変形してフォノンの分布関数に対する運動学的方程式を微視的に導き，その衝突項の表式を不純物濃度についての巾級数に展開し，展開の2次まで具体的に計算する。その結果，衝突項は長波長，低振動数極限において，振動数依存性のある緩和時間，$\tau(k\omega) = \tau_0(k)(1+(\omega\tau_0(k))^{-1}\ln(\omega\tau_0(k)^{-1})^{-1}$，の形で表わされることがわかった。ただし$\tau_0(k)$は通常のレーリー散乱型のフォノンの緩和時間で，2次元では，k^{-3}に比例している。カッコ内の第2項がフォノン局在の前駆現象を表わす(と考えられる)。このときディスプレイスメントについての非線型効果は無視した。

次に，このようにして求めた運動学的方程式を用いて，フォノン局在の(前駆現象の)熱伝導への効果を計算した。結果は，$\kappa = (A/T)\cdot(1+BT^2\ln T)$の形に表わされる。ここで$T$は温度，$A$，$B$は定数である。この$\kappa$の表式を求める際には，先の非線型効果を，考慮に入れた。これは，この効果を入れないで不純物散乱だけでフォノンによる熱伝導を計算すると，κが発散してしまう，というよく知られた困難を避けるためである。

ところが一方，このようにフォノン・不純物とフォノン・フォノン散乱の両方を計算の中に取り入れると，2つの効果の入りまじった効果の中に，(問題になっているκの補正項が上のように表わされる温度領域で)上記の補正項より大きな項が出てくる。このため，現実に実験で上記のκの補正項を見出すのはかなり困難なことと思われる。この辺りの事情は電子系の場合と異なるところであるが，詳細は本文を参照して下さい。

§1. Introduction

In this paper, we consider the vibration of crystal lattice containing impurity atoms in two dimensions (d=2). As we shall see shortly, we can expect that in this system all of the normal mode of the vibrations are localized, except for those the wave-lengths of which are of order L(L: the system size). Our purpose is then to calculate the effect of such localizations on the lattice thermal conductivity.

We now present the reason why those normal modes will be localized in the system. For this we recapitulate the argument in Ref. 1), in which it is shown that the excitation of lattice wave and electronic excitation have many mathematical features in common. Let us first consider the vibration of the lattice. Suppose that the system has a configuration of minimum potential energy in which the i-th atom would be at $\boldsymbol{R}_{i0}$. And we assume that a small displacement $\boldsymbol{x}_i$ of the atom are subject to restoring force that are linear in the relative displacement of nearly atoms. Then the equation of motion for these displacement takes the form,

$$\sum_{\beta}(\lambda_i^{\alpha\beta}-\lambda\delta_{\alpha\beta})\,\tilde{x}_i^{\beta}+\sum_{\beta}\sum_{j\neq i}\xi_{ij}^{\alpha\beta}\,\tilde{x}_j^{\beta}=0, \tag{1·1}$$

where

$$\lambda_i^{\alpha\beta}=\phi_{ii}^{\alpha\beta}/m_i, \quad \xi_{ij}^{\alpha\beta}=\phi_{ij}^{\alpha\beta}/\sqrt{m_i m_j}, \quad \lambda=\omega^2$$

and $\tilde{\boldsymbol{x}}_i=\sqrt{m_i}\boldsymbol{x}_i$ with m_i being the mass of the atom, $\phi_{ij}^{\alpha\beta}$ measuring the forces produced at the site $\boldsymbol{R}_{i0}$ by displacement of the atom at $\boldsymbol{R}_{j0}$, and ω being the frequency of the normal mode. When the system contains impurity atoms, m_i depends on i at random, and $\lambda_i^{\alpha\beta}$ and $\xi_{ij}^{\alpha\beta}$ become random variables. Next, consider the tight-binding model for the electron states of a condensed system, in which the wavefunction for one electron is approximated as $\Psi(\boldsymbol{r})=\sum_{i\alpha}\tilde{x}^{\alpha}\,\psi_i^{\alpha}(\boldsymbol{r}-\boldsymbol{R}_{i0})$; $\psi_i^{\alpha}(\boldsymbol{r})$ are the atomic orbitals corresponding to the atomic levels E_i^{α} at site i. Then the amplitude $\tilde{x}_i^{\alpha}$ again satisfy Eq. (1.1) with $\lambda_i^{\alpha\beta}$ being interpreted as $E_i^{\alpha}\delta_{\alpha\beta}$, $\xi_{ij}^{\alpha\beta}$ as the overlap integrals and λ as the energy of an electron eigenstate of the Hamiltonian of the whole system. The $\lambda_i^{\alpha\beta}$ and $\xi_{ij}^{\alpha\beta}$ thus defined also become random variables when the electron system contains various kinds of imperfections. Then, both problems of the excitation of lattice wave and the electronic excitation are mathematically equivalent: diagonalizing the random matrix, $\lambda_i^{\alpha\beta}\,\delta_{ij}+\xi_{ij}^{\alpha\beta}$. There is of course a subtle difference between them: $\lambda_i^{\alpha\beta}=0$ $(\alpha\neq\beta)$ for the electron system,

but $\lambda_i^{\alpha\beta} \neq 0$ $(\alpha \neq \beta)$ for the lattice vibration one.

These arguments are essentially given in Ref. 1). On the other hand, according to the recent theories on the Anderson localization for independent electrons subject to random fields, all of the eigenfunctions of the electrons are localized in d=2 no matter how the magnitude of the random field is small. [2~4] Moreover it is believed that this conclusion does not depend on microscopic details of the random field*). Thus we can consider that all of the normal modes of the lattice vibrations which satisfy Eq. (1.1) are also localized, neglecting the subtle difference in the matrix elements $\lambda_i^{\alpha\beta}$ mentioned previously.

We now notice a special feature in the lattice vibration problem; that is, the long wavelength plane waves are not influenced by the imperfections contained in the lattice, and remain being the normal modes even in the system considered here. This is because a plane wave with the wavelength k is scattered by a imperfection with the cross section $\sigma \sim k^3$ (Rayleigh's law in d=2) and σ is vanishingly small for the waves with $k \sim 1/L$. We can understand this from Eq. (1.1), too. Indeed, multiplying m_i on both sides of Eq. (1.1), we see that m_i being the origin of the disorder in Eq. (1.1) apears in the equation together with ω^2. If we now suppose that the plane wave with $k \sim 1/L$ is normal mode, ω should be replaced by ck. Then, for the wave with $k \sim 1/L$, the disorder arising from the imperfection in m_i vanishes in the equation to determine the behavior of the normal modes; this consistently assures the previous assumption, the plane wave with $k \sim 1/L$ being the normal mode of the system.

In this way, all of the normal modes in two-dimensional lattice containing the impurity atoms, are expected to be localized, except for the plane waves with $k \sim 1/L$ (from now on we call these the localization of the phonons, too).

The organization of this paper is as follows: in §2 we give the Hamiltonian treated in this paper. In §3, using linear response theory, we study the distribution function of phonon, $f_{\boldsymbol{p}\lambda}(\boldsymbol{k}\omega)$, under temperature gradient, and express it in terms of response functions. In §4, the response functions are investigated to evaluate a correction to the relaxation time of $f_{\boldsymbol{p}\lambda}(\boldsymbol{k}\omega)$ and obtain a term proportional to $\ln\omega$. In §5, using the kinetic equation, we calculate the lattice thermal conductivity. Then we take account of terms due to phonon-phonon interaction. In §6, we give discussions on the result.

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*) In fact the arguments in Ref. 3) do not make use of any special properties of the random field, other than the characteristic length of the variations of the field being far smaller than L.

§2. Hamiltonian

We consider a two-dimensional lattice, which posseses N atoms, of equilibrium position $\boldsymbol{R}_{i0}$ and a particle interaction specified by $V(\boldsymbol{R}_i - \boldsymbol{R}_j)$. The system Hamiltonian is then given by

$$H=\sum_i \frac{\boldsymbol{P}_i^2}{2m_i} + \sum_{i\neq j}\frac{1}{2}V(\boldsymbol{R}_i-\boldsymbol{R}_j). \tag{2·1}$$

We suppose the system has perfect isotropic disorder, where the masses m_i are not the same on every equivalent lattice site. For simplicity we use the binary alloy model, where A- and B-type atoms, of masses m_A and m_B, are distributed at random on a regular lattice.

Denoting m_A by m and m_B by $m+\delta m$, we separate H to free phonon Hamiltonian H_0 and interaction Hamiltonian H' for phonon-impurity scattering. We now expand the potential V in a power series in the small displacement δR_i denoting $R_i - R_{i0}$ and introduce the normal modes,

$$\delta R_i^\alpha = \frac{1}{\sqrt{Nm}}\sum_{\boldsymbol{p}\lambda} q_{\boldsymbol{p}\lambda}\varepsilon^\alpha_{\boldsymbol{p}\lambda}\, e^{i\boldsymbol{p}\cdot\boldsymbol{R}_{i0}}, \tag{2·2}$$

$$P_i^\alpha = \sqrt{\frac{m}{N}}\sum_{\boldsymbol{p}\lambda} p_{\boldsymbol{p}\lambda}\,\varepsilon^\alpha_{\boldsymbol{p}\lambda}\, e^{i\boldsymbol{p}\cdot\boldsymbol{R}_{i0}}, \tag{2·3}$$

to obtain

$$H = H_0 + H', \tag{2·4}$$

$$H_0 = \frac{1}{2}\sum_{\boldsymbol{p}\lambda}(p_{\boldsymbol{p}\lambda}p_{-\boldsymbol{p}\lambda} + \omega_{\boldsymbol{p}\lambda}^2 q_{\boldsymbol{p}\lambda}q_{-\boldsymbol{p}\lambda}), \tag{2·5}$$

$$H' = \frac{1}{2N}\sum_a\sum_{\boldsymbol{p}'\lambda'}\sum_{\boldsymbol{p}''\lambda''} u_{\boldsymbol{p}'\lambda',\boldsymbol{p}''\lambda''} p_{\boldsymbol{p}'\lambda'}p_{\boldsymbol{p}''\lambda''}\, e^{-i(\boldsymbol{p}'+\boldsymbol{p}'')\cdot\boldsymbol{R}_{a0}}, \tag{2·6}$$

where $\varepsilon_{\boldsymbol{p}\lambda}$ is a unit polarization vector with λ=1,2 indicating longitudinal and transverse components, and we suppose $\omega_{\boldsymbol{p}\lambda} = c_\lambda p$, since we consider only temperature much lower than Debye temperature; in Eq. (2.6), $\sum_a$ indicates the summation over the impurity sites, i.e. the sites of B-type atom, and $u_{\boldsymbol{p}'\lambda',\boldsymbol{p}''\lambda''} = -(\delta m/m)\cdot(\varepsilon_{\boldsymbol{p}'\lambda'}\cdot\varepsilon_{\boldsymbol{p}''\lambda''})$. We suppose of course the commutation relations such as $[p_{\boldsymbol{p}\lambda}, q_{\boldsymbol{p}'\lambda'}] = -i\delta_{\lambda\lambda'}\delta_{\boldsymbol{p}+\boldsymbol{p}'}$ hold everywhere.

§3. Distribution function of phonons under temperature gradient

Let us now consider the distribution function of phonons $f_{p\lambda}(k, \omega)$ under temperature gradient; by making use of linear response theory, we express $f_{p\lambda}(k, \omega)$ in term of a response function.

We assume temperature varies slowly both spatially and temporally, and there is a well-defined temperature $T(r, t)$ at each point and each time. Then we suppose the density matrix at time t to be as follows:*)

$$\rho(t) = \exp[-\beta\{H + \sum_i \delta\bar{\beta}_i(t) H_i\}] , \tag{3·1}$$

where $\delta\bar{\beta}_i(t) = (\beta_i(t) - \beta)/\beta << 1$, and H_i is the energy "density" at i-site.

Using familiar technique of linear response theory, we find, for the distribution function of phonons,

$$\begin{aligned} f_{\boldsymbol{p}\lambda}(\boldsymbol{k}, \omega) &= \int_{-\infty}^{\infty} dt \{ \mathrm{tr}(\rho(t) F_{\boldsymbol{p}\lambda}(\boldsymbol{k})) - \mathrm{tr}(\rho_c F_{\boldsymbol{p}\lambda}(\boldsymbol{k})) \} e^{-i\omega t} \\ &= -\frac{1}{N} \sum_{\alpha} \int_{-\infty}^{\infty} dt (e^{-i\omega t} - 1) i\theta(t) < [F_{\boldsymbol{p}\lambda}(\boldsymbol{k}, t), j_{\alpha}^{\varepsilon}(-\boldsymbol{k})] > V_{-\boldsymbol{k}}^{\alpha}(\omega), \end{aligned} \tag{3·2}$$

where $F_{p\lambda}(k) = a^{+}_{p-k/2,\lambda} a_{p+k/2,\lambda}$ with $a_{p\lambda} = \sqrt{\omega_{p\lambda}/2}\,(q_{p\lambda} + i p_{p\lambda}/\omega_{p\lambda})$ and $a^{+}_{p\lambda} = \sqrt{\omega_{p\lambda}/2}\,(q_{-p\lambda} - i p_{-p\lambda}/\omega_{p\lambda})$, ρ_c is the density matrix of the equilibrium, and $j^{\varepsilon}_{\alpha}(-\boldsymbol{k})$ is the Fourier component of the energy current density as

$$j_{\alpha}^{\varepsilon}(-\boldsymbol{k}) = -i \sum_{\boldsymbol{p}\lambda} (c_{\lambda}^2 p^{\alpha} q_{\boldsymbol{p}\lambda} p_{\boldsymbol{k}-\boldsymbol{p},\lambda} + \sum_{\beta=1,2} a_{\lambda\bar{\lambda}}^{\alpha\beta}(\boldsymbol{p}) p^{\beta} q_{\boldsymbol{p}\lambda} p_{\boldsymbol{k}-\boldsymbol{p},\bar{\lambda}}), \tag{3·3}^{**)}$$

with

$$a_{\lambda\bar{\lambda}}^{\alpha\beta}(\boldsymbol{p}) = m^{-1} \sum_{j} R_{j_0}^{\alpha} R_{j_0}^{\beta} \varepsilon_{\boldsymbol{p}\lambda}^{\gamma} \varepsilon_{\boldsymbol{p}\bar{\lambda}}^{\delta} \nabla_{\gamma} \nabla_{\delta} V(\boldsymbol{R}_{j_0}),$$

and $\bar{\lambda}$ representing the polarization index different from λ ($\bar{\lambda}=2$ for $\lambda=1$ and vice versa); furthermore

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*) Temperatures are expressed in energy units ($k_B = 1$), so that β means $1/T$. For simplicity we treat in this paper $\sum_i \delta\bar{\beta}_i(t) H_i$ as if it were the dynamical external field. In fact, the expectation values of macroscopic variables given by Eq. (3.1) agree with those by more sophisticated arguments (e.g. see §2.12 of Ref. 6), if the temperature varies slowly.

**) The quantity $j_{\alpha}^{\varepsilon}(k)$ is defined through the equation $\partial H_k/\partial t = -ik^{\alpha} j_{\alpha}^{\varepsilon}(k)$ with $H_k = \sum_i H_i \exp(-ik \cdot R_{i0})$.

$$V^{\alpha}_{-\boldsymbol{k}}(\omega) = \frac{\boldsymbol{k}^{\alpha}\delta\beta_{-\boldsymbol{k}}(\omega)}{\omega} \tag{3·4}$$

For simplicity we calculate $f_{\boldsymbol{p}\lambda}(\boldsymbol{k}, \omega)$ only up to order $O(k)$, assuming $k\to 0$. We can then put $k=0$ in the expectation value $<\cdots\cdots>$ on the right hand side of Eq. (3.2) since external field $V^{\alpha}_{-\boldsymbol{k}}$ is already proportional to k^{α}. Let us substitute Eq. (3.3) into Eq. (3.2), and rewrite $a_{\boldsymbol{p}}$ and $a^{+}_{\boldsymbol{p}}$ in terms of $p_{\boldsymbol{p}}$ and $q_{\boldsymbol{p}}$. Then Eq. (3.2) leads to

$$f_{\boldsymbol{p}\lambda}(\boldsymbol{k}, \omega) = -\frac{1}{N}\sum_{\boldsymbol{p}'\lambda'}\{(K^{R}_{\boldsymbol{p}\lambda,\boldsymbol{p}'\lambda'}(\omega) - K^{R}_{\boldsymbol{p}\lambda,\boldsymbol{p}'\lambda'}(0))V_{\boldsymbol{p}'\lambda'}(\boldsymbol{k}, \omega)$$

$$+ (K'^{R}_{\boldsymbol{p}\lambda,\boldsymbol{p}'\lambda'}(\omega) - K'^{R}_{\boldsymbol{p}\lambda,\boldsymbol{p}'\lambda'}(0))V'_{\boldsymbol{p}'\lambda'}(\boldsymbol{k}, \omega)\}, \tag{3·5}$$

where

$$K^{R}_{\boldsymbol{p}\lambda,\boldsymbol{p}'\lambda'}(t) = \mathrm{i}\theta(t)<[q_{-\boldsymbol{p}\lambda}(t)p_{\boldsymbol{p}\lambda}(t), q_{\boldsymbol{p}'\lambda'}p_{-\boldsymbol{p}'\lambda'}]>, \tag{3·6}$$

$$K'^{R}_{\boldsymbol{p}\lambda,\boldsymbol{p}'\lambda'}(t) = \mathrm{i}\theta(t)<[q_{-\boldsymbol{p}\lambda}(t)p_{\boldsymbol{p}\lambda}(t), q_{\boldsymbol{p}'\lambda'}p_{-\boldsymbol{p}'\bar{\lambda}'}]>, \tag{3·7}$$

and

$$V_{\boldsymbol{p}\lambda}(\boldsymbol{k}, \omega) = \sum_{\alpha} c^{2}_{\lambda}p^{\alpha}V^{\alpha}_{\boldsymbol{k}}(\omega), \tag{3·8}$$

$$V'_{\boldsymbol{p}\lambda}(\boldsymbol{k}, \omega) = \sum_{\alpha} a^{\alpha\beta}_{\lambda\bar{\lambda}}p^{\beta}V^{\alpha}_{\boldsymbol{k}}(\omega). \tag{3·9}$$

§4. Genelarized Boltzmann equation

Two-particle temperature Green's function

From Eq. (3.5) we now derive a genelarized Boltzmann equation for $f_{\boldsymbol{p}\lambda}(\boldsymbol{k}, \omega)$. To do this, let us consider the two-particle temperature Green's function,

$$\mathcal{H}_{\boldsymbol{p}\lambda,\boldsymbol{p}'\lambda'}(\tau) = <T(q_{-\boldsymbol{p}\lambda}(\tau)p_{\boldsymbol{p}\lambda}(\tau), q_{\boldsymbol{p}'\lambda'}p_{-\boldsymbol{p}'\lambda'})>. \tag{4·1}$$

As is well known, the retarded function $K^{R}_{\boldsymbol{p}\lambda,\boldsymbol{p}'\lambda'}(\omega)$ is obtained from $\mathcal{H}_{\boldsymbol{p}\lambda,\boldsymbol{p}'\lambda'}(\omega_m)$ by analytic continuation $\mathrm{i}\omega_m\to\omega+\mathrm{i}\delta$.

Let us now treat H' in Eq. (2.6) as a perturbation and expand $\mathcal{H}_{p\lambda,p'\lambda'}(\tau)$ in powers of $u_{p\lambda,p'\lambda'}$ in Eq. (2.6). After averaging over impurity configurations, the expansion parameter turn out to be a quantity such as $n_i u^2_{p\lambda,p'\lambda'}$, where $n_i = N_i/N$ with N_i being the number of B-atom; we of course consider the case $n_i u^2_{p\lambda,p'\lambda'} << 1$. On the other hand the imaginary part of the self-energy of the retarded phonon Green's function γ_λ is also proportional to n_i, as is shown in Eq. (A.4), so that γ_λ is another small parameter. For simplicity, we thus denote the order of magnitude of various terms appeared in the perturbation expansion by the power of γ_λ instead of $n_i u^2_{p\lambda,p'\lambda'}$, simply writing γ_λ as γ.

Then $\mathcal{H}_{p\lambda,p'\lambda'}(\tau)$ yields two kinds of contribution: $\mathcal{H}^a_{p\lambda,p'\lambda'}(\tau)$ and $\mathcal{H}^b_{p\lambda,p'\lambda'}(\tau)$ (see later). We find for $\mathcal{H}^a_{p\lambda,p'\lambda'}(\tau)$

$$\mathcal{I}^a_{p\lambda,\,p'\lambda'}(\omega_m) = T\sum_{\varepsilon_n}\{\delta_{p-p'}\mathcal{G}^{11}_{\lambda'\lambda}(p,\,\varepsilon_n)\mathcal{G}^{22}_{\lambda\lambda'}(p,\,\varepsilon_n+\omega_m)$$

$$+N^{-1}\mathcal{G}^{21}_{\mu\lambda}(p,\,\varepsilon_n)\mathcal{G}^{22}_{\lambda\nu}(p,\,\varepsilon_n+\omega_m)L^{\nu\mu,\,\nu'\mu'}_{pp'}(\omega_m;\,\varepsilon_n)\mathcal{G}^{12}_{\lambda'\mu'}(p',\,\varepsilon_n)\mathcal{G}^{22}_{\nu'\lambda'}(p',\varepsilon_n$$

$$+\omega_m)\} = T\sum_{\varepsilon_n}\tilde{\mathcal{I}}^a_{p\lambda,\,p'\lambda'}(\,i\varepsilon_n+i\omega_m,\,i\varepsilon_n)\,, \qquad (4\cdot2)$$

where the second equality defines the function $\tilde{\mathcal{H}}^a_{p\lambda,p'\lambda'}$ $(i\varepsilon_n+i\omega_m,\,i\varepsilon_n)$, and we provide the definition and the evaluation of the phonon Green's functions $\mathcal{G}^{\alpha\beta}_{\lambda'\lambda}(p,\,\varepsilon_n)$ in Appendix. Figure 1 shows the diagram for $K^a_{p\lambda,p'\lambda'}(\omega_m,\,\varepsilon_n)$. As is observed, K^a is the set of all contributions in which outer line (2λ) on the left hand side is connected by phonon lines to one $(2\lambda')$ on the right hand side, and similarly line (1λ) to one $(1\lambda')$. Together with $\mathcal{H}^a$ we will later take account of the contribution $\mathcal{H}^b$, in which outer lines on both hands are connected diagonally by phonon lines.

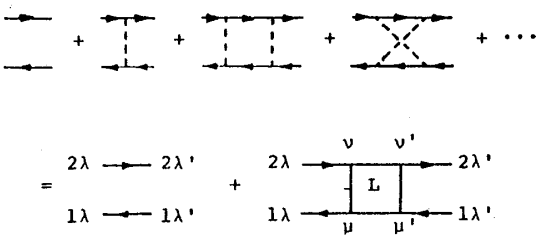

Fig. 1. Diagrams for $\mathcal{H}^a_{p\lambda,p\lambda'}(\omega_m,\varepsilon_n)$. The full lines refer to $\mathcal{G}^{\alpha\beta}_{\lambda\lambda'}(p,\varepsilon_n)$, where index 1 or 2 at the end of lines represent upper suffix α,β of $\mathcal{G}^{\alpha\beta}_{\lambda\lambda'}$; the dotted lines refer to quantities like $n_i u^2_{p\lambda,p'\lambda'}$. The arrows on the phonon lines are drawn in order to perform our calculations in the same way as that for particle system.

Equation for $\phi(\omega;p,\,\varepsilon)$

Let us now consider a analytic continuation of $\mathcal{H}^a_{p\lambda,p'\lambda'}(\omega_m)$ in upper half plane of ω

to obtain $K^{aR}_{p\lambda,\,p'\lambda'}(\omega)$. Then we have

$$K^{aR}_{\boldsymbol{p}\lambda,\,\boldsymbol{p}'\lambda'}(\omega)=\frac{1}{2\pi i}\int d\varepsilon\,\{(f^0(\varepsilon+\omega)-f^0(\varepsilon))\widetilde{\mathcal{K}}^{a}_{\boldsymbol{p}\lambda,\,\boldsymbol{p}'\lambda'}(\varepsilon+\omega+i\delta,\ \varepsilon-i\delta)$$

$$+f^0(\varepsilon)\widetilde{\mathcal{K}}^{a}_{\boldsymbol{p}\lambda,\,\boldsymbol{p}'\lambda'}(\varepsilon+\omega+i\delta,\ \varepsilon+i\delta)-f^0(\varepsilon+\omega)\widetilde{\mathcal{K}}^{a}_{\boldsymbol{p}\lambda,\,\boldsymbol{p}'\lambda'}(\varepsilon+\omega-i\delta,\ \varepsilon-i\delta)\},\tag{4·3}$$

where $f^0(\varepsilon)=1/[\exp(\beta\varepsilon)-1]$ and $\int d\varepsilon(\cdots)$ means principal value of the integration over ε; in the following, however, we abbreviate the sign indicating to take a principal value. As we shall see later, only first two terms on the right hand side of Eq. (4.3) contribute to the Boltzmann equation for $f_{\boldsymbol{p}\lambda}(\boldsymbol{k},\omega)$, so that in what follows the third and fourth terms are neglected.

We insert Eq. (4.2) into Eq. (4.3), then substitute Eq. (4.3) into Eq. (3.5), and take a limit $\omega\to0$, obtaining for such contribution to $f_{\boldsymbol{p}\lambda}$ that comes from K^a,

$$f^a_{\boldsymbol{p}\lambda}(\boldsymbol{k},\omega)=-N^{-1}\frac{\omega}{2\pi i}\int d\varepsilon\frac{\partial f^0}{\partial\varepsilon}\sum_{\lambda'}(G^{22,R}_{\lambda\lambda'}(\boldsymbol{p},\varepsilon+\omega)G^{11,A}_{\lambda'\lambda}(\boldsymbol{p},\varepsilon)V_{\boldsymbol{p}\lambda'}(\boldsymbol{k},\omega)$$

$$+G^{22,R}_{\lambda\upsilon}(\boldsymbol{p},\varepsilon+\omega)G^{21,A}_{\mu\lambda}(\boldsymbol{p},\varepsilon)\frac{1}{N}\sum_{\boldsymbol{p}'}L^{\upsilon\mu,\upsilon'\mu'}_{\boldsymbol{p}\boldsymbol{p}'}(\omega;\varepsilon)G^{22,R}_{\upsilon'\lambda'}(\boldsymbol{p}',\varepsilon+\omega)G^{12,A}_{\lambda'\mu'}(\boldsymbol{p}',$$

$$\varepsilon)V_{\boldsymbol{p}'\lambda'}(\boldsymbol{k},\omega)),\tag{4·4}$$

where $G^{\alpha\beta,R}_{\lambda\upsilon}(\boldsymbol{p},\varepsilon)$ and $G^{\alpha\beta,A}_{\lambda\upsilon}(\boldsymbol{p},\varepsilon)$ are analytic continuation of $\mathcal{G}^{\alpha\beta}_{\lambda\mu}(\boldsymbol{p},\varepsilon_n)$ in upper and lower half plane of ε, respectively.

Among contributions to the vertex part L, let us consider those shown in Fig. 2. In this case, for $\omega\to0$, the poles of two phonon Green's functions come together from different side of the real axis. As a result magnitude of these contributions turn out to be of order $0(1/\gamma)$. Since we consider $\gamma\ll1$, these terms are dominant ones in L and require special consideration.*) To separate out these parts of L, we single out the contribution from all the diagrams that do not have any parallel pairs of lines with nearly equal value of the poles. We denote by U this part of the function L, which has no singularity at $\omega=\gamma=0$. Then,

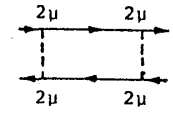

Fig. 2. Diagram for $L^{\lambda\lambda,\lambda'\lambda'}_{\boldsymbol{p}\boldsymbol{p}'}$.

*) The quantities $K^a_{p\lambda,\,p'\lambda'}(\varepsilon+\omega+i\delta,\varepsilon+i\delta)$ and $K^a_{p\lambda,\,p'\lambda'}(\varepsilon+\omega-i\delta,\varepsilon-i\delta)$ of Eq. (4.3) include no such a pair of Green's function, so that they are ignored.

$$L^{\lambda\lambda,\lambda'\lambda'}_{\boldsymbol{p}\boldsymbol{p}'}(\omega;\varepsilon)=U^{\lambda\lambda,\lambda'\lambda'}_{\boldsymbol{p}\boldsymbol{p}'}(\omega;\varepsilon)+\frac{1}{N}\sum_{\boldsymbol{p}''\ \nu}U^{\lambda\lambda,\nu\nu}_{\boldsymbol{p}\boldsymbol{p}''}(\omega;\varepsilon)$$

$$\times G^{22,R}_{\nu\nu}(\boldsymbol{p}'',\varepsilon+\omega)G^{22,A}_{\nu\nu}(\boldsymbol{p}'',\varepsilon)L^{\nu\nu,\lambda'\lambda'}_{\boldsymbol{p}''\boldsymbol{p}'}(\omega;\varepsilon)\,. \tag{4·5}$$

We now let $\phi^{\lambda\lambda'}_{21,\,21}(\omega;\boldsymbol{p},\varepsilon)$ be the terms in the parenthesis of Eq. (4.4) and take account of Eq. (4.5) to find

$$\phi^{\lambda\lambda'}_{21,\,21}(\omega;\boldsymbol{p},\varepsilon)=G^{22,R}_{\lambda\lambda}(\boldsymbol{p},\varepsilon+\omega)G^{11,A}_{\lambda\lambda}(\boldsymbol{p},\varepsilon)V_{\boldsymbol{p}\lambda}(\boldsymbol{k},\omega)\delta_{\lambda\lambda'}$$

$$+G^{22,R}_{\lambda\lambda}(\boldsymbol{p},\varepsilon+\omega)G^{22,A}_{\lambda\lambda}(\boldsymbol{p},\varepsilon)\frac{1}{N}\sum_{\boldsymbol{p}''\ \lambda''}U^{\lambda\lambda,\lambda''\lambda''}_{\boldsymbol{p}\boldsymbol{p}''}(\omega;\varepsilon)\phi^{\lambda''\lambda'}_{21,\,21}(\omega;\boldsymbol{p}'',\varepsilon)\,, \tag{4·6}$$

where we neglect the terms which are order $O(\gamma)$ less than the first term on the r.h.s. of Eq. (4.6), and employed the relation,

$$G^{21,A}_{\lambda\lambda}(\boldsymbol{p},\varepsilon)G^{12,A}_{\lambda'\lambda'}(\boldsymbol{p}',\varepsilon)\cong G^{22,A}_{\lambda\lambda}(\boldsymbol{p},\varepsilon)G^{11,A}_{\lambda'\lambda'}(\boldsymbol{p}',\varepsilon)\,, \tag{4·7}$$

which holds for $\gamma\ll1$.

Similarly we obtain such contribution to $f_{\boldsymbol{p}\lambda}(\boldsymbol{k},\omega)$ that come from $\mathcal{H}^{b}_{\boldsymbol{p}\lambda,\boldsymbol{p}'\lambda'}(\tau)$. Then adding $\phi^{\lambda\lambda}_{21,\,21}$ and one coming from $\mathcal{H}^{b}_{\boldsymbol{p}\lambda,\boldsymbol{p}'\lambda'}$ (written as $\phi^{\lambda\lambda}_{21,\,12}$), and using identity, $G^RG^A=-(G^R-G^A)/[\,(G^R)^{-1}-(G^A)^{-1}]$, we have

$$\mathrm{i}\omega\phi^{\lambda\lambda'}(\omega;\boldsymbol{p},\varepsilon)=-\,\mathrm{sgn}\varepsilon\cdot\gamma_{\boldsymbol{p}\lambda}\phi^{\lambda\lambda'}(\omega;\boldsymbol{p},\varepsilon)$$

$$+2\,\mathrm{sgn}\varepsilon\cdot\mathrm{Im}G^{22,R}_{\lambda\lambda}(\boldsymbol{p},\varepsilon)\frac{1}{\omega_{\boldsymbol{p}\lambda}}V_{\boldsymbol{p}\lambda}(\boldsymbol{k},\omega)\delta_{\lambda\lambda'}$$

$$+\,\mathrm{sgn}\varepsilon\cdot\omega_{\boldsymbol{p}\lambda}\,\mathrm{Im}\,G^{22,R}_{\lambda\lambda}(\boldsymbol{p},\varepsilon)\frac{1}{N}\sum_{\boldsymbol{p}''\ \lambda''}U^{\lambda\lambda,\lambda''\lambda''}_{\boldsymbol{p}\boldsymbol{p}''}(\omega;\varepsilon)\phi^{\lambda''\lambda'}(\omega;\boldsymbol{p}'',\varepsilon) \tag{4·8}$$

where sgn ε is 1 for $\varepsilon>0$ and -1 for $\varepsilon<0$, and

$$\phi^{\lambda\lambda'}(\omega;\boldsymbol{p},\varepsilon)=\phi^{\lambda\lambda'}_{21,\,21}(\omega;\boldsymbol{p},\varepsilon)+\phi^{\lambda\lambda'}_{21,\,12}(\omega;\boldsymbol{p},\varepsilon)\,.$$

Equation for $f_{p\lambda}$ (k, ω)

Let us now rewrite Eq. (4.8) into the equation for $f_{p\lambda}(k, \omega)$. To do this we note that $\phi^{\lambda\lambda'}(\omega;p,\varepsilon)$ sharply varies with respect to ε and takes finite value only near $\varepsilon=\omega_{p\lambda}$; we thus separate a sharply varying part from $\phi^{\lambda\lambda'}(\omega;p,\varepsilon)$, such that

$$\phi^{\lambda\lambda'}(\omega;\boldsymbol{p},\varepsilon)=\mathrm{sgn}\varepsilon\cdot \mathrm{Im}\,G^{22,R}_{\lambda\lambda}(\boldsymbol{p},\varepsilon)\,\tilde{\phi}^{\lambda\lambda'}(\omega;\boldsymbol{p},\varepsilon)\ . \tag{4·9}$$

After inserting Eq. (4.9) into Eq. (4.8), we multiply both sides of Eq. (4.8) by $-(\omega/2\pi i)(\partial f^0/\partial\varepsilon)$, and perform the integration and summation over ε and λ'respectively. As a result we have

$$\begin{aligned} i\omega f_{\boldsymbol{p}\lambda}(\boldsymbol{k},\omega)=\omega^3_{\boldsymbol{p}\lambda}\gamma'_\lambda f_{\boldsymbol{p}\lambda}(\boldsymbol{k},\omega)-i\omega\frac{\partial f^0}{\partial\omega_{\boldsymbol{p}\lambda}}N^{-1}V_{\boldsymbol{p}\lambda}(\boldsymbol{k},\omega) \\ -\frac{\omega_{\boldsymbol{p}\lambda}}{2|\gamma_\lambda|}\frac{1}{N}\sum_{\boldsymbol{p}'}U^{\lambda\lambda,\lambda\lambda}_{\boldsymbol{p}\boldsymbol{p}'}(\omega)f_{\boldsymbol{p}'\lambda}(\boldsymbol{k},\omega) \end{aligned} \tag{4·10}$$

where $\gamma_{\lambda'}$ is given by Eq. (A.5).

Let us here estimate the other contribution to $f_{p\lambda}(k, \omega)$ i.e. those coming from K'^R in Eq. (3.5); figure 3, shows a set of examples. We first consider the contribution given by the diagram in Fig. 3(a). Since it contains a Green's function $G^{\alpha\beta}_{\lambda\bar{\lambda}}$ carrying a factor of order $0(\gamma)$, it yield a contribution to $f_{p\lambda}$ of order $0(\gamma^0)$; we write this one as $f'_{p\lambda}$. On the other hand the third term on the right hand side of Eq. (4.10) yield to $f_{p\lambda}$ a contribution of order $0(\gamma^0 \ln\omega)$, as we shall see later in Eq. (4.14) with Eq. (4.13); this contribution to $f_{p\lambda}$ is just what we concerned with in this paper. Therefore we can neglect $f'_{p\lambda}$, since when $\omega\to 0$ it is smaller by factor $\ln\omega$ than that contribution to $f_{p\lambda}$ mentioned just above. Contributions coming from diagrams in Fig. 3(b) are more safely neglected, since they yield still smaller contributions to $f_{p\lambda}$ than $f'_{p\lambda}$.

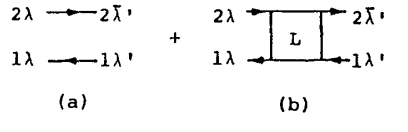

Fig. 3. Diagram for relevant to $K'_{pp'}(t)$.

Let us now a little bit simplify Eq. (4.10). We first note that as is showed in Eq.(B.12), the function $U^{\lambda\lambda,\lambda\lambda}_{pp'}(\omega)$ diverges with $(p+p')\to 0$ as $(p+p')^{-2}$ when $\omega=0$. Therefore the last term on the right hand side of Eq. (4.10) can be approximated as

$-\frac{\omega_{p\lambda}}{2|\gamma_\lambda|} f_{-p\lambda}(k, \omega) N^{-1} \sum_{p'} U_{pp'}^{\lambda\lambda,\lambda\lambda}(\omega)$. Secondly, note that if we neglect the third term on the right hand side of Eq. (4.10), which is indeed smaller than others by a factor of order $0(\gamma)$, then we find $f_{p\lambda}(k, \omega)$ to be a odd function of p. We can thus rewrite Eq. (4.10) as

$$i\omega f_{p\lambda}(k, \omega) = \frac{1}{\tau_R} f_{p\lambda}(k, \omega) - i\omega \frac{\partial f^0}{\partial \omega_{p\lambda}} N^{-1} V_{p\lambda}(k, \omega) , \tag{4·11}$$

neglecting errors of order $0(\gamma^2)$, where

$$\frac{1}{\tau_R} = \frac{1}{\tau_0} + \frac{\omega_{p\lambda}}{2|\gamma_\lambda|} \frac{1}{N} \sum_{p} U_{pp}^{\lambda\lambda,\lambda\lambda}(\omega) , \tag{4·12}$$

with τ_0 being $1/\gamma'\omega_{p\lambda}^3$. Furthermore, inserting Eq. (B.12) into Eq. (4.12), and performing the integration over p with a ultraviolet cut off of order $1/c_\lambda\tau_0$ since Eq. (B.12) was derived for $|p_1+p_2| \ll 1/c_\lambda\tau_0$, we have

$$\frac{1}{\tau_R} = \frac{1}{\tau_0} \left(1 + \frac{\tilde{\gamma}}{\pi} \ln \frac{1}{\omega\tau_0}\right) , \tag{4·13}$$

where $1/\tilde{\gamma} = 1/|\gamma_1| + 1/|\gamma_2|$, and we used approximations $c_1 \cong c_2$ and $\gamma_1 \cong \gamma_2$ in the argument of logarithms.

We note that the correction to τ_R is proportional to $\ln(\omega\tau_0)$, diverging with $\omega \to 0$. This is similar to the correction, $-(1/2\pi E_F\tau)\ln\omega\tau$, to the relaxation time $\tau(\omega)$ of independent electrons in $d=2$; E_F is the Fermi energy, τ is the bare relaxation time of electrons, and ω the frequency of the electric field[4]. The latter correction to $\tau(\omega)$ represents the effect of weak localization (a precursor to strong localization at $\omega=0$) of two-dimensional electrons interacting with impurities.[3,4] Therefore, we can also regard the correction to τ_R in Eq. (4.13) as a effect of the localization of the phonons, taking account of the arguments presented in §1, which shows the intimate relation between the lattice vibration problem and the electron excitation problem.

At the end of this section we rewrite $V_{p\lambda}(k,\omega)$ in terms of the temperature gradient by making use of Eqs. (3.4) and (3.8). After carrying out a Fourier transformation with respect to k on both sides of Eq. (4.11), we have

$$i\omega f_{p\lambda}(R_{i0}, \omega) = \tau_R^{-1} f_{p\lambda}(R_{i0}, \omega) + \nabla T \cdot c_{p\lambda} N^{-1} \frac{\partial f^0}{\partial T} , \tag{4·14}$$

where $c_{p\lambda} = c_\lambda p/|p|$. We thus have the convenient genelarized Boltzmann equation to calculate thermal conductivity in §5.

§5. Thermal conductivity in Callaway formulation

In this section we calculate thermal conductivity by making use of Eq. (4.14) with Eq. (4.13).

As is well known, if we only take account of the phonon scattering by impurities, the mean free path of the phonons diverges at long-wavelength as p^{-3} in two-dimension; as a result thermal conductivity also diverges. To avoid this, following Callaway, we introduce into Eq. (4.14) normal phonon-phonon scattering processes.*) After taking a limit $\omega \to 0$, we then have[7]

$$-\nabla T \cdot \boldsymbol{c}_{\boldsymbol{p}\lambda} \frac{\partial f^0}{\partial T} = \frac{f_{\boldsymbol{p}\lambda} - f^{\alpha}_{\boldsymbol{p}\lambda}}{\tau_N} + \frac{f_{\boldsymbol{p}\lambda} - f^0_{\boldsymbol{p}\lambda}}{\tau_R} \quad (5\cdot 1)$$

**)

Here we took account of the following condition: since normal processes conserve the total momentum, they bring phonons only into local equilibrium described by the distribution function, $f^{\alpha}_{\boldsymbol{p}\lambda} = 1/[\exp\{-\beta(\omega_{\boldsymbol{p}\lambda} - \boldsymbol{\alpha}\cdot\boldsymbol{p})\} - 1]$ with a chemical potential $\boldsymbol{\alpha}\cdot\boldsymbol{p}$, which is determined later and found to be proportional to ∇T. Expanding the right hand side of the expression for $f^{\alpha}_{\boldsymbol{p}\lambda}$ with respect to the chemical potential $\boldsymbol{\alpha}\cdot\boldsymbol{p}$, we get,

$$f^{\alpha}_{\boldsymbol{p}\lambda} = f^0_{\boldsymbol{p}\lambda} - \boldsymbol{\alpha}\cdot\boldsymbol{p}\frac{\partial f^0_{\boldsymbol{p}\lambda}}{\partial \omega_{\boldsymbol{p}\lambda}} \quad . \quad (5\cdot 2)$$

Let us now substitute Eq. (5.2) into Eq. (5.1) and denote $(f_{\boldsymbol{p}\lambda} - f^0_{\boldsymbol{p}\lambda})$ by $g_{\boldsymbol{p}\lambda}$ in order to solve Eq. (5.2) for $g_{\boldsymbol{p}\lambda}$. We then have

$$g_{\boldsymbol{p}\lambda} = -\tilde{\tau}_{\boldsymbol{p}\lambda}\frac{\partial f^0}{\partial T}\left(\nabla T \cdot \boldsymbol{c}_{\boldsymbol{p}\lambda} - \boldsymbol{\alpha}\cdot\boldsymbol{p}\frac{T}{\omega_{\boldsymbol{p}\lambda}\tau_N}\right), \quad (5\cdot 3)$$

where $1/\tilde{\tau} = 1/\tau_N + 1/\tau_R$. The quantity $\boldsymbol{\alpha}$ is determined so that the normal phonon-phonon scattering may conserve the total momentum. Actually, substituting Eq. (5.3) into Eq. (5.1), multiplying the both sides of Eq. (5.1) by $\boldsymbol{p}$, and then performing summation over $\boldsymbol{p}$, we obtain

---

*) We consider the thermal conductivity at temperatures so lower than the Debye temperatures that the Umklapp processes are neglected at all in this paper.

**) Here we define $f_{\boldsymbol{p}\lambda}(\omega) = \sum_i f_{\boldsymbol{p}\lambda}(R_{i0},\omega)$, assuming ∇T being independent of R_{i0}.

$$\alpha = -\nabla T \sum_{\boldsymbol{p}\lambda} \frac{\tilde{\tau}}{\tau_N} \omega_{\boldsymbol{p}\lambda} \frac{\partial f^0}{\partial T} \Big/ \sum_{\boldsymbol{p}\lambda} \frac{\tilde{\tau}}{\tau_R \tau_N} \frac{\boldsymbol{p}^2}{\omega_{\boldsymbol{p}\lambda}} T \frac{\partial f^0}{\partial T} \quad . \tag{5·4}$$

Let us now calculate the heat current by making use of expressions (5.3) and (5.4). The energy current density $j^{\varepsilon}(\boldsymbol{q})$ obtained in Eq. (3.3) may be rewritten in terms of a and a^{+}, such that

$$j^{\varepsilon}_{\alpha}(\boldsymbol{q}\sim 0) = \sum_{\boldsymbol{p}\lambda} c^{\alpha}_{\boldsymbol{p}\lambda}\, \omega_{\boldsymbol{p}\lambda}\, a^{+}_{\boldsymbol{p}\lambda}\, a_{\boldsymbol{p}\lambda} + \sum_{\boldsymbol{p}\lambda}\sum_{\beta} a^{\alpha\beta}_{\lambda\lambda}\, p^{\beta}\, a^{+}_{\boldsymbol{p}\lambda}\, a_{\boldsymbol{p}\lambda} \quad , \tag{5·5}$$

at the long-wavelength limit. Here, we have a term $a^{+}_{\boldsymbol{p}\lambda} a_{\boldsymbol{p}\bar{\lambda}}$, of which expectation value has not been considered so far. However, the contribution of this term to the energy current density turn out to be smaller than that of $\langle a^{+}_{\boldsymbol{p}\lambda} a_{\boldsymbol{p}\lambda}\rangle$ for a reason in the following. For example we give in Fig. 4 diagram for $\phi'_{21,21}$ which is relevant to $\langle a^{+}_{\boldsymbol{p}\lambda} a_{\boldsymbol{p}\bar{\lambda}}\rangle$. As one observes, the outer lines of these diagrams do not possess parallel pairs of lines with nearly equal value of pole. We thus find that the lowest order diagram for $\phi'_{21,21}$ (Fig. 4(a)) yield to $\langle a^{+}_{\boldsymbol{p}\lambda} a_{\boldsymbol{p}\bar{\lambda}}\rangle$ a contribution of order $0(\gamma^0)$. This is again smaller than those correction terms to the $f_{\boldsymbol{p}\lambda}$ which appeared on the right hand side of Eq. (4.10), since the latter was of order $0(\gamma^0 \ln\omega)$. The contributions coming from Fig. 4(b) are still smaller than that from Fig. 4(a) and are therefore ignored. These facts allow us to neglect the second term of expression (5.5).

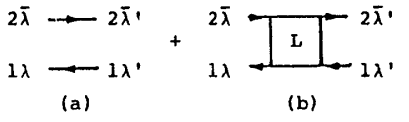

Fig. 4. Diagram for $\phi'_{21,21}$.

Let us now proceed to the calculation of the expectation value of j^{ε}. After taking ensemble average of j^{ε}, we substitute Eq. (5.3) with Eq. (5.4) into Eq. (5.5) and assume the temperature gradient is parallel to the x-axis to get

$$\langle j^{\varepsilon}_{x}\rangle = -\frac{1}{3} \nabla_x T \sum_{\boldsymbol{p}\lambda} \omega_{\boldsymbol{p}\lambda} \tilde{\tau}(\boldsymbol{p}\lambda) \frac{\partial f^0}{\partial T} c^2_{\lambda}$$

$$\times \Big\{ 1 + \frac{1}{c^2_{\lambda}\tau_N(\boldsymbol{p}\lambda)} \frac{\sum_{\boldsymbol{p}'\lambda'} (\tilde{\tau}(\boldsymbol{p}'\lambda')/\tau_N(\boldsymbol{p}'\lambda'))\, \omega_{\boldsymbol{p}'\lambda'} (\partial f^0/\partial T)}{\sum_{\boldsymbol{p}'\lambda'} (\tilde{\tau}(\boldsymbol{p}'\lambda')/\tau_R(\boldsymbol{p}'\lambda')\, \tau_N(\boldsymbol{p}'\lambda'))\, (\boldsymbol{p}'^2/\omega_{\boldsymbol{p}'\lambda'})\, (\partial f^0/\partial T)} \Big\}, \tag{5·6}$$

where we explicitly write the fact that $\tilde{\tau}$, τ_N and τ_R depend on $\boldsymbol{p}$ and λ.

We now estimate a magnitude of τ_N. Supposing that among various normal processes

three phonon scattering processes are dominant, we have

$$\frac{1}{\tau_N} \sim \frac{pT^3}{ma\theta^3} \quad , \tag{5·7}$$

where we write a for the lattice constant and θ for the Debye temperature, and we used the approximations $c_1 = c_2$ and $\theta_1 = \theta_2$ for simplicity. Equation (5.7) is easily derived from §69 of Ref. 7) with replacing three-dimentional integrations over momentums by two-dimensional ones. We now require $\tau_N << \tau_R$, since we assumed in the first place of this section that the distribution function of phonons first relaxes to local equilibrium due to normal processes, and then relaxes to true equilibrium due to the phonon-impurity scattering. Using T/c instead of p in Eq. (5.7), we thus have the condition

$$T >> n_i (\delta m/m)^2 mc^2 \quad . \tag{5·8}$$

Under the condition (5.8) we have $\tilde{\tau} \cong \tau_N$. Then from Eq. (5.6) we find, for thermal conductivity,

$$\kappa = \frac{1}{2}\{\frac{1}{V}\sum_{\boldsymbol{p}\lambda} \omega_{\boldsymbol{p}\lambda}(\partial f^0/\partial T)\}^2 / \frac{1}{V}\sum_{\boldsymbol{p}\lambda} \tau_R^{-1}(\omega_{\boldsymbol{p}\lambda}/c_\lambda^2)(\partial f^0/\partial T) \quad . \tag{5·9}$$

We finally substitute Eq. (4.13) into Eq. (5.9). Upon carrying out the integration over p and taking account of the fact that we consider the temperature much lower than the Debye temperature, we have

$$\kappa = A\frac{(\sum_\lambda (\Theta_\lambda/c_\lambda)^2 (T/\Theta_\lambda)^2)^2}{\sum_\lambda \gamma'_\lambda (\Theta_\lambda^5/c_\lambda^4)(T/\Theta_\lambda)^5} \times \{1 - \frac{28\pi}{5}\tilde{\gamma}'' \frac{\sum_\lambda \gamma'_\lambda (\Theta_\lambda^7/c_\lambda^6)(T/\Theta_\lambda)^7 \ln(\gamma'_\lambda T^3/\omega)}{\sum_\lambda \gamma'_\lambda (\Theta_\lambda^5/c_\lambda^4)(T/\Theta_\lambda)^5}\} , \tag{5·10}$$

where we expand the denominator of Eq. (5.9) in power series in γ, ignoring errors of order $0(\gamma)$; $A = 1701\zeta^2(3)/64\pi^2$, the Debye temperature Θ_λ is given by $c_\lambda \Lambda$, where Λ is the momentum at zone boundary, $\gamma' = c_1^2 c_2^2 \gamma'_1 \gamma'_2/(c_1^2\gamma'_1 + c_2^2\gamma'_2)$, and $\zeta(n)$ is the Riemann zeta function. In order to see qualitative features of Eq. (5.10), let us again ignore any dependence of the quantities on the polarization indices. Then Eq. (5.10) yields

$$\kappa \cong \frac{2A}{\gamma' T}\left(1-\frac{14\pi}{5}\gamma' T^2 \ln\left(\frac{\gamma' T^3}{\omega}\right)\right) . \qquad (5\cdot 11)$$

Here the second term in the bracket represents the effect of the localization of the phonons.

The divergence of κ at $\omega=0$ in Eq. (5.11) is surpressed by taking account of inelastic scatterings in the calculation of the vertex part $U_{pp'}^{\lambda\lambda,\lambda\lambda}$ in Appendix B. To see this, following Ref. 8), we evaluate the contributions of the diagrams shown in Fig. 5, in which the first diagram represents Eq. (B.12) yielding Eq. (5.11), and the others represent the effects of the three phonon interactions. Then we get same expression for $U_{pp'}^{\lambda\lambda,\lambda\lambda}$ as Eq. (B.12) except $i\omega$ in Eq. (B.12) being replaced by $(i\omega - 1/\tau_N)$. Inserting this new expression into Eq. (4.12), we find

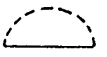

Fig. 5. Diagrams for the vertex part $\bar{M}$, which gives the expression for U including three phonon interactions.

$$\kappa = \frac{2A}{\gamma' T}\left(1-\frac{14\pi}{5}\gamma' T^2 \ln\frac{1}{T}\right) \qquad (5\cdot 12)$$

where we used Eq. (5.7) for τ_N with substituting T/c for p. In conclusion, for $T<<\Theta$, we get the correction to the lattice thermal conductivity, $\Delta\kappa \propto T\ln T$ due to the localizations of phonons, which takes place in $d=2$ in the lattice containing impurity atoms.

§6. Discussions

In this paper, we have evaluated the correction to κ only due to the localizations of the phonons, and dropped various ones other than that; we here make a comment on the latter. Among others, we omitted corrections of order $(\gamma' T)^{-1}$ $(\tau_N T)^{-1}$. These will be introduced, for example, by taking account of the three phonon interaction in the calculation of Σ in Eq. (A.2). We now recall that the correction to κ due to the localizations of the phonons is of order $(\gamma' T)^{-1}$ $(T\tau_0)^{-1}\ln(T\tau_0)^{-1}$, and the temperature region $\tau_0>>\tau_N$ is considered in this paper. then, comparing $(\gamma' T)^{-1}$ $(T\tau_0)^{-1}\ln(T\tau_0)^{-1}$ and $(\gamma' T)^{-1}$ $(\tau_N T)^{-1}$, we find that the former correction evaluated in this paper is smaller than the latter ones; this makes it difficult to detect the correction $\Delta\kappa \propto T\ln T$ experimentally. Nevertheless, since the neglected corrections will depend on temperature as T^2, being different from the one in question, $T\ln T$, we can still have a hope to observe the latter, providing the temperature-dependence of κ will be precisely determined in experiments in the future.

Acknowledgment

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Appendix A

Green's function

The one-particle temperature Green's functions used in this paper are defined by

$$\hat{\mathcal{G}}_{\lambda\lambda'}(\boldsymbol{p}, \boldsymbol{p}'; \tau) = \begin{pmatrix} \mathcal{G}^{11}_{\lambda\lambda'}, & \mathcal{G}^{12}_{\lambda\lambda'} \\ \mathcal{G}^{21}_{\lambda\lambda'}, & \mathcal{G}^{22}_{\lambda\lambda'} \end{pmatrix}$$

$$= -\begin{pmatrix} <T(q_{\boldsymbol{p}\lambda}(\tau)\, q_{\boldsymbol{p}'\lambda'})>, & <T(q_{\boldsymbol{p}\lambda}(\tau) p_{\boldsymbol{p}'\lambda'})>. \\ <T(p_{\boldsymbol{p}\lambda}(\tau)\, q_{\boldsymbol{p}'\lambda'})>, & <T(p_{\boldsymbol{p}\lambda}(\tau) p_{\boldsymbol{p}'\lambda'})> \end{pmatrix}. \qquad (A\cdot 1)$$

Using Eqs. (2.4), (2.5) and (2.6) in Eq. (A.1), then expanding $\mathcal{G}_{\lambda\lambda'}$ in powers of $u_{p\lambda,p'\lambda'}$ in Eq. (2.6), and averaging over impurity configurations, we obtain up to the lowest non-trivial order in the impurity concentration n_i,

$$\hat{\mathcal{G}}_{\lambda\lambda'}(\boldsymbol{p}, \varepsilon_n) = \frac{-\delta_{\lambda\lambda'}}{\varepsilon_n^2 + \omega^2_{\boldsymbol{p}\lambda}\,(1+\Sigma_\lambda(\varepsilon_n))} \begin{pmatrix} 1 & \varepsilon_n \\ -\varepsilon_n & \omega^2_{\boldsymbol{p}\lambda} \end{pmatrix}, \qquad (A\cdot 2)$$

where

$$\Sigma_\lambda(\varepsilon_n) = n_i a^2 \sum_{\lambda'} \int \frac{d^2p'}{(2\pi)^2}\, u^2_{\boldsymbol{p}\lambda,\boldsymbol{p}'\lambda'} \frac{-\omega^2_{\boldsymbol{p}'\lambda'}}{\varepsilon_n^2 + \omega^2_{\boldsymbol{p}'\lambda'}}, \qquad (A\cdot 3)$$

with a being the lattice spacing; Fig. 6 shows the diagram for Σ_λ. Analytic continuation

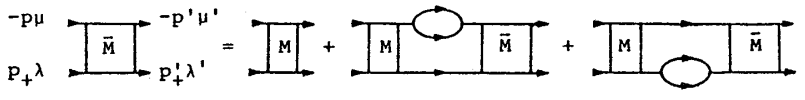

Fig. 6. Diagrams for $\Sigma_\lambda(\varepsilon_n)$.

$i\varepsilon_n \to \varepsilon + i\delta$ of $\Sigma_\lambda(\varepsilon_n)$ yield the self-energy of the retarded Green's functions, $\Sigma^R_\lambda(\varepsilon)$. Since the real parts of $\Sigma^R_\lambda(\varepsilon)$ give only small shifts of the sound velocities, we neglect them everywhere. Then Eq. (A. 3) yield

$$\mathrm{Im}.\Sigma_\lambda^{\mathrm{R}}(\varepsilon)=\gamma_\lambda=-\gamma'_\lambda\,\varepsilon^2\,\mathrm{sgn}\,\varepsilon \quad , \tag{A·4}$$

where

$$\gamma'_\lambda=\frac{n_i a^2}{4}\left(\frac{u_{1\lambda}^2}{c_1^2}+\frac{u_{2\lambda}^2}{c_2^2}\right) \quad , \tag{A·5}$$

with the definition

$$u_{\lambda\lambda'}^2=\left(\frac{\delta m}{m}\right)^2\sum_{\alpha\beta}\varepsilon_{\boldsymbol{p}\lambda}^{\alpha}\varepsilon_{\boldsymbol{p}\lambda}^{\beta}\int\frac{\mathrm{d}\theta_{\boldsymbol{p}'}}{2\pi}\varepsilon_{\boldsymbol{p}'\lambda'}^{\alpha}\varepsilon_{\boldsymbol{p}'\lambda'}^{\beta} \quad ,$$

$\theta_{\boldsymbol{p}'}$ being the angle between $\boldsymbol{p}'$ and x-axis. For practical purpose we neglect the momentum dependence of $u_{\lambda\lambda'}^2$.

Appendix B

–Irreducible Vertex Part–

The "particle-hole" irreducible vertex part U are shown by Fig. 7(a) in the lowest approximation in γ. They are "particle-particle" ladder diagrams as in Fig. 7(b), and so all have same order of magnitude in γ. More complicated diagrams have higher order in γ compared with the contributions of Fig. 7(b); we see this, for instance, by calculating that the contribution of Fig. 8 (b) to U is one order of magnitude less than that of Fig. 8(a).

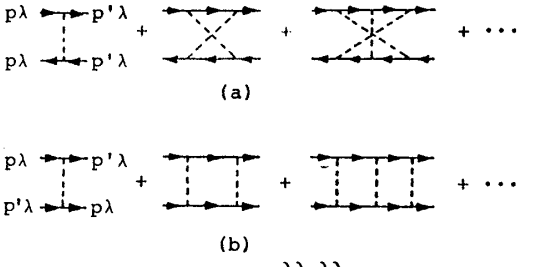

Fig. 7. Diagrams for $U_{pp'}^{\lambda\lambda,\lambda\lambda}$ in the lowest order in γ.

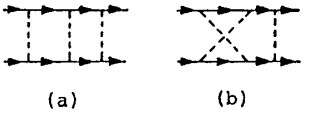

Fig. 8. (a). A contribution to U in the lowest order in γ. (b). A contribution to U which is one order of magnitude less than that of (a).

In this appendix, instead of calculating directly the contribution of Fig. 7(b) itself, we consider the "particle-particle" complete vertex part M, of which singular part agrees with that of Fig. 7(b) in the lowest approximation in γ. Then it is shown that M has a form of a diffusion propagator in general. After that we use a perturbation expansion in γ to calculate various constants appeared in the diffusion propagator.

Let us now consider the vertex part M shown in Fig. 9.

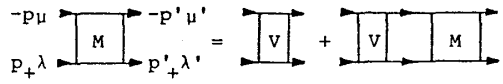

Fig. 9. Diagrams for the vertex part M.

$$M_{\boldsymbol{pp'}}^{\lambda\mu,\lambda'\mu'}(\boldsymbol{q},\omega)=V_{\boldsymbol{pp'}}^{\lambda\mu,\lambda'\mu'}(\boldsymbol{q},\omega)$$

$$+\sum_{\boldsymbol{p''}}V_{\boldsymbol{pp'}}^{\lambda\mu,\xi'\nu'}(\boldsymbol{q},\omega)\,G_{\xi'\xi}^{22,R}(\boldsymbol{p''}+\boldsymbol{q},\varepsilon+\omega)\,G_{\nu'\nu}^{22,A}(-\boldsymbol{p''},\varepsilon)\,M_{\boldsymbol{p''p'}}^{\xi\nu,\lambda'\mu'}(\boldsymbol{q},\omega)\quad, \tag{B·1}$$

where V is the "particle-particle" irreducible vertex part; here and in what follows we assume to sum over any repeated Greek index and omit the summation sign. By defining a function ψ as

$$\psi_{\boldsymbol{pp'}}^{\alpha\beta,\lambda'\mu'}(\boldsymbol{q},\omega)=G_{\alpha\lambda}^{22,R}(\boldsymbol{p}+\boldsymbol{q},\varepsilon+\omega)G_{\beta\mu}^{22,A}(-\boldsymbol{p},\varepsilon)M_{\boldsymbol{pp}}^{\lambda\mu,\lambda'\mu'}(\boldsymbol{q},\omega)\quad, \tag{B·2}$$

Eq. (B.1) yield

$$\psi_{\boldsymbol{pp'}}^{\alpha\beta,\lambda'\mu'}(\boldsymbol{q},\omega)=G_{\alpha\lambda}^{R}(\boldsymbol{p}_+)\,G_{\beta\mu}^{A}(-\boldsymbol{p})\,V_{\boldsymbol{pp}}^{\lambda\mu,\lambda'\mu'}(\boldsymbol{q},\omega)$$

$$+G_{\alpha\lambda}^{R}(\boldsymbol{p}_+)G_{\beta\mu}^{A}(-\boldsymbol{p})\sum_{\boldsymbol{p''}}V_{\boldsymbol{pp''}}^{\lambda\mu,\xi'\nu'}(\boldsymbol{q},\omega)\,\psi_{\boldsymbol{p''p'}}^{\xi'\nu',\lambda'\mu'}(\boldsymbol{q},\omega)\quad, \tag{B·3}$$

where the subscripts 22 on $G_{\alpha\beta}^{22,R}$ and $G_{\alpha\beta}^{22,A}$ are dropped and $\boldsymbol{p}+\boldsymbol{q}$ are denoted as $\boldsymbol{p}_+$. We multiply the both sides of Eq. (B.3) by $(G^R(\boldsymbol{p}_+))_{\beta\alpha}^{-1}$ and $(G^A(-\boldsymbol{p}))_{\alpha\beta}^{-1}$ to get two equations; then subtracting the former equation from the latter one, we have

$$-\sum_{\boldsymbol{p}}\{(G^R(\boldsymbol{p}_+)_{\beta\alpha}^{-1}-(G^A(-\boldsymbol{p}))_{\alpha\beta}^{-1}\}\,\psi_{\boldsymbol{pp'}}^{\alpha\beta,\lambda'\mu'}(\boldsymbol{q},\omega)$$

$$=\sum_{\boldsymbol{p}}(G_{\alpha\lambda}^{R}(\boldsymbol{p}_+)-G_{\lambda\alpha}^{A}(-\boldsymbol{p}))\,V_{\boldsymbol{pp'}}^{\lambda\alpha,\lambda'\mu'}(\boldsymbol{q},\omega)$$

$$+\sum_{\boldsymbol{pp''}}(G_{\alpha\lambda}^{R}(\boldsymbol{p}_+)-G_{\lambda\alpha}^{A}(-\boldsymbol{p}))\,V_{\boldsymbol{pp''}}^{\lambda\alpha,\xi'\nu'}(\boldsymbol{q},\omega)\,\psi_{\boldsymbol{p''p'}}^{\xi'\nu',\lambda'\mu'}(\boldsymbol{q},\omega)\quad. \tag{B·4}$$

Here let us use two relations:

(i) $(G^R(\boldsymbol{p}_+))^{-1}_{\alpha\beta} - (G^A(-\boldsymbol{p}))^{-1}_{\beta\alpha}$

$$= -\Omega_{\alpha\beta} + (\Sigma^R_{\alpha\beta}(\boldsymbol{p}+\boldsymbol{q},\ \varepsilon+\omega) - \Sigma^A_{\beta\alpha}(-\boldsymbol{p},\ \varepsilon)) \quad , \tag{B·5}$$

for $q,\ \omega \to 0$, where $\Omega_{\alpha\beta}=\delta_{\alpha\beta}\ (2\varepsilon^2/c_\alpha p^2)\ (\omega/\varepsilon - \boldsymbol{p}\cdot\boldsymbol{q}/p^2)$; this is given by using the expressions for the free phonon Green's functions, which we find in Eq. (A.2) with $\Sigma_\lambda=0$, and the general definition for the self-energy of the one-particle Green's function.*)

(ii) The second is the relation between the self-energy and the irreducible vertex part V:

$$\Sigma^R_{\beta\alpha}(\boldsymbol{p},\ \varepsilon+\omega) - \Sigma^A_{\alpha\beta}(-\boldsymbol{p},\ \varepsilon)$$

$$= \frac{1}{N}\sum_{\boldsymbol{p}'} (G^R_{\beta'\alpha'}(\boldsymbol{p},\ \varepsilon+\omega) - G^A_{\alpha'\beta'}(-\boldsymbol{p},\ \varepsilon)) V^{\alpha'\beta';\ \alpha\beta}_{\boldsymbol{p}'\boldsymbol{p}}(\boldsymbol{q}=0,\ \omega) \quad , \tag{B·6}$$

(a version of Ward-Takahashi indentity) which we derive by using the same technique as in Ref. 9) and 10).

Let us insert Eq. (B.5) into Eq. (B.4); then put $q=0$ at the first term on the right hand side of Eq. (B.4), and expand all functions multiplying ψ in powers of q up to order $0(q)$ in order to find the equation for ψ in the limit $q \to 0$. After that, using Eq. (B.6), we have

$$\frac{1}{N}\sum_{\boldsymbol{p}} (\Omega_{\alpha\beta} + \boldsymbol{q}\cdot\boldsymbol{B}_{\alpha\beta}(\boldsymbol{p}))\, \psi^{\alpha\beta,\lambda'\mu'}_{\boldsymbol{p}\boldsymbol{p}'}(\boldsymbol{q},\ \omega)$$

$$= \Sigma^R_{\mu'\lambda'}(\boldsymbol{p}') - \Sigma^A_{\lambda'\mu'}(-\boldsymbol{p}') \quad , \tag{B·7}$$

where $\boldsymbol{q}\cdot\boldsymbol{B}_{\alpha\beta}(\boldsymbol{p})$ represents the first order terms in Taylor expansion in q carried out above. We note that $\boldsymbol{B}_{\alpha\beta}(\boldsymbol{p})$ has the same signature -1 as $\boldsymbol{p}$ under space invesion (i.e. $\boldsymbol{p}\to-\boldsymbol{p}$); this is because it contain operators like $\partial_{\boldsymbol{p}}$ only once and the relation $\varepsilon_{\boldsymbol{p}\lambda}=\varepsilon_{-\boldsymbol{p}\lambda}$ holds in it. The latter relation comes from reality condition for $\boldsymbol{P}_i$ and $\delta\boldsymbol{R}_i$ in Eqs. (2.2) and (2.3). Thus we can regard $\boldsymbol{q}\cdot\boldsymbol{B}_{\alpha\beta}(\boldsymbol{p})$ as a simple correction to $\delta_{\alpha\beta}\times(2\varepsilon^2/c_\alpha p^2)(\boldsymbol{p}\cdot\boldsymbol{q}/p^2)$ of $\Omega_{\alpha\beta'}$ and write $\Omega'_{\alpha\beta}=\Omega_{\alpha\beta}+\boldsymbol{q}\cdot\boldsymbol{B}_{\alpha\beta}(\boldsymbol{p})$. Substituting Eq. (B.2) into Eq. (B.7) gives

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*) The self-energy $\Sigma^R_\lambda(\varepsilon)$ in Eq. (A. 4) is given by putting $\lambda=\mu$ in $\Sigma^R_{\lambda\mu}(p,\ \varepsilon)$.

$$\frac{1}{N}\sum_{\boldsymbol{p}}\Omega'_{\alpha\beta}G^R_{\alpha\lambda}(\boldsymbol{p}_+)G^A_{\beta\mu}(-\boldsymbol{p})M^{\lambda\mu,\lambda'\mu'}_{\boldsymbol{pp'}}(\boldsymbol{q},\omega)=\Delta\Sigma_{\mu'\lambda'}(\boldsymbol{p'}) \quad , \tag{B·8}$$

with

$$\Delta\Sigma_{\mu'\lambda'}(\boldsymbol{p'})=\Sigma^R_{\mu'\lambda'}(\boldsymbol{p'})-\Sigma^A_{\lambda'\mu'}(-\boldsymbol{p'}) \quad .$$

In order to find the solution of Eq. (B.8), let us now put

$$M^{\lambda\mu,\lambda'\mu'}_{\boldsymbol{pp'}}(\boldsymbol{q},\omega)=\Delta\Sigma_{\mu\lambda}(\boldsymbol{p})A(\boldsymbol{q},\omega)\Delta\Sigma_{\mu'\lambda'}(\boldsymbol{p'}) \quad . \tag{B·9}$$

Then we have

$$A(\boldsymbol{q},\omega)=((1/N)\sum_{\boldsymbol{p}}\Omega'_{\alpha\beta}G^R_{\alpha\lambda}(\boldsymbol{p}_+)G^A_{\beta\mu}(-\boldsymbol{p})\Delta\Sigma_{\mu\lambda}(\boldsymbol{p}))^{-1} \quad . \tag{B·10}$$

It is easy to see that, in the denominator of Eq. (B.10), the terms which are proportional to $\boldsymbol{q}$ vanish, since such terms in the summation of $\Sigma_{\boldsymbol{p}}$ change their sign under the replacement, $\boldsymbol{p}\rightarrow-\boldsymbol{p}$. We therefore understand that the denominater has a form (const.) x $(\omega+iDq^2)$ in general, and so the vertex M has a diffusion pole.

So far we have introduced no approximations except for taking limits q, $\omega\rightarrow0$. Let us now evaluate the diffusion constant and the intensity of the diffusion propagator by using perturbation theory in γ and neglecting the momentum dependence of $\Delta\Sigma_{\mu\lambda}(\boldsymbol{p})$. Inserting into Eq. (B.10) the expressions for G^R and Σ^R etc. obtained in Appendix A, and performing the integration over $\boldsymbol{p}$ give, for q, $\omega\rightarrow0$.

$$A(\boldsymbol{q},\omega)\cong a^{-2}\{\mathrm{i}\left(\frac{1}{c_1^2}+\frac{1}{c_2^2}\right)|\varepsilon|\omega-\frac{1}{2}\left(\frac{1}{|r_1|}+\frac{1}{|r_2|}\right)q^2\}^{-1} \quad . \tag{B·11}$$

We have then

$$U^{\lambda\lambda,\lambda\lambda}_{\boldsymbol{pp'}}=\frac{1}{a^2}\frac{-4r_\lambda^2}{\mathrm{i}\left(\frac{1}{c_1^2}+\frac{1}{c_2^2}\right)|\varepsilon|\omega-\frac{1}{2}\left(\frac{1}{|r_1|}+\frac{1}{|r_2|}\right)(\boldsymbol{p}+\boldsymbol{p'})^2} \quad , \tag{B·12}$$

by substituting $(\boldsymbol{p}+\boldsymbol{p'})$ for q in the expression for $M^{\lambda\lambda,\lambda\lambda}_{\boldsymbol{pp'}}(\boldsymbol{q},\omega)$ which is given by Ea. (B.9)

and (B.11); here we use the fact that, in the lowest order in γ, the singular part of M is same as that of U.

In order to check the solution thus obtained, we may calculate directly the contributions shown in Fig. 7(a) using the "isotropic medium model" i.e. $\varepsilon_{p\ell}=\hat{p}$ and $\varepsilon_{pt}=\hat{z}\times\hat{p}$, together with the perturbation expansion in γ; here subscripts ℓ and t means longitudinal and transverse respectively, and $\hat{p}$ and $\hat{z}$ are unit vectors along p and z-axis. This calculation is straightfoward, so that we do not show the detail explicitly but only state that the result agree with Eq. (B.11).

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