

Superfluidity of a perfect quantum crystal II

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Abstract. This paper continues the work begun in a previous paper [Eur. Phys. J. B 71, 85 (2009)]. To treat the equations that describe a crystal with condensate that can be superfluid, a method termed the Kirkwood approximation is used. Earlier, the method was found to be rather seminal when applied to a classical crystal. In the case of a simple cubic lattice, solutions to the equations under study can be expressed in terms of the well-known Mathieu functions. A more realistic case of the face centered cubic lattice is also considered although in this case the three-dimensional equations cannot be reduced to one-dimensional ones. Condensate crystals without superfluidity are studied first and then the same crystals in a superfluid state. It is shown in particular that a crystal in which the condensate is formed is energetically preferable with respect to the same quantum crystal without condensate at absolute zero of temperature. Therefore, on lowering the temperature there must somewhere occur Bose-Einstein condensation in the crystal. In the concluding section, we discuss various physical aspects of the problem.

1 Introduction

In a previous paper [1] (hereafter referred to as I), the possibility of superfluidity in a crystalline solid was investigated with the help of the approach in equilibrium quantum statistical mechanics proposed in [2] (see also [3]). The approach is based upon a hierarchy of equations for reduced density matrices obtained from the quantum mechanical Liouville equation, the hierarchy going over, in the classical limit, into the well-known equilibrium Bogolyubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy. In I, it was shown that below the Bose-Einstein condensation point the hierarchy admits solutions relevant to a perfect crystal (immobile) in which there is a frictionless flow of atoms, which amounts to saying that the perfect quantum crystal can be superfluid. The solutions were studied with the help of the bifurcation method and some their peculiarities were found out.

The present paper continues the work begun in I. Seeing that the bifurcation method provides only limited possibilities for studying periodic solutions of the equations describing a crystal, in the present paper we resort to another method, namely, to an approximation termed the Kirkwood approximation in [4]. In the case of a classical crystal, the approximation enables one to solve exactly the equations under study and to obtain a wide variety of results concerning the crystal [4,5].

In Section 2 of this paper, we present the basic equations that will be treated in the following sections, and formulate the Kirkwood approximation. Section 3 is devoted to a simple cubic lattice. Although crystals with the

simple cubic lattice are rare in occurrence, the lattice is interesting from the theoretical point of view because in this case solutions to the equations under study can be expressed in terms of known functions, the Mathieu functions. In Section 4, we consider a more realistic case of the face centered cubic lattice. In these two sections, first we consider crystals without superfluidity (although in the state with a condensate), and then the same crystals in a superfluid state. The results obtained are discussed in the concluding section.

For the sake of convenience, when referring to an equation of paper I we shall place I in front; so we shall write, e.g., (I.28) implying equation (28) of I.

2 Basic equations

We consider a system of N spinless bosons enclosed in a volume V . The particles of mass m interact via a two-body potential $K(|\mathbf{r}_j - \mathbf{r}_k|)$. In the present paper, we shall imply the case of zero temperature upon presuming that the condensate comprises all particles (see I). In this case the spatial number density of particles is given by equation (I.28), namely,

$$\rho(\mathbf{r}) = \rho_0 |u(\mathbf{r})|^2, \quad (1)$$

where $\rho_0 = N/V$ is the average density. The function $u(\mathbf{r})$ satisfies equation (I.29):

$$\frac{\hbar^2}{2m} \nabla^2 u(\mathbf{r}) + \frac{i\hbar \mathbf{p}_0}{m} \nabla u(\mathbf{r}) + \left[\varepsilon_{(1)} - \frac{\mathbf{p}_0^2}{2m} - U(\mathbf{r}) \right] u(\mathbf{r}) = 0. \quad (2)$$

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The normalization condition for $u(\mathbf{r}) \equiv u_1(\mathbf{r})$, equation (I.16), can be conveniently written in the form

$$\frac{1}{v_0} \int_{v_0} |u(\mathbf{r})|^2 d\mathbf{r} = 1, \quad (3)$$

where the integration is carried out over the volume of the elementary cell v_0 .

The vector \mathbf{p}_0 determines the superflow in the crystal by (I.27). If $\mathbf{p}_0 = 0$, we have a crystal without superfluidity although the particles of the crystal are in the condensate state.

With the same approximation for the pair correlation function $g(\mathbf{r}_1, \mathbf{r}_2)$ as in I, the effective potential $U(\mathbf{r})$ is given by equation (I.32):

$$U(\mathbf{r}) = \int K_g(|\mathbf{r} - \mathbf{r}'|) \rho(\mathbf{r}') d\mathbf{r}', \quad (4)$$

in which

$$K_g(r) = \int_0^r \frac{dK(r')}{dr'} g(r') dr'. \quad (5)$$

The periodic crystal density of (1) can be represented by a Fourier series:

$$\rho(\mathbf{r}) = \sum_{l,m,n} a_{lmn} e^{i\mathbf{A}\mathbf{r}}, \quad (6)$$

where $\mathbf{A} = l\mathbf{a}_1 + m\mathbf{a}_2 + n\mathbf{a}_3$ with the basic reciprocal-lattice vectors $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$, and $a_{000} = \rho_0$. In this case, equation (4) yields (see (I.37))

$$U(\mathbf{r}) = \sum_{l,m,n} a_{lmn} \sigma(A) e^{i\mathbf{A}\mathbf{r}}, \quad (7)$$

where

$$\sigma(k) = \frac{4\pi}{k} \int_0^\infty r K_g(r) \sin kr dr. \quad (8)$$

One of the way to simplify the matter is to put $\sigma(k) = 0$ if $k \geq k_m$, in which case the infinite series in (7) will be cut off and will contain a finite numbers of terms. Such an approximation was introduced for the first time in reference [6] and was called Kirkwood's approximation in [4]. The productivity of this approximation in the case of a classical crystal is demonstrated by references [4,5]. The behaviour of the function $\sigma(k)$ in the quantum case is presented in Figure 2 of I, being similar to the one in the classical case depicted in Figure 1 of [5] (see curve 1). The function $\sigma(k)$ diminishes rather rapidly with k . What is more, owing to the oscillating behaviour of $\sigma(k)$, different terms in sums containing $\sigma(k)$ have differing signs and cancel one another to some degree or other. For this reason, cutting off the sums made with the Kirkwood approximation may affect the result insignificantly.

If the sum in (7) is cut off, the potential $U(\mathbf{r})$ will acquire rather a simple form dependent on the type of the crystal lattice, which will be considered in the next

sections. In this case equation (2) may lend itself to a standard mathematical treatment. Sometimes the equation can even be reduced to the well-known Mathieu equation.

Combined with the Kirkwood approximation, it is convenient to put $g(r) = 1$, i.e., to use the Vlasov approximation that is reasonably good in the statistical theory of crystals [3]. This greatly simplifies the matter. If $g(r) = 1$, equation (5) yields $K_g(r) = K(r)$, and we shall have $\sigma_\varepsilon(A) = \sigma(A)/2$ in (I.42). As a result, the energy of the crystal given by (I.42) will acquire the form

$$E = \varepsilon_{(1)}N - \frac{V}{2} \sum_{l,m,n} |a_{lmn}|^2 \sigma(A). \quad (9)$$

If the Kirkwood approximation is used, the last sum will be cut off as well.

We turn now to the stress tensor that was not considered in I. The quantum mechanical stress tensor σ_{ij} is specified by the formula [3,7]

$$\sigma_{ij} = \frac{\hbar^2}{mV} \int \left[\frac{\partial^2}{\partial x_i \partial x_j} R_1(\mathbf{r}, \mathbf{r}') \right]_{\mathbf{r}'=\mathbf{r}} d\mathbf{r} + \frac{1}{2} \int x_j \frac{\partial K(|\mathbf{r}|)}{\partial x_i} \langle \rho_2(\mathbf{r}', \mathbf{r}' + \mathbf{r}) \rangle d\mathbf{r}, \quad (10)$$

in which $R_1(\mathbf{r}, \mathbf{r}')$ is the singlet density matrix and $\langle \dots \rangle$ denotes a space average of the diagonal elements of the pair density matrix $\rho_2(\mathbf{r}_1, \mathbf{r}_2)$ according to

$$\langle \rho_2(\mathbf{r}', \mathbf{r}' + \mathbf{r}) \rangle = \frac{1}{V} \int \rho_2(\mathbf{r}', \mathbf{r}' + \mathbf{r}) d\mathbf{r}'. \quad (11)$$

We substitute the first term of (I.25) into the first term of (10) and utilize the Fourier series for $u(\mathbf{r}) \equiv u_1(\mathbf{r})$ defined by (I.34). The second term in (10) can be treated by analogy with reference [8]. As a result, we get

$$\sigma_{ij} = -\frac{\rho_0}{m} \sum_{l,m,n} (p_{0i} + \hbar A_i)(p_{0j} + \hbar A_j) |c_{lmn}|^2 - \frac{1}{2} \sum_{l,m,n} |a_{lmn}|^2 [\delta_{ij} \sigma(A) + A_i A_j \sigma'(A)/A], \quad (12)$$

where p_{0i}, p_{0j}, A_i, A_j are the components of the vectors \mathbf{p}_0 and \mathbf{A} respectively, c_{lmn} are the Fourier coefficients of $u(\mathbf{r})$, and the prime over σ denotes differentiation with respect to the argument A . In the Kirkwood approximation, the last sum will contain a finite numbers of terms as in (9). It will be noted that the form of the last term in (12) is valid not only when $g(r) = 1$ but also in a more general approximation used in [8].

3 Simple cubic lattice

When considering the simple cubic (SC) lattice, we shall imply the symmorphic space group of the highest symmetry, namely, $O_h^1 = Pm\bar{3}m$, and denote

$a = |\mathbf{a}_1| = |\mathbf{a}_2| = |\mathbf{a}_3|$. Resorting to the Kirkwood approximation we assume that $\sigma(\nu a) = 0$ if $\nu \geq \sqrt{2}$. In this case, according to Appendix of [4] the effective potential is of the form

$$U(\mathbf{r}) = \rho_0 \sigma_0 + 2\alpha_1 \sigma_a (\cos ax + \cos ay + \cos az), \quad (13)$$

where $\sigma_0 = \sigma(0)$, $\sigma_a = \sigma(a)$, $\alpha_1 = a_{\pm 100} = a_{0\pm 10} = a_{00\pm 1}$. The first terms in the Fourier series for the density of (6) are

$$\rho(\mathbf{r}) = \rho_0 \left[1 + \frac{2\alpha_1}{\rho_0} (\cos ax + \cos ay + \cos az) + \dots \right]. \quad (14)$$

For definiteness sake, we shall assume that one of the maximums of the density lies at $x = y = z = 0$, for which it is necessary that $\alpha_1 > 0$. It is clear that the potential should have a minimum there, so that $\sigma_a < 0$.

We write down also the energy per one particle $E_1 = E/N$ that in this case in view of (9) is

$$E_1 = \varepsilon_{(1)} - \frac{1}{2} \rho_0 \sigma_0 - \frac{3}{\rho_0} \alpha_1^2 \sigma_a. \quad (15)$$

3.1 Nonsuperfluid crystal

We set $\mathbf{p}_0 = 0$ in equation (2) and substitute (13) with the result

$$\frac{\hbar^2}{2m} \nabla^2 u(\mathbf{r}) + [\varepsilon_{(1)} - \rho_0 \sigma_0 - 2\alpha_1 \sigma_a (\cos ax + \cos ay + \cos az)] u(\mathbf{r}) = 0. \quad (16)$$

An equation of this type admits separation of variables, that is to say, its solution can be sought in the form

$$u(\mathbf{r}) = f_1(x) f_2(y) f_3(z). \quad (17)$$

Substituting into (16) yields the equation for $f_1(x)$

$$\frac{\hbar^2}{2m} \frac{d^2 f_1}{dx^2} + (c_1 - 2\alpha_1 \sigma_a \cos ax) f_1(x) = 0 \quad (18)$$

and identical equations for $f_2(y)$ and $f_3(z)$ whereas

$$\varepsilon_{(1)} = \rho_0 \sigma_0 + c_1 + c_2 + c_3. \quad (19)$$

The normalization of $f_1(x)$ follows from (3) and (17) (the period $d = 2\pi/a$):

$$\frac{a}{2\pi} \int_0^{2\pi/a} f_1^2 dx = 1. \quad (20)$$

We introduce now the following dimensionless quantities

$$\xi = ax, \quad c = \frac{2m}{\hbar^2 a^2} c_1, \quad q = \frac{2m}{\hbar^2 a^2} \alpha_1 \sigma_a. \quad (21)$$

As a consequence, equation (18) takes the form of the well-known Mathieu equation

$$\frac{d^2 f_1}{d\xi^2} + (c - 2q \cos \xi) f_1(\xi) = 0. \quad (22)$$

The equation has various periodic solutions. We are interested in the solution that gives a minimum of the energy specified by (15) and (19), for which the least possible value of c is required. The relevant solution of equation (18) will be

$$f_1 = \sqrt{2} c e_0 \left(\frac{ax}{2}, 4q \right). \quad (23)$$

Hereinafter we adopt the definition of the Mathieu functions as in [9]. It should be noted that the form of the Mathieu equation and the normalization in [9] differ slightly from (22) and (20), which is reflected in (23). Besides, some formulae and figures in [9] are given assuming that $q > 0$ whereas our $q < 0$ since $\sigma_a < 0$ (see above). The sign of q in (22) can be inverted by the transformation $\xi \rightarrow \xi + \pi$.

The value of q in (23) is not arbitrary in our case as long as we must have (14). We place (17) with (23) in (1) (the functions $f_2(y)$ and $f_3(z)$ have a form analogous with (23)) and expand $c e_0(ax/2, 4q)$ in powers of q [9] with the result that

$$\rho(\mathbf{r}) = \rho_0 [1 - (4q - 14q^3 + \dots) (\cos ax + \cos ay + \cos az) + \dots]. \quad (24)$$

Comparing this with (14) and recalling that q is defined in (21) one obtains an equation for α_1 . In a first approximation (upon discarding terms of order α_1^4 and higher) the equation is

$$1 + \frac{4m\rho_0\sigma_a}{\hbar^2 a^2} = \frac{56m^3\rho_0}{\hbar^6 a^6} \alpha_1^2 \sigma_a^3. \quad (25)$$

Inasmuch as $\sigma_a < 0$, this equation for α_1 has a solution only if its left-hand side is negative. Since $\rho_0 = 1/d^3 = a^3/8\pi^3$ for the SC lattice, the condition for the solution to exist takes the form

$$1 + \frac{m}{2\pi^3 \hbar^2} a \sigma_a < 0. \quad (26)$$

If this condition holds, the condensate crystalline phase exists. The exact value of α_1 can be calculated if the complete coefficient of the cosines in (24) is utilized according to (23).

If the interaction between atoms is weak, i.e., $|\sigma_a|$ is small, the condition of (26) cannot be fulfilled. At the same time, the lattice period $d = 2\pi/a$ and thereby the quantity $a\sigma_a \equiv a\sigma(a)$ depend upon the pressure (the quantity $\sigma(a)$ may also depend on the pressure via the pair correlation function $g(\mathbf{r}_1, \mathbf{r}_2)$); however in the present study we assume that $g = 1$). It may happen that, when the pressure changes, the condition of (26) begins to hold. In this case we shall have a phase transition from a liquid state to the condensate crystalline state. A similar transition occurs in helium that becomes solid only at sufficiently high pressures (recall that the case of zero temperature is considered). It should be remarked, however, that the result just obtained cannot be applied directly to helium since the crystal lattice of helium is not simple cubic.

Nevertheless, it is of interest to discuss the question as to whether the condition of (26) is realistic for helium and other rare gases. To this end, we denote the dimensionless quantity that figures in (25) and (26) as

$$s_a = \frac{4m\rho_0\sigma_a}{\hbar^2 a^2} = \frac{ma\sigma_a}{2\pi^3\hbar^2}. \quad (27)$$

Now the condition of (26) assumes the form $s_a < -1$. The quantity $\sigma_a \equiv \sigma(a)$ can be expressed in terms of the dimensionless quantity $\tilde{\sigma} = \sigma/(\varepsilon r_m^3)$ with the parameters ε and r_m that characterize the Lennard-Jones potential (see I). The value of the period can be estimated as $d \sim r_m$, so that $a \sim 2\pi/r_m$. All of these, when inserted into (27), give

$$s_a \sim \frac{m\varepsilon r_m^2}{\pi^2\hbar^2} \tilde{\sigma}(a) = \frac{\zeta}{\pi^2} \tilde{\sigma}(a), \quad (28)$$

where the dimensionless parameter ζ of (I.45) has been used. For helium, $\zeta = 6.9$ and the minimum value of $\tilde{\sigma}(a)$ is -4.5 (see I); in this case, $s_a \sim -3.1$ and the condition of (26) is fulfilled. When the pressure is low, the lattice period d increases and $a = 2\pi/d$ decreases. The value of $\tilde{\sigma}(a)$ decreases as well (and even vanishes at point A of Fig. 2 of I). In this case the condition of (26) will not be fulfilled and the crystal will not exist. As to other rare gases, the parameter ζ is substantially greater (see I) and $|s_a|$ is large for them, so that (26) is always fulfilled. For this reason, these rare gases are solid at any pressure (and zero temperature implied here).

To investigate in greater detail the phase transition when (26) begins to hold let us consider the energy. The eigenvalue c in equation (22) relevant to the eigenfunction of (23) is $c = a_0(4q)/4$ where a_0 is to be taken from [9]:

$$c = -2q^2 + \frac{7}{2}q^4 - \dots \quad (29)$$

If this and (19) are inserted into (15), we shall arrive at

$$E_1 = \frac{1}{2}\rho_0\sigma_0 - \frac{3\sigma_a\alpha_1^2}{\rho_0} \left(1 + \frac{4m\rho_0\sigma_a}{\hbar^2 a^2} \right) + \frac{84m^3}{\hbar^6 a^6} \alpha_1^4 \sigma_a^4. \quad (30)$$

If we minimize this energy with respect to α_1 , we shall get equation (25). Therefore the solution obtained above corresponds to a minimum of the energy which is, after substituting (25),

$$E_1 = \frac{1}{2}\rho_0\sigma_0 - \frac{3\hbar^6 a^6}{112m^3\rho_0^2\sigma_a^2} \left(1 + \frac{4m\rho_0\sigma_a}{\hbar^2 a^2} \right)^2. \quad (31)$$

If, when the pressure changes, the condition of (26) begins to hold, the energy will commence to decrease continuously from the energy of the liquid state $E_1 = 1/2\rho_0\sigma_0$ according to (31). Here we have a typical second-order phase transition. It is interesting to note that in the classical case the phase transition from the liquid to a crystal with the SC lattice should be second order as well [10]. In actual fact, however, the second-order phase transition from a classical liquid to a classical crystal is impossible because on cooling the liquid becomes unstable before the transition could occur [4].

3.2 Superfluid crystal

If $\mathbf{p}_0 \neq 0$, the crystal will be deformed (see I), the lattice will cease to be cubic, and the potential $U(\mathbf{r})$ will change its form as compared with (13). The variables in equation (2) will no longer be separated, which greatly complicates matters. For simplicity's sake we shall assume that the crystal is subjected to external stresses such that the lattice restores the cubic form. The necessary stresses can be computed if the solution obtained is placed in equation (12) for the stress tensor.

If (13) is substituted into (2), the solution can be sought again in the form of (17), and instead of (18) one gets

$$\frac{\hbar^2}{2m} \frac{d^2 f_1}{dx^2} + \frac{i\hbar}{m} p_{0x} \frac{df_1}{dx} + (c_1 - 2\alpha_1\sigma_a \cos ax) f_1(x) = 0. \quad (32)$$

The equations for $f_2(y)$ and $f_3(z)$ will be analogous, and

$$\varepsilon_{(1)} = \rho_0\sigma_0 + \frac{\mathbf{p}_0^2}{2m} + c_1 + c_2 + c_3. \quad (33)$$

We introduce again the dimensionless quantities of (21) and $p = p_{0x}/(\hbar a)$ with the result

$$\frac{d^2 f_1}{d\xi^2} + 2ip \frac{df_1}{d\xi} + (c - 2q \cos \xi) f_1(\xi) = 0. \quad (34)$$

The solutions of this equation can be expressed in terms of nonperiodic Mathieu functions (the equation can be obtained from (22) if we look for a solution in the form $f_1 = e^{ip\xi} \tilde{f}_1$ and replace $c - p^2 \rightarrow c$). To have the solution in a form suited for our purposes we resort to a standard method for solving the Mathieu equation, namely, expansion in powers of q [11]. First of all we remark that the constant term in $f_1(\xi)$ can be put equal to unity since, if the term does not equal unity, we can always divide $f_1(\xi)$ by the term so that it will become unity. Secondly, if $q = 0$, we must have $c = 0$ in view of (29) because we look for a solution that goes over into (23) and (29) when $p = 0$. As a consequence, we seek the solution to (34) in the form

$$f_1 = 1 + qu_1(\xi) + q^2 u_2(\xi) + q^3 u_3(\xi) + q^4 u_4(\xi) + \dots, \quad (35)$$

$$c = qa_1 + q^2 a_2 + q^3 a_3 + q^4 a_4 + \dots,$$

on condition that no constant term is present in $u_i(\xi)$.

The terms in (34) linear in q yield

$$\frac{d^2 u_1}{d\xi^2} + 2ip \frac{du_1}{d\xi} = -a_1 + 2 \cos \xi. \quad (36)$$

The right-hand side should contain no constant terms otherwise a nonperiodic term increasing with ξ will appear in $u_1(\xi)$; therefore $a_1 = 0$. Now it is easily seen that the periodic solution of (36) is of the form

$$u_1 = \frac{2}{4p^2 - 1} \cos \xi - \frac{4ip}{4p^2 - 1} \sin \xi. \quad (37)$$

The solution loses its meaning at $p = 1/2$, that is, at $p_{0x}/\hbar = a/2$. The value of $p_{0x}/\hbar = a/2$ corresponds to

the boundary of the Brillouin zone. We presume for the moment that $p < 1/2$, the case $p = 1/2$ being treated later.

In analogous way, one can calculate other terms in (35). For example,

$$u_2 = \frac{1 + 2p^2}{2(4p^2 - 1)(p^2 - 1)} \cos 2\xi - \frac{3ip}{2(4p^2 - 1)(p^2 - 1)} \sin 2\xi; \quad (38)$$

$$a_2 = \frac{2}{4p^2 - 1}, a_3 = 0, a_4 = \frac{7 + 20p^2}{2(4p^2 - 1)^3(p^2 - 1)}. \quad (39)$$

The next step is to normalize f_1 according to (3) (see also (20)). Let us write down the first terms in the modulus squared of the normalized f_1 :

$$|f_1(x)|^2 = 1 + \frac{2q}{4p^2 - 1} \left[2 + \frac{7 + 20p^2}{(4p^2 - 1)^2(p^2 - 1)} q^2 \right] \times \cos ax + \dots \quad (40)$$

With account taken of (17) we compare this with (14), which yields the equation for α_1 that replaces (25) if $p \neq 0$:

$$1 + \frac{4m\rho_0\sigma_a}{\hbar^2 a^2(1 - 4p^2)} = \frac{8m^3\rho_0(7 + 20p^2)}{\hbar^6 a^6(1 - 4p^2)^3(1 - p^2)} \alpha_1^2 \sigma_a^3. \quad (41)$$

Instead of (26), we have the following condition for the solution of (41) to exist

$$1 + \frac{m}{2\pi^3 \hbar^2(1 - 4p^2)} a \sigma_a < 0. \quad (42)$$

This condition demonstrates an interesting situation. If σ_a is such that (26) is not fulfilled, there always exists $p \neq 0$ when (42) will hold. This amounts to saying that, even if the interatomic interaction is such that the nonsuperfluid crystal cannot exist, a superfluid crystal can be formed nevertheless.

To clarify the situation we calculate the energy. For definiteness, we assume that $p_{0x} = p_{0y} = p_{0z} = p_0/\sqrt{3}$ (other directions of the vector \mathbf{p}_0 can be treated analogously). In this case, the functions $f_2(y)$ and $f_3(z)$ will be identical in form with $f_1(x)$, and $c_1 = c_2 = c_3$. With use made of (39) we place (33) in (15), which gives (cf. (30))

$$E_1 = \frac{1}{2}\rho_0\sigma_0 + \frac{p_0^2}{2m} - \frac{3\sigma_a\alpha_1^2}{\rho_0} \left[1 + \frac{4m\rho_0\sigma_a}{\hbar^2 a^2(1 - 4p^2)} \right] + \frac{12m^3(7 + 20p^2)}{\hbar^6 a^6(1 - 4p^2)^3(1 - p^2)} \alpha_1^4 \sigma_a^4. \quad (43)$$

If one minimizes this energy with respect to α_1 , one will obtain (41). Substituting α_1 given by (41) into (43) yields

$$E_1 = \frac{1}{2}\rho_0\sigma_0 + \frac{3\hbar^2 a^2}{m} \left[\frac{p^2}{2} - \frac{(1 - 4p^2)^3(1 - p^2)}{(7 + 20p^2)s_a^2} \left(1 + \frac{s_a}{1 - 4p^2} \right)^2 \right], \quad (44)$$

where the quantity s_a of (27) is employed.

Investigation of this energy shows that, if (42) is fulfilled while (26) does not hold, E_1 exceeds the energy $1/2\rho_0\sigma_0$ of the liquid, that is to say, the liquid is energetically preferable. If (26) holds (then (42) is fulfilled, of course), the energy E_1 is minimum at $p = 0$, that is to say, the nonsuperfluid crystal is energetically preferable in this instance. It should be emphasized that this conclusion is valid only if p is not close to $1/2$.

Let us calculate also the momentum flow given by (I.27). Substituting (17) with f_i obtained above yields, in a first approximation,

$$\mathbf{P} = N\mathbf{p}_0 \left[1 - \frac{8q^2}{(1 - 4p^2)^2} \right]. \quad (45)$$

If $|q|$ augments, the flow diminishes.

It remains now to be seen what happens at $p = 1/2$ where the above formulae fail (other singularities lie outside the first Brillouin zone). If we set $p = 1/2$ in (34), the equation becomes

$$\frac{d^2 f_1}{d\xi^2} + i \frac{df_1}{d\xi} = -(c - 2q \cos \xi) f_1(\xi). \quad (46)$$

In the zeroth approximation ($q = c = 0$), the equation admits a periodic solution of the form

$$u_0 = 1 + \gamma e^{-i\xi}, \quad (47)$$

instead of 1 in (35), the constant γ being arbitrary. We continue solving equation (46) according to (35) with the new u_0 now. The terms linear in q yield

$$\frac{d^2 u_1}{d\xi^2} + i \frac{du_1}{d\xi} = -a_1 + \gamma + (1 - \gamma a_1) e^{-i\xi} + e^{i\xi} + \gamma e^{-2i\xi}. \quad (48)$$

The right side must not contain constant terms and terms with $e^{-i\xi}$ which will lead to nonperiodic solutions. Therefore, $a_1 = \gamma$ and $\gamma = \pm 1$. The remaining terms give

$$u_1 = -\frac{1}{2} e^{i\xi} - \frac{\gamma}{2} e^{-2i\xi} + \gamma_1 e^{-i\xi} \quad (49)$$

with a new constant γ_1 . In the next approximation, we compute γ_1 , a_2 and u_2 and so on:

$$\gamma_1 = \gamma_2 = 0, a_2 = -\frac{1}{2}, a_3 = -\frac{\gamma}{4}. \quad (50)$$

Next, we normalize f_1 as above with the result

$$|f_1(x)|^2 = 1 + \gamma \cos ax - q(\cos ax + \gamma \cos 2ax) - \frac{q^2}{12}(9\gamma \cos ax + 4 \cos 2ax - 5 \cos 3ax). \quad (51)$$

We compare this with (14) as above and get the equation for α_1

$$\frac{3m^2}{\hbar^4 a^4} \alpha_1^2 \sigma_a^2 + \frac{2\gamma\alpha_1}{\rho_0} \left(1 + \frac{m\rho_0\sigma_a}{\hbar^2 a^2} \right) - 1 = 0. \quad (52)$$

This equation always admits two real solutions for α_1 .

We calculate now the energy by (15) with use made of (50), (35) and (17) upon putting $p = 1/2$ (we assume that $p_{0x} = p_{0y} = p_{0z} = p_0/\sqrt{3}$ as before):

$$E_1 = \frac{1}{2}\rho_0\sigma_0 + \frac{3\hbar^2 a^2}{8m} + 3\gamma\alpha_1\sigma_a - \frac{3\sigma_a\alpha_1^2}{\rho_0} \left(1 + \frac{m\rho_0\sigma_a}{\hbar^2 a^2}\right) - \frac{3\gamma m^2}{\hbar^4 a^4} \alpha_1^3 \sigma_a^3. \quad (53)$$

This E_1 has a minimum and maximum for which α_1 is specified by (52) while the minimum corresponds to $\gamma = +1$ since $\alpha_1 > 0$, which will be implied in the following.

To analyze E_1 we solve (52) for α_1 and place in (53):

$$E_1 = \frac{1}{2}\rho_0\sigma_0 + \frac{3\hbar^2 a^2}{216ms_a^3} \left[128(4 + 2s_a + s_a^2)^{3/2} - 1024 - 768s_a - 480s_a^2 - 61s_a^3\right], \quad (54)$$

where s_a of (27) is used. Numerical calculation shows that this E_1 becomes less than the energy of the liquid $1/2\rho_0\sigma_0$ when $s_a < -1.451$, and this E_1 becomes less than E_1 of (31) when $s_a < -1.660$. In the latter case, the crystal with $p = 1/2$ is energetically preferable with respect to the one of the preceding subsection with $p = 0$. It should be emphasized that these results must be considered to be only tentative as long as the corresponding values of q are rather large ($q \approx -0.5$) and subsequent terms in the above expansions in powers of q may play a role.

The values of s_a obtained just above are quite realistic for the rare gas solids in view of the above estimates (although their lattices are not SC). If $|s_a|$ is small at low pressures (the case analogous to helium), we have a liquid. When $|s_a|$ augments with the pressure, there occurs a second-order phase transition to a nonsuperfluid condensate crystal at $s_a = -1$. If $|s_a|$ continues to increase, we shall have a first-order phase transition to a crystal with $p = 1/2$ when $s_a = -1.660$ (p jumps from 0 to $1/2$). In the case analogous to heavier rare gases, the $p = 1/2$ crystal should exist at all pressures. Two remarks need to be made at this point. Firstly, the case where p is not small but $p \neq 1/2$ was not investigated here while this case may be interesting. Secondly, we have studied only the direction of the vector \mathbf{p}_0 when $p_{0x} = p_{0y} = p_{0z}$. Other directions of the vector may happen to be energetically preferable.

It is of interest to calculate the momentum flow. A calculation akin to that which leads to (45) shows that the two terms in equation (I.27) compensate each other in the present case, so that $\mathbf{P} = 0$. This result can be explained by the fact that, if $p = 1/2$, one has a standing wave owing to Bragg reflection met with when the Brillouin zone boundary is concerned. According to (45), the momentum flow \mathbf{P} first augments as p_0 increases, then diminishes and vanishes at $p = 1/2$ as we have just seen. In actual fact, we have a nonsuperfluid crystal in the last instance as long as $\mathbf{P} = 0$ although $\mathbf{p}_0 \neq 0$.

Still another question should be clarified. From the condition of (42) it follows that, if $p \rightarrow 1/2$, the condition holds even if $\sigma_a \rightarrow 0$ for any a , whereas the case

$\sigma_a \equiv 0$ corresponds to noninteracting particles. A similar results stems also from equation (52) that has a solution $\alpha_1 = \rho_0/2$ (with $\gamma = +1$) if $\sigma_a = 0$. A crystal formed by the noninteracting particles seems strange. The resolution of this paradox consists in the following. If $\sigma(k) \equiv 0$, equation (16) becomes the Schrödinger equation for a free particle. This equation admits, of course, solutions in the form of de Broglie waves (in the present case we have a standing de Broglie wave with the same spatial period as in (47)). The energy of the free particle is $p_0^2/2m$, which is in accord with (43) if $\sigma(k) \equiv 0$. Hence, our solution goes over into the solution for the free particle if $\sigma_a \rightarrow 0$, this last solution being of no interest for our problem.

3.3 Change in symmetry

If $\mathbf{P} \neq 0$, the crystal symmetry should change (see I). In particular, the inversion of the coordinate axes should now affect the formula for the density $\rho(\mathbf{r})$. At the same time, the above formulae for the density remain unaltered under the transformation $x \rightarrow -x$. This is due to a shortcoming of the approximation of (13) where $U(\mathbf{r})$ is always symmetric. To reflect the change of the crystal symmetry further terms in $U(\mathbf{r})$ are to be taken into account.

Let us perform first a general analysis. We shall assume that the vector \mathbf{p}_0 is directed along the z -axis and the initial space group is O_h^1 as above. If $\mathbf{p}_0 \neq 0$, all symmetry transformations that touch upon the direction of the z -axis will be lost. As a result, we arrive at space group $C_{4v}^1 = P4mm$. An analysis akin to the one carried out in Appendix of [4] shows that, in the Kirkwood approximation when $\sigma(\nu a) = 0$ and $\sigma(\nu b) = 0$ if $\nu > 2$, the potential $U(\mathbf{r})$ is

$$\begin{aligned} U(\mathbf{r}) = & \rho_0\sigma_0 + 2\alpha_1\sigma(a)(\cos ax + \cos ay) \\ & + 2\alpha'_1\sigma(b)\cos bz + 4\alpha_2\sigma\left(a\sqrt{2}\right)\cos ax\cos ay \\ & + 4\alpha'_2\sigma\left(\sqrt{a^2 + b^2}\right)(\cos ax + \cos ay)\cos bz \\ & + 4\alpha''_2\sigma\left(\sqrt{a^2 + b^2}\right)(\cos ax + \cos ay)\sin bz \\ & + 8\alpha_3\sigma\left(\sqrt{2a^2 + b^2}\right)\cos ax\cos ay\cos bz \\ & + 8\alpha'_3\sigma\left(\sqrt{2a^2 + b^2}\right)\cos ax\cos ay\sin bz \\ & + 2\alpha_4\sigma(2a)(\cos 2ax + \cos 2ay) \\ & + 2\alpha'_4\sigma(2b)\cos 2bz + 2\alpha''_4\sigma(2b)\sin 2bz. \end{aligned} \quad (55)$$

Here the coordinate origin is chosen such the term with $\sin bz$ is absent.

This section is devoted only to cases in which equation (2) can be reduced to a one-dimensional form. With this in mind we shall suppose that the crystal is so compressed perpendicularly to the z -axis that a becomes sufficiently large and we can neglect all $\sigma(k)$'s with $k > a$ (in the Kirkwood approximation again). In this case the

potential (55) will become

$$U(\mathbf{r}) = \rho_0 \sigma_0 + 2\alpha_1 \sigma_a (\cos ax + \cos ay) + 2\alpha'_1 \sigma_b \cos bz \\ + 2\alpha'_4 \sigma_{2b} \cos 2bz + 2\alpha''_4 \sigma_{2b} \sin 2bz, \quad (56)$$

where $\sigma_b = \sigma(b)$, $\sigma_{2b} = \sigma(2b)$ and the notation from (13) is used. The first terms in the Fourier series for the density are

$$\rho(\mathbf{r}) = \rho_0 \left[1 + \frac{2\alpha_1}{\rho_0} (\cos ax + \cos ay) + \frac{2\alpha'_1}{\rho_0} \cos bz \\ + \frac{2\alpha'_4}{\rho_0} \cos 2bz + \frac{2\alpha''_4}{\rho_0} \sin 2bz + \dots \right]. \quad (57)$$

When (56) is placed in (2), the solution can again be sought in the form of (17). Since the vector \mathbf{p}_0 is directed along the z -axis, the equations for $f_1(x)$ and $f_2(y)$ will remain as before while the equation for $f_3(z)$ will take the form

$$\frac{\hbar^2}{2m} \frac{d^2 f_3}{dz^2} + \frac{i\hbar}{m} p_0 \frac{df_3}{dz} + (c_3 - 2\alpha'_1 \sigma_b \cos bz \\ - 2\alpha'_4 \sigma_{2b} \cos 2bz - 2\alpha''_4 \sigma_{2b} \sin 2bz) f_3(z) = 0, \quad (58)$$

the quantity $\varepsilon_{(1)}$ being given by (33).

After introducing the dimensionless quantities

$$\xi = bz, \quad c = \frac{2m}{\hbar^2 b^2} c_3, \quad q_1 = \frac{2m}{\hbar^2 b^2} \alpha'_1 \sigma_b, \\ q_2 = \frac{2m}{\hbar^2 b^2} \alpha'_4 \sigma_{2b}, \quad q_3 = \frac{2m}{\hbar^2 b^2} \alpha''_4 \sigma_{2b}, \quad p = \frac{p_0}{\hbar b}, \quad (59)$$

equation (58) becomes

$$\frac{d^2 f_3}{d\xi^2} + 2ip \frac{df_3}{d\xi} + (c - 2q_1 \cos \xi \\ - 2q_2 \cos 2\xi - 2q_3 \sin 2\xi) f_3(\xi) = 0. \quad (60)$$

It is convenient to introduce a parameter q such that $q_1 = qg_1$, $q_2 = qg_2$, and $q_3 = qg_3$. We can now look for a solution to equation (60) in the form of (35) again. The terms linear in q give

$$\frac{d^2 u_1}{d\xi^2} + 2ip \frac{du_1}{d\xi} = -a_1 + 2(g_1 \cos \xi + g_2 \cos 2\xi + g_3 \sin 2\xi). \quad (61)$$

By analogy with equation (36) one obtains that $a_1 = 0$ and

$$u_1 = \frac{2g_1}{4p^2 - 1} \cos \xi - \frac{4ipg_1}{4p^2 - 1} \sin \xi + \frac{g_2 + ipg_3}{2(p^2 - 1)} \cos 2\xi \\ + \frac{g_3 - ipg_2}{2(p^2 - 1)} \sin 2\xi. \quad (62)$$

The calculations, while rather cumbersome, are carried out in much the same way as for equation (34). We shall

not write down unwieldy formulae restricting ourselves to

$$a_2 = \frac{2g_1^2}{4p^2 - 1} + \frac{g_2^2 + g_3^2}{2(p^2 - 1)}, \quad a_3 = \frac{3g_1^2 g_2}{(4p^2 - 1)(p^2 - 1)}, \\ a_4 = \frac{(7 + 20p^2) g_1^4}{2(4p^2 - 1)^3 (p^2 - 1)} + \frac{20g_1^2 (g_2^2 + g_3^2)}{(4p^2 - 1)(p^2 - 1)(4p^2 - 9)} \\ + \frac{(7 + 5p^2) (g_2^2 + g_3^2)^2}{32(p^2 - 1)^3 (p^2 - 4)}. \quad (63)$$

The first terms in the modulus squared of the normalized f_3 are

$$|f_3(z)|^2 = 1 + \frac{2q_1}{4p^2 - 1} \left\{ 2 + \frac{3q_2}{p^2 - 1} \right. \\ \left. + \frac{1}{p^2 - 1} \left[\frac{7 + 20p^2}{(4p^2 - 1)^2} q_1^2 + \frac{20(q_2^2 + q_3^2)}{4p^2 - 9} \right] \right\} \cos bz \\ + \frac{q_1 q_3}{(4p^2 - 1)(p^2 - 1)} \left[6 + \frac{16(17 + 28p^2)}{(4p^2 - 1)^2 (4p^2 - 9)} q_1^2 \right. \\ \left. - \frac{9(3 - 7p^2)}{4(p^2 - 1)^2 (p^2 - 4)} (q_2^2 + q_3^2) \right] \sin bz \\ + \frac{1}{p^2 - 1} \left\{ q_2 + \frac{3q_1^2}{4p^2 - 1} + q_2 \left[\frac{40q_1^2}{(4p^2 - 1)(4p^2 - 9)} \right. \right. \\ \left. \left. + \frac{(7 + 5p^2)(q_2^2 + q_3^2)}{8(p^2 - 1)^2 (p^2 - 4)} \right] \right\} \cos 2bz \\ + \frac{q_3}{p^2 - 1} \left[1 + \frac{40q_1^2}{(4p^2 - 1)(4p^2 - 9)} \right. \\ \left. + \frac{(7 + 5p^2)(q_2^2 + q_3^2)}{8(p^2 - 1)^2 (p^2 - 4)} \right] \sin 2bz. \quad (64)$$

A comparison between this and (57) furnishes four equations. We shall not write down the equations since they are of little interest because they can be fulfilled only if $|q_1|$, $|q_2|$ and $|q_3|$ are sufficiently large. This is seen at once if we put the coefficient of $\sin bz$ in (64) equal to zero, as in (57), with $q_1 \neq 0$ and $q_3 \neq 0$ (recall that the above series are valid in case p is not close to $1/2$). It may be observed in passing that the equation that follows from the coefficient of $\sin bz$ put equal to zero is a consequence of the other three equations. The first terms in the series can be employed only if $|q_1|$, $|q_2|$ and $|q_3|$ are small. To obtain trustworthy equations for q_1 , q_2 and q_3 it is necessary to know an expression for f_3 of the type (64) for large $|q_1|$, $|q_2|$ and $|q_3|$. This can most likely be achieved only with use made of numerical methods. It may be added that the above three equations can also be obtained by minimizing the energy with respect to α'_1 , α'_4 , α''_4 (or q_1 , q_2 , q_3), the energy in the present instance being of the form

$$E_1 = \frac{1}{2} \rho_0 \sigma_0 + \frac{p_0^2}{2m} + \frac{\hbar^2 b^2}{2m} c - \alpha'^2_1 \frac{\sigma_b}{\rho_0} \\ - \left(\alpha'^2_4 + \alpha''^2_4 \right) \frac{\sigma_{2b}}{\rho_0} + E_1(\alpha_1), \quad (65)$$

where $E_1(\alpha_1)$ is the part of the energy that depends on the parameter α_1 in (56).

It should be emphasized that we have utilized the simplified potential of (56) whereas even the full potential of (55) is of little physical interest because the SC lattice are rare in nature. The main aim in the present subsection was to elaborate a mathematical method for treating the change in crystal symmetry induced by the superflow using a simple example that can be reduced to a one-dimensional problem. It may turn out that crystals (with arbitrary lattices) superfluid in the ground state are few and far between, in which case the equations obtainable with the method of the section will have solutions only for peculiar types of the interatomic potential.

4 Face centred cubic lattice

When considering the face centred cubic (FCC) lattice, we shall imply the symmorphic space group of the highest symmetry, namely, $O_h^5 = Fm\bar{3}m$, and take the vectors $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ to be directed along the axes of a rectangular coordinate system with $a = |\mathbf{a}_1| = |\mathbf{a}_2| = |\mathbf{a}_3|$. Note that in I the vectors $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ were chosen otherwise; they corresponded to the smallest lattice periods and were not mutually orthogonal. Resorting to the Kirkwood approximation we assume that $\sigma(\nu a) = 0$ if $\nu \geq 2$. In this case, according to Appendix of [4] the effective potential is of the form

$$U(\mathbf{r}) = \rho_0 \sigma_0 + 8\alpha_3 \sigma_3 \cos ax \cos ay \cos az, \quad (66)$$

where $\sigma_0 = \sigma(0)$, $\sigma_3 = \sigma(a\sqrt{3})$, $\alpha_3 = a_{\pm 1 \pm 1 \pm 1}$. The first terms in the Fourier series for the density are

$$\rho(\mathbf{r}) = \rho_0 \left[1 + \frac{8\alpha_3}{\rho_0} \cos ax \cos ay \cos az + \dots \right]. \quad (67)$$

We shall assume that one of the maximums of the density lies at $x = y = z = 0$, for which it is necessary that $\alpha_3 > 0$. Since the potential should have a minimum there, we have $\sigma_3 < 0$.

We write down also the energy per one particle $E_1 = E/N$ that in view of (9) is

$$E_1 = \varepsilon_{(1)} - \frac{1}{2}\rho_0\sigma_0 - \frac{4}{\rho_0}\alpha_3^2\sigma_3. \quad (68)$$

4.1 Nonsuperfluid crystal

We set $\mathbf{p}_0 = 0$ in equation (2) and substitute (66) with the result

$$\frac{\hbar^2}{2m} \nabla^2 u(\mathbf{r}) + \left[\varepsilon_{(1)} - \rho_0 \sigma_0 - 8\alpha_3 \sigma_3 \cos ax \cos ay \cos az \right] u(\mathbf{r}) = 0. \quad (69)$$

The variables in this equation cannot be separated unlike equation (16). The author does not know any study on

three-dimensional differential equations of this type. For this reason, equation (69) will be solved leaning upon the method used above.

We first define dimensionless quantities according to

$$\begin{aligned} \tilde{x} &= ax, & \tilde{y} &= ay, & \tilde{z} &= az, \\ c &= \frac{2m}{\hbar^2 a^2} [\varepsilon_{(1)} - \rho_0 \sigma_0], & q &= \frac{2m}{\hbar^2 a^2} \alpha_3 \sigma_3. \end{aligned} \quad (70)$$

Now equation (69) can be recast in the form

$$\frac{\partial^2 u}{\partial \tilde{x}^2} + \frac{\partial^2 u}{\partial \tilde{y}^2} + \frac{\partial^2 u}{\partial \tilde{z}^2} = -cu(\tilde{\mathbf{r}}) + 8q \cos \tilde{x} \cos \tilde{y} \cos \tilde{z} u(\tilde{\mathbf{r}}). \quad (71)$$

By analogy with (35), we look for a solution to (71) in terms of expansions in powers of q :

$$\begin{aligned} u &= 1 + qu_1(\tilde{\mathbf{r}}) + q^2 u_2(\tilde{\mathbf{r}}) + q^3 u_3(\tilde{\mathbf{r}}) + q^4 u_4(\tilde{\mathbf{r}}) + \dots, \\ c &= qa_1 + q^2 a_2 + q^3 a_3 + q^4 a_4 + \dots \end{aligned} \quad (72)$$

The terms in (71) linear in q give

$$\frac{\partial^2 u_1}{\partial \tilde{x}^2} + \frac{\partial^2 u_1}{\partial \tilde{y}^2} + \frac{\partial^2 u_1}{\partial \tilde{z}^2} = -a_1 + 8 \cos \tilde{x} \cos \tilde{y} \cos \tilde{z}. \quad (73)$$

The right-hand side should contain no constant terms by the same reasoning as for (36); therefore $a_1 = 0$. The periodic solution to (73) is of the form

$$u_1 = -\frac{8}{3} \cos \tilde{x} \cos \tilde{y} \cos \tilde{z}. \quad (74)$$

In an analogous way, one can calculate other terms in the expansions of (72). For example, $a_2 = -8/3$, $a_3 = 0$, $a_4 = -28/27$ and

$$\begin{aligned} u_2 &= \frac{2}{3} (\cos 2\tilde{x} + \cos 2\tilde{y} + \cos 2\tilde{z}) + \frac{1}{3} (\cos 2\tilde{x} \cos 2\tilde{y} \\ &+ \cos 2\tilde{y} \cos 2\tilde{z} + \cos 2\tilde{x} \cos 2\tilde{z}) + \frac{2}{9} \cos 2\tilde{x} \cos 2\tilde{y} \cos 2\tilde{z}. \end{aligned} \quad (75)$$

The next step is to normalize u according to (3). Let us write down the terms in the modulus squared of the normalized u that are needed for our purposes:

$$|u(\mathbf{r})|^2 = 1 - \frac{16}{3}q \left(1 + \frac{7}{9}q^2 \right) \cos ax \cos ay \cos az + \dots \quad (76)$$

With account taken of (1) we compare this with (67), which yields the following equation for α_3

$$1 + \frac{4m\rho_0\sigma_3}{3\hbar^2 a^2} = -\frac{112m^3\rho_0}{27\hbar^6 a^6} \alpha_3^2 \sigma_3^3. \quad (77)$$

Seeing that $\sigma_3 < 0$, we have the following condition for the solution to exist

$$1 + \frac{4m\rho_0\sigma_3}{3\hbar^2 a^2} > 0. \quad (78)$$

In contradistinction to (26), this condition can be fulfilled only if $|\sigma_3|$ is small. To clarify the situation we compute

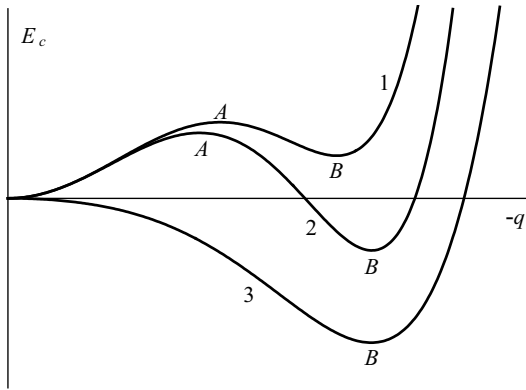


Fig. 1. Energy $E_c = E_1 - 1/2\rho_0\sigma_0$ for the FCC lattice as a function of q . The abscissa axis is inverted for convenience since $q < 0$.

the energy. We place $\varepsilon_{(1)}$ taken from (70) with regard to (72) in (68). It is convenient to express the result in terms of q :

$$E_1 = \frac{1}{2}\rho_0\sigma_0 - \frac{\hbar^4 a^4}{m^2 \rho_0 \sigma_3} \left(1 + \frac{4m\rho_0\sigma_3}{3\hbar^2 a^2} \right) q^2 - \frac{14\hbar^2 a^2}{27m} q^4. \quad (79)$$

When the condition of (78) is fulfilled, the coefficient of q^2 in (79) is positive and the energy first increases with $|q|$ and then begins to decrease limitlessly owing to the last term. At the same time the energy must be limited from below. To obtain this one may try and calculate subsequent terms in the expansion of E_1 in powers of q . Such a procedure will not be of much benefit, however, insofar as the subsequent terms may have different signs and we shall not be sure that uncalculated terms will leave the situation unchanged. To resolve the problem we can resort to a result obtained below in Section 4.3 according to which $\varepsilon_{(1)}$ is proportional to $8q$ as $|q| \rightarrow \infty$. Now we see that the last term in (68) which is positive and proportional to q^2 will dominate over the first term in the limit as $|q| \rightarrow \infty$ so that $E_1 \propto +q^2$ in this limit. The resulting schematic picture is presented in Figure 1.

When $|\sigma_3|$ is small and (78) holds, we have curves 1 or 2, equation (77) being relevant to the maximum at point A. When $|\sigma_3|$ is large and the inequality of (78) breaks down, the maximum disappears and we have curve 3. If $\sigma_3 = \sigma(a\sqrt{3})$ changes with the pressure (see Sect. 3.1), we shall have a first-order phase transition from the liquid state to the condensate crystalline state when point B touches the abscissa. To study the phase transition it needs to know the parameter α_3 and the energy E_1 in the neighbourhood of the minimum of E_1 at point B where $|q|$ is not small. The expansions in powers of q are of little use there.

It is interesting to observe that in the classical case the phase transition from the liquid to a FCC crystal described by the same potential as in (66) is first order as well [4]. In this last reference, the transition is studied in detail. In this context, it is worthwhile to discuss in brief still another type of the cubic lattices, namely, the body centered cubic (BCC) lattice. In the case of the

symmorphic BCC space group of the highest symmetry $O_h^9 = Im\bar{3}m$, the effective potential is specified by equation (A.7) of [4] (we put $\gamma_4 = 0$ and denote the first Fourier coefficient by α_2). This potential can be treated in perfect analogy with (66) revealing two important dissimilarities in the results. Firstly, in an equation of the type (25) or (77), the right-hand side will be linear in α_2 instead of being quadratic in α_1 or α_3 and thereby no condition of the type (26) or (78) will exist. Secondly, in the formula for the energy of the type (30) or (79) there will be a cubic in α_2 (or q) term. All of these signify that the peculiarities of the phase transition from a liquid to the BCC condensate crystal will be analogous to the ones in the case of a classical crystal considered in detail in Section 4.1 of [4].

4.2 Superfluid crystal

In order to find out principal details in the case where $\mathbf{p}_0 \neq 0$, for the sake of simplicity, we shall not take explicit account of the symmetry change due to the vector \mathbf{p}_0 . For definiteness, we shall assume that the vector \mathbf{p}_0 is directed along the z -axis. We shall suppose also that the crystal is subjected to external stresses such that the crystal cell remains cubic.

If (66) is placed in (2), we get

$$\frac{\hbar^2}{2m} \nabla^2 u(\mathbf{r}) + \frac{i\hbar p_0}{m} \frac{\partial u}{\partial z} + \left[\varepsilon_{(1)} - \frac{p_0^2}{2m} - \rho_0 \sigma_0 - 8\alpha_3 \sigma_3 \cos ax \cos ay \cos az \right] u(\mathbf{r}) = 0. \quad (80)$$

Upon introducing $\tilde{\mathbf{r}}$, q analogously with (70), and also $\mathbf{p} = \mathbf{p}_0/\hbar a$ and

$$c = \frac{2m}{\hbar^2 a^2} \left[\varepsilon_{(1)} - \frac{p_0^2}{2m} - \rho_0 \sigma_0 \right], \quad (81)$$

equation (80) becomes

$$\tilde{\nabla}^2 u(\mathbf{r}) + 2ip \frac{\partial u}{\partial \tilde{z}} + [c - 8q \cos \tilde{x} \cos \tilde{y} \cos \tilde{z}] u(\tilde{\mathbf{r}}) = 0. \quad (82)$$

The procedure of solving this equation is fully analogous with the one used for (71) (and especially for (34)). Let us write down only the expression for the eigenvalue c :

$$c = \frac{24}{4p^2 - 9} q^2 - \eta(p) q^4 + \dots; \quad \eta(p) = 6 \frac{4536 - 3636p^2 + 3687p^4 - 559p^6 + 12p^8}{(4p^2 - 9)^3 (p^2 - 1) (p^2 - 4) (p^2 - 9)}, \quad (83)$$

and the first terms in the modulus squared of the normalized u :

$$|u(\mathbf{r})|^2 = 1 + q \left[\frac{48}{4p^2 - 9} - 4\eta(p)q^2 \right] \times \cos ax \cos ay \cos az + \dots \quad (84)$$

These formulae demonstrate the character of corrections to the formulae of the preceding subsection in the case

where $\mathbf{p}_0 \neq 0$. We shall not discuss the corrections inasmuch as they are relevant to small values of $|q|$, whereas the physically interesting region lies in the neighbourhood of the minimum of the energy at point B in Figure 1. In this subsection, we were interested first of all in the procedure of treating the equations for a FCC superfluid crystal.

4.3 Strongly localized particles

If $|\alpha_3\sigma_3|$ in equation (69) (and consequently, $|q|$ of (70)) is very large, each atom will be in a deep potential well and will oscillate near the bottom of the well. If we take, for example, the atom that is located near the site at $x = y = z = 0$, the cosines in equation (71) can be replaced by the first terms of the Maclaurin series, so that

$$\tilde{\nabla}^2 u(\tilde{\mathbf{r}}) + [c - 8q + 4q(\tilde{x}^2 + \tilde{y}^2 + \tilde{z}^2)] u(\tilde{\mathbf{r}}) = 0. \quad (85)$$

This is the Schrödinger equation (in a dimensionless form) for a three-dimensional harmonic oscillator. The solution for the ground state is of the form

$$u = Be^{-\beta\tilde{\mathbf{r}}^2}. \quad (86)$$

Substituting into (85) yields

$$\beta = \sqrt{-q}, c = 8q + 6\sqrt{-q}. \quad (87)$$

The first term of this last formula for c was used above when discussing the energy represented in Figure 1.

Now it is necessary to normalize u . In the volume $v_0 = d^3 = 8\pi^3/a^3$ of the cubic FCC cell there are 4 particles. When making use of (3) we can integrate over the overall space upon neglecting exponentially small terms once $|q|$ and thereby $\beta \rightarrow \infty$. As a result,

$$B = 2^{5/4}\pi^{3/4}(-q)^{3/8}. \quad (88)$$

The next step is to obtain an equation for $\alpha_3 = a_{\pm 1 \pm 1 \pm 1}$ that figures in the above formulae. The Fourier coefficients of the density $\rho(\mathbf{r})$ are defined by [12]

$$a_{lmn} = \frac{1}{v_0} \int \rho(\mathbf{r}) e^{-i\mathbf{A}\mathbf{r}} d\mathbf{r}, \quad (89)$$

where \mathbf{A} is the same as in (6). When (1) with (86) are inserted into (89), one can again integrate over the overall space:

$$a_{lmn} = \rho_0 \exp\left(-\frac{A^2}{8\beta a^2}\right). \quad (90)$$

Putting here $l = m = n = 1$ (then $A^2 = 3a^2$) and taking β from (87) one obtains the equation sought for α_3 as long as q depends on α_3 by (70):

$$\alpha_3 = \rho_0 \exp\left(-\frac{3}{8\sqrt{-q}}\right). \quad (91)$$

According to the foregoing this equation is meaningful only when $|q|$ is large. Expanding the exponential in powers of $1/|q|$ yields finally

$$\frac{\alpha_3}{\rho_0} = 1 - \frac{3}{8} \sqrt{-\frac{\hbar^2 a^2}{2m\sigma_3\alpha_3}}. \quad (92)$$

This equation completes the solution of the problem in the case of strongly localized particles. The equation always has real roots for α_3 when $|\sigma_3|$ is large. The crystal density can be obtained by periodical continuation of the function u from (86).

We turn now to the energy. If $\varepsilon_{(1)}$ from (70) with account taken of (87) is placed in (68), there results

$$E_1 = \frac{1}{2}\rho_0\sigma_0 - \frac{4}{\rho_0}\alpha_3^2\sigma_3 + 8\alpha_3\sigma_3 + 3\sqrt{-\frac{2\hbar^2 a^2}{m}}\alpha_3\sigma_3. \quad (93)$$

If one puts the derivative $dE_1/d\alpha_3$ equal to zero, one will get just equation (92). The greater root of (92) corresponds to a minimum of E_1 . Thus, we have obtained point B in Figure 1 going from large $|q|$. If $\sigma_3 = \sigma(a\sqrt{3})$ changes with the pressure, the first-order phase transition from the liquid state to the condensate crystalline state occurs when point B touches the abscissa. One can get the relevant value of σ_3 if one eliminates α_3 from two equations, $E_1 - 1/2\rho_0\sigma_0 = 0$ and (92).

It is of interest to compare the energy of the condensate crystalline state with the energy of an ordinary crystal at absolute zero of temperature ($T = 0$). The ordinary quantum crystal in the framework of the approach proposed in [2] was considered in reference [8]. The case of low temperatures is treated in Section 6 of [8]. We need the function $\tilde{K}(\mathbf{r})$ defined in (6.19) of [8]. It should be remarked that the approximation of nearest neighbours utilized in Section 6 of [8] is necessary only for $T \neq 0$. If $T = 0$, we can sum over all lattice sites, then

$$\tilde{K}(\mathbf{r}) = \sum_{l,m,n} K(|\mathbf{r} - \mathbf{D}|), \quad (94)$$

with $\mathbf{D} = l\mathbf{d}_1 + m\mathbf{d}_2 + n\mathbf{d}_3$ in which $\mathbf{d}_1, \mathbf{d}_2, \mathbf{d}_3$ are the crystal periods. By analogy with $U(\mathbf{r})$ in (7) this function $\tilde{K}(\mathbf{r})$ can be represented by the Fourier series (an equation of the type (89) is to be used)

$$\tilde{K}(\mathbf{r}) = \rho_0 \sum_{l,m,n} \sigma(A) e^{i\mathbf{A}\mathbf{r}}. \quad (95)$$

In the same approximation in which (66) is written, equation (95) yields

$$\tilde{K}(\mathbf{r}) = \rho_0\sigma_0 + 8\rho_0\sigma_3 \cos ax \cos ay \cos az. \quad (96)$$

Now we are able to calculate the quantities defined in (6.20) of [8]:

$$\begin{aligned} K_0 &= \tilde{K}(0) = \rho_0\sigma_0 + 8\rho_0\sigma_3, \\ K_{21} &= \tilde{K}''_{xx}(0) = -8\rho_0\sigma_3 a^2. \end{aligned} \quad (97)$$

Substituting this into equation (6.33) of [8] for the energy of the ordinary quantum crystal at $\theta = T = 0$ yields

$$E_1^{(ord)} = \frac{1}{2}\rho_0\sigma_0 + 4\rho_0\sigma_3 + 3\sqrt{-\frac{2\hbar^2 a^2}{m}\rho_0\sigma_3}. \quad (98)$$

We have to compare this energy with (93). To this end we eliminate the square root from (93) with the help of (92):

$$E_1 = \frac{1}{2}\rho_0\sigma_0 + \frac{12}{\rho_0}\alpha_3^2\sigma_3 - 8\alpha_3\sigma_3. \quad (99)$$

The right side of this equation is a minimum when α_3 satisfies (92). If, instead of this α_3 , one takes $\alpha_3 = \rho_0$, one only augments the right side; therefore

$$E_1 < \frac{1}{2}\rho_0\sigma_0 + 4\rho_0\sigma_3. \quad (100)$$

Comparing this with (98) we see clearly that $E_1 < E_1^{(ord)}$, which amounts to saying that the condensate crystal is energetically more preferable than the ordinary quantum crystal at $T = 0$. Therefore, on lowering the temperature there must somewhere occur a phase transition from an ordinary crystalline state to the state with condensate. It may be remarked that the character of motion of atoms near the lattice sites at $T = 0$ closely resembles each other in both the cases in a first approximation because equations (86) and (6.11) of [8] are similar. In the condensate phase, nevertheless, there exist especial correlations between the atoms that give rise to off-diagonal long range order (ODLRO) described by equation (I.25).

It remains for us to consider the superfluid crystal where $\mathbf{p}_0 \neq 0$. The direction of the vector \mathbf{p}_0 plays no role in the present approximation. For this reason, after the manipulations that have led to (85), we rewrite equation (82) in a more general form

$$\tilde{\nabla}^2 u(\tilde{\mathbf{r}}) + 2i\mathbf{p} \frac{\partial u}{\partial \tilde{\mathbf{r}}} + [c - 8q + 4q(\tilde{x}^2 + \tilde{y}^2 + \tilde{z}^2)] u(\tilde{\mathbf{r}}) = 0. \quad (101)$$

The solution of this equation that goes over into (86) as $\mathbf{p}_0 \rightarrow 0$ is

$$u = B e^{-\beta\tilde{\mathbf{r}}^2 + i\mathbf{g}\tilde{\mathbf{r}}}. \quad (102)$$

Substituting into (101) gives

$$\beta = \sqrt{-q}, \quad \mathbf{g} = -\mathbf{p}, \quad c = 8q + 6\sqrt{-q} - \mathbf{p}^2. \quad (103)$$

These results can be anticipated in advance. As a matter of fact, the function $\varphi_1(\mathbf{r})$ of (I.15) has a factor $\exp(i\mathbf{p}_0\mathbf{r}/\hbar)$ that cancels out when (102) is put into (I.15), and one arrives at equation (I.14) for $u_1(\mathbf{r}) \equiv u(\mathbf{r})$ that will lead to (85). It should be emphasized that the cancellation of the factor $\exp(i\mathbf{p}_0\mathbf{r}/\hbar)$ occurs only at the lattice site $x = y = z = 0$. When the function $u(\mathbf{r})$ of (102) is periodically continued in space (the continuation is performed by the replacement $\mathbf{r} \rightarrow \mathbf{r} - \mathbf{D}$), there will remain the factor $\exp(i\mathbf{p}_0\mathbf{D}/\hbar)$ at other sites. To treat the $\mathbf{p}_0 \neq 0$ case for the strongly localized particles a more sophisticated approximation should be worked out.

Nevertheless the above results point to an important fact. When c of (103) is placed in $\varepsilon_{(1)}$ taken from (81), the term $p_0^2/2m$ will disappear. The term essentially augments the energy of the superfluid crystal. This is seen, for example, from equation (44): if the term $p^2/2$ in the square brackets is deleted, the energy of the superfluid crystal will always be less than that of the liquid. When the energy of the superfluid crystal is calculated with the help of the above-mentioned sophisticated approximation, it seems quite possible that this energy without the term $p_0^2/2m$ will be less than the one of the nonsuperfluid crystal.

There is yet another fact worthwhile to be mentioned. If one calculates the momentum flow given by equation (I.27) with use made of (102), one will see that the two terms in (I.27) cancel each other out with the result that $\mathbf{P} = 0$. Here again the approximation used above is not sufficient for calculating \mathbf{P} .

5 Concluding remarks

In nature, there is only one liquid, namely, liquid helium II, that exhibits Bose-Einstein condensation. All other substances are solid at such temperatures. The results of I and of the present paper demonstrate that the Bose-Einstein condensation can occur in the solid state as well¹. Moreover, in Section 4.3 it was shown that a crystal in which the condensate is formed is energetically preferable with respect to the same quantum crystal without condensate at $T = 0$ (at least in the case treated in that subsection). Therefore, on lowering the temperature of the crystal there must somewhere happen Bose-Einstein condensation as in liquid helium, which should manifest itself in the temperature behaviour of various physical quantities. This opens a huge field for experimental investigations of Bose-Einstein condensation and of its influence on properties of the solids. An estimate for the Bose-Einstein condensation point in solid neon can be found in I.

The next intriguing question arises as to whether the condensate crystals can be superfluid. Let us first recall the interpretation of superfluidity proposed in [7] and different from the well-known Landau mechanism (remarks on Landau's mechanism can be found in the full version of reference [7]). We start from an analogy with atoms. Many atoms in the ground state possess an orbital angular momentum \mathbf{L} , only electrons of the outermost shells contributing to \mathbf{L} [14] (note that atoms with many electrons can have a significant orbital momentum). The movement of these electrons is in fact a superflow, and thereby the atoms can be regarded as tiny superfluid systems (more precisely, superconducting systems since the electrons are charged and their movement is an electric current). The circular flow of \mathbf{L} in the atoms persists perpetually without any dissipation. This purely quantum effect can manifest itself in macroscopic bodies as well. A superfluid body

¹ The present study is restricted to spinless bosons. A modification of the approach used with account taken of the spin can be found in [13].

may be regarded as a gigantic atom formed by ordinary atoms in which the orbital motion is converted to a rectilinear characterized by a linear momentum \mathbf{P} , only atoms of the condensate contributing to \mathbf{P} . We shall not speak here of further details and analogies concerning this interpretation of superfluidity referring to [7].

We can point out an experimental fact that supports the above interpretation of superfluidity. If helium II is placed in an open vessel, it always crawls up the wall, out of the vessel [15]. Why should the liquid creep up the wall against the force of gravity if its sole property is the absence of viscosity? This fact can be readily explained if we presume that the thermodynamically equilibrium state of helium II is characterized by the presence of an intrinsic superflow whose magnitude is fixed by thermodynamics [7]. It is clear that the superflow tries and chooses a rectilinear trajectory and for this reason moves along the wall despite the gravity. In an analogous fashion, one can explain the fountain effect [15]. The effect is more involved because of a temperature gradient that occurs here. Owing to the gradient, however, the closed streamlines [7] can open and the spontaneous superflow will flow up through the capillary tube placed in the container with helium II.

We now return to the crystals. The results of I and of the present paper show that the spontaneous superflow can exist in perfect crystals as well, the magnitude of the superflow being given by (I.27). The question as to whether the superflow can exist in a state of thermodynamic equilibrium (or in the ground state at $T = 0$) of the crystal is still open (in the present paper we could not answer the question). In [7] it was observed that the potential of interaction between helium atoms has a peculiarity. It is not excluded that just to this peculiarity is due the fact that helium II is superfluid in the thermodynamically equilibrium state. If this is the case, the condensate crystals will be superfluid in thermodynamic equilibrium only if their interatomic potential has a similar peculiarity. At the same time other peculiarities in the interatomic potentials that would lead to superfluidity are not inconceivable as well.

If we revert to the atoms, an atom that has $\mathbf{L} = 0$ in the ground state can pass into an excited state where $\mathbf{L} \neq 0$. Analogously, a condensate crystal whose thermodynamically equilibrium state is not superfluid ($\mathbf{P} = 0$) may pass into a superfluid metastable state where $\mathbf{P} \neq 0$ (such states do exist according the results of I and of this paper).

The role of the exciting agent in this case can be played by a temperature or pressure gradient. This can also occur if the crystal is placed in a rotating container as discussed in I. The lifetime of the excited state of the atom is very short, which is due to the action of the electromagnetic field created by the electron upon the electron itself. This quantum electrodynamicical effect is absent in the case of neutral atoms, so that the lifetime of the superfluid metastable state may be rather long.

An interesting situation may occur in metals in which the positive ions that form the crystal lattice are bosons (this depends upon the number of neutrons in the nucleus). The ionic system may well pass into a condensate state that might turn out superfluid (perhaps, metastable²). In this case we shall have ionic superconductivity because the ions have a charge. Therefore, along with electronic superconductivity a metal can possess ionic superconductivity. The case is not inconceivable in which a metal is an ionic superconductor without being an electronic superconductor.

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² In the metals, the role of the exciting agent may be played not only by an external voltage but also by a contact potential as noted in [7].