COHERENT CRYSTALLIZATION OF QUANTUM LIQUID

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The inhomogeneous state of Fermi and Bose systems of special nature, resulting from long-range attraction between particles, is investigated with simple models as examples. This state corresponds to a crystal lattice whose parameter is determined not by the particle concentration but by the law governing their interaction. In this case the particles are not localized at the lattice sites and are capable of moving throughout the volume of the crystal. The type of permissible lattices and the character of the "liquid-crystal" phase transition are determined. It is shown that the shear modulus differs from zero, making it possible to regard the discussed type of crystals as a special modification of a solid.

1. INTRODUCTION

IT is well known that at increased pressure the quantum liquids He^3 and He^4 go over into the crystalline state. It is very probable that at definite, albeit difficultly-attainable conditions an analogous transition can also be experienced by other quantum liquids, such as that of electrons, nucleons, etc. One can raise the question whether the crystalline state encountered in all the cases is similar to the state of the ordinary crystal or whether under certain conditions we encounter a crystal of a qualitatively different type. The same question pertains also to the character of the "liquid–crystal" phase transition itself. An attempt to answer these questions is the subject of this and succeeding articles.

It turns out that the answer depends significantly on the type of the interaction between the particles (quasiparticles) of the system. One can point to two different mechanisms capable of leading to spontaneous violation of translational symmetry. If sufficiently strong repulsion forces act at small distances between the particles, then the tendency of the particles in each pair to stay as far away from each other as possible gives rise to an ordered structure corresponding to a minimum overlap of the wave functions of the particles, and consequently to an energy minimum. As a result, owing to such correlations, the particles turn out to be localized at the sites of a regular three-dimensional lattice. We emphasize that in order for the structure in question to be formed, it is the repulsion forces that play an important role. It suffices to state that at high pressures even the hard-sphere system crystallizes. The role of the attraction forces needed for the crystal to exist at zero pressure, is mainly to keep the system from flying apart.[1)] The described mechanism serves as the basis for the occurrence of the state of the "ordinary" crystal (OC); this covers both the majority of solid-state structures and, for example, the "Wigner crystal"—an electron crystal in a system with a positive compensating background.[1]

The occurence of a periodic structure of an entirely different nature is possible, in principle, if the interaction between the particle has sufficiently large Fourier components $\nu(\mathbf{k}) < 0$ (attraction) in some region of the momentum transfer $k \sim k_0$; in addition, this interaction should be long-range and, as a consequence, should be well described by the self-consistent-field approximation. In this approximation, the interaction energy can be written in the form

$$E_{int} = {}^1/_2 \int d^3k\, \nu(\mathbf{k})\, |n_k|^2,$$

where n_k is the Fourier component of the particle-number density. It is clear from this equation that the minimum energy corresponds to a state with such spatial periodicity that the components n_k with $k \sim k_0$ differ from zero.[2)] Such a state, in contrast to the OC, is not due to correlations but constitutes a stable inhomogeneous state of a system in a self-consistent field, and the periodic density distribution and the periodic field maintain each other. It can be stated that in this state a separate particle of the system is already a crystal. We shall call this a coherent crystal (CC), bearing in mind that the corresponding state is covered by the general definition of coherent states (see [2] and Sec. 3 below).

In describing the physical differences between OC and CC, we note first that in CC the particles are not localized and can move freely through the system. For this reason, the quantitative characteristics of the CC depend strongly on whether it is made up of Bose or Fermi particles. Further, the CC lattice parameter is determined not by the particle concentration, as in the case of OC, but principally by the form of the interaction between them. In particular, long-wave structures are possible, the period of which spans a large number

[1)] The attraction forces can be replaced by enclosing the system in a box and applying an external pressure, as will be assumed later.

[2)] Conceivably, the periodic distribution is not the only possible stable state of a system that has lost translational symmetry. Thus, the quantity E_{int} can be expanded not only in the eigenfunctions of the operators p_x, p_y, and p_z, but in eigenfunctions of another triad of operators that commute with one another and are constructed of generators of the motion group of a homogeneous and isotropic system, for example $p^2 M^2$, and M_z, where p is the momentum and M the angular momentum. If the corresponding component ν_{klm} of the interaction potential is negative and sufficiently large, then the resultant state has the form of a rosette (details will be given in a separate article).

of particles. Accordingly, weakly-damped oscillations with wavelength much shorter than the lattice period can propagate through the CC. There are also other differences, among which we mention the coexistence in a single-component CC of "solid" sound (lattice vibrations) and "liquid" sound (vibrations of the density with the lattice remaining unchanged), and also the stability of a one-dimensional CC. These questions will be discussed separately.

There is, of course, no unbridgeable gulf between the OC and CC states. These states constitute only two limiting cases. It is possible, apparently, also to realize intermediate structures corresponding, for example, to particle motion that can be described as successive "jumps" from one point of temporary localization of the particle to another such point. This is precisely the character possessed by the motion of a particle diffusing in a solid. It is therefore conceivable that an OC with sufficiently large vacancy concentration could manifest certain properties of CC. Favoring this assumption are recent investigations by Andreev and I. Lifshitz,[3] who established the presence of special excitations of the "liquid" sound type (see above) in such crystals.

As to the CC in pure form, it is at present difficult to point to such objects. It may turn out that they do not exist at all. However, the probability of the existence of crystals with predominantly coherent mechanism is not quite small. It is possible that one should expect the appearance of such structures in multinucleon systems, for example in the interiors of the recently discovered neutron stars (pulsars).

Insofar as we know, the correct relation between CC and OC has not been established in the scanty literature on CC.[4-10] In some papers (for example, in the pioneer work of Vlasov,[4] where the self-consistent-field method was applied in noncritical fashion to classical systems with ordinary molecular forces), these states were actually regarded as identical, whereas in others, to the contrary, they were regarded as being radically opposite. Thus, Gross[5] has stated that the CC is not a solid, since he was unable to observe transverse sound; a similar statement was made in [6]. Actually, however, the CC, if it is actually realized as a locally stable state of the system, exhibits a nonzero shear elasticity (see Sec. 5 below).

In a number of papers, starting with the present article and serving as a continuation of a preceding publication by the authors,[7][3)] we shall describe the results of a systematic investigation of coherent crystallization of a quantum liquid. The present article serves as an introduction. It considers only the main features of the phenomenon in question, namely the periodic character of the resultant structure (Sec. 3), the types of possible lattices, the character of the phase transition as a function of the type of lattice (Fig. 4), and the stability against shear (Sec. 5). In this paper we consider only the case T = 0. In succeeding articles we shall consider other singularities of coherent crystallization, and will also discuss questions only touched upon in this article, namely the dependence of the character of the phase transition on the type of the interaction, the stability of a one-dimensional CC, the spectrum of the collective excitations, the properties of the system near the critical point, the role of the correlation effects, etc.

2. INSTABILITY OF A HOMOGENEOUS STATE OF A SYSTEM

The transition of a system into an inhomogeneous state corresponds, as a rule, to the appearance of instability of the homogeneous state against infinitesimally small density perturbations that upset the homogeneity. Information concerning such an instability is contained in the corresponding linear response function, which depends on the 4-momentum transfer. The instability of a given state of a system becomes manifest in the occurrence in this function of anomalous singularities in the frequency, leading to perturbations that grow in time. Similar singularities (but with respect to the total 4-momentum) arise in the response function to a change of the density of the condensate for the normal state of a superconductor at a temperature below critical.[11]

To describe the CC, we choose a model in which the coherent mechanism appears in purest form and which, on the other hand, can be calculated without difficulty. The interaction potential, or more accurately its Fourier transform, is given by Fig. 1 (see also [7]). The following conditions are assumed satisfied:

$$v(0) > 0, \quad \int d^3k\, v(\mathbf{k}) > 0,$$

and make collapse of the system impossible. The system is assumed to be "compressed," and the characteristic momentum transfer k_0 is small compared with the reciprocal distance between the particles $n^{1/3}$. Further, the interaction energy of a particle pair is assumed to be small compared with the characteristic kinetic energy, but the total interaction energy per particle pair can be of the order of or larger than the kinetic energy.[4)] The foregoing conditions, written out separately for Fermi systems (F) and Bose systems (B), are

$$k_0 n^{-1/3} \ll 1,\ m|v|k_0^3 n^{-2/3} \ll 1,\ m|v|n^{1/3} \gtrsim 1, \qquad (1F)$$
$$k_0 n^{-1/3} \ll 1,\ m|v|k_0 \ll 1,\quad m|v|nk_0^{-2} \gtrsim 1. \qquad (1B)$$

In the latter case, the smallness of the parameter $m|\nu|n^{1/3}$ makes it possible to neglect the excitation of the condensate (in this case n coincides with its density).

When conditions (1) are satisfied, the system (including the region adjacent to the phase-transition point) can be described in the Hartree approximation.

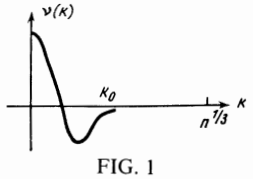

FIG. 1

[3)] In the cited article, an attempt was made to attribute the anomalous behavior of the specific heat of He^3 to its coherent crystallization.

[4)] In a compressed system, there are many particles inside the action radius of the forces, so that these conditions do not contradict each other.

This can readily be verified by recognizing that the corresponding corrections—exchange and correlation—are determined by the second of the parameters entering in (1); only the term corresponding to the direct self-consistent interaction describes the interaction of the given particle with all the remaining particles located in the sphere of action of the forces, and is determined by the large third parameter.

For Fermi systems, the Green's function in the Hartree approximation is given by

$$\left[\omega - \frac{\hat{p}^2}{2m} - \int dx'' n(x'') V(x-x'')\right] G(x, x', \omega) = \delta(x-x'), \quad (2F)$$

where the particle-number density is

$$n(x) = -2i \int \frac{d\omega}{2\pi} G(x, x, \omega). \quad (3F)$$

For Bose systems, we can neglect the excitation of the condensate; introducing its wave function $\xi(x)$, we get

$$\left(\mu - \frac{\hat{p}^2}{2m} - \int dx' n(x') V(x-x')\right) \xi(x) = 0, \quad (2B)$$

where

$$n(x) = \xi^2(x) \quad (3B)$$

and μ is the chemical potential. The foregoing equations are nonlinear and each can have several solutions.

The system energy can be written in the form

$$E = E_{kin} + E_{int}, \quad E_{int} = \frac{1}{2} \int dx\, dx'\, n(x) n(x') V(x-x'),$$

where

$$E_{kin} = -2i \int dx \int \frac{d\omega}{2\pi} \lim_{x' \to x} \frac{p^2}{2m} G(x, x', \omega), \quad (4F)$$

$$E_{kin} = \int dx\, \xi(x) \frac{\hat{p}^2}{2m} \xi(x). \quad (4B)$$

We introduce further in (2) an infinitesimally small time-dependent external field δU and relate it to the corresponding change of density with the aid of the response function χ:

$$\delta n(x, \omega) = \int dx' \chi(x, x', \omega) \delta U(x', \omega).$$

Simple calculation yields for χ the equation

$$\chi(x, x', \omega) = \Pi(x, x', \omega) + \int dx''\, dx''' \Pi(x, x'', \omega) V(x'' - x''') \chi(x''', x', \omega), \quad (5)$$

where the polarization operator is

$$\Pi(x, x', \omega) = -2i \int \frac{d\omega'}{2\pi} G(x, x', \omega') G(x', x, \omega' + \omega), \quad (6F)$$

$$\Pi(x, x', \omega) = -\xi(x)\xi(x') [G(x, x', \omega - \mu) + G(x', x, \mu - \omega)]. \quad (6B)$$

By G is meant here the solution of Eq. (2F) with circuiting rules determined by the type of the statistics, i.e., the single-particle Green's function in the self-consistent field. For a Bose system, the function G has the meaning of the propagation function of the condensate particle. In diagram language, Eq. (5) corresponds to summation of the sequences of diagrams shown in Fig. 2 (Fermi system) and Fig. 3 (Bose system). The dashed line corresponds to the interaction line and the wavy line to the condensate.

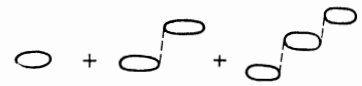

FIG. 2

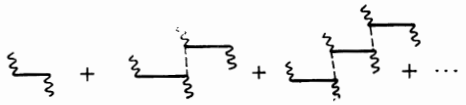

FIG. 3

Being interested in the stability of the homogeneous state, let us separate the translationally-symmetrical solution of Eqs. (2)

$$n(x) = n, \quad G^{-1}(k, \omega) = \omega - \frac{k^2}{2m} - n\nu(0), \quad \mu = n\nu(0), \quad \xi = \sqrt{n}.$$

Equation (5) yields

$$\chi(k, \omega) \propto [1 - \nu(k)\Pi(k, \omega)]^{-1}, \quad (5')$$

where

$$\Pi(k, \omega) = \frac{mp_0}{\pi^2} \int_0^1 \frac{dx\, x^2}{m^2\omega^2/p_0^2k^2 - x^2 + i\delta}, \quad (7F)$$

$$\Pi(k, \omega) = \frac{nk^2/m}{\omega^2 - (k^2/2m)^2 + i\delta}. \quad (7B)$$

(Here p_0 is the limiting Fermi momentum). For pure imaginary values of ω, the right-hand sides of (7) are correspondingly larger than $-mp_0/\pi^2$ and $-4mn/k^2$. Therefore, when the following conditions are satisfied[6]

$$\gamma(k) \equiv -(1 + mp_0\nu(k)/\pi^2) > 0, \quad (8F)$$

$$\gamma(k) \equiv -(1 + 4mn\nu(k)/k^2) > 0; \quad (8B)$$

$\chi(k, \omega)$ has an anomalous pole at imaginary frequency, contradicting the spectral formulas and leading to an increase of the perturbations with time.[7]

Unlike in a superconductor, this pole does not arise at arbitrarily weak attraction, and there is a certain finite threshold for it. The reason is that on going over to the inhomogeneous state (see below) there must occur an increase of the kinetic energy, which can be compensated for by decreasing the interaction energy only at a sufficiently large value of $|\nu(k)|$. It follows from (8), in particular, that when

$$n < n_{cr} = -\pi^4/3m^3(v_{min})^3, \quad (9F)$$

$$n < n_{cr} = -\tfrac{1}{4} m^{-1} [\nu(k)/k^2]_{min}^{-1}, \quad (9B)$$

the homogeneous state is certainly stable. A phase transition to the CC state occurs thus with increasing pressure at a density equal to n_{cr}.

The interpretation of the results is quite simple. The Hartree equations (2) and (3) constitute, as is well

[5] We omit the factor $\delta_{\sigma\sigma'}$ of G and add an extra factor 2 when taking the trace. In the formulas that follow, the contours of integration with respect to the frequency are closed by a large circle in the upper half-plane.

[6] The criterion (8B) can be obtained directly from the Bogolyubov spectrum of a weakly-nonideal Bose gas [12] $\omega^2 = k^2(k^2/2m + 2n\nu(k))/2m$.

[7] An analogous pole also arises in the response function of the OC (see [13]). In this case, however, it is brought about by short-range correlations connected with repulsion.

known, the conditions for an extremum (not necessarily a minimum!) of the energy with respect to small variations of the density $\delta_1 E = 0$. At the same time, the sign of the second variation $\delta_2 E$, which determines the type of this extremum, is opposite to the sign of γ. In fact, if one introduces a small external field U(x), then derivations similar to those leading to (5) and (6) yield

$$\delta_2 E = \frac{1}{2}\int d^3k \frac{|U(\mathbf{k})|^2}{\nu(\mathbf{k}) + \pi^2/mp_0}, \tag{F}$$

$$\delta_2 E = \frac{1}{2}\int d^3k \frac{|U(\mathbf{k})|^2}{\nu(\mathbf{k}) + k^2/4mn} \tag{B}$$

(For the particular case of a δ-function interaction see [14]).

Therefore, when $\gamma < 0$ the homogeneous state realizes the minimum of the energy and is stable. On the other hand, when $\gamma > 0$, the homogeneous solution corresponds to a maximum of the energy and there exists another inhomogeneous solution which is the stable one.[8)]

Thus, when the condition $\gamma < 0$ is violated, inhomogeneity in the particle distribution arises in the system. We note that the second variation of the energy corresponds to the first variation of the Hartree equation, which, in turn, as is well known, corresponds to the equations for zero sound (Fermi system) or for ordinary sound (Bose system). Therefore the instability in question becomes manifest in the fact that these excitations increase in time, and are transformed in final analysis to "congealed" waves in the density distribution.

3. CRYSTALLINE CHARACTER OF A STABLE STATE OF THE SYSTEM

As seen from (8) and (9), when the critical density is reached the stability condition is violated first for the Fourier component with $k = k^0$, where k^0 is the point of the minimum of the function $\nu(k)$ (Fermi system) or $\nu(k)/k^2$ (Bose system):

$$\nu(k)|_{k^0} = \min, \tag{10F}$$

$$\nu(k)/k^2|_{k^0} = \min. \tag{10B}$$

With further increase of the density, an entire interval of k is reached in which the system is unstable. This raises the question whether the resultant inhomogeneity in the particle distribution has Fourier components in this entire interval, or whether the system "prefers" to choose only certain discrete vector values k, with moduli lying in this interval. In other words, the question is whether the density distribution has a periodic character.

For simplicity we consider the case of a Bose system (the result for the Fermi system is the same) and determine the possible forms of violation of translational symmetry of the systems, on the basis of the considerations advanced above. We turn to the Fourier transform of the wave function of the condensate $\xi(\mathbf{k}) = \xi_0\delta^3(\mathbf{k}) + \varphi(\mathbf{k})$, where we have separated the homogeneous term in the function $\xi(\mathbf{x})$.

It is easy to verify that if the function $\varphi(\mathbf{k})$ has singularities of degree lower than the third[9)] (and, in particular, if it is continuous), then its contribution to $\xi(\mathbf{x})$ is a function that attenuates at large x, and its contribution to the system energy increases more slowly than the first power of the volume V. A function $\varphi(\mathbf{k})$ of this type describes a local violation of homogeneity. One can advance arguments indicating that such violations do not correspond to a minimum of the energy. In fact, if this were so, then it would be more convenient to produce as many violations of this type as possible, with a number that increases in proportion to the volume of the system. But then their contribution to the energy would be proportional to V, and we would then deal with the case of stronger singularities.

On the other hand, if the degree of the singularity of $\varphi(\mathbf{k})$ exceeds 3, the contribution to the energy increases more rapidly than V, i.e., the system becomes unstable. It is therefore meaningful to consider singularities of the third degree only. There are only two types of integrable singularities of this degree, $\delta^3(\mathbf{k} - \mathbf{k}_n)$ and $P[1/((\mathbf{k} - \mathbf{k}_n)\mathbf{n}_1)((\mathbf{k} - \mathbf{k}_n)\mathbf{n}_2)((\mathbf{k} - \mathbf{k}_n)\mathbf{n}_3)]$, where $\mathbf{k}_n$ is a certain fixed vector, P is the principal-value symbol, and $\mathbf{n}_{1,2,3}$ are noncomplanar unit vectors. Mixed singularities of the type $\delta((\mathbf{k} - \mathbf{k}_n)\mathbf{n}_1)P[1/((\mathbf{k} - \mathbf{k}_n)\mathbf{n}_2) \times ((\mathbf{k} - \mathbf{k}_n)\mathbf{n}_3)]$ are also possible, but their study yields nothing new.

Let us consider first the first case, corresponding to

$$\xi(\mathbf{x}) = \sqrt{n}\left(a_0 + \sum_n a_n e^{i\mathbf{k}_n\mathbf{x}}\right), \tag{11}$$

where $\{\mathbf{k}_n\}$ is a certain set of fixed vectors containing the zero vector $\mathbf{k}_n = 0$ (the term a_0)[10)]. Substituting (11) in (2B) and (3B), we readily see that the sums of any pairs of vectors from $\{\mathbf{k}_n\}$ should belong to the same set. In particular, the reciprocal vector $-\mathbf{k}_n$ also belongs to the set. Therefore the set $\{\mathbf{k}_n\}$ forms a discrete vector group, and in accord with the well known theorem,[15] the vector $\mathbf{k}_n$ can be represented in the form

$$\mathbf{k}_n = N_1\mathbf{k}_1 + N_2\mathbf{k}_2 + N_3\mathbf{k}_3, \tag{12}$$

where $\mathbf{k}_{1,2,3}$ are the basis vectors and $N_{1,2,3}$ are integer coefficients. Thus, the density distribution in the case under consideration is spatially periodic (with the reciprocal-lattice basis $\mathbf{k}_{1,2,3}$).

Let us show that we are dealing in essence here with a unique "condensation" of bosons (or "particle-hole" pairs in the case of a Fermi system) in a state with a definite value of the momentum transfer k. A "smearing" over the continuous interval k would lead to a noticeable lowering of the energy gain, by virtue of the nonlinear dependence of the interaction energy on $\xi(\mathbf{x})$. We note in this connection that substitution of (11) in (2B) and (3B) leads to equations that contain the Fourier

[8)] We note that the indicated connection between the position of the pole of the response function and the sign of $\delta_2 E$ has a general character. Therefore, if an inhomogeneous solution corresponding to the minimum of the energy is found for Eqs. (2) and (3), then one can be assured that the corresponding response function has no anomalous singularities, and vice versa.

[9)] The degree n of the singularity of the function $\varphi(\mathbf{k})$ at the point $\mathbf{k} = \mathbf{k}_n$ is determined by the relation $\varphi(\mathbf{k}) \to \alpha^{-n}\varphi(\mathbf{k})$ as $\mathbf{k} - \mathbf{k}_n \to \alpha(\mathbf{k} - \mathbf{k}_n)$ (k is assumed to be close to $\mathbf{k}_n$).

[10)] The normalization $\int d\mathbf{x}\xi^2(\mathbf{x}) = N$ yields $|a_0|^2 + \sum_n |a_n|^2 = 1$.

components of the interaction potential $\nu(\mathbf{k}_n)$ themselves (and not their integral over $\mathbf{k}$-space). Therefore the state in question arises when the potential reduces to a single unique Fourier component (and consequently, it is not manifest in any way in the scattering experiments). This is the typical many-particle effect resulting from the infinite number of particles in the system and reducing to the already mentioned condensation in a state with $\mathbf{k} = \mathbf{k}_n$. This effect is very similar in its nature to superconductivity (condensation of fermion pairs in a state with total momentum $\mathbf{p} = 0$),[11] and also to the Ruelle-Fisher instability,[16] where the system condenses in space about two or several centers as a result of an infinitesimally narrow negative potential "spike."

The presence of a macroscopic number of bosons (or Bose complexes) in the state $\mathbf{k}_n$ with a single wavelength and phase makes it possible to regard the corresponding state of the system as the static analog of coherent scattering.[2] We have in mind here the maximally classical state of the "density oscillator" $a^+_{\mathbf{k}_n} a_0$ (for the Bose system) or $a^+_{\mathbf{p}+\mathbf{k}_n} a_{\mathbf{p}}$ (for the Fermi system). It can be shown that this state also satisfies all the formal requirements that are valid for coherent states. It is, in particular, the eigenstate of the indicated operators, which have the meaning of annihilation operators for the density oscillations.

Let us turn now to the terms of $\varphi(\mathbf{k})$ whose singularities have the form of principal values. Changing over to $\mathbf{x}$-space, we can readily see that we deal, as before, with a periodic state, but one characterized by a "collapse" of the phase on planes whose normals coincide with the vectors $\mathbf{n}_1$, $\mathbf{n}_2$, and $\mathbf{n}_3$. Thus, in the one-dimensional case, $1/(k - k_n)$ corresponds to the function $\epsilon(x)\exp(ik_n x)$. Thus, we actually deal with a polycrystal. Even without ascertaining whether such states satisfy the Hartree equation, they can be rejected by indicating that the phase discontinuity surfaces correspond to a positive addition to the kinetic energy (surface energy).

Let us stop to consider in conclusion the possible CC lattice types. It is natural to assume that if the criterion (8) is satisfied and the inhomogeneous state becomes stable, a three-dimensional crystalline structure appears, in which, in comparison with the one-dimensional or two-dimensional structure, the largest energy gain is ensured.[12] In addition, owing to the symmetry of the problem in k-space ($\nu(\mathbf{k})$ depends only on $|\mathbf{k}|$), all the vectors $\mathbf{k}_{1,2,3}$ will be equal to one another in absolute magnitude. This makes it possible to pick out the crystal systems to which the CC can belong. These are the cubic system (primitive PC, face-centered FCC, and body-centered BCC), rhombohedral R, and hexagonal H (with a definite ratio of the height to the side of the base of the prism). In all other cases, the reciprocal-lattice basis vectors have different lengths.

The magnitude of these vectors should itself obviously fall in the interval referred to at the beginning of this section; in particular, near the transition point $|\mathbf{k}_{1,2,3}| \approx k^0$ (see (10)). Even this shows that the CC lattice period is determined not by the density but by the type of interaction between the particles. Another most important difference between CC and OC is connected with the fact that CC particles, obeying the Hartree equation, behave like particles in an external periodic field, i.e., they move practically independently of one another in the entire volume of the crystal.

4. PHASE TRANSITION TO THE CC STATE

To determine the type of the phase transition to the CC state (see (9)), it is useful to introduce the concept of fundamental reciprocal-lattice vectors. These will include, besides the basis vectors $\mathbf{k}_1$, $\mathbf{k}_2$, and $\mathbf{k}_3$, also the reciprocal-lattice vectors (see (12)), which have the same length. Denoting their number by s, we present expressions for the fundamental vectors in Cartesian coordinates, assuming the basis vector length to be unity:[18]

$$
\begin{aligned}
&\text{FC}, \quad s=6, \quad (\pm\mathbf{i}, \pm\mathbf{j}, \pm\mathbf{k}),\\
&\text{BCC}, \quad s=12, \quad \frac{1}{\sqrt{2}}(\pm\mathbf{i}\pm\mathbf{j},\ \pm\mathbf{i}\pm\mathbf{k},\ \pm\mathbf{j}\pm\mathbf{k}),\\
&\text{FCC}, \quad s=8, \quad \frac{1}{\sqrt{3}}(\pm\mathbf{i},\ \pm\mathbf{j},\ \pm\mathbf{k}).\\
&\text{H}, \quad s=8, \quad \left(\pm\mathbf{i}\frac{\sqrt{3}}{2}\pm\mathbf{j},\ \pm\mathbf{j},\ \pm\mathbf{k}\right),\\
&\text{P}, \quad s=6, \quad (\pm(\mathbf{i}+a(\mathbf{j}+\mathbf{k})),\ \pm(a(\mathbf{i}+\mathbf{k})+\mathbf{j}),\\
&\qquad\qquad \pm(a(\mathbf{i}+\mathbf{j})+\mathbf{k})).
\end{aligned}
\tag{13}
$$

The ± signs combine here independently.

It turns out that the type of the phase transition depends on whether it is possible to find among the fundamental vectors at least one triad forming a closed triangle. If there are no such triads (type I), then the transition to the CC state can be a second-order transition: the lattice first appears in the system with infinitesimally small amplitude, which increases with increasing distance from the critical point.[13] On the other hand, if there are closed triads of the fundamental vectors (type II), then we deal of necessity with a first-order transition. It follows from (13) that type I consists of the systems BCC, H, and R (the latter at $a = -\frac{1}{2}$, i.e., when the angle between the basis vectors is 120°).

We shall carry out the analysis near the critical point, i.e., at $\gamma(k) \ll 1$ (see (8)) but far enough from it to be able to neglect correlation effects. We emphasize that in a compressed system the correlation effects are small (see, for example, [19,20]), and we are therefore dealing with the very close vicinity of the critical point; accordingly, when speaking of a first- or second-order transition, we have in mind the behavior of the phase curve outside this vicinity. The investigation of the role

[11] We note in this connection that to describe the CC we can successfully use in practice any method of superconductivity theory, with the particle-particle pairing replaced by particle-hole pairing.

[12] The known considerations concerning the instability of one- and two-dimensional crystals [17] are not applicable directly to CC (details will be given in a separate article).

[13] The reason why the well-known Landau theorem [17], that a second-order "solid–liquid" transition is impossible, does not apply in this case is that the energy terms of third order in the amplitude of the inhomogeneity vanish identically.

of correlation effects will be the subject of a separate article.

Confining ourselves to the simpler case of a Bose system, we find, first, an expression for the thermodynamic potential $\Phi = E + pV$, the variation of which at constant p and N yields the necessary information on the phase transition. From Eq. (2B) we have

$$\Phi = \mu N = E_{\text{kin}} + 2E_{int},$$

whence $p = E_{\text{int}}/V$. Substituting (11) in (4B) and the expression for E_{int}, we obtain after changing over to Fourier components

$$E_{\text{kin}} = N\sum_i |a_i|^2 \frac{k_i^2}{2m},$$

$$E_{int} = \frac{N^2}{V}\Big\{2\sum_i \nu(\mathbf{k}_i)|a_i|^2|a_0|^2 + \sum_{ijk}\nu(\mathbf{k}_i-\mathbf{k}_j)a_i^*a_j^*a_ka_0 + \sum_{ijkl}\nu(\mathbf{k}_i-\mathbf{k}_j)a_i^*a_j^*a_ka_l\Big\}.$$

Here and below, the symbol ijk under the summation sign denotes summation over the reciprocal-lattice vectors satisfying the condition $\mathbf{k}_i + \mathbf{k}_j + \mathbf{k}_k = 0$, and analogously for ijk*l*. Expressing the volume in terms of the pressure $p = n^2\nu(0)/2$, we have

$$\frac{\Phi}{N} = \sum_i |a_i|^2\frac{k_i^2}{2m} + n\nu(0)\Big\{1 + 4\sum_i |a_i|^2|a_0|^2\frac{\nu(\mathbf{k}_i)}{\nu(0)} + 2\sum_{ijk} a_i^*a_j^*a_ka_0\frac{\nu(\mathbf{k}_i-\mathbf{k}_j)}{\nu(0)} + 2\sum_{ijkl} a_i^*a_j^*a_ka_i\frac{\nu(\mathbf{k}_i-\mathbf{k}_j)}{\nu(0)}\Big\}^{1/2}. \quad (14)$$

Near the critical point, we seek a weakly-inhomogeneous state of the system $|a_i| \ll a_0 \approx 1$. Accordingly, we expand the curly bracket in (14) and obtain

$$\frac{\Phi}{N} = n\nu(0) + \sum_i |a_i|^2\Big(\frac{k_i^2}{2m} + 2\nu(\mathbf{k}_i)|a_0|^2 n\Big) + n\sum_{ijk} a_i^*a_j^*a_ka_0\nu(\mathbf{k}_i-\mathbf{k}_j) + n\sum_{ijkl} a_i^*a_j^*a_ka_i\nu(\mathbf{k}_i-\mathbf{k}_j) + \ldots \quad (14')$$

Let us examine the second term of (14′), and mark the fundamental vectors with a tilde. In our case their length is close to k^0 (see (10)). Therefore in the sum over i we separate the terms corresponding to summation over the fundamental vectors and containing the small factor $\tilde{k}_i^2/2m + 2\nu(\tilde{k}_i)|a_0|^2 \sim \gamma(\tilde{k}_i) \ll 1$. We assume (as will be subsequently confirmed) that the largest of all the a_i are the coefficients $\tilde{a}_i$ corresponding to the fundamental vectors, and that for the remaining vectors we have $a/\tilde{a} \lesssim \tilde{a}$. Accordingly, in the third and fourth terms of (14′) the principal role will be played by the sum over the fundamental vectors. For a lattice of the type I (there are no triads of fundamental vectors) the principal part of the third term drops out, and the main role is assumed by the second and fourth terms of (14′). The second term turns out here to be of the order of $\tilde{a}_i^2\gamma(\tilde{k}_i)$, and the fourth of the order $\tilde{a}_i^4$. Hence, varying with respect to $\tilde{a}_i$, we get

$$\tilde{a}_i \sim \sqrt{\gamma(\tilde{k}_i)} \sim \sqrt{(n-n_{\text{cr}})/n_{\text{cr}}}. \quad (15)$$

The energy correction connected with the inhomogeneity turns out to be of the order of $\tilde{k}^2\gamma^2(\tilde{k})$.[14] We are therefore dealing with a typical second-order phase transition. For nonfundamental vectors that are sums of two fundamental ones, we obtain the estimate $a \sim \gamma(\tilde{k})$, and for the remainder we obtain an even smaller quantity, in agreement with the assumption made above.

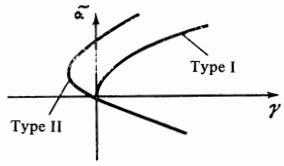

FIG. 4

On the other hand, if the lattice is of type II, then the principal role is played by the third term in (14′), the order of which is $\tilde{a}^3$.

Hence

$$\tilde{a} \sim \gamma(\tilde{k}). \quad (16)$$

and the correction to the energy is of the order of $\gamma^3(\tilde{k})$. At first glance it appears from a comparison of (15) and (16) that the formation of a lattice of type I is favored energywise. However, in the considered case of an isotropic interaction potential $\nu(|k|)$, the weakly-inhomogeneous solution (15) is unstable. Namely, if we produce besides the lattice (16) also a pair of one-dimensional lattices such that closed triangles appear in the aggregate in the reciprocal lattice, then such a configuration will have a lower energy. It can be shown that in such a situation the sign of the third term in the curly brackets of (14) is negative, and the absolute minimum of the thermodynamic potential corresponds to competition between the third and fourth terms in these brackets. This obviously, leads to $\tilde{a} \sim 1$. In this case, the inhomogeneous solution enters the region $\gamma < 0$, where it competes with the homogeneous one (an analog of a superheated crystal). The foregoing is illustrated by Fig. 4.

It follows from all the foregoing that a stable state of the CC corresponds to a lattice of type II (BCC, H, and R with $a = -1/2$). The choice between these systems calls for a complicated energy calculation which has not yet been performed.

5. SHEAR MODULI OF CC

We shall demonstrate that CC has nonzero shear moduli, i.e., that it is a solid body, using as an example a weakly-inhomogeneous PC lattice. Such a lattice has shear elasticity, although, as indicated at the end of Sec. 4, it is unstable in other respects. A cubic lattice has two shear moduli, which enter in the elastic energy of the crystal in the following manner:[21]

$$E_{\text{упр}}/V = 1/2(\lambda_1 u_{xx}^2 + \lambda_2 u_{xy}^2). \quad (17)$$

The coordinate axes are assumed here to coincide with the fourfold axes, and the deformations different from zero were chosen to be u_{xx}, $u_{yy} = -u_{xx}$ and $u_{xy} = u_{yx}$.

We do not present here the details of the calculations, and indicate only the path followed in the calculations and the result. The problem consists of determining the energy of the system in the case of the weakly-deformed lattice. This can be done by minimizing the energy at given deformations. The difference between the obtained expression and the energy of the undeformed lat-

[14] Even this indicates that the length of the fundamental vector is close to k^0: the condition for minimizing the energy with respect to this length yields for $(d/dk)(\nu(k)/k^2)|_k$ a small quantity of the order of $\gamma(\tilde{k})$.

tice yields, when compared with (17), the values of the shear modulus. We obtain

$$\lambda_1 = \frac{n\tilde{k}^2}{m}\left(1 + \frac{\tilde{k}^2 v''(\tilde{k})}{2|v(\tilde{k})|}\right)\tilde{a}^2, \qquad (18)$$

And the modulus λ_2 turns out to be of the order of $\tilde{a}^4$.

Thus, the shear elasticity of the CC is finite, although it tends to zero on approaching the critical density. We therefore cannot agree with the statement that the CC is not a solid.

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[1] E. Wigner, Trans. Faraday Soc. 34, 678 (1938).
[2] R. Glauber, Translation in Kvantovaya optika i kvantovaya radiofizika (Quantum Optics and Quantum Radiophysics), Mir, 1966, p. 91.
[3] A. F. Andreev and I. M. Lifshitz, Abstracts of All-Union Conference on Solid-State Theory, Moscow, 1969.
[4] A. A. Vlasov, Uch. zapiski (Science Notes), Moscow State University 75, 30 (1945).
[5] E. Gross, Phys. Rev. Lett. 4, 599 (1960). Ann. of Phys. 4, 57 (1958); 9, 292 (1960).
[6] L. Kadanoff and G. Baym, Quantum Statistical Mechanics, Benjamin, 1962.
[7] D. A. Kirzhnits and Yu. A. Nepomnyashchiĭ, ZhETF Pis. Red. 4, 86 (1966) [JETP Lett. 4, 58 (1966)].
[8] G. Ochirbat, Vestnik, Moscow State University, No. 3, 1967 and No. 1, 1968.
[9] A. Overhauser, Phys. Rev. Lett. 4, 415 (1960).
[10] A. de Luca, L. M. Riccardi, and H. Umezawa, Physica 40, 61 (1968).
[11] A. A. Abrikosov, L. P. Gor'kov, and I. E. Dzyaloshinskiĭ, Metody kvantovoĭ teorii polya v statisticheskoĭ fizike (Quantum Field-Theoretical Methods in Statistical Physics), Fizmatgiz, 1962 [Pergamon, 1965].
[12] N. N. Bogolyubov, Izv. AN SSSR, Ser. Fiz. 11, 77 (1947).
[13] R. Brout, Phase Transitions, Benjamin, 1965.
[14] D. J. Thouless, Quantum Mechanics of Many-Body Systems, Academic Press, 1961.
[15] G. Ya. Lyubarskiĭ, Teoriya grupp i ee primeneniya v fizike (Group Theory and Its Applications to Physics), Fizmatgiz, 1958.
[16] M. Fisher and D. Ruelle, J. Math. Phys. 7, 260 (1966).
[17] L. D. Landau and E. M. Lifshitz, Statistical Physics, Nauka, 1964 [Addison-Wesley].
[18] C. Kittel, Elementary Solid State Physics, Wiley, 1962.
[19] D. A. Kirzhnits, Polevye metody teorii mnogikh chastits (Field Methods of Many-Particle Theory), Atomizdat, 1963.
[20] S. T. Belyaev, Zh. Eksp. Teor. Fiz. 34, 417, 433 (1958) [Sov. Phys.-JETP 7, 289, 299 (1958)].
[21] L. D. Landau and E. M. Lifshitz, Teoriya uprugosti (Theory of Elasticity), Nauka, 1965 [Addison-Wesley].

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