Theory of Bose quantum crystals

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A theory of crystals consisting of Bose particles of a single type (e.g., He^4) is developed by quantum field theory methods. Under the assumption that single-particle excitations in such crystals form a Bose condensate, the collective excitation spectra are determined and a number of exact relations are derived, e. g., the relation (1.4) between the normal and the superfluid densities.

1. INTRODUCTION

In our previous works [1,2] carried out in cooperation with Levchenkov (in what follows [2] will be referred to as I, and equations from it as (I, ...)) we used methods of the quantum field theory to build a theory of crystals consisting of Fermi particles (e.g., He^3). We have examined most extensively the case when the Fermi crystal contains low-lying single-particle excitations forming a Fermi liquid at T = 0. The possibility of such situation was first suggested by Andreev and Lifshitz [3]. Our results differ from those of Andreev and Lifshitz in that they regarded the Fermi excitations as crystal defects ("vacancions" and "impuritons"), assumed that their number is small, and treated the whole problem in the gas approximation, whereas our results depended neither on the number of Fermi excitations (there could be at least one of them per unit cell) nor on the intensity of interaction.

The idea of Andreev and Lifshitz holds also for the case of crystals consisting of Bose particles (e.g., He^4). Treating the problem phenomenologically [3], they derived a system of hydrodynamic equations for a crystal possessing the property of superfluidity. Furthermore, within the framework of the gas approximation, they have studied the thermodynamic properties of a Bose crystal with a small number of defectons.

In the present work we consider the properties of a Bose crystal at T = 0 by methods of the quantum field theory for an arbitrary number of bosons in the condensate and for an arbitrary interaction strength.

The main physical results consist in the following. If a fraction of the particles in a Bose crystal are in the condensate, of density n_0, and, moreover, if the distribution of the condensate particles is nonuniform, i.e., the "wave-function" of a particle in the condensate is periodic with the crystal period **a**, i.e.,

$$\varphi_0(\mathbf{r}+\mathbf{a})=\varphi_0(\mathbf{r}), \tag{1.1}$$

then in such a crystal there exist four branches of collective low-frequency excitation, and their spectrum is given by the following system of dispersion equations:

$$\begin{aligned}&(\omega^2-c_{lm}k_lk_m)\varphi-i\varkappa_{il}k_i\omega u_i=0,\\&(\rho_{ij}^{(n)}\omega^2-\lambda_{iljm}k_lk_m)u_j+i\varkappa_{il}k_i\omega\varphi=0,\end{aligned} \tag{1.2}$$

where c_{ij} and κ_{ij} are tensors having the symmetry of the crystal, $\rho_{ij}^{(n)}$ is the normal-density tensor of the crystal, and λ is the lattice elastic-moduli tensor (cf. I, (4.18), (4.19), and (4.20)).

One of the branches in (1.2), which corresponds to the variable φ, stems from the phonon branch in a uniform superfluid Bose system. The other three, described by the vector u_i, are genetically connected with the three acoustic modes of vibration in ordinary crystals. As is apparent from (1.2), these two groups of excitations are coupled together in a Bose crystal with condensate. Their interaction is described by tensor κ_{ij}.

Along with the normal density there exists the superfluid density

$$\rho_{ij}^{(s)}=m^2c_{ij}/a, \tag{1.3}$$

where c_{ij} is the tensor that appears in the system of equations (1.2) for the excitation spectrum, m is the mass of the free atom, and a is a new constant. The tensors $\rho_{ij}^{(n)}$ and $\rho_{ij}^{(s)}$ satisfy the obvious relation

$$\rho_{ij}^{(n)}+\rho_{ij}^{(s)}=mn\delta_{ij}, \tag{1.4}$$

where n is the particle-number density of the crystal, so that $\rho = mn$ is its specific weight.

The superfluid current is related to the superfluid veloicty by the usual expression

$$j_i^{(s)}=\rho_{ij}^{(s)}v_j^{(s)}=m^2a^{-1}c_{ij}v_j^{(s)}. \tag{1.5}$$

As in the case of a fluid, rotation of the crystal can be shown to cause dragging of only the normal part of its density.

Finally, a physical interpretation of the constant a in (1.3) is given by the expression for compressibility (cf. I, (5.20)):

$$\frac{\partial P}{\partial\rho}=\frac{n/m}{a^{-1}+\eta_{ij}\Lambda_{ijlm}\eta_{lm}}. \tag{1.6}$$

The tensors Λ and η are basically defined as in I.

On going to the case of a liquid, $\eta_{ij} \sim \rho \to 0$, $\kappa_{ij} \to 0$, and $c_{ij} \to c\delta_{ij}$. The expresisons (1.3), (1.4) and (1.6) yield

$$c=\frac{\rho^{(s)}a}{m^2}=\frac{an}{m},\qquad a=\frac{m}{n}\frac{\partial P}{\partial\rho}$$

whence one obtains the familiar result for the spectrum (1.2):

$$\omega^2=\frac{\partial P}{\partial\rho}k^2.$$

In the absence of condensate, Λ is the inverse of the elastic moduli tensor λ, $\eta_{ij} = n\delta_{ij}$, and (1.6) reduces to the trivial relation for the bulk modulus:

$$\Lambda_{iijj}=\frac{1}{\rho}\frac{\partial\rho}{\partial P}.$$

The existence of four gapless branches of the Bose spectrum, described by the dispersion system (1.2), follows from a well-known theorem by Goldstone [4] about broken symmetry. The branch corresponding to param-

eter φ is due to the noninvariance of the state with condensate under the wave-function transformation $\varphi_0(\mathbf{r}) \to \varphi_0(\mathbf{r})e^{i\alpha}$. An equivalent formulation of this property is given by the Pines-Hugengoltz theorem [5] (see also [6], Sec. 25). The other three branches of the spectrum are brought about by the broken symmetry of the system under the operations of infinitesimal translation; this type of broken symmetry has been already considered in I. Peculiar features of the effect of broken symmetry in the case of Bose systems are discussed in Sec. 2. The system of dispersion equations (1.2) is derived in Sec. 3. In Sec. 4 the relation (1.3) for the superfluid density is derived. According to the results of Sec. 3, in the presence of condensate all the four excitation branches of a Bose crystal are determined by poles of the single-particle Green's function. It is clear that as $n_0 \to 0$ at least three of the four branches persist. The only difference is that at $n_0 = 0$ their spectrum is determined by the poles of the two-particle (four-point) functions. In the last section, the density and current correlation functions are obtained, the formula (1.4) is proved, and the limit as $n_0 \to 0$ is discussed.

2. GREEN'S FUNCTIONS

In the presence of the Bose condensate the particle creation and annihilation operators $\hat{\psi}^+(x)$ and $\hat{\psi}(x)$ (where $x = (\mathbf{r}, t)$ is the space-time coordinate) averaged over the ground state with a given chemical potential, remain finite in the infinite-system limit

$$\xi(\mathbf{r}) = \langle\hat{\psi}(x)\rangle \neq 0, \quad \xi^*(\mathbf{r}) = \langle\hat{\psi}^+(x)\rangle \neq 0. \tag{2.1}$$

Owing to this circumstance, the usual form of the quantum field theory technique fails to describe the Bose systems with condensate. The necessary formalism was developed by Belyaev [7]. The appropriate derivation was carried out for uniform systems, but it can be readily generalized to the case of Bose crystals, since the uniformity is not an essential factor.

The starting point of Belyaev's formalism is splitting the Heisenberg operators $\hat{\psi}$ and $\hat{\psi}^*$ into two parts:

$$\hat{\psi}(x) = \xi(\mathbf{r}) + \hat{\psi}'(x), \quad \hat{\psi}^+(x) = \xi^*(\mathbf{r}) + \hat{\psi}'^+(x), \tag{2.2}$$

where the functions $\xi(\mathbf{r})$ and $\xi^*(\mathbf{r})$, defined by (2.1), describe the state of the condensate and are c-numbers in the thermodynamic limit, and the operators $\hat{\psi}'(x)$ and $\hat{\psi}'^+(x)$ correspond to the annihilation and creation of above-condensate particles.

On substituting (2.2) in the Hamiltonian of the system the diagram expansion assumes its conventional form. The quantities $\xi(\mathbf{r})$ and $\xi^*(\mathbf{r})$ in this case play the role of external fields which are determined from the condition that the ground-state energy E be a minimum for a given number of particles N.

According to the definition (2.1), the quantities $\xi(\mathbf{r})$ and $\xi^*(\mathbf{r})$ have the symmetry of the system's ground state and reduce for the uniform case to the constants $\xi(\mathbf{r}) = \xi^*(\mathbf{r}) = n_0^{1/2}$ (n_0 being the condensate particle density). On the other hand, in crystal these quantities assume the form:

$$\xi(\mathbf{r}) = n_0^{1/2}\varphi_0(\mathbf{r}), \quad \xi^*(\mathbf{r}) = n_0^{1/2}\varphi_0^*(\mathbf{r}), \tag{2.3}$$

where the function $\varphi_0(\mathbf{r})$, normalized to unit volume, is an invariant of the space group of the lattice. Owing to the symmetry of the system with respect to time reversal, the quantities $\xi(\mathbf{r})$ and $\xi^*(\mathbf{r})$ must be equal apart from a coordinate-independent phase factor. Having the freedom of choice for this factor, in what follows we shall use the gauge corresponding to a real condensate wave function

$$\varphi_0^*(\mathbf{r}) = \varphi_0(\mathbf{r}).$$

As in the case of uniform Bose systems, in addition to the normal Green's function $G(x, x') = -i\langle T(\hat{\psi}'(x)\hat{\psi}'^+(x'))\rangle$ (T is the time-ordering operator) in a crystal with a condensate there exist also the anomalous functions

$$\check{G}(x, x') = -i\langle T(\hat{\psi}'(x)\hat{\psi}'(x'))\rangle, \quad \hat{G}(x, x') = -i\langle T(\hat{\psi}'^+(x)\hat{\psi}'^+(x'))\rangle.$$

For convenience we shall use the Nambu [8] matrix formulation in which the Green's functions are combined to form the matrix

$$G_{\alpha\beta}(x, x') = -i\langle T(\hat{\psi}_\alpha'(x)\hat{\psi}_\beta'^+(x'))\rangle, \quad \hat{\psi}_1' = \hat{\psi}', \quad \hat{\psi}_2' = \hat{\psi}'^+. \tag{2.4}$$

From the symmetry of the system with respect to time reversal and from the definition (2.4) we have the following relations:

$$\begin{gathered} G_{11}(\mathbf{r}, t; \mathbf{r}', t') = G_{11}(\mathbf{r}', -t'; \mathbf{r}, -t), \quad G_{22}(\mathbf{r}, t; \mathbf{r}', t') = G_{22}(\mathbf{r}', -t'; \mathbf{r}, -t), \\ G_{12}(\mathbf{r}, t; \mathbf{r}', t') = G_{21}(\mathbf{r}', -t'; \mathbf{r}, -t), \quad G_{11}(\mathbf{r}, t; \mathbf{r}', t') = G_{22}(\mathbf{r}', t'; \mathbf{r}, t), \\ G_{12}(\mathbf{r}, t; \mathbf{r}', t') = G_{12}(\mathbf{r}', t'; \mathbf{r}, t). \end{gathered} \tag{2.5}$$

In the absence of external fields, taking into account the translational properties of the system, the Green's function $G_{\alpha\beta}(x, x')$ can be represented in the form

$$\begin{aligned} G_{\alpha\beta}(x, x') &= \int \frac{dk}{(2\pi)^4} G_{\alpha\beta}(\omega, \mathbf{k}; \mathbf{r}, \mathbf{r}') e^{ik(x-x')} \\ &= \int \frac{dk}{(2\pi)^4} G_{\alpha\beta}^{nm}(\omega, \mathbf{k})\varphi_n(\mathbf{r})\varphi_m^*(\mathbf{r}') e^{ik(x-x')}, \end{aligned} \tag{2.6}$$

where $k = (\mathbf{k}, \omega)$, $kx = \mathbf{k}\cdot\mathbf{r} - \omega t$, $dk = d\mathbf{k}d\omega$, we integrate over ω from $-\infty$ to ∞, and the integration over $\mathbf{k}$ is bounded by the volume of a unit cell of the reciprocal lattice (the Brillouin zone). $\{\phi_n(\mathbf{r})\}$ is an arbitrary complete orthonormal set of functions invariant with respect to the lattice translation group. In (2.6) and below we use the convention that repeated indices are to be summed over.

For convenience in the following analysis, we shall choose the basis $\{\phi_n(\mathbf{r})\}$ so as to include the condensate wave function $\phi(\mathbf{r})$ ($n = 0$) as one of its components. Three more components of the basis $\phi_i(\mathbf{r})$ ($i = 1, 2, 3$) will be taken to be proportional to $\partial\phi_0/\partial r_i$. We shall choose the coordinate axes in such a way that the functions ϕ_i and ϕ_j ($i \neq j = 1, 2, 3$) will also be orthogonal to each other. The other components of the basis $\phi_n(\mathbf{r})$ ($n \neq 0, 1, 2, 3$) will be regarded as arbitrary. In what follows $\phi_0(\mathbf{r})$ will be referred to as the scalar and the set $\phi_i(\mathbf{r})$ as the vector components of the basis $\{\phi_n(\mathbf{r})\}$.

The function $G_{\alpha\beta}^{nm}(\omega, \mathbf{k})$ is related to the Green's function $\hat{G}^{(0)}$ of the noninteracting system by the Dyson equation

$$\hat{G} = \hat{G}^{(0)} + \hat{G}^{(0)}\hat{\Sigma}\hat{G}. \tag{2.7}$$

In the coordinate representation the self-energy part $\Sigma_{\alpha\beta}(x, x')$ satisfies the same symmetry relations that the Green's function (2.5). It is convenient to define the bare Green's function $\hat{G}_0$ then takes the form

$$\begin{gathered} G_{11}^{(0)nm}(\omega, \mathbf{k}) = \frac{\delta_{nm}}{\omega + \mu}, \quad G_{22}^{(0)nm}(\omega, \mathbf{k}) = \frac{\delta_{nm}}{-\omega + \mu}, \\ G_{12}^{(0)nm}(\omega, \mathbf{k}) = G_{21}^{(0)nm}(\omega, \mathbf{k}) = 0, \end{gathered} \tag{2.8}$$

where μ is the chemical potential.

Let us now proceed to derive the relations which follow from the broken symmetry property of the system with respect to gauge and translational transformations. We note first that since $\xi(\mathbf{r})$ and $\xi^*(\mathbf{r})$ minimize the energy E of the system at a constant total number of parti-

cles N, the thermodynamic potential $\Omega = E - N\mu$ satisfies the conditions

$$\left(\frac{\delta\Omega}{\delta\xi^*(\mathbf{r})}\right)_\mu = 0, \quad \left(\frac{\delta\Omega}{\delta\xi(\mathbf{r})}\right)_\mu = 0. \tag{2.9}$$

These relations, as well as the quantities E and Ω, are invariant under the gauge transformation

$$\xi(\mathbf{r}) \to \xi(\mathbf{r}) e^{i\alpha}, \quad \xi^*(\mathbf{r}) \to \xi^*(\mathbf{r}) e^{-i\alpha}.$$

We subject the relations (2.9) to this transformation, and then, since α is arbitrary, differentiate them with respect to α and thereupon let $\alpha = 0$. As the result, we obtain

$$\mu\delta_{0l} = \Sigma_{11}^{0l}(0, 0) - \Sigma_{12}^{0l}(0,0). \tag{2.10}$$

We have taken into account here the fact that the quantities $\delta^2 E/\delta\xi^*(\mathbf{r})\delta\xi(\mathbf{r}')$ and $\delta^2 E/\delta\xi^*(\mathbf{r})\delta\xi^*(\mathbf{r}')$ are determined by sets of G-line-irreducible graphs containing, respectively, an incoming and outgoing or else two outgoing G-lines, and, therefore,

$$\begin{aligned} \delta^2 E/\delta\xi^*(\mathbf{r})\delta\xi(\mathbf{r}') &= \Sigma_{11}(0, 0; \mathbf{r}, \mathbf{r}'), \\ \delta^2 E/\delta\xi^*(\mathbf{r})\delta\xi^*(\mathbf{r}') &= \Sigma_{12}(0, 0; \mathbf{r}, \mathbf{r}'). \end{aligned} \tag{2.11}$$

The energy and the thermodynamic potential of the system, and hence the expressions (2.9), also remain invariant under a displacement of the crystal by an arbitrary vector **a**. Upon doing the transformation

$$\xi(\mathbf{r}) \to \xi(\mathbf{r}+\mathbf{a}), \quad \xi^*(\mathbf{r}) \to \xi^*(\mathbf{r}+\mathbf{a}),$$

we differentiate (2.9) with respect to **a**, and then let **a** = 0. As the result, taking (2.11) into account, we obtain

$$\mu\delta_{il} = \Sigma_{11}^{il}(0, 0) + \Sigma_{12}^{il}(0, 0). \tag{2.12}$$

We recall that subscripts i = 1, 2, 3 correspond to the functions $\partial\varphi_0/\partial r_i$.

Let us emphasize that the relation (2.10), being a consequence of the broken symmetry of the ground state with respect to gauge transformations, is a generalization of the Pines-Hugengoltz theorem[5] to the crystal case. Relation (2.12) results from the broken symmetry of the ground state of the system with respect to arbitrary translations. It has no analog in the case of uniform systems.

3. EXCITATION SPECTRUM

Let us investigate the singularities of the Green's functions which, as is well-known[6], determine the excitation spectrum of a system. We shall first prove that $G_{\alpha\beta}(\omega, \mathbf{k}; \mathbf{r}, \mathbf{r}')$ has a fourfold degenerate pole at ω, $\mathbf{k} = 0$. To do so, we observe that the poles of this function correspond to nontrivial solutions of the system of homogeneous equations.

$$\int d\mathbf{r}' G_{\alpha\beta}^{-1}(\omega, \mathbf{k}; \mathbf{r}, \mathbf{r}') X_\beta(\mathbf{r}') = 0, \tag{3.1}$$

$$G_{\alpha\beta}^{-1}(\omega, \mathbf{k}; \mathbf{r}, \mathbf{r}') = G_{\alpha\beta}^{(0)-1}(\omega, \mathbf{k}; \mathbf{r}, \mathbf{r}') - \Sigma_{\alpha\beta}(\omega, \mathbf{k}; \mathbf{r}, \mathbf{r}'). \tag{3.2}$$

Whence, taking into consideration (2.8) and (2.10), we see that one of the solutions of (3.1) at ω, $\mathbf{k} = 0$ is

$$\hat{X}^0(\mathbf{r}) = \varphi_0(\mathbf{r}) \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

Three more solutions of the system (3.1) at ω, $\mathbf{k} = 0$ follow from the theorem (2.12):

$$\hat{X}^i(\mathbf{r}) = \frac{\partial\varphi_0(\mathbf{r})}{\partial r_i} \begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

The residues of the Green's functions at the above poles are obviously proportional to bilinear combinations of the functions $\hat{X}^0(\mathbf{r})$, $\hat{X}^i(\mathbf{r})$ with $\hat{X}^0(\mathbf{r}')$, $\hat{X}^i(\mathbf{r}')$.

In order to elucidate the structure of the poles at ω, $\mathbf{k} \neq 0$, we determine the self-energy part $\overline{\Sigma}_{\alpha\beta}^{mn}(\omega, \mathbf{k})$ which is irreducible in the scalar and vector components of the bare function $G_{\alpha\beta}^{(0)nm}$ (n, m = 0, 1, 2, 3) and reducible in all its other components. The function $\overline{\Sigma}_{\alpha\beta}^{mn}$ is connected with the irreducible self-energy part $\Sigma_{\alpha\beta}^{mn}$ by the obvious equation

$$\overline{\Sigma}_{\alpha\beta}^{nm} = \Sigma_{\alpha\beta}^{nm} + \sum_{l\neq 0,1,2,3} \Sigma_{\alpha\gamma}^{nl} G_{\gamma\delta}^{(0)} \overline{\Sigma}_{\delta\beta}^{lm}. \tag{3.3}$$

If we now change from Σ to $\overline{\Sigma}$ in the Dyson equation (2.7) we can then isolate in the infinite system of equations (2.7) an independent finite subsystem for the functions $G_{\alpha\beta}^{\mu\nu}(\omega, \mathbf{k})$ (μ, ν = 0, 1, 2, 3):

$$G_{\alpha\beta}^{\mu\nu}(\omega, \mathbf{k}) = G_{\alpha\beta}^{(0)}(\omega, \mathbf{k})\delta_{\mu\nu} + G_{\alpha\gamma}^{(0)}(\omega, \mathbf{k})\overline{\Sigma}_{\gamma\delta}^{\mu\mu'}(\omega, \mathbf{k}) G_{\gamma\delta}^{\mu'\nu}(\omega, \mathbf{k}). \tag{3.4}$$

We consider first the case $\mathbf{k} = 0$, $\omega \neq 0$. Because of the symmetry, the quantities $\overline{\Sigma}_{\alpha\beta}^{0i}(\omega, 0)$ and $\overline{\Sigma}_{\alpha\beta}^{i0}(\omega, 0)$ (i = 1, 2, 3) vanish, and the system (3.4) splits into two subsystems:

$$\begin{aligned} G_{\alpha\beta}^{00}(\omega, 0) &= G_{\alpha\beta}^{(0)}(\omega, 0) + G_{\alpha\gamma}^{(0)}(\omega, 0)\overline{\Sigma}_{\gamma\delta}^{00}(\omega, 0) G_{\delta\beta}^{00}(\omega, 0), \\ G_{\alpha\beta}^{ij}(\omega, 0) &= G_{\alpha\beta}^{(0)}(\omega, 0)\delta_{ij} + G_{\alpha\gamma}^{(0)}(\omega, 0)\overline{\Sigma}_{\gamma\delta}^{ii'}(\omega, 0) G_{\delta\beta}^{i'j}(\omega, 0). \end{aligned} \tag{3.5}$$

It can be readily seen with the help of (3.3) that the relations (2.10) and (2.12) also remain valid if we replace Σ by $\overline{\Sigma}$. In view of this, the solution of (3.5), to within terms nonsingular at $\omega \to 0$, can be written in the form:

$$\begin{aligned} G_{11}^{00}(\omega, 0) &= G_{22}^{00}(-\omega, 0) = \frac{a}{\omega^2} n_0 \left(1 + \omega \frac{1 - \Pi_{11}^{00}}{\overline{\Sigma}_{12}^{00}}\right), \\ G_{12}^{00}(\omega, 0) &= G_{21}^{00}(\omega, 0) = -\frac{a}{\omega^2} n_0, \\ G_{11}^{ij}(\omega, 0) &= G_{22}^{ij}(-\omega, 0) = \frac{n_0}{\omega^2}\{\hat{\rho}^{(n)-1}[\hat{1} - \hat{\Sigma}_{12}^{-1}(\hat{1} - \hat{\Pi}_{11})\omega]\}_{ij}, \\ G_{12}^{ij}(\omega, 0) &= G_{21}^{ij}(\omega, 0) = \frac{n_0}{\omega^2}\hat{\rho}_{ij}^{(n)-1}. \end{aligned} \tag{3.6}$$

We have here used the notation

$$\begin{aligned} a^{-1} &= \frac{n_0}{\overline{\Sigma}_{12}^{00}}[(1 - \Pi_{11}^{00}) - \overline{\Sigma}_{12}^{00}(P_{11}^{00} - P_{12}^{00})], \\ \rho_{ij}^{(n)} &= n_0\{\hat{\Sigma}_{12}^{-1}[(1 - \hat{\Pi}_{11})^2 + \hat{\Sigma}_{12}(\hat{P}_{11} + \hat{P}_{12})]\}_{ij}, \\ \overline{\Sigma}_{\alpha\beta}^{00} &= \overline{\Sigma}_{\alpha\beta}^{00}(0, 0), \quad (\hat{\Sigma}_{\alpha\beta})_{ij} = \overline{\Sigma}_{\alpha\beta}^{ij}, \\ \Pi_{\alpha\beta}^{00} &= \frac{\partial}{\partial\omega}\overline{\Sigma}_{\alpha\beta}^{00}|_{\omega=0}, \quad \hat{\Pi}_{\alpha\beta} = \frac{\partial}{\partial\omega}\hat{\Sigma}_{\alpha\beta}|_{\omega=0}, \\ P_{\alpha\beta}^{00} &= \frac{\partial^2}{\partial\omega^2}\overline{\Sigma}_{\alpha\beta}^{00}|_{\omega=0}, \quad \hat{P}_{\alpha\beta} = \frac{\partial^2}{\partial\omega^2}\hat{\Sigma}_{\alpha\beta}|_{\omega=0}. \end{aligned}$$

In deriving the expressions for $G_{\alpha\beta}^{ij}(\omega, 0)$ use has been made of the fact that the crystal structure of solid He^4 is either cubic or hexagonal. Due to the appropriate symmetry, all the components $\hat{\Sigma}_{\alpha\beta}(\omega, 0)$ are symmetrical tensors which can be brought into diagonal form in a common coordinate system.

The functions $G_{\alpha\beta}^{\mu\nu}(\omega, 0)$ in (3.6), to within terms regular at $\omega \to 0$, can be written in the form

$$G_{\alpha\beta}^{\mu\nu}(\omega, 0) = S_\alpha^{\mu\mu'}(\omega) D_{\mu'\nu'}(\omega, 0) S_\beta^{\nu'\nu}(\omega); \tag{3.7}$$

$$\begin{aligned} D_{00}(\omega, 0) &= \frac{a}{\omega^2}, \quad D_{ij}(\omega, 0) = \rho_{ij}^{(n)-1}\frac{1}{\omega^2}, \\ D_{i0}(\omega, 0) &= D_{0i}(\omega, 0) = 0; \\ S_1^{00}(\omega) &= -S_2^{00}(-\omega) = n_0^{1/2}\left(1 + \omega\frac{1 - \Pi_{11}^{00}}{2\overline{\Sigma}_{12}^{00}}\right), \end{aligned} \tag{3.8}$$

$$S_1^{ij}(\omega)=S_2^{ij}(-\omega)=n_0^{1/2}\left[\delta_{ij}-\frac{\omega}{2}(\hat{\tilde{\Sigma}}_{12}^{-1}(\hat{1}-\hat{\Pi}_{11}))_{ij}\right], \quad (3.9)$$
$$S_\alpha^{0i}(\omega)=S_\alpha^{i0}(\omega)=0.$$

An examination of (3.4) shows that the factorization form of $G^{\mu\nu}_{\alpha\beta}$ in terms of the subscripts α and β is preserved as we go over to the case k = 0:

$$G_{\alpha\beta}^{\mu\nu}(\omega,\mathbf{k})=S_\alpha^{\mu\mu'}(\omega)D_{\mu'\nu'}(\omega,\mathbf{k})S_\beta^{\nu'\nu}(\omega). \quad (3.10)$$

A substitution of this expression in (3.4) leads to the following system of equations for $D_{\mu\nu}(\omega, \mathbf{k})$:

$$\begin{aligned}
D_{00}(\omega,\mathbf{k})&=D_{00}^0(\omega,\mathbf{k})+D_{00}^0(\omega,\mathbf{k})a^{-1/2}\varkappa_i(\omega,\mathbf{k})D_{i0}(\omega,\mathbf{k}),\\
D_{i0}(\omega,\mathbf{k})&=D_{ii'}(\omega,\mathbf{k})a^{-1/2}\varkappa_{i'}(\omega,\mathbf{k})D_{00}(\omega,\mathbf{k}), \quad (3.11)\\
D_{ij}(\omega,\mathbf{k})&=D_{ij}^0(\omega,\mathbf{k})-D_{ii'}(\omega,\mathbf{k})a^{-1/2}\varkappa_{i'}(\omega,\mathbf{k})D_{0j}(\omega,\mathbf{k}),\\
D_{0i}(\omega,\mathbf{k})&=D_{00}^0(\omega,\mathbf{k})a^{-1/2}\varkappa_{i'}(\omega,\mathbf{k})D_{i'i}(\omega,\mathbf{k}),
\end{aligned}$$

where the functions $D_{00}^0(\omega, \mathbf{k})$ and $D_{ij}(\omega, \mathbf{k})$ are defined by

$$\begin{aligned}
D_{00}^0(\omega,\mathbf{k})&=\frac{a}{\omega^2-c_{lm}k_lk_m},\\
\hat{D}_{ij}^{0-1}(\omega,\mathbf{k})&=\rho_{ij}^{(n)}\omega^2-\lambda_{ilmj}k_lk_m,
\end{aligned} \quad (3.12)$$

and the quantities c_{lm}, λ_{ilmj}, and $\varkappa_i(\omega, \mathbf{k})$ are equal to

$$\begin{aligned}
c_{lm}&=an_0\frac{\partial^2}{\partial k_l\,\partial k_m}(\overline{\Sigma}_{11}^{00}(0,\mathbf{k})-\overline{\Sigma}_{12}^{00}(0,\mathbf{k}))|_{k=0},\\
\lambda_{ilmj}&=n_0\frac{\partial^2}{\partial k_l\,\partial k_m}(\overline{\Sigma}_{11}^{ij}(0,\mathbf{k})+\overline{\Sigma}_{12}^{ij}(0,\mathbf{k}))|_{k=0}, \quad (3.13)\\
\varkappa_i(\omega,\mathbf{k})&=a^{1/2}n_0S_\alpha^{ii'}(\omega)\Sigma_{\alpha\beta}^{i'0}(\omega,\mathbf{k})S_\beta^{00}(\omega).
\end{aligned}$$

Using (3.9) and the symmetry conditions (2.5) we find easily that $\varkappa_i(\omega, \mathbf{k})$ is an odd function of frequency. Therefore, to within the required accuracy it can be written in the form:

$$\varkappa_i(\omega,\mathbf{k})=i\omega\varkappa_{il}k_l. \quad (3.14)$$

The dependence of the frequency on the wave vector at the poles of $D_{\mu\nu}(\omega, \mathbf{k})$ is given by the requirement that a nontrivial solution exist for the homogeneous system corresponding to (3.11). Taking (3.12) and (3.14) into account, this system assumes the form (1.2), which gives the sought system of dispersion equations for four low-frequency excitation branches of the Bose crystal. All are the result of the broken symmetry of the system (gauge invariance and translational symmetry). Let us emphasize that the dispersion law of the four branches is linear:

$$\omega_\mu(\mathbf{k})=c_\mu(\mathbf{k}/|\mathbf{k}|)|\mathbf{k}|.$$

It should be noted that the system of dispersion equations (1.2), which we obtained on the basis of a microscopic theory, is identical in its structure to the appropriate system of Andreev and Lifshitz [3]. The parameters they use have the following correspondence to the constants introduced in the present section:

$$\left(\frac{\partial\rho}{\partial\mu}\right)_{u_{il}}=\frac{m^2}{a}, \quad \left(\frac{\partial\rho}{\partial u_{il}}\right)_\mu+\rho_{il}^{(n)}=\frac{m^2}{a}\varkappa_{il}$$

(u_{il} is the lattice deformation tensor).

4. SUPERFLUIDITY

As is well-known [9], systems of interacting Bose particles, containing the Bose condensate, possess the property of superfluidity. Let us determine the Bose-crystal macroscopic mass-current density $\mathbf{j}^{(s)}$ which corresponds to the motion of the superfluid component with a given velocity $\mathbf{v}^{(s)}$.

In the linear approximation this relation should be of the form:

$$j_i^{(s)}=\rho_{ij}^{(s)}v_j^{(s)}, \quad (4.1)$$

where $\rho_{ij}^{(s)}$ is a symmetrical second-rank tensor which can be naturally called the density tensor of the crystal's superfluid component.

In order to relate the tensor $\rho_{ij}^{(s)}$ with the constants that have already been introduced in the theory, we note that, since in the diagram technique the condensate plays the role of an external field, the vector j_i is a functional of the quantities $\xi(\mathbf{r})$ and $\xi^*(\mathbf{r})$: $j_i = j_i\{\xi, \xi^*\}$. In the absence of true external fields, $j_i = 0$ for static boundary conditions and for a condensate at rest. If we keep the first two conditions and go over to the case of slowly moving condensate, the current density will then take the form:

$$j_i^{(s)}=\int d\mathbf{r}\left[\frac{\delta j_i\{\xi,\xi^*\}}{\delta\xi(\mathbf{r})}\delta\xi(\mathbf{r})+\frac{\delta j_i\{\xi,\xi^*\}}{\delta\xi^*(\mathbf{r})}\delta\xi^*(\mathbf{r})\right].$$

Since the indicated transition corresponds to the transformation

$$\begin{aligned}
\xi(\mathbf{r})&\to\xi(\mathbf{r})\exp(im\mathbf{v}^{(s)}\mathbf{r})=n_0^{1/2}\varphi_0(\mathbf{r})\exp(im\mathbf{v}^{(s)}\mathbf{r}),\\
\xi^*(\mathbf{r})&\to\xi^*(\mathbf{r})\exp(-im\mathbf{v}^{(s)}\mathbf{r})=n_0^{1/2}\varphi_0(\mathbf{r})\exp(-im\mathbf{v}^{(s)}\mathbf{r}),
\end{aligned}$$

we obtain the following expression for the current density in the approximation linear in $\mathbf{v}^{(s)}$:

$$j_i^{(s)}=mv_j^{(s)}\lim_{k\to0}\frac{\partial}{\partial k_j}\int d\mathbf{r}\,n_0^{1/2}\varphi_0(\mathbf{r})e^{-i\mathbf{kr}}\left(\frac{\delta j_i\{\xi,\xi^*\}}{\delta\xi^*(\mathbf{r})}-\frac{\delta j_i\{\xi,\xi^*\}}{\delta\xi(\mathbf{r})}\right) \quad (4.2)$$

In writing this formula we have used the fact that, according to the symmetry conditions, the integral

$$\int d\mathbf{r}\frac{\delta j_i\{\xi,\xi^*\}}{\delta\xi(\mathbf{r})}\varphi_0(\mathbf{r})e^{i\mathbf{kr}}$$

is an odd function of $\mathbf{k}$ as $\mathbf{k}\to0$. Comparing (4.2) with the relation (A.14) derived in the Appendix and keeping in mind that j_i stands for the quantity $\langle\hat{j}_i(\mathbf{x})\rangle$ averaged over the dimensions of unit cell, we obtain

$$j_i^{(s)}=m^2c_{ij}v_j^{(s)}/a.$$

whence, from the definition (4.1), we find the expression for the superfluid density tensor of the crystal.

5. CORRELATION FUNCTIONS

We introduce the correlation functions $R_{\mu\nu}(\mathbf{x}, \mathbf{x}')$ (μ, ν = 0, 1, 2, 3) by the formulae

$$\begin{aligned}
R_{00}(x,x')&=-i\langle T(\hat{n}(x)\hat{n}(x'))\rangle, \quad R_{0i}(x,x')=-i\langle T(\hat{n}(x)\hat{j}_i(x'))\rangle,\\
R_{i0}(x,x')&=-i\langle T(\hat{j}_i(x)\hat{n}(x'))\rangle, \quad R_{ij}(x,x')=-i\langle T(\hat{j}_i(x)\hat{j}_j(x'))\rangle,
\end{aligned} \quad (5.1)$$

where

$$\begin{aligned}
\hat{n}(x)&=\hat{\psi}^+(x)\hat{\psi}(x),\\
j_i(x)&=\frac{1}{2i}\left(\hat{\psi}^+(x)\frac{\partial\hat{\psi}(x)}{\partial r_i}-\frac{\partial\hat{\psi}^+(x)}{\partial r_i}\hat{\psi}(x)\right)
\end{aligned}$$

are the particle-density and mass-flux-density operators.

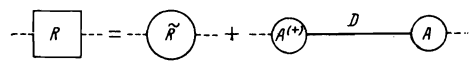
We are interested in expressions for the functions

$$R_{\mu\nu}(\omega,\mathbf{k})=\int_{v_c}\frac{d\mathbf{r}}{v_c}\int dx'\,e^{-ik(x-x')}R_{\mu\nu}(x,x') \quad (5.2)$$

in the long-wave and low-frequency domain ($\omega, \mathbf{k}\to0$); v_c is the volume of the lattice unit cell.

It is clear that each function $R_{\mu\nu}$ corresponds to a set of diagrams having one incoming and one outgoing line for interactions with either the scalar of the vector field, depending on the values of μ and ν.

It is convenient to represent $R_{\mu\nu}$ as a sum of two terms, one irreducible and the other reducible with respect to the Green's function:



or in the equivalent analytic form:

$$R_{\mu\nu}(\omega, \mathbf{k}) = \tilde{R}_{\mu\nu} + A^{(+)}_{\mu\mu'}(\omega, \mathbf{k}) D_{\mu'\nu'}(\omega, \mathbf{k}) A_{\nu'\nu}(\omega, \mathbf{k}). \quad (5.3)$$

As $\omega, \mathbf{k} \to 0$, the Green's functions $D_{\mu\nu}$ are the only source of singularities of the correlation functions. The irreducible part $\tilde{R}_{\mu\nu}$ can therefore be regarded as a constant equal to its value at $\omega, \mathbf{k} = 0$.

$A_{\mu\nu}(\omega, \mathbf{k})$ is given by a set of graphs which have one incoming line for the D-function and one outgoing line for the interaction with an external field. The latter is either a scalar or a vector, depending on whether the subscript ν takes the value 0 or 1, 2, 3. Similarly, $A^{(+)}_{\mu\nu}$ is given by a set of diagrams each having one incoming line for the μ-th component of external field and an outgoing line for the D-functions.

The symmetry property of the system with respect to time reversal enables us to establish the following relations:

$$A_{00}(\omega, \mathbf{k}) = -A_{00}(-\omega, \mathbf{k}), \quad A_{0i}(\omega, \mathbf{k}) = A_{0i}(-\omega, \mathbf{k}), \quad A_{i0}(\omega, \mathbf{k}) = A_{i0}(-\omega, \mathbf{k}),$$
$$A_{ij}(\omega, \mathbf{k}) = -A_{ij}(-\omega, \mathbf{k}), \quad A^{(+)}_{\mu i}(\omega, \mathbf{k}) = -A_{i\mu}(\omega, \mathbf{k}), \quad A^{(+)}_{\mu 0}(\omega, \mathbf{k}) = A_{0\mu}(\omega, \mathbf{k}); \quad (5.4)$$

i, j = 1, 2, 3; μ = 0, 1, 2, 3. From this, and using the equality

$$A_{\mu\nu}(0, 0) = A^{(+)}_{\mu\nu}(0, 0) = 0,$$

which follows from the physical requirement that $R_{\mu\nu}(0, \mathbf{k})$ and $R_{\mu\nu}(\omega, 0)$ be finite, we obtain in the long-wave and low-frequency limit

$$A_{00} = b\omega, \quad A_{0i} = d_{il}k_l,$$
$$A_{i0} = -i\eta_{il}k_l, \quad A_{ij} = -ih_{ij}\omega, \quad (5.5)$$

where d_{il}, η_{il}, and h_{il} are symmetrical second-rank tensors.

The constants b, d_{il}, η_{il}, and h_{il} are not really independent, and can be expressed in terms of the constants introduced before. It is shown in the Appendix [(A.4), (A.8), (A.12)] that

$$b = a^{-1}, \quad d_{ij} = mc_{ij}/a, \quad h_{ij} = \rho^{(n)}_{ij}. \quad (5.6)$$

From the conservation of total particle number and total momentum it follows that

$$R_{\mu\nu}(\omega, 0) = 0,$$

whence, in view of the equalities (5.3)—(5.6), we have

$$\tilde{R}_{00} = -a^{-1}, \quad \tilde{R}_{0i} = \tilde{R}_{i0} = 0, \quad \tilde{R}_{ij} = -\rho^{(n)}_{ij}. \quad (5.7)$$

Two more relations follow from the identities

$$m\omega R_{00} - k_i R_{i0} = 0,$$
$$m^2\omega^2 R_{00} - k_i k_j R_{ij} = nm\delta_{ij}, \quad (5.8)$$

which are a consequence of the continuity equation satisfied by the operators $m\hat{n}(x)$ and $\hat{j}_j(x)$. Substituting (5.3) in (5.8) and using (5.4)—(5.7), (3.11), and (3.12), we obtain

$$\eta_{ij} = m^{-1}\rho^{(n)}_{ij} - a^{-1/2}\varkappa_{ij}, \quad (5.9)$$

$$\rho^{(n)}_{ij} + m^2 a^{-1} c_{ij} = nm\delta_{ij}. \quad (5.10)$$

In view of the formula (1.3) proved in the preceding section, Eq. (5.10) reduces to (1.4). The expressions (5.3)—(5.10) give a complete solution to the problem of Bose-crystal correlation functions. Using these results, we shall prove the statement that only the normal part of the density is carried along by a crystal's rotation. To do so, we note that the increment of the system's Hamiltonian, which arises from the rotation and is linear in its angular velocity $\boldsymbol{\Omega}$, is of the form

$$\hat{H}_1 = -\int d\mathbf{r}\, \hat{j}_i(x) v_i(\mathbf{r}), \quad \mathbf{v}(\mathbf{r}) = [\mathbf{r} \times \boldsymbol{\Omega}].$$

Hence, if we turn on the rotation adiabatically slowly at $t \to -\infty$, the average value of the mass-flux density will then, according to linear-response theory and definitions (5.1) and (5.2), be equal to

$$j_i = -\int d\mathbf{r}' \int \frac{d\mathbf{k}}{(2\pi)^3} R_{ij}(0, \mathbf{k}) e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}')} v_j(\mathbf{r}').$$

Substituting here the expression

$$R_{ij}(0, \mathbf{k}) = -\rho^{(n)}_{ij} - \frac{m^2}{a}\frac{c_{il}k_l c_{jm}k_m}{c_{rs}k_r k_s},$$

which follows from (5.3)—(5.7), we obtain the formula

$$j_i = \rho^{(n)}_{ij} v_j,$$

which proves the above statement.

Let us now derive the compressibility formula (1.6). For this purpose we make use of the expression for $R_{00}(0, \mathbf{k})$ which, according to (5.3)—(5.9), is equal to

$$R_{00}(0, \mathbf{k}) = -a^{-1} + \eta_{il}k_l D_{ij}(0, \mathbf{k}) \eta_{jm}k_m, \quad (5.11)$$

where, in agreement with (3.11), (3.12), and (3.14)

$$D_{ij}^{-1}(0, \mathbf{k}) = -\lambda_{ilmj}k_l k_m.$$

Next, we pass to the limit $\mathbf{k} \to 0$ in (5.11) taking into account the effect of the finite size of the crystal. Substitution of the result into the formula

$$\frac{\partial P}{\partial \rho} = \frac{n}{m}\left(\frac{\partial n}{\partial \mu}\right)^{-1} = -\frac{n}{m}[\lim_{\mathbf{k}\to 0} R_{00}(0, \mathbf{k})]^{-1}$$

(which follows from the thermodynamics) leads to (1.6).

As another application of the correlation functions we determine the linear response of the lattice structure to an external scalar field $\delta\varphi e^{i\mathbf{kx}}$. To do this, one should follow the method applied in I to exactly the same problem for the case of a Fermi crystal. Omitting the details of the derivation, we present only the final result for the deformation tensor

$$w_{ik}(\mathbf{R}, t) = \partial u_k(\mathbf{R}, t)/\partial R_i$$

(where $\mathbf{u}(\mathbf{R}, t)$ is the displacement vector of the lattice sites and $\mathbf{R}$ the macroscopic coordinate):

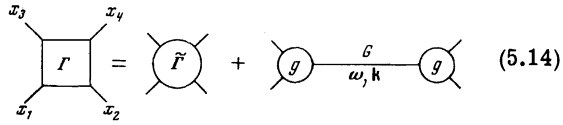
$$w_{ik}(\mathbf{R}, t) = k_k D_{ij}(\omega, \mathbf{k}) \eta_{jm}(\omega, \mathbf{k}) k_m \delta\varphi e^{i(\mathbf{kR}-\omega t)}, \quad (5.12)$$

where the function $\eta_{jm}(\omega, \mathbf{k})$ is of the form:

$$\eta_{jm}(\omega, \mathbf{k}) = \eta_{jm} + a^{-1/2}\varkappa_{jm}\frac{\omega^2}{\omega^2 - c_{rs}k_r k_s}. \quad (5.13)$$

In conclusion, we shall discuss the limiting case of vanishing density of the Bose condensate, $n_0 \to 0$. In the absence of condensate there exists only one type of broken symmetry, namely with respect to arbitrary translations. Therefore, at $n_0 = 0$ there are grounds for only three gapless excitation branches, corresponding in this case to acoustic phonons. At $n_0 \neq 0$ the poles as-

sociated with these branches are contained in the single-particle G-function. Since three-point vertices exist at $n_0 \neq 0$, the indicated poles also belong to the two-particle vertex part of Γ:



(5.14)

According to the results of Sec. 3 the singular terms in the G-functions are proportional to n_0. Let us prove now that the poles associated with acoustic phonons, which vanish in the G-functions, nonetheless remain in the vertex Γ. It is essential here that the singular part of Γ turns out to be equal to the limit to which the second term in (5.14) tends. To proceed with the proof, we observe that a simultaneous displacement of both space arguments of the self-energy part $\Sigma(x, x')$ as well as of the arguments of functions $\xi(\mathbf{r})$, $\xi^*(\mathbf{r})$ (of which Σ is a functional) by an infinitesimal distance $\delta\mathbf{a}$ leaves the function $\Sigma(x, x')$ invariant. This implies that

$$\frac{\partial\Sigma(x_1,x_3)}{\partial r_1^{\,i}}+\frac{\partial\Sigma(x_1,x_3)}{\partial r_3^{\,i}}+\sqrt{n_0}\int d\mathbf{r}'\,\frac{\partial\varphi_0(\mathbf{r}')}{\partial r_i'}\left[\frac{\delta\Sigma(x_1,x_3)}{\delta\xi(\mathbf{r}')}+\frac{\delta\Sigma(x_1,x_3)}{\delta\xi^*(\mathbf{r}')}\right]=0.$$

From this equality, in view of the remark made in the Appendix in derivation of (A.14), it follows that at $k = 0$ the three-point vertex $g_i(x_1, x_3; k)$ is equal to

$$g_i(x_1,x_3;0)=-n_0^{-1/2}\left[\frac{\partial\Sigma(x_1,x_3)}{\partial r_1^{\,i}}+\frac{\partial\Sigma(x_1,x_3)}{\partial r_3^{\,i}}\right].$$

The factor n_0^{-1} arising from the product $g_i(x_1, x_3; k)$ $g_j(x_2, x_4; -k)$ cancels the factor n_0 to which the G-function at the pole in the second term of (5.14) is proportional. Therefore, the contribution to the pole due to the second term in (5.14) remains finite as $n_0 \to 0$. In this case, the residue of Γ at $\mathbf{k}$, $\omega = 0$ can be readily seen to coincide with the residue of Γ in the case of Fermi crystal (see I, (3.13)).

APPENDIX

We shall prove here a number of the above-employed identities which follow from general symmetry properties of the system.

To establish the first of them, we consider a uniform external scalar field $\delta\varphi e^{-i\omega t}$ whose interaction with the system is described by a Hamiltonian of the form:

$$H_{int}=\delta\varphi e^{-i\omega t}\hat{N},\quad \hat{N}=\int d\mathbf{r}\,\hat{\psi}^+(x)\hat{\psi}(x), \tag{A.1}$$

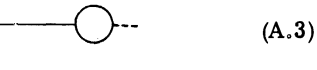
Since the total particle-number operator $\hat{N}$ commutes with the main Hamiltonian of the system, we note that, as this field is turned on, the Heisenberg operator $\hat{\psi}(x)$ transforms according to the following law

$$\hat{\psi}(x)\to\hat{\psi}(x)\exp\left(\frac{\delta\varphi}{\omega}e^{-i\omega t}\right).$$

Whence the linear response of $\langle\hat{\psi}(x)\rangle$ to the field (A.1) is of the form

$$\delta\langle\hat{\psi}(x)\rangle=\frac{\delta\varphi}{\omega}e^{-i\omega t}n_0^{1/2}\varphi_0(\mathbf{r}). \tag{A.2}$$

On the other hand, by virtue of the general diagram technique, this quantity is determined by a set of graphs each having one incoming line for the particle field and one outgoing line for interaction with the external scalar field:

$\delta\langle\hat{\psi}(x)\rangle =$  (A.3)

The circle in the graph stands for the quantity $A_{00}(\omega, 0) = b\omega$, introduced in Sec. 5. Comparing the equalities (A.2) and (A.3), in view of (3.8), (3.9), we obtain the identity

$$b=a^{-1}. \tag{A.4}$$

The second relation will be derived by considering the linear response of the system to a uniform external vector field of the form

$$\hat{H}_{int}=\delta v_i e^{-i\omega t}\int d\mathbf{r}\,\hat{j}_i(x) \tag{A.5}$$

(where $\hat{j}_i(x)$ is the mass-flux density operator of the system). Taking into account that the total mass flux coincides with the total momentum and the latter operator commutes with the main Hamiltonian of the crystal, we obtain the following expression for the linear response of $\langle\hat{\psi}(x)\rangle$

$$\delta\langle\hat{\psi}(x)\rangle=-i\frac{\delta v_i}{\omega}e^{-i\omega t}n_0^{1/2}\frac{\partial\varphi_0(\mathbf{r})}{\partial r_i}. \tag{A.6}$$

This quantity can also be determined by considering the vector component of the diagram relation (A.3). In this case, the line with the arrow will correspond to the expression $S_1^{ii'}(\omega)D_{i'j'}(\omega, 0)$, and the circle will correspond to the quantity $A_{ij}(\omega, 0) = -ih_{ij}\omega$ defined in Sec. 5:

$$\delta\langle\hat{\psi}(x)\rangle=-i\frac{\partial\varphi_0}{\partial r_i}S_1^{\alpha\alpha'}(\omega)D_{i'j'}(\omega,0)A_{j'j}(\omega,0)\delta v_j e^{-i\omega t}. \tag{A.7}$$

Comparing (A.6) and (A.7), and taking (3.8) and (3.9) into account, we obtain

$$h_{ij}=\rho_{ij}^{(n)}. \tag{A.8}$$

One more identity will be established by considering the response of the system to a static vector field

$$\hat{H}_{int}=\delta v_i\int d\mathbf{r}\,e^{i\mathbf{k}\mathbf{r}}\hat{j}_i(x). \tag{A.9}$$

As $\mathbf{k} \to 0$ the switching-on of such a field is equivalent to changing to a coordinate frame which moves with the velocity δv_i, and, therefore, the appropriate transformation of the operator $\hat{\psi}(x)$ is of the form

$$\hat{\psi}(x)\to\hat{\psi}(x)e^{-im\delta\mathbf{v}\mathbf{r}},$$

where m is the mass of an isolated crystal atom. This gives us an expression for the linear response of the average value of the ψ-operator:

$$\delta\langle\hat{\psi}(x)\rangle=-i\mathbf{r}\delta v n_0^{1/2}\varphi_0(\mathbf{r})m. \tag{A.10}$$

On the other hand, the scalar component of the diagram relation, in the case of interaction with the field (A.9), yields

$$\delta\langle\hat{\psi}(x)\rangle=-n_0^{1/2}e^{i\mathbf{k}\mathbf{r}}\varphi_0(\mathbf{r})a\frac{\delta v_i d_{il}k_l}{c_{rs}k_r k_s}. \tag{A.11}$$

We have recognized that in this case the circle in (A.3) corresponds to the quantity $A_{0i}(0, \mathbf{k}) = d_{il}k_l$ and the function $D_{00}(0, \mathbf{k})$, according to (3.11), (3.12), and (3.14), is equal to $-a/c_{rs}k_r k_s$.

Going over in (A.11) to the coordinate representation, and then assuming that the typical dimensions of nonuniformity of the external field ($\sim|\mathbf{k}|^{-1}$) exceed the size of the system, we obtain, on comparison with (A.10),

$$d_{ij}=mc_{ij}/a. \tag{A.12}$$

According to (2.1), the quantities ξ and ξ^* enter in the Hamiltonian of the system symmetrically with the operators $\hat{\psi}'$ and $\hat{\psi}'^+$. Therefore, if we have two sets of

diagrams $\mathscr{P}$ and Q which differ only in that the graphs Q have an additional input for the scalar line D_{00} at $\omega = 0$, then, in view of (3.9) and (3.1), the analytic expressions for $\mathscr{P}$ and Q are connected by

$$Q = \int d\mathbf{r}\, n_0^{1/2} \varphi_0(\mathbf{r}) e^{-i\mathbf{k}\mathbf{r}} \left(\frac{\delta \mathscr{P}}{\delta \xi^*(\mathbf{r})} - \frac{\delta \mathscr{P}}{\delta \xi(\mathbf{r})} \right). \quad \text{(A.13)}$$

We now take as $\mathscr{P}$ the set of diagrams for the mass current $j_i(x) = \langle \hat{j}_i(x) \rangle$. Then, considering the definition of $A_{0j}(\omega, \mathbf{k})$, given in Sec. 5, and the formulae (A.12), we obtain from (A.13)

$$\frac{mc_{ij}k_j}{a} = \frac{1}{v_c} \int_c d\mathbf{r} \int d\mathbf{r}'\, e^{ik(\mathbf{r}-\mathbf{r}')} n_0^{1/2} \varphi_0(\mathbf{r}') \left[\frac{\delta \langle \hat{j}_i(x) \rangle}{\delta \xi^*(\mathbf{r}')} - \frac{\delta \langle \hat{j}_i(x) \rangle}{\delta \xi(\mathbf{r}')} \right]. \quad \text{(A.14)}$$

In this expression, as in all preceding derivations, the long-wave limit is assumed for the quantities involved. Symbol c under the integral denotes integration over the volume of a unit cell of the crystal, which is equal to v_c.

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