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DYNAMICS THEORY OF QUANTUM CRYSTALS WITH DELOCALIZED DEFECTS

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1. INTRODUCTION

Quantum crystal is a really unique object possessing simultaneously properties typical of solids and liquids. On a parallel with the presence of a crystal lattice, a "percolation" of point defects (vacancies, impurities, etc.) is observed owing to their delocalization and transformation into quasiparticles (defectons /1-3/ or mass-fluctuation waves /4/). Such delocalized defects are characterized not by their lattice positions (or coordinates), but by their quasimomentum k and dispersion law $\mathcal{E}(k)$. In deriving the quantum crystal dynamics, the role of the defecton excitations can be important and has to be taken into account. A phenomenological set of hydrodynamics equations of defect quantum crystals has been considered by Andreev and Lifshitz /1/ and Liu /5/ when treating the problem of superfluidity. Following Landau an equation for superflow has been added. However, the pure hydrodynamic approach used in these works is not able to take into account the specific features in the quasiparticle gas behaviour. A nondissipative set of hydrodynamics equations, in which the role of the defecton gas quasimomentum and dispersion law is accounted for, has been obtained by the author /6/ and the possibility of defecton second sound propagation has been cosidered.

The purpose of this work is to derive the exact nonlinear set of equations consisting of bonded equations of the elasticity theory and the kinetic equation for the quasiparticle gas. An equation of motion for the quasimomentum density in nonstationarily deformed periodic structure is extracted. The results obtained may be applied also to a wide class of problems when uncharged quasiparticle behaviour in deformable dielectric crystals is studied.

2. NONLINEAR ELASTICITY THEORY OF AN IDEAL CRYSTAL

In deriving the nonlinear theory of elasticity, it is convenient to introduce a local frame with bases vectors $\vec{a}_\alpha$ (α = 1,2,3) which coincide with the lattice translation vectors. In such a description each lattice site is determined by three coordinate numbers N^α indicating the number of steps (each equal to the local value of $\vec{a}_\alpha(\vec{r},t)$) along the coordinate axes to the lattice site (compare also with [7]). Then, the vector between two lattice sites separated at a fixed moment in time by a distance large compared to the lattice constant but small compared to the characteristic variations in space may be written in the form

$$d\vec{r} = \vec{a}_\alpha dN^\alpha. \tag{1}$$

The time evolution of $\vec{a}_\alpha$ can be obtained from plain geometrical considerations and may be expressed by the following equation:

$$\dot{\vec{a}}_\alpha + (\dot{\vec{u}}\nabla)\vec{a}_\alpha - (\vec{a}_\alpha\nabla)\dot{\vec{u}} = 0, \tag{2}$$

where $\vec{u}(\vec{r},t)$ is the displacement vector.

Equation (2) automatically conserves $\vec{a}_\alpha$-vector lines. In fact, the $\vec{a}_\alpha$-line conservation condition consists in collinearity of $\vec{a}_\alpha$ to the left-hand side of (2), which is obviously satisfied.

If the crystal lattice is free of dislocations, the functions $N^\alpha(\vec{r},t)$ introduced are one-valued and equation (2) describes completely the evolution of the lattice configuration. The presence of delocalized defects (e.g., vacancions) does not change the method of description because the lattice sites remain to be well defined.

Let us introduce also the reciprocal lattice vectors $\vec{a}^\alpha$. They satisfy the conditions

$$\vec{a}^\alpha \vec{a}_\beta = \delta_{\alpha\beta}, \qquad a^\alpha_i a_{\alpha k} = \delta_{ik}. \tag{3}$$

Making use of (3) one can rewrite (1) in the form

$$\vec{a}^\alpha d\vec{r} = dN^\alpha$$

and therefore the reciprocal vectors $\vec{a}^\alpha$ can be expressed by means of coordinate functions N^α:

$$\vec{a}^\alpha = \nabla N^\alpha. \tag{4}$$

Multiplying (2) by $\vec{a}^\alpha$ and taking into account (3) and (4) yield the evolution equation for $\vec{a}^\alpha$:

$$\dot{\vec{a}}^\alpha + \nabla(\vec{a}^\alpha \dot{\vec{u}}) = 0 \tag{5}$$

and the expression for the deformation velocity

$$\dot{\vec{u}} = -\vec{a}_\alpha \dot{N}^\alpha. \tag{6}$$

For later convenience introduce also the metrical tensor $g_{\alpha\beta} = \vec{a}_\alpha \vec{a}_\beta$ and its reciprocal tensor $g^{\alpha\beta} = \vec{a}^\alpha \vec{a}^\beta$. Then the lattice cell volume is equal to $\sqrt{g}$, where $g = det|g_{\alpha\beta}|$.

In this notation the density of an ideal (free of defects) crystal may be written in the form

$$\rho_0 = M/\sqrt{g}$$

(M being the total mass of the cell atoms). The equation of continuity can be now obtained by time differentiation of ρ_0. Making use of the identity

$$dg = -g\, g_{\alpha\beta}\, dg^{\alpha\beta} \tag{7}$$

and of equations (2-5) yields

$$\rho_0 + div\, \vec{j} = 0, \tag{8}$$

where the mass current $\vec{j} = \rho_0 \dot{\vec{u}}$.

The fluxes of energy $\vec{Q}$ and momentum $\tilde{\Pi}_{ik}$ can be derived following the standard procedure. The continuity equation (8), the momentum conservation law

$$\frac{\partial j_i}{\partial t} + \frac{\partial \tilde{\Pi}_{ik}}{\partial x_k} = 0, \tag{9}$$

and the law of increase of entropy

$$\dot{S} + div(S\dot{\vec{u}} + \vec{q}/T) = R/T \tag{10}$$

(where R is the dissipative function) have to be consistent with the redundant energy conservation law

$$\dot{E} + div\, \vec{Q} = 0. \tag{11}$$

The energy E in the laboratory system is a sum of the kinetic energy and the internal energy E_0 supposed to be a function of metrical tensor components $g^{\alpha\beta}$ and entropy. Hence,

$$\dot{E} = \frac{1}{2}\frac{\partial}{\partial t}(\rho_0 \dot{u}^2) + T\dot{S} - \frac{1}{2}\sigma_{\alpha\beta}\dot{g}^{\alpha\beta}, \tag{12}$$

where

$$\sigma_{\alpha\beta} = -2\left(\frac{\partial E_0}{\partial g^{\alpha\beta}}\right)_S.$$

Time derivatives of the kinetic energy and entropy can be replaced by space derivatives according to (8) and (10). The last term in (12) is transformed by means of (5):

$$\frac{1}{2}\sigma_{\alpha\beta}\,\dot g^{\alpha\beta} = \sigma_{\alpha\beta}\, a_i^{\beta}\Big(v_k \frac{\partial a_i^{\alpha}}{\partial x_k} + a_k^{\alpha}\frac{\partial \dot u_k}{\partial x_i}\Big). \tag{13}$$

On the other hand

$$\nabla_k E_0 = -\sigma_{\alpha\beta}\,\vec a^{\beta}\,\nabla_k \vec a^{\alpha} + T\nabla_k S. \tag{14}$$

Using (13) and (14) yields

$$\dot E_0 = T(\dot S + \mathrm{div}(S\dot{\vec u})) - \mathrm{div}(E_0\dot{\vec u}) + (\sigma_{\alpha\beta} + F g_{\alpha\beta})\,a_i^{\alpha} a_k^{\beta}\frac{\partial \dot u_i}{\partial x_k},$$

where $F = E - TS$ is the Helmholtz free energy per unit volume, equal (up to a sign) in virtue of the Duhem-Gibbs relation to the pressure ($P = -F$). Finally, the energy conservation law (12) takes the form

$$\dot E + \nabla_k\Big\{\frac{1}{2}\rho_0\dot u^2\dot u_k + \dot u_i(\tilde\Pi_{ik} - \rho\dot u_i\dot u_k + E_0\delta_{ik}) + q_k\Big\} =$$

$$= R + \vec q\,\frac{\nabla T}{T} + \Big\{\tilde\Pi_{ik} - \rho_0\dot u_i\dot u_k + F\delta_{ik} + \sigma_{\alpha\beta}a_i^{\alpha}a_k^{\beta}\Big\}\frac{\partial \dot u_i}{\partial x_k}.$$

Hence the flux of momentum has the form

$$\tilde\Pi_{ik} = \rho_0\dot u_i\dot u_k - (\sigma_{\alpha\beta} + F g_{\alpha\beta})\,a_i^{\alpha}a_k^{\beta} + \pi_{ik}$$

and the energy current is given by the expression

$$\vec Q = \frac{1}{2}\rho_0\dot u^2\dot{\vec u} + \vec a^{\alpha}(\vec a^{\beta}\dot{\vec u})\,\sigma_{\alpha\beta} + TS\dot{\vec u} + \vec q.$$

The dissipative function has the usual form

$$R = -\vec q\,\frac{\nabla T}{T} - \pi_{ik}\frac{\partial \dot u_i}{\partial x_k}.$$

It follows from the symmetry of $\tilde\Pi_{ik}$ that π_{ik} is also symmetric, and therefore, R depends only on the symmetric part of $\partial\dot u_i/\partial x_k$ i.e., on $\dot u_{ik} \equiv \frac{1}{2}\Big(\frac{\partial \dot u_i}{\partial x_k} + \frac{\partial \dot u_k}{\partial x_i}\Big).$

Due to the Onsager symmetry principle the dissipative function takes finally the form

$$R = \varkappa_{ik}\frac{\partial T}{\partial x_i}\frac{\partial T}{\partial x_k} + \eta_{iklm}\,\dot u_{ik}\,\dot u_{lm},$$

where $\varkappa_{ik}$ and η_{iklm} are positive definite matricies. We shall not examine here their properties in detail.

3. KINETIC EQUATION

The kinetic equation for the defecton distribution function $f(\vec p, \vec z, t)$ in the laboratory system has the form

$$\frac{\partial f}{\partial t} + \frac{\partial f}{\partial \vec z}\frac{\partial H}{\partial \vec p} - \frac{\partial f}{\partial \vec p}\Big(\frac{\partial H}{\partial \vec z} - \vec F\Big) = \hat I(f), \tag{15}$$

where $\hat I(f)$ is the collision integral, $\vec p$ is the defecton "quasi-momentum" (see below), $\vec F$ are external forces, and H is the Hamiltonian function.

Here some explanations have to be made, concerning the description of every quasiparticle gas in a deformable periodic structure. Strictly speaking, quasiwave vector and dispersion law (as a periodical function of the quasimomentum) may be introduced only in the case of an ideal periodic lattice. However,the dispersion law is established whitin a distance of several lattice constants while the scale of deformations is always large compared to interatomic distances. That is why in every small volume ("point") one can determine a local dispersion law in the comoving system as a function of the local value of quasimomentum defined by local lattice translation vectors $\vec a_{\alpha}(\vec z, t)$. In this sense the quantity $\vec p$ being the canonically conjugate to the coordinates $\vec z$ is not a real quasimomentum of any quasiparticle. It is of interest therefore to derive a kinetic equation containing as a variable the excitation quasimomentum $\vec k$ conjugate canonically to the "discrete coordinate" N^{α} (compare with /8/). Note also that the energy of the quasiparticle must be a periodic function of k both in the laboratory system and in the comoving local frame, and the kinetic equation has to be invariant under a shift $\vec k \to \vec k + 2\pi\vec a^{\alpha}$. Unfortunately, all these circumstances have not been correctly accounted for in the most previous works (see,e.g., /9-10/). As a result, the kinetic equation turned out to be inconsistent with the conservation laws, a dificulty hindering the derivation of a nonlinear selfconsistent theory. In linear theories such a difficulty has been overcome by introducing artificially some terms in quasiparticle energy breaking in this way the Galilean transformations for the mean energy.

To derive a consistent theory along the lines mentioned above, one has to keep in mind that the translation vectors $\vec{a}_\alpha$ and the velocity of deformation vary slowly in space in time. Therefore, the Hamiltonian and the energy of a quasiparticle in the laboratory system may be obtained (analogously to the hydrodynamic fluxes) from their values in the comoving system by considering formally $\vec{a}_\alpha$ and $\dot{\vec{u}}$ as constants, i.e., with the help of Galilean transformations. This leads to the following expression for the energy:

$$\mathcal{E} = \varepsilon(\vec{k}, g^{\alpha\beta}) + m\dot{\vec{u}}\frac{\partial\varepsilon}{\partial\vec{k}} + \frac{m\dot{u}^2}{2}, \tag{16}$$

where ε and $\mathcal{E}$ are the energy values in the comoving and laboratory systems respectively, m is the mass of a defect (in the case of vacancies $m = -m_0$, m_0 being the atomic mass), and $m\,\partial\varepsilon/\partial\vec{k}$ is the mean defecton momentum (mass current) in the comoving system. Obviously, $\mathcal{E}$ has the same periodicity in k-space as the dispersion law in the local frame $\varepsilon(\vec{k}, g^{\alpha\beta})$.

In contrast to the energy and all other physical quantities (f , mass and moment fluxes, etc.) the Hamiltonian $H(\vec{p},\vec{r},t)$ is not necessarily periodic in k-space. Moreover, the invariance of the kinetic equation required can be reached only with the help of a nonperiodic H . The Hamiltonian has only to generate right equations of motion and its choice, in general, is not unique. Since in the comoving local frame the Hamiltonian coincides with the dispersion law $\varepsilon(\vec{k}, g^{\alpha\beta})$, $H(\vec{p},\vec{r},t)$ may be obtained by a canonical transformation with the substitution function

$$\Phi = (\vec{p} - m\vec{v})\vec{r}_0 + (\vec{p} - \tfrac{1}{2}m\vec{v})\vec{v}t \tag{17}$$

corresponding to the "Galilean transformations"

$$\vec{r} = \vec{r}_0 + \vec{v}t \quad , \quad \vec{k} = \vec{p} - m\vec{v}.$$

As a result

$$H = \varepsilon(\vec{p} - m\vec{v}, g^{\alpha\beta}) + \vec{p}\vec{v} - \tfrac{1}{2}mv^2. \tag{18}$$

Where $\vec{v} \equiv \dot{\vec{u}}(\vec{r},t)$ and $\vec{r}_0$ are coordinates in the comoving system. A comparison of (18) and (16) gives the relationship

$$H = \mathcal{E} + (\vec{p} - m\frac{\partial\varepsilon}{\partial\vec{p}})\dot{\vec{u}} - \tfrac{1}{2}m\dot{u}^2. \tag{19}$$

If the velocity of deformation $\dot{\vec{u}}$ is small enough, (18) gives in the linear approximation the expression

$$\tilde{H} = \varepsilon(\vec{p}, g^{\alpha\beta}) + (\vec{p} - m\frac{\partial\varepsilon}{\partial\vec{p}})$$

obtained first by Landau, and used in many works as exact one. However, $m\dot{\vec{u}}$ is not necessarily small, and in the case of a defecton gas can be large due to the big atomic mass m.

Having derived H and $\mathcal{E}$ as functions of $\vec{p}, \vec{r}, t$, and $\vec{p}$, $\vec{r}$ as functions of $\vec{k}$ and $\vec{r}_0$ we have, in fact, completely defined the kinetic equation (15).

To write the kinetic equation in an invariant form with respect to a shift by a reciprocal lattice constant let us introduce an "invariant quasimomentum" with components k_α measured in units of the reciprocal lattice periods $\vec{a}^\alpha$. So

$$k_\alpha = \vec{k}\vec{a}_\alpha = \vec{a}_\alpha(\vec{p} - m\dot{\vec{u}})$$

$$\vec{k} = k_\alpha \vec{a}^\alpha.$$

In these variables (canonically conjugate to coordinate functions N^α, not to $\vec{r}$) the Hamiltonian takes the form

$$H = \varepsilon(k_\alpha, g^{\alpha\beta}) + k_\alpha \vec{a}^\alpha \dot{\vec{u}} + \tfrac{1}{2}m\dot{u}^2. \tag{20}$$

To transform equation (15) the following relations are useful:

$$\frac{\partial f}{\partial\vec{p}} = \frac{\partial f}{\partial k_\alpha}\vec{a}_\alpha$$

$$\left(\frac{\partial f}{\partial t}\right)_{\vec{p}} = \left(\frac{\partial f}{\partial t}\right)_{k_\alpha} + \frac{\partial f}{\partial k_\alpha}\left\{k_\beta \vec{a}_\alpha \nabla(\vec{a}^\beta\dot{\vec{u}}) - m\ddot{\vec{u}}\vec{a}_\alpha\right\}$$

$$\left(\frac{\partial H}{\partial\vec{r}}\right)_{\vec{p}} = \left(\frac{\partial H}{\partial\vec{r}}\right)_{k_\alpha} + \frac{\partial H}{\partial k_\alpha}\left\{k_\beta a^\beta_\kappa \nabla a_{\alpha\kappa} - m a_{\alpha\kappa}\nabla\dot{u}_\kappa\right\}$$

$$\frac{\partial H}{\partial\vec{p}} = \vec{a}_\alpha\frac{\partial\varepsilon}{\partial k_\alpha} + \vec{a}_\alpha(\dot{\vec{u}}\vec{a}_\alpha).$$

After further transformations the kinetic equation (15) takes the form:

$$\frac{df}{dt} + \vec{a}_\alpha\frac{\partial\varepsilon}{\partial k_\alpha}\left(\frac{\partial f}{\partial\vec{r}}\right)_{k_\alpha} - \frac{\partial f}{\partial k_\alpha}\left\{m\frac{d\dot{\vec{u}}}{dt} + \left(\frac{\partial\varepsilon}{\partial\vec{r}}\right)_{k_\alpha} - m\frac{\partial\varepsilon}{\partial k_\beta}[\vec{a}_\beta\,\mathrm{rot}\,\dot{\vec{u}}] - \vec{F}\right\} = \hat{I}(f), \tag{21}$$

where $\frac{d}{dt} = \frac{\partial}{\partial t} + (\dot{\vec{u}}\nabla)$.

The term $\frac{d\dot{u}}{dt}$ takes into account the noninertial moving of the local frame in a quite natural way.

In this form the kinetic equation does not contain any non-periodic terms. Note, that according to (18) the quasiparticle velocity $\vec{v} = \partial H/\partial \vec{p}$ is also periodic in $\vec{p}$ and, therefore, the external forces $\vec{F}$ in (21) may be dependent on the velocity and its derivatives.

Further it will be necessary to integrate diverse physical quantities over the Brillouin zone, to transform such integrals by parts as well as to perform differentiation with respect to time and space. However the Brillouin zone boundaries in our case are also space and time dependent and, therefore, the differentiation does not commutate with integrating over the Brillouin zone. This can be of great importance in nonequilibrium systems as well as at high temperatures compared to the energy band width. In such cases, typical of defecton gases in quantum crystals, the distribution function values on the boundaries are nonvanishing, and noncommutativity may not be neglected. This inconvenience can be eliminated by introducing the renormalized distribution function $\varphi = f/\sqrt{g}$. By means of formulae (2,4,5,7) the kinetic equation takes the form

$$\dot{\varphi} + div\left\{\left(\dot{\vec{u}} + \vec{a}_\alpha \frac{\partial \varepsilon}{\partial K_\alpha}\right)\varphi\right\} - \frac{\partial}{\partial K_\alpha}\left\{\varphi \vec{a}_\alpha \left(\nabla\varepsilon - m\frac{d\dot{\vec{u}}}{dt}\right) - m\varphi\frac{\partial \varepsilon}{\partial K_\beta}[\vec{a}_\alpha \vec{a}_\beta]\, rot\, \dot{\vec{u}} - \vec{a}_\alpha \vec{F}\right\} = \hat{I}(\varphi) \quad (22)$$

In this notation the differentiation with respect to t and $\vec{r}$ is carried out at constant K_α and, hence, commutates with $\int d^3K_\alpha$. The result obtained by such a procedure can easily by rewritten in the previously adopted variables by the substitution

$$\vec{a}_\alpha \frac{\partial}{\partial K_\alpha} \rightarrow \frac{\partial}{\partial \vec{K}} \rightarrow \frac{\partial}{\partial \vec{p}} .$$

The corresponding integrals over the Brillouin zone are transformed as follows:

$$\langle f\ldots\rangle \equiv \int \frac{d^3p}{(2\pi\hbar)^3} f(\vec{p},\vec{r},t)\ldots = \frac{1}{\sqrt{g}}\int\frac{d^3K_\alpha}{(2\pi\hbar)^3} f(K_\alpha,\vec{r},t)\ldots = \int\frac{d^3K_\alpha}{(2\pi\hbar)^3}\varphi\ldots \equiv \langle\!\langle \varphi \rangle\!\rangle . \quad (23)$$

In the same way

$$\int d^3r\ldots = \int d^3N^\alpha \sqrt{g}\ldots$$

It follows from all the above considerations that the right results may be obtained also directly from (15) or (21) if all fluxes through the Brillouin zone boundaries appearing as a result of integrating by parts formally equal zero in spite of the nonperiodic form of the integrand. By way of illustration let us calculate the time derivative of the defecton energy

$$\frac{\partial}{\partial t}\langle \varepsilon f\rangle = \langle\!\langle \dot{\varepsilon}\varphi \rangle\!\rangle + \langle\!\langle \varepsilon\dot{\varphi} \rangle\!\rangle ,$$

where

$$\dot{\varepsilon} = \left(\frac{\partial \varepsilon}{\partial t}\right)_{K_\alpha} = \frac{1}{2}\lambda_{\alpha\beta}\dot{g}^{\alpha\beta} = -\lambda_{\alpha\beta}a_i^\alpha a_K^\beta \frac{\partial \dot{u}_i}{\partial x_K} - \dot{\vec{u}}(\nabla\varepsilon)_{K_\alpha}$$

$$\lambda_{\alpha\beta} = 2\frac{\partial \varepsilon}{\partial g^{\alpha\beta}} = \lambda_{\beta\alpha}$$

and $\dot{\varphi}$ is given by (22).

Consequently

$$\frac{\partial}{\partial t}\langle \varepsilon f\rangle = \langle\!\langle \varepsilon\hat{I}(\varphi)\rangle\!\rangle - div\left\{\dot{\vec{u}}\langle\!\langle \varepsilon\varphi\rangle\!\rangle + \vec{a}_\alpha\langle\!\langle \varphi\varepsilon\frac{\partial\varepsilon}{\partial K_\alpha}\rangle\!\rangle\right\} + \vec{a}_\alpha\langle\!\langle \vec{F}\frac{\partial\varepsilon}{\partial K_\alpha}\varphi\rangle\!\rangle -$$

$$- m\ddot{\vec{u}}\vec{a}_\alpha\langle\!\langle \frac{\partial\varepsilon}{\partial K_\alpha}\varphi\rangle\!\rangle - \frac{\partial\dot{u}_i}{\partial x_K}\left\{m\dot{u}_K a_{\alpha i}\langle\!\langle \frac{\partial\varepsilon}{\partial K_\alpha}\varphi\rangle\!\rangle + a_i^\alpha a_K^\beta\langle\!\langle \lambda_{\alpha\beta}\varphi\rangle\!\rangle\right\} =$$

$$= \langle \varepsilon\hat{I}(f)\rangle - div\left\{\dot{\vec{u}}\langle \varepsilon f\rangle + \vec{a}_\alpha\langle \varepsilon\frac{\partial\varepsilon}{\partial K_\alpha}f\rangle\right\} + \vec{a}_\alpha\langle \vec{F}\frac{\partial\varepsilon}{\partial K_\alpha}f\rangle - \quad (24)$$

$$- m\ddot{\vec{u}}\langle \frac{\partial\varepsilon}{\partial\vec{p}}f\rangle - \frac{\partial\dot{u}_i}{\partial x_K}\left\{m\dot{u}_K\langle \frac{\partial\varepsilon}{\partial p_i}f\rangle + \langle \lambda_{\alpha\beta}f\rangle a_i^\alpha a_K^\beta\right\} .$$

4. CONSERVATION LAWS AND DYNAMICS EQUATIONS

The equation of continuity for the defecton gas follows directly from the kinetic equation (22). Integrating yields:

$$m\dot{n} + div\,\vec{J}_0 = 0 . \quad (25)$$

where $n = \langle\!\langle \varphi\rangle\!\rangle = \langle f\rangle$ is the defecton number density and the quasiparticle gas momentum density (mass current) is equal to

$$\vec{J}_0 = mn\dot{\vec{u}} + \vec{j}_0 , \quad \vec{j}_0 = m\langle \frac{\partial\varepsilon}{\partial\vec{p}}f\rangle . \quad (26)$$

The total mass current is

$$\vec{J} = \vec{J}_0 + \vec{j} = \rho\dot{\vec{u}} + \vec{j}_0 ,$$

where $\rho = \rho_0 + mn$ is the density of the crystal.

To derive a selfconsistent closed set of dynamics equations, momentum and energy fluxes Π_{iK} and $\vec{Q}$ have to be defined. Following the standard procedure described briefly in Sec.1 , we write down the conservation laws

$$\dot{J}_i + \nabla_K \Pi_{iK} = 0 , \tag{27}$$

$$\dot{E} + div\,\vec{Q} = 0 , \tag{28}$$

where the total energy E is of the form

$$E = \frac{1}{2}\rho_o \dot{u}^2 + E_o(g^{\alpha\beta}) + \langle \mathcal{E} f \rangle \tag{29}$$

with $\mathcal{E}$ given by (16). In view of further applications to quantum crystals at low temperatures when the main contribution to the entropy is due to defectons the strain energy $E_o(g^{\alpha\beta})$ is supposed to depend only on the metrical tensor components. Differentiating (29) with respect to time and replacing all time derivatives by space derivatives with the help of equations (8),(22),(24) and (27) yilds after some transformations

$$\dot{E} + \nabla_K \Big\{ \frac{1}{2}\rho\dot{u}^2\dot{u}_K + \dot{u}_i\big[\Pi_{iK} - \rho\dot{u}_i\dot{u}_K + E_o\delta_{iK} + \langle\varepsilon f\rangle\delta_{iK}\big] - $$
$$- \frac{1}{2}m\dot{u}^2\langle\frac{\partial\varepsilon}{\partial p_K} f\rangle + \langle\varepsilon\frac{\partial\varepsilon}{\partial p_K} f\rangle \Big\} = \langle\varepsilon\hat{I}(f)\rangle +$$
$$+ \frac{\partial\dot{u}_i}{\partial x_K}\Big\{\Pi_{iK} - \rho\dot{u}_i\dot{u}_K + \sigma_{\alpha\beta}a_i^\alpha a_K^\beta - \langle\lambda_{\alpha\beta}f\rangle a_i^\alpha a_K^\beta + E_o\delta_{iK} - \dot{u}_i j_{oK} - \dot{u}_K j_{oi}\Big\}.$$

Comparing this equation with (28) gives unambiguously the fluxes in the form

$$\Pi_{iK} = -(\sigma_{\alpha\beta} + E_o g_{\alpha\beta} - \langle\lambda_{\alpha\beta}f\rangle)a_i^\alpha a_K^\beta + \rho\dot{u}_i\dot{u}_K + \dot{u}_i j_{oK} + \dot{u}_K j_{oi} \tag{30}$$

$$\vec{Q} = \dot{\vec{u}}\Big(\rho\frac{\dot{u}^2}{2} + \langle\varepsilon f\rangle + \dot{\vec{u}}\vec{j}_o\Big) + \vec{a}^\alpha(\vec{a}^\beta\dot{\vec{u}})(\langle\lambda_{\alpha\beta}f\rangle - \sigma_{\alpha\beta}) + \langle f\frac{\partial\varepsilon}{\partial\vec{p}}(\varepsilon - \frac{m}{2}\dot{u}^2)\rangle. \tag{31}$$

Therefore, the exact complete nonlinear set of equations consists of the equation of continity (8), the kinetic equation and equations (27) with Π_{iK} given in (30). The equations of the theory of elasticity follow from (27) :

$$\frac{\partial}{\partial t}(\rho\dot{u}_i) = -\frac{\partial\Pi_{iK}}{\partial x_K} - \frac{\partial j_{oi}}{\partial t} . \tag{32}$$

The second term in the right-hand side written in the form of a time derivative of the quasiparticle current $\vec{j}_o$ cannot be expressed as a divergence of any tensor. It represents the driving force acting upon the lattice by defectons. The term $\langle\lambda_{\alpha\beta}f\rangle$ describes mainly the defecton contribution to the elastic constant tensor and may be called the deformation force.

In the case when defectons are the only quasiparticles, only defecton-defecton collisions take place and energy is conserved. In this case $\langle\varepsilon\hat{I}\rangle = 0$ and the equilibrium distribution function can be obtained from the entropy maximum condition at conserved energy and quasiparticle number (if conserved). If defectons obey the Bose-Einstein statistics this leads to

$$f_o = \Big(exp\big(\frac{\varepsilon-\mu}{T}\big) - 1\Big)^{-1}. \tag{33}$$

In the zero order approximation with respect to defecton mean free path ℓ , the solution of the kinetic equation is given by the local equilibrium function $f_o(\varepsilon-\mu(\vec{r},t))$. In this approximation $\vec{j}_o = 0$, defectons are carried by the lattice, and their effect reduces to changing of the strain constants. Equation (32) takes then the form

$$\frac{\partial}{\partial t}(\rho\dot{u}_i) = \frac{\partial\Sigma_{iK}}{\partial x_K} ,$$

where

$$\Sigma_{iK} = (\sigma_{\alpha\beta} + E_o g_{\alpha\beta} - \langle\lambda_{\alpha\beta}f\rangle)a_i^\alpha a_K^\beta .$$

If the defecton quasimomentum is also conserved (due to the non-effective umclapp collisions), the local-equilibrium function is of the form /6/:

$$\tilde{f} = f_o(\varepsilon - \vec{p}\vec{V} - \mu) . \tag{34}$$

Then, in first approximation with respect to small $\vec{V}$

$$j_{oi} = -mV_K\langle p_K\frac{\partial\varepsilon}{\partial p_i}\frac{\partial f_o}{\partial\varepsilon}\rangle = mnV_i .$$

Substituting into (32) shows that in a statically deformed crystal defectons are subjected to a force

$$mn\dot{V}_i = \frac{\partial\Sigma_{iK}}{\partial x_K} ,$$

5. QUASIMOMENTUM EQUATION OF MOTION

Since quasimomentum is a characteristic of great importance, it is of interest to derive an equation of its behaviour. Multiplying (22) by $\vec k$ and integrating over the Brillouin zone yield

$$\dot P_i + \nabla_k\left(L_{ik} + P_i \dot u_k\right) - \langle \varepsilon \nabla_i f\rangle = \langle p_i \hat I(f)\rangle , \tag{35}$$

where $\vec P = \langle \vec p f\rangle$ is the quasimomentum density, and

$$L_{ik} = \langle p_i \frac{\partial \varepsilon}{\partial p_k} f\rangle + \langle \varepsilon f\rangle \delta_{ik}$$

may be called the quasimomentum flux tensor. This tensor is diagonal independently of the dispersion law and lattice symmetry because the energy is invariant under trasformation $\vec k \to -\vec k$ due only to the time inverse symmetry. If the deviation of the distribution function from the equilibrium one is small L_{ik} can be expressed by the thermodynamics function $\Omega(T,\mu)$ /6/. Making use of the local distribution function (34) yields after integrating by parts:

$$\langle p_i \frac{\partial \varepsilon}{\partial p_k} f\rangle = T\langle \ln(1+f)\rangle \delta_{ik} = -\Omega\, \delta_{ik} .$$

On the other hand substituting (34) into the expression for the entropy of a Bose-gas

$$S = \langle s\rangle \quad , \quad s = (1+f)\ln(1+f) - f\ln f \tag{36}$$

one obtains

$$TS = T\langle \ln(1+f)\rangle + \langle(\varepsilon - \mu - \vec p \vec V) f\rangle = -\Omega - \mu n - \vec P \vec V + \langle \varepsilon f\rangle$$

and hence

$$L_{ik} = (TS + \mu n + \vec P \vec V)\delta_{ik} . \tag{37}$$

The term $\langle \varepsilon \nabla f\rangle$ can be transformed analogously. Differentiating of (36) yields

$$\nabla s = \ln\frac{1+f}{f}\nabla f = \frac{\varepsilon - \mu - \vec p \vec V}{T}\nabla f$$

and therefore,

$$\langle \varepsilon \nabla f\rangle = T\nabla S + \mu \nabla n + V_k \nabla P_k .$$

Finally, the quasimomentum equation of motion with a local-equilibrium function (34) takes the form

$$\dot P_i + S\nabla_i T + n\nabla_i \mu + \vec P \nabla_i \vec V = -\nabla_k (P_i \dot u_k) . \tag{38}$$

In the linear approximation with respect to $\vec V$

$$P_i = \rho_{i\ell} V_\ell ,$$

where $\rho_{i\ell} = -\left(\frac{\partial^2 \Omega}{\partial V_i \partial V_\ell}\right)_{T,\mu}$ and (38) together with the continuity equation for the quasiparticles (25) and the energy conservation law (28) forms a closed set of equations used in /6/ in the defection second sound considerations.

6. DEFECTON DISTRIBUTION IN A ROTATING ^{4}He

As an application of the nonlinear theory developed, consider the defecton distribution in quantum solids rotating with a constant velocity $\vec\omega$. This problem cannot be solved in a linear theory because of not small velocities $\dot{\vec u}$.

According to the very low temperatures of interest, we assume that a cylinder of solid ^{4}He is rotating in superfluid ^{4}He (with vanishing normal density $\rho_n = 0$). Then, the vacancy concentration on the boundary is determined by thermal equilibrium conditions and hence $\mu(R) = 0$ (R being the radius of the cylinder).

As a rotation with a constant velocity $\vec\omega = \frac{1}{2}\,\mathrm{rot}\,\dot{\vec u}$ is an equilibrium one, the distribution function may be taken in the form $f = f_0(\varepsilon(\vec z) - \mu(\vec z))$. Then, the kinetic equation (21) yields

$$\dot{\vec u}\nabla f - \frac{\partial f}{\partial k_\alpha}\left\{m\ddot{\vec u}\vec a_\alpha + \vec a_\alpha(\dot{\vec u}\nabla)\dot{\vec u} + \vec a_\alpha \nabla\mu - 2m\frac{\partial \varepsilon}{\partial k_\beta}\vec\omega[\vec a_\alpha \vec a_\beta]\right\} = 0 . \tag{39}$$

The first term vanishes due to the radial symmetry, the last one is zero as it can be seen from its rewritten form

$$\frac{\partial f}{\partial k_\alpha}\frac{\partial \varepsilon}{\partial k_\beta}[\vec a_\alpha \vec a_\beta] = \frac{\partial f}{\partial \varepsilon}\left[\frac{\partial \varepsilon}{\partial \vec k}\frac{\partial \varepsilon}{\partial \vec k}\right] = 0 .$$

Substituting $\dot{\vec u} = [\vec\omega \vec z]$ in (39) then yields

$$\nabla\mu = -m[\vec\omega[\vec\omega \vec z]]$$

and hence,

$$\mu = \frac{m}{2}\omega^2(r^2 - R^2) . \tag{40}$$

To obtain the distribution function one needs to know the defecton energy as a function of deformation. The equations of elasticity for our case have the form

$$\frac{\partial \Sigma_{ik}}{\partial x_k} + F_i = 0 , \tag{41}$$

where $\vec{F} = \rho[\vec{\omega}[\vec{r}\vec{\omega}]]$ is the centrifugal force, and

$$\Sigma_{ik} = \left(\sigma_{\alpha\beta} + E_o g_{\alpha\beta} - \langle \lambda_{\alpha\beta} f_o \rangle\right) a_i^{\alpha} a_k^{\beta}$$

are the elastic matrix elements influenced by the presence of defectons, i.e., the matrix elements as obtained from experiments. As the elastic deformations are always small, we can restrict ourselves within the linear theory of elasticity. For simplicity we consider the ^{4}He sample as an isotropic medium. Then

$$\Sigma_{ik} = \frac{E'}{1+\sigma}\left(u_{ik} + \frac{\sigma}{1-2\sigma} u_{ll}\delta_{ik}\right). \tag{42}$$

where σ and E' are Poisson's and Young's modulus respectively. The solution of (41) can easily be obtained in cylindrical coordinates

$$u_r = \alpha\rho\omega^2 r\left\{(3-2\sigma)R^2 - r^2\right\}, \tag{43}$$

where $\alpha = \dfrac{1+\sigma}{24K(1-\sigma)}$ and $K = \dfrac{E'}{3(1-2\sigma)}$ is the modulus of dilatation. This is the solution which satisfies the boundary condition

$$\Sigma_{rr}(R) = 0 .$$

Hence, the nonzero deformation tensor components are

$$u_{rr} = \alpha\rho\omega^2\left\{3(R^2 - r^2) - 2\sigma R^2\right\} , \quad u_{\varphi\varphi} = \frac{u_r}{r} \tag{44}$$

and the local volume change is

$$\operatorname{div}\vec{u} = 2\alpha\rho\omega^2\left\{(3-2\sigma)R^2 - 2r^2\right\} .$$

The local defecton dispersion law in an isotropic medium may be written in the form

$$\varepsilon(\vec{k}, u_{ik}) = \left(\eta K + \lambda(k)\right)\operatorname{div}\vec{u} + \varepsilon_o(\vec{k}),$$

where η describes the change of the volume due to the presence of the defect, and $\lambda(k)$ is the change of the band spectrum. Owing to the small energy band width it may turn out to be

$$T < \lambda < \eta K .$$

In such a case Boltzmann statistics is preferable and the vacancions density varies as

$$n(r) = n(R)\exp\left\{-\frac{\varkappa(r)}{T}\omega^2\right\} ,$$

where

$$n(R) \sim \exp\left\{-\frac{\eta\rho(1+\sigma)}{6T}R^2\omega^2\right\}$$

is the vacancy concentration at the solid - liquid boundary, and

$$\varkappa(r) = \left(\eta\rho\frac{1+\sigma}{12(1-\sigma)} - \frac{m_o}{2}\right)(R^2 - r^2).$$

It is seen, that $\varkappa(r)$ can be positive or negative depending both on the sign and on the value of η , as well as on Poisson's modulus σ . If $\varkappa(r) > 0$ the vacancy concentration should have its maximum at the boundary, not in the cylinder axis. However such a situation can hardly be realized because of relatively small values of $\eta\rho < m_o$.

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Пушкаров Д.И. E17-85-531

Динамическая теория квантовых кристаллов с делокализованными дефектами

Построена динамическая теория квантовых кристаллов с делокализованными дефектами /дефектонами/. Получена точная нелинейная система, состоящая из уравнений теории упругости и кинетического уравнения. Полученные уравнения могут применяться к любому квазичастичному газу /или смеси газов/ с произвольным законом дисперсии в деформируемом кристалле. Корректно учтена роль квазиимпульса; для него получено уравнение движения. Вычислена функция распределения дефектов во вращающемся квантовом кристалле.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

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Pushkarov D.I. E17-85-531

Dynamics Theory of Quantum Crystals with Delocalized Defects

Dynamics theory of quantum crystals with delocalized defects (defectons) is developed. An exact, nonlinear set, consisting of elasticity theory and kinetic equations is derived. The equations deduced may be applied to every uncharged quasiparticle gas (or gases) with an arbitrary dispersion law in deformable solids. The quasiwave vector role is correctly taken into account, and its equation of motion is obtained. The defecton distribution function in a rotating quantum solid is calculated.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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