Quasimomentum in the theory of elasticity and its conservation

V. L. Gurevich* and A. Thellung
Institut für Theoretische Physik der Universität Zürich, Schönberggasse 9, CH-8001 Zürich, Switzerland
(Received 3 May 1990)

It is shown that, in the nonlinear theory of elasticity for a macroscopically homogeneous anisotropic medium, there exists, together with the energy, a vector quantity that is conserved. Its properties are investigated, and a physical interpretation is given. If one considers the dynamical interaction of the elastic strain field with the phonon gas of an ideal crystal, the sum of that vector quantity and the well-known quasimomentum (also called crystal momentum) of the phonons is conserved as long as one can neglect the umklapp processes in phonon-phonon collisions. For that reason the conserved quantity in the theory of elasticity is also called quasimomentum. Possible applications of this conservation law to various physical phenomena are mentioned.

I. INTRODUCTION

The purpose of this paper is to show that in the general, nonlinear theory of elasticity, apart from the usual integrals of the motion, there is another conservation law concerning some vector quantity which, for reasons we shall explain in detail below, we call quasimomentum. It reflects the fact that the medium is supposed to be macroscopically homogeneous in space. This conservation law is important for the description of the dynamical properties of a system of long-wavelength acoustic waves interacting via elastic anharmonicities. The interaction is described in terms of a generalized strain tensor. It is only in a *nonlinear* theory that such interactions occur.

We shall also treat the interaction of this elastic strain field with short-wavelength (thermal) phonons. (Such systems have been investigated, for instance, by Götze and Michel.[1]) The phonons will be described in terms of a distribution function $N(\mathbf{k},\mathbf{r},t)$, which is a function of wave vector $\mathbf{k}$, position in space $\mathbf{r}$, and time t, and obeys the Boltzmann equation. If umklapp processes[2] can be neglected, it will turn out that the sum of the well-known phonon quasimomentum[3,4] (also called crystal momentum[4,5]) and the quasimomentum of the elastic medium is conserved in this combined system.

On the one hand, it is interesting to investigate the interaction between a strain field and a phonon field because it permits one to study such physical phenomena as, for instance, (nonlinear) interaction between ordinary sound and second sound or phonon drag caused by an acoustic wave. On the other hand, a systematic treatment of this interaction permits one to gain more physical insight into the nature of the investigated elastic quasimomentum.

It has been shown by one of the authors[6] that phonons in a liquid can be defined as carrying (ordinary) momentum $\hbar\mathbf{k}$ (Eulerian phonons) or zero momentum (Lagrangian phonons). In contrast to this, in the considered case of a solid, where it is natural to assume that the center of mass is at rest, the net flow of mass is zero and therefore the ordinary momentum vanishes. Thus in solids the *quasi*momentum of the elastic vibrations (together with the energy) remains the only interesting integral of the motion.

We believe that Gilbert and Mollow[7] were the first to consider quasimomentum in the phenomenological theory of elasticity. Their analysis was restricted to the case of longitudinal waves in a one-dimensional system in the linear approximation. Kobussen and Paszkiewicz[8] extended the discussion of quasimomentum and ordinary momentum to three-dimensional anisotropic elastic media, but they still retained the linear approximation.

In Sec. II we start by treating the nonlinear anisotropic macroscopic elastic medium and show that, besides the energy integral, there exists a conserved vector quantity. In order to gain physical insight into its meaning, we consider in Sec. III the dynamical interaction of the elastic strain field with a gas of (thermal) phonons. We arrive at the conclusion that the conserved quantity has to be interpreted as the quasimomentum of the elastic medium. In Sec. IV the results are summarized and further examples of systems interacting with strain fields are given. Possible implications for other physical phenomena are indicated.

II. CONSERVATION LAWS IN A NONLINEAR ELASTIC MEDIUM

We start from the equation of motion[9]

$$\rho_0 \ddot{u}_i = \frac{\partial}{\partial x_l} \frac{\partial E^{(0)}}{\partial u_{i,l}} . \tag{2.1}$$

Here, x_l $(l=1,2,3)$ are the Lagrangian (material) coordinates, u_i are the components of the displacement vector, and $E^{(0)}$ is the density of the elastic energy considered to be an arbitrary function of the generalized strain tensor components $u_{i,l}=\partial u_i/\partial x_l$. ρ_0 is the *constant* mass density of the (homogeneous) medium in the space of Lagrangian variables. Here and henceforth the Einstein summation convention is applied.

A. Energy conservation

As an illustration, let us recall that energy conservation is obtained by multiplying Eq. (2.1) by $\dot{u}_i$. The familiar transformations then lead to the continuity equation

$$\frac{\partial}{\partial t}\left(\tfrac{1}{2}\rho_0 \dot{\mathbf{u}}^2 + E^{(0)}\right) + \operatorname{div}\mathbf{Q}^{(0)} = 0 , \tag{2.2}$$

where

$$Q_l^{(0)} = -\frac{\partial E^{(0)}}{\partial u_{i,l}}\dot{u}_i \tag{2.3}$$

are the components of the energy flux vector.

B. Quasimomentum conservation

We multiply Eq. (2.1) by $u_{i,n}$ and obtain

$$\rho_0 \ddot{u}_i u_{i,n} = \left[\frac{\partial}{\partial x_l}\frac{\partial E^{(0)}}{\partial u_{i,l}}\right] u_{i,n} . \tag{2.4}$$

The left-hand side of Eq. (2.4) can be written as

$$\rho_0 \ddot{u}_i u_{i,n} = \frac{\partial}{\partial t}(\rho_0 \dot{u}_i u_{i,n}) - \rho_0 \dot{u}_i \dot{u}_{i,n}$$
$$= \frac{\partial}{\partial t}(\rho_0 \dot{u}_i u_{i,n}) - \frac{\partial}{\partial x_n}\left(\tfrac{1}{2}\rho_0 \dot{u}_i^2\right) .$$

The right-hand side of Eq. (2.4) is transformed as follows:

$$\left[\frac{\partial}{\partial x_l}\frac{\partial E^{(0)}}{\partial u_{i,l}}\right] u_{i,n} = \frac{\partial}{\partial x_l}\left[\frac{\partial E^{(0)}}{\partial u_{i,l}} u_{i,n}\right] - \frac{\partial E^{(0)}}{\partial u_{i,l}}\frac{\partial^2 u_i}{\partial x_n \partial x_l}$$
$$= \frac{\partial}{\partial x_l}\left[\frac{\partial E^{(0)}}{\partial u_{i,l}} u_{i,n}\right] - \frac{\partial E^{(0)}}{\partial x_n} .$$

The result is a local conservation law

$$-\frac{\partial}{\partial t}(\rho_0 \dot{u}_i u_{i,n}) + \frac{\partial F_{nl}^{(0)}}{\partial x_l} = 0 , \tag{2.5}$$

where

$$F_{nl}^{(0)} = \frac{\partial E^{(0)}}{\partial u_{i,l}} u_{i,n} + \delta_{nl}\left(\tfrac{1}{2}\rho_0 \dot{\mathbf{u}}^2 - E^{(0)}\right) \tag{2.6}$$

is a flux tensor, and $-\rho_0 \dot{u}_i u_{i,n}$ is the density of a conserved quantity whose physical meaning will become clear in the next section when we consider the interaction of the strain field with the phonons.

The conservation law (2.5) can also be obtained with the help of Noether's theorem.[7] It is the consequence of the invariance of the Lagrangian $\mathcal{L} = \int d^3 r \left(\tfrac{1}{2}\rho_0 \dot{\mathbf{u}}^2 - E^{(0)}\right)$ with respect to a displacement in space of the deformation pattern $u_i(\mathbf{r},t)$ by an infinitesimal amount ϵ, together with a displacement of the region of integration by the same amount, i.e.,

$$u_i(\mathbf{r},t) \rightarrow u_i(\mathbf{r}-\epsilon, t), \quad \delta\mathbf{r} = \epsilon$$
$$\delta u_i = -u_{i,l}\epsilon_l, \quad \delta t = 0 .$$

This symmetry property of $\mathcal{L}$ reflects the fact that the medium is supposed to be (macroscopically) homogeneous.

The elastic energy density $E^{(0)}$ has been assumed to be a function only of the strain tensor components $\partial u_i/\partial x_l$, as is normally done in the theory of elasticity.[9] However, our analysis can be extended to cases where $E^{(0)}$ also depends on higher-order derivatives of u_i. In that case, too, a conservation law of the form (2.5) can be derived with a generalized flux tensor $F_{nl}^{(0)}$ containing additional terms.

III. INTERACTION OF PHONONS IN A CRYSTAL WITH A STRAIN FIELD

A. Phonons in a strain field

We assume the phonon frequencies Ω to depend, as usual, on the wave vector $\mathbf{k}$ and a branch index j (which we shall omit). Following Akhieser,[10] we assume that Ω also depends on space and time coordinates via the strain tensor $u_{i,l}(\mathbf{r},t)$. The latter is supposed to be slowly varying in time and space, in such a way that the following inequalities are satisfied:[11]

$$|\dot{u}_{i,l}|/|u_{i,l}| \ll \Omega, \quad \left|\frac{\partial u_{i,l}}{\partial x_k}\right| \Big/ |u_{i,l}| \ll k . \tag{3.1}$$

(The first inequality is usually referred to as the adiabatic approximation.)

Under these conditions the phonon distribution function N satisfies the Boltzmann equation[12,13,11]

$$\frac{\partial N}{\partial t} + \frac{\partial \Omega}{\partial \mathbf{k}}\frac{\partial N}{\partial \mathbf{r}} - \frac{\partial \Omega}{\partial \mathbf{r}}\frac{\partial N}{\partial \mathbf{k}} = \left[\frac{\partial N}{\partial t}\right]_{\text{coll}} . \tag{3.2}$$

The third term on the left-hand side describes the rate of change of the phonon distribution function due to the coordinate dependence of the phonon frequencies.

We consider an ideal crystal and the case of low temperatures so that the umklapp processes can be neglected. Then the right-hand side of Eq. (3.2) describes the phonon-phonon collisions in which the phonon wave vector is conserved.

B. The elastic medium in the presence of phonons

Equation (2.1) now has to be supplemented by a term describing an extra stress due to the phonon contribution, which is derived in the Appendix. This leads to the equation

$$\rho_0 \ddot{u}_i = \frac{\partial}{\partial x_l}\frac{\partial E^{(0)}}{\partial u_{i,l}} + \frac{\partial}{\partial x_l}\int d\xi_k N \frac{\partial(\hbar\Omega)}{\partial u_{i,l}} . \tag{3.3}$$

Here,

$$\int d\xi_k \equiv \sum_j \int \frac{d^3 k}{(2\pi)^3}$$

denotes integration over the phonon vectors $\mathbf{k}$ and summation over the phonon branches j.

As in Sec. II B, we multiply Eq. (3.3) by $u_{i,n}$ and obtain Eq. (2.5) with an additional term, i.e.,

$$-\frac{\partial}{\partial t}(\rho_0 \dot{u}_i u_{i,n}) + \frac{\partial F_{nl}^{(0)}}{\partial x_l} + u_{i,n}\frac{\partial}{\partial x_l}\int d\xi_k N \frac{\partial(\hbar\Omega)}{\partial u_{i,l}} = 0 . \tag{3.4}$$

This is a continuity equation with a source term due to the phonons. It can be evaluated by using Eq. (3.2).

C. Quasimomentum conservation for the combined system of the phonons and the strain field

Multiplying the Boltzmann equation (3.2) by $\hbar k_n$ and integrating over $d\xi_k$ and remembering that we assumed the wave vector to be conserved in phonon-phonon collisions, we obtain

$$\frac{\partial}{\partial t}\int d\xi_k N\hbar k_n+\frac{\partial}{\partial x_l}\int d\xi_k N\hbar k_n\frac{\partial\Omega}{\partial k_l} -\int d\xi_k \hbar k_n\frac{\partial}{\partial k_l}\left[N\frac{\partial\Omega}{\partial x_l}\right]=0 . \quad (3.5)$$

Thereby in Eq. (3.2) we have employed the identity

$$\frac{\partial\Omega}{\partial k_l}\frac{\partial N}{\partial x_l}-\frac{\partial\Omega}{\partial x_l}\frac{\partial N}{\partial k_l}=\frac{\partial}{\partial x_l}\left[N\frac{\partial\Omega}{\partial k_l}\right]-\frac{\partial}{\partial k_l}\left[N\frac{\partial\Omega}{\partial x_l}\right] .$$

The third term in Eq. (3.5) can be integrated by parts to give

$$\begin{aligned}\int d\xi_k N\frac{\partial(\hbar\Omega)}{\partial x_n}&=\int d\xi_k N\frac{\partial(\hbar\Omega)}{\partial u_{i,l}}\frac{\partial^2 u_i}{\partial x_l\partial x_n}\\&=\frac{\partial}{\partial x_l}\int d\xi_k N\frac{\partial(\hbar\Omega)}{\partial u_{i,l}}u_{i,n}\\&\quad-u_{i,n}\frac{\partial}{\partial x_l}\int d\xi_k N\frac{\partial(\hbar\Omega)}{\partial u_{i,l}} .\end{aligned}$$

Substitution of this expression for the third term in Eq. (3.5) yields

$$\begin{aligned}\frac{\partial}{\partial t}\int d\xi_k N\hbar k_n&+\frac{\partial}{\partial x_l}\int d\xi_k N\hbar k_n\frac{\partial\Omega}{\partial k_l}\\&+\frac{\partial}{\partial x_l}\int d\xi_k N\frac{\partial(\hbar\Omega)}{\partial u_{i,l}}u_{i,n}\\&-u_{i,n}\frac{\partial}{\partial x_l}\int d\xi_k N\frac{\partial(\hbar\Omega)}{\partial u_{i,l}}=0 . \quad (3.6)\end{aligned}$$

Addition of Eqs. (3.4) and (3.6) shows that the source terms cancel and we obtain the following conservation law:

$$\frac{\partial P_n}{\partial t}+\frac{\partial F_{nl}}{\partial x_l}=0 \quad (3.7)$$

with the flux tensor

$$F_{nl}=F_{nl}^{(0)}+\int d\,\xi_k N\hbar k_n\frac{\partial\Omega}{\partial k_l}+\int d\,\xi_k N\frac{\partial(\hbar\Omega)}{\partial u_{i,l}}u_{i,n} . \quad (3.8)$$

The density of the conserved quantity $\mathbf{P}$ is now given by

$$P_n=-\rho_0\dot{u}_i u_{i,n}+\int d\xi_k N\hbar k_n . \quad (3.9)$$

Clearly, the second term on the right-hand side of Eq. (3.9) is what is called quasimomentum[3,4] (or crystal momentum[4,5]) density of the phonons propagating in a crystal. This is the reason why we obviously should call the first term on the right-hand side of Eq. (3.9) the quasimomentum density of the (macroscopic) elastic medium (not to be confused with the ordinary momentum density $\rho_0\dot{u}_n$).

In a similar way, the conservation of the total energy can be derived (cf. Ref. 11 for the linear approximation)

$$\frac{\partial W}{\partial t}+\mathrm{div}\mathbf{Q}=0 , \quad (3.10)$$

with

$$W=(\tfrac{1}{2}\rho_0\dot{\mathbf{u}}^2+E^{(0)})+\int d\xi_k N\hbar\Omega , \quad (3.11)$$

$$Q_l=-\frac{\partial E^{(0)}}{\partial u_{i,l}}\dot{u}_i+\int d\xi_k N\hbar\Omega\frac{\partial\Omega}{\partial k_l}-\dot{u}_i\int d\xi_k N\frac{\partial(\hbar\Omega)}{\partial u_{i,l}} . \quad (3.12)$$

Each of the densities (3.9) and (3.11) is additively composed of two separate contributions, one stemming from the elastic medium, the other from the phonons. On the other hand, each of the fluxes (3.8) and (3.12) contains, in addition, a third term depending on both the phonon and the elastic medium variables.

IV. SUMMARY AND OUTLOOK

We have demonstrated [Eq. (2.5)] that the conservation law found by other authors in the linearized version of the theory of elasticity is in fact valid in the general nonlinear theory of anisotropic elastic media. The physical significance of this integral of motion has become clear by discussing the coupling with a gas of high-frequency phonons. It turns out to be nothing else than the quasimomentum of the elastic medium.

The same result could be obtained for a pure crystalline metal by considering the interaction of the strain field with the conduction electrons.

One might also consider a three-component system consisting of electrons and phonons interacting with each other and with an elastic strain field. If the Fermi surface is closed and the temperature is low so that the quasimomentum is conserved in electron-phonon collisions (as well as in phonon-phonon collisions), it is possible to prove conservation of the total quasimomentum of electrons, phonons, and the elastic medium.

The considerations employing quasimomentum conservation for the interaction of long-wavelength acoustic waves with conduction electrons of a metal or a semiconductor may be very useful for the analysis of such phenomena as the acoustoelectric effect, i.e., the dc current due to conduction electrons dragged along by a traveling acoustic wave. For the case of linear (intensity-independent) ultrasonic absorption, a quasimomentum-conservation analysis of this phenomenon has been carried out by Weinreich.[14] This approach, however, can also be used for intensity-dependent (nonlinear) absorption.

The same considerations can be applied to investigate an analogous effect in crystalline dielectrics. A traveling acoustic wave in the course of its absorption should transfer its energy and momentum to the phonon system.

As a result, a temperature difference may appear across a sample where the traveling acoustic wave propagates. This difference can also be analyzed in the same way as in Ref. 14, i.e., by using quasimomentum conservation.

The quasimomentum integral for the elastic strain field may prove to be useful for an even wider class of physical systems such as, e.g., amorphous dielectrics.

There, the high-frequency phonons, as a rule, cannot be described by a wave vector. However, considerations based on energy and momentum conservation can be used in regard to the elastic strain field itself.

A further example of this sort is crystalline dielectrics at high temperatures. Here the quasimomentum within the phonon system is not conserved. However, it still may be possible to describe the motion of the elastic continuum by the (nonlinear) equations of the theory of elasticity as long as the dissipative terms due to viscosity and heat conduction are negligible.

Another problem for which the quasimomentum integral may turn out to be helpful is the derivation and discussion of two-fluid equations for Lagrangian phonons.[6]

One may conclude that the analysis of the quasimomentum integral of motion in the nonlinear theory of elasticity and clear understanding of its physical origin may help to treat a number of nonequilibrium phenomena in solids.

ACKNOWLEDGMENTS

One of us (V.L.G.) wishes to express his sincere gratitude to the Institute of Theoretical Physics of Zürich University for the hospitality extended to him while the work on this paper was done and to the Schweizerischer Nationalfonds for financial support.

APPENDIX: PHONON CONTRIBUTION TO THE STRESS TENSOR

Here we are going to derive the extra term in Eq. (3.3) due to the phonons.

Let us assume that in a crystal, together with the real deformation $u_{i,l}(\mathbf{r},t)$, some virtual deformation $\delta u_{i,l}(\mathbf{r},t)$ is created. The latter is supposed to be created during a time interval δt short enough for the real deformation to remain unchanged. This means in fact that we consider a virtual deformation in the presence of a *constant* real deformation. The virtual deformation is supposed to obey the inequalities (3.1).

Our purpose is to calculate the variation of the total energy $\mathcal{E}^{(\mathrm{ph})}$ of the phonons linear in $\delta u_{i,l}$. This can be written as

$$\delta\mathcal{E}^{(\mathrm{ph})}=\int d^3r\,\sigma_{il}^{(\mathrm{ph})}\delta u_{i,l}\ . \tag{A1}$$

We are going to express it in terms of the phonon distribution function N and thus find the phonon contribution to the stress tensor, $\sigma_{il}^{(\mathrm{ph})}$.

The derivation proceeds along the same lines as in Ref. 11, with the difference that the phonon frequencies Ω are now considered to be nonlinear functions of the generalized strain $u_{i,l}$, while the tensor $\sigma_{il}^{(\mathrm{ph})}$ is, in general, asymmetric (cf. Ref. 9).

The energy of the phonon system is given by

$$\mathcal{E}^{(\mathrm{ph})}=\int d^3r\int d\xi_k\,\hbar\tilde{\Omega}\tilde{N}\ , \tag{A2}$$

where $\tilde{N}$ and $\tilde{\Omega}$ are the phonon distribution function and the phonon frequency in the presence of both the real and the virtual deformation.

The change in the energy of the phonon system caused by the virtual deformation during a time interval δt is given by

$$\delta\mathcal{E}^{(\mathrm{ph})}=\int_0^{\delta t}dt\,\dot{\mathcal{E}}^{(\mathrm{ph})}=\int_0^{\delta t}dt\int d^3r\int d\xi_k\,\hbar(\dot{\tilde{\Omega}}\tilde{N}+\tilde{\Omega}\dot{\tilde{N}})\ . \tag{A3}$$

According to our assumptions the virtual deformation is slow enough that the first inequality (3.1) is satisfied. Then it does not change directly the occupation numbers of the phonon states. Indeed, the occupation numbers $\tilde{N}$ are adiabatic invariants that remain unchanged under the action of slow perturbations.

In such a case, the change of the phonon distribution, $\dot{\tilde{N}}$, can be found from the Boltzmann equation

$$\dot{\tilde{N}}+\frac{\partial\tilde{\Omega}}{\partial\mathbf{k}}\frac{\partial\tilde{N}}{\partial\mathbf{r}}-\frac{\partial\tilde{\Omega}}{\partial\mathbf{r}}\frac{\partial\tilde{N}}{\partial\mathbf{k}}=\left[\frac{\partial\tilde{N}}{\partial t}\right]_{\mathrm{coll}}\ .$$

It follows from this equation that the integral of the second term in the parentheses of Eq. (A3) vanishes. Indeed, the term

$$\int d\xi_k\,\hbar\tilde{\Omega}\left[\frac{\partial\tilde{N}}{\partial t}\right]_{\mathrm{coll}}$$

is zero because of conservation of the total energy of the phonon system under phonon-phonon (as well as phonon-defect) collisions. The difference

$$-\hbar\tilde{\Omega}\frac{\partial\tilde{\Omega}}{\partial\mathbf{k}}\frac{\partial\tilde{N}}{\partial\mathbf{r}}+\hbar\tilde{\Omega}\frac{\partial\tilde{\Omega}}{\partial\mathbf{r}}\frac{\partial\tilde{N}}{\partial\mathbf{k}}$$

can be written as

$$-\frac{\hbar}{2}\frac{\partial}{\partial\mathbf{r}}\left[\frac{\partial\tilde{\Omega}^2}{\partial\mathbf{k}}\tilde{N}\right]+\frac{\hbar}{2}\frac{\partial}{\partial\mathbf{k}}\left[\frac{\partial\tilde{\Omega}^2}{\partial\mathbf{r}}\tilde{N}\right]\ .$$

The integral of the first term over d^3r is transformed into the surface integral of the normal component of the energy flux carried by the phonons. We assume it to vanish. In the second term, the integral over the volume of the first Brillouin zone,

$$\int d^3k\frac{\partial}{\partial\mathbf{k}}\left[\frac{\partial\tilde{\Omega}^2}{\partial\mathbf{r}}\tilde{N}\right]\ ,$$

is transformed into an integral over its surface. It vanishes if one takes into account periodicity of the integrand as a function of $\mathbf{k}$ at opposite faces of the Brillouin zone.

Now we are going to calculate the contribution of the first term in the parentheses of Eq. (A3). In this term, we should replace $\tilde{N}$ by the actual phonon distribution function, N, since we are interested only in the linear terms in

$\delta u_{i,l}$. Integrating over time, we have

$$\delta\mathcal{E}^{(\mathrm{ph})}=\int d^3r\int d\xi_k\hbar\delta\Omega N ,$$

where

$$\delta\Omega=\frac{\partial\Omega}{\partial u_{i,l}}\delta u_{i,l} .$$

Comparison with Eq. (A1) yields

$$\sigma_{il}^{(\mathrm{ph})}=\int d\xi_k\hbar N\frac{\partial\Omega}{\partial u_{i,l}} . \tag{A4}$$

Thus, the extra term to be added in Eq. (3.3) turns out to be

$$\frac{\partial\sigma_{il}^{(\mathrm{ph})}}{\partial x_l}=\frac{\partial}{\partial x_l}\int d\xi_k N\frac{\partial(\hbar\Omega)}{\partial u_{i,l}} . \tag{A5}$$

*Permanent address: A. F. Ioffe Institute for Physics and Engineering, 194021 Leningrad, U.S.S.R.

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