Zeitschrift: Helvetica Physica Acta

Band: 49 (1976)

Heft: 4

Artikel: Local and substantial fluxes for energy, linear momentum and quasi momentum in systems with a non-local internal interaction

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DOI: https://doi.org/10.5169/seals-114784

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Local and Substantial Fluxes for Energy, Linear Momentum and Quasi Momentum in Systems with a Non-local Internal Interaction

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(16. II. 1976)

Abstract. The dynamics of a continuous inhomogeneous system with a non-linear non-local internal interaction is described. This is done in terms of a Lagrangian density by means of local as well as substantial coordinates. In both coordinate systems the conservation laws for energy and linear momentum are derived. Additionally, a balance equation for a quantity, which may be termed quasi momentum, has been constructed. The expressions in both coordinate systems are mutually related.

1. Introduction

In many problems in physics it is not obvious what physical quantities must be taken as the independent variables, the coordinates. In the description of the dynamics of a compressible fluid one may use local coordinates, also called Eulerian coordinates, or substantial coordinates, also termed Lagrangian or material coordinates. In solid state physics the same problem is met.

In hydrodynamics as well as solid state physics local quantities mixed up with substantial quantities are generally used. Mass densities and energy densities are usually local densities. On the other hand, the velocities used in the same discussions are time derivatives of substantial quantities. This mixing up of two different descriptions hinders the formulation of the dynamics in terms of a Lagrangian or a Hamiltonian. One has to find suitable field variables first.

Recently we studied the conversion from substantial into local coordinates in terms of a Lagrangian and Hamiltonian formulation of fluid motion (Ref. [1] and Ref. [2], chapters 6 and 7). In the present paper we study the same problem for a continuous inhomogeneous dynamical system with a non-linear non-local internal interaction. The Lagrangian of the model has been chosen such that, for a special choice of the mass density and the potential energy function, the system may describe both local interaction and the dynamics of a crystal lattice as limiting cases.

In Section 2 of this paper a Lagrangian density is introduced in terms of substantial coordinates. On the basis of invariant infinitesimal transformations of the field variable (Noether's theorem) expressions for substantial energy density and flux, substantial linear-momentum density and flux are found. With a modification of

[1]) Work supported by the Swiss National Foundation.

Noether's theorem expressions for what can be called quasi-momentum density, flux and production density are derived. In Section 3 we convert the formalism of Section 2 into local coordinates. The transformation for this is analogous to the transformation used in [1] and [2] for the hydrodynamical case. The transformation used is purely geometrical, i.e. it does not depend explicitly on the dynamics. In Section 4 we give a concise discussion and comparison of the results of Sections 2 and 3. In a forthcoming paper we will apply the present results to the dynamics of a crystal lattice; there, a comparison will be given with results of other authors who use methods familiar in the field of solid state physics.

2. Substantial Description

Let the state of a continuous dynamical system with dimensionality d be realized by fixing the components of the field vector $u = u(m) = (u_1(m), u_2(m), \ldots, u_d(m))$ and the field velocity $\dot{u} = \dot{u}(m) = (\dot{u}_1(m), \dot{u}_2(m), \ldots, \dot{u}_d(m))$ as a function of the coordinate $m = (m_1, m_2, \ldots, m_d)$. The coordinate m itself will be interpreted as a substantial coordinate, indicating material points of the system. For example one can take the position, at time $t = 0$ or in another reference situation, of some material point as the corresponding coordinate m.

The system dynamics is described by a function of time: $u(m, t)$. This function gives the time evolution of the field vector u. The field velocity then takes the form $\dot{u} = (du/dt)_m$. Finally, we assume that admissible fields $u = u(m, t)$ are prescribed by solutions of the Euler–Lagrange equations following from the substantial Lagrangian density (i.e. Lagrangian density in m space)

$$L(m) = \tfrac{1}{2}\rho_0(m)\dot{u}_i\dot{u}_i - \int d\mu V(z(m, \mu), m, \mu), \tag{2.1}$$

where

$$z(m, \mu) = u(m + \mu) - u(m) + \mu. \tag{2.2}$$

(Summation over repeated Latin indices is implied over $1, 2, \ldots, d$.) The quantity $\rho_0(m)$ is a non-negative scalar function of m and can be interpreted as the mass density in the substantial coordinate m-space. $\rho_0(m)$ will be termed substantial mass density. The function $V(z, m, \mu)$ is a real scalar function of the three d-tuples z, m and μ and may be interpreted as the potential energy density in m, μ-space. Furthermore $\int d\mu$ denotes the multiple integral $\int d\mu_1 \int d\mu_2 \ldots \int d\mu_d$. The integration over μ has to be carried out over the entire volume of the system. As a rule we will not write the argument of the function u explicitly if $u(m)$ is meant.

The potential energy density in m space $\int d\mu V(z(m, \mu), m, \mu)$ describes the interaction between material points with coordinates m and $(m + \mu)$ of distance $z(m, \mu) = \mu + u(m + \mu) - u$. Additionally certain conditions ensuring a decent behaviour, such as differentiability and integrability, should be imposed, but we will not specify, and in the following not even mention, these conditions.

In general any dynamical system can be described by a class of Lagrangian densities. In applications one does not have to worry about this, because what can be derived from one particular Lagrangian density can be derived from any suitable Lagrangian density. Therefore we did not try to give the most general Lagrangian to describe the same system, as e.g. Marnelius [3] recently did for systems with a non-local internal interaction. On the contrary, we tried to introduce a Lagrangian density that is easily manageable with a minimal loss of generality concerning applications to different systems.

Let $x = (x_1, x_2, \ldots, x_d), y = (y_1, y_2, \ldots, y_d)$ and $d/dx = d/dx_1\, d/dx_2 \ldots d/dx_d$; then for any function $F(x)$ holds:

$$F(x) = -d/dx \int_{C_x} F(y)\, dy = -d/dx \int_{C_0} F(x + y)\, dy$$

and analogously

$$F(x - z) = -d/dx \int_{C_{x-z}} F(y)\, dy = -d/dx \int_{C_{-z}} F(x + y)\, dy.$$

Subtraction of both equations gives

$$F(x) - F(x - z) = d/dx \int_{D_z} F(x + y)\, dy. \tag{2.3}$$

Here $D_z = C_{-z} \backslash C_0$ is the first 'octant' $C_{-z} = \{y \mid y_i > -z_i\}$ in y-space with the center in $y = -z$ minus the first 'octant' $C_0 = \{y \mid y_i > 0\}$ with the center in the origin $y = 0$. We note that in (2.3) the function F is not necessarily a scalar function.

In order to derive from (2.1) the equations of motion (Euler–Lagrange equations) and various conservation laws we must be able to translate arguments of functions. Equation (2.3) makes this possible.

We shall use the following notations

$$u_{j,i} = (\partial/\partial m_i\, u_j(m))_{m_l \neq i, t},$$
$$\rho_{0,i}(m) = (\partial/\partial m_i\, \rho_0(m))_{m_j \neq i},$$
$$V_{,i}(\alpha, \beta, \gamma) = (\partial/\partial \alpha_i\, V(\alpha, \beta, \gamma))_{\alpha_j \neq i, \beta, \gamma},$$
$$V_{;i}(\alpha, \beta, \gamma) = (\partial/\partial \beta_i\, V(\alpha, \beta, \gamma))_{\alpha, \beta_j \neq i, \gamma},$$

where the comma in $V_{,i}(\alpha, \beta, \gamma)$ means differentiation with respect to the first variable, and the semi-colon in $V_{;i}(\alpha, \beta, \gamma)$ means differentiation with respect to the second variable. From (2.1) we can derive the equation of motion

$$\rho_0(m)\ddot{u}_i \doteq \int d\mu (V_{,i}(z(m, \mu), m, \mu) - V_{,i}(z(m - \mu, \mu), m - \mu, \mu)), \tag{2.4}$$

which leaves for the first-order variation $\delta L(m)$ of $L(m)$

$$\delta L(m) \doteq d/dt\, (\rho_0(m)\dot{u}_i \delta u_i)$$
$$- d/dm \int d\mu \int_{D_\mu} d\eta V_{,i}(z(m + \eta, \mu), m + \eta, \mu)\delta u_i(m + \mu + \eta). \tag{2.5}$$

Note that here d/dt means differentiation with constant m. The symbol $\doteq$ denotes the so called weak identity only valid for solutions u of the equations of motion.

From the definition (2.1) of $L(m)$ it is readily seen that the infinitesimal translation in u-space ($\delta u_i = \epsilon_i$, ϵ_i being vanishingly small constants) leaves the Lagrangian density $L(m)$ invariant:

$$\delta u_i = \epsilon_i \rightarrow \delta L = 0.$$

So from (2.5) we obtain the set of local conservation laws:

$$d/dt\, (\rho_0(m)\dot{u}_i) - d/dm \int d\mu \int_{D_\mu} d\eta V_{,i}(z(m + \eta, \mu), m + \eta, \mu) \doteq 0. \tag{2.6}$$

With the interpretation of u_i as a deviation of a material point in the ith direction and $\rho_0(m)$ as the substantial mass density, the quantity $\int_\Omega \rho_0(m)\dot{u}\, dm$ clearly represents the total linear momentum in the volume Ω. Consequently (2.6) is the local conservation law for the linear momentum in substantial coordinates. In fact this derivation is equivalent to Noether's theorem (Ref. [2], section (3.4)).

In the same way we may deduce the conservation law for the energy by the infinitesimal translation in t-space (ϵ being an infinitesimal scalar)

$$\delta u = \epsilon \dot{u} \rightarrow \delta L(m) = \epsilon d/dt L(m),$$

So with (2.5) we find the local conservation law for the energy:

$$d/dt \left(\tfrac{1}{2}\rho_0(m)\dot{u}_i\dot{u}_i + \int d\mu V(z(m, \mu), m, \mu)\right)$$
$$- d/dm \int d\mu \int_{D_\mu} d\eta V_{,i}(z(m + \eta, \mu), m + \eta, \mu)\dot{u}_i(m + \mu + \eta) \doteq 0. \tag{2.7}$$

If the system described by (2.1) were homogeneous, the infinitesimal translation in m-space would also be a Noetherian variation: If $\rho_{0,i}(m) = 0$ and $V_{;i}(z, m, \mu) = 0$ then $\delta u_i = \epsilon_j u_{i,j}$ yields $\delta L(m) = \epsilon_j d/dm_j\, L(m)$. In the general inhomogeneous case the variation $\delta u_i = \epsilon_j u_{i,j}$ does not leave $L(m)$ invariant up to a total derivative, but there are other terms containing $\rho_{0,i}(m)$ and $V_{;i}(z, m, \mu)$. The result is not a local conservation law but a local balance equation, i.e. a local conservation law with a non-zero right-hand side (source term).

$$\delta u_i = \epsilon_j u_{i,j} \rightarrow \delta L(m) = \epsilon_j \left\{ d/dm_j\, L(m) - \tfrac{1}{2}\rho_{0,j}(m)\dot{u}_i\dot{u}_i + \int d\mu V_{;j}(z(m, \mu), m, \mu)\right\}.$$

With (2.5) we then obtain

$$d/dt\,(-\rho_0(m)\dot{u}_i u_{i,j}) + d/dm_j \left(\tfrac{1}{2}\rho_0(m)\dot{u}_i\dot{u}_i - \int d\mu V(z(m, \mu), m, \mu)\right)$$
$$+ d/dm \int d\mu \int_{D_\mu} d\eta V_{,i}(z(m + \eta, \mu), m + \eta, \mu)u_{i,j}(m + \mu + \eta)$$
$$\doteq \tfrac{1}{2}\rho_{0,j}(m)\dot{u}_i\dot{u}_i - \int d\mu V_{;j}(z(m, \mu), m, \mu). \tag{2.8}$$

This equation, obviously a local balance equation in substantial coordinates, will be interpreted as a description of the balance of 'quasi momentum'. One reason for this is that for homogeneous media (2.8) changes to a conservation law that is usually identified with the conservation law for quasi momentum. Another argument is found in the specialization of (2.1) for crystal lattices. Then using an appropriate continuum representation for u and suitable phonon variables, the total quasi momentum $-\int dm\rho_0(m)\dot{u}_i u_{i,j}$ can be written as $\sum_{\mathbf{k}} k_j N_{\mathbf{k}s}$. Here $\mathbf{k} = (k_1, k_2, \ldots, k_d)$ is the wave vector of a phonon, $N_{\mathbf{k}s}$ the number of phonons with wave vector $\mathbf{k}$ and mode/polarization s. In solid state physics such a quantity is called quasi momentum (if it is not simply called momentum). In a forthcoming paper we will come back to this subject.

Any of the equations (2.6), (2.7) and (2.8) contain a term of the form $d/dm \int d\mu \int_{D_\mu} d\eta F(m + \eta, \mu)$, which is the divergence of some flux term:

$$\operatorname{div} G = d/dm_i\, G_i = d/dm_1 \ldots d/dm_d \int d\mu \int_{D_\mu} F(m + \eta, \mu)\, d\eta. \tag{2.9}$$

The components G_i of the flux term are not defined uniquely by this equation. A divergence-free term may always be added to G_i. To obtain symmetrically looking expressions one may write

$$G_1 = d/dm_2 \cdots d/dm_d \left\{ \int d\mu \int_{-\mu_1}^{0} d\eta_1 \int_0^{\infty} d\eta_2 \cdots \int_0^{\infty} d\eta_d F(m+\eta, \mu) + 1/d \int d\mu \int_{-\mu_1}^{0} d\eta_1 \int_{-\mu_2}^{0} d\eta_2 \cdots \int_{-\mu_d}^{0} d\eta_d F(m+\eta, \mu) \right\} \quad (2.10)$$

and similar expressions for $G_2, G_3, \ldots, G_d$. From (2.10), we obtain easily

$$\int dm G_i = (-)^{d-1} \iint dm\, d\mu \mu_i F(m, \mu) \quad (2.11)$$

where the integration over m is done over the entire system. The factor $(-)^{d-1}$ comes from integrating by parts $(d-1)$ times. The second term of (2.10) does not give a contribution to $\int G_1\, dm$. The equations (2.6), (2.7) and (2.8) may now be written in the usual form

$$d/dt\, p_i(m) + d/dm_j\, \pi_{ij}(m) \doteq 0, \quad (2.12)$$

$$d/dt\, e(m) + d/dm_j\, s_j(m) \doteq 0, \quad (2.13)$$

and

$$d/dt\, \hat{p}_i(m) + d/dm_j\, \hat{\pi}_{ij}(m) \doteq Q_i(m), \quad (2.14)$$

respectively. Here

$$p_i(m) = \rho_0(m)\dot{u}_i, \quad (2.15)$$

$$e(m) = \tfrac{1}{2}\rho_0(m)\dot{u}_i\dot{u}_i + \int d\mu V(z(m, \mu), m, \mu), \quad (2.16)$$

and

$$\hat{p}_i(m) = -\rho_0(m)\dot{u}_k u_{k,i} \quad (2.17)$$

are the substantial linear-momentum density, the substantial energy density and the substantial quasi-momentum density, respectively. For the substantial linear-momentum flux $\pi_{ij}(m)$, the substantial energy flux $s_j(m)$ and the substantial quasi-momentum flux $\hat{\pi}_{ij}(m)$, we give only the value of the integral over the entire volume.

$$\int \pi_{ij}(m)\, dm = (-)^d \iint dm\, d\mu \mu_j V_{,i}(z(m, \mu), m, \mu), \quad (2.18)$$

$$\int s_j(m)\, dm = (-)^d \iint dm\, d\mu \mu_j \dot{u}_i(m+\mu) V_{,i}(z(m, \mu), m, \mu), \quad (2.19)$$

$$\int \hat{\pi}_{ij}(m)\, dm = \int dm \tfrac{1}{2}\rho_0(m)\dot{u}_k\dot{u}_k\delta_{ij} - \iint dm\, d\mu V(z(m, \mu), m, \mu)\delta_{ij} - (-)^d \iint dm\, d\mu \mu_j u_{k,i}(m+\mu) V_{,k}(z(m, \mu), m, \mu), \quad (2.20)$$

where δ_{ij} is the usual Kronecker delta symbol

$$\delta_{ij} = 1\ (i = j); \quad \delta_{ij} = 0\ (i \neq j).$$

We can write down the expressions for the fluxes themselves. Nevertheless, we prefer to give the integrated value only, because these expressions are simpler and are sufficient for many physical applications. The source density of the balance equation for the quasi momentum reads

$$Q_i(m) = \tfrac{1}{2}\rho_{0,i}(m)\dot{u}_k\dot{u}_k - \int d\mu V_{;i}(z(m, \mu), m, \mu). \tag{2.21}$$

3. Local Description

If in the foregoing section the substantial coordinate m describes the position of a material point in some reference situation and the field vector $u(m)$ is the deviation from this reference situation, the local positions of the material points are given by

$$x = q(m) = m + u(m). \tag{3.1}$$

In analogy to the procedure in [1] and [2] we now define the new field vector $v(x) = (v_1(x), v_2(x), \ldots, v_d(x))$ by introducing $\tilde{q}(x)$, the set of inverse functions of $q(m)$:

$$m = \tilde{q}(x) = x + v(x), \tag{3.2}$$

where

$$x = q(\tilde{q}(x)); \quad m = \tilde{q}(q(m)). \tag{3.3}$$

Note that the transformation $u(m) \to v(x)$ is a purely geometrical transformation, i.e. the transformation does not depend on the dynamics of the system. Inserting (3.1) and (3.2) into (3.3) we obtain

$$x = \tilde{q}(x) + u(\tilde{q}(x)) = x + v(x) + u(x + v(x)),$$
$$m = q(m) + v(q(m)) = m + u(m) + v(m + u(m)),$$

or

$$v(x) + u(x + v(x)) = 0, \tag{3.4}$$

$$u(m) + v(m + u(m)) = 0. \tag{3.5}$$

In general we shall not write the arguments of u and v explicitly, unless confusion might arise. Thus, writing u or v, we mean the functions $u(m)$ or $v(x)$, respectively.

In analogy to (3.2) we put

$$m + \mu = \tilde{q}(x + z) = x + z + v(x + z). \tag{3.6}$$

Then, with (3.2) we get

$$\mu = z + v(x + z) - v(x). \tag{3.7}$$

On the other hand, from (3.1), (3.3) and (3.6) we obtain

$$x + z = q(m + \mu) = m + \mu + u(m + \mu),$$

or again with (3.1)

$$z = q(m + \mu) - q(m) = \mu + u(m + \mu) - u(m). \tag{3.8}$$

The Jacobian of the transformation $m \to x$ is

$$J(x) = \frac{\partial(m_1, \ldots, m_d)}{\partial(x_1, \ldots, x_d)} = \det\left(\frac{\partial m_i}{\partial x_j}\right) = \det\left(\frac{\partial \tilde{q}_i(x)}{\partial x_j}\right),$$

and because of (3.2)

$$J(x) = \det(\delta_{ij} + v_{i,j}(x)). \tag{3.9}$$

Analogously the Jacobian of the transformation from the pair of variables (m, μ) to (x, z), given by (3.2) and (3.7), is

$$\frac{\partial(m_1, \ldots, m_d, \mu_1, \ldots, \mu_d)}{\partial(x_1, \ldots, x_d, z_1, \ldots, z_d)} = \det\begin{pmatrix} \partial m_i/\partial x_j & \partial \mu_i/\partial x_j \\ \partial m_i/\partial z_j & \partial \mu_i/\partial z_j \end{pmatrix} = J(x)J(x + z). \tag{3.10}$$

The relation between the substantial field velocity $\dot{u}$ and the local field velocity $\dot{v}$ is obtained by differentiating equation (3.5) with respect to time. In this way we find

$$\dot{u}_i + \dot{v}_i + v_{i,j}\dot{u}_j = \dot{u}_j(\delta_{ij} + v_{i,j}) + \dot{v}_i = 0.$$

Now we introduce the inverse of the matrix $(\delta_{ij} + v_{i,j})$:

$$A_{li}(\delta_{ij} + v_{i,j}) = \delta_{lj}. \tag{3.11}$$

Then

$$\dot{u}_l = -A_{li}\dot{v}_i. \tag{3.12}$$

Analogously we can find

$$u_{l,k} = -A_{li}v_{i,k}. \tag{3.13}$$

Now enough preliminary work has been done to convert the substantial Lagrangian density $L(m)$ into a local Lagrangian density $\bar{L}(x)$. This has to be done in such a way that the Lagrangian functionals $\int L(m)\, dm$ and $\int \bar{L}(x)\, dx$ are equal (Ref. [2], section (3.2)). From (2.1) and (2.2) we see

$$\mathscr{L} = \int dm \tfrac{1}{2}\rho_0(m)\dot{u}_i\dot{u}_i - \iint dm\, d\mu V(\mu + u(m + \mu) - u(m), m, \mu). \tag{3.14}$$

With (3.9) and (3.10), the substitution of (3.2), (3.7), (3.8) and (3.12) into (3.14) gives

$$\mathscr{L} = \int dx \tfrac{1}{2}J(x)\rho_0(x + v)A_{ij}A_{il}\dot{v}_j\dot{v}_l - \iint dx\, dz J(x)J(x + z) \times V(z, x + v, z + v(x + z) - v(x)).$$

So with $\mathscr{L} = \int \bar{L}(x)\, dx$ we find for the local Lagrangian density $\bar{L}(x)$

$$\bar{L}(x) = \tfrac{1}{2}J(x)\rho_0(x + v)A_{ij}A_{il}\dot{v}_j\dot{v}_l - J(x)\int dz J(x + z)V(z, x + v, z + v(x + z) - v). \tag{3.15}$$

Note that $J(x)$ depends explicitly on $v_{i,j}$. Therefore, for variations δv the variation $\delta J(x)$ of $J(x)$ is

$$\delta J(x) = \frac{\partial J(x)}{\partial v_{i,l}}\, \delta v_{i,l}. \tag{3.16}$$

From (3.11) and the properties of determinants one easily verifies

$$\frac{\partial J(x)}{\partial v_{i,l}} = J(x)A_{li}. \tag{3.17}$$

Hence

$$\delta J(x) = J(x)A_{li}\delta v_{i,l}. \tag{3.18}$$

Analogously the variation of the matrix element A_{ik} is

$$\delta A_{ik} = \frac{\partial A_{ik}}{\partial v_{l,m}}\,\delta v_{l,m}. \tag{3.19}$$

Differentiating (3.11) with respect to $v_{l,m}$ gives

$$\frac{\partial A_{ik}}{\partial v_{l,m}} = -A_{il}A_{mk}. \tag{3.20}$$

We have calculated the variation $\delta L(m)$ for arbitrary variations δu in Section 2. Analogously we may calculate the variation $\delta\bar{L}(x)$ for variations δv. Before doing this we note that the expression (3.15) for $\bar{L}(x)$ is much more complicated than (2.1) for $L(m)$. Furthermore we do not need the full expression for $\delta\bar{L}(x)$ but only the analogue of (2.5), for we shall not need an explicit expression for the equation of motion in local variables. Therefore in the elaboration of the expression for $\delta\bar{L}(x)$ we have to collect only terms that give a contribution to terms which are derivatives with respect to time t (at constant x) or to x_i (at constant t, $x_{j\neq i}$). The calculation becomes less complicated by writing

$$\begin{aligned}\bar{L}(x) = {} & \tfrac{1}{2}J(x)\rho_0(x+v)\dot{u}_i(x+v)\dot{u}_i(x+v)\\ & - J(x)\int d\mu V(\mu + u(x+v+\mu) - u(x+v), x+v, \mu)\end{aligned} \tag{3.21}$$

instead of (3.15). This is allowed because $1/J(x+z)$ is the Jacobian of the transformation of the integration variable z into μ (fixed x, m) as is readily seen with (3.7).

Using (3.21) instead of (3.15) we need additionally the relation between δv_i and the variations of u_k and $\dot{u}_i$. From (3.5) and (3.11) it follows

$$\delta u_k = -A_{ki}\delta v_i. \tag{3.22}$$

From (3.12) we see

$$\delta\dot{u}_i = -A_{ik}\delta\dot{v}_k - \dot{v}_k\frac{\partial A_{ik}}{\partial v_{l,n}}\,\delta v_{l,n}$$

or with (3.20) and again with (3.12)

$$\delta\dot{u}_i = -A_{ik}\delta\dot{v}_k - \dot{u}_n A_{il}\delta v_{l,n}. \tag{3.23}$$

For $\delta\bar{L}(x)$ we obtain finally

$$\begin{aligned}\delta\bar{L}(x) \doteq {} & d/dt\,(\rho(x)\dot{u}_i\delta u_i) + d/dx_j\,(-\tfrac{1}{2}\rho(x)\dot{u}_i\dot{u}_i\delta u_j + \rho(x)\dot{u}_i\dot{u}_j\delta u_i\\ & + J(x)\delta u_j\int d\mu V(z(x+v,\mu), x+v, \mu))\\ & - d/dx\int d\mu\int_{D_\mu} d\eta\,\delta u_i(x+v+\eta+\mu)\\ & \times V_{,i}(z(x+v+\eta),\mu), x+v+\eta, \mu),\end{aligned} \tag{3.24}$$

where

d/dt is the differentiation with respect to t at constant x,

$$u_i = u_i(x + v), \quad \dot{u}_i = \dot{u}_i(x + v), \quad \delta u_j = \delta u_j(x + v), \tag{3.25}$$

$\rho(x) = J(x)\rho_0(x + v)$ is the hydrodynamical local mass density, (3.26)

$d/dx = d/dx_1\, d/dx_2 \ldots d/dx_d$,

$D_\mu = C_{-\mu}\backslash C_0 = \{\eta \mid \eta_i > -\mu_i\}\backslash\{\eta \mid \eta_i > 0\}$ and

$$z(m, \mu) = \mu + u(m + \mu) - u(m). \tag{2.2}$$

For further reference we note that the last term in (3.24) may also be written as

$$-d/dx \int dz \int_{D_z} dy J(x + z)J(x + y + z)A_{il}(x + y + z)\delta v_l(x + y + z)$$
$$\times V_{,i}(z, x + y + v(x + y), z + v(x + y + z) - v(x + y)). \tag{3.27}$$

In Section 2 the conservation of linear momentum has been derived by means of the variation $\delta u_i = \epsilon_i$. From (3.22) and (3.11) the equivalence of the variations

$$\delta u_i = \epsilon_i \quad \text{and} \quad \delta v_i = -\epsilon_j(\delta_{ij} + v_{i,j}) \tag{3.28}$$

follows. Using (3.15), (3.16) and (3.19) for the variation (3.28), we obtain

$$\delta\bar{L}(x) = -\epsilon_j\, d/dx_j\, \bar{L}(x). \tag{3.29}$$

Equations (3.24) and (3.28) yield

$$\delta\bar{L}(x) \doteq \epsilon_k\, d/dt\, (\rho(x)\dot{u}_k) + \epsilon_k\, d/dx_j\, (-\tfrac{1}{2}\rho(x)\dot{u}_i\dot{u}_i\delta_{jk} + \rho(x)\dot{u}_k\dot{u}_j$$
$$+ J(x)\delta_{jk} \int d\mu V(z(x + v, \mu), x + v, \mu))$$
$$- \epsilon_k\, d/dx \int d\mu \int_{D_\mu} d\eta V_{,k}(z(x + v + \eta, \mu), x + v + \eta, \mu). \tag{3.30}$$

On the other hand we obtain with (3.29), (3.21), (3.25) and (3.26)

$$\delta\bar{L}(x) = \epsilon_k d/dx_j\, (-\tfrac{1}{2}\rho(x)\dot{u}_i\dot{u}_i\delta_{jk} + J(x)\delta_{jk} \int d\mu V(z(x + v, \mu), x + v, \mu)). \tag{3.31}$$

From (3.30) and (3.31), we get then the local conservation law in local coordinates

$$d/dt\, (\rho(x)\dot{u}_k) + d/dx_j\, (\rho(x)\dot{u}_k\dot{u}_j)$$
$$- d/dx \int d\mu \int_{D_\mu} d\eta V_{,k}\, (z(x + v + \eta), x + v + \eta, \mu) \doteq 0. \tag{3.32}$$

In analogy to (2.12) we write

$$d/dt\, p_i^l(x) + d/dx_j\, \pi_{ij}^l(x) \doteq 0 \tag{3.33}$$

instead of (3.32). Here

$$p_i^l(x) = \rho(x)\dot{u}_i. \tag{3.34}$$

With (2.15) and (3.26) it follows

$$p_i(x + v)J(x) = p_i^l(x) \tag{3.35}$$

and consequently

$$\int p_i^l(x)\,dx = \int p_i(x+v)J(x)\,dx = \int p_i(m)\,dm.$$

Therefore (3.32) is the local conservation law for the linear momentum in local coordinates, $p_i^l(x)$ being the local linear-momentum density and $\pi_{ij}^l(x)$ being the local linear-momentum flux. For the integrated value of the local linear-momentum flux $\int \pi_{ij}^l(x)\,dx$ we can write (c.f. (3.27) and (2.9)–(2.11))

$$\int \pi_{ij}^l(x)\,dx = \int dm\rho_0(m)\dot{u}_i\dot{u}_j + (-)^d \iint dm d\mu(\mu_j + u_j(m+\mu) - u_j(m)) \times V_{,i}(z(m,\mu), m, \mu). \tag{3.36}$$

With the variation $\delta u_i = \epsilon\dot{u}_i$ the conservation of energy has been derived in Section 2. The variation $\delta v_i = \epsilon\dot{v}_i$ is equivalent to the variation $\delta u_i = \epsilon\dot{u}_i$ (c.f. equation (3.22) and (3.12)). Because $\bar{L}(x)$ does not depend on time explicitly, under the variation $\delta v_i = \epsilon\dot{v}_i$ we obtain for $\delta\bar{L}(x)$

$$\delta\bar{L}(x) = \epsilon\, d/dt\, \bar{L}(x) = \epsilon\, d/dt\, (\tfrac{1}{2}\rho(x)\dot{u}_i\dot{u}_i - J(x)\int d\mu V(z(x+v,\mu), x+v, \mu)). \tag{3.37}$$

On the other hand, with (3.24) we get

$$\begin{aligned}\delta\bar{L}(x) \doteq{}& \epsilon\, d/dt\, (\rho(x)\dot{u}_i\dot{u}_i)\\ &+ \epsilon\, d/dx_j\, (\tfrac{1}{2}\rho(x)\dot{u}_i\dot{u}_i\dot{u}_j + J(x)\dot{u}_j \int d\mu V(z(x+v,\mu), x+v,\mu))\\ &- \epsilon\, d/dx \int d\mu \int_{D_\mu} d\eta \dot{u}_i(x+v+\eta+\mu)V_{,i}(z(x+v+\eta,\mu), x+v+\eta,\mu).\end{aligned} \tag{3.38}$$

Subtracting these two equations we obtain

$$\begin{aligned}&d/dt\, (\tfrac{1}{2}\rho(x)\dot{u}_i\dot{u}_i + J(x)\int d\mu V(z(x+v,\mu), x+v,\mu))\\ &\quad + d/dx_j\, (\tfrac{1}{2}\rho(x)\dot{u}_i\dot{u}_i\dot{u}_j + J(x)\dot{u}_j \int d\mu V(z(x+v,\mu), x+v,\mu))\\ &\quad - d/dx \int d\mu \int_{D_\mu} d\eta \dot{u}_i(x+v+\eta+\mu)V_{,i}(z(x+v+\eta,\mu), x+v+\eta,\mu) \doteq 0.\end{aligned} \tag{3.39}$$

In analogy to (2.13) we write now

$$d/dt\, e^l(x) + d/dx_j\, s_j^l(x) \doteq 0, \tag{3.40}$$

where (c.f. equation (2.16))

$$e^l(x) = \tfrac{1}{2}\rho(x)\dot{u}_i\dot{u}_i + J(x)\int d\mu V(z(x+v,\mu), x+v,\mu) = J(x)e(x+v), \tag{3.41}$$

and therefore $\int e^l(x)\,dx = \int e(m)\,dm$. This implies that (3.39)–(3.40) is the local conservation law for the energy in local coordinates, $e^l(x)$ being the local energy density

and $s_j^l(x)$ the local energy flux. Analogously to what we did for the integrated value of the local energy flux we may write

$$\int s_j^l(x)\,dx = \int dm \tfrac{1}{2}\rho_0(m)\dot{u}_i\dot{u}_i\dot{u}_j + \iint dm\,d\mu\dot{u}_j V(z(m,\mu), m, \mu)$$
$$+ (-)^d \iint dm\,d\mu(\mu_j + u_j(m+\mu) - u_j)\dot{u}_i(m+\mu)V_{,i}(z(m,\mu), m, \mu). \quad (3.42)$$

The balance equation for the quasi momentum has been derived in substantial coordinates by the variation $\delta u_i = \epsilon_j u_{i,j}$. The variation $\delta v_i = \epsilon_j v_{i,j}$ is equivalent to that variation as a consequence of (3.13) and (3.22). From (3.15) and (3.26) we then obtain

$$\delta\bar{L}(x) = \epsilon_j\, d/dx_j\,(\tfrac{1}{2}\rho(x)\dot{u}_i\dot{u}_i - J(x)\int d\mu V(z(x+v,\mu), x+v, \mu))$$
$$- \rho_{0,j}(x+v)J(x)\dot{u}_i\dot{u}_i + J(x)\int d\mu V_{;j}(z(x+v,\mu), x+v, \mu). \quad (3.43)$$

On the other hand (3.24) yields

$$\delta\bar{L}(x) \doteq \epsilon_k\, d/dt\,(\rho(x)\dot{u}_i u_{i,k}) + \epsilon_k\, d/dx_j\,(-\tfrac{1}{2}\rho(x)\dot{u}_i\dot{u}_i u_{j,k}$$
$$+ \rho(x)\dot{u}_i\dot{u}_j u_{i,k} + J(x)u_{j,k}\int d\mu V(z(x+v,\mu), x+v, \mu))$$
$$- \epsilon_k\, d/dx \int d\mu \int_{D_\mu} d\eta u_{i,k}(x+v+\eta+\mu)$$
$$\times V_{,i}(z(x+v+\eta,\mu), x+v+\eta, \mu). \quad (3.44)$$

Subtracting (3.43) and (3.44) we get the balance equation

$$d/dt\,(-\rho(x)\dot{u}_i u_{i,k}) + d/dx_j\,(\tfrac{1}{2}\rho(x)\dot{u}_i\dot{u}_i(u_{j,k} + \delta_{jk}) - \rho(x)\dot{u}_i\dot{u}_j u_{i,k})$$
$$- d/dx_j\,((u_{j,k} + \delta_{jk})J(x)\int d\mu V(z(x+v,\mu), x+v, \mu))$$
$$+ d/dx \int d\mu \int_{D_\mu} d\eta u_{i,k}(x+v+\eta+\mu)V_{,i}(z(x+v+\eta,\mu), x+v+\eta, \mu)$$
$$\doteq \rho_{0,k}(x+v)J(x)\dot{u}_i\dot{u}_i - J(x)\int d\mu V_{;k}(z(x+v,\mu), x+v, \mu). \quad (3.45)$$

In analogy to (2.14) we write

$$d/dt\,\hat{p}_k^l(x) + d/dx_j\,\hat{\pi}_{kj}^l(x) \doteq Q_k^l(x), \quad (3.46)$$

where (c.f. equations (2.17) and (2.21))

$$\hat{p}_k^l(x) = -\rho(x)\dot{u}_i u_{i,k} = J(x)\hat{p}_k(x+v), \quad (3.47)$$

$$Q_k^l(x) = \rho_{0,k}(x+v)J(x)\dot{u}_i\dot{u}_i - J(x)\int d\mu V_{;k}(z(x+v,\mu), x+v, \mu)$$
$$= J(x)Q_k(x+v), \quad (3.48)$$

and therefore $\int \hat{p}_k^l(x)\,dx = \int \hat{p}_k(m)\,dm$; $\int Q_k^l(x)\,dx = \int Q_k(m)\,dm$, so that (3.45)–(3.46) is the balance equation for the quasi momentum in terms of local coordinates, $p^l(x)$ being the local quasi-momentum density, $\hat{\pi}^l(x)$ being the local quasi-momentum flux, and $Q^l(x)$ the local production-density of quasi momentum.

For the integrated value of the quasi-momentum flux we find

$$\int \hat{\pi}^l_{kj}(x)dx = \int dm\{\tfrac{1}{2}\rho_0(m)\dot{u}_i\dot{u}_i(u_{j,k} + \delta_{jk}) - \rho_0(m)\dot{u}_i\dot{u}_j u_{i,k}\}$$
$$- \iint dm\, d\mu(u_{j,k} + \delta_{jk})V(z(m, \mu), m, \mu)$$
$$- (-)^d \iint dm\, d\mu(\mu_j + u_j(m + \mu) - u_j)u_{i,k}(m + \mu)V_{,i}(z(m, \mu), m, \mu). \quad (3.49)$$

4. Discussion and Final Remarks

In several places in the foregoing sections we have interpreted the state $u = 0$, $\dot{u} = 0$ of the system as an equilibrium state. This interpretation is only possible if $u(m, t) = 0$ is a solution of the equation of motion (2.4). A necessary and sufficient condition for this is

$$\int d\mu(V_{,i}(\mu, m, \mu) - V_{,i}(\mu, m - \mu, \mu)) = 0. \quad (4.1)$$

In many models of physical systems one takes a form of the potential energy that does not contain terms linear in u. In our notation:

$$V_{,i}(\mu, m, \mu) = 0. \quad (4.2)$$

This condition is much stronger than (4.1). It implies that the equilibrium state $u(m, t) = 0$ does not correspond only to a minimum of the total potential energy of the system, but rather to a simultaneous minimum of the potential energy of any of the different two-particle interactions. We note this point because the linear terms of V contribute to the harmonic terms of the local fluxes for linear momentum, energy and quasi momentum.

Another familiar assumption is that one has no macroscopic motion of the system, i.e. no motion of the center of mass of the system:

$$d/dt \int x\rho(x)\, dx = d/dt \int (m + u)\rho_0(m)\, dm = \int \rho_0(m)\dot{u}\, dm = 0. \quad (4.3)$$

Therefore this assumption implies that the total linear momentum is zero. A consequence hereof is that elementary excitations of the system (phonons) do not carry any linear momentum unless such an elementary excitation is related to a motion of the center of mass. This statement seems trivial. Nevertheless we pointed this out in order to emphasize that the **k** vector of a phonon in a crystal lattice defined in the usual way has nothing to do with the linear momentum.

Unless (4.3) yields a zero total linear momentum, the linear-momentum flux does not vanish, neither does its volume average. From (2.18) it is readily seen that $\int \pi_{ij}(m)\, dm$ vanishes only for linear systems (i.e. $V_{,ijk} = 0$). The harmonic terms of the integrated substantial linear-momentum flux depend on the cubic terms of the potential energy. Comparing (2.18) and (3.36) one deduces

$$\int \pi^l_{ij}(x)\, dx - \int \pi_{ij}(m)\, dm = \int dm\rho_0(m)\dot{u}_i\dot{u}_j + (-)^d$$
$$\times \iint dm\, d\mu(u_j(m + \mu) - u_j)V_{,i}(z(m, \mu), m, \mu). \quad (4.4)$$

For many physical applications one is mainly interested in the harmonic terms of the fluxes or its integrated values. From (4.4) it is seen that the difference of the harmonic terms of the substantial and the local flux is not zero. Nevertheless it can be shown that for long enough periods the time average of (4.4) vanishes.

The relation between the integrated values of substantial and local energy flux is obtained by comparison of (2.19) and (3.42):

$$\int s_j^l(x)\,dx - \int s_j(m)\,dm = \int dm \tfrac{1}{2}\rho_0(m)\dot{u}_i\dot{u}_i\dot{u}_j + \iint dm\,d\mu\dot{u}_j V(z(m,\mu),m,\mu)$$
$$+(-)^d \iint dm\,d\mu(u_j(m+\mu)-u_j)\dot{u}_i(m+\mu)V_{,i}(z(m,\mu),m,\mu). \tag{4.5}$$

under the assumption (4.2) the harmonic terms of $\int s_i^l(x)\,dx$ and $\int s_i(m)\,dm$ are identical. In general these harmonic terms differ by

$$\int {}^2s_j^l(x)\,dx - \int {}^2s_j(m)\,dm = \iint dm\,d\mu\dot{u}_j(u_i(m+\mu)-u_i)V_{,i}(\mu,m,\mu)$$
$$+(-)^d \iint dm\,d\mu\dot{u}_i(m+\mu)(u_j(m+\mu)-u_j)V_{,i}(\mu,m,\mu). \tag{4.6}$$

We have an analogous situation for the integrated value of the quasi-momentum flux. Comparison of (2.20) and (3.49) yields

$$\int \hat{\pi}_{kj}^l(x)\,dx - \int \hat{\pi}_{kj}(m)\,dm = \int dm \tfrac{1}{2}\rho_0(m)\dot{u}_i(\dot{u}_i u_{j,k} - 2\dot{u}_j u_{i,k})$$
$$-\iint dm\,d\mu u_{j,k}V(z(m,\mu),m,\mu)$$
$$-(-)^d \iint dm\,d\mu u_{i,k}(m+\mu)(u_j(m+\mu)-u_j)V_{,i}(z(m,\mu),m,\mu). \tag{4.7}$$

If we only consider the harmonic terms we have

$$\int {}^2\hat{\pi}_{kj}^l(x)\,dx - \int {}^2\hat{\pi}_{kj}(m)\,dm = -\iint dm\,d\mu u_{j,k}(u_i(m+\mu)-u_i)V_{,i}(\mu,m,\mu)$$
$$-(-)^d \iint dm\,d\mu u_{i,k}(m+\mu)u_j(m+\mu)-u_j)V_{,i}(\mu,m,\mu). \tag{4.8}$$

The present results can be applied to crystal lattices. Several authors have already worked in this field: For Bravais lattices Choquard [4] discussed the substantial energy flux, whereas Hardy [5] discussed the local energy flux. De Vault [6] applied Hardy's method to the local linear-momentum flux, Enz [7] generalized the method to non-Bravais lattices. Pokrovsky and Sergeev [8] have given a rather general discussion of local fluxes in crystals. Furthermore they have described a transformation from the local flux to the flux in a material description, as they called it.

An application of the present theory to crystal lattices permits a more general approach of fluxes in crystals. Local as well as substantial fluxes can be calculated for energy, linear momentum and for quasi momentum. This is the program for a forthcoming paper [9]. There we will also give a comparison of our results and those of the cited authors. Without going into details about the discrete crystal structure here we can discuss Pokrovsky's and Sergeev's transformation of a local flux into a 'flux in a material description'.

Let a quantity $\bar{j}_k(m)$ be given in substantial coordinates. Then, we have because of (3.2), (3.9) and (3.11)

$$\begin{aligned}\int dm\, d/dm_k\, \bar{j}_k(m) &= \int dx J(x)\, d/dm_k\, \bar{j}_k(m)\\ &= -\int dx J(x) A_{lk}\, d/dx_k\, \bar{j}_k(x+v)\\ &= -\int dx\, d/dx_l\, (-A_{lk} J(x) \bar{j}_k(x+v))\\ &\quad + \int \bar{j}_k(x+v)\, d/dx_l\, (J(x) A_{lk}).\end{aligned} \tag{4.9}$$

Furthermore we note that

$$\frac{d}{dx_l}(J(x)A_{lk}) = \frac{\partial J(x)}{\partial v_{i,j}} v_{i,jl} A_{lk} + J(x) \frac{\partial A_{lk}}{\partial v_{i,j}} v_{i,jl} \tag{4.10}$$

or with (3.17) and (3.20)

$$d/dx_l\, (J(x)A_{lk}) = J(x) v_{i,jl}(A_{ji}A_{lk} - A_{li}A_{jk}) = 0. \tag{4.11}$$

From (4.9)–(4.11) it follows

$$\int dm\, d/dm_k\, \bar{j}_k(m) = \int dx\, d/dx_l\, j_l(x), \tag{4.12}$$

where

$$j_l(x) = -A_{lk} J(x) \bar{j}_k(x+v). \tag{4.13}$$

If $j_k(x)$ is the flux in a local description, it is, according to Pokrovsky and Sergeev, natural to define $\bar{j}_k(m)$ as the flux in a material description. This formulation may insinuate that $\bar{j}(m)$ is a substantial flux if $j(x)$ is a local flux. But this is not true. A local or a substantial flux has to be related to local conservation laws (balance equations) in local or substantial coordinates, respectively. In the paper of Pokrovsky and Sergeev the flux $j(x)$ in a local description corresponds to our local flux, i.e. a flux through a local point x. On the other hand $\bar{j}(m)$ is not a substantial flux, i.e. a flux through a material point m, but rather the same local flux in another coordinate system. Therefore physically $j(x)$ and $\bar{j}(m)$ are the same. The reason why $\bar{j}(m)$ is not a substantial flux is that the time derivative d/dt in a local conservation law in local coordinates has to be taken at constant x. On the other hand in a local conservation law in substantial coordinates d/dt means differentiation with respect to t at constant m.

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