Quasi-particle kinetic equation in a deformable material continuum

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THE KINETIC MODEL of interaction between a deformation field of a material continuum and a system of quasi-particles is discussed. The crystal structure of the material body is described by fields of local base vectors what allows to write the quasi-particle kinetic equation in the actual configuration. In the particular case of a one-dimensional system with a linear dispersion curve, it is possible to obtain a closed system of equations for the deformation field and for the moments of the phonon distribution function defining the density of the internal energy and of the heat flux.

1. Introduction

IN THE PAPER [1] GUSEV discussed the problem of interactions between a system of quasi-particles (phonons) with a deformation field of a material continuum. The dynamics of quasi-particles was described by means of a Boltzmann kinetic equation, and equations of motion were composed of a kinetic equation for quasi-particles and of a balance of a linear momentum for material continuum. The coupling between quasi-particles and continuum was introduced by means of corresponding additional assumptions; according to GUSEV, quasi-particles introduce an additional term to the stress tensor and, simultaneusly, the quasi-particle dispersion curve depends on deformation. Such a coupling is the simplest and is a direct generalization of the one applied in solid state physics in the case of small deformations [2]. However, in [1] the kinetic equation was written in a reference configuration, and therefore the treatment presented there cannot be considered as fully satisfactory. In fact, quasi-particle excitations are naturally defined on the actual configuration of the material body and a more systematic approach should take this configuration (related with the points of Galilean space-time, occupied actually by the material points of a continuum) as a starting point.

In this paper we discuss a problem of interactions between a material continuum and a system of quasi-particles, starting from the geometry of local base vectors of a crystal lattice, with the motion of the material continuum described by a four-velocity field defined on the Galilean space-time and the crystal structure of a material body given by three fields of spatial vectors, assigning to each space-time point the corresponding local base vectors of a crystal lattice. Such an approach is similar to the one well-founded within the framework of the theory of continuously distributed defects [3, 4], and was applied previously to the description of transport processes in a rigid material body containing continuously distributed defects of a crystal lattice [5]. In this approach we apply a localization procedure which treats infinitesimal elements of a material body as pieces of

an ideal crystal and postulates that the description of dissipative processes in a continuum can be locally approximated by means of a kinetic model, developed within the framework of solid state physics of ideal crystals. From a physical point of view, such an approach can be justified if a mean free path of colliding quasi-particles is small compared to the spatial scale on which base vectors of a crystal lattice can be treated as approximately constant. From a formal point of view, such localisational approach states the problem of construction of a quasi-particle kinetic equation defined on a sum (with the set of space-time points as the index set) of local Brillouin Zones. Such a sum has a canonical phase-space structure and a Liouville equation, implied by it, determines the form of a quasi-particle kinetic equation (the kinetic equation is formally understood as a Liouville equation with a source term; compare [5]). This kinetic equation transformed to the reference configuration in which the body assumes the form of an ideal crystal becomes identical with the kinetic equation postulated by GUSEV [1].

The construction of the kinetic equation discussed in this paper is nearly identical to the one concerning the case of a rigid body containing continuously distributed defects and in a big part of Sect. 3 we simply repeat the reasoning presented in [5]. However, the case of a deformable material continuum subject to finite deformations and interacting with the gas of quasi-particles is important from the physical point of view because it serves as the microscopic model of transport and dissipation processes in solids, and that is why it seems to deserve a separate treatment. Physical problems which can be analysed on the basis of this kinetic model, such as the relations of moment identities with macroscopic conservation laws or derivation of macroscopic field theories, shall be discussed elsewhere. The only exception is the example of a one-dimensional material continuum with a linear dispersion curve, which has a unique property that the moment equations, corresponding to it, form a closed system (Sect. 4). As a consequence, for this case one immediately obtains the field equations describing transport processes arbitrary far from thermodynamical equilibrium and these field equations are exact (that is, they give the same evolution of the energy density, the heat flux and the deformation field of a material continuum, which is determined by exact solutions of a kinetic equation). Then from the time-independent solutions we can determine the expression relating the heat flux with the internal energy gradient, the deformation gradient and the relaxation time. After introducing the effective temperature as a function of the internal energy and the deformation gradient, this expression takes a form similar to the classical Fourier law. If we postulate, that the formula for the heat flux, obtained in that manner, is valid also in the time-dependent case (that is, if we treat it as a "constitutive law" of a Fourier type) then we obtain a field theory in which the state of the system is described by the fields of deformation and temperature. Such a field theory corresponds to the description of traditional thermomechanics. The interesting problem is whether (and in what sense) such a thermomechanical theory is an approximation of the exact nonequilibrium description (in which the state of the system is specified by the fields of the internal energy, the heat flux and the deformation). However, the discussion of this problem is outside the scope of this paper. In Sect. 2 we recall briefly basic notions related with the motion of a material continuum through Galilean space-time. The construction of the quasi-particle kinetic equation and its transformation to the reference configuration are described in Sect. 3 and 4. In Sect. 5 we discuss the coupling between the motion of the material continuum and the dynamics of the quasi-particles gas. The coupling discussed there is known in literature [1, 2], but we introduce it in a slightly modified order: instead of postulating

the form of the coupling on the basis of physical arguments, we simply search for such closing relations which lead to the conservation of the total energy. The simplest possible solution corresponds to that known in literature [1, 2] (it should be noted, however, that other kinds of closing relations can be of some interest too, especially for the description of a "nonadiabatic" coupling between the deformation and the quasi-particle gas [2]). In Sect. 6 we discuss the case of a one-dimensional deformable material continuum inhabited by phonons with a linear dispersion curve.

2. Motion of material continuum through Galilean space-time

In this section we shall briefly recall basic notions, related with the motion of a material continuum through Galilean space-time.

By a Galilean space-time we mean an ordered quadruple $(G, T_G, \gamma, \cdot)$ where (G, T_G) is a four-dimensional real affine space (G is a set of points of affine space, and T_G is a corresponding translation space), γ is a non-zero form on T_G (that is, $\gamma \in T_G^*$, where T_G^* is a vector space dual to T_G), and $\cdot$ is a scalar product in the space S, where $S := \{\mathbf{w} \in T_G ; \gamma(\mathbf{w}) = 0\}$ [6]. The elements of S are called spatial vectors. The absolute time of point $p \in G$ with respect to the point $p' \in G$ is given by $\gamma(p - p')$ (from the definition of an affine space it follows, that $p - p'$ is a vector from T_G).

By a frame in (G, T_G) we mean a pair (O, b) where $O \in G$ and $b = (\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3, \mathbf{e}_4)$ is a basis in T_G. By inertial reper in G we mean a frame (O, b) which is such that

$$
\begin{align}
&1) &&\gamma(\mathbf{e}_4) = 1, \\
(2.1) \quad &2) &&\gamma(\mathbf{e}_\alpha) = 0 &&\text{for} &&\alpha = 1, 2, 3, \\
&3) &&\mathbf{e}_\alpha \cdot \mathbf{e}_\beta = \delta_{\alpha\beta} &&\text{for} &&\alpha, \beta = 1, 2, 3.
\end{align}
$$

Every inertial reper defines a chart on G given by

$$
(2.2) \qquad \mathbf{R}^4 \ni (t, x_1, x_2, x_3) \to O + t\mathbf{e}_4 + \sum_{\alpha=1}^{3} x_\alpha \mathbf{e}_\alpha,
$$

where $\mathbf{R}$ denotes the set of real numbers. Coordinates on G introduced by (2.2) correspond to the observations of an inertial observer, with t being a time coordinate and $\sum_{\alpha=1}^{3} x_\alpha \mathbf{e}_\alpha$ being an Euclidean radius vector.

Hyperplanes in G, composed of simultaneous events, are given as equivalence classes of a relation

$$
(2.3) \qquad p, p' \in G, p \sim p' \equiv p - p' \in S.
$$

We shall choose an arbitrary point $\tilde{p}$ of G and compute an absolute time of any other space-time point with respect to $\tilde{p}$. This allows us to identify the domain of the time variable with the set of real numbers, and to specify a unique relation between the values of the time parameter and the classes of the relation (2.3) (to each class we assign the number $\gamma(p - \tilde{p})$, with p being an arbitrary representative of the considered equivalence class). The equivalence class of the relation (2.3) corresponding to the absolute time instant t shall be denoted by H_t.

The motion of a material point through a Galilean space-time can be described by a smooth curve in G, which intersects each hyperplane H_t only once. In consequence, points along such a curve can be bijectively parametrized by a set of absolute time instants. In

the following, such curves (which shall be called world lines) shall be always parametrized in that manner. If $\xi(t) : \mathbf{R} \to G$ is a world line of a material point, then $d\xi(t)\,/\,dt$ is called its four-velocity. The set of all admissible four-velocities of material points can be identified with a hyperplane in T_G, given by $W := \{\mathbf{w} \in T_G;\ \gamma(\mathbf{w}) = 1\}$ [6]. The motion of a material body through the Galilean space-time is described by a family of diffeomorphisms $\psi_t, t \in \mathbf{R}$ of the body manifold $\mathcal{B}$ with open subsets of H_t (compare [7]). We assume, that ψ_t is a smooth function of the time variable and that for each time instant t the body fills up the whole space H_t. The motion of the continuum can be alternatively described as a congruence of the world lines of the individual material points of the body. After parametrizing the congruence lines in terms of the absolute time and computing the corresponding tangent vectors, we obtain the four-velocity field, describing the motion of the material continuum. Conversely, the motion of the material continuum can be also defined by a smooth, globally defined and complete field of four-velocity. The motion of the individual material points is then determined by integral curves of such a four-velocity field.

In mechanics, a crystalline structure of a perfect crystal is usually described by introducing in the material body a particular coordinate system, called crystallographic coordinates: distances along coordinate lines are then measured by lattice step counting [3]. In our discussion, we shall restrict ourselves to the case of perfect crystals. We shall also assume that the body is infinite in the sense, that the domain of crystallographic coordinates is $\mathbf{R}^3$. Then the crystallographic coordinate system in the body manifold

$$(2.4) \qquad\qquad \mathbf{R}^3 \ni (s_1, s_2, s_3) \to X(s_1, s_2, s_3) \in \mathcal{B}$$

together with the motion ψ_t of the body $\mathcal{B}$ define a coordinate system on the Galilean space-time

$$(2.5) \qquad\qquad \mathbf{R}^4 \ni (s_1, s_2, s_3, t) \to \psi_t(X(s_1, s_2, s_3)) \in G.$$

Vector fields, tangent to the coordinate lines of the coordinate system (2.5), shall be denoted by $\partial_t, \partial_{s_\alpha}, \alpha = 1, 2, 3$. Then ∂_t determines a field of a four-velocity, describing the motion of the material continuum, whereas spatial vectors $\partial_{s_\alpha}, \alpha = 1, 2, 3$, determine, for a fixed value of the time parameter t, fields of local base vectors of a primitive crystal lattice, defined on H_t (compare [3]). Let $\mathbf{u}$ denote the four-velocity field of the material continuum (of course, the four-velocity field can be defined also for the material bodies which do not possess the crystal structure). In order to discuss the balance of a linear momentum corresponding to a subbody $\mathcal{C}$ of the material $\mathcal{B}$, we shall define the linear four-momentum of $\mathcal{C}$ at the time instant t

$$(2.6) \qquad\qquad \mathbf{P}(\mathcal{C}, t) := \int_{\psi_t(\mathcal{C})} \rho_t \mathbf{u}\, d\nu_t,$$

where $d\nu_t$ denotes the integration with respect to the Euclidean volume measure on H_t and ρ_t denotes the mass density of the material continuum; ρ_t defines a real function on H_t, which is assumed to be smooth. The vector $\mathbf{P}(\mathcal{C}, t)$, as defined by Eq. (2.6), is not a spatial vector; however, its time derivative is spatial. The balance of a linear momentum states, that the time derivative of $\mathbf{P}(\mathcal{C}, t)$ is equal to the spatial vector $\mathbf{b}(\mathcal{C}, t)$, which is called the total force acting on the subbody $\mathcal{C}$ at the time instant t:

$$(2.7) \qquad\qquad \frac{d}{dt}\mathbf{P}(\mathcal{C}, t) = \mathbf{b}(\mathcal{C}, t) .$$

Writing the formula (2.7) in the coordinates, corresponding to the choice of an arbitrary inertial frame, we can easily state its equivalence with the balance of a linear momentum of the form usually applied in continuum mechanics [7]. For the world line $\xi(t)$ of a fixed material point of the continuum we can define the acceleration $\mathbf{a}(\xi, (t))$ by the formula $\mathbf{a}(\xi(t)) = \dfrac{d^2\xi(t)}{dt^2}$. Since, in our case, any point of the space-time belongs to the world line of a certain material point, then the motion of the continuum defines the acceleration field $\mathbf{a} : G \to S$ on G. The time derivative of a linear four-momentum of the subbody $\mathcal{C} \subset \mathcal{B}$ is then related with the acceleration field $\mathbf{a}$ by the formula

$$(2.8) \qquad \frac{d}{dt}\mathbf{P}(\mathcal{C}, t) = \int\limits_{\psi_t(\mathcal{C})} \mathbf{a}\rho_t\, d\nu_t .$$

In this paper, we shall discuss only the case, when the total force acting on the subbody $\mathcal{C} \subset \mathcal{B}$ has a form of a divergence of a tensor field $\mathbf{T}$:

$$(2.9) \qquad \mathbf{b}(\mathcal{C}, t) = \int\limits_{\psi_t(\mathcal{C})} \mathrm{div}\mathbf{T}\, d\nu_t ,$$

where div means the Euclidean divergence operator on the space H_t. The tensor field $\mathbf{T}$, satisfying (2.9), is called the field of Cauchy stress tensor. Note that in this formulation we do not have to introduce the notion of an inertial frame, and the price for that is that the linear momentum, as defined by (2.6), is not a spatial vector.

3. Quasi-particle kinetic equation

The motion of the material continuum through the Galilean space-time imposes time-dependent constraints on the system of quasi-particles. In order to determine the structure of a Liouville operator, which in turn implies the form of a corresponding quasi-particle kinetic equation (see Introduction), we shall start with the Hamiltonian description of the systems with time-dependent constraints. We shall make use of the formulation, based on the notion of the so-called Heisenberg Picture [9].

DEFINITION 1. *By a Heisenberg Picture in mechanics we mean a fibre bundle (F, M, Π) over a one-dimensional contractable manifold M together with a closed 2-form $\omega_{\mathcal{F}}$ which is such that for every $m \in M$, $\omega_{\mathcal{F}|\Pi^{-1}(m)}$ is a symplectic form (F is a space of a bundle, M is its base, and Π is a bundle projection).*

Base vectors of a local inverse lattice $\mathbf{G}^j(g)$, $j = 1, 2, 3$ at the point g of Galilean space-time shall be defined as spatial vectors, satisfying the following relation

$$(3.1) \qquad \partial_{s_i}(g) \cdot \mathbf{G}^j(g) = 2\pi\delta_i^j, \qquad i, j = 1, 2, 3.$$

In order to construct a Heisenberg Picture, corresponding to the quasiparticle gas in a deformable medium, we shall repeat the reasoning known from [5]. A local Brillouin Zone, assigned to the point g, is defined as a quotient space T_g^3, composed of the equivalence classes of the relation

$$(3.2) \qquad \mathbf{w}, \mathbf{w}' \in S, \mathbf{w} \underset{g}{\sim} \mathbf{w}' \equiv \mathbf{w} - \mathbf{w}' = \sum_{j=1}^{3} z_j\mathbf{G}^j(g) ,$$

where z_j are arbitrary integers.

An equivalence class of the element $\mathbf{w} \in S$ in the relation (3.2) shall be denoted by $[\mathbf{w}]_g$. The space T_g^3 has a natural structure of a torus group, with the composition law defined by the rule $[\mathbf{w}]_g + [\mathbf{w}']_g = [\mathbf{w} + \mathbf{w}']_g$. Note that this composition rule, written in terms of vector representatives, becomes identical with the rule of addition of quasi-particle wave vectors (that is, with addition of vectors modulo an integer linear combination of local base vectors of an inverse lattice) [10].

Let V be a three-dimensional real vector space with a given basis $\mathbf{v}_i$, $i = 1, 2, 3$. We shall introduce in V an equivalence relation, analogous to (3.2):

$$(3.3) \qquad \mathbf{v}, \mathbf{v}' \in V, \mathbf{v} \sim \mathbf{v}' \equiv \mathbf{v} - \mathbf{v}' = \sum_{j=1}^{3} z_j \mathbf{v}_j$$

(z_j are arbitrary integers).

An equivalence class of the element $\mathbf{v} \in V$ in the relation (3.2) shall be denoted $[\mathbf{v}]$ and the group action in $T_v^3 := \bigcup_{\mathbf{v} \in V} [\mathbf{v}]$ shall be defined similarly as in the case of T_g^3. Let us denote by $\mathcal{Z}$ a sum of local Brillouin Zones, taken with respect to all space-time points:

$$(3.4) \qquad \mathcal{Z} := \bigcup_{g \in G} T_g^3.$$

Let $\mathcal{A}_{[\mathbf{v}]}$ denote a map, given by

$$(3.5) \qquad \mathcal{A}_{[\mathbf{v}]} : \mathbf{R}^4 \times (-\pi, \pi)^3 \ni (t, s_1, s_2, s_3, \varepsilon_1, \varepsilon_2, \varepsilon_3)$$

$$\to \Big[\sum_{j=1}^{3} \Big(v^j + \frac{\varepsilon^j}{2\pi} \Big) \mathbf{G}^j (g(s_i, t)) \Big]_{g(s_i, t)} \in \mathcal{Z},$$

where $g(s_i, t)$ denotes the point $\psi_t(X(s_i))$ of the Galilean space-time, occupied at the time t by the point $X(s_i)$ of the material body

$$(3.6) \qquad g(s_i, t) \equiv \psi_t(X(s_i)),$$

and v^j are components of any representative $\sum_{j=1}^{3} v^j \mathbf{v}_j$ of $[\mathbf{v}]$ in the basis $\{\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3\}$. A C — compatible atlas $\mathcal{A}$,

$$(3.7) \qquad \mathcal{A} := \{\mathcal{A}_{[\mathbf{v}]}; [\mathbf{v}] \in T_v^3\}$$

gives $\mathcal{Z}$ a structure of a smooth manifold.

Let us define the projection $P : \mathcal{Z} \to G$,

$$(3.8) \qquad P([\mathbf{w}]_g) := g,$$

and the action of T_v^3 on $\mathcal{Z}$

$$T_v^3 \times \mathcal{Z} \ni ([\mathbf{v}], [\mathbf{w}]_g) \to [\mathbf{v}] \times [\mathbf{w}]_g := \Big[\sum_{j=1}^{3} (v^j + w^j) \mathbf{G}^j (g) \Big]_g \in \mathcal{Z},$$

where v^j are the components of $\mathbf{v}$ in the basis $\mathbf{v}_j$, $j = 1, 2, 3$ of V and w^j are the components of $\mathbf{w}$ in the basis $\mathbf{G}^j(g)$ of S.

A triple $(\mathcal{Z}, G, P)$ forms a principal fibre bundle with T_V^3 as a structure group. Each of the coordinate system $\mathcal{A}_{[\mathbf{v}]}$ from the atlas $\mathcal{A}$ defines seven vector fields $\partial_{t,[\mathbf{v}]}, \partial_{s_i,[\mathbf{v}]}, \partial_{\varepsilon_j,[\mathbf{v}]}$, $i, j = 1, 2, 3$, tangent to its corresponding coordinate lines. These vector fields are not defined globally on $\mathcal{Z}$, since none of the coordinate systems $\mathcal{A}_{[\mathbf{v}]}$ is defined globally on $\mathcal{Z}$. However, all such vector fields are the restrictions (to the coordinate domains of a given coordinate system $\mathcal{A}_{[\mathbf{v}]}$ from the atlas $\mathcal{A}$) of seven vector fields $\partial_{\tilde{t}}, \partial_{\tilde{s}_i}, \partial_{\varepsilon_j}, i, j = 1, 2, 3$ defined globally on $\mathcal{Z}$. A tilde over t and s_i is introduced in order to distinguish those vector fields from the natural base vectors $\partial_t, \partial_{s_j}, j = 1, 2, 3$ of the coordinate system (2.5) in the Galilean space-time. The fields of forms, defined on $\mathcal{Z}$ and dual to $\partial_{\tilde{t}}, \partial_{\tilde{s}_i}, \partial_{\varepsilon_j}$, $i, j = 1, 2, 3$ are denoted by $d\tilde{t}, d\tilde{s}^i, d\varepsilon^j, i, j = 1, 2, 3$. The action of these forms is defined by

$$
(3.9) \quad
\begin{array}{lll}
\langle d\tilde{s}^i, \partial_{s_j} \rangle = \delta_j^i, & \langle d\varepsilon^i, \partial_{\varepsilon_j} \rangle = \delta_j^i, & \langle d\tilde{t}, \partial_{\tilde{t}} \rangle = 1, \\
\langle d\tilde{s}^i, \partial_{\varepsilon_j} \rangle = 0, & \langle d\varepsilon^i, \partial_{s_j} \rangle = 0, & \langle d\tilde{t}, \partial_{\tilde{s}_i} \rangle = 0, \\
\langle d\tilde{s}^i, \partial_{\tilde{t}} \rangle = 0, & \langle d\varepsilon^i, \partial_{\tilde{t}} \rangle = 0, & \langle d\tilde{t}, \partial_{\varepsilon_j} \rangle = 0,
\end{array}
$$

where the bracket $\langle, \rangle$ denotes the action of the form on the vector. Let $\tilde{P}$ denote the projection, assigning to the points of the Galilean space-time G the corresponding absolute time instants. The specification of the form γ and the choice of the event, the time of which is equal to zero, allows us to identify the set of absolute time instants with the real axis (see [7]). By means of the mapping $\tilde{P}$ we can define projection $\hat{P}, \hat{P} : \mathcal{Z} \to \mathbf{R}$

$$
(3.10) \quad \hat{P}([\mathbf{w}]_g) := \tilde{P}(g) \in \mathbf{R}.
$$

Let ω denote a smooth function, defined on $\mathcal{Z}$. A triple $\left(\mathcal{Z}, \mathbf{R}, \hat{P} \right)$ forms a fibre bundle which satisfies the definition of the Heisenberg Picture, with the form $\omega_{\mathcal{Z}}$ given by

$$
(3.11) \quad \omega_{\mathcal{Z}} = d\varepsilon^i \wedge d\tilde{s}^i - d\omega \wedge \tilde{t},
$$

where $\wedge$ denotes an external product and the summation with respect to repeated indices is assumed (from the comparison with the formulae of solid state physics it will become clear that ω corresponds to the dispersion curve of quasi-particles).

A fibre $\hat{P}^{-1}(t)$ is a manifold, which is a sum of all local Brillouin Zones, corresponding to the space-time points from H_t:

$$
(3.12) \quad \hat{P}^{-1}(t) = \bigcup_{g \in H_t} T_g^3,
$$

with the atlas $\mathcal{A}_t$ composed of the mappings $\mathcal{A}_{t,[\mathbf{v}]}$

$$
(3.13) \quad \mathcal{A}_t = \{ \mathcal{A}_{t,[\mathbf{v}]}; [\mathbf{v}] \in T_v^3 \}
$$

(the mappings $\mathcal{A}_{t,[\mathbf{v}]}$ are obtained by fixing the time coordinate in the charts $\mathcal{A}_{[\mathbf{v}]}$ from the atlas $\mathcal{A}$).

Vector fields $\partial_{\tilde{s}_i}, \partial_{\varepsilon_j}, i, j = 1, 2, 3$ which are composed of vertical vectors of the bundle $(\mathcal{Z}, \mathbf{R}, \hat{P})$ can be naturally restricted to $\hat{P}^{-1}(t)$. Moreover, form fields on $\hat{P}^{-1}(t)$, dual to these restrictions, are given by restrictions (to $\hat{P}^{-1}(t)$) of the form fields $d\tilde{s}^i, d\varepsilon^j$, $i, j = 1, 2, 3$ on $\mathcal{Z}$. The restriction of $\omega_{\mathcal{Z}}$ to $\hat{P}^{-1}(t)$ is given by

$$
(3.14) \quad \omega_{\mathcal{Z}|\hat{P}^{-1}(t)} = d\varepsilon^i \wedge d\tilde{s}^i_{|\hat{P}^{-1}(t)}.
$$

It can easily be shown that Eq. (3.14) defines a symplectic form on $\hat{\mathcal{P}}^{-1}(t)$. By repeating the reasoning given in [5], it is possible to show that this symplectic form is canonical (this fact is not quite trivial, since $\hat{\mathcal{P}}^{-1}(t)$ is not a cotangent bundle). Let h denote a local, smooth cross-section of the bundle $(\mathcal{Z}, \mathbf{R}, \hat{\mathcal{P}})$ over a time interval $I \subset \mathbf{R}$ (I is open in $\mathbf{R}$). By h' we shall denote the derivative of h which, by definition, assigns to each time instant $t \in I$ the linear mapping $h'(t)$ from $T_t(\mathbf{R})$ into $T_{h(t)}(\mathcal{Z})$ ($T_{h(t)}(\mathcal{Z})$ is a vector space tangent to $\mathcal{Z}$ at $h(t)$ and $T_t(\mathbf{R})$ denotes the vector space tangent to $\mathbf{R}$ at $t \in \mathbf{R}$; as it is well-known, $T_t(\mathbf{R})$ can be identified with $\mathbf{R}$).

DEFINITION 2. *A smooth cross-section h of the bundle $(\mathcal{Z}, \mathbf{R}, \hat{\mathcal{P}})$ is called a quasi-particle trajectory if h' belongs to the kernel of $\omega_\mathcal{Z}$ (compare [12, 13]).*

From the standard discussion (see, for example, [13]) it follows that in the coordinates of the chart $\mathcal{A}_{[v]}$ from the atlas $\mathcal{A}$, the quasi-particle trajectory is described by the mapping $t \rightarrow (t, s_i(t), \varepsilon_j(t))$, $i, j = 1, 2, 3$ where $s_i(t), \varepsilon_j(t)$ satisfy Hamilton equations:

(3.15)
$$\frac{\partial \varepsilon_j}{\partial t} = -\frac{\partial \omega}{\partial s_j},$$
$$\frac{\partial s_j}{\partial t} = \frac{\partial \omega}{\partial \varepsilon_j}.$$

It should be noted that in the case of quasi-particles the solutions of Hamilton equations exist only for sufficiently small time intervals, that is, in general we cannot assume that Hamiltonian vector fields for quasi-particles are complete (compare [12]).

From Hamiltonian equations we immediately obtain a Liouville equation, governing the time evolution of the phase density f. In turn, the Liouville equation determines the structure of a kinetic equation (understood as the Liouville equation with a source term; see Introduction). We assume, that the structure of the source term $J(f)$, corresponding to the collision integral of the kinetic equation, is locally identical with the one known from the case of ideal crystals (compare [5, 10]).

Hence we arrive at the final form of the kinetic equations for quasi-particles in a deformable medium

(3.16)
$$\mathcal{L}_{\partial_{\tilde{t}}} f + \underset{(1,3)}{\mathrm{Tr}} \underset{(2,4)}{\mathrm{Tr}} \left(\partial_{\varepsilon_i} \wedge \partial_{\tilde{s}_i} \right) \otimes d\omega \otimes df = J(f),$$

where $\mathcal{L}_{\partial_{\tilde{t}}}$ denotes a Lie derivative along the vector field $\partial_{\tilde{t}}$, $\otimes$ is a tensor product and Tr denotes the trace operation with respect to the indices, listed below.

In the coordinates (t, s_i, ε_j) of the chart $\mathcal{A}_{[v]}$ from the atlas $\mathcal{A}$, the kinetic equation (3.16) takes the form

(3.17)
$$\frac{\partial f}{\partial t} + \frac{\partial \omega}{\partial \varepsilon_i} \frac{\partial f}{\partial s_i} - \frac{\partial \omega}{\partial s_i} \frac{\partial f}{\partial \varepsilon_i} = J(f)$$

(in. Eq.(3.17), as well as in the rest of this paper, we assume summation with respect to repeated indices).

4. Transition to reference configuration

The kinetic equation (3.16) governing the behaviour of the distribution function, is written in terms of tensor fields on $\mathcal{Z}$ by means of operations like Lie derivative and

contractions of tensors, and therefore it can be equivalently written on any manifold, diffeomorphic with $\mathcal{Z}$. Since our kinetic equation is just a Liouville equation with a source term, then such transformations are identical to transformations of phase spaces, discussed in textbooks on mechanics (where the diffeomorphism of the manifold on which the phase space structure is defined induce a new isomorphic phase space [12,13]). In mechanics of continua, one often defines tensor fields, related with the motion of the material continuum, on the so-called reference configuration [7]. We shall write the kinetic equation (3.16) in the form corresponding to the reference configuration in which the body assumes a form of an ideal crystal. As the Euclidean point space, chosen for the construction of the reference configuration, we can take H_0, that is, the space of simultaneous events at the time instant equal to zero.

Let Θ be a fixed point of H_0 and let $\mathbf{E}_i$, $i = 1, 2, 3$ be an arbitrary basis in the translation space of H_0.

The reference configuration of the material body $\mathcal{B}$ shall be defined by means of a diffeomorphism κ of $\mathcal{B}$ onto H_0, given by

$$(4.1) \qquad \mathcal{B} \ni X \to \kappa(X) = \Theta + s_i(X)\mathbf{E}_i \in H_0,$$

where $s_i(X)$, $i = 1, 2, 3$ are the values of the crystal coordinates assigned to the point X of the material body $\mathcal{B}$, and Θ is an arbitrary point of H_0 (of course, the configuration ψ_0 assumed by the material body at the time instant $t = 0$ is not related in any way with κ). By the deformation from the configuration κ to the configuration ψ_t we mean a mapping φ_t, $\varphi_t : H_0 \to H_t$ given by

$$(4.2) \qquad \varphi_t := \psi_t \circ \kappa^{-1},$$

and the deformation gradient $\mathbf{F}_t$ is defined as a derivative of φ_t [7]. In the reference configuration (4.1), the vectors $\mathbf{E}_i$, $i = 1, 2, 3$, are base vectors of a primitive crystal lattice of an ideal crystal [3]. Let us denote by $\mathbf{G}_\kappa^j$, $j = 1, 2, 3$, the corresponding base vectors of the inverse lattice (that is, $\mathbf{G}_\kappa^j$ are determined by the condition $\mathbf{E}_i \cdot \mathbf{G}_\kappa^j = 2\pi\delta_i^j$). Let T_κ^3 denote the Brillouin Zone, determined by $\mathbf{G}_\kappa^j$; T_κ^3 is a quotient space defined by the relation analogous to (3.2) and the equivalence classes of this relation shall be denoted by $[\cdot]_\kappa$. The kinetic equation (3.16), transformed to the reference configuration, takes a form of an equation for quasi-particles in a rigid ideal crystal with the space-and time-dependent quasi-particle dispersion curve [2]. Such a transformation can be done formally by defining a Heisenberg Picture analogous to the previously discussed one but with the product $\mathcal{Z}_\kappa := T_\kappa^3 \times H_0 \times \mathbb{R}$ as a base space; $\mathcal{Z}$ and $\mathcal{Z}_\kappa$ are then related by a diffeomorphism $\mathcal{D}$, $\mathcal{D} : \mathcal{Z} \to \mathcal{Z}_\kappa$

$$(4.3) \qquad \mathcal{D}([\beta_i\mathbf{G}^i(g)]_g) = ([\beta_i\mathbf{G}_\kappa^i]_\kappa, \tilde{\kappa}(g), \mathcal{P}(g)) \in T_\kappa^3 \times H_0 \times \mathbb{R} \equiv \mathcal{Z}_\kappa,$$

where $\beta_i\mathbf{G}^i(g)$ is an arbitrary representative of the point $[\beta_i\mathbf{G}^i(g)]_g$ of $\mathcal{Z}$ and $\tilde{\kappa}(g)$ denotes the point of H_0 occupied in the reference configuration by this material point, the world line of which goes through the space-time point g. Under the action of $\mathcal{D}$, the distribution function and the dispersion curve are transformed as scalar, whereas the 2-form corresponding to the Heisenberg Picture on $\mathcal{Z}_\kappa$ is given by the pull-back of $\omega_\mathcal{Z}$, induced by the inverse of $\mathcal{D}$ [12,13]. For the quasi-particle kinetic equation written in the reference configuration of an ideal crystal we shall apply a standard convention of solid state physics where one treats quasi-particle wave-vector as the elements of the Euclidean vector space (what is valid with accuracy to the set of a measure zero) [10]. The spatial

points in the reference configuration shall be determined by the radius-vector $\mathbf{r}$. In this notation, the kinetic equation is given by

(4.4) $\dfrac{\partial}{\partial t} f(\mathbf{r}, \mathbf{k}, t) + \nabla_\mathbf{k} \omega(\mathbf{r}, \mathbf{k}, t) \cdot \nabla_\mathbf{r} f(\mathbf{r}, \mathbf{k}, t) - \nabla_\mathbf{r} f(\mathbf{r}, \mathbf{k}, t) \cdot \nabla_\mathbf{k} f(\mathbf{r}, \mathbf{k}, t)$

$$= I(f(\mathbf{r}, \mathbf{k}, t)),$$

where $\nabla_\mathbf{k}$ denotes the gradient computed with respect to the wave-vector $\mathbf{k}$ of quasi-particle, $\nabla_\mathbf{r}$ is the gradient computed with respect to the spatial variable $\mathbf{r}$, $f(\mathbf{r}, \mathbf{k}, t)$ is the distribution function, $\omega(\mathbf{r}, \mathbf{k}, t)$ is the dispersion curve and $J(f)$ is the collision integral of the kinetic equation.

In the rest of our paper we shall write the kinetic equation and the tensor fields describing the motion of the material continuum in a fixed reference configuration (of the kind described by (4.1)). As a consequence, in Sect. 5 and 6 we shall mean by $\mathbf{a}$ and $\mathbf{v}$ the acceleration and the velocity fields, defined on this reference configuration (compare [7]). Moreover, we shall assume that the density of the material continuum in the reference configuration is constant. This density shall be denoted by ρ.

5. Coupling between motion of continuum and dynamics of quasi-particle gas

A form of the coupling between the evolution of the quasiparticle system and the motion of the material continuum follows from two assumptions.

The first assumption is that the stress tensor depends on the deformation gradient and on the quasiparticle distribution function, and that the evolution of the quasiparticles is related to the motion of the material continuum via the local dependence of the dispersion curve and of the collision rates of the collision integral on the deformation gradient. It means that the system of coupled equations takes in the reference configuration the following form

(5.1) $\begin{cases} \rho \mathbf{a} - \operatorname{div} \mathcal{T}(\mathbf{F}, f) = 0, \\ \dfrac{\partial f}{\partial t} + \nabla_\mathbf{k} \omega \cdot \nabla_\mathbf{r} f - \nabla_\mathbf{r} \omega \cdot \nabla_\mathbf{k} f = J(f), \end{cases}$

where $\mathbf{a}$ is the acceleration, ρ is the mass density in the reference configuration, $\mathcal{T}(\mathbf{F}, f)$ is the Piola–Kirchhoff stress tensor and $\omega = \omega(\mathbf{F}, \mathbf{k})$ denotes the dispersion curve.

The second assumption is that the total energy of the system is additive in the sense that it is a sum of the energy of continuum (composed of the kinetic energy and of the elastic energy, given by a hyperelastic potential), and of the internal energy of the quasiparticle gas. The expression for the energy of quasiparticles contained in a given subbody of the material body shall be computed in the reference configuration (it can easily be shown that the expression for the energy of quasiparticles, defined in that way, does not depend on the choice of the reference configuration). Hence, the spatial density of the total energy written in the reference configuration is given by

(5.2) $$\mathcal{E} = \frac{1}{2} \rho \mathbf{v} \cdot \mathbf{v} + \varphi(\mathbf{F}) + \int \hbar \omega f \frac{d^3 \mathbf{k}}{(2\pi)^3},$$

where $\mathbf{v}$ is the velocity of the medium, $\varphi(\mathbf{F})$ is a hyperelastic potential, $2\pi\hbar$ is Planck's

constant and the third term on the r.h.s. of Eq. (5.2) describes the energy density of the quasiparticle gas (compare [2]).

The total energy $\mathcal{E}(\mathcal{C})$ of a given subbody $\mathcal{C}$ of the material body $\mathcal{B}$ is defined as a volume integral over $\kappa(\mathcal{C})$ of $\mathcal{E}$. The time derivative of $\mathcal{E}(\mathcal{C})$ satisfies the following relation

$$(5.3) \qquad \frac{\partial}{\partial t}\mathcal{E}(\mathcal{C}) + \int\limits_{\kappa(\mathcal{C})} \operatorname{div}\left\{ \mathbf{g} - \mathbf{v}\cdot\left(\rho\frac{d\varphi}{d\mathbf{F}} + \int\limits_{T_\kappa^3} f\frac{d\hbar\omega}{d\mathbf{F}}\frac{d^3\mathbf{k}}{(2\pi)^3} \right) \right\} d^3\mathbf{r}$$

$$= \int\limits_{\kappa(\mathcal{C})} \left\{ \mathbf{v}\cdot\left[\rho\mathbf{a} - \operatorname{div}\left(\rho\frac{d\varphi}{d\mathbf{F}} + \int\limits_{T_\kappa^3} f\frac{d\hbar\omega}{d\mathbf{F}}\frac{d^3\mathbf{k}}{(2\pi)^3} \right) \right] \right\} d^3\mathbf{r},$$

where div denotes the Euclidean divergence,

$$(5.4) \qquad \mathbf{g} = \int\limits_{T_\kappa^3} f\hbar\omega\nabla_\mathbf{k}\omega\frac{d^3\mathbf{k}}{(2\pi)^3}$$

is the moment expression for the heat flux, and $d^3\mathbf{r}$ denotes the integration with respect to the Euclidean volume element in the reference configuration. The time derivative of $\mathcal{E}(\mathcal{C})$ is equal to the surface integral over the surface of $\kappa(\mathcal{C})$ if the term on the r.h.s. of Eq. (5.3) is equal to zero. This, in turn, is assured if

$$(5.5) \qquad \rho\mathbf{a} - \operatorname{div}\left(\rho\frac{d\varphi}{d\mathbf{F}} + \int\limits_{T_\kappa^3} f\frac{d\hbar\omega}{d\mathbf{F}}\frac{d^3\mathbf{k}}{(2\pi)^3} \right) = 0.$$

Equation (5.5) has the form of the balance of a linear momentum of material continuum with the stress tensor given by

$$(5.6) \qquad \mathcal{T}(\mathbf{F}, f) = \rho\frac{d\varphi}{d\mathbf{F}} + \int\limits_{T_\kappa^3} f\frac{d\hbar\omega}{d\mathbf{F}}\frac{d^3\mathbf{k}}{(2\pi)^3}.$$

From the formula (5.3) we also see that

$$(5.7) \qquad \mathbf{q}_{\text{tot}} = \mathbf{q} - \mathbf{v}\cdot\mathcal{T}(\mathbf{F}, f)$$

describes the flux of the total energy.

The form of the stress tensor (5.6) can be interpreted in this way that a single excitation gives a contribution $\hbar\omega$ to the hyperelastic energy of the medium and that the contribution of the whole quasi-particle gas is additive, that is, it is given by the integral of the terms introduced by individual excitations.

By analogy to mechanics, we can impose the following restrictions on the form of φ and ω

$$(5.8) \qquad \begin{aligned} \varphi(\mathbf{Q}*\mathbf{F}) &= \varphi(\mathbf{F}), \\ \omega(\mathbf{Q}*\mathbf{F}, \mathbf{k}) &= \omega(\mathbf{F}, \mathbf{k}), \end{aligned}$$

where Q is the rotation tensor and $Q*$ means the action of the rotation on the tensor argument [7]. Then, from the considerations given in Wang's monograph ([7], vol. I, Sect. 20), it follows that the Cauchy stress tensor corresponding to the Piola - Kirchoff stress tensor of the form (5.6) is symmetric.

6. One-dimensional material continuum with linear dispersion curve

In some cases, such as the description of the low-temperature effects or the transition from the discrete crystal to the continuum limit, one assumes that quasiparticle wave vectors are not restricted to the Brillouin Zone, but belong to the whole Euclidean vector space [2]. Quasi-particles with such a property can be obtained also without any approximations or limit procedures if, as the starting point for defining quasiparticles, one takes a quantization of the elastic continuum [10]. We can imagine a transition from the Brillouin Zone to the three-dimensional Euclidean vector space as a "limit", in which local base vectors of a crystal lattice become infinitely small and the Brillouin Zone tends to infinity.

In this section we shall discuss a one-dimensional material continuum containing phonons with quasiparticle wave vectors belonging to a one-dimensional vector space. We shall assume, that the dispersion curve is given by

$$(6.1) \qquad \omega(F, k) = c(F)|k|,$$

where F is the deformation gradient, $c(F)$ is the velocity of sound (depending on F) and $|k|$ is a modulus of the quasiparticle wave vector [2].

The dynamics of the system shall be described by the one-dimensional counterpart of the kinetic equation, discussed in Sect. 5, with the additional assumption that the collision integral $J(f)$ has a form

$$(6.2) \qquad J(f) = -\frac{1}{\tau(\varepsilon, F)}(f - f_0(\varepsilon, F)) + \tilde{J}(f),$$

where the first term on the r.h.s. of Eq.(6.2) corresponds to the collision process described by a single relaxation time $\tau(\varepsilon, F)$ (which is assumed to depend on F and on the energy density ε of the phonon gas). The second term on the r.h.s. of Eq.(6.2) corresponds to such collisions of quasiparticles, which conserve the total quasimomentum of the colliding excitations, that is, for every distribution function f the following identity holds

$$(6.3) \qquad \int k\tilde{J}(f)\,dk = 0.$$

The function $f_0(\varepsilon, F)$ is given by

$$(6.4) \qquad f_0(\varepsilon, F) = \frac{1}{e^{\frac{\hbar c(F)|k|}{k_B T}} - 1},$$

where $T(\varepsilon, F)$ is uniquely determined from the condition

$$(6.5) \qquad \varepsilon = \int \hbar c(F)|k|f\frac{dk}{2\pi} = \int \frac{\hbar c(F)|k|}{\exp\left[\dfrac{\hbar c(F)|k|}{k_B T(\varepsilon, F)}\right] - 1}\frac{dk}{2\pi},$$

and k_B denotes Planck's constant.

The decomposition of the collision integral of the form (6.2) is frequently applied in solid state physics [2]. The physical meaning of the function $f_0(\varepsilon, F)$ is that it corresponds to such a locally equilibrium distribution function which gives, for a fixed value of F, the same energy density as the distribution function f. The function $T = T(\varepsilon, F)$ given by Eq. (6.5) defines the effective temperature as a function of the energy density ε and of the deformation gradient F.

In order to obtain a closed system of equations for the moments of the distribution function coupled with the motion of the material continuum for the system, specified by

the choice of the collision integral of the form (6.2) and of the dispersion curve of the form (6.1), we multiply the kinetic equation by $\hbar c\,(F)\,|k|$ and $\hbar c^2\,(F)\,k$ correspondingly, integrate it with respect to the variable k and change the order of integration and differentiation. We also divide the result, obtained in that manner, by 2π and assume that for large k the distribution function vanishes more rapidly than the inverse of polynomials.

As a result, we obtain the following set of equations

$$\frac{\partial}{\partial t}\int \hbar c|k|f\frac{dk}{2\pi} + \frac{\partial}{\partial x}\int \hbar c^2 k f\frac{dk}{2\pi} = \left\{\int f\hbar|k|\frac{\partial c}{\partial F}\frac{dk}{2\pi}\right\}\cdot\frac{\partial F}{\partial t}\,,$$

(6.6)
$$\frac{\partial}{\partial t}\int \hbar c^2 k f\frac{dk}{2\pi} + \frac{\partial}{\partial x}\int \hbar c^3|k|f\frac{dk}{2\pi} = \int \hbar|k|c^2\frac{\partial c}{\partial x}f\frac{dk}{2\pi}$$
$$-\frac{1}{\tau(\varepsilon,F)}\int \hbar c^2 k f\frac{dk}{2\pi}\,,$$

$$\rho\frac{\partial v}{\partial t} - \frac{\partial}{\partial x}\left(\rho\frac{d\varphi(F)}{dF} + \int f\frac{d(\hbar c(F)|k|)}{dF}\frac{dk}{2\pi}\right) = 0\,.$$

From solid state physics we know that the moment expression for the heat flux in a one-dimensional system with the quasi-particle dispersion curve (6.1) reads

(6.7)
$$q = \int \hbar c^2 k f\frac{dk}{2\pi}\,.$$

All integrals in the system(6.6) can be expressed in terms of the energy density ε (formula (6.5)) and of the heat flux (given by Eq.(6.7)). This allows us to write (6.6) in the following equivalent form:

$$\frac{\partial}{\partial t}\varepsilon + \frac{\partial}{\partial x}q = \frac{\varepsilon}{c(F)}\frac{\partial c(F)}{\partial F}\frac{\partial F}{\partial t}\,,$$

(6.8)
$$\frac{\partial}{\partial t}q + \frac{\partial}{\partial x}c^2\varepsilon = \varepsilon c(F)\frac{\partial c(F)}{\partial x} - \frac{1}{\tau(\varepsilon,F)}q\,,$$

$$\rho\frac{\partial v}{\partial t} - \frac{\partial}{\partial x}\left(\rho\frac{\partial\varphi(F)}{\partial F} + \frac{\varepsilon}{c(F)}\frac{\partial c(F)}{\partial F}\right) = 0\,.$$

These equations can be supplemented by the formula

(6.9)
$$\frac{\partial F}{\partial t} = \nabla v$$

relating the deformation gradient F to the velocity field v. The important property of Eqs. (6.8)$_1$, (6.8)$_2$, (6.8)$_3$ and (6.9) is that they form a closed system. Let us consider a stationary solution of this system. From Eq.(6.8)$_2$ we can determine the formula for the heat flux

(6.10)
$$q = -\tau(\varepsilon,F)c(F)\frac{\partial}{\partial x}\{c(F)\varepsilon\}\,.$$

After inserting Eq. (6.5) into Eq. (6.10) we can determine the heat flux q in terms of the

effective temperature T and of the deformation gradient F

(6.11)
$$q = -\tau(T, F)c(F)\frac{2k_B^2 T}{\hbar\pi}\frac{\partial T}{\partial x}\left(\int_0^\infty \frac{z\,dz}{e^z - 1}\right)$$

$$= -\tau(T, F)c(F)\frac{2}{3}\frac{\pi k_B^2 T}{\hbar}\frac{\partial T}{\partial x}.$$

If we postulate that this formula is valid also in the time-dependent case (that is, if we treat it as a "constitutive law" of the Fourier type) then, combining it with Eqs. (6.8)$_1$, (6.8)$_3$, (6.9) and expressing the energy density in terms of the effective temperature and the deformation, we obtain a field theory, in which the state of the system is described in terms of the deformation and the temperature. Such a field theory corresponds to the description of traditional thermomechanics. The interesting problem is whether (and in what sense) such a thermomechanical theory is an approximation of the exact nonequilibrium description given by Eqs. (6.8) and (6.9) (in which the state of the system is specified by the fields of energy density, heat flux and deformation). However, this problem shall not be discussed here.

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