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# The scattering of phonons by the strain and rotation fields of crystal defects

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**Abstract.** The scattering of long-wavelength phonons due to the spatial variation of elastic moduli that is produced by the inhomogeneous elastic strain and rotation fields of static crystal defects is calculated in terms of the second- and third-order elastic constants of the undeformed crystal. The present theory is distinguished from those of previous authors by its ability to deal with rotation angles that are not necessarily small, such as those associated with large-angle grain boundaries or macroscopically bent or twisted crystals. For small rotations the classical equations of motion and the second-quantised Hamiltonian obtained by previous authors are rederived and the modifications appropriate to large rotations are discussed. Approximate, but simple, expressions for scattering cross sections, etc, are obtained; these facilitate subsequent calculations of transport coefficients and lead to estimates of lattice thermal resistivities in dislocated crystals that are in good agreement with experiment. Previous theoretical studies of the strain-field scattering problem are reviewed.

## 1. Introduction

This paper presents the results of a theoretical investigation of the scattering of phonons by the elastic‡ strain and rotation fields of crystal defects. It lays the foundations for subsequent calculations of phonon transport properties in crystals containing point, line and (internal) surface defects, including large-angle grain boundaries. The formulation to be described can also deal with the large elastic rotations present in crystals that have been bent or twisted on a macroscopic scale.

The importance of the strain-field§ scattering mechanism for phonons, at least in dislocated crystals, is strongly suggested by the frequent observation of a lattice thermal resistivity component having a temperature dependence proportional to  $T^{-2}$  at low temperatures (typically  $\sim 10$  K) in deformed crystals (Klemens 1955). Although only this, amongst several, proposed phonon–defect scattering mechanisms can account for such a temperature dependence (Wasserbach 1978), the repeated failure of early

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‡ An elastic continuum model is perfectly adequate for the long-wavelength phonons that dominate the lattice conduction at temperatures below, say, 10 K.

§ Here and henceforth we will frequently follow common usage in describing the scattering due to both strain and rotation fields as ‘strain-field scattering’. The distinction between strains and rotations will be made explicit where necessary.

theories of strain-field scattering to explain the *magnitude* of the observed resistivity increment has been a long-standing source of uncertainty, with one being forced to assume that the discrepancies were due to the crude descriptions of the crystal anharmonicities that were unavoidable in the early calculations. The situation prior to the improved calculations of Kogure and Hiki (1974, 1975; henceforth KH) and Eckhardt and Wasserbäch (1978, henceforth EW) is reviewed by Berman (1976) and some further discussion of the early theories may be found in the Appendix.

The more recent calculations of KH and EW employ a seemingly adequate description of the anharmonic interaction in terms of the complete set of third-order elastic (TOE) moduli, measured values of which are now widely available. However these calculations have not clarified the role of the strain-field scattering mechanism, for while EW are able to account satisfactorily for the measured low-temperature lattice thermal resistivity of deformed Nb (Wasserbäch 1978) examination of the KH results shows (Brown 1983a) that their calculated resistivities are too small to account for the data on deformed Cu, Si and LiF. This suggests that a re-examination and close comparison of the two theories may be desirable.

The KH and EW formulations are difficult to compare at the analytic level because that of the former authors is purely classical while that of the latter emphasises the quantum features. Furthermore, while EW take other sources of phonon scattering into account, KH ignore all but the scattering by parallel groups of identical dislocations. The latter procedure is expected (Brown 1983a) to lead to significant underestimates of thermal resistivity but it is not immediately clear whether this alone is responsible for the different outcomes of the two calculations. Comparisons at the numerical level are not possible because of the disparate crystals considered. A further complication concerns the role of 'global' scattering, due to extensive bending of the crystal, which was calculated by EW and which was used by Wasserbäch (1978) to account for a  $T^3$  temperature dependence of the thermal conductivity  $\kappa$  in the less strongly deformed Nb samples. Some aspects of the global scattering will be discussed in the present paper, and an improved method of dealing with it will be developed, but a detailed study of this and other examples which involve large elastic rotation angles will be deferred to a further publication. The present work is principally a study of 'local' strain-field scattering† by isolated dislocations, all theories of which agree in predicting  $\kappa \propto T^2$  at low temperatures (Klemens 1955, 1958, 1969, Carruthers 1961, Bross 1962, 1966, Bross *et al* 1963a, b, 1965, Seeger *et al* 1964, Gruner 1965a, b, 1968, 1970, Gruner and Bross 1968, Ohashi 1968, KH 1974, 1975, EW 1978).

The present paper has three principal aims. The first aim is to derive the classical and quantum equations describing strain- and rotation-field scattering in such a way that large angles of rotation (e.g. those associated with large-angle grain boundaries and macroscopically bent and twisted crystals) can be included. This is done by studying wave propagation in a crystal whose elastic constants vary with position as a result of the static strains and rotations, an approach that has the advantage of simplicity and requires a more modest mathematical effort than those of KH and EW, to which it is in most respects equivalent. However, its most important feature is that it deals separately with the effects of strains and rotations on the propagation, in a way that allows large rotation angles to be conveniently handled. The resulting form of the scattering Hamiltonian is valid for small strains but arbitrary rotations, being linear in the former but periodic (period  $2\pi$ ) in the latter.

† We use the terms 'local' and 'global' in the sense of EW.

Our second aim is to use the method developed herein to rederive the classical (KH) and quantum (EW) equations that apply when both strains and rotations are small. This serves to verify the soundness of the present method and, equally, as an independent check on the results of KH and EW. Comparison of the latter two treatments shows that the quantum formulation has definite advantages, both conceptual and mathematical.

The third aim is to prepare the way for subsequent numerical estimation of transport coefficients, without the need for the sophisticated machine calculations of KH and EW, so that the theory can be readily tested by applying it to a wider spectrum of crystals. This is achieved (for the case of small distortions) by deriving simplified approximate expressions for scattering probabilities, etc, that retain adequate dependence on the full set of second-order elastic (SOE) and TOE constants, and on the full set of strain and rotation components. Particularly simple results, e.g. equation (5.8), are obtained for cubic crystals, and these have been shown (Brown 1981, 1982, 1983b) to lead to good agreement with experimental thermal conductivity data. These formulae distinguish between the contributions to the scattering from lattice strains and rotations, a distinction that is useful because the former, which involve the TOE constants, typically contribute terms to the scattering amplitude that are an order of magnitude bigger than those arising from the rotations (which enter through the SOE constants only). The latter terms may therefore frequently be neglected, leading to further simplification of the formulae. Also, in certain applications, e.g. to scattering by grain boundaries, energy considerations imply that all strains vanish, leaving only rotations, and again a significant simplification is obtained.

The basic theory is developed in §§ 2 and 3 (classical) and § 4 (quantum). Approximate expressions for scattering probabilities are derived in § 5. Our conclusions are summarised in § 6 and the relationship of earlier theories to the present one is explored in the Appendix.

## 2. Small vibrations about a pre-strained equilibrium state

A statically deformed body is obtained by displacing the material elements that are situated at positions  $a_i$  ( $i = 1, 2, 3$ ) in the 'natural' state (i.e. in the perfectly periodic, stress-free crystal) to positions  $X_i = a_i + U_i$ , thereby defining the static displacements  $U_i$ . We will confine our attention to those configurations  $\{X_i\}$  that represent equilibrium states. Vibrations of the deformed body are then described by additional time-dependent displacements  $u_i(X, t)$  measured from the 'intermediate' state  $\{X_i\}$ . Throughout this paper it is understood that the coordinates  $a_i$ ,  $X_i$ , etc, will be measured with respect to a single fixed set of cartesian axes.

The essential effect of the static deformation is to make the elastic moduli vary with position  $X$  in the body, and the equations of motion for the  $u_i(X, t)$  in terms of these position-dependent moduli may be derived as follows. First we define the *Lagrangian strains*

$$\eta_{ij}(X, t) \equiv \frac{1}{2}(u_{i,j} + u_{j,i} + u_{k,i}u_{k,j}) = \eta_{ji}(X, t) \quad (2.1)$$

where  $u_{i,j} \equiv \partial u_i(X, t)/\partial X_j$  and the repeated-index summation convention is adopted (and will apply elsewhere also, unless otherwise stated). The  $\eta_{ij}$  represent the changes in the size and shape of the unit cell of the intermediate state at  $X$  that are brought about by the additional dynamic displacements. As usual, we assume that the elastic potential energy  $V$  (per unit mass) associated with the vibration is determined by the local strains and

write

$$V = V\{C(X), \boldsymbol{\eta}(X, t)\}. \quad (2.2)$$

The first argument reminds us that the elastic moduli, denoted collectively by  $C$ , depend on position. More general energy functions that involve higher derivatives of the displacement and include the work done by 'couple stresses' during rotational deformations have been discussed by Huntington (1958), Toupin (1962), Mindlin and Tiersten (1962), Krumhansl (1965), Kröner (1970) and Kröner and Datta (1970). The additional terms may be important for very small crystals displaying permanent magnetic or electric polarisation (Hirth and Lothe 1968). They are not important (Krumhansl 1965) for simple metallic and ionic crystals.

Given the function (2.2) the equations of motion may be obtained in the form

$$\rho(X)\ddot{u}_i(X, t) = (\partial/\partial X_j)\{\rho\alpha_{ik}\partial V/\partial\eta_{kj}\} \quad (2.3)$$

where the mass density  $\rho(X)$  of the intermediate state and

$$\alpha_{ij} \equiv \delta_{ij} + u_{i,j} \equiv \alpha_{ij}(X, t) \quad (2.4)$$

are introduced. The equations (2.3) follow from equations (232A.3) and (232A.4) of Truesdell and Toupin (1960) on writing their strain energy function  $\sigma\{X, \boldsymbol{\alpha}\}$  as  $V\{C, \boldsymbol{\eta}\}$ , and using  $\eta_{ij} \equiv \frac{1}{2}(\alpha_{ki}\alpha_{kj} - \delta_{ij})$  and  $\partial/\partial\alpha_{ik} \equiv \alpha_{il}\partial/\partial\eta_{kl}$ .

To proceed further we follow Wallace (1970) and expand the energy density as a power series in the strains:

$$\rho(X)V\{C, \boldsymbol{\eta}\} = C_{ij}(X)\eta_{ij} + \frac{1}{2}C_{ijkl}(X)\eta_{ij}\eta_{kl} + O(\eta^3) \quad (2.5)$$

where

$$C_{ij}(X) = \rho(X)(\partial V/\partial\eta_{ij}) = C_{ji} \quad (2.6)$$

$$C_{ijkl}(X) = \rho(X)(\partial^2 V/\partial\eta_{ij}\partial\eta_{kl}) = C_{jikl} = C_{klij}.$$

The strain derivatives in (2.6) are to be evaluated at  $\boldsymbol{\eta} = 0$ . We need not distinguish between adiabatic, isothermal and 'mixed' elastic moduli, since these are virtually identical for crystals at low temperatures (Wallace 1970, Thurston and Brugger 1964). It is significant that in the present formulation the phonon-defect interactions appear in the *second*-order terms of (2.5) while the phonon-phonon interactions in the deformed crystal first appear in the terms of third order in  $u_{i,j}$ . This clear distinction between the two phonon-scattering mechanisms, both of which are ascribed to lattice anharmonicities, is not so evident in those formulations that are based on the ideal crystal as reference state (e.g. Klemens 1955, 1958, 1969).

The functions  $C_{ij}(X)$  are simply the components  $T_{ij}(X)$  of the stress tensor at  $X$  in the intermediate state (Wallace 1970). Since this is an equilibrium state we have

$$C_{ij,j} = T_{ij,j} = 0 \quad (2.7)$$

and substituting (2.5) and (2.7) into (2.3) we readily obtain

$$\rho(X)\ddot{u}_i = u_{i,kj}T_{kj}(X) + u_{k,ij}C_{klji}(X) + u_{k,i}C_{klji,j}(X). \quad (2.8)$$

Our equations so far have made no reference to the 'natural' (undeformed) state of the body, but we must now express the stress  $T_{kj}(X)$  and the elastic moduli  $C_{klji}(X)$  in terms of the strains

$$n_{ij}(X) \equiv \frac{1}{2}(U_{i,j} + U_{j,i} + U_{k,i}U_{k,j}) = n_{ji} \quad (2.9)$$

and rotations

$$\omega_{ij}(X) \equiv \frac{1}{2}(U_{i,j} - U_{j,i}) = -\omega_{ji} \quad (2.10)$$

associated with the deformation from the natural to the intermediate state. Since it is desirable to work with the conventionally tabulated elastic constants of the natural state we will henceforth suppose that the fixed axes  $\{X_i\}$  are chosen to lie along the conventional symmetry directions of the crystal in its natural state (e.g. along the unit cell edges of a cubic crystal). Provided the quantities (2.10) are *small* we can regard the deformed unit cell at  $X$  as being obtained from the initially undeformed cell by first *rotating* the axes through the angles (2.10) to form a rotated but still orthogonal set  $\{\tilde{X}_i\}$ , and then *straining* the rotated cell. Then the state of stress produced by the strain is specified by the tensor components†

$$\tilde{T}_{\alpha\beta}(X) = \bar{c}_{\alpha\beta\gamma\delta}\bar{n}_{\gamma\delta}(X) + O(\bar{n}^2) \quad (2.11)$$

where the bars indicate that all tensors are expressed with respect to the  $\{\tilde{X}_i\}$  axes. Since the latter lie along the conventional symmetry directions for the unit cell at  $X$  it is clear that the  $\bar{c}_{\alpha\beta\gamma\delta}$  are the *conventional* second-order elastic (SOE) constants. To get the stress components  $T_{ij}(X)$  in the  $\{X_i\}$  system, which are required in (2.8), we use the usual laws of transformation of cartesian tensors to obtain

$$T_{ij} = \rho_{\alpha i}\rho_{\beta j}\tilde{T}_{\alpha\beta} \quad n_{ij} = \rho_{\alpha i}\rho_{\beta j}\bar{n}_{\alpha\beta} \quad (2.12)$$

where  $\rho_{\alpha i} \equiv \partial\tilde{X}_\alpha/\partial X_i$  satisfy the orthogonality conditions

$$\rho_{\alpha i}\rho_{\alpha j} = \delta_{ij}. \quad (2.13)$$

Use of (2.13) and (2.12) in (2.11) readily yields

$$T_{ij} = c_{ijkl}n_{kl} + O(n^2) \equiv C_{ij} \quad (2.14)$$

where

$$c_{ijkl} = \bar{c}_{\alpha\beta\gamma\delta}\rho_{\alpha i}\rho_{\beta j}\rho_{\gamma k}\rho_{\delta l} = c_{ijkl}(X) \quad (2.15)$$

are the components, with respect to the  $\{X_i\}$  axes, of the elastic modulus tensor of an undeformed crystal whose orientation is that of the unit cell at position  $X$  in the deformed crystal. They depend on  $X$  through the rotation matrices  $\rho_{\alpha i}(X)$ , which have the form

$$\rho_{\alpha i}(X) = \delta_{\alpha i} - \omega_{\alpha i}(X) + O(\omega^2) \quad (2.16)$$

for small  $\omega_{\alpha i}$ . Since we envisage applications to situations where  $\omega$  is small and of the same order as  $n$  (e.g. in dislocated crystals), or where  $n \equiv 0$  and  $|\omega| \ll 1$  (e.g. small-angle grain boundaries), the use of (2.16) in (2.14) yields

$$T_{ij}(X) = \bar{c}_{ijkl}n_{kl}(X) + O(n^2, \omega n, \omega^2) \quad (2.17)$$

where the second-order terms are negligible.

For the  $C_{ijkl}(X)$  we first of all use equation (8.20) of Wallace (1970) to obtain the elastic modulus tensor  $\bar{C}_{\alpha\beta\gamma\delta}(X)$  in terms of the rotated but unstrained system  $\{\tilde{X}_i\}$ :

$$\begin{aligned} \bar{C}_{\alpha\beta\gamma\delta}(X) = & \bar{c}_{\alpha\beta\gamma\delta} - \bar{c}_{\alpha\beta\gamma\delta}\bar{n}_{pp} + \bar{c}_{\alpha\beta\gamma p}\bar{n}_{\delta p} + \bar{c}_{\alpha\beta p\delta}\bar{n}_{\gamma p} \\ & + \bar{c}_{\alpha p\gamma\delta}\bar{n}_{\beta p} + \bar{c}_{p\beta\gamma\delta}\bar{n}_{\alpha p} + \bar{c}_{\alpha\beta\gamma\delta p q}\bar{n}_{p q} + O(n^2). \end{aligned} \quad (2.18)$$

† Greek indices take values (1, 2, 3) just like italic indices.

The  $\bar{c}_{\alpha\beta\gamma\delta\rho q}$  are the (conventional) third-order elastic constants. On transforming to the fixed system  $\{X_i\}$  we obtain, just as in (2.15),

$$C_{ijkl}(X) = \rho_{\alpha i} \rho_{\beta j} \rho_{\gamma k} \rho_{\delta l} \bar{C}_{\alpha\beta\gamma\delta}(X). \quad (2.19)$$

Using (2.16) and the inverse of (2.12) in (2.19) then yields

$$C_{ijkl}(X) = \bar{c}_{ijkl} + S_{ijkl}(X) + R_{ijkl}(X) + O(n^2, \omega n, \omega^2) \quad (2.20)$$

where

$$S_{ijkl}(X) = -\bar{c}_{ijk} n_{pp} + \bar{c}_{ijkp} n_{lp} + \bar{c}_{ijpl} n_{kp} + \bar{c}_{ipkl} n_{jp} + \bar{c}_{pikl} n_{ip} + \bar{c}_{ijkpq} n_{pq} \quad (2.21)$$

depends only on the strains, and

$$R_{ijkl}(X) = \bar{c}_{ijkp} \omega_{lp} + \bar{c}_{pjkl} \omega_{lp} + \bar{c}_{ipkl} \omega_{jp} + \bar{c}_{ijpl} \omega_{kp} \quad (2.22)$$

depends only on the rotations.

If we introduce the constant density  $\rho_0$  of the natural state and write  $\rho(X) = \rho_0(1 - n_{pp} + O(n^2))$ , and also use (2.18) and (2.20), the equations of motion (2.8) become, to leading order,

$$\begin{aligned} \rho_0 \ddot{u}_i - \bar{c}_{klji} u_{k,lj} = & \bar{c}_{kijlm} n_{lm} u_{i,kj} + (\bar{c}_{klji} n_{pp} + S_{klji} \\ & + R_{klji}) u_{k,lj} + (S_{klji,j} + R_{klji,j}) u_{k,l} \end{aligned} \quad (2.23)$$

where the terms involving the static deformation are collected on the right-hand side. These equations are suitable for a classical treatment of scattering by *small* strains and rotations. We observe that the static rotations that enter (2.23) via (2.22) are associated only with the SOE constants, but the static strains are associated, in (2.21), with the TOE constants as well. Since the latter are usually an order of magnitude larger than the SOE constants we expect that the contribution of the rotations to the scattering will frequently be negligible. An important exception is when all  $n_{ij}$  vanish but  $\omega_{ij} \neq 0$ , which is frequently the case for grain boundaries.

Application of (2.23) will normally be to systems in which the strains and rotations are localised to some extent, for example in the vicinity of a crystal defect. However the equations also describe propagation in a *uniformly* strained and/or rotated crystal, in which cases the terms on the right-hand side simply define the (position-independent) elastic constants appropriate to the new unit-cell orientation and morphology.

Equations (2.23) are similar to equations (16) of KH (1974). They differ firstly by the appearance of  $\partial U_i / \partial a_j$  in the latter where, by virtue of (2.9), (2.10), (2.20) and (2.21),  $\partial U_i / \partial X_j$  appears in the former. This difference is not important since the two derivatives differ only by terms of second order in the static strains and rotations and such terms have already been omitted from both (2.23) and equation (16) in KH (1974). The only real difference between (2.23) and equation (16) in KH (1974) concerns the absence from the latter of the last terms of the former. These terms, which are proportional to the gradients of the static strains and rotations, complicate the classical analysis and were dropped from equation (5) of KH (1974) for reasons of convenience. Their omission may be justifiable (on the grounds that these terms decrease more rapidly with distance from the defect than do the terms that were retained) but KH do not explicitly show their effects to be negligible. It is one of several attractive features of the quantum formulation (§ 4) that these difficulties do not arise, so rather than pursue the classical solutions of (2.23) it is preferable to quantise the elastic vibration field. This leads us

first to consider the classical Hamiltonian and its associated normal coordinates and their conjugate momenta.

We emphasise that (2.16)–(2.23) apply only when the strains and rotations are *both* small enough to make second-order terms negligible. The case of large rotation angles will be discussed following equation (4.6).

### 3. The classical Hamiltonian

In terms of (2.2) the Lagrangian density is

$$\mathcal{L} = \frac{1}{2}\rho(X)\dot{u}_i\dot{u}_i - \rho(X)V\{C, \eta\} \quad (3.1)$$

so that the momentum density conjugate to  $u_i$  is

$$p_i \equiv \partial\mathcal{L}/\partial\dot{u}_i = \rho(X)\dot{u}_i. \quad (3.2)$$

In terms of these conjugate variables the Hamiltonian is

$$H = \int_{\Omega} (\frac{1}{2}\rho^{-1}p_i p_i + \rho V) d^3X \quad (3.3)$$

where the integral is over the volume  $\Omega$  of the statically deformed body.

Upon using (2.1), (2.5), (2.17) and (2.20)–(2.22) in (3.3) we find

$$H = H_0 + H' + O(u_{i,j}^3) \quad (3.4)$$

where

$$H_0 = \frac{1}{2} \int_{\Omega} (\rho_0^{-1} p_i p_i + \bar{c}_{ijkl} u_{i,j} u_{k,l}) d^3X \quad (3.5)$$

$$H' = \frac{1}{2} \int_{\Omega} [n_{ii} p_j p_j / \rho_0 + \bar{c}_{ijkl} n_{kl} (2u_{i,j} + u_{m,i} u_{m,j}) + (S_{ijkl} + R_{ijkl}) u_{i,j} u_{k,l}] d^3X \quad (3.6)$$

and terms higher than second order in the  $u_{i,j}$  and higher than first order in the  $U_{i,j}$  have been discarded.

The term linear in  $u_{i,j}$  can be transformed, using the divergence theorem and the equilibrium condition (2.7), to the form

$$\int_{\Omega} \bar{c}_{ijkl} n_{kl} u_{i,j} d^3X = \int_S \bar{c}_{ijkl} n_{kl} u_i dS_j \quad (3.7)$$

where  $S$  is the surface of the statically deformed body. This represents the work done during the dynamic displacement  $u_i$  by the surface tractions acting on the statically stressed body. Hence (3.7) vanishes for the usual case where the body has a free surface. It also vanishes if the surface is constrained so that  $u_i(S) = 0$ . For other boundary conditions it may not vanish but it can be shown to make no contribution to the elastic scattering, because of the energy conservation requirement of time-dependent perturbation theory. This term will henceforth be dropped from (3.6).

The fact that the  $H_0$  defined by (3.5) is not the Hamiltonian of the body in its undeformed state (because the  $u_i$  are not displacements from the natural state and the volume  $\Omega$  is not in general that of the undeformed body) deserves emphasis, as this is characteristic of strain-field scattering. Rather,  $H_0$  is the Hamiltonian of a (fictitious) body filling the volume  $\Omega$  of the deformed body and having the same elastic constants



and density, and therefore the same dispersion relations, as the natural state. However, from (3.4)–(3.6) we see that the energy–momentum eigenfunctions of  $H_0$  (or, classically, its normal modes) provide a convenient set of base states that allow us to describe the vibrational properties of the deformed crystal within the usual framework of time-dependent perturbation theory and its associated concepts of transition rates, scattering cross sections, etc.

To proceed towards quantisation we need to introduce classical normal coordinates for the system described by  $H_0$ . Thus we write the continuous function  $u_\alpha(X, t)$  as the Fourier integral

$$u_\alpha(X, t) = \frac{1}{8\pi^3} \left( \frac{\Omega}{\rho_0} \right)^{1/2} \int F_\alpha(\mathbf{k}, t) \exp(i\mathbf{k} \cdot \mathbf{X}) d^3k. \quad (3.8)$$

The integration in (3.8) is over all  $\mathbf{k}$ -space. However, adoption of a continuum model already implies that only slowly varying displacements will be considered, so without further approximation we may assume that the  $F_\alpha$  are appreciable only for small  $|\mathbf{k}|$  and restrict the integration to the first Brillouin zone of the undeformed crystal. As is well known, the classical treatment of the Hamiltonian  $H_0$  leads to the result (Callaway 1974) that the  $F_\alpha$  are linear combinations of the eigenvectors  $e_\alpha^i(\mathbf{k})$  of the dynamical matrix

$$D_{\alpha\gamma}(\mathbf{k}) = \bar{c}_{\alpha\beta\gamma\delta} k_\beta k_\delta / \rho_0 = D_{\alpha\gamma}^*(\mathbf{k}) = D_{\gamma\alpha}(\mathbf{k}) = D_{\alpha\gamma}(-\mathbf{k}) \quad (3.9)$$

i.e.

$$F_\alpha(\mathbf{k}, t) = e_\alpha^j(\mathbf{k}) Q_j(\mathbf{k}, t) \quad (3.10)$$

where

$$\omega_j^2(\mathbf{k}) e_\alpha^j(\mathbf{k}) = D_{\alpha\gamma}(\mathbf{k}) e_\gamma^j(\mathbf{k}). \quad (3.11)$$

The sum in (3.11) is over all components  $\gamma$  but not over the polarisation branches  $j = 1, 2, 3$ . Without loss of generality we can choose (Callaway 1974)

$$\omega_j(\mathbf{k}) = \omega_j(-\mathbf{k}) \equiv \omega_{jk} \quad e_\alpha^j(\mathbf{k}) = e_\alpha^{j*}(-\mathbf{k}) \quad (3.12)$$

so that for real displacements  $u_\alpha$  we have from (3.8)–(3.11)

$$Q_j^*(\mathbf{k}, t) = Q_j(-\mathbf{k}, t) \equiv Q_{jk}^*. \quad (3.13)$$

We record the orthonormality and closure relations (Callaway 1974)

$$e_\alpha^{j*}(\mathbf{k}) e_\alpha^i(\mathbf{k}) = \delta_{ij} \quad e_\alpha^{j*}(\mathbf{k}) e_\beta^j(\mathbf{k}) = \delta_{\alpha\beta} \quad (3.14)$$

and we will also find it convenient to use

$$\delta(\mathbf{k}) = \lim_{\Omega \rightarrow \infty} \frac{1}{8\pi^3} \int_\Omega \exp(i\mathbf{k} \cdot \mathbf{X}) d^3X. \quad (3.15)$$

Finally, on substituting (3.2) and (3.8) into (3.5), and using (3.10)–(3.15) we obtain

$$\mathcal{H}_0 = \frac{H_0}{\Omega} = \frac{1}{2} \sum_{j=1}^3 \int (|\dot{Q}_{jk}|^2 + \omega_{jk}^2 |Q_{jk}|^2) \frac{d^3k}{8\pi^3}. \quad (3.16)$$

The Lagrangian  $L_0$  corresponding to  $H_0$  is obtained by changing the sign of the last term in (3.16). It yields the ‘momentum’ conjugate to the normal coordinate  $Q_{jk}$  as

$$P_{jk} \equiv \partial L_0 / \dot{Q}_{jk} = \dot{Q}_{jk} \quad (3.17)$$

and on introducing this into (3.16) we have

$$H_0 = \frac{1}{2} \sum_{j=1}^3 \int (|P_{jk}|^2 + \omega_{jk}^2 |Q_{jk}|^2) \frac{d^3k}{8\pi^3}. \quad (3.18)$$

Similarly the part (3.6) of the Hamiltonian that is responsible for transitions between the modes of  $H_0$  leads to

$$\begin{aligned} \mathcal{H}' = \frac{H'}{2\rho_0} = \frac{1}{2\rho_0} \iint \{ & k'_\beta k_\delta Q_{j'k'} Q_{jk}^* [(\tilde{S}_{\alpha\beta\gamma\delta} + \tilde{R}_{\alpha\beta\gamma\delta}) e_\alpha^{j'}(\mathbf{k}') e_\gamma^{j*}(\mathbf{k}) + \tilde{c}_{\beta\delta\gamma\alpha} \tilde{n}_{\gamma\alpha} e_\tau^{j'}(\mathbf{k}') e_\tau^{j*}(\mathbf{k})] \\ & + \rho_0 \tilde{n}_{\alpha\alpha} e_\beta^{j'}(\mathbf{k}') e_\beta^{j*}(\mathbf{k}) P_{j'k'} P_{jk}^* \} d^3k d^3k' / (8\pi^3)^2 \end{aligned} \quad (3.19)$$

where the tilde indicates the Fourier transform of argument  $(\mathbf{k}' - \mathbf{k})$ , e. g.

$$\tilde{n}_{\alpha\beta} \equiv \tilde{n}_{\alpha\beta}(\mathbf{k}' - \mathbf{k}) = \lim_{\Omega \rightarrow \infty} \int_{\Omega} \exp[i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{X}] n_{\alpha\beta}(\mathbf{X}) d^3X. \quad (3.20)$$

The normalisation of (3.20) has been chosen to agree with that of Klemens (1958, equation (5.22)), and it is assumed that the strains and rotations are sufficiently localised for the integral in (3.20) to converge to a volume-independent value as  $\Omega$  increases. Hence, this formulation is suitable for distortions due to isolated (point) defects, which are localised in three dimensions. For isolated line and surface defects (e.g. dislocations and grain boundaries) and for the practically interesting cases which involve a finite concentration of point, line or surface imperfections, the strain and rotation fields extend throughout the crystal volume with undiminished amplitude in at least one dimension. These cases may be dealt with in a straightforward manner by working with a crystal of finite volume or by deferring the limiting process in (3.20) to a later stage in the calculation. If desired, the defect concentration may then be introduced in a natural way for a uniform distribution of defects. In a finite-crystal formulation it may sometimes be convenient to replace the integrals in (3.18) and (3.19) by sums over the quasicontinuous distribution of wavevectors according to

$$\int d^3k = \frac{8\pi^3}{\Omega} \sum_{\mathbf{k}}. \quad (3.21)$$

#### 4. Quantisation

The quantisation of (3.18) and (3.19) can now be carried out in the usual way by replacing the classical  $P_{jk}$  and  $Q_{jk}$  by *operators* (and their complex conjugates by the Hermitian conjugate operators) that are independent of time in the Schrödinger picture and satisfy the commutation rules (see, e.g., Callaway 1974)

$$\begin{aligned} [Q_{jk}^*, P_{j'k'}] &= -[Q_{jk}, P_{j'k'}^\dagger] = i\hbar \delta_{jj'} \delta(\mathbf{k} - \mathbf{k}') \\ [Q_{jk}, Q_{j'k'}^\dagger] &= [P_{jk}, P_{j'k'}^\dagger] = [Q_{jk}, P_{j'k'}] = 0. \end{aligned} \quad (4.1)$$

The annihilation and creation operators,  $b_{jk}$  and  $b_{jk}^\dagger$  respectively, are defined by

$$b_{jk} = (\omega_{jk}/2\hbar)^{1/2} Q_{jk} + i(2\hbar\omega_{jk})^{-1/2} P_{jk} \quad (4.2)$$

and its Hermitian conjugate. By using the operator equivalents of (3.13) and (3.17) the

inverse transformations

$$Q_{jk} = (\hbar/2\omega_{jk})^{1/2}(b_{jk} + b_{j,-k}^\dagger) \quad P_{jk} = -i(\hbar\omega_{jk}/2)^{1/2}(b_{jk} - b_{j,-k}^\dagger) \quad (4.3)$$

are readily obtained. On using these in (3.18) and (3.19), and employing the commutation relations (4.1), we find

$$\mathcal{H}_0 = \sum_j \int \hbar\omega_{jk}(b_{jk}^\dagger b_{jk} + \frac{1}{2}) d^3k/8\pi^3 \quad (4.4)$$

and

$$\mathcal{H}' = \sum_{jj'} \int \int (h_{jj'}(\mathbf{k}, \mathbf{k}') b_{jk} b_{j'k'}^\dagger + h_{jj'}^*(\mathbf{k}, \mathbf{k}') b_{jk}^\dagger b_{j'k'}) \frac{d^3k d^3k'}{(8\pi^3)^2} \quad (4.5)$$

where terms of type  $bb$  and  $b^\dagger b^\dagger$ , which do not contribute to the two-phonon scattering, have been dropped from the latter equation. The two-phonon scattering amplitude in (4.5) is given by

$$h_{jj}^*(\mathbf{k}, \mathbf{k}') = h_{jj}(\mathbf{k}', \mathbf{k}) = [\hbar(\omega\omega')^{1/2}/4] \bar{D}(\mathbf{k}' - \mathbf{k}) e_{\alpha}^{j'}(\mathbf{k}') e_{\alpha}^{j*}(\mathbf{k}) \\ + [\hbar k_{\beta} k'_{\delta} / 4\rho_0(\omega\omega')^{1/2}] e_{\alpha}^{j*}(\mathbf{k}) e_{\gamma}^{j'}(\mathbf{k}') (\bar{S}_{\alpha\beta\gamma\delta}(\mathbf{k}' - \mathbf{k}) + \bar{R}_{\alpha\beta\gamma\delta}(\mathbf{k}' - \mathbf{k})). \quad (4.6)$$

We have written  $\bar{D} \equiv \bar{n}_{\alpha\alpha} + (k_{\alpha} k'_{\beta} / \rho_0 \omega \omega') \bar{c}_{\alpha\beta\gamma\delta} \bar{n}_{\gamma\delta}$  and  $\omega_{jk} \equiv \omega$ ,  $\omega_{j'k'} \equiv \omega'$ .

We emphasise that the expression (4.6) for the scattering amplitude for two-phonon processes is *exact* (to first order in the static strains and rotations). As shown in the Appendix, it bears a close relationship to the third of Klemens' estimates (Klemens 1969).

The matrix elements (4.6) are linear in the static strains and rotations, and it is clear from their derivation that they are only applicable when both strains and rotations are small. The same remarks apply to the classical equations (3.19) and (2.23). The limitation to small *strains* cannot be removed in any obvious way, but there is little need to do so since energy considerations will generally ensure that strains remain small. Large rotations can be dealt with by using the exact rotation matrices  $\rho_{ij}$  in place of the small-angle expressions (2.16). To specify the functions  $\rho_{ij}(\mathbf{X})$  we imagine removing a small volume element surrounding the point  $\mathbf{X}$  in the deformed body and letting it relax so that its atoms undergo further displacements  $\bar{U}_i$  corresponding to the strains  $\bar{n}_{ij} \equiv -n_{ij}(\mathbf{X})$ . This additional strain, which returns the previously strained element to its natural state, is essentially homogeneous since it is implicit in our theory that strains (and rotations) undergo only small fractional changes over distances of the order of the phonon wavelength. Consequently we can achieve this with *no further rotational deformation*, a condition that is assured if  $\bar{U}_i(\mathbf{X}, \mathbf{X}')$  is chosen to satisfy  $\partial \bar{U}_i / \partial X_j' = \partial \bar{U}_j / \partial X_i'$ ; here  $\mathbf{X}'$  labels positions within the element removed from the neighbourhood of  $\mathbf{X}$ . Under these conditions the final relaxed orientations of the (cubic) unit-cell edges define the directions of the axes  $\bar{X}_i$  (see the discussion following (2.10)) at the point  $\mathbf{X}$  and hence the quantities  $\rho_{\alpha i} \equiv \partial \bar{X}_{\alpha} / \partial X_i$ .

The above procedure shows that the  $\rho_{\alpha i}$  are well defined and can be calculated, but explicit expressions for the  $\rho_{\alpha i}$  in terms of the  $U_{i,j}$  are not obtainable in general. This is because transformations that involve large rotations<sup>†</sup> cannot be described in terms of *independent* (i.e. commuting) rotations about the three coordinate axes. Nevertheless

<sup>†</sup> It is the commutation of infinitesimal rotations that makes the simple representation (2.16) possible.

there are situations of physical interest, such as tilt and twist grain boundaries and uniformly bent or twisted crystals, that involve rotations about one direction only, say that of the  $X_3$  axis. Phonon scattering by these distortions can be studied by using

$$\rho = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \psi & \sin \psi \\ 0 & -\sin \psi & \cos \psi \end{pmatrix} \quad (4.7)$$

in place of (2.16). Here  $\psi(X)$  represents the angle of rotation of a short fibre at  $X$  that before deformation was perpendicular to the  $X_3$  axis. When used in (2.15) and (2.19), equation (4.7) leads to differential equations (cf (2.23)) and a scattering Hamiltonian (cf (3.19) and (4.6)) that are linear in the strains but are periodic, as they clearly should be, in the rotation angle  $\psi$ . One must distinguish between the (average) angles of rotation,  $\psi(X)$ , of material fibres at  $X$  and the quantity  $\omega_{21}(X)$  defined in terms of the displacement gradients by (2.10), since these two quantities are identical only for small angles. The precise relationship between  $\psi$  and  $\omega_{21}$  (henceforth  $\omega$ ) is investigated by Novozhilov (1961, ch 1, § 10). Corresponding to his equations (10.13) we find that the values of  $\cos \psi$  and  $\sin \psi$ , averaged over fibres of all orientations at  $X$ , are given by

$$\begin{aligned} \langle \cos \psi \rangle &= \left( \frac{(1 + U_{1,1})(1 + U_{2,2}) - \frac{1}{4}(U_{1,2} + U_{2,1})^2}{\omega^2 + (1 + U_{1,1})(1 + U_{2,2}) - \frac{1}{4}(U_{1,2} + U_{2,1})^2} \right)^{1/2} \\ \langle \sin \psi \rangle &= \omega [\omega^2 + (1 + U_{1,1})(1 + U_{2,2}) - \frac{1}{4}(U_{1,2} + U_{2,1})^2]^{-1/2}. \end{aligned} \quad (4.8)$$

Our assumption that the strains (2.9) are small will ordinarily imply that the combinations  $(U_{i,j} + U_{j,i})$  are small so that (4.8) reduces to

$$\begin{aligned} \langle \cos \psi \rangle &\simeq (1 + \omega^2)^{-1/2} [1 + \omega^2(U_{1,1} + U_{2,2})/2(1 + \omega^2)] \\ \langle \sin \psi \rangle &\simeq \omega(1 + \omega^2)^{-1/2} [1 - (U_{1,1} + U_{2,2})/2(1 + \omega^2)]. \end{aligned} \quad (4.9)$$

Furthermore, for the uniaxial deformation considered we will generally have  $U_{3,3} = 0$ , and it then follows from Novozhilov (1961, ch 1, equations (13.3) and (5.6)) that (4.9) take the form

$$\begin{aligned} \langle \cos \psi \rangle &\simeq (1 + \omega^2)^{-1/2} [1 + \omega^2(\Delta - \omega^2)/2(1 + \omega^2)] \\ \langle \sin \psi \rangle &\simeq \omega(1 + \omega^2)^{-1/2} [1 + (\omega^2 - \Delta)/2(1 + \omega^2)] \end{aligned} \quad (4.10)$$

where  $\Delta(X)$  is the dilatation. In many cases the latter may be negligibly small. The approximation involved in (4.9) and (4.10) consists of the omission from the square bracket of terms that are quadratic in the shear strains. The application of the above formulae to the study of phonon scattering in crystals subject to large angular deformations will be considered in a later publication.

Finally, for uniform strains and rigid rotations both (4.6) and the large-angle version of it yield scattering amplitudes proportional to  $\delta(\mathbf{k}' - \mathbf{k})$ . This indicates the obvious fact that a plane wave will propagate without scattering in any perfect crystal, whatever its symmetry or orientation (at least for small wavevectors far from Brillouin-zone boundaries).

To complete this section we present some expressions for transition rates, scattering cross sections, etc, in terms of the matrix elements (4.6). It will be convenient to consider a deformed body of large but finite volume  $\Omega$  and to include polarisation and wavevector in the single label  $\kappa \equiv j\mathbf{k}$ . The many-phonon eigenstates of  $H_0$  that correspond to  $N_\kappa$

phonons in each state  $\kappa$  are denoted by  $|\dots, N_\kappa, \dots\rangle$ . The matrix elements of  $H'$  are readily evaluated from (4.6) using (Callaway 1974)

$$\begin{aligned} b_\kappa |\dots, N_\kappa, \dots\rangle &= N_\kappa^{1/2} |\dots, N_\kappa - 1, \dots\rangle \\ b_\kappa^\dagger |\dots, N_\kappa, \dots\rangle &= (N_\kappa + 1)^{1/2} |\dots, N_\kappa + 1, \dots\rangle \end{aligned} \quad (4.11)$$

The only non-zero matrix elements are those of the form

$$\begin{aligned} H'_{\kappa\kappa'} &= \langle \dots, N_\kappa - 1, \dots, N_{\kappa'} + 1, \dots | H' | \dots, N_\kappa, \dots, N_{\kappa'} \dots \rangle \\ &= (2h_{\kappa\kappa'}/\Omega) [N_\kappa(N_{\kappa'} + 1)]^{1/2} \end{aligned} \quad (4.12)$$

which correspond to the scattering of a phonon from state  $\kappa$  to state  $\kappa'$ . Standard time-dependent perturbation theory (see e.g. Schiff 1968) yields for the transition rate induced by  $H'$

$$\frac{dN_\kappa}{dt} = \frac{2\pi\Omega}{\hbar^2} \sum_{j'} \int_{S'} \frac{dS'}{8\pi^3} \frac{|H'_{\kappa\kappa'}|^2 - |H'_{\kappa'\kappa}|^2}{|\nabla_{\mathbf{k}'}\omega_{\kappa'}|} \quad (4.13)$$

where the integration is over the surface  $\omega_{\kappa'} = \omega_\kappa$ . Use of (4.12) gives

$$\frac{dN_\kappa}{dt} = \frac{8\pi}{\hbar^2\Omega} \sum_{j'} \int_{S'} \frac{dS'}{8\pi^3} \frac{h_{\kappa\kappa'}^2 (N_{\kappa'} - N_\kappa)}{|\nabla_{\mathbf{k}'}\omega_{\kappa'}|}. \quad (4.14)$$

The relaxation rate which describes the return of the phonon distribution from  $N_\kappa \equiv N^0 + n_\kappa$  to the Bose-Einstein equilibrium value  $N^0(\omega) = 1/[\exp(\hbar\omega/kT) - 1]$  is, according to (4.14),

$$\tau_\kappa^{-1} \equiv -\frac{1}{n_\kappa} \frac{dn_\kappa}{dt} = \frac{8\pi}{\hbar^2\Omega} \sum_{j'} \int_{S'} \frac{dS'}{8\pi^3} |h_{\kappa\kappa'}|^2 \frac{(1 - n_{\kappa'}/n_\kappa)}{|\nabla_{\mathbf{k}'}\omega_{\kappa'}|} \quad (4.15)$$

Scattering cross sections can similarly be calculated. For example, in ballistics experiments where a large incident flux of phonons centred on state  $\kappa = j\mathbf{k}$  is injected, the number of phonons per second per unit incident flux  $(v_\kappa N_\kappa/\Omega)$  scattered into all final states  $\kappa'$  of a single polarisation  $j'$  is

$$\sigma(j\mathbf{k} \rightarrow j') = \frac{8\pi}{\hbar^2 v_\kappa} (N^0 + 1) \int_{S'} \frac{dS'}{8\pi^3} |h_{\kappa\kappa'}|^2 |\nabla_{\mathbf{k}'}\omega_{\kappa'}| \quad (4.16)$$

where the final states were assumed to be in thermal equilibrium, i.e.  $N_{\kappa'} = N^0(\omega_{\kappa'})$ . In the approximation,  $\omega_{j\mathbf{k}} = v_j|\mathbf{k}|$ , this becomes

$$\sigma(j\mathbf{k} \rightarrow j') = (8\pi/\hbar^2 v_j v_{j'}) \int_{S'} (dS'/8\pi^3) |h_{\kappa\kappa'}|^2. \quad (4.17)$$

The corresponding differential cross sections are obtained by restricting the integration to a small element  $\delta S'$  centred on a particular  $\mathbf{k}'$ .

In view of intended applications to scattering by line defects in crystals we need to specialise (4.13)–(4.17) to the case

$$h_{jj'}(\mathbf{k}, \mathbf{k}') = h_{jj'k_3}(\mathbf{k}_*, \mathbf{k}_*) \delta_{k_3k'_3} \quad (4.18)$$

where  $\mathbf{k}_* \equiv \mathbf{k} - \mathbf{k}_3$  and the component  $k_3$  of the wavevector parallel to the line defect (chosen as the  $X_3$  axis) is conserved in the scattering process. We find, for a crystal of length  $L$  in the  $X_3$  direction, that the appropriate formulae are obtained from (4.13)–

(4.17) by replacing the surface integral by

$$\int_{S'} dS'/8\pi^3 \rightarrow \frac{1}{L} \oint_{\lambda'(k_3)} dl'/4\pi^2 \quad (4.19)$$

and replacing  $\nabla\omega$  by its projection perpendicular to the line defect, and of course setting  $k'_3 = k_3$ . The line integral in (4.19) is around the curve  $\lambda'(k_3)$  of intersection of the plane  $k'_3 = k_3$  with the surface  $\omega_{K'} = \omega_K$ .

## 5. Reduction of $|h_{KK'}|^2$

The absolute square of (4.6) is the sum of more than  $3^{12}$  terms, each of which depends on the wavevectors and polarisations of both initial and final states as well as on the Fourier transforms of static strain and rotation components. Clearly, the exact calculation of scattering cross sections, etc, demands sophisticated computing techniques. Such calculations are capable of yielding valuable insights into the detailed angular distribution of the scattering due to specific crystal defects (KH 1974, 1975). However, the results must be used with care in deducing the transport properties of deformed crystals in which other scattering processes also play a significant role in limiting phonon mean free paths. This is especially true (Brown 1983a) in cases where the scattering is strongly anisotropic, as it is for scattering by single straight dislocations (KH 1974). In such cases it may appear to be highly inappropriate to replace the differential cross section by an average value, independent of propagation directions and polarisations. On the contrary, it has been argued (Brown 1983a) that the *failure* to do so can lead to considerable overestimates of lattice thermal conductivity of crystals having 'real' (i.e. multidirectional, multicharacterised) dislocation distributions. The same applies even for crystals having a single set of identical parallel dislocations unless one takes proper account of other scattering mechanisms, e.g. boundaries, impurities and three-phonon processes, which limit the mean free paths of those modes for which dislocation scattering is particularly weak.

The above considerations lead us to endorse the procedures of Klemens (1955, 1958, 1969), Carruthers (1961) and others who have worked with directional and polarisation-averaged transition probabilities.

We can average  $|h_{KK'}|^2$  over polarisations by applying the closure relation (3.14) to the absolute square of (4.6). We find

$$\begin{aligned} \langle |h_{kk'}|^2 \rangle &= \frac{1}{6} \sum_{jj'} |h_{jj'}(\mathbf{k}, \mathbf{k}')|^2 \\ &= \frac{1}{3} (\hbar\omega/4)^2 |\bar{D}|^2 + (\hbar^2 k'_\beta k_\delta / 144 \rho_0) (\bar{D} T_{\alpha\beta\alpha\delta}^* + \bar{D}^* \bar{T}_{\alpha\beta\alpha\delta}) \\ &\quad + (\hbar/12 \rho_0 \omega)^2 k'_\beta k'_\eta k_\delta k_\zeta \bar{T}_{\alpha\beta\gamma\delta} \bar{T}_{\alpha\eta\gamma\zeta}^* \end{aligned} \quad (5.1)$$

where

$$\bar{T}_{\alpha\beta\gamma\delta} \equiv \bar{S}_{\alpha\beta\gamma\delta} + \bar{R}_{\alpha\beta\gamma\delta} \quad (5.2)$$

and we have set  $\omega' = \omega = \text{constant}$ , independent of  $(j, \mathbf{k})$ . It is understood that the argument of each Fourier transform in (5.1) and (5.2) is  $(\mathbf{k}' - \mathbf{k})$ .

The result (5.1) is exact, but in typical applications one may actually require an average  $|h|^2$  that differs from (5.1) by the appearance of weighting factors in the summand that involve the propagation velocities of the  $j\mathbf{k}$  and  $j'\mathbf{k}'$  modes. In such cases

an appropriately defined average velocity must be adopted together with (5.1). A detailed study of (4.6) shows that individual values of  $|h_{\mathbf{k}\mathbf{k}'}|^2$  can differ from (5.1) by quite large factors. In fact the  $j = j' = 1$  (longitudinal mode) term is invariably larger than (5.1), by a factor that may be as large as three for certain types of deformation. The four (longitudinal, transverse) terms are also generally larger than (5.1), by factors that may be as high as 1.5, while the four (transverse, transverse) terms are smaller than (5.1) by amounts sufficient to make (5.1) an exact average.

Ordinarily the final term in (5.1) dominates the expression since the absolute values of the TOE constants that appear in  $\hat{T}$  are typically an order of magnitude greater than the SOE constants that appear in  $\hat{D}$ . Estimates for dislocation strain fields show that the first term in (5.1) accounts for less than 0.3% of the total while the middle-term contribution fluctuates in sign, as the directions of  $\mathbf{k}$  and  $\mathbf{k}'$  vary, with amplitude less than 2% of the total. Taking these estimates as typical we conclude that to a good approximation (2% error), which becomes excellent (0.3% error) if an angular average is subsequently taken, (5.1) reduces to

$$\langle |h_{\mathbf{k}\mathbf{k}'}|^2 \rangle = (\hbar/12\rho_0\omega)^2 k'_\beta k'_\eta k_\delta k_\zeta \hat{T}_{\alpha\beta\gamma\delta} \hat{T}_{\alpha\eta\gamma\zeta}^* \quad (5.3)$$

Further reduction of (5.3) relies on the fact that it is still the sum of a large number ( $3^6 = 729$ ) of terms, and the factors that make up each term fluctuate in sign as the varying indices pick out different components of the initial and final wavevectors as well as the Fourier transforms of various components of the static strain tensor and rotation vector. We conclude that (5.3) will fluctuate about the 'random-phase' value

$$|h_{\mathbf{k}\mathbf{k}'}^2|_{\text{ave}} = (\hbar/12\rho_0\omega)^2 \sum_{\alpha\beta\gamma\delta} |k'_\beta k'_\delta \hat{T}_{\alpha\beta\gamma\delta}(\mathbf{k}' - \mathbf{k})|^2 \quad (5.4)$$

as the directions of  $\mathbf{k}$  and  $\mathbf{k}'$  vary. In fact (5.4) can be identified as an angular average of (5.3) over the incident and scattered directions, in so far as all cross terms of type  $k_\delta k_{\delta'}$  ( $\delta \neq \delta'$ ) have been dropped. If we follow Klemens (1955, 1958, 1969) and Carruthers (1961) and complete this averaging process by replacing each  $k_\delta^2$  by its RMS value of  $k^2/3$ , equation (5.4) becomes

$$|h_{\mathbf{k}\mathbf{k}'}^2|_{\text{RMS}} = (\hbar k k'/36\rho_0\omega)^2 \sum_{\alpha\beta\gamma\delta} |\hat{T}_{\alpha\beta\gamma\delta}(\mathbf{k}' - \mathbf{k})|^2 \quad (5.5)$$

This approximation is completely analogous to that adopted by Klemens (1955, 1958, 1969) and Carruthers (1961), except that the anharmonic interaction is represented accurately by the second and third-order elastic constants that appear in the quantities  $\hat{T}_{\alpha\beta\gamma\delta}$  by virtue of (5.2), (3.20), (2.21) and (2.22).

For cubic crystals the symmetry of the elastic constants allows a further substantial simplification of (5.5) when we write  $\hat{T} = \hat{S} + \hat{R}$ . For cubic symmetry it is well known (see e.g., Leibfried and Breuer 1978) that  $\hat{c}_{\alpha\beta\gamma\delta}$  and  $\hat{c}_{\alpha\beta\gamma\delta\zeta\eta}$  vanish unless the indices appear in pairs, and all moduli obtained by permutation or by cyclic interchange of cartesian indices are equal. As a result there are only three independent SOE constants and six independent TOE constants. In Voigt notation these are  $c_{11}$ ,  $c_{12}$ ,  $c_{44}$ ,  $c_{111}$ ,  $c_{112}$ ,  $c_{166}$ ,  $c_{144}$ ,  $c_{654}$  and  $c_{123}$ , where it is understood that the  $c_{ij}$  and  $c_{ijk}$  refer to axes directed along the edges of the cubic unit cell. One readily checks from (2.22) that there are only 24 non-vanishing  $R_{\alpha\beta\gamma\delta}$ . Their Fourier transforms are

$$\begin{aligned} \hat{R}_{1112} = \hat{R}_{1121} = \hat{R}_{1211} = \hat{R}_{2111} &= G\omega_{21} = -\hat{R}_{2221} = -\hat{R}_{2212} \\ &= -\hat{R}_{2122} = -\hat{R}_{1222} \end{aligned} \quad (5.6)$$

with the other 16 being obtained by cyclic permutation of the indices. We have introduced

$$G \equiv c_{11} - c_{12} - 2c_{44}. \quad (5.7)$$

On the other hand (2.21) shows that  $\tilde{S}_{1112} = \tilde{S}_{2221}$ , etc, for cubic crystals, so (5.6) implies that there are *no cross terms* of type  $(\tilde{S}\tilde{R}^* + \tilde{R}\tilde{S}^*)$  in the expansion of  $|\tilde{T}|^2 = |\tilde{S} + \tilde{R}|^2$ ; i.e. for cubic crystals the static strain and rotation contribute *independently* to the scattering cross section in the approximation (5.5). In fact a straightforward but rather tedious analysis shows that for cubic crystals (5.5) becomes

$$\begin{aligned} |h_{kk'}^2|_{\text{RMS}} = & (\hbar k k' / 36 \rho_0 \omega)^2 \{ A(|\tilde{n}_{11}|^2 + |\tilde{n}_{22}|^2 + |\tilde{n}_{33}|^2) + B(|\tilde{n}_{12}|^2 + |\tilde{n}_{23}|^2 + |\tilde{n}_{31}|^2) \\ & + C[(\tilde{n}_{11}\tilde{n}_{22}^* + \tilde{n}_{22}\tilde{n}_{33}^* + \tilde{n}_{33}\tilde{n}_{11}^*) + \text{complex conjugate}] \\ & + 8G^2(|\tilde{\omega}_{12}|^2 + |\tilde{\omega}_{23}|^2 + |\tilde{\omega}_{31}|^2) \} \end{aligned} \quad (5.8)$$

where

$$\begin{aligned} A = & (c_{111} + 3c_{11})^2 + 4(c_{112} + c_{12})^2 + 2(c_{123} - c_{12})^2 + 2(c_{112} - c_{11})^2 \\ & + 8(c_{166} + c_{44})^2 + 4(c_{144} - c_{44})^2 \\ B = & 8(2c_{166} + c_{11} + c_{12} + 2c_{44})^2 + 16(c_{144} + c_{12})^2 + 32(c_{654} + c_{44})^2 \\ C = & (c_{111} + 3c_{11})(c_{112} - c_{11}) + 4(c_{112} + c_{12})^2 + 2(c_{123} - c_{12})(c_{112} + c_{12}) \\ & + 8(c_{166} + c_{44})^2 + 4(c_{166} + c_{44})(c_{144} - c_{44}). \end{aligned} \quad (5.9)$$

and we caution that the omission of the SOE constants from (5.9) would lead to significant overestimates of  $A$ ,  $B$  and  $C$ . The constant  $G$ , which is given by (5.7), vanishes for crystals that are elastically isotropic, so (5.8) is consistent with the obvious requirement that rotations should not effect the propagation of elastic waves in such crystals. It has already been remarked, following (2.23), that the contribution of the static rotations to the scattering will normally be very much less than that of the strains. Numerical estimates (Brown 1983b) show that the rotations contribute less than 2% of the lattice thermal resistivity due to dislocations (both edge and screw).

## 6. Summary and conclusion

We considered the elastic vibrations of an internally stressed body whose position-dependent Hooke's law moduli are functions of the elastic strains and rotations, measured from the initial stress-free state. Our approach encompassed rotations of arbitrary magnitude. For small rotations we rederived the classical equations (2.23) of KH (1974) and the second-quantised Hamiltonian density (4.4 and 4.5) of EW (1978). The relationship of the present theory to those of earlier workers is considered in the Appendix.

The quantum version of the theory, which is conceptually and mathematically simpler than the classical, at least for scattering phenomena, led first to the expression (4.6) for the scattering amplitude between arbitrary phonon modes, in terms of the second- and third-order elastic constants, the wavevectors and polarisation vectors of the incident and scattered phonons, and the Fourier transforms of the (small) static strains and rotations. This expression is exact, to first order in the static strains and rotations, given that the energy of deformation is determined by the strains alone. Expressions (4.13)–



(4.17) for transition rates and scattering cross sections were also presented. The extension of the theory to include large rotations was discussed following (4.6).

In § 5 we considered several useful approximations for the absolute square of the scattering amplitude, suitable for numerical estimation of scattering cross sections, etc. This led penultimately to (5.5), an approximation that is in most respects equivalent to those adopted by Klemens (1955, 1958, 1969) and Carruthers (1961), but is distinguished by the more or less exact description of the anharmonic interaction that is afforded by the SOE and TOE constants that appear in (5.5). By detailed discussion of the several steps leading to (5.5) from the exact expression (4.6) we have attempted to make the assessment of the approximate expressions more objective and their ultimate adoption more palatable. Of course these approximate expressions, equations (5.1)–(5.5), are averages that only have physical significance when used to calculate quantities that actually represent some sort of average over various scattering events—e.g. thermal transport coefficients. In individual applications it may be convenient to modify or dispense with some of the steps involved in passing from (4.6) to (5.5). In any event the averaging processes should be deferred to as late a stage in a calculation as is practicable.

Finally, for the important case of cubic symmetry, we derived the simple expression (5.8) for the square of the scattering amplitude. Straightforward application of this expression to the calculation of lattice thermal resistivity in deformed crystals has led (Brown 1982, 1983a, b) to good agreement with experiment.

## Appendix. Comparison with previous theories

In contrast to most of the earlier calculations, thermal conductivity estimates (Brown 1982, 1983a, b) based on (5.8) turn out to be in good agreement with experiment. For this reason it is important to explore the relationships between earlier theories and the present one.

Previous theories of strain-field scattering may be divided into three broad groups according to their representation of the anharmonic interaction responsible for the scattering. Thus Klemens (1955, 1958, 1969), Carruthers (1961) and Ohashi (1968) were forced, by the limited experimental data then available concerning non-linear elastic moduli, to describe the anharmonic interaction in terms of a single parameter, e.g. the average Grüneisen parameter,  $\gamma$ . Bross (1962, 1966), Bross *et al* (1963a, b, 1965), Seeger *et al* (1964), Gruner (1965a, b, 1968, 1970) and Gruner and Bross (1968) presented calculations for elastically isotropic crystals which have three independent TOE constants, while, as previously discussed, KH and EW took advantage of the availability of complete sets of six TOE constants for a number of cubic crystals, following the measurements of Bogardus (1965), Chang (1965), Hiki and Granato (1966) and others. We discuss each group of theories in turn.

### A1. Single-parameter theories

The Klemens (1955) theory assumed anharmonic linkages between nearest-neighbour atoms in a simple cubic structure. The change of the lattice vibration frequencies with compression that was implied by this model was used to express the anharmonic components of the interatomic forces in terms of the single Grüneisen parameter obtained from thermal expansion measurements. We observe from equation (35) of Klemens

(1955) that each (of three) rotation component contributes roughly twice as much to the energy of deformation (and hence four times as much to the scattering cross section) as a dilatation of the same magnitude. Consequently rotations tend to dominate the estimates by Klemens (1955) of dislocation scattering and this results in approximately equal resistivity contributions from screws and edges. This is at odds with our result (5.8), in which the contribution of rotations is negligible compared with that of strains and the resistivity due to screw dislocations turns out to be significantly less than that due to edges.

The Klemens (1955) estimate of dislocation scattering turned out to be far too small (Moss 1966, Klemens 1958), and was supplanted by a considerably larger estimate (Klemens 1958, equation (5.24)). This second estimate was based on a less specific model than that of Klemens (1955) and its precise basis is difficult to establish; it appears to underestimate the strength of dislocation-phonon scattering by a factor of about five (Klemens 1958, § 18, Brown 1983b). Some insight into the Klemens (1958) calculation is provided by that of Klemens (1969, § IIIA), although it seems that in the latter only strains, not rotations, contribute.

We can establish a close relationship between the Klemens (1969) calculation and that of the present paper by using (3.14) and (3.15), together with the commutation relations for the creation and annihilation operators (which follow from equations (4.1) and (4.2)) to rewrite (4.4) as

$$\mathcal{H}_0 = \frac{1}{2} \int_{\Omega} d^3X \sum_{jj'} \iint e_{\alpha}^{j*}(\mathbf{k}) e_{\alpha}^{j'}(\mathbf{k}') \hbar(\omega\omega')^{1/2} \exp[i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{X}] (b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}'} + b_{\mathbf{k}'} b_{\mathbf{k}}^{\dagger}) d^3k d^3k' / (8\pi^3)^2. \quad (\text{A1})$$

If we now follow the Klemens (1969) procedure and replace  $\omega$  by its Debye approximation  $\omega_j(\mathbf{k}) = v_j|\mathbf{k}| \equiv v_j k$ , the Hamiltonian appropriate to the *deformed* crystal may be inferred by assuming that the velocities  $v_j$  vary with position in response to the spatial variation of the elastic constants. This leads to the Hamiltonian density  $\mathcal{H} = \mathcal{H}_0 + \delta\mathcal{H}$ , where

$$\delta\mathcal{H} = \frac{\hbar}{4} \sum_{jj'} \int_{\Omega} d^3X \iint e_{\alpha}^{j*}(\mathbf{k}) e_{\alpha}^{j'}(\mathbf{k}') \left( \frac{kk'}{v_j v_{j'}} \right)^{1/2} (v_j \delta v_{j'} + v_{j'} \delta v_j) \times \exp[i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{X}] (b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}'} + b_{\mathbf{k}'} b_{\mathbf{k}}^{\dagger}) d^3k d^3k' / (8\pi^3)^2 \quad (\text{A2})$$

and the velocity change  $\delta v_j(\mathbf{X})$  depends on the SOE and TOE constants and the static strains and rotations. For our purposes of comparison it is sufficient to retain only the terms involving the TOE constants, which in any case tend to dominate (A2). Then, using the results of Wallace (1970, equation (10.9)) we have

$$\delta v_j = k^{-1} \delta \omega_j(\mathbf{k}) = c_{\alpha\beta\gamma\delta\zeta\eta} n_{\zeta\eta}(\mathbf{X}) k_{\beta} k_{\delta} e_{\alpha}^{j*}(\mathbf{k}) e_{\gamma}^{j'}(\mathbf{k}') / 2\rho_0 k \omega_j(\mathbf{k}) \quad (\text{A3})$$

where no summation is implied over the index  $j$ . Upon substituting this into (A2) we find, setting  $\omega = \omega'$  for elastic scattering,

$$\delta\mathcal{H} = \frac{\hbar}{8\rho_0\omega} \sum_{jj'} \iint c_{\alpha\beta\gamma\delta\zeta\eta} \tilde{n}_{\zeta\eta}(\mathbf{k}' - \mathbf{k}) e_{\alpha}^{j*}(\mathbf{k}) e_{\alpha}^{j'}(\mathbf{k}') (b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}'} + b_{\mathbf{k}'} b_{\mathbf{k}}^{\dagger}) \times (k_{\beta} k_{\delta} e_{\alpha}^{j*}(\mathbf{k}) e_{\gamma}^{j'}(\mathbf{k}') + k'_{\beta} k'_{\delta} e_{\alpha}^{j'}(\mathbf{k}') e_{\gamma}^{j*}(\mathbf{k})) d^3k d^3k' / (8\pi^3)^2. \quad (\text{A4})$$

This is broadly similar, although *not* identical, to those terms of (4.5) that involve TOE constants. However one can readily check that in the approximation equivalent to

(5.3) the two models are identical, so that the only essential difference between the model of Klemens (1969) and ours is due to the replacement of the true position dependence of the velocities by the simple, and generally inadequate approximation (Klemens 1969, equation (65))

$$\delta v/v = -\gamma\Delta(X) \quad \text{independent of } j \quad (\text{A5})$$

with  $\gamma$  an average Gruneisen constant and  $\Delta$  the dilatation, or some (ill defined) component of shear strain.

The theories of Carruthers (1961) and Ohashi (1968) differ from those of Klemens principally by their methods of estimating the magnitude of the single parameter used to represent the anharmonic interaction. Both authors obtained calculated thermal resistivities for dislocated crystals that were significantly larger than the first estimate of Klemens (1955). Moss (1966) has compared the calculations of Klemens and Carruthers with experimental data for alkali halide crystals and finds that large discrepancies remain. This may be largely due, however, to the effects of narrow dislocation dipoles (Kneezel and Granato 1982, Brown 1983a), which were not revealed by the etching experiments. The resistivities calculated by Ohashi were in quite good agreement with experimental data on alkali halide crystals. This agreement, which is due in part to the unrealistic assumption of no coupling between the three components of the displacement, must be regarded as fortuitous, since it is evident from (5.8) that no single-parameter description of the anharmonicities can suffice.

## A2. The isotropic model

The general results (4.6), (5.8), etc, can be specialised to the isotropic case by substituting (Thurston 1964)

$$\begin{aligned} c_{11} &= \lambda + 2\mu & c_{12} &= \lambda & c_{44} &= \mu \\ c_{123} &= \nu_1 & c_{144} &= \nu_2 & c_{456} &= \nu_3 \\ c_{111} &= \nu_1 + 6\nu_2 + 8\nu_3 & c_{112} &= \nu_1 + 2\nu_2 & c_{166} &= \nu_2 + 2\nu_3 \end{aligned} \quad (\text{A6})$$

where  $\lambda$  and  $\mu$  are the Lamé constants of the linear theory and the  $\nu_i$  are the third-order Lamé constants defined by Toupin and Bernstein (1961). In this case our theory reduces to that of Bross (1962) and related papers. However it seems that the values adopted by the German school for the third-order constants†

$$\begin{aligned} A_3 &= (\nu_1 - 18\nu_2 - 40\nu_3 - 80\mu)/144 & A_4 &= (\nu_2 + \nu_3 + 4\mu)/2 \\ A_5 &= (\nu_3 + 2\mu)/2 \end{aligned} \quad (\text{A7})$$

bear little relation to those measured for real polycrystalline samples. For example, in the case of copper we have evaluated (table 1) the  $A_i$  using both the Voigt-averaged Lamé constants proposed by Hamilton and Parrott (1968) and also those proposed by Chang (1967). The latter were calculated using the single-crystal moduli measured by Salama and Alers (1967). The two resulting sets of  $A_i$  are in order-of-magnitude agreement, but are an order of magnitude smaller than the values quoted by Bross *et al*

† Equations (A7) follow from the Gruner (1965a) definition of the  $A_i$  in terms of the Murnaghan (1951)  $l, m, n$ , which were then expressed in terms of the  $\nu_i$  using the table on p 230 of Truesdell and Noll (1965).

**Table 1.** Pseudo-isotropic TOE constants for copper ( $10^{12}$  dyn cm $^{-2}$ ).

Source	$A_3$	$A_4$	$A_5$
Hamilton and Parrott (1968)	0.39	-1.52	-0.42
Chang (1967)	0.31	-1.39	-0.09
Bross <i>et al</i> (1963a)	-4.58	12.2	-15.6

(1963a). This leads one to expect the thermal resistivities calculated by the German workers to be of the order of 100 times those measured. However they obtained much *weaker* scattering (see KH 1975, § 5) than both experiment, and calculation (Brown 1982, 1983a, b) based on the present theory, indicate. The reasons for these discrepancies are not clear.

### A3. Exact descriptions of anharmonicities

Models such as those of KH and EW, which employ the full set of SOE and TOE constants to describe the crystal anharmonicities within a continuum approximation, must be regarded as exact, at least for the description of sufficiently long waves. Some relatively minor differences between the classical equations of KH and our (2.23) were discussed following the latter. The low resistivities calculated by these authors are due primarily to the adoption of an incorrect Green function when calculating scattering amplitudes and to the neglect of other scattering processes that serve to limit the mean free paths of phonons that are not strongly scattered by a given type of dislocation. These points have been discussed in detail elsewhere (Brown 1983b).

The formulation of the present paper is very similar to that of EW and the results of the two calculations, for small strains and rotations, are identical if we ignore the scattering due to dislocation motion that was included by EW. However, whereas applications of the EW theory demand sophisticated computer calculations, the simplified formulae derived in § 5 of the present work enable useful estimates of transport coefficients, which turn out to be in good agreement with experiments (Brown 1982, 1983a, b), to be obtained easily with nothing more elaborate than a hand-held calculator.

The 'global' scattering due to the macroscopic bending of the lattice associated with a uniform density of identical edge dislocations was calculated by EW. These authors used a scattering Hamiltonian essentially identical to (3.19) which is valid only for small distortions, despite the fact that the rotations increase linearly with distance into the crystal (normal to the bending axis). Hence the scattering Hamiltonian for a large crystal does not remain small and perturbation theory cannot properly be used. Faced with a (physically dubious) transition rate which increased linearly with distance into the crystal EW were forced to artificially limit the size of the crystal. Although they recognise (see their discussion following their equation (9)) that their theory is valid only for small distortions it is not easy to see how their method of derivation can be extended to cope with large rotations. This extension is readily carried out using the methods of the present paper—see the discussion following (4.6).

The contribution of dynamic scattering, which was considered by EW, can be appended to our Hamiltonian (4.6) in an obvious way. However, a feature of EW's analysis that should be noted is their neglect of the change in core energy during dislocation motion. This prevents their theory from giving an adequate description of

the oscillations of a dislocation in its Peierls potential well but would appear to describe adequately the effects of dislocation glide.

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