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Local and Substantial Fluxes for Energy, Linear Momentum and Quasi Momentum in Crystals

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Abstract. The dynamics of a crystal lattice with an internal two-particle interaction is described as a limiting case of a continuous dynamical system with a non-local internal interaction. The explicit expressions for the densities and fluxes of linear momentum, energy and quasi momentum are given. This is done in terms of substantial as well as local coordinates.

1. Introduction

In electromagnetic (e.m.) theory the concept of elementary excitations of the e.m. field as quasi particles, termed photons, has been shown to be very useful. For a great class of applications, an elementary excitation of the e.m. field characterized by the wave vector $\mathbf{k}$ and polarization s behaves like a particle with an energy $\hbar\omega_s(\mathbf{k})$ and a linear momentum $\hbar\mathbf{k}$ which is, apart from a constant factor c^2, also the energy flux. The total energy of the e.m. field can be written as $\sum_{\mathbf{k}} \sum_s \hbar\omega_s(\mathbf{k})N_{\mathbf{k}s}$, the total linear momentum of the e.m. field as $\sum_{\mathbf{k}} \sum_s \hbar\mathbf{k}N_{\mathbf{k}s}$. Here $N_{\mathbf{k}s}$ is the number of elementary excitations (photons) of the e.m. field, with polarization s and wave vector $\mathbf{k}$; $\omega_s(\mathbf{k})$ represents the dispersion relation $\omega = c|\mathbf{k}|$ of the e.m. field.

There is a close analogy between the theories of the e.m. field, of lattice vibrations in crystals and of waves in fluids. Therefore it has been very tempting to extend the photon concept to the theory of fluid waves and of crystal vibrations. One meets in the literature, often without further explanation, the assumption that an elementary excitation of the crystal or fluid (here termed phonon), characterized by the wave vector $\mathbf{k}$ and polarization s, carries not only an energy $\hbar\omega_s(\mathbf{k})$, but also a linear momentum $\hbar\mathbf{k}$, the energy current tensor being $\hbar\mathbf{k} \times d/d\mathbf{k}\ \omega_s(\mathbf{k})$.

In spite of the analogy between the theory of the e.m. field on the one hand and the theories of crystal vibrations and fluid waves on the other hand, there are also many essential differences:

(i) The e.m. field theory is a covariant theory. Consequently the linear momentum density is proportional to the energy current. On the other side, crystal vibrations and fluid waves are usually treated non-relativistically. Therefore in these theories linear momentum and energy current are different concepts.

(ii) In e.m. field theory photons with a zero wave vector have no physical

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meaning. For fluids and for crystals the elementary excitations with a zero wave vector represent (in most papers) a macroscopic motion of the entire system. The mechanically defined linear momentum is related to this macroscopic motion and therefore to phonons with $\mathbf{k} = 0$. The physical meaning of the statement 'a phonon carries a linear momentum $\hbar\mathbf{k}$' remains rather unclear.

As far as we know the first authors who discussed these problems thoroughly were Leibfried [1], Brenig [2] and Süssmann [3]. They clarified that any phonon with $\mathbf{k} \neq 0$ carries a zero linear momentum. The quantity $\hbar\mathbf{k}$ connected with a phonon is then called 'quasi momentum'. Brenig [2] and later Gilbert and Mollow [4] discuss the connection between linear momentum and quasi momentum. The physical meaning of the concept of the quasi momentum, however, has not been explained. Süssmann [3] tackles the problem by means of invariance properties of the Hamilton operator of the crystal. The conservation of the linear momentum of a crystal is due to some continuous invariance group of the crystal, the selection rule for the quasi momentum is due to some discrete invariance group.

Nevertheless, all this is only a part of the truth. The relations between invariance groups, constants of the motion and elementary excitations depend essentially on the formalism in use. An elucidating example hereof is found in the paper of Kronig and Thellung [5]. These authors discuss a formalism for fluid waves in local coordinates. Phonons with a wave vector $\mathbf{k}$, defined in this formalism, carry a mechanically defined momentum $\hbar\mathbf{k}$. This does not contradict the result of Leibfried, Brenig and Süssmann, it shows only the influence of the formalism in use.

For the calculation of transport coefficients in solids (e.g. heat conduction and viscosity) it is necessary to know the currents of energy and linear momentum in the solid. There are two obvious ways to define these currents. One can define the current of some quantity either through a material point (point fixed in the medium) or through a local point (point fixed in the laboratory). Corresponding to these possibilities we speak about substantial and about local fluxes, respectively. For Bravais lattices Choquard [6] discussed the substantial energy flux, Hardy [7] the local energy flux. De Vault [8] applied Hardy's method to the local linear-momentum flux, Enz [9] generalized the method to non-Bravais lattices. Pokrovsky and Sergeev [10] gave a rather general discussion of local fluxes in crystals. Furthermore, they gave a transformation of the local flux in what they call 'a flux in a material description'. As we already pointed out in a previous paper [11] (hereafter referred to as I), this flux is still a local flux.

In Section 2 of this paper we describe the dynamics of a crystal lattice as a limiting case of the dynamics of a continuous medium with a non-local internal interaction, which we have discussed in I. For later use and to fasten down the notation, the Bloch functions for a crystal lattice are introduced in Section 3. In Section 4 the results of I are used to discuss the density and the flux of linear momentum in a crystal lattice. These results are also related to some earlier papers. The discussion is given in terms of substantial as well as local coordinates. In a similar way the energy density and flux are discussed in Section 5, and the balance of quasi momentum in Section 6. Finally, we give in Section 7 an evaluation of the present results.

2. Non-Bravais Crystal Lattices

Let the equilibrium positions of the atoms of an elementary cell of an ideal crystal that contains g atoms, be given by the set of 3-tuples $\mathbf{C} = \{\alpha^1, \alpha^2, \ldots, \alpha^g\}$.

The mass of an atom with an equilibrium position $m = \alpha$ shall be M_α. The primitive translation vectors of an elementary cell are taken to be given by the 3-tuples $(a_1, 0, 0)$, $(0, a_2, 0)$ and $(0, 0, a_3)$. The set $\mathbf{T}$ of all translation vectors of the crystal is then represented by

$$\mathbf{T} = \{\xi = (\xi_1, \xi_2, \xi_3) \mid \xi_i = n_i a_i, n_i \in \mathbf{Z}_{N_i}\}. \tag{2.1}$$

Here $\mathbf{Z}_{N_i}$ is the cyclic group of all integers modulo $N_i = L_i/a_i$ and $L = (L_1, L_2, L_3)$ denotes the linear dimensions of the crystal. Note that the 3-tuples $\alpha \in \mathbf{C}$ and $\xi \in \mathbf{T}$ represent the components of vectors with respect to some coordinate system, which in general is non-orthogonal. The (substantial) coordinates of an arbitrary atom in the crystal are now $m = \alpha + \xi$ where $\alpha \in \mathbf{C}$ and $\xi \in \mathbf{T}$.

A suitable field vector for the description of the crystal dynamics is $u(m) = (u_1(m), u_2(m), u_3(m))$, i.e. the deviation from the equilibrium position of the atom with substantial coordinate (equilibrium position) m, the field velocity vector being $\dot{u}(m) = (d/dt\, u(m))_m$. We impose periodic boundary conditions for u.

The substantial mass density of the crystal is given by

$$\rho_0(m) = \sum_{\alpha \in \mathbf{C}} \sum_{\xi \in \mathbf{T}} M_\alpha \delta(m - \alpha - \xi). \tag{2.2}$$

Here $\delta(m - \alpha)$ is the three-dimensional Dirac delta function $\delta(m_1 - \alpha_1)\delta(m_2 - \alpha_2)$ $\delta(m_3 - \alpha_3)$.

We assume that the total potential energy of the crystal may be written as a sum of two-particle interaction energies:

$$\sum_{\alpha, \beta \in \mathbf{C}} \sum_{\xi, \zeta \in \mathbf{T}} f_{\alpha\beta}^{\xi - \zeta}(z(\alpha + \xi, \alpha + \xi - \beta - \zeta)) = \iint dm\, d\mu V(z(m, \mu), m, \mu),$$

where (c.f. (2.2) of I)

$$z(m, \mu) = u(m + \mu) - u(m) + \mu, \tag{2.3}$$

so that

$$V(z, m, \mu) = f_{\alpha\beta}^{\xi - \zeta}(z)\delta(m - \alpha - \xi)\delta(\mu + \alpha + \xi - \beta - \zeta). \tag{2.4}$$

Here a summation over $\alpha, \beta \in \mathbf{C}$ and $\xi, \zeta \in \mathbf{T}$ is implied. Furthermore we assume

$$f_{\alpha\beta}^{\xi - \zeta}(z) = f_{\alpha\beta}^{\xi - \zeta}(-z) = f_{\alpha\beta}^{\zeta - \xi}(z) = f_{\beta\alpha}^{\xi - \zeta}(z). \tag{2.5}$$

The derivatives of $f_{\alpha\beta}^{\xi - \zeta}(z)$ will be indicated as

$$f_{\alpha\beta,i}^{\xi - \zeta}(z) = d/dz_i f_{\alpha\beta}^{\xi - \zeta}(z); \quad f_{\alpha\beta,ij}^{\xi - \zeta}(z) = d/dz_i\, d/dz_j f_{\alpha\beta}^{\xi - \zeta}(z), \quad \text{etc.}$$

From (2.5) it follows

$$f_{\alpha\beta,i}^{\xi - \zeta}(z) = -f_{\alpha\beta,i}^{\xi - \zeta}(-z); \quad f_{\alpha\beta,ij}^{\xi - \zeta}(z) = f_{\alpha\beta,ij}^{\xi - \zeta}(-z), \quad \text{etc.} \tag{2.6}$$

With (2.2) and (2.4) we can now apply the results of I. Then, for the equation of motion (c.f. (2.4) of I) we find

$$M_\alpha \ddot{u}_i(\alpha + \xi) - \sum_{\beta \in \mathbf{C}} \sum_{\zeta \in \mathbf{T}} 2 f_{\alpha\beta,i}^{\xi - \zeta}(\alpha + \xi - \beta - \zeta + u(\alpha + \xi) - u(\beta + \zeta)) \doteq 0. \tag{2.7}$$

This expression clearly represents the equation of motion of an arbitrary periodic crystal with a general two-particle interaction.

We have interpreted u as the deviation from equilibrium, therefore $u = \dot{u} = 0$ must satisfy (2.7) or:

$$\sum_{\beta\in\mathbf{C}} \sum_{\zeta\in\mathbf{T}} F_{\alpha\beta,i}^{\xi-\zeta} = 0, \tag{2.8}$$

where we use the short-hand notation

$$F_{\alpha\beta,i}^{\xi-\zeta} = f_{\alpha\beta,i}^{\xi-\zeta}(\alpha - \beta + \xi - \zeta). \tag{2.9}$$

A similar abbreviation will be used for the higher order derivatives of $f_{\alpha\beta}^{\xi-\zeta}(z)$. Equation (2.8) states that the total force on each atom is zero when the crystal is in equilibrium. For $u = 0$ the potential energy of the crystal may be chosen to be zero:

$$\sum_{\alpha,\beta\in\mathbf{C}} \sum_{\xi,\zeta\in\mathbf{T}} F_{\alpha\beta}^{\xi-\zeta} = 0. \tag{2.10}$$

For reasons of completeness we note that, as we will see in Section 4, the additional requirement

$$\sum_{\alpha,\beta\in\mathbf{C}} \sum_{\zeta\in\mathbf{T}} (\alpha - \beta + \xi - \zeta) F_{\alpha\beta,i}^{\xi-\zeta} = 0 \tag{2.11}$$

assures that the linear-momentum flux through the crystal, averaged over the entire volume, vanishes for $u = \dot{u} = 0$.

In literature one often meets a much stronger condition than (2.8) and (2.11) namely

$$F_{\alpha\beta,i}^{\xi-\zeta} = 0. \tag{2.12}$$

A deeper discussion of the equilibrium conditions for crystals is for example given by Leibfried and Ludwig [12].

3. Bloch Functions and the Dispersion Relation

According to Bloch's theorem for periodic structures the functions $u(\alpha + \xi)$ may be written as

$$u(\alpha + \xi) = (\Omega M_\alpha)^{-1/2} \sum_{\kappa\in\mathbf{B}} w(\alpha, k) \exp[ik\cdot(\alpha + \xi)]. \tag{3.1}$$

Here Ω is the number of elementary cells in the crystal and $k = (k_1, k_2, k_3)$ is the wave number 3-tuple from the first Brioullin zone $\mathbf{B}$:

$$\mathbf{B} = \{k = (k_1, k_2, k_3) \mid k_i = 2\pi n_i/L_i;\ n_i \in \mathbf{Z},\ -\tfrac{1}{2}N_i < n_i \leqslant \tfrac{1}{2}N_i\}$$

with $\mathbf{Z}$ is the set of all integers, a dot between 3-tuples denotes contraction:

$$k\cdot(\alpha + \xi) = \sum_i k_i(\alpha + \xi)_i.$$

The components k_i of the 3-tuple k can be interpreted as the contra-variant components of the usual $\mathbf{k}$ vector. For the Bloch functions $w(\alpha, k)$ we have the reality condition

$$w(\alpha, k) = w(\alpha, -k)^*, \tag{3.2}$$

where the asterisk denotes complex conjugation.

We shall make use of the following identity

$$\sum_{\xi \in \mathbf{T}} \exp[i(k + k')\cdot \xi] = \Omega \Delta_{k+k'} \tag{3.3}$$

where

$$\Delta_k = 0(k \notin \mathbf{K}),$$
$$\Delta_k = 1(k \in \mathbf{K}),$$
$$\mathbf{K} = \{K = (K_1, K_2, K_3) \mid K_i = 2\pi n_i/a_i, n_i \in \mathbf{Z}_{N_i}\}.$$

If the components K_i of $K \in \mathbf{K}$ are interpreted as the contra-variant components of some vector, the set $\mathbf{K}$ is the usual reciprocal lattice. With (2.9) a linearization of the equation of motion (2.7) for small values of u_i yields

$$M_\alpha \ddot{u}_i(\alpha + \xi) + \sum_{\beta \in \mathbf{C}} \sum_{\zeta \in \mathbf{T}} 2F^{\xi-\zeta}_{\alpha\beta,ij}(u_j(\alpha + \xi) - u_j(\beta + \zeta)) \doteq 0. \tag{3.4}$$

(Summation over $j = 1, 2, 3$ is implied.) Substitution of (3.1) into (3.4), afterwards multiplication of the equation with $M_\alpha^{-1/2} \exp[-ik'\cdot(\alpha + \xi)]$, summation of the first two terms with (3.3) for $\xi \in \mathbf{T}$, then substitution of $\eta = \xi - \zeta$ into the third term and finally summation over $\xi \in \mathbf{T}$ gives

$$w_i(\alpha, k) + \sum_{\beta \in \mathbf{C}} W_{\alpha\beta ij}(k) w_j(\beta, k) \doteq 0 \tag{3.5}$$

where

$$W_{\alpha\beta ij}(k) = 2 \sum_\eta \left\{ \sum_{\gamma \in \mathbf{C}} M_\alpha^{-1} F^\eta_{\beta\gamma,ij} \delta_{\beta\alpha} - (M_\alpha M_\beta)^{-1/2} F^\eta_{\alpha\beta,ij} \exp[-ik\cdot(\alpha - \beta + \eta)] \right\}. \tag{3.6}$$

The Kronecker symbol $\delta_{\beta\alpha}$ is defined in the usual way:

$$\delta_{\beta\alpha} = 0(\beta \neq \alpha), \quad \delta_{\beta\alpha} = 1(\beta = \alpha).$$

With (2.5) and (3.6) we find

$$W_{\alpha\beta ij}(k) = W^*_{\beta\alpha ji}(k) = W_{\beta\alpha ji}(-k). \tag{3.7}$$

Thus, the matrix W is Hermitian and has therefore real eigenvalues. The set of eigenvectors of W is a complete set.

If (3.5) represents the first-order approximation to the equation of motion of a real crystal we have to require additionally that $W(k)$ is a non-negative matrix. The eigenvalue problem for $W(k)$ can then be written as:

$$W_{\alpha\beta ij}(k) X_{i\beta s}(k) = \omega_s^2(k) X_{j\alpha s}(k). \tag{3.8}$$

(Summation over $\beta \in \mathbf{C}$ and $i = 1, 2, 3$ is implied.) Here the index s, running from 1 to $3g$, counts the three different polarizations as well as the g different modes. Because of the orthonormality of the eigenvectors we have

$$X_{i\alpha s}(k) X^*_{i\alpha s'}(k) = \delta_{ss'} \tag{3.9}$$

and from (3.8) it follows

$$X^*_{i\alpha s}(k) W_{\alpha\beta ij}(k) X_{j\beta s'}(k) = \omega_s^2(k) \delta_{ss'}. \tag{3.10}$$

By interchanging the dummy variables α and β in (3.10) it is easily verified that

$$X^*_{i\alpha s}(k) = X_{i\alpha s}(-k) \tag{3.11}$$

and

$$\omega_s^2(k) = \omega_s^2(-k). \tag{3.12}$$

Furthermore because of the completeness of the set of eigenvectors, any $w(\alpha, k)$ can be written as

$$w_i(\alpha, k) = \sum_s c_s(k) X_{i\alpha s}(k). \tag{3.13}$$

With (3.11) and the reality condition (3.2) we see that

$$c_s(k) = c_s^*(-k). \tag{3.14}$$

With (3.8), the substitution of (3.13) into (3.5) yields

$$\ddot{c}_s(k) X_{i\alpha s}(k) + W_{\alpha\beta ij}(k) X_{j\beta s}(k) c_s(k) = -\omega_s^2(k) X_{i\alpha s}(k).$$

(Summation over $s = 1, 2, \ldots, 3g$ is implied.) So

$$\ddot{c}_s(k) + \omega_s^2(k) c_s(k) \doteq 0. \tag{3.15}$$

Functions of the form $c_s(k) X_{i\alpha s}(k)$ (no summation over k and s) for which $c_s(k)$ satisfies (3.15) will be termed substantial phonons. We use the adjective substantial to indicate that the linearization of the equation of motion has been performed in terms of the substantial variable u.

For the classical analogues of the creation and annihilation operators we may write

$$\begin{aligned} a_{ks} &= \sqrt{\tfrac{1}{2}\omega_s(k)}\, c_s(k) + i\sqrt{\tfrac{1}{2}\omega_s(k)}\, \dot{c}_s(k), \\ a^+_{ks} &= \sqrt{\tfrac{1}{2}\omega_s(k)}\, c_s(-k) - i\sqrt{\tfrac{1}{2}\omega_s(k)}\, \dot{c}_s(-k), \end{aligned} \tag{3.16}$$

or inversely

$$\begin{aligned} \dot{c}_s(k) &= i\sqrt{\tfrac{1}{2}\omega_s(k)}\,(a_{ks} - a^+_{-ks}), \\ c_s(k) &= \sqrt{\tfrac{1}{2}\omega_s(k)}\,(a_{ks} + a^+_{-ks}). \end{aligned} \tag{3.17}$$

From these formulas one obtains easily

$$c_s(k) c_s(-k) = 1/\omega_s(k)(N_{ks} + S_{ks}), \tag{3.18}$$

$$\dot{c}_s(k) \dot{c}_s(-k) = \omega_s(k)(N_{ks} - S_{ks}), \tag{3.19}$$

$$c_s(k) \dot{c}_s(-k) = \tfrac{1}{2} i (a_{ks} a^+_{ks} - a^+_{-ks} a_{-ks}) - \tfrac{1}{2} i (a_{ks} a_{-ks} - a^+_{-ks} a^+_{ks}), \tag{3.20}$$

where

$$N_{ks} = a^+_{ks} a_{ks} \tag{3.21}$$

is the classical analogue of the substantial phonon number operator for a substantial phonon with wave number k and polarization/mode s, and

$$S_{ks} = S_{-ks} = \tfrac{1}{2}(a_{ks} a_{-ks} + a^+_{ks} a^+_{-ks}). \tag{3.22}$$

In the following, we assume that the center of mass of the crystal is at rest, for which we get with (3.1) the condition

$$w(\alpha, 0) = 0. \tag{3.23}$$

In Section 2 we have shown that, with respect to the dynamics, a crystal lattice can be considered as a limiting case of a continuous dynamical system. For continuous systems $u(m)$ is defined for all m, whereas for the crystal $u(m)$ is only defined for $m = \alpha + \xi$, $\alpha \in \mathbf{C}$, $\xi \in \mathbf{T}$. Consequently the derivatives $u_{i,j}(m)$ are not defined. Therefore we have to define some continuation of $u(\alpha + \xi)$ in order to apply the formalism of I to full extent. In principle such a continuum representation is arbitrary. We shall assume that the desired continuum representation yields (c.f. equation (3.1))

$$u_{i,j}(\alpha + \xi) = (\Omega M_\alpha)^{-1/2} i k_j w_i(\alpha, k) \exp[ik \cdot (\alpha + \xi)]. \tag{3.24}$$

(Summation over $k \in \mathbf{B}$ is implied.) A further specification of the continuum representation is not needed.

4. The Conservation of Linear Momentum

In I we have derived the local conservation law for the linear momentum in terms of substantial as well as local coordinates. In the special case of a crystal lattice (see (2.2) and (2.4)), the substantial linear-momentum flux density (2.15) of I reads

$$p_i(m) = M_\alpha \dot{u}_i(\alpha + \xi)\delta(m - \alpha - \xi). \tag{4.1}$$

Analogously the local linear-momentum density (cf. (3.26), (3.34) of I) is

$$\begin{aligned} p_i^l(x) &= M_\alpha \dot{u}_i(\alpha + \xi)\delta(x + v(x) - \alpha - \xi)J(x) \\ &= M_\alpha \dot{u}_i(\alpha + \xi)\delta(x - q(\alpha + \xi)), \end{aligned} \tag{4.2}$$

where

$$q + v(q) = \alpha + \xi \tag{4.3}$$

and

$$J(x) = \det(\delta_{ij} + v_{i,j}(x)).$$

With (2.2)–(2.5) the integrated value of the substantial linear momentum flux (2.18) of I reads

$$\int \pi_{ij}(m)\, dm = (\alpha - \beta + \xi - \zeta)_i f_{\alpha\beta,j}^{\xi-\zeta}(\alpha - \beta + \xi - \zeta + u(\alpha + \xi) - u(\beta + \zeta)). \tag{4.4}$$

(Summation over $\alpha, \beta \in \mathbf{C}$; $\xi, \zeta \in \mathbf{T}$ is implied.) We can expand this expression in powers of u. The constant and linear term are zero because of (2.11) and (3.23). With (2.5) and (2.9) we find for the quadratic term

$$\int {}^2\pi_{ij}(m)\, dm = (\alpha - \beta + \xi - \zeta)_i F_{\alpha\beta,jln}^{\xi-\zeta} u_l(\alpha + \xi) u_n(\beta + \zeta). \tag{4.5}$$

Now we substitute (3.1) twice into (4.5), put $\eta = \xi - \zeta$ and replace the summation

over ξ and ζ by a sum over ζ and η. Then with (3.3), the summation over ζ can be done explicitly. We obtain

$$\int {}^2\pi_{ij}(m)\, dm = -(\alpha - \beta + \eta)_i F^{\eta}_{\alpha\beta,jln}(M_\alpha M_\beta)^{1/2} \exp[ik\cdot(\alpha - \beta + \eta)] \times w_l(\alpha, k) w_n(\beta, -k). \tag{4.6}$$

(Summation over α, β, η and k is implied.) With (3.13), equation (4.6) reads

$$\int {}^2\pi_{ij}(m)\, dm = -(M_\alpha M_\beta)^{-1/2}(\alpha - \beta + \eta)_i F^{\eta}_{\alpha\beta,jln} \exp[ik\cdot(\alpha - \beta + \eta)] \times X_{n\beta s'}(-k) X_{l\alpha s}(k) c_s(k) c_{s'}(-k). \tag{4.7}$$

(Summation over s and s'.) For the difference of the integrated values of the substantial and the local linear-momentum flux one finds (cf. equation (4.4) of I)

$$\int \pi^l_{ij}(x)\, dx - \int \pi_{ij}(m)\, dm = M_\alpha \dot{u}_i(\alpha + \xi)\dot{u}_j(\alpha + \xi) - (u_j(\beta + \zeta) - u_j(\alpha + \xi)) f^{\xi-\zeta}_{\alpha\beta,i}(\alpha - \beta + \xi - \zeta + u(\alpha + \xi) - u(\beta + \zeta)).$$

We may also expand (4.8) in a power series in u. The constant term is zero and the linear term vanishes because of (3.23). With (2.5) and (2.9) we find for the quadratic term

$$\begin{aligned}\int {}^2\pi^l_{ij}(x)\, dx - \int {}^2\pi_{ij}(m)\, dm &= M_\alpha \dot{u}_i(\alpha + \xi)\dot{u}_j(\alpha + \xi) \\ &\quad - (u_j(\beta + \zeta) - u_j(\alpha + \xi))(u_l(\alpha + \xi) - u_l(\beta + \zeta)) F^{\xi-\zeta}_{\alpha\beta,il} \\ &= M_\alpha \dot{u}_i(\alpha + \xi)\dot{u}_j(\alpha + \xi) + 2(u_j(\alpha + \xi) u_l(\alpha + \xi) \\ &\quad - u_j(\alpha + \xi) u_l(\beta + \zeta)) F^{\xi-\zeta}_{\alpha\beta,il}.\end{aligned}$$

Now we insert (3.1) twice, put $\eta = \xi - \zeta$, replace the summation over ξ and ζ by a sum over ζ and η, use (3.3) and (3.6), and obtain finally

$$\int {}^2\pi^l_{ij}(x)\, dx - \int {}^2\pi_{ij}(m)\, dm = \dot{w}_i(\alpha, k)\dot{w}_j(\alpha, -k) + 2W_{\beta\alpha il}(k) w_j(\alpha, k) w_l(\beta, -k). \tag{4.9}$$

With (3.7), (3.8) and (3.12), equation (3.13) yields

$$\int {}^2\pi^l_{ij}(x)\, dx - \int {}^2\pi_{ij}(m)\, dm = X_{i\alpha s}(k) X_{j\alpha s'}(-k) \dot{c}_s(k) \dot{c}_{s'}(-k) + 2\omega_s^2(k) X_{j\alpha s}(k) X_{l\beta s'}(-k) c_s(k) c_{s'}(-k). \tag{4.10}$$

From (4.1) and (4.2) it is easily verified that $\int p(m)\, dm = \int p^l(x)\, dx = 0$. This conclusion agrees with Leibfried's result [1], but disagrees with that of Bassett and Pryce [13] and that of Lewis [14]. Bassett and Pryce discuss the so-called localized running waves. These waves are just a linear combination of our substantial phonons. In terms of displacements of the lattice, the authors define a certain quantity and call it 'momentum'. They show that this 'momentum' is proportional to the **k** vector of the 'localized phonon' with a factor that is a measure for the anharmonicity of the lattice. On the other side, we have defined the linear momentum as the product of mass and velocity. In general these two definitions disagree. In our opinion the terming of Bassett and Pryce is therefore rather misleading.

An analogous jumbling of concepts leading to wrong conclusions, is found in the paper by Lewis [14]. In order to define the 'momentum' the author introduces the sound pressure. This sound pressure is thereupon identified with the product of the momentum and the phonon velocity (which is, in the model of Lewis, the Debye velocity). But, the sound pressure must be related to the linear-momentum flux. The result of Lewis corrected in this way agrees with our results (4.7) and (4.8).

We have derived expression (4.2) for the local linear momentum density. An analogous expression is used as a starting point in the discussion of de Vault [8]. The expressions for the momentum flux found by this author corresponds also with our results of the local linear-momentum flux (4.7) and (4.8).

5. The Conservation of Energy

In I expressions for the substantial and for the local energy densities have been derived. For the crystal lattice defined by (2.2) and (2.4), the substantial energy density reads (cf. (2.16) of I)

$$\begin{aligned} e(m) = {} & (\tfrac{1}{2}M_\alpha \dot{u}_j(\alpha + \xi)\dot{u}_j(\alpha + \xi) \\ & + f_{\alpha\beta}^{\xi-\zeta}(\alpha - \beta + \xi - \zeta + u(\alpha + \xi) - u(\beta + \zeta)))\delta(m - \alpha + \xi). \end{aligned} \tag{5.1}$$

(Summation over $j = 1, 2, 3$; $\alpha, \beta \in \mathbf{C}$ and $\xi, \zeta \in \mathbf{T}$ is implied.) The corresponding expression for the local energy density is (cf. (4.3))

$$\begin{aligned} e^l(x) = {} & (\tfrac{1}{2}M_\alpha \dot{u}_j(\alpha + \xi)\dot{u}_j(\alpha + \xi) \\ & + f_{\alpha\beta}^{\xi-\zeta}(\alpha - \beta + \xi - \zeta + u(\alpha + \xi) - u(\beta + \zeta)))\delta(x - q(\alpha + \xi)). \end{aligned} \tag{5.2}$$

Consequently we have

$$\int e(m)\, dm = \int e^l(x)\, dx,$$

which gives an alternative definition of the total energy.

It is a usual procedure to expand the total energy in a power series in u. Because of (2.10), the constant term in the series vanishes and the linear term is zero because of (3.23). By straightforward calculations the quadratic terms can be brought into the form

$$\int {}^2e(m)\, dm = \int {}^2e^l(x)\, dx = \omega_s(k)N_{ks}. \tag{5.3}$$

(Summation over s and $k \in \mathbf{B}$.) For the lattice, the integrated value of the substantial energy flux (cf. (2.19) of I) reads

$$\begin{aligned} \int s_i(m)\, dm = {} & -(\alpha - \beta + \xi - \zeta)_i \dot{u}_j(\beta + \zeta) \\ & \times f_{\alpha\beta,j}^{\xi-\zeta}(\alpha - \beta + \xi - \zeta + u(\alpha + \xi) - u(\beta + \zeta)). \end{aligned} \tag{5.4}$$

Here again the constant and the linear term of the power series expansion vanish. Using (2.5) and (2.9) for the term quadratic in u we find

$$\int {}^2s_i(m)\, dm = -(\alpha - \beta + \xi - \zeta)_i \dot{u}_j(\beta + \zeta)u_l(\alpha + \xi)F_{\alpha\beta,jl}^{\xi-\zeta}. \tag{5.5}$$

With the aid of (3.3) the introduction of the Bloch functions by (3.1) yields

$$\int {}^2s_i(m)\,dm = -(\alpha - \beta + \eta)_i F^{\eta}_{\alpha\beta,jl}(M_\alpha M_\beta)^{-1/2}\dot{w}_j(\beta, -k)w_l(\alpha, k) \times \exp[ik\cdot(\alpha - \beta + \eta)],$$

or with (3.6)

$$\int {}^2s_i(m)\,dm = -\tfrac{1}{2}i\, d/dk_i\, W_{\alpha\beta jl}(-k)\dot{w}_j(\beta, -k)w_l(\alpha, k). \tag{5.6}$$

Using (3.13) we may write

$$\int {}^2s_i(m)\,dm = -\tfrac{1}{2}i\, d/dk_i\, W_{\alpha\beta jl}(-k)X_{j\beta s'}X_{l\alpha s}(k)\dot{c}_s(-k)c_s(k).$$

With the chain rule for differentiation and the equations (3.8), (3.9) and (3.11) we obtain

$$\int {}^2s_i(m)\,dm = \tfrac{1}{2}i\dot{c}_{s'}(-k)c_s(k) \times \{-d/dk_i\, \omega_s^2(k)\delta_{ss'} + W_{\alpha\beta jl}(-k)\, d/dk_i\, (X_{j\beta s'}(-k)X_{l\alpha s}(k))\}. \tag{5.7}$$

Applying (3.8) twice and using (3.9) we get

$$\int {}^2s_i(m)\,dm = \tfrac{1}{2}i\dot{c}_{s'}(-k)c_s(k) \times \{-d/dk_i\, \omega_s^2(k)\delta_{ss'} + (\omega_s^2(k) - \omega_{s'}^2(k))X_{l\alpha s}(k)\, d/dk_i\, X_{l\alpha s'}(-k)\}, \tag{5.8}$$

or with (3.20)–(3.22)

$$\int {}^2s_i(m)\,dm = \omega_s(k)\, d/dk_i\, \omega_s(k)N_{ks} + \tfrac{1}{2}i(\omega_s^2(k) - \omega_{s'}^2(k))X_{l\alpha s}(k)\, d/dk_i\, X_{l\alpha s'}(-k)\dot{c}_{s'}(-k)c_s(k). \tag{5.9}$$

The difference between the integrated values of the local and the substantial energy flux is (cf. equation (4.5) of I)

$$\begin{aligned}\int s_i^l(x)\,dx - \int s_i(m)\,dm = {} & \tfrac{1}{2}M_\alpha\dot{u}_j(\alpha + \xi)\dot{u}_j(\alpha + \xi)\dot{u}_i(\alpha + \xi) \\ & + \dot{u}_i(\alpha + \xi)f^{\xi-\zeta}_{\alpha\beta}(\alpha - \beta + \xi - \zeta + u(\alpha + \xi) - u(\beta + \zeta)) \\ & - (u_i(\beta + \zeta) - u_i(\alpha + \xi)) \\ & \times \dot{u}_j(\beta + \zeta)f^{\xi-\zeta}_{\alpha\beta,j}(\alpha - \beta + \xi - \zeta + u(\alpha + \xi) - u(\beta + \zeta)).\end{aligned} \tag{5.10}$$

The constant and the linear term of the series expansion in powers of u are zero. For the quadratic terms (cf. also (4.6) of I) we find

$$\begin{aligned}\int {}^2s_i^l(x)\,dx - \int {}^2s_i(m)\,dm = {} & -\dot{u}_i(\alpha + \xi)(u_j(\alpha + \xi) - u_j(\beta + \zeta))F^{\xi-\zeta}_{\alpha\beta,i} \\ & + \dot{u}_j(\beta + \zeta)(u_i(\alpha + \xi) - u_i(\beta + \zeta))F^{\xi-\zeta}_{\alpha\beta,i}\end{aligned} \tag{5.11}$$

which vanishes in the special case (2.12).

The results of this section are compatible with the literature: Our expression for the substantial energy flux agrees with Choquard's expression for the energy current [6]. The local energy density is the starting point for Hardy [7] and Enz [9]. The

expressions for the local energy flux also agrees with the energy fluxes of Hardy and Enz. A discussion of the meaning of the terms of (5.8) is given there.

6. The Balance of Quasi Momentum

With a modification of Noether's theorem, we have derived in I a local balance equation by means of an infinitesimal translation in m-space. This balance equation reads in substantial coordinates

$$d/dt\, \hat{p}_i(m) + d/dm_j\, \hat{\pi}_{ij}(m) \doteq Q_i(m) \tag{6.1}$$

and in local coordinates

$$d/dt\, \hat{p}_i^l(x) + d/dx_j\, \hat{\pi}_{ij}^l(x) \doteq Q_i^l(x). \tag{6.2}$$

For the crystal lattice the substantial and local densities become (cf. equations (2.17) and (3.47) of I and (4.3))

$$\hat{p}_i(m) = -M_\alpha \dot{u}_j(\alpha + \xi) u_{j,i}(\alpha + \xi)\delta(m - \alpha - \xi), \tag{6.3}$$

$$\hat{p}_i^l(x) = -M_\alpha \dot{u}_j(\alpha + \xi) u_{j,i}(\alpha + \xi)\delta(x - q(\alpha + \xi)). \tag{6.4}$$

(Summation over $j = 1, 2, 3$; $\alpha \in \mathbf{C}$, $\xi \in \mathbf{T}$ is implied.) With (3.1), (3.24) and (3.3) one obtains easily

$$\int \hat{p}_i(m)\, dm = \int \hat{p}_i^l(x)\, dx = -ik_i \dot{w}_j(\alpha, -k) w_j(\alpha, k). \tag{6.5}$$

(Summation over $k \in \mathbf{B}$.) This can be transformed to

$$\begin{aligned}\int \hat{p}_i(m)\, dm = \int \hat{p}_i^l(x)\, dx &= -ik_i X_{j\alpha s}(-k) X_{j\alpha s'}(k) \dot{c}_s(-k) c_{s'}(k) \\ &= -ik_i \dot{c}_s(-k) c_s(k) = k_i N_{ks}.\end{aligned} \tag{6.6}$$

Thus, the quantities $\hat{p}_i(m)$ and $\hat{p}_i^l(x)$ resemble the linear momentum density of the e.m. field. Therefore, following Leibfried et al., the equations (6.1) and (6.2) are interpreted as the balance equations for the 'quasi momentum' of the crystal. This naming agrees with the terming for homogeneous media. For these mediums, the analogues of (6.1) and (6.2) are the conservation laws for the quasi momentum.

For the crystal lattice, the substantial quasi-momentum production density reads (cf. equation (2.21) of I)

$$\begin{aligned}Q_i(m) = (\tfrac{1}{2} M_\alpha \dot{u}_j(m) \dot{u}_j(m) - f_{\alpha\beta}^{\xi-\zeta}(m - \beta - \zeta + u(m) \\ - u(m - \alpha - \xi + \beta + \zeta))\, d/dm_i\, \delta(m - \alpha - \xi).\end{aligned} \tag{6.7}$$

An analogous expression holds for the local quasi momentum production density (cf. (3.48) of I). The integrated values of both quantities are

$$\begin{aligned}\int Q_i(m)\, dm = \int Q_i^l(x)\, dx &= -M_\alpha \dot{u}_j(\alpha + \xi) \dot{u}_{j,i}(\alpha + \xi) \\ &+ (u_{j,i}(\alpha + \xi) - u_{j,i}(\beta + \zeta)) f_{\alpha\beta,ij}^{\xi-\zeta}(\alpha - \beta + \xi - \zeta + u(\alpha + \xi) - u(\beta + \zeta)).\end{aligned}$$

With the cyclic boundary condition one sees easily

$$\int Q_i(m)\, dm = \int Q_i^l(x)\, dx = 0. \tag{6.8}$$

Thus, although the quasi momentum is not a locally conserved quantity, i.e. there exists no local conservation law but only a local balance equation, globally the quasi momentum is a constant of the motion, as follows from (6.1), (6.2) and (6.8):

$$d/dt \int \hat{p}_i(m)\, dm = d/dt \int \hat{p}_i^l(x)\, dx \doteq 0. \tag{6.9}$$

For the crystal, the substantial quasi-momentum flux integrated over the volume reads (cf. equation (2.20) of I)

$$\begin{aligned}\int \hat{\pi}_{ij}(m)\, dm &= (\alpha - \beta + \xi - \zeta)_j u_{l,i}(\beta + \zeta) \\ &\quad \times f_{\alpha\beta,l}^{\xi-\zeta}(\alpha - \beta + \xi - \zeta + u(\alpha + \xi) - u(\beta + \zeta)) \\ &\quad + \delta_{ij}(\tfrac{1}{2}M_\alpha \dot{u}_l(\alpha + \xi)\dot{u}_l(\alpha + \xi) - f_{\alpha\beta}(\alpha - \beta + \xi - \zeta + u(\alpha + \xi) \\ &\quad - u(\beta + \zeta))).\end{aligned} \tag{6.10}$$

Here again, the constant and the linear term in the power-series expansion vanish. The quadratic terms can be treated in a way analogous to the calculation of the energy and the energy flux. In this way we obtain

$$\begin{aligned}\int {}^2\pi_{ij}(m)\, dm &= -\omega_s(k)S_{ks}\delta_{ij} + k_i\, d/dk_j\, \omega_s(k)(N_{ks} + S_{ks}) \\ &\quad + \tfrac{1}{2}(\omega_s^2(k) - \omega_{s'}^2(k))X_{n\alpha s}(k)\, d/dk_j\, X_{n\alpha s'}(-k)c_s(k)c_{s'}(-k).\end{aligned} \tag{6.11}$$

The difference of the integrated values of the local and the substantial quasi-momentum flux is (cf. equation (4.7) of I)

$$\begin{aligned}\int \hat{\pi}_{ij}^l(x)\, dx - \int \hat{\pi}_{ij}(m)\, dm &= \tfrac{1}{2}M_\alpha \dot{u}_l(\alpha + \xi)(\dot{u}_l(\alpha + \xi)u_{j,i}(\alpha + \xi) \\ &\quad - 2\dot{u}_j(\alpha + \xi)u_{l,i}(\alpha + \xi)) - u_{j,i}(\alpha + \xi)f_{\alpha\beta}^{\xi-\zeta}(\alpha - \beta + \xi - \zeta + u(\alpha + \xi) \\ &\quad - u(\beta + \zeta)) + u_{l,i}(\beta + \zeta)(u_j(\beta + \zeta) - u_j(\alpha + \xi)) \\ &\quad \times f_{\alpha\beta,i}^{\xi-\zeta}(\alpha - \beta + \xi - \zeta + u(\alpha + \xi) - u(\beta + \zeta)).\end{aligned} \tag{6.12}$$

In the special case (2.12) the harmonic terms of (6.12) vanish.

Let us now discuss (6.11). The term $k_i\, d/dk_j\, \omega_s(k)N_{ks}$ corresponds to the transport of the quasi momentum in a crystal with the group velocity $d/dk_j\, \omega_s(k)$. In most papers this term is the only one that is considered. The last term in (6.11) which is proportional to $(\omega_s^2(k) - \omega_{s'}^2(k))$, describes the influence of the interference of two non-degenerate modes or polarizations on the flux of the quasi momentum. This term finds its analogue in the expression (5.9) for the volume averaged energy flux. Furthermore, we have the term

$$(k_i\, d/dk_j\, \omega_s(k) - \delta_{ij}\omega_s(k))S_{ks}. \tag{6.13}$$

This term appears also in the theory of homogeneous media. It vanishes for dispersion-free one-dimensional systems. Moreover, it is easily proved that the time average of S_k over a long enough period approaches zero. For many physical applications, it is sufficient to know the time average of the volume averaged flux. For those cases the term (6.13) can be left out.

7. Evaluation and Final Remarks

With something that may be called 'physical intuition' one may feel the leaning or even the prospensity to write for the volume average of the energy flux in the harmonic approximation

$$\int {}^2 s_i(m)\, dm = \omega_s(k)\, d/dk_i\, \omega_s(k) N_{ks}. \tag{7.1}$$

The same physical intuition leads to the expression

$$k_i\, d/dk_j\, \omega_s(k) N_{ks} \tag{7.2}$$

for the volume average of the linear momentum flux, or if it is known that this is wrong, for the quasi-momentum flux. Our results and earlier results of other authors show that such a physical intuition is misleading.

Using the results of I, in this paper a crystal has been described as the limiting case of a continuous system. Methods used in continuum physics could therefore be applied to the crystal. Using substantial coordinates m, we have described in terms of a Lagrangian density L the dynamics of a crystal. With a transformation of the field variable $u(m) \to v(x)$ we have obtained an other Lagrangian density $\bar{L}$ which describes the crystal dynamics in terms of local coordinates x. The explicit form of both Lagrangian densities allowed us to use Noether's theorem in order to derive several local conservation laws and a local balance equation in terms of substantial as well as local coordinates.

With the infinitesimal transformation $\delta u_i(m) = \epsilon_i$ and $\delta v_i(x) = -\epsilon_j(\delta_{ij} + v_{i,j})$ we have derived (in substantial and in local coordinates, respectively) local conservation laws that describe the conservation of some quantity, which has been identified with the linear momentum of the crystal. The description in local coordinates corresponds to that of de Vault [8].

With an infinitesimal time shift ($\delta t = \epsilon$ or equivalently $\delta u_i = \epsilon \dot{u}_i$ and $\delta v_i = \epsilon \dot{v}_i$, respectively) the conservation of energy has been derived in terms of substantial and local coordinates. The description in substantial coordinates corresponds to that of Choquard [6], the description in local coordinates to the discussion of Hardy [7] and Enz [9].

With an infinitesimal shift of the lattice points ($\delta m_j = \epsilon_j$ or equivalently $\delta u_i(m) = \epsilon_j u_{i,j}$ and $\delta v_i(x) = \epsilon_j v_{i,j}$, respectively) we have derived a balance equation for a quantity that resembles the linear momentum of the e.m. field and has therefore been called 'quasi momentum'.

In order to clarify some aspects of the physical meaning of the concept of quasi momentum, we shall make a number of remarks:

(i) The definition of quasi momentum has been chosen such that the total quasi momentum of a crystal can be written as $\sum_k k_i N_{ks}$. As the total linear momentum is zero, we could also have taken a linear combination of the balance equation of the linear momentum and the balance equation of quasi momentum as an alternative definition of the balance equation of quasi momentum. Then the resulting expressions would have been more complicated, i.e. the anharmonicity of the crystal would have contributed to the harmonic part of the flux (cf. equations (4.7) and (6.11)). Thus, our choice is the simplest choice.

(ii) After linearization, the equations of motion in local and in substantial coordinates are identical. Then it is not clear in advance whether the independent coordinate is of substantial or of local nature. Consequently, a linear combination of linear momentum and quasi momentum may appear where only the linear momentum is expected.

(iii) One may obtain a better understanding of the concept of the quasi momentum of a crystal in a situation where the crystal interacts with its environment. For example, we can take a single particle interacting with the crystal. Then the crystal and the particle together constitute the dynamical system. The interaction energy of particle and crystal is in general of the form

$$\sum_{\xi\in\mathbf{T}}\sum_{\alpha\in\mathbf{C}} g(\alpha + \xi + u(\alpha + \xi) - q) \tag{7.3}$$

where $q = (q_1, q_2, q_3)$ denotes the position of the particle. With this form of the interaction energy it is easily seen that the sum of the linear momentum of the crystal and that of the particle is a conserved quantity. Similarly, one shows easily that the sum of the linear momentum of the particle and the quasi momentum of the crystal is conserved. (The same assumptions as in Section 6 have to be made.) Therefore we may say that the linear momentum of the particle is additively transferable to the linear momentum as well as to the quasi momentum of the crystal. (See the discussion on additive transferability of constants of the motion in [15], chapter 4.) Therefore the linear momentum and the quasi momentum of the crystal have the same 'particle analogue', in some sense. Furthermore it follows, also in the case where the crystal interacts with another particle, that the linear momentum and the quasi momentum are numerically equal (apart from a constant term).

(iv) In the whole discussion it has not been necessary to treat the so called 'Umklapp' processes. About this point the following remarks can be made: Because the values allowed for k are restricted to the first Brioullin zone $\mathbf{B}$, the definition (3.24) of $u_{j,i}(\alpha + \xi)$ is rather arbitrary. With another choice for $\mathbf{B}$ other values of $u_{j,i}(\alpha + \xi)$ are obtained. Consequently the value of $\int \hat{p}(m)\, dm$ depends essentially on the choice of $\mathbf{B}$. In fact, the use of the quantity $u_{j,i}$ in the discussion of the quasi momentum requires some continuum representation of u, for example

$$u(\alpha + \xi) \to u_\alpha(m) = M_\alpha^{-1/2} w(\alpha, k) \exp[ik\cdot(\alpha + m)]. \tag{7.4}$$

The restriction of the values of k to $\mathbf{B}$ becomes then inadequate. For example, one could take

$$k \in \{k = (k_1, k_2, k_3) \mid k_i = 2\pi n_i/L_i, n_i \in \mathbf{Z}\}. \tag{7.5}$$

With (7.4), a summation over ξ transforms into an integral over m. Instead of (3.3) we use then the identity

$$\int dm \exp[i(k - k')\cdot m] = \lambda\delta_{kk'}, \qquad \lambda = L_1L_2L_3 \tag{7.6}$$

and substantial phonons with $k \notin \mathbf{B}$ may appear in the description. Afterwards k can be reduced again to the first Brioullin zone:

$$\begin{aligned} &w(\alpha, k) \to w'(\alpha, k) = 0, \qquad k \notin \mathbf{B} \\ &w'(\alpha, k) = \sum_{K\in\mathbf{K}} w(\alpha, k + K), \qquad k \in \mathbf{B}. \end{aligned} \tag{7.7}$$

This restriction to **B** does not make any difference for the values of u at the lattice points, but it does for the derivatives. The consequence is that the quasi momentum changes in the same way as by 'Umklapp' processes. Therefore, 'Umklapp' processes enter the discussion of 'quasi momentum' in crystals because of the lack of its unique definition.

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