01.70.03 EJ2

IL NUOVO CIMENTO Vol. LXIX B N. 1 11 Settembre 1970

Collective-Variable Description of the Dynamics of Crystals.

B. Alascio and A. López Dávalos

Centro Atómico Bariloche, Comisión Nacional de Energía Atómica
Instituto de Fisica « Dr. José A. Balseiro », Universidad Nacional de Cuyo
San Carlos de Bariloche, Rio Negro

(ricevuto il 3 Febbraio 1970)

Summary. — A description is given of the dynamics of crystals by means of collective variables, namely the Fourier transforms of the divergence and curl of the current. It is shown that, in the harmonic approximation, the classical equations of motion are reduced to a set of three equations involving only the collective variables themselves. From these equations the usual result for the frequency of phonons is obtained. Furthermore, the quantum-mechanical equations of motion can again be reduced, in a suitable approximation, to a set of three coupled equations in the collective variables. A relationship between frequency and wave number is derived for the excitations of the system from them.

1. – Introduction.

The use of collective variables for the description of quantum liquids has been exploited by Landau (¹) in his discussion of the properties of superfluid He. A more formal basis for quantum hydrodynamics was then given by Kroning and Thellung but restricted to the description of irrotational flow. This was later extended by Thellung (³) and by Ziman (⁴) to rotational flow.

(¹) L. D. Landau: *Journ. Phys. USSR*, **5**, 71 (1941).
(²) R. Kroning and A. Thellung: *Physica*, **18**, 749 (1952).
(³) A. Thellung: *Physica*, **19**, 217 (1953).
(⁴) J. M. Ziman: *Proc. Roy. Soc.*, A **219**, 257 (1953).

On the other hand ZWANZIG (5) in a discussion on the existence of longitudinal and transverse phonon modes in a classical liquid has also used collective variables (the components of the momentum density) to describe the system.

Recently, YEE (6) has proposed a current algebra formulation of quantum hydrodynamics, and rederived to lowest order the Hamiltonian obtained by ZIMAN.

We use here the Fourier transform of the divergence and rotational of the current $\boldsymbol{j}(\boldsymbol{r})$ to describe collective excitations in a many-body system, and show that they can be used for the description of phonons in classical crystals. The application of the method to quantum crystals is also discussed.

Since the variables are particularly suitable for the description of liquids (both, quantum and classical) it seems reasonable to assume that they could be used with advantage to describe the dynamics of systems near or at the liquid-solid transition.

In Sect. 2, we define the variables in terms of the classical individual particle variables, obtaining equations for them from a general Hamiltonian with pair interaction.

We then show that, in the harmonic approximation, they reduce to a set of equations connecting the $\boldsymbol{k}$-th Fourier component of the divergence $D_{\boldsymbol{k}}(t)$ with the two independent components of the rotational $\boldsymbol{C}_{\boldsymbol{k}}$ for the same $\boldsymbol{k}$. The ensuing third-order secular equation can be shown to be identical with the secular equation determining the phonon frequencies in the usual description of the dynamics of a crystal by the displacements of the particles from their equilibrium positions.

In Sect. 3 the corresponding quantum-mechanical variables are defined and their equations of motion determined. They are then approximated on the assumption that the state of the system is similar to a ground state in which each particle is considered to be in a bound state whose center of mass coincides with its equilibrium poistion in the crystal (*). It is found that in that way a third-order equation can again be obtained to determine the eigenfrequencies corresponding to the collective modes. For low $\boldsymbol{k}$ these eigenfrequencies are very similar to those obtained in ref. (7) for quantum crystals, but they depart from them considerably for high $\boldsymbol{k}$.

As a consequence of the use of $D_{\boldsymbol{k}}$ and $\boldsymbol{C}_{\boldsymbol{k}}$ as dynamical variables the frequencies are not periodic in reciprocal space. This feature is also discussed in Sect. 3.

---

(5) R. ZWANZIG: *Phys. Rev.*, **156**, 190 (1967).

(6) D. D. H. YEE: *Phys. Rev.*, **184**, 196 (1969).

(*) This, plus the assumption that the ground and first excited states are those corresponding to the harmonic oscillator, were used by WERTHAMER and NOSANOW (7) to calculate the phonon frequencies in quantum crystals.

(7) B. H. NOSANOW and N. R. WERTHAMER: *Phys. Rev. Lett.*, **15**, 618 (1965).

2. - Classical description.

Given a classical system of N particles whose positions and velocities are characterized by $\boldsymbol{r}_j$ and $\boldsymbol{v}_j$, we can define a local density and current in the usual form

$$\varrho(\boldsymbol{r}) = \sum_j \delta(\boldsymbol{r} - \boldsymbol{r}_j)\,, \tag{2.1}$$

$$j(\boldsymbol{r}) = \sum_j \boldsymbol{v}_j\, \delta(\boldsymbol{r} - \boldsymbol{r}_j)\,. \tag{2.2}$$

As is known (4,8) longitudinal vibrations are described by fluctuations in $\varrho(\boldsymbol{r})$. Through the continuity equation

$$\varrho(\boldsymbol{r}) + \operatorname{div}\boldsymbol{j}(\boldsymbol{r}) = 0\,, \tag{2.3}$$

these oscillations are connected to fluctuations of the quantity $D(\boldsymbol{r})$ defined by

$$D(\boldsymbol{r}) = \operatorname{div}\boldsymbol{j}(r)\,. \tag{2.4}$$

For a system that can also support transverse excitations, we can have a unified description by introducing a quantity $\boldsymbol{C}(\boldsymbol{r})$ independent of $D(\boldsymbol{r})$, given by

$$\boldsymbol{C}(\boldsymbol{r}) = \operatorname{curl}\boldsymbol{j}(\boldsymbol{r})\,. \tag{2.5}$$

The longitudinal and transverse character of the excitations described by $D(\boldsymbol{r})$ and $\boldsymbol{C}(\boldsymbol{r})$ is clearly seen in the Fourier transforms

$$D_{\boldsymbol{k}}(t) = \int \mathrm{d}^3 r \exp[i\boldsymbol{k}\cdot\boldsymbol{r}]\, D(\boldsymbol{r}, t) = -\,i \sum_j \boldsymbol{k}\cdot\boldsymbol{v}_j \exp[i\boldsymbol{k}\cdot\boldsymbol{r}]\,, \tag{2.6}$$

$$\boldsymbol{C}_{\boldsymbol{k}}(t) = \int \mathrm{d}^3 r \exp[i\boldsymbol{k}\cdot\boldsymbol{r}]\, \boldsymbol{C}(\boldsymbol{r}, t) = -\,i \sum_j \boldsymbol{k}\times\boldsymbol{v}_j \exp[i\boldsymbol{k}\cdot\boldsymbol{r}]\,. \tag{2.7}$$

Taking a Hamiltonian of the form

$$H = \sum_j \frac{p_j^2}{2m} + \frac{1}{2} \sum_{i \neq j} V(|\boldsymbol{r}_i - \boldsymbol{r}_j|)\,, \tag{2.8}$$

where $\boldsymbol{p}_j = m\boldsymbol{x}_j$, and using the fact that the time derivative of any dynamical

---

(8) O. Penrose: *Phil. Mag.*, **45**, 80 (1954).

quantity A is given by

$$\dot{A}(t) = \{A, H\}\,, \tag{2.9}$$

where $\{A, B\}$ indicates the Poisson brackets of A and B, we obtain

$$\ddot{D}_{\boldsymbol{k}} = -i \sum_{j} [(\boldsymbol{k}\cdot\ddot{\boldsymbol{v}}_j) + 3i(\boldsymbol{k}\cdot\boldsymbol{v}_j)(\boldsymbol{k}\cdot\dot{\boldsymbol{v}}_j) - (\boldsymbol{k}\cdot\boldsymbol{v}_j)^3] \exp[i\boldsymbol{k}\boldsymbol{r}_j] \tag{2.10}$$

and

$$\begin{aligned}\boldsymbol{C}_{\boldsymbol{k}} = -i \sum_{j} [(\boldsymbol{k}\times\ddot{\boldsymbol{v}}_j) + 2i(\boldsymbol{k}\times\dot{\boldsymbol{v}}_j)(\boldsymbol{k}\cdot\boldsymbol{v}_j) +\\ + i(\boldsymbol{k}\times\boldsymbol{v}_j)(\boldsymbol{k}\cdot\ddot{\boldsymbol{v}}_j) - (\boldsymbol{k}\times\boldsymbol{v}_j)(\boldsymbol{k}\cdot\boldsymbol{v}_j)^2] \exp[i\boldsymbol{k}\boldsymbol{r}_j]\,.\end{aligned} \tag{2.11}$$

Restricting ourselves to the description of the system in a region of phase space in the neighbourhood of the point of equilibrium, we can neglect third-order terms in the velocity.

Within this approximation, eqs. (2.10) and (2.11) can be written

$$\ddot{D}_{\boldsymbol{k}} = \sum_{\boldsymbol{k}} \varrho_{\boldsymbol{k}'} \{a_{\boldsymbol{k}\boldsymbol{k}'} D_{\boldsymbol{k}-\boldsymbol{k}'} + \boldsymbol{b}_{\boldsymbol{k}\boldsymbol{k}'} \boldsymbol{C}_{\boldsymbol{k}-\boldsymbol{k}'}\} \tag{2.12a}$$

and

$$\ddot{\boldsymbol{C}}_{\boldsymbol{k}} = \sum_{\boldsymbol{k}} \varrho_{\boldsymbol{k}'} \{\boldsymbol{d}_{\boldsymbol{k}\boldsymbol{k}'} D_{\boldsymbol{k}-\boldsymbol{k}'} + e_{\boldsymbol{k}\boldsymbol{k}'} \boldsymbol{C}_{\boldsymbol{k}-\boldsymbol{k}'} + (\mathbf{f}_{\boldsymbol{k}\boldsymbol{k}'}\cdot\boldsymbol{C}_{\boldsymbol{k}-\boldsymbol{k}'})\}\,, \tag{2.12b}$$

where

$$a_{\boldsymbol{k}\boldsymbol{k}'} = -\frac{1}{mV}\left[\left(k^2 - (\boldsymbol{k}\cdot\boldsymbol{k}')\right) V_{\boldsymbol{k}-\boldsymbol{k}'} + \frac{\left((3\boldsymbol{k}-\boldsymbol{k}')\cdot(\boldsymbol{k}-\boldsymbol{k}')\right)}{(\boldsymbol{k}-\boldsymbol{k}')^2}(\boldsymbol{k}\cdot\boldsymbol{k}')\, V_{\boldsymbol{k}'}\right], \tag{2.13a}$$

$$\boldsymbol{b}_{\boldsymbol{k}\boldsymbol{k}'} = \frac{1}{mV}\, 2(\boldsymbol{k}\cdot\boldsymbol{k}')\frac{(\boldsymbol{k}'\times\boldsymbol{k})}{(\boldsymbol{k}-\boldsymbol{k}')^2} V_{\boldsymbol{k}'}\,, \tag{2.13b}$$

$$\boldsymbol{d}_{\boldsymbol{k}\boldsymbol{k}'} = \frac{1}{mV}(\boldsymbol{k}\times\boldsymbol{k}')\left[\left(\frac{k'^2}{(\boldsymbol{k}-\boldsymbol{k}')^2} - 2\right) V_{\boldsymbol{k}'} + V_{\boldsymbol{k}-\boldsymbol{k}'}\right], \tag{2.13c}$$

$$e_{\boldsymbol{k}\boldsymbol{k}'} = -\frac{1}{mV}\frac{(\boldsymbol{k}\cdot\boldsymbol{k}')}{(\boldsymbol{k}-\boldsymbol{k}')^2}\left(\boldsymbol{k}\cdot(\boldsymbol{k}-\boldsymbol{k}')\right) V_{\boldsymbol{k}'} \tag{2.13d}$$

and the dyadic

$$\mathbf{f}_{\boldsymbol{k}\boldsymbol{k}'} = \frac{1}{mV}\frac{(\boldsymbol{k}\cdot\boldsymbol{k}')^2}{(\boldsymbol{k}-\boldsymbol{k}')}(\boldsymbol{k}-\boldsymbol{k}')\,\boldsymbol{k} V_{\boldsymbol{k}'}\,. \tag{2.13e}$$

Here $V_{\boldsymbol{k}}$ is the Fourier transform of the potential

$$V(\boldsymbol{r}) = \frac{1}{V}\sum_{\boldsymbol{q}} V_{\boldsymbol{q}} \exp[-i\boldsymbol{q}\boldsymbol{r}]\,.$$

We now want to apply eq. (12) to a crystalline solid and show that in the harmonic approximation the ensuing secular equation coincides with the secular equation obtained by describing the excitations directly by means of the atomic displacements.

To do this we replace $\varrho_{\boldsymbol{k}}$ in the right-hand side of eqs. (12) by its equilibrium value $\varrho_{\boldsymbol{k}}^0$, which for a crystal is given by

$$\varrho_{\boldsymbol{k}}^0 = N \sum_{\boldsymbol{G}} \delta(\boldsymbol{k} - \boldsymbol{G}) \,, \tag{2.14}$$

where the G's are the reciprocal lattice vectors.

Substituting (2.14) into eqs. (2.12) we get a coupling between $D_{\boldsymbol{k}}$ and $\boldsymbol{C}_{\boldsymbol{k}}$ on one side and $D_{\boldsymbol{k}+\boldsymbol{G}}$ and $C_{\boldsymbol{k}+\boldsymbol{G}}$ for all G's on the other. These relations can be further simplified by noting that

$$D_{\boldsymbol{k}+\boldsymbol{G}} = -i \sum_{j} \big((\boldsymbol{k} + \boldsymbol{G}) \cdot \boldsymbol{v}_j\big) \exp\,[i(\boldsymbol{k} + \boldsymbol{G}) \cdot \boldsymbol{r}_j]$$

and that to lowest order in the deviation from equilibrium

$$D_{\boldsymbol{k}+\boldsymbol{G}} \simeq -i \sum_{j} \big((\boldsymbol{k} + \boldsymbol{G}) \cdot \boldsymbol{v}_j\big) \exp\,[i\boldsymbol{k}\boldsymbol{r}_j^0] = \left(1 + \frac{(\boldsymbol{k} \cdot \boldsymbol{G})}{k^2}\right) D_{\boldsymbol{k}} + \frac{1}{k^2}\big((\boldsymbol{k} \times \boldsymbol{G}) \cdot \boldsymbol{C}_{\boldsymbol{k}}\big) \tag{2.15}$$

and similarly (*)

$$\boldsymbol{C}_{\boldsymbol{k}+\boldsymbol{G}} \simeq \left(1 + \frac{(\boldsymbol{k} \cdot \boldsymbol{G})}{k^2}\right) \boldsymbol{C}_{\boldsymbol{k}} - \frac{(\boldsymbol{k} \times \boldsymbol{G})}{k^2} D_{\boldsymbol{k}} - \frac{\boldsymbol{k}}{k^2} (\boldsymbol{G} \cdot \boldsymbol{C}_{\boldsymbol{k}}) \,. \tag{2.16}$$

Combining (2.14), (2.15) and (2.16) with the equations of motion (2.12) we obtain

$$\begin{aligned} \ddot{D}_{\boldsymbol{k}} = -\frac{N}{mV} \sum_{\boldsymbol{G}} \Bigg\{ \left[\frac{(\boldsymbol{k} \cdot \boldsymbol{G})}{k^2} V_{\boldsymbol{G}} + \frac{(\boldsymbol{k} \cdot (\boldsymbol{k} - \boldsymbol{G}))}{k^2} V_{\boldsymbol{k}-\boldsymbol{G}}\right] \big(\boldsymbol{G} \cdot (\boldsymbol{k} \times \boldsymbol{C}_{\boldsymbol{k}})\big) \,+ \\ + \frac{1}{k^2} \big[(\boldsymbol{k} \cdot (\boldsymbol{k} - \boldsymbol{G}))^2 V_{\boldsymbol{k}-\boldsymbol{G}} - (\boldsymbol{k} - \boldsymbol{G})^2 V_{\boldsymbol{G}}\big] D_{\boldsymbol{k}} \Bigg\} \end{aligned} \tag{2.17a}$$

and

$$\begin{aligned} \ddot{\boldsymbol{C}}_{\boldsymbol{k}} = \frac{N}{mV} \sum_{\boldsymbol{G}} \Bigg\{ \frac{\boldsymbol{k} \times \boldsymbol{G}}{k^2} (V_{\boldsymbol{k}-\boldsymbol{G}} - V_{\boldsymbol{G}}) \big(\boldsymbol{G} \cdot (\boldsymbol{k} \times \boldsymbol{C}_{\boldsymbol{k}})\big) \,+ \\ + (\boldsymbol{k} \times \boldsymbol{G}) \left[V_{\boldsymbol{k}-\boldsymbol{G}} - \frac{(\boldsymbol{k} \cdot \boldsymbol{G})}{k^2} (V_{\boldsymbol{k}-\boldsymbol{G}} - V_{\boldsymbol{G}})\right] D_{\boldsymbol{k}} \Bigg\} \,. \end{aligned} \tag{2.17b}$$

(*) In deriving (2.16) we have used the following vector identity:

$$\boldsymbol{A}^2(\boldsymbol{B} \times \boldsymbol{C}) = (\boldsymbol{A} \cdot \boldsymbol{B})(\boldsymbol{A} \times \boldsymbol{C}) - (\boldsymbol{A} \cdot \boldsymbol{C})(\boldsymbol{A} \times \boldsymbol{B}) - \big(\boldsymbol{B} \cdot (\boldsymbol{A} \times \boldsymbol{C})\big)\boldsymbol{A} \,.$$

Since $\boldsymbol{C}_k$ is normal to $\boldsymbol{k}$, we can completely characterize it by giving its components relative to a pair of orthogonal unit vectors $\boldsymbol{e}_1$, $\boldsymbol{e}_2$ in the plane normal to $\boldsymbol{k}$. Calling these components $C_k^{(1)}$ and $C_k^{(2)}$ eqs. (2.17) can be written as

$$\ddot{D}_k = X_k D_k + Y_k^{(1)} C_{k,1} + Y_k^{(2)} C_{k,2}\,, \tag{2.18a}$$

$$\ddot{C}_{k,i} = Z_k^{(i)} D_k + W_k^{(i)(1)} C_{k,1} + W_k^{(i)(2)} C_{k,2}\,, \tag{2.18b}$$

where

$$k^2 X_k = -\frac{N}{mV}\sum_{\boldsymbol{G}}\left[\left(\boldsymbol{k}\cdot(\boldsymbol{k}-\boldsymbol{G})\right)^2 V_{k-G} - (\boldsymbol{k}\cdot\boldsymbol{G})^2 V_G\right], \tag{2.19a}$$

$$kY_k^{(i)} = \frac{N}{mV}(-1)^i \sum_{\boldsymbol{G}}\left[\left(\boldsymbol{k}\cdot(\boldsymbol{k}-\boldsymbol{G})\right)V_{k-G} + (\boldsymbol{k}\cdot\boldsymbol{G})\,V_G\right](\boldsymbol{G}\cdot\boldsymbol{e}_{i'}) \quad (i\neq i')\,, \tag{2.19b}$$

$$kZ_k^{(i)} = \frac{N}{mV}\sum_{\boldsymbol{G}}\left(e_i\cdot(\boldsymbol{k}\times\boldsymbol{G})\right)\left(kV_{k-G} - (\boldsymbol{k}\cdot\boldsymbol{G})(V_{k-G}-V_G)\right), \tag{2.19c}$$

$$k^2 W^{(i)(j)} = (-1)^{j+1}\frac{N}{mV}\sum_{\boldsymbol{G}}(\boldsymbol{e}_i\cdot\boldsymbol{k}\times\boldsymbol{G})(\boldsymbol{G}\cdot\boldsymbol{e}_j)\,V_{k-G} \qquad (j'\neq j)\,. \tag{2.19d}$$

Equations (18) above can be shown to be identical to those obtained in the usual approach (^{9}).

3. – Quantum-mechanical description.

In this Section we write the quantum-mechanical expressions corresponding to the dynamical variables $\boldsymbol{D}_k$ and $\boldsymbol{C}_k$ and derive equations of motion for them in the Heisenberg representation. The equations of motion thus obtained are approximated assuming that the system is in a state « close » to the ground state. The resulting equations, harmonic in $\boldsymbol{D}_k$ and $\boldsymbol{C}_k$, provide the eigenfrequencies of the system.

The expressions for $\boldsymbol{D}_k$ and $\boldsymbol{C}_k$ in the notation of second quantization are

$$D_k = \frac{\hbar}{2im}\sum_{\boldsymbol{k}'}\left[(\boldsymbol{k}+\boldsymbol{k}')^2 - k'^2\right]a^\dagger_{k+k'}a_{k'}\,, \tag{3.1}$$

$$\boldsymbol{C}_k = \frac{\hbar}{im}\sum_{\boldsymbol{k}'}(\boldsymbol{k}\times\boldsymbol{k}')\,a^\dagger_{k+k'}a_{k'}\,, \tag{3.2}$$

where $a_k^\dagger$ and a_k are the creation and annihilation operators for a particle in the $\boldsymbol{k}$-th eigenstate of the linear momentum.

(^{9}) D. PINES: *Elementary Excitations in Solids* (New York, 1964).

In the Heisenberg representation, the time derivative of an operator A is

$$i\hbar\dot{A} = [A, H] .$$

Separating H into its kinetic (T) and potential (V) energies we have

$$T = \sum_{\boldsymbol{k}} \frac{\hbar^2 k^2}{2m} a^\dagger_{\boldsymbol{k}} a_{\boldsymbol{k}} \tag{3.3}$$

and

$$V = \frac{1}{2V} \sum_{\boldsymbol{k}} V_{\boldsymbol{k}} \varrho_{\boldsymbol{k}} \varrho_{-\boldsymbol{k}} - \frac{1}{2} V_0 \varrho_0 , \tag{3.4}$$

where $V_{\boldsymbol{k}}$ is the Fourier transform of the two-particle potential and $\varrho_{\boldsymbol{k}}$ is the density operator

$$\varrho_{\boldsymbol{k}} = \sum_{\boldsymbol{k}'} a^\dagger_{\boldsymbol{k}+\boldsymbol{k}'} a_{\boldsymbol{k}'} , \tag{3.5}$$

using (3.2) to (3.5) and after considerable algebra we obtain

$$-\hbar^2 \ddot{D}_{\boldsymbol{k}} = \big[[D_{\boldsymbol{k}}, T], T\big] + \hbar^2 \sum_{\boldsymbol{k}'} \big\{a_{\boldsymbol{k}',\boldsymbol{k}} \mathscr{D}_{\boldsymbol{k},\boldsymbol{k}'} + \big(\boldsymbol{b}_{\boldsymbol{k},\boldsymbol{k}'} \cdot (\boldsymbol{k} \times \mathscr{C}_{\boldsymbol{k},\boldsymbol{k}'})\big)\big\} \tag{3.6}$$

and

$$-\hbar^2 \ddot{C}_{\boldsymbol{k}} = \big[[C_{\boldsymbol{k}}, T], T\big] + \hbar^2 \sum_{\boldsymbol{k}'} \big\{d_{\boldsymbol{k}',\boldsymbol{k}'} \mathscr{D}_{\boldsymbol{k},\boldsymbol{k}'} + e_{\boldsymbol{k},\boldsymbol{k}'} \mathscr{C}_{\boldsymbol{k},\boldsymbol{k}'} + f_{\boldsymbol{k}',\boldsymbol{k}} \cdot \mathscr{C}_{\boldsymbol{k},\boldsymbol{k}'}\big\} , \tag{3.7}$$

where

$$\mathscr{D}_{\boldsymbol{k},\boldsymbol{k}'} = \frac{\varrho_{\boldsymbol{k}'} D_{\boldsymbol{k}-\boldsymbol{k}'} + D_{\boldsymbol{k}-\boldsymbol{k}'} \varrho_{\boldsymbol{k}'}}{2} \tag{3.8}$$

and

$$\mathscr{C}_{\boldsymbol{k}\boldsymbol{k}'} = \frac{\varrho_{\boldsymbol{k}'} C_{\boldsymbol{k}-\boldsymbol{k}'} + C_{\boldsymbol{k}-\boldsymbol{k}'} \varrho_{\boldsymbol{k}'}}{2} \tag{3.9}$$

are the quantum-mechanical equivalents of the correctly symmetrized classical variables $\varrho_{\boldsymbol{k}'} D_{\boldsymbol{k}-\boldsymbol{k}'}$ and $\varrho_{\boldsymbol{k}'} C_{\boldsymbol{k}-\boldsymbol{k}'}$ and $a_{\boldsymbol{k},\boldsymbol{k}'}$, $\boldsymbol{b}_{\boldsymbol{k},\boldsymbol{k}'}$, $\boldsymbol{d}_{\boldsymbol{k},\boldsymbol{k}'}$, $e_{\boldsymbol{k},\boldsymbol{k}'}$ and $f_{\boldsymbol{k},\boldsymbol{k}'}$ coincide with the coefficients obtained in the classical equations and are given by formulae (2.13).

We will now proceed to approximate eqs. (3.6) and (3.7) so that they will correspond to the excitations of a quantum-mechanical crystalline system. In order to do this, we will calculate the expectation value of $\varrho_{\boldsymbol{k}}$, $\boldsymbol{D}_{\boldsymbol{k}}$ and $C_{\boldsymbol{k}}$ using wave functions obtained by making small changes in the ground-state wave function Ψ_0 and linearizing in the deviations.

As in ref. (7), Ψ_0 is taken as an unsymmetrized product of real one-particle wave functions, all with the same form, localized, and centred about different equilibirum positions $\boldsymbol{r}_l^0$:

$$\Psi_0(\boldsymbol{r}_1, \boldsymbol{r}_2, \dots, \boldsymbol{r}_N) = \varphi(\boldsymbol{r}_1 - \boldsymbol{r}_1^0)\,\varphi(\boldsymbol{r}_2 - \boldsymbol{r}_2^0) \dots \varphi(\boldsymbol{r}_N - \boldsymbol{r}_N^0)\,. \tag{3.10}$$

We will assume the overlap of the φ's negligible, so that the lack of symmetry is inconsequential. The N-particle wave function Ψ used to evaluate the expectation values is obtained from Ψ_0 by multiplying it by a phase factor $\exp\left[i\sum_l \boldsymbol{k}_l \boldsymbol{r}_l\right]$. Furthermore we approximate $\langle \varrho D + D\varrho\rangle$ by $2\langle D\rangle\langle\varrho\rangle$, with the wave function described above and the expression

$$\varrho(\boldsymbol{r}) = \sum_l \delta(\boldsymbol{r} - \boldsymbol{r}_l)$$

we obtain

$$\varrho_{\boldsymbol{k}} = \sum_{\boldsymbol{G}} \delta(\boldsymbol{k} - \boldsymbol{G})\,\chi_{\boldsymbol{k}}\,, \tag{3.11}$$

where the G's indicate reciprocal lattice vectors, and χ_k is the Fourier transform of $[\varphi(\boldsymbol{r})]^2$.

Taking now the expectation value of

$$\boldsymbol{j}(\boldsymbol{r}) = \frac{1}{2m}\sum_l [\boldsymbol{p}_l\,\delta(\boldsymbol{r} - \boldsymbol{r}_l) + \delta(\boldsymbol{r} - \boldsymbol{r}_l)\boldsymbol{p}_l]$$

($\boldsymbol{p}_l$ are the one-particle momentum operators), we obtain

$$\boldsymbol{j}_k = \sum_l \frac{\hbar \boldsymbol{k}_l}{m} \exp[i\boldsymbol{k}\boldsymbol{r}_l^0]\,\chi_k\,. \tag{3.12}$$

Using the relations between $\boldsymbol{j}_k$ and D_k and $\boldsymbol{C}_k$ we see that

$$\langle D_k\rangle = -i\boldsymbol{k}\langle \boldsymbol{j}_k\rangle = -i\boldsymbol{k}\sum_l \frac{\hbar \boldsymbol{k}_l}{m}\exp[i\boldsymbol{k}\boldsymbol{r}_l^0]\,\chi_k \tag{3.13}$$

and

$$\langle \boldsymbol{C}_k\rangle = -i\boldsymbol{k}\times\langle \boldsymbol{j}_k\rangle = -i\boldsymbol{k}\times\sum_l \frac{\hbar \boldsymbol{k}_l}{m}\exp[i\boldsymbol{k}\boldsymbol{r}_l^0]\,\chi_k \tag{3.14}$$

and from these, with no further approximations,

$$\langle D_{k+G}\rangle = \frac{\chi_{k-G}}{\chi_k}\left\{\left(1 - \frac{(\boldsymbol{k}\cdot\boldsymbol{G})}{k^2}\right)\langle D_k\rangle - \frac{(\boldsymbol{k}\times\boldsymbol{G})\cdot\langle \boldsymbol{C}_k\rangle}{k^2}\right\} \tag{3.15}$$

and

$$(3.16)\qquad \langle \boldsymbol{C}_{k+G}\rangle = \frac{\chi_{k-G}}{\chi_k}\left\{\left(1-\frac{(\boldsymbol{k}\cdot\boldsymbol{G})}{k^2}\right)\langle \boldsymbol{C}_k\rangle + \frac{(\boldsymbol{k}\times\boldsymbol{G})}{k^2}D_k + \frac{\boldsymbol{k}}{k^2}(\boldsymbol{G}\cdot\boldsymbol{C}_k)\right\}$$

replacing now (3.11), (3.15), (3.16) in (3.6) and (3.7) we obtain the following equations relating the time Fourier transform of D_k and C_k:

$$(3.17)\qquad -\omega^2 D_k = \frac{N}{mV}\sum_{G}\frac{\chi_G\chi_{k-G}}{\chi_k}\left\{\left[-(3k^2-\boldsymbol{k}\boldsymbol{G})(\boldsymbol{k}\cdot\boldsymbol{G})V_G-(\boldsymbol{k}\cdot(\boldsymbol{k}-\boldsymbol{G}))^2V_{k-G}\right]\frac{D_k}{k^2}+\right.$$
$$\left.+\frac{1}{k^2}\left[(\boldsymbol{k}\cdot\boldsymbol{G})V_G+\boldsymbol{k}(\boldsymbol{k}-\boldsymbol{G})V_{k-G}\right]\left((\boldsymbol{k}\times\boldsymbol{G})\cdot\boldsymbol{C}_k\right)\right\}-\frac{1}{\hbar^2}[[D_k,T],T]$$

and

$$(3.18)\quad -\omega^2\boldsymbol{C}_k = \frac{N}{mV}\sum_{G}\frac{\chi_G\chi_{k-G}}{\chi_k}\left\{\left[\left(1-\frac{\boldsymbol{k}\cdot\boldsymbol{G}}{k^2}\right)V_{k-G}-\left(2-\frac{\boldsymbol{k}\cdot\boldsymbol{G}}{k^2}\right)V_G\right](\boldsymbol{k}\times\boldsymbol{G})D_k+\right.$$
$$\left.+\frac{1}{k^2}\left[(V_{k-G}-V_G)(\boldsymbol{k}\times\boldsymbol{G})\right](\boldsymbol{G}\times\boldsymbol{k})\boldsymbol{C}_k-(\boldsymbol{k}\cdot\boldsymbol{G})V_G\boldsymbol{C}_k\right\}-\frac{1}{\hbar^2}[[C_k,T],T]\,.$$

The last terms in the right-hand side of eqs. (3.17) and (3.18) stem from the kinetic-energy part of the Hamiltonian. They can be written in the form

$$(3.19)\qquad -\frac{1}{\hbar^2}[[D_k,T],T] = \left(\frac{\hbar^2k^2}{2m}\right)^2 D_k + \text{one-particle terms}\,,$$

$$(3.20)\qquad -\frac{1}{\hbar^2}[[\boldsymbol{C}_k,T],T] = \left(\frac{\hbar^2k^2}{2m}\right)^2 \boldsymbol{C}_k + \text{one-particle terms}\,.$$

The first term is a purely quantum term as evidenced by the fact that it vanishes as $\hbar$ goes to zero. This term is obtained also in different treatments of the degenerate imperfect Bose gas (*) ([10,11]), and in the Bohm and Pines treatment of the interacting electron gas ([9]). The other terms are not expressible in terms of the collective variables. In the case of the electron gas they give rise to the k^2 dependence of the plasma frequency and to the electron-plasmon coupling ([9]).

Unlike the classical case, the secular determinant obtained from eqs. (3.17) and (3.18) for the $\boldsymbol{k}$-th mode is different from the one obtained for the $\boldsymbol{k}+\boldsymbol{G}$

(*) Notice that if the quantum-mechanical spread is comparable to the lattice spacing, this term contributes an energy of the order of the localization energy of the particle for $\boldsymbol{k}$ near the Brillouin-zone boundary.

([10]) R. D. ETTERS: *Nuovo Cimento*, **44** B, 68 (1966).

([11]) N. BOGOLIUBOV: *Journ. Phys. USSR*, **11**, 23 (1947).

mode, the nonperiodicity of the ω^2-function in reciprocal space arising from the kinetic-energy terms as well as from the χ_k factors. This feature is a consequence of the description of the system by the collective variables $\boldsymbol{D}_k$ and $\boldsymbol{C}_k$: the periodicity of ω^2 in the usual treatment results from the fact that the normal mode $k + G$ describes exactly the same physical situation as the $\boldsymbol{k}$-th normal mode, the information contained in them concerning only the deviation of the mean value of the position operator from equilibrium. Since the information contained in $\boldsymbol{D}_k$ or $\boldsymbol{C}_k$ involves also the spread of the particles about their mean position through the χ_k factors, this is not so in our description.

Since the collective variables do not depend critically on the deviation of the position of the particles from a fixed equilibrium point as discussed by ZWANZIG (5), they are also suitable for the description of quantum liquids, consequently they could be useful in the description of the solid-liquid transition in He for example.

We should also mention that the neutron scattering cross-section is related to the Fourier transform of the density-density correlation function $\langle \varrho(\boldsymbol{r}, t)\, \varrho(\boldsymbol{r}, 0)\rangle$ (12).

The time derivative of $\varrho(\boldsymbol{r}, t)$ is related to $D(\boldsymbol{r}, t)$ through the continuity equation (*) $\dot{\varrho}(\boldsymbol{r}, t) + D(\boldsymbol{r}, t) = 0$. Therefore it seems reasonable to expect that the results of neutron scattering measurements in quantum crystals can be compared more easily with the predictions of eqs. (3.17) and (3.18) than with the results obtained by the usual method.

---

(12) L. VAN HOVE: *Phys. Rev.*, 95, 249 (1954).

(*) As is known (see ref. (6) for example) this equation is obtained directly from the commutator $[\varrho, H]$ and the definitions of ϱ and D.

RIASSUNTO (*)

Si dà una descrizione della dinamica dei cristalli tramite variabili collettive, cioè le trasformate di Fourier della divergenza e della rotazione della corrente. Si dimostra che, nell'approssimazione armonica, le equazioni classiche del moto sono ridotte ad un insieme di tre equazioni che legano solo le variabili collettive stesse. Per queste equazioni si ottiene il solito risultato per la frequenza dei fononi. Inoltre si possono ancora ridurre le equazioni quantomeccaniche, in una approssimazione opportuna, ad un insieme di tre equazioni accoppiate nelle variabili collettive. Si ricava un'equazione fra la frequenza ed il numero d'onda per le eccitazioni del sistema.

(*) *Traduzione a cura della Redazione.*

Описание динамики кристаллов с помощью коллективных переменных.

Резюме (*). — Приводится описание динамики кристаллов с помощью коллективных переменных, а именно, фурье преобразований дивергенции и ротора тока. Показывается, что в гармоническом приближении их классические уравнения движения сводятся к системе трех уравнений, которые включают только сами коллективные переменные. Из этих уравнений получается обычный результат для частоты фононов. Кроме того, квантовомеханические уравнения движения также могут быть сведены, в соответствующем приближении, к системе трех связанных уравнений по коллективным переменным. Из этих уравнений выводится связь между частотой и волновым вектором для рассматриваемых возбуждений.

(*) *Переведено редакцией.*