

Quasiparticle Kinetic Equation in Geometry of Local Base Vectors

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Kinetic equations for quasiparticle excitations in ideal crystals, known from solid state physics, are generalized to the case of material bodies the crystal structure of which is distorted by the existence of continuously distributed defects. Distribution of defects is described by a field of local base vectors of a primitive crystal lattice. The form of conservation laws implied by such kinetic equations is discussed using the example of energy balance in a phonon system. It is shown that energy balance can be written either with respect to lattice connection or with respect to the Euclidean connection, having a vanishing source term in both cases. Transition from one version to another involves a redefinition of the heat flux vector.

1. INTRODUCTION

Transport processes in solids are described from a microscopic point of view in terms of quasiparticle excitations (Umezawa *et al.*, 1982; Fetter and Walecka, 1971). In turn, quasiparticle systems are often described by kinetic equations (Ziman, 1962; Gurevich, 1980). In solid state physics such equations are applied, in particular, to the description of effects caused by lattice imperfections (Gurevich, 1980; Reissland, 1973). The presence of imperfections is then taken into account by introducing additional collision processes into the collision integral. In such an approach, based on the geometry of an ideal crystal, one does not take into account that lattice imperfections can destroy the long-range order of a crystal. In order to include effects resulting from the lack of a long-range order, we have to reconsider the whole structure of the quasiparticle kinetic equation.

In mechanics, continuously distributed dislocations are frequently described by means of fields of local base vectors of a primitive crystal lattice

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(Kroner, 1986; Trzęsowski, 1987). Our aim here is to derive a form of a quasiparticle kinetic equation implied by such a description. Our approach is based on a localization procedure leading to the replacement of the product of the Brillouin zone and the three-dimensional Euclidian point space (which is the domain of a quasiparticle distribution function in the case of an ideal crystal) by the sum of local Brillouin zones (with the set of spatial points as the index set). From a physical point of view, such an approach is justified if the mean free path of excitations is small compared with the spatial scale on which base vectors of the local primitive lattice can be considered as approximately constant.

For a perfect crystal a sum of local Brillouin zones is endowed with a canonical symplectic structure. Hence, a kinetic equation for quasiparticles in a perfect crystal can be obtained formally, from the requirement that its structure is given by a Liouville equation with a source term (a Liouvillian part of such an equation describes single-particle evolution, while the collision integral approximates the effects of the many-body interactions). Such a kinetic equation is identical to the one obtained heuristically by writing the kinetic equation for quasiparticles in an ideal crystal in lattice coordinates and deforming the ideal crystal into a perfect crystal (keeping fixed the form of kinetic equation, written in convected coordinates).

A discussion of the quasiparticle kinetic equation in the case of crystalline bodies, with crystal structure described by fields of local base vectors of a crystal lattice, is based on the observation that differential operators defining the structure of a quasiparticle kinetic equation in the case of a perfect crystal can be represented as cross sections of a certain vector bundle and that such cross sections are functions of vector fields, defining a local crystal structure of a material body. Such mapping, assigning to the crystal structure of a material body (represented by a field of local base vectors) the differential operator (which defines a form of a kinetic equation) has a unique extension to the case of anholonomic vector fields. The kinetic equation obtained in that manner corresponds to the replacement of partial derivatives computed along the lines of crystallographic coordinates by directional derivatives along local base vectors of a crystal lattice.

Balance laws implied by such a kinetic equation are discussed using the example of the energy balance of a phonon system. It is shown that energy balance can be alternatively written in two forms, either with respect to the lattice connection or with respect to the Euclidian connection, having a vanishing source term in both forms. Transition from one version to another involves a redefinition of the heat flux vector.

2. KINETIC EQUATION

Let us consider a fixed configuration of a crystalline material body B , in which the body is mapped on a three-dimensional Euclidian point space

E. The material points of the body will be identified with elements of the Euclidian space occupied by them. The translation space of *E* will be denoted by Ξ . Local base vectors of a primitive crystal lattice are described by three linearly independent, globally defined, and smooth vector fields $\mathbf{a}_I, I=1, 2, 3$, on *E* with values in Ξ . Let $y_j, j=1, 2, 3$, be coordinates of a curvilinear coordinate system on *E*. Then the vector fields \mathbf{a}_I , the fields of dual base vectors $\mathbf{F}^J, J=1, 2, 3$ [defined by $(\mathbf{a}_I, \mathbf{F}^J) = \delta_I^J, I, J=1, 2, 3$, with (\cdot, \cdot) being the scalar product in Ξ], and the natural base vectors ∂y_i and base forms $\mathbf{d}y^j, i, j=1, 2, 3$, of the coordinates y_i are related via the matrix functions A_I^j and A_j^I on *E* according to the well-known formulas (Kroner, 1986; Trzesowski, 1987):

$$\begin{aligned} \mathbf{a}_I &= A_I^j \partial_{y_j} & A_I^j A_j^I &= \delta_I^I \\ A_I^j A_j^I &= \delta_I^I & \mathbf{F}^J &= A_j^J \mathbf{d}y^j \\ \mathbf{d}y^j &= A_j^I \mathbf{F}^J & \partial y_i &= A_i^I \mathbf{a}_I \end{aligned} \tag{1}$$

In (1), as well as in the rest of this paper, we apply Einstein's convention, assuming summation with respect to repeated indices. The "vector" notation $\mathbf{d}y^j$ for base forms follows from the fact that in the considered case of Euclidian geometry forms are canonically isomorphic with vectors. Local base vectors of the inverse lattice $\mathbf{G}^J, J=1, 2, 3$, will be defined as $\mathbf{G}^J = 2\pi \mathbf{F}^J$ and the local Brillouin zone T_x^3 , corresponding to the point $x, x \in E$, will be defined as the quotient space E/\sim_x , where \sim_x is the following equivalence relation:

$$X \in E, \quad \mathbf{w}, \mathbf{w}' \in \Xi, \quad \mathbf{w} \sim_x \mathbf{w}' \equiv \mathbf{w} - \mathbf{w}' = \sum_{J=1}^3 z_J \mathbf{G}^J(x) \tag{2}$$

with z_J being arbitrary integers (Ziman, 1962). The equivalence class, corresponding to the vector $\mathbf{w} \in \Xi$, will be denoted as $[\mathbf{w}]_x$. The space $T_x^3 \equiv \Xi/\sim_x$ endowed with the quotient topology has a natural structure of a compact Abelian Lie group with a topological structure of a three-dimensional torus (the group action is induced by the operation of adding vectors in Ξ).

Let us introduce a sum of all local Brillouin zones

$$\mathcal{F} := \bigcup_{x \in E} T_x^3 \tag{3}$$

Let *V* be a three-dimensional real vector space with a fixed basis $\mathbf{v}_i, i=1, 2, 3$. After introducing in *V* an equivalence relation, analogous to (2),

$$\mathbf{v}, \mathbf{v}' \in V, \quad \mathbf{v} \sim \mathbf{v}' \equiv \mathbf{v} - \mathbf{v}' = \sum_{j=1}^3 z_j \mathbf{v}_j \tag{4}$$

where z_j are arbitrary integers, we obtain a quotient space $T_V^3 \equiv \bigcup_{\mathbf{v} \in V} [\mathbf{v}]$, where $[\mathbf{v}]$ denotes the equivalence class of \mathbf{v} in the relation (4). The space

T_V^3 carries a Lie group structure isomorphic to that of T_x^3 . The action of T_V^3 on \mathcal{F} can be defined according to

$$T_V^3 \times \mathcal{F} \ni ([\mathbf{v}], [\mathbf{w}]_x) \rightarrow [\mathbf{v}] \cdot [\mathbf{w}]_x := [(v^J + w^J)\mathbf{G}^J(x)]_x \in \mathcal{F} \tag{5}$$

where $v^J \mathbf{v}_J$ and $w^J \mathbf{G}^J(x)$ are arbitrary representatives of $[\mathbf{v}]$ and $[\mathbf{w}]_x$.

Let us introduce the set W_x of vectors, defined as

$$W_x := \left\{ \mathbf{i} \in \mathbb{Z}^3; \mathbf{i} = \frac{\varepsilon_J \mathbf{G}^J(x)}{2\pi}, |\varepsilon_J| < \pi, J = 1, 2, 3 \right\} \tag{6}$$

(W_x contains quasiparticle wave vectors from the interior of the local Brillouin zone).

Let us assume that the coordinate system y_i on E is given by a diffeomorphism between E and \mathbb{R}^3 (\mathbb{R} denotes a set of real numbers).

The subset $U_{x,[0]}$ of T_x^3 will be defined as

$$U_{x,[0]} := \{[\mathbf{i}]; \mathbf{i} \in W_x\} \tag{7}$$

and $U_{x,[\mathbf{v}]}$ will denote the image of $U_{x,[0]}$ under the action of $[\mathbf{v}] \in T_x^3$. On the subset $U_{E,[\mathbf{v}]}$ of \mathcal{F} , defined as

$$U_{E,[\mathbf{v}]} := \bigcup_{x \in E} U_{x,[\mathbf{v}]} \tag{8}$$

we can introduce a coordinate system

$$\begin{aligned} \mathcal{A}_{E,[\mathbf{v}]}: \quad \mathbb{R}^3 \times (-\pi, \pi)^3 \ni (y_1, y_2, y_3, \varepsilon_1, \varepsilon_2, \varepsilon_3) \\ \rightarrow \left[\left(v^J + \frac{\varepsilon^J}{2\pi} \right) \mathbf{G}^J(x(y_j)) \right]_{x(y_j)} \in U_{E,[\mathbf{v}]} \subset \mathcal{F} \end{aligned} \tag{9}$$

(v^J are components of an arbitrary representative $v^J \mathbf{v}_J$ of $[\mathbf{v}]$ in the basis $\{\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3\}$).

A set of coordinate systems

$$\mathcal{A}_E := \{ \mathcal{A}_{E,[\mathbf{v}]}; [\mathbf{v}] \in T_V^3 \} \tag{10}$$

is a C^∞ -compatible atlas on \mathcal{F} , which gives \mathcal{F} a structure of a smooth manifold. Let us define a function $\mathcal{P}, \mathcal{P}: \mathcal{F} \rightarrow E$, as

$$\mathcal{P}([\mathbf{w}]_x) := x \tag{11}$$

A triple $(\mathcal{F}, E, \mathcal{P})$ forms a principal fiber bundle with T_V^3 as a structure group. Vectors tangent to the coordinate lines of charts from the atlas \mathcal{A}_E form six globally defined, smooth vector fields on \mathcal{F} , which shall be denoted by $\partial y_i, \partial \varepsilon_j, i, j = 1, 2, 3$ (we apply here the same symbol ∂y_i for vector fields on \mathcal{F} and E , since, on account of the triviality of the bundle \mathcal{F} , they can be canonically identified). By μ_x we shall denote the invariant measure on

T_x^3 , normalized in such a way that the “volume” of T_x^3 is equal to the volume of an elementary cell of a local inverse lattice.

For a perfect crystal, local base vectors of a crystal lattice are natural base vectors of a particular coordinate system, called crystallographic coordinates (Kroner, 1986). A mapping $S: \mathbb{R}^3 \rightarrow E$

$$S: \mathbb{R}^3 \ni (s_1, s_2, s_3) \rightarrow x(s_i) \in E \tag{12}$$

defining crystallographic coordinates allows us to parametrize the cotangent bundle $T^*(E)$ of E by means of parameters (s_i, β_j) , $i, j = 1, 2, 3$,

$$\mathbb{R}^6 \ni (s_i, \beta_j) \rightarrow \beta_j ds^j(x(s_i)) \in T^*(E) \tag{13}$$

where ds^j are natural base forms corresponding to crystallographic coordinates. Note that $2\pi ds^j$ can be identified with a field of local base vectors \mathbf{G}^j of the inverse lattice of a perfect crystal. Taking this identification into account, we can define a function $M: T^*(E) \rightarrow \mathcal{F}$ given by

$$T_{x(s_i)}^*(E) \ni \beta_j ds^j(x(s_i)) \rightarrow [\beta_j ds^j(x(s_i))]_{x(s_i)} \in \mathcal{F} \tag{14}$$

A triple $(T^*(E), \mathcal{F}, M)$ forms a covering space, with M as a covering mapping. For $|\beta_j| < \pi$ the mapping M acts as a diffeomorphism, the image of which is $U_{E,[0]}$ [compare (8)]. The mapping M , restricted to $|\beta_j| < \pi$, allows us to assign to a canonical symplectic form on $T^*(E)$ [implied by a cotangent bundle structure (Sławianowski, 1975)] a corresponding symplectic form on $U_{E,[0]}$. This symplectic form on $U_{E,[0]}$ can be uniquely extended to the symplectic form on \mathcal{F} , invariant under the action of T_V^3 on \mathcal{F} . The inverse of this symplectic form on \mathcal{F} , taken with a minus sign, is given by a tensor field

$$\Omega = \partial_{e_j} \wedge \partial_{s_j} \tag{15}$$

where \wedge denotes an exterior product and $\partial_{s_j}, j = 1, 2, 3$, are vector fields on \mathcal{F} , induced by crystallographic coordinates on E [the relation between fields ∂_{s_j} on \mathcal{F} and crystallographic coordinates on E is identical with the relation between vector fields $\partial_{y_j}, j = 1, 2, 3$, on \mathcal{F} , introduced after the formula (11), and curvilinear coordinates y_i on E]. The form of a Liouville equation implied by such a phase space structure determines a structure of a corresponding kinetic equation for quasiparticles in an ideal crystal

$$\frac{\partial f}{\partial t} + \text{Tr}_{(1,3)} \text{Tr}_{(2,4)} (\partial_{e_j} \wedge \partial_{s_j}) \otimes d\omega \otimes df = J(f) \tag{16}$$

where f denotes the phase density (identical with the quasiparticle distribution function). Tr denotes contraction with respect to the indices listed below, \otimes denotes a tensor product, ω is a Hamiltonian function (identical

with the quasiparticle dispersion curve), and $J(f)$ denotes the collision integral. For simplicity, we restrict ourselves to the case when only one branch of quasiparticle excitations is present. The form of the collision integral on the rhs of (16) is identical with the one known from the ideal crystal case; it can be obtained simply by replacing the integration with respect to the vectors from the Brillouin zone by integration with respect to the invariant measure μ_x on T_x^3 . In our construction the collision rates defining the explicit form of the collision integral and the dispersion curve remain unspecified. They have to be given by constitutive functions or derived from a microscopic theory (the dispersion curve can be, in principle, determined from diffraction experiments).

Now we shall discuss the problem of the generalization of the quasiparticle kinetic equation to the case of crystalline bodies containing continuously distributed defects which are described by means of a field of local base vectors of a primitive crystal lattice (Kroner, 1986; Trzęsowski, 1987). We shall assume that in the case of continuously distributed defects it is still possible to introduce a quasiparticle distribution function and a quasiparticle dispersion curve, both defined on the manifold \mathcal{F} (that is, on a sum of local Brillouin zones). From a physical point of view, such an assumption is justified if the mean free path of excitations is small compared with the spatial scale on which base vectors of the local primitive crystal lattice can be considered as approximately constant. A mapping

$$\mathcal{F} \ni [v^i \mathbf{G}^i(x)]_x \rightarrow ([v^i \mathbf{v}_i], x) \in T_V^3 \times E \quad (17)$$

{with $v^i \mathbf{G}^i(x)$ being an arbitrary representative of the point $[v^i \mathbf{G}^i(x)]_x$ of T_x^3 } diffeomorphically relates the manifold \mathcal{F} with the product of a material body (which is, in our case, identified with the Euclidian point space E) and of a torus group T_V^3 . As a consequence, the domain of quasiparticle distribution function can be parametrized by a pair of variables, one parametrizing points of T_V^3 (and measuring the quasiparticle wave vector in terms of local base vectors of the inverse lattice), and the second, specifying the space point occupied by quasiparticle.

From the fact that the tensor field $\partial_{\varepsilon_i} \wedge \partial_{s_i}$, which defines the lhs of the kinetic equation in the case of perfect crystal, is invariant under the action of T_V^3 , it follows that it can be represented as a cross section of a vector bundle W ,

$$W := \bigcup_{x \in E} A \{ (\mathcal{L} \oplus T_x(E)) \otimes (\mathcal{L} \oplus T_x(E)) \} \quad (18)$$

where \mathcal{L} denotes a Lie algebra of T_V^3 , $T_x(E)$ is a vector space tangent to E at x , \oplus denotes a direct sum of vector spaces, and A is a symbol of

antisymmetrization. To construct this cross section explicitly, let us parametrize a certain neighborhood of the neutral element of the torus group T_V^3 by means of parameters $\gamma_1, \gamma_2, \gamma_3$ according to the relation

$$(\gamma_1, \gamma_2, \gamma_3) \rightarrow \left[\frac{\gamma_i}{2\pi} \mathbf{v}_i \right] \in T_V^3 \tag{19}$$

Vectors tangent to the coordinate lines of the coordinate system (19) at $\gamma_i = 0, i = 1, 2, 3$, shall be denoted by $\partial_{\gamma_i(0)}$. If $\partial_{s_i}, i = 1, 2, 3$, form a field of local base vectors tangent to coordinate lines of crystal coordinates, then the tensor field $\partial_{\varepsilon_i} \wedge \partial_{s_i}$ [which defines a differential operator on the lhs of (16)] can be represented as the section $E \ni x \rightarrow \partial_{\gamma_i(0)} \wedge \partial_{s_i}(x)$ of the bundle W . We can now look at the form of a kinetic equation for quasiparticles in a perfect crystal as a result of a mapping which assigns to a crystal structure of a material body (which is given by fields of local base vectors) a manifold \mathcal{F} with a tensor field $\partial_{\varepsilon_i} \wedge \partial_{s_i}$ invariant under the action of T_V^3 . However, all operations defining this mapping act “locally” on the fields of local base vectors (in the sense that they do not distinguish whether fields of local base vectors are holonomic or not) and can be uniquely generalized to the case of anholonomic fields. Namely, let $\mathbf{a}_I, I = 1, 2, 3$, define a triple of globally defined and smooth fields of local base vectors on E , which in curvilinear coordinates $y_i, i = 1, 2, 3$, are given by formulas (1). Then a corresponding cross section of W given by $E \ni x \rightarrow \partial_{\gamma_i(0)} \wedge \mathbf{a}_I(x)$ determines a tensor field $\partial_{\varepsilon_i} \wedge \mathbf{a}_I$ on \mathcal{F} , invariant under the action of T_V^3 [\mathcal{F} denotes a sum of local Brillouin zones corresponding to the field of bases $\mathbf{a}_I, I = 1, 2, 3$, on E , whereas $\partial_{\varepsilon_i} \wedge \mathbf{a}_I$ is the exterior product of vector fields ∂_{ε_i} and $\mathbf{a}_I = A_I^i \partial_{y_i}$ on \mathcal{F} : for simplicity, we apply here the same symbols \mathbf{a}_I for vector fields on \mathcal{F} and on E , which is possible because of the triviality of the bundle \mathcal{F} ; see comments after the formula (11)].

In turn, the tensor field $\partial_{\varepsilon_i} \wedge \mathbf{a}_I$ determines the final form of the kinetic equation for quasiparticles in a crystalline body, the crystal structure of which is described by a field of local base vectors

$$\frac{\partial f}{\partial t} + \text{Tr}_{(1,3)} \text{Tr}_{(2,4)} (\partial_{\varepsilon_i} \wedge \mathbf{a}_I) \otimes d\omega \otimes df = J(f) \tag{20}$$

In an arbitrary chart from the atlas \mathcal{A}_E , equation (20) takes the form

$$\frac{\partial f}{\partial t} + A_I^i \left(\frac{\partial \omega}{\partial \varepsilon_I} \frac{\partial f}{\partial y_i} - \frac{\partial f}{\partial \varepsilon_I} \frac{\partial \omega}{\partial y_i} \right) = J(f) \tag{21}$$

Note that (21) can be obtained directly from the kinetic equation corresponding to the case of a perfect crystal by means of a heuristic procedure

of replacing partial derivatives, computed along the lines of crystallographic coordinates, by directional derivatives along local base vectors of a crystal lattice.

3. ENERGY BALANCE OF A PHONON GAS

In kinetic theory, conservation laws are obtained as the moment equations corresponding to summational invariants (Grad, 1958) (by summational invariants one means functions which, multiplied by the collision integral and integrated with respect to “momentum” variable, give, for every distribution function, identically zero). We shall illustrate a construction of the conservation law implied by a kinetic equation of the form (20) by the example of a phonon gas. In the case of the kinetic equation for phonons in an ideal crystal, phonon energy $\hbar\omega$, where $2\pi\hbar$ is the Planck constant, is a summational invariant, and the corresponding energy balance of a phonon gas has a well-known form (Gurevich, 1980). In order to obtain an energy balance law in the case of a geometry of local base vectors, we assume that $\hbar\omega$ remains a summational invariant also in the case of nonideal crystal structure. We multiply both sides of the kinetic equation (20) by $\hbar\omega$, integrate it with respect to the measure μ_x over the local Brillouin zone, integrate the result over a volume of a subbody $H \subset E$, change the order of integration and differentiation, and make use of the definition of the lattice connection (Kroner, 1986; Trzęsowski, 1987) (that is, the connection uniquely defined by the condition that vector fields \mathbf{a}_r are absolutely parallel). After dividing our result by $(2\pi)^3$, we obtain

$$\int_{y_i(H)} \left\{ \frac{\partial}{\partial t} \frac{\int_{T_x^3} \hbar\omega f d\mu_x}{\int_{T_x^3} d\mu_x} + \text{Div} \frac{\int_{T_x^3} \hbar\omega f \mathbf{v}_g d\mu_x}{\int_{T_x^3} d\mu_x} \right\} \det(A'_i) d^3y = 0 \quad (22)$$

where $y_i, i = 1, 2, 3$, are coordinates of a curvilinear coordinate system on E , $\det(A'_i)$ is a determinant of the matrix A'_i [introduced by formulas (1)], $y_i(H)$ denotes the domain of variables y_i parametrizing a subbody H , the vector field \mathbf{v}_g , given by

$$\mathbf{v}_g = \text{Tr}_{(2,3)} \mathbf{a}_r \otimes \partial_{\epsilon_r} \otimes d\omega \quad (23)$$

has a meaning of a group velocity of quasiparticles, and Div means a divergence taken with respect to the lattice connection. In deriving (22) we have taken into account that the product of volumes of elementary cells of primitive and of inverse lattices is equal to $(2\pi)^3$ (Gurevich, 1980).

From (22) we can immediately obtain a corresponding balance equation in a local form

$$\frac{\partial}{\partial t} \frac{\int_{T_x^3} \hbar \omega f d\mu_x}{\int_{T_x^3} d\mu_x} + \text{Div} \frac{\int_{T_x^3} \hbar \omega f \mathbf{v}_g d\mu_x}{\int_{T_x^3} d\mu_x} = 0 \quad (24)$$

However, (22) implies also an alternative form of the local balance law, written with respect to the "Euclidian" connection. In order to find such alternative form of the local balance equation, we replace covariant divergence in (22) by a divergence defined by a volume form $F^1 \wedge F^2 \wedge F^3$ (where F^J , $J=1, 2, 3$, are forms dual to the local base vectors \mathbf{a}_I , $I=1, 2, 3$), write the divergence term in (22) as the surface integral over ∂H , and apply Stokes' theorem; such transformations are discussed, for example, in Schutz (1982, Chapters 4 and 6). As a result, we obtain an identity

$$\frac{\partial}{\partial t} \int_{T_x^3} \hbar \omega f \frac{d\mu_x}{(2\pi)^3} + \text{div} \int_{T_x^3} \hbar \omega f \mathbf{v}_g \frac{d\mu_x}{(2\pi)^3} = 0 \quad (25)$$

where div denotes the Euclidian divergence. Hence, from the kinetic equation we can derive two alternative forms of a local balance equation, with the definition of a flux vector depending on the connection. The Euclidian form of energy balance (25) is analogous to the one known from the case of ideal crystals (Gurevich, 1980), and shows that the kinetic equation (20) is consistent with the macroscopic conservation laws.

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