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Lattice effects in the quasiparticle dynamics and kinetics

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Abstract. In this work we present a full selfconsistent set of nonlinear equations which unifies the nonlinear elasticity theory equations, the Boltzmannn transport theory and the Maxwell equations for quasiparticles with arbitrary dispersion laws in nonstationarily deformed crystals with arbitrary (but linear) constitutive relations. Transformations to replace the Galilean ones are obtained, the quasiparticle mechanics in a Hamiltonian form is deduced, and a Boltzmann-type transport equation (valid in the whole Brillouin zone) is derived. The theory may be applied to metals, semiconductors, quantum crystals, low-dimensional structures etc.

PACS. 05.60.-k Transport processes – 05.20.-y Classical statistical mechanics – 41.20.-q Applied classical electromagnetism

1 Introduction

Solids are that right physical system where the geometry plays a fundamental role. It changes the form of the basic conservation laws related to the properties of the space. The periodicity of the crystal lattice breaks the homogeneity of the space. As a result, the momentum is not conserved. It becomes a bad quantum number and the energy spectrum and quantum states are classified in terms of the quasimomentum, $\mathbf{k}$. The state of the elementary excitations (the quasiparticles) are described not by their positions and velocities, but by the corresponding wave function and dispersion relation $\varepsilon(\mathbf{k})$. Both these quantities are strongly dependent on the lattice geometry. There is a fundamental difference between particles and quasiparticles in continuous media and those in crystalline bodies. The crystal lattice is a *privileged (and not inertial) coordinate frame*. The quasiparticles are well defined only in a given ideal periodic lattice and *there are no Galilean transformations* to any other lattice frame. Hence, the mechanical equations for quasiparticles in lattice structures have to be rederived. They must be expressed in terms of the dispersion law and quasimomentum, and transformation relations to replace Galilean ones must be found. Another fundamental problem is the behavior of the quasiparticles in real structures that are always deformed (due to elastic waves, defects, external fields etc.) In such systems the quasimomentum is not completely conserved. And, finally, one needs a new scattering theory and new transport equation which solutions must satisfy the periodicity conditions applied by the lattice.

The situation becomes even more complicated for charged quasiparticles in electromagnetic fields. Two typical problems come to life immediately. One comes from the electrodynamics of macroscopic bodies where there is still no consensus about the form of the field momentum and the corresponding electromagnetic stress tensor [1–3] (this problem is known as Minkowski-Abraham controversy as well). The other is a typical solid state problem related to the momentum-quasimomentum duality in quasiparticle and photon description (put by Blount [4] and Peierls [5,6]). Let us mention that even the form of the Lorentz force on a (quasi-) electron in conducting or valence band becomes questionable. In fact, these open questions show that the electrodynamics of crystalline bodies is still far from its perfection.

These problems are as old as the quantum theory of solids itself. There were many attempts to solve them, but unfortunately not consistent enough and in the frame of a linear approximation only. More information and a critical review can be found in [8] and the bibliography cited there.

2 Quasiparticle mechanics

Our starting point in deriving the quasiparticle (say, conducting electron) mechanics is that the dispersion law $\varepsilon(\mathbf{k})$ plays the role of both Hamiltonian and energy in a lattice frame in rest (or moving with a constant velocity). This is a privileged frame. In this frame all physical quantities (energy, momentum etc.) are periodic functions in k-space. If the lattice is deformed, then the dispersion law becomes a function of coordinates. Such a description *(known as local lattice approach)* is justified by the fact that the dispersion relation is established in a region of several lattice constants while the characteristic length of the deformation is much larger (otherwise the deformations are not elastic as supposed here). The dependence on the

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coordinates enters into the dispersion relation by means of the deformations. In case of small deformations

$$\varepsilon(\mathbf{k}, u_{ik}) = \varepsilon(\mathbf{k}) + \lambda_{ik}(\mathbf{k}) u_{ik} \tag{1}$$

where $\lambda_{ik}(\mathbf{k})$ are known as *deformation potential constants*. In this notation the Hamilton equations of motion have the form:

$$\dot{\mathbf{r}}' = \frac{\partial \varepsilon}{\partial \mathbf{k}} \qquad \dot{\mathbf{k}} = \frac{\partial \varepsilon}{\partial \mathbf{r}'} \tag{2}$$

where $\mathbf{r}'$ and $\mathbf{k}$ are the coordinates and quasimomentum in the lattice frame. A generalization [9–11] of equation (1) is a dispersion law depending on the metrical tensor g_{ik} instead of the tensor of small deformations u_{ik}. The relation between g_{ik} and the full deformation tensor w_{ik} is $w_{ik} = (1/2)(g_{ik} - \overset{\circ}{g}_{ik})$ where $\overset{\circ}{g}_{ik}$ corresponds to the undeformed crystal lattice [7].

Equations (2) are written using canonically conjugate variables $\mathbf{r}'$ and $\mathbf{k}$. They have the same form as in a homogeneous media with $\mathbf{r}'$ and $\mathbf{k}$ for coordinates and momentum respectively. However, quasimomentum appears as a result of the lattice discreteness and hence cannot be conjugate to the ordinary continuous coordinate. Strictly speaking [12], it is conjugate to a *discrete* coordinate $\mathbf{r_N} = N^\alpha \mathbf{a}_\alpha$ assigned to the lattice site number $\mathbf{N}$ (where $\mathbf{a}_\alpha$ are the lattice vectors). These are the same quantities as in the Wannier wave-function

$$W(\mathbf{r} - \mathbf{r_N}) = \frac{1}{\sqrt{\mathcal{N}}} \sum_{\mathbf{k}} \exp(-\mathrm{i}\mathbf{k}\mathbf{r_N}) \psi_{\mathbf{k}}(\mathbf{r})$$

where $\mathcal{N}$ is the number of lattice cells and $\psi_{\mathbf{k}}(\mathbf{r})$ is the Bloch function. In a continuum limit $\mathbf{r_N}$ and $\mathbf{k}$ can be considered as smooth conjugate variables. The physical infinitesimal distance (small compared with the characteristic deformation length but large compared to the interatomic distances) can be written then in the form [9]:

$$\mathrm{d}\mathbf{r} = \mathbf{a}_\alpha \mathrm{d}N^\alpha + \dot{\mathbf{u}} \mathrm{d}t \tag{3}$$

where $\dot{\mathbf{u}}$ is the lattice velocity. In a deformed crystal the lattice vectors $\mathbf{a}_\alpha(\mathbf{r}, t)$ are functions of the coordinates and the time. Their time-evolution equations can be found from plain geometrical considerations [9] and read:

$$\dot{\mathbf{a}}_\alpha + (\dot{\mathbf{u}}\nabla)\mathbf{a}_\alpha - (\mathbf{a}_\alpha \nabla)\dot{\mathbf{u}} = 0. \tag{4}$$

We introduce also the reciprocal lattice vectors $\mathbf{a}^\alpha(\mathbf{r}, t)$. They satisfy the relations

$$\mathbf{a}^\alpha . \mathbf{a}_\beta = \delta^\alpha_\beta, \qquad a^\alpha_i a_{\alpha k} = \delta_{ik} \tag{5}$$

and the time evolution equation

$$\dot{\mathbf{a}}^\alpha + \nabla(\mathbf{a}^\alpha \dot{\mathbf{u}}) = 0. \tag{6}$$

The metrical tensors describing the deformations in the real and reciprocal spaces are $g_{\alpha\beta} = \mathbf{a}_\alpha \mathbf{a}_\beta$ and $g^{\alpha\beta} = \mathbf{a}^\alpha \mathbf{a}^\beta$ respectively.

It follows from (3) that

$$\mathbf{a}^\alpha = \nabla N^\alpha, \qquad \mathbf{a}_\alpha = \frac{\partial \mathbf{r}}{\partial N^\alpha}, \qquad \dot{\mathbf{u}} = -\mathbf{a}_\alpha \dot{N}^\alpha. \tag{7}$$

Hence, the functions $N^\alpha(\mathbf{r}, t)$ fully describe the lattice geometry. They give the number of steps in the lattice (each of them being equal to the corresponding local value of the lattice vector $\mathbf{a}_\alpha$). We call these quantities *discrete coordinates*. The canonically conjugate variables are the *invariant quasimomentum* components and will be denoted by $\boldsymbol{\kappa}$. In this dimensionless notation the dispersion law has the form $\varepsilon(\boldsymbol{\kappa}, g^{\alpha\beta})$ and all physical quantities have a constant period in the κ-space 2π (not $2\pi\mathbf{a}^\alpha$).

The Hamilton equations of motion in this notation were derived in [9] (see also Ref. [13,8]). In L-system they read:

$$\dot{\mathbf{r}} = \frac{\partial H(\mathbf{p}, \mathbf{r}, t)}{\partial \mathbf{p}}, \quad \dot{\mathbf{p}} = -\frac{\partial H(\mathbf{p}, \mathbf{r}, t)}{\partial \mathbf{r}} \tag{8}$$

where the Hamiltonian is a function of the coordinates $\mathbf{r}$ and quasimomentum $\mathbf{p}$ in the L-system according to the relations:

$$\mathbf{r} = \mathbf{r}' + \dot{\mathbf{u}}, \quad \mathbf{p} = \kappa_\alpha \mathbf{a}^\alpha + m\dot{\mathbf{u}} \tag{9}$$

$$H(\mathbf{p}, \mathbf{r}, t) = \varepsilon(\kappa, g^{\alpha\beta}) + \mathbf{p}\dot{\mathbf{u}} - \frac{m\dot{u}^2}{2} \tag{10}$$

and $\varepsilon = \varepsilon(\mathbf{a}_\alpha(\mathbf{p} - m\dot{\mathbf{u}}), g^{\alpha\beta})$ is the dispersion law in which the components of the invariant quasimomentum κ are replaced by

$$\kappa_\alpha = \mathbf{a}_\alpha(\mathbf{p} - m\dot{\mathbf{u}}) = \mathbf{k}\mathbf{a}_\alpha \tag{11}$$

according to (9). $\varepsilon(\mathbf{a}_\alpha(\mathbf{p} - m\dot{\mathbf{u}}), g^{\alpha\beta})$ is a periodic function of $\mathbf{p}$ with periods $2\pi\hbar\mathbf{a}^\alpha$ determined by the reciprocal lattice vectors corresponding to the deformed local lattice. This is the reason to call $\mathbf{p}$ *the quasimomentum of the quasiparticle in L-system*. Let us note that the dispersion law is 'originally' dependent on the *invariant quasimomentum* $\boldsymbol{\kappa}$, not on the quasimomentum $\mathbf{k}$.

Equations (9) are the *generalized Galilean transformations* for quasiparticles. The energy in L-system is

$$\mathcal{E} = \frac{m\dot{u}^2}{2} + m\dot{\mathbf{u}}\frac{\partial \varepsilon}{\partial \mathbf{p}} + \varepsilon = \frac{m\dot{u}^2}{2} + \mathbf{p}_0\dot{\mathbf{u}} + \varepsilon \tag{12}$$

where $\mathbf{p}_0 = m\frac{\partial \varepsilon}{\partial \mathbf{p}}$ is the average momentum (the mass flow) in C-system. Expression (12) is a periodic function of $\mathbf{p}$ and is in agreement with the Galilean principle.

3 Boltzmann equation

Boltzmann equation for a quasiparticle distribution function $f(\mathbf{p}, \mathbf{r}, t)$ in L system can be derived by the condition that the full derivative of this function be equal to its change due to the collisions:

$$\frac{\partial f}{\partial t}+\frac{\partial f}{\partial \mathbf{r}}\dot{\mathbf{r}}+\frac{\partial f}{\partial \mathbf{p}}\dot{\mathbf{p}}=\hat{I}f \tag{13}$$

where $\hat{I}$ is the collision operator. The derivatives $\dot{\mathbf{r}}$ and $\dot{\mathbf{p}}$ are replaced using Hamilton equations. This gives

$$\frac{\partial f}{\partial t}+\frac{\partial f}{\partial \mathbf{r}}\frac{\partial H}{\partial \mathbf{p}}-\frac{\partial f}{\partial \mathbf{p}}\left(\frac{\partial H}{\partial \mathbf{r}}-\mathbf{F}\right)=\hat{I}f. \tag{14}$$

For real gases the left-hand side of this equation is well defined by the classical Hamilton equations. In the case of quasiparticles under consideration equations (2) with Hamiltonian of the form (10) have to be used.

It can be shown [9,8] that the solution of the Boltzmann equation (14) is a periodic function $f(\mathbf{p},\mathbf{r},t)=f\left(\mathbf{p}+2\pi\hbar\mathbf{a}^{\alpha}(\mathbf{r},t),\mathbf{r},t\right)$ although the Hamiltonian (10) contains aperiodic terms $\left(\frac{\partial f}{\partial \mathbf{p}}\frac{\partial H}{\partial \mathbf{r}}\right)$.

The transformation to the new variables can be done using the following relations, obtained by means of the evolution equations (4, 6):

$$\dot{\kappa}_\alpha=\mathbf{a}_\alpha\left(\kappa_\beta\nabla(\mathbf{a}^\beta\dot{\mathbf{u}})-m\ddot{\mathbf{u}}\right) \tag{15}$$

$$\frac{\partial}{\partial \mathbf{p}}=\mathbf{a}_\alpha\frac{\partial}{\partial \kappa_\alpha} \tag{16}$$

$$\left(\frac{\partial}{\partial \mathbf{r}}\right)_{\mathbf{p}}=\left(\frac{\partial}{\partial \mathbf{r}}\right)_{\kappa}+\left(\kappa_\beta\mathbf{a}^\beta\nabla a_{\alpha k}-ma_{\alpha k}\nabla\dot{u}_k\right)\frac{\partial}{\partial\kappa_\alpha} \tag{17}$$

$$\left(\frac{\partial}{\partial t}\right)_{\mathbf{p}}=\left(\frac{\partial}{\partial t}\right)_{\kappa}+\left(\kappa_\beta\mathbf{a}_\alpha\nabla(\mathbf{a}^\beta\dot{\mathbf{u}})-m\mathbf{a}_\alpha\ddot{\mathbf{u}}\right)\frac{\partial}{\partial\kappa_\alpha}\cdot \tag{18}$$

As a result, the kinetic equation for the partition function $f(\boldsymbol{\kappa},\mathbf{r},t)$ takes the form:

$$\frac{\mathrm{d}f}{\mathrm{d}t}+\mathbf{a}_\alpha\frac{\partial\varepsilon}{\partial\kappa_\alpha}\left(\frac{\partial f}{\partial \mathbf{r}}\right)_{\boldsymbol{\kappa}}-\mathbf{a}_\alpha\frac{\partial f}{\partial\kappa_\alpha}\left\{m\frac{\mathrm{d}\dot{\mathbf{u}}}{\mathrm{d}t}+\left(\frac{\partial\varepsilon}{\partial \mathbf{r}}\right)_{\boldsymbol{\kappa}}-m\frac{\partial\varepsilon}{\partial\kappa_\beta}\mathbf{a}_\beta\times\operatorname{curl}\dot{\mathbf{u}}-\mathbf{F}\right\}=\hat{I}f \tag{19}$$

where $\frac{\mathrm{d}}{\mathrm{d}t}=\frac{\partial}{\partial t}+(\dot{\mathbf{u}}\nabla)$, $\mathbf{F}$ is the external force, and all quantities are differentiated with respect to the coordinates and the time at constant $\boldsymbol{\kappa}$. The term $m\frac{\mathrm{d}\dot{\mathbf{u}}}{\mathrm{d}t}$ takes into account noninertial properties of the local frame. This is the term which is responsible for the Stewart-Tolman effect in metals.

The term

$$m\frac{\partial\varepsilon}{\partial\kappa_\beta}\mathbf{a}_\beta\times\operatorname{curl}\dot{\mathbf{u}} \tag{20}$$

is of *essentially new kind* and cannot be obtained in linear theories. It is proportional to the bare mass m and, hence, is also responsible for noninertial effects. In fact, $\mathbf{a}_\beta\frac{\partial\varepsilon}{\partial\kappa_\beta}$ is the quasiparticle velocity with respect to the lattice. If the body rotates with a constant velocity $\boldsymbol{\Omega}$, then $\operatorname{curl}\dot{\mathbf{u}}=2\boldsymbol{\Omega}$ and the expression (20) represents the Coriolis force.

Equation (19) does not contain any nonperiodic terms. It follows from the form of the Hamiltonian (10) that the velocity $\partial H/\partial\mathbf{p}$ is a periodic function. Hence, external forces $\mathbf{F}$ which depend on the velocity and its derivatives are permissible. A force of this kind is the Lorentz force. In our notation it has the form:

$$\mathbf{F_L}=-e\mathbf{E}-\frac{e}{c}\frac{\partial\varepsilon}{\partial\kappa_\alpha}\mathbf{a}_\alpha\times\mathbf{B}-\frac{e}{c}\dot{\mathbf{u}}\times\mathbf{B} \tag{21}$$

(the electron charge is taken equal to $-e$, $e>0$). Substituting $\mathbf{F}_L$ into (19) yields

$$\frac{\partial f}{\partial t}+\left(\dot{\mathbf{u}}+\mathbf{a}_\alpha\frac{\partial\varepsilon}{\partial\kappa_\alpha}\right)(\boldsymbol{\nabla}f)_{\boldsymbol{\kappa}}-\mathbf{a}_\alpha\frac{\partial f}{\partial\kappa_\alpha}\left\{\boldsymbol{\nabla}\left(\varepsilon+\frac{m\dot{\mathbf{u}}^2}{2}\right)_{\boldsymbol{\kappa}}+\frac{e}{c}\left(\dot{\mathbf{u}}+\mathbf{a}_\alpha\frac{\partial\varepsilon}{\partial\kappa_\alpha}\right)\times\tilde{\mathbf{B}}+e\mathbf{E}+m\ddot{\mathbf{u}}\right\}=\hat{I}f. \tag{22}$$

The quantity $\tilde{\mathbf{V}}=\dot{\mathbf{u}}+\mathbf{a}_\beta\frac{\partial\varepsilon}{\partial\kappa_\beta}=\frac{\partial H}{\partial\mathbf{p}}$ is the velocity of the quasiparticle in L-system. It is worth noting that the sum $\varepsilon+m\dot{u}^2/2$ in (22) is not the quasiparticle energy $\mathcal{E}$ (12) in L-system. For equations (10–12) one has:

$$\varepsilon+\frac{m\dot{u}^2}{2}=\mathcal{E}-\mathbf{p_0}\dot{\mathbf{u}}=H-\mathbf{k}\dot{\mathbf{u}}$$

The magnetic field enters in the transport equation only in a combination

$$\tilde{\mathbf{B}}=\mathbf{B}-\frac{mc}{e}\operatorname{curl}\dot{\mathbf{u}}. \tag{23}$$

If one introduces the vector potential $\mathbf{A}$ ($\mathbf{B}=\operatorname{curl}\mathbf{A}$), then the right hand side of (23) takes the form

$$-\frac{c}{e}\left(m\dot{\mathbf{u}}-\frac{e}{c}\mathbf{A}\right)=-\frac{c}{e}\mathcal{P} \tag{24}$$

where $\mathcal{P}$ is the well known generalized momentum.

An essential part of any theoretical work in quasiparticle kinetics is integrating of diverse physical quantities over the Brillouin zone, transforming such integrals by parts, as well as differentiating with respect to coordinates and the time. However, in a nonstationary case the boundaries of the Brillouin zone are moving under the time-varying deformations and become dependent not only on a deformation in a given instant but also on the velocity of the lattice. As a result, the integration over the Brillouin zone does not commutate with the differentiation with respect to $\mathbf{r}$ and t. This noncommutativity manifests itself in some fluxes through the zone boundaries. This effect is important for nonequilibrium systems, open Fermi surfaces as well as for all cases when the distribution function or its derivatives do not vanish on the zone boundaries. This kind of difficulties can be passed over by introducing a *renormalized partition function*

$$\varphi(\boldsymbol{\kappa},\mathbf{r},t)=f/\sqrt{g}. \tag{25}$$

The Boltzmann kinetic equation for $\varphi(\boldsymbol{\kappa}, \mathbf{r}, t)$ has the form

$$\dot{\varphi} + \operatorname{div}\left\{\left(\dot{\mathbf{u}} + \mathbf{a}_\alpha \frac{\partial \varepsilon}{\partial \kappa_\alpha}\right)\varphi\right\} - \mathbf{a}_\alpha \frac{\partial}{\partial \kappa_\alpha}\varphi\left\{\nabla\left(\varepsilon + \frac{m\dot{\mathbf{u}}^2}{2}\right)_{\boldsymbol{\kappa}} - m\left(\dot{\mathbf{u}} + \frac{\partial \varepsilon}{\partial \kappa_\beta}\mathbf{a}_\beta\right) \times \operatorname{curl}\dot{\mathbf{u}} + m\ddot{\mathbf{u}} - \mathbf{F}\right\} = \hat{I}\varphi. \quad (26)$$

4 Electrodynamics of deformable solids

In this section we derive the full set of equations describing the behavior of deformable crystalline bodies with quasiparticle excitations in electromagnetic fields. The case of metals was considered in [9,13]. The general case was considered in [8,14]. We shall pay attention here to the most interesting case of dielectrics. In fact, the Maxwell equations in their general form

$$\operatorname{curl}\mathbf{E} = -\frac{1}{c}\frac{\partial \mathbf{B}}{\partial t}, \qquad \operatorname{curl}\mathbf{H} = \frac{4\pi}{c}\mathbf{j}_e + \frac{1}{c}\frac{\partial \mathbf{D}}{\partial t}, \quad (27)$$

$$\operatorname{div}\mathbf{D} = 4\pi q, \qquad \operatorname{div}\mathbf{B} = 0, \quad (28)$$

have a limited application. The two currents in the right hand site of the Ampère law (27) can be considered as a decomposition with respect to the electric field $\mathbf{j}_e = \sigma\mathbf{E}$ and its time derivative $\dot{\mathbf{D}} \sim \omega\mathbf{E}$. Usually, these two terms are of different order of magnitude. In metals the displacement current is neglected (due to large conductivity σ) while in dielectrics it dominates. Therefore, we shall neglect the current $\mathbf{j}$ and the extraneous charges q in (27) and (28). We suppose also linear constitutive relations $\mathbf{D}' = \epsilon\mathbf{E}'$ and $\mathbf{B}' = \mu\mathbf{H}'$. The permeabilities $\mu(g^{\alpha\beta})$ and $\epsilon(g^{\alpha\beta})$ are functions of time dependent deformations and this dependence is in general anisotropic. This means that the derivatives $\epsilon_{\alpha\beta} = 2\frac{\partial\epsilon}{\partial g^{\alpha\beta}}$ and $\mu_{\alpha\beta} = 2\dfrac{\partial \mu}{\partial g^{\alpha\beta}}$ are matrices. The primes are used to show that the constitutive relations refer to the co-moving lattice frame. In L-system they read

$$\mathbf{D} + \frac{1}{c}\dot{\mathbf{u}} \times \mathbf{H} = \epsilon\left\{\mathbf{E} + \frac{1}{c}\dot{\mathbf{u}} \times \mathbf{B}\right\} \quad (29)$$

$$\mathbf{B} - \frac{1}{c}\dot{\mathbf{u}} \times \mathbf{E} = \mu\left\{\mathbf{H} - \frac{1}{c}\dot{\mathbf{u}} \times \mathbf{D}\right\}.$$

A full selfconsistent set of equations has to contain Maxwell's equations, Boltzmann equation and a dynamic (elasticity theory) equation. To derive it we turn to the conservation laws. The mass conservation law (continuity equation) is

$$m\dot{n} + \operatorname{div}\mathbf{j}_0 = 0 \quad (30)$$

where

$$n = \langle f \rangle, \quad \mathbf{j}_0 = m\left\langle \frac{\partial H}{\partial \mathbf{p}} f\right\rangle = m\left\langle \frac{\partial \varepsilon}{\partial \mathbf{p}} f\right\rangle + mn\dot{\mathbf{u}} \quad (31)$$

and $\langle ... \rangle = \int \mathrm{d}^3k \ldots$ stands for integral over the Brillouin zone. Alternatively, $\langle\langle \ldots \rangle\rangle = \int \mathrm{d}^3\kappa_\alpha$. Equation (30) follows directly from the Boltzmann equation [13].

The total mass current is

$$\mathbf{J}_0 = \rho\dot{\mathbf{u}} + \mathbf{j}'_0, \qquad \mathbf{j}'_0 = m\left\langle \frac{\partial \varepsilon}{\partial \mathbf{p}} f\right\rangle \quad (32)$$

where $\rho = \rho_0 + mn$ is a sum of the densities of the lattice, ρ_0, and quasiparticles.

The quantities ρ and $\mathbf{J}_0$ satisfy the mass continuity equation

$$\dot{\rho} + \operatorname{div}\mathbf{J}_0 = 0. \quad (33)$$

The full momentum $\mathbf{J}$ is a sum of $\mathbf{J}_0$ and the field momentum $\mathbf{g}$:

$$\mathbf{J} = \mathbf{J}_0 + \mathbf{g}. \quad (34)$$

Note, that in this case *the full momentum does not coincide with the mass flow!*

Our aim is to determine momentum and energy fluxes Π_{ik} and $\mathbf{Q}$ in a way as to satisfy the continuity equation (33), the momentum conservation law

$$\dot{J}_i + \nabla_k \Pi_{ik} = 0, \quad (35)$$

and the energy conservation law

$$\dot{E} + \operatorname{div}\mathbf{Q} = 0. \quad (36)$$

The energy in L-system is given by the expression

$$E = \frac{1}{2}\rho_0\dot{\mathbf{u}}^2 + E_0(g^{\alpha\beta}) + \langle\langle \mathcal{E}\varphi \rangle\rangle + W, \quad (37)$$

where $E_0(g^{\alpha\beta})$ is the strain energy in C-system, and W is the field energy.

The time derivative of the energy (37) is then

$$\dot{E} = \rho\dot{\mathbf{u}}\ddot{\mathbf{u}} + \frac{1}{2}\dot{\rho}\dot{u}^2 + \frac{\partial}{\partial t}\langle\langle \varepsilon\varphi \rangle\rangle + m\ddot{\mathbf{u}}\mathbf{a}_\alpha\left\langle\left\langle \varphi\frac{\partial \varepsilon}{\partial k_\alpha}\right\rangle\right\rangle + \dot{E}_0 + m\dot{\mathbf{u}}\dot{\mathbf{a}}_\alpha\left\langle\left\langle \varphi\frac{\partial \varepsilon}{\partial k_\alpha}\right\rangle\right\rangle + m\dot{\mathbf{u}}\mathbf{a}_\alpha\left\langle\left\langle \varphi\frac{\partial \dot{\varepsilon}}{\partial k_\alpha}\right\rangle\right\rangle + m\dot{\mathbf{u}}\mathbf{a}_\alpha\left\langle\left\langle \dot{\varphi}\frac{\partial \varepsilon}{\partial k_\alpha}\right\rangle\right\rangle + \dot{W}. \quad (38)$$

The time derivative of the elastic energy $E_0(g^{\alpha\beta})$ (as well as of any function of $g^{\alpha\beta}$) can be taken making use of the identity

$$\mathrm{d}g = -g g_{\alpha\beta}\mathrm{d}g^{\alpha\beta}. \quad (39)$$

Therefore,

$$\dot{g} = -g g_{\alpha\beta}\dot{g}^{\alpha\beta} = -g\mathbf{a}_\alpha\mathbf{a}_\beta(\dot{\mathbf{a}}^\alpha\mathbf{a}^\beta + \mathbf{a}^\alpha\dot{\mathbf{a}}^\beta)$$

The time derivatives can be eliminated using the evolution equation (6). This yields

$$\dot{E}_0 = \sigma_{\alpha\beta}a_i^\alpha a_k^\beta\frac{\partial \dot{u}_i}{\partial x_k} - \dot{\mathbf{u}}\nabla E_0. \quad (40)$$

All other time derivatives in (38) can be transformed to space derivatives using conservation laws, Boltzmann equation and evolution equations. Finally, the time derivative of the energy (38) can be written in the form

$$\dot{E} + \nabla_k \Bigg\{ \frac{1}{2}\rho \dot{u}^2 \dot{u}_k + \dot{u}_i \left(\Pi_{ik} - \rho \dot{u}_i \dot{u}_k + E_0 \delta_{ik} + \langle\langle \varepsilon f \rangle\rangle \delta_{ik} \right) - \frac{1}{2} m \dot{u}^2 \left\langle \frac{\partial \varepsilon}{\partial p_k} f \right\rangle + \left\langle \varepsilon \frac{\partial \epsilon}{\partial p_k} f \right\rangle \Bigg\} = \frac{\partial \dot{u}_i}{\partial x_k} \Bigg\{ \Pi_{ik} - \rho \dot{u}_i \dot{u}_k + \sigma_{ik} - \langle \lambda_{ik} f \rangle + E_0 \delta_{ik} - \dot{u}_i j_{0i} - \dot{u}_k j_{0i} \Bigg\} + \langle \varepsilon \hat{I} f \rangle + \left\langle \mathbf{F}_L \frac{\partial \varepsilon}{\partial \mathbf{p}} f \right\rangle + \dot{W} - \dot{\mathbf{u}} \dot{\mathbf{g}} \quad (41)$$

where

$$\lambda_{ik} = 2 \frac{\partial \varepsilon}{\partial g^{\alpha\beta}} a_i^\alpha a_k^\beta \qquad \sigma_{ik} = -2 \frac{\partial E_0}{\partial g^{\alpha\beta}} a_i^\alpha a_k^\beta. \quad (42)$$

The last three terms in (41) describe the change of the field energy, field momentum and the effect of external forces. They depend on the concrete type of interaction and should be omitted if there are no external fields. Let us first consider this case.

In the absence of energy dissipation equation (41) must coincide with the energy conservation law. On the other hand the fluxes of energy and momentum are functions of the thermodynamic variables and velocities, but do not depend on their time and space derivatives. This enables us to obtain from (41) unique expressions for the desired quantities

$$Q_i = E \dot{u}_i + \left\langle \varepsilon \frac{\partial H}{\partial p_i} f \right\rangle - \frac{1}{2} \dot{u}^2 J_i + \Pi_{ik} \dot{u}_k \quad (43)$$

and

$$\Pi_{ik} = -(\sigma_{ik} + E_0 \delta_{ik}) + \rho \dot{u}_i \dot{u}_k + \langle \lambda_{ik} f \rangle - m \left\langle f \frac{\partial \varepsilon}{\partial p_i} \frac{\partial \varepsilon}{\partial p_k} \right\rangle + m \left\langle f \frac{\partial H}{\partial p_i} \frac{\partial H}{\partial p_k} \right\rangle \cdot \quad (44)$$

The momentum flux tensor consists of two parts, L_{ik} and P_{ik}, which correspond to the contributions of the lattice and quasiparticles respectively:

$$L_{ik} = -(\sigma_{ik} + E_0 \delta_{ik}) + \rho_0 \dot{u}_i \dot{u}_k \quad (45)$$

$$P_{ik} = \langle \lambda_{ik}^0 f \rangle + m \left\langle f \frac{\partial H}{\partial p_i} \frac{\partial H}{\partial p_k} \right\rangle \quad (46)$$

where

$$\langle \lambda_{ik}^0 f \rangle = \langle \lambda_{ik} f \rangle - m \left\langle f \frac{\partial \varepsilon}{\partial p_i} \frac{\partial \varepsilon}{\partial p_k} \right\rangle \quad (47)$$

is the quasiparticle momentum flux tensor (the quasiparticle stress tensor) in the system of center of mass while $\langle \lambda_{ik} f \rangle$ corresponds to the co-moving frame. It can be shown [8] that the sum $\sigma_{ik} + E_0 \delta_{ik}$ corresponds (but coincides in linear approximation only) to the stress tensor of the linear elasticity theory and turns into pressure for isotropic media.

Finally, the equation of the elasticity theory for an elastic crystalline body with quasiparticle excitations in the absence of external fields takes the form:

$$\frac{\partial}{\partial t}(\rho \dot{u}_i) = -\frac{\partial L_{ik}}{\partial x_k} - \frac{\partial P_{ik}}{\partial x_k} - \frac{\partial j_{0i}}{\partial t} \cdot \quad (48)$$

The last term in the right-hand side describes the force which appears when varying the quasiparticle mass current (32) with respect to the lattice.

Let us consider now the contribution of the field terms

$$\left\langle \mathbf{F}_L \frac{\partial \varepsilon}{\partial \mathbf{p}} f \right\rangle + \dot{W} - \dot{\mathbf{u}} \dot{\mathbf{g}}. \quad (49)$$

We restrict ourselves to the linear (with respect to $\dot{u}/c$) terms. Then, the quantity

$$\left\langle \mathbf{F}_L \frac{\partial \varepsilon}{\partial \mathbf{p}} f \right\rangle = \mathbf{j}'_e \left(\mathbf{E} + \frac{\dot{\mathbf{u}}}{c} \times \mathbf{B} \right) = \mathbf{j}'_\mathbf{e} \mathbf{E}'. \quad (50)$$

This term equals zero for $\mathbf{j}'_e = 0$. To calculate $\dot{W}$ let us first consider the variation of the field energy $W' = (1/4\pi)(\mathbf{E}'\mathbf{D}' + \mathbf{H}'\mathbf{B}')$ in the lattice frame. By definition

$$\delta W'_E = \frac{1}{4\pi} \mathbf{E}' \delta \mathbf{D}' = \frac{1}{4\pi} \left\{ \mathbf{E}'^2 \delta \epsilon + \epsilon \mathbf{E}' \delta \mathbf{E}' \right\} = \frac{\mathbf{E}'^2}{8\pi} \delta \epsilon + \delta \frac{\epsilon \mathbf{E}'^2}{8\pi} \cdot \quad (51)$$

Therefore, the variation of W in time is:

$$\dot{W} = \frac{1}{4\pi} (\mathbf{E}\dot{\mathbf{D}} + \mathbf{H}\dot{\mathbf{B}}) = \frac{1}{4\pi} \left(\mathbf{E}' - \frac{\dot{\mathbf{u}}}{c} \times \mathbf{B} \right) \left(\dot{\mathbf{D}}' - \frac{\dot{\mathbf{u}}}{c} \times \dot{\mathbf{H}} \right) + \frac{1}{4\pi} \left(\mathbf{H}' + \frac{\dot{\mathbf{u}}}{c} \times \mathbf{D} \right) \left(\dot{\mathbf{B}}' - \frac{\dot{\mathbf{u}}}{c} \times \dot{\mathbf{E}} \right) = \frac{\partial}{\partial t} \frac{\epsilon E'^2 + \mu H'^2}{8\pi} + \frac{E'^2}{8\pi} \dot{\epsilon} + \frac{H'^2}{8\pi} \dot{\mu} + \dot{\mathbf{u}}(\dot{\mathbf{g}} + \dot{\mathbf{G}}) \quad (52)$$

where

$$\mathbf{g} = \frac{\mathbf{E} \times \mathbf{H}}{4\pi c}, \qquad \mathbf{G} = \frac{\mathbf{D} \times \mathbf{B}}{4\pi c} \cdot \quad (53)$$

The time derivatives $\dot{\varepsilon}$ and $\dot{\mu}$ are calculated in the same manner as (40):

$$\dot{\epsilon} = -\epsilon_{ik} \frac{\partial \dot{u}_i}{\partial x_k} - \dot{\mathbf{u}} \nabla \epsilon, \qquad \dot{\mu} = -\mu_{ik} \frac{\partial \dot{u}_i}{\partial x_k} - \dot{\mathbf{u}} \nabla \mu. \quad (54)$$

Substituting (54) in (52) and making use of the Poynting theorem one obtains

$$\dot{W} - \dot{\mathbf{u}} \dot{\mathbf{g}} = -\mathrm{div}\, \mathbf{S}' - \left(\frac{\mathbf{E}'^2}{8\pi} \epsilon_{ik} + \frac{\mathbf{H}'^2}{8\pi} \mu_{ik} \right) \frac{\partial \dot{u}_i}{\partial x_k} - \dot{\mathbf{u}} \left(\frac{\mathbf{E}'^2}{8\pi} \nabla \epsilon + \frac{\mathbf{H}'^2}{8\pi} \nabla \mu \right) + \dot{\mathbf{u}} \dot{\mathbf{G}}. \quad (55)$$

Neglecting terms of the order $0(v^2/c^2)$ in (52) means that one may replace $\dot{\mathbf{G}}$ by $\dot{\mathbf{G}}'$. The time derivative $\dot{\mathbf{G}}'$ can be transformed using Maxwell's equations in the co-moving frame. This yields:

$$\dot{\mathbf{u}}\dot{\mathbf{G}}' = \dot{u}_i \nabla_k t'_{ik} + \dot{\mathbf{u}} \left(\frac{\mathbf{E}'^2}{8\pi} \nabla \epsilon + \frac{\mathbf{H}'^2}{8\pi} \nabla \mu \right) \quad (56)$$

where

$$t'_{ik} = \frac{\epsilon}{4\pi} \left(E'_i E'_k - \frac{E'^2}{2} \delta_{ik} \right) + \frac{\mu}{4\pi} \left(H'_i H'_k - \frac{H'^2}{2} \delta_{ik} \right) \quad (57)$$

is the Maxwell's stress tensor in the co-moving frame. Finally,

$$\dot{W}_f = -\mathrm{div}\, \mathbf{S}' + \nabla_k \dot{u}_i t'_{ik} - T'_{ik} \frac{\partial \dot{u}_i}{\partial x_k} \quad (58)$$

where

$$T'_{ik} = \frac{1}{4\pi} \left\{ \epsilon E'_i E'_k + \frac{E'^2}{2} (\epsilon_{ik} - \epsilon \delta_{ik}) + \mu H'_i H'_k + \frac{H'^2}{2} (\mu_{ik} - \mu \delta_{ik}) \right\} \cdot \quad (59)$$

Hence, one has to add the term

$$Q_i^f = S'_i - \dot{u}_k t'_{ik} = S_i - \dot{u}_i W \quad (60)$$

to the energy flux density in (43), as well as the term $-T'_{ik}$ to the momentum flux tensor Π_{ik} in (44).

The elasticity theory equation takes then the form:

$$\frac{\partial}{\partial t}(\rho \dot{u}_i) = -\frac{\partial L_{ik}}{\partial x_k} - \frac{\partial P_{ik}}{\partial x_k} + \frac{\partial T'_{ik}}{\partial x_k} - \frac{\partial g_i}{\partial t} \cdot \quad (61)$$

The electromagnetic stress tensor $\hat{T}'$ is written in the lattice frame. In L-system it has the form:

$$T_{ik} = \frac{1}{4\pi} (\epsilon E_i E_k + \mu H_i H_k) + (\epsilon_{ik} - \epsilon \delta_{ik}) \frac{E^2}{8\pi} + (\mu_{ik} - \mu \delta_{ik}) \frac{H^2}{8\pi} + \dot{u}_i G_k + \dot{u}_k G_i - \dot{u}_i g_k - \dot{u}_k g_i. \quad (62)$$

The last four terms are of the order $\dot{u}/c$ smaller, and can actually be neglected for all reasonable problems of the solid state physics.

The full system of equations of electrodynamics of crystalline dielectrics with quasiparticle excitations consists of the elasticity theory equation (61), Boltzmann equation (22) or (26) and Maxwell's equations supplemented with corresponding constitutive relations.

A significant difference between T_{ik} and the Maxwell-Abraham stress tensor is the presence of the derivatives ϵ_{ik} and μ_{ik}. In an isotropic media the operator [8]

$$2a_i^\alpha a_k^\beta \frac{\partial}{\partial g^{\alpha\beta}} \quad \rightarrow \quad \delta_{ik} \rho \frac{\partial}{\partial \rho} \cdot \quad (63)$$

5 Conclusion remarks

We derived a general nonlinear self-consistent set of equations applicable to both crystalline and homogeneous continuous media with quasiparticle excitations. Some instructive examples can be found elsewhere (see *e.g.* [8,14,15]). In particular, at $T = 0$ the Boltzmann equation can be replaced by the Schrödinger equation. The quantity $|\psi|^2$ plays then the role of the distribution function. With this ansatz the theory of Davydov solitons follows [8,10,11]. It is known that the attempts to generalize the method of Davydov to nonzero temperatures have failed. We believe that if soliton-type excitations exist at $T \neq 0$, they should be solutions of the nonlinear set of equations presented here. In addition the effect of electromagnetic fields as well as of other external forces on the soliton motion can be considered.

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