Two-dimensional and layered crystals

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A two-dimensional atomic system is considered by means of the method developed in the theory of strongly anharmonic crystals.[7] It is shown that although long-range order is absent in such systems at low temperatures, there exist elastic moduli, including the shear modulus, and their behavior as functions of temperature is determined. The long-range crystal order which arises in a stack of such layers is studied as a function of the interplane interaction constant. The resonance frequency in inelastic scattering of thermal neutrons by a two-dimensional lattice is the branch point for the dynamic structure factor. The temperature dependence of the order of the branch point is calculated.

1. INTRODUCTION

It is well known that there is no long-range order in two-dimensional systems at finite temperature. As noted already by Peierls[1], the absence of crystalline ordering in the two-dimensional case at finite temperature follows from the divergence of the mean-squared deviations of the atoms from the equilibrium position with increasing sample dimensions. Namely, in the harmonic approximation we have

$$\langle \mathbf{u}_i^2 \rangle = \frac{\hbar}{2mN} \sum_{\mathbf{k},\lambda} \frac{1}{\omega_\lambda(\mathbf{k})} \operatorname{cth} \frac{\hbar\omega_\lambda(\mathbf{k})}{2T} \approx \frac{Ta^2\nu}{\pi m u^2} \ln \frac{R}{a}. \tag{1.1}$$

Here m is the mass of the atom, $\omega_\lambda(\mathbf{k})$ is the frequency of the λ-th mode of the oscillations, a is the average distance between atoms, u is the average speed of sound, ν is a geometric factor equal to unity for a square lattice and to $\sqrt{3}/2$ for a triangular lattice, and R is the dimension of the sample. Outside the framework of the harmonic approximation, the impossibility of the existence of two-dimensional crystals was proved by Mermin[2].

However, if the mean-squared deviation of the atom from the equilibrium position diverges logarithmically with increasing sample dimension, then the mean squared difference of the deviations of two atoms

$$\langle (\mathbf{u}_i - \mathbf{u}_j)^2 \rangle = \frac{\hbar}{mN} \sum_{\mathbf{k},\lambda} \frac{1-\exp(i\mathbf{k}\mathbf{R}_{ij})}{\omega_\lambda(\mathbf{k})} \operatorname{cth} \frac{\hbar\omega_\lambda(\mathbf{k})}{2T} \tag{1.2}$$

is finite for each finite value of the distance $\mathbf{R}_{ij}$ between them. At large $\mathbf{R}_{ij}$, equation (1) behaves asymptotically like

$$\frac{2Ta^2\nu}{\pi m u^2} \ln \frac{R_{ij}}{a}.$$

Comparing this quantity with a^2, we find that for sections with dimensions smaller than

$$\rho \approx a \exp(\pi m u^2 / 2\nu T) \tag{1.3}$$

it can be assumed that the crystal retains the memory of the long-range order that was present at zero temperature[1)].

This circumstance leads to a power-law decrease of the correlator of the position of two particles

$$\langle \exp[i\mathbf{q}(\mathbf{r}_i - \mathbf{r}_j)] \rangle \sim R_{ij}^{-2\Delta}. \tag{1.4}$$

Here $\mathbf{q}$ is the reciprocal-lattice vector, and $\Delta = \nu T a^2 q^2 / 4\pi m u^2$. It follows from (1.4) that in the two-dimensional case, below a certain temperature $T_c = 4\pi m u^2 / \nu a^2 q^2$ the static structure factor becomes infinite with increasing sample dimension R (see[3,4]):

$$N^{-1} \langle \rho(\mathbf{q}) \rho(-\mathbf{q}) \rangle \sim R^{2(1-\Delta)}. \tag{1.5}$$

For $T > T_c$, the structure factor becomes finite, as is assumed also in the case of liquids. Berezinskiĭ[5] has demonstrated that in the two-dimensional case there occurs in the low-temperature phase a "transverse rigidity" (shear modulus for a crystal), which is here an order parameter, and indicated the connection between the exponent Δ and this quantity.

All the results[3-5], however, were obtained in the harmonic approximation where, as is well known, there is no temperature dependence of the interatomic distances and of the force constants, and consequently there is no melting. Pokrovskiĭ and Uĭmin[6] have developed a self-consistent method of summing the anharmonicities for the calculation of the dependence of the "transverse rigidity" on the temperature in the model of a flat planar magnet. In this paper, using a self-consistent procedure similar to that used in[6], we investigate the behavior of flat[2)] and layered crystal structures, with weak interaction between layers, below the phase transition temperature T_m. The question of the character of the transition and of the temperature dependence of the thermodynamic functions near the transition point remains open and will not be discussed.

2. TWO-DIMENSIONAL CRYSTAL

We consider a system of atoms on a plane; these atoms interact with one another via paired central forces. The Hamiltonian of this system is

$$H = \sum_i \left(-\frac{\hbar^2}{2m} \nabla_i^2 \right) + \frac{1}{2} \sum_{i \neq j} v(\mathbf{r}_i - \mathbf{r}_j). \tag{2.1}$$

At zero temperature, the system of atoms in the plane forms a crystal lattice. As follows from (1.1)—(1.3), at nonzero temperatures the main contribution to the breaking of the crystal order is made by long-wave fluctuations. It can therefore be assumed, in the limit of long-wave fluctuations, that the system is described by a certain harmonic Hamiltonian

$$H_h = \sum_i \left(-\frac{\hbar}{2m} \nabla_i^2 \right) + \frac{1}{2} \sum_{\substack{i \neq j \\ \alpha,\beta}} \frac{1}{2} u_{ij}^\alpha \Phi_{ij}^{\alpha\beta} u_{ij}^\beta, \tag{2.2}$$

$$u_{ij}^\alpha = u_i^\alpha - u_j^\alpha = r_i^\alpha - r_j^\alpha - R_{ij}^\alpha;\ \alpha, \beta = x, y, z;$$

where $\mathbf{R}_{ij} = \mathbf{R}_i - \mathbf{R}_j$ is a certain average distance between the i-th and j-th atoms. As already noted in the introduction, for large differences $i - j$ the distance is not defined, but if we take into account the interaction of a given atom only with sufficiently near neighbors, then we can introduce an average distance between close atoms.

The force constants $\Phi_{ij}^{\alpha\beta}$ are chosen such that at a given temperature the harmonic Hamiltonian (2.2) ap-

proximates in the best manner the initial Hamiltonian (2.1). This problem was solved by various methods in the theory of anharmonic crystals (see, e.g., [7], where it is solved by a variational principle). For the frequencies $\omega_\lambda(k)$, for the mean-squared deviations $D_{ij}^{\alpha\beta} = \langle u_{ij}^\alpha u_{ij}^\beta \rangle$, and for the force constants Φ_{ij}, we obtain the following self-consistent system of equations

$$\omega_\lambda^2(\mathbf{k}) e_\lambda^\alpha(\mathbf{k}) = \frac{1}{m}\sum_j (1-\exp(i\mathbf{k}\mathbf{R}_{ij})) e_\lambda^\beta(\mathbf{k}) \Phi_{ij}^{\alpha\beta},$$

$$D_{ij}^{\alpha\beta} = \frac{\hbar}{mN}\sum_{\mathbf{k},\lambda} (1-\exp(i\mathbf{k}\mathbf{R}_{ij})) \frac{e_\lambda^\alpha(\mathbf{k}) e_\lambda^\beta(\mathbf{k})}{\omega_\lambda(\mathbf{k})} \operatorname{cth}\frac{\hbar\omega_\lambda(\mathbf{k})}{2T}, \tag{2.3}$$

$$\Phi_{ij}^{\alpha\beta} = \frac{\partial^2 w_{ij}(\mathbf{r})}{\partial r_\alpha \partial r_\beta}\Big|_{\mathbf{r}=\mathbf{R}_{ij}},$$

$$w_{ij}(\mathbf{r}) = \frac{1}{[(2\pi)^2 \det D_{ij}^{\alpha\beta}]^{1/2}} \int d^2u\, v(\mathbf{r}+\mathbf{u}) \exp\left\{-\frac{1}{2} u^\alpha (D_{ij}^{\alpha\beta})^{-1} u^\beta\right\}.$$

Here $e_\lambda(k)$ are the polarization vectors. We note that in the derivation of (2.3) we did not use anywhere the assumption that the atoms form a regular lattice. We use throughout not the absolute positions of the atoms $\mathbf{R}_i$, but the distances between atoms $\mathbf{R}_{ij}$. The possibility of diagonalizing the quadratic form (2.2) in order to derive equations for the frequencies is due to the fact that $\Phi_{ij}^{\alpha\beta}$ depend only on the differences $i-j$.

Assume that at zero temperature the lattice was trigonal with distances a_0 between neighboring atoms. For simplicity we assume also that only the nearest neighbors interact. Then (2.3) can be rewritten in the form

$$\omega_\lambda^2(\mathbf{k}) = \frac{1}{m}\sum_{\mathbf{a}} (1-e^{i\mathbf{k}\mathbf{a}}) \frac{(\mathbf{e}_\lambda(\mathbf{k})\mathbf{a})^2}{a^2} \frac{\partial^2 w(\mathbf{a})}{\partial a^2},$$

$$D_a = \frac{D_a^{\alpha\beta} a^\alpha a^\beta}{a^2} = \frac{\hbar}{mN}\sum_{\mathbf{k}\lambda} (1-e^{i\mathbf{k}\mathbf{a}}) \frac{(\mathbf{e}_\lambda(\mathbf{k})\mathbf{a})^2}{a^2\omega_\lambda(\mathbf{k})} \operatorname{cth}\frac{\hbar\omega_\lambda(\mathbf{k})}{2T}, \tag{2.4}$$

$$w(\mathbf{a}) = \frac{1}{2\pi}\int d^2u \exp\left(-\frac{u^2}{2}\right) v(\mathbf{a}+\mathbf{u}D_a^{1/2}).$$

We now define the average equilibrium distance between the nearest neighbors, at a given temperature, as the distance over which the bonds between the atoms are not stretched, i.e.,

$$w'(\mathbf{a}) = 0. \tag{2.5}$$

We shall solve the system[3] (2.4). We specify the interaction between the atoms in the form

$$v(\mathbf{r}) = v_0[\exp[-2\alpha(r^2-a_0^2)]-2\exp[-\alpha(r^2-a_0^2)]]. \tag{2.6}$$

A potential in the form (2.6) is chosen exclusively for the sake of making the integration convenient and of being able to carry through the solution to conclusion in analytic form.

From (2.4) and (2.5) we have

$$w(\mathbf{r}) = \exp(-4\alpha^2 D_a a_0^2) v_0(\exp[-2\alpha(r^2-a^2)]-2\exp[-\alpha(r^2-a^2)]), \tag{2.7}$$

$$a^2 = a_0^2 + 6a_0^2\alpha D_a. \tag{2.8}$$

Expressions (2.7) and (2.8) were obtained under the condition $\alpha D_a \ll 1$, and this will be shown below to be valid always at $\alpha a_0^2 \gg 1$.

From (2.4) we can also obtain

$$ZD_a \frac{\partial^2 w}{\partial r^2}\Big|_{r=a} = \frac{\hbar}{N}\sum_{\mathbf{k},\lambda} \omega_\lambda(\mathbf{k}) \operatorname{cth}\frac{\hbar\omega_\lambda(\mathbf{k})}{2T}. \tag{2.9}$$

Here Z is the number of nearest neighbors, Z = 6 for a triangular lattice. Equation (2.9) will be solved in two limiting cases: a) $T \gg \Theta$; b) $T \ll \Theta$. The Debye temperature is $\Theta \approx 3\hbar(w''/m)^{1/2}$.

Case a). In this case[4] we can use the high-temperature expansion of the cotangent. We have

$$Zv_0 \exp(-4\alpha^2 D_a a_0^2)\cdot 8\alpha^2 D_a a^2 = 4T.$$

If we introduce the symbol $x = 4\alpha^2 D_0 a_0^2$, then at $(a-a_0)/a_0 \ll 1$ (see below) this expression can be written in the form

$$xe^{-x} = 2T/Zv_0. \tag{2.10}$$

We see that real solutions of (2.10) exist only at sufficiently low temperature. The transition temperature can be obtained from the condition that at $T = T_m$ the left-hand side of (2.10) is equal to the right-hand side at the point of its maximum, whence

$$x_m = 1, \quad T_m = Zv_0/2e. \tag{2.11}$$

Let us verify the satisfaction of the employed inequality $\alpha D_a \ll 1$: $1 = \max(\alpha^2 D_a a_0^2)$, whence $\alpha D_a \ll 1$ at $\alpha a_0^2 \gg 1$, and consequently

$$\max\left(\frac{a-a_0}{a_0}\right) \approx \frac{3}{4\alpha a_0^2} \ll 1.$$

The elastic constant w'', which is the order parameter in the two-dimensional crystal structure,

$$w'' = 8\alpha^2 a_0^2 v_0 e^{-x}, \tag{2.12}$$

changes by a factor e when T changes from zero to T_m. The shear modulus is $\mu = Za^2 w''$.

Case b). We obtain from (2.9)

$$2Zv_0 xe^{-x} = {}^4/_3\Theta + 19.2T^3/\Theta^2. \tag{2.13}$$

Since at $r = a_0$ Eqs. (2.6) and (2.7) yield $(a-a_0)/a_0 \ll 1$, $w'' = e^{-x}v''$, it follows that $\Theta = e^{-x/2}\Theta_0$, where Θ_0 is the Debye temperature in the harmonic approximation. Thus, we can rewrite (2.13) in the form

$$xe^{-2x} - \gamma e^{-3x/2} = 14.4\gamma(T/\Theta_0)^3, \qquad \gamma = 2\Theta_0/3Zv_0. \tag{2.14}$$

The solution of (2.14) even at T = 0 exists only for not too large γ. For simplicity we assume that $\gamma \ll 1$ (the mass of the atom m is large). Then $x_0 \approx \gamma$ at T = 0. In analogy with case a), we obtain the transition point:

$$x_m \approx {}^1/_2, \quad T_m \approx (28.8e\gamma)^{-1/3}\Theta_0. \tag{2.15}$$

The elastic constant (2.12) decreases when the temperature changes from T = 0 to $T = T_m$ by a factor $e^{1/2-\gamma}$.

It is easy to verify that the inequality $(a-a_0)/a_0 \ll 1$ holds true up to the transition point at $\alpha a_0^2 \gg 1$.

In accordance with (1.5), $\langle \rho(q)\rho(-q)\rangle/N$ becomes infinite at $T < T_c$ with increasing sample dimensions. Let us estimate $T_c = 4\pi mu^2/\nu a^2 q^2$. If u_l and u_t are the longitudinal and transverse sound velocities, then, using (3.2),

$$u^2 = \frac{2u_l^2 u_t^2}{u_l^2+u_t^2} = \frac{3Za^2 w''(a)}{32m},$$

$$T_c = \frac{3\pi Z}{\nu(aq)^2}(\alpha a_0^2)^2 v_0 e^{-x}.$$

It is easy to see, since $a \approx 2\pi$ and $\alpha a_0^2 \gg 1$, that $T_m \ll T_c$ in cases a) and b).

Thus, in the entire region of the stability of a two-dimensional crystal (and T_m is the upper bound of this region) the correlator of the position of two particles and the static structure factor are given by expressions (1.4) and (1.5), while the exponent Δ is given by

$$\Delta=\frac{v(aq)^2Te^x}{3\pi Z(\alpha a_0^2)^2v_0}. \qquad (2.16)$$

We note that up to T_m we have $\Delta \ll 1$.

3. LAYERED CRYSTAL

We consider a system of atoms consisting of monmonatomic plane layers that are equidistant from one another. As already noted, at such an arbitrarily strong interaction between the atoms that are situated in one plane, there is no long-range crystal order. However, turning on an arbitrarily weak interaction between the layers makes the system three-dimensional and leads to the appearance of crystal ordering in the planes.

The task of the present section is to establish how the degree of ordering in the plane depends on the constant of the interplanar interaction at a given temperature. To this end, we consider a hexagonal lattice, the interaction between the layers of which is much less than the interaction inside the layers. As shown by I. Lifshitz [10], the spectrum of the oscillations of such a lattice can be written in the long-wave limit in the form

$$\omega_1^2=u_1^2\varkappa^2+u_3^2k_z^2, \qquad \omega_2^2=u_2^2\varkappa^2+u_3^2k_z^2,$$
$$\omega_3^2=u_3^2\varkappa^2+u_4^2k_z^2+\xi\varkappa^4.$$

The z axis is directed here perpendicular to the layers, $\kappa^2 = k_x^2 + k_y^2$, and $u_3 \lesssim u_4 \ll u_1 \approx u_2$. Oscillations whose displacement vector lies in the XOY plane correspond to the first two modes $\omega_{1,2}$. The last mode corresponds to flexural oscillations of the planes.

Since we are interested only in the establishment of order in a plane, we consider a crystal model in which only oscillations with a displacement vector lying in the XOY plane are allowed. Such a crystal has a simple hexagonal lattice, with interaction only between the nearest neighbors, such that in the plane the atoms interact via the central potential $v(\mathbf{r})$ ($\mathbf{r} = (x, y)$), and between the planes they interact by a noncentral potential $f(\mathbf{r})$.[5] For this crystal, the spectrum of the oscillations takes in the long-wave limit the form

$$\omega_1^2=u_1^2\varkappa^2+u_3^2k_z^2, \qquad \omega_2^2=u_2^2\varkappa^2+u_3^2k_z^2, \qquad (3.1)$$

where

$$^1/_3u_1^2=u_2^2=Za^2w''(a)/16m, \qquad u_3^2=c^2g''(0)/m, \qquad (3.2)$$

a is the distance between the nearest neighbors in the plane, Z = 6 is the number of nearest neighbors in the plane, $w''(a)$ is the strength constant in the plane, c is the distance between layers, $g''(0)$ is the strength constant between layers, m is the mass of the atom.

To calculate the force constants, we use a system of self-consistent equations, analogous to (2.4). We have

$$w(\mathbf{r})=\frac{1}{2\pi}\int d^2u\exp\left(-\frac{u^2}{2}\right)v(\mathbf{r}+\mathbf{u}D_a^{1/2}),$$
$$g(\mathbf{r})=\frac{1}{2\pi}\int d^2u\exp\left(-\frac{u^2}{2}\right)f(\mathbf{r}+\mathbf{u}D_c^{1/2}); \qquad (3.3)$$

$$D_a=\frac{\hbar}{mN}\sum_{\mathbf{k},\lambda}(1-e^{i\mathbf{k}\mathbf{a}})\frac{(\mathbf{e}_\lambda(\mathbf{k})\mathbf{a})^2}{a^2\omega_\lambda(\mathbf{k})}\operatorname{cth}\frac{\hbar\omega_\lambda(\mathbf{k})}{2T},$$
$$D_c=\frac{\hbar}{mN}\sum_{\mathbf{k},\lambda}\frac{1-\exp(ik_zc)}{\omega_\lambda(\mathbf{k})}\operatorname{cth}\frac{\hbar\omega_\lambda(\mathbf{k})}{2T}. \qquad (3.4)$$

The distance a is determined from the condition $w'(a) = 0$.

For $v(\mathbf{r})$ we use expression (2.6), and we take $f(\mathbf{r})$ in the form

$$f(\mathbf{r})=-f_0\exp(-\beta r^2). \qquad (3.5)$$

Then from (3.3) and (3.5) at $\alpha D_a \ll 1$ we have again formula (2.7) for $w(\mathbf{r})$, and

$$g(\mathbf{r})=-\frac{f_0}{1+2\beta D_c}\exp\left[-\frac{\beta r^2}{1+2\beta D_c}\right]. \qquad (3.6)$$

From the condition $w'(a)$ we obtain $a^2 = a_0^2 + 6a_0^2\alpha D_a$, and from (2.7) and (3.6) we get

$$w''(\mathbf{a})=8\alpha^2a_0^2v_0e^{-x}, \qquad (3.7)$$

$$g''(0)=2f_0\beta/(1+2\beta D_c)^2. \qquad (3.8)$$

we recall that $x = 4\alpha^2 D_a a_0^2$.

To find D_a and D_c, it is necessary to substitute (3.7) and (3.8) in Eqs. (3.1), and these in turn must be substituted in (3.4). We thus obtain a system of two equations with two unknowns, D_a and D_c. We note that to solve the first of these equations we can use the fact that, by assumption, the coupling between layers is weak, i.e., $u_3 \ll u_1$. We then have in the zeroth approximation in u_3

$$(\omega_1^0)^2=u_1^2\varkappa^2, \qquad (\omega_2^0)^2=u_2^2\varkappa^2. \qquad (3.9)$$

From (3.9), from the first equation of (3.4) and also from (3.7) we obtain Eq. (2.9) for the pure planar case. Thus, the force constant $w''(\mathbf{a})$ is given by expression (3.7), and the temperature dependence of D_a was investigated in the preceding section.

The second equation of (3.4) cannot be treated in this fashion, for if we take the frequencies in the form (3.9), then the sum over k begins to diverge at small k. Therefore it is necessary to substitute in the second equation of (3.4) the exact expression for the frequencies (3.1), with allowance for the already known force constant $w''(\mathbf{a})$. The second equation of (3.4) will be investigated in two limiting cases: a) $T \gg \Theta$ and b) $T \ll \Theta$; Θ is the Debye temperature in the plane, $\Theta \approx 3h(w''/m)^{1/2}$.

Case a). Carrying out the high-temperature expansion of the cotangent, we have

$$D_c=\frac{2Tc^2}{\varkappa_D^2k_{zD}m}\int_0^{\varkappa_D}\varkappa\,d\varkappa\int_{-k_{zD}/2}^{k_{zD}/2}k_z^2\,dk_z\left(\frac{1}{u_1^2\varkappa^2+u_3^2k_z^2}+\frac{1}{u_2^2\varkappa^2+u_3^2k_z^2}\right).$$

Here $\kappa_D^2 = 8\pi/3^{1/2}a^2$ and $k_{zD} = 2\pi/c$. Retaining in the integration only the large logarithms, we obtain with logarithmic accuracy

$$D_c\approx\frac{4Tc^2k_{zD}^2}{9u_2^2m\varkappa_D^2}\ln\left(\frac{\varkappa_Du_2}{k_{zD}u_3}\right). \qquad (3.10)$$

We note that in the temperature region where the real D_a is determined (see (2.10) and (2.11)) the solution of (3.10) always exists (see (3.2), (3.7), and (3.8)). Consequently, if we confine ourselves, as before, to the zeroth approximation in u_3 to determine D_a, then the transition temperature in the layered case remains unchanged in comparison with the pure two-dimensional case. It is easy to write out the solution for D_c in the case $D_c\beta \ll 1$. Namely, from (3.10) we obtain with logarithmic accuracy

$$D_c\approx\frac{\pi\sqrt{3}\,T}{9Zv_0\alpha^2a_0^2}\ln\left(\frac{v_0\alpha^2a_0^2e^{-x}}{f_0\beta}\right).$$

As is well known, the order parameter for the crystal is the mean value of the Fourier component of the density:

$$\frac{1}{N}\langle\rho(\mathbf{q})\rangle=\exp\left\{-\frac{\hbar}{2mN}\sum_{\mathbf{k},\lambda}\frac{(\mathbf{q}\mathbf{e}_\lambda(\mathbf{k}))^2}{\omega_\lambda(\mathbf{k})}\operatorname{cth}\frac{\hbar\omega_\lambda(\mathbf{k})}{2T}\right\}. \qquad (3.11)$$

Here $\mathbf{q}$ is the reciprocal-lattice vector. This is a directly-measurable quantity, since it yields the inten-

sity of the maxima of elastic scattering of x rays by the lattice (see, e.g., [12]). For vectors $\mathbf{q}$ lying in the XOY plane, the quantity $\langle \rho(\mathbf{q}) \rangle / N$ yields the degree of ordering in the plane. At $T \gg \Theta$, carrying out a high-temperature expansion of the cotangent and calculating the integrals, we obtain with logarithmic accuracy

$$\frac{1}{N}\langle \rho(\mathbf{q}) \rangle \approx \left(\frac{16\pi v g''(0)}{Z w''(a)} \right)^{\Delta}. \qquad (3.12)$$

Here Δ is determined by (2.16). We note that $\langle \rho(\mathbf{q}) \rangle / N$ tends to zero when $g''(0)$ tends to zero, as it should.

Case b). Separating in the second equation (3.4) the temperature-independent terms, we obtain

$$D_c = \frac{\hbar c^2}{m k_{zD} \varkappa_D^2} \int_0^{\varkappa_D} \varkappa \, d\varkappa \int_{-k_{zD}/2}^{k_{zD}/2} k_z^2 \, dk_z \Big\{ \frac{1}{(u_1^2\varkappa^2 + u_3^2 k_z^2)^{1/2}} \times \Big[1 + \frac{2}{\exp[\hbar(u_1^2\varkappa^2 + u_3^2 k_z^2)^{1/2}/T] - 1} \Big] + \frac{1}{(u_2^2\varkappa^2 + u_3^2 k_z^2)^{1/2}} \times \Big[1 + \frac{2}{\exp[\hbar(u_2^2\varkappa^2 + u_3^2 k_z^2)^{1/2}/T] - 1} \Big] \Big\}. \qquad (3.13)$$

We can integrate (3.13) in two limiting cases, $\hbar u_3 k_{zD}/T \ll 1$ and $\hbar u_3 k_{zD}/T \gg 1$. The second case actually means $T = 0$, and we therefore consider only the first. In (3.13), the temperature-independent terms can be integrated at $u_3 = 0$, and in the temperature dependent terms we can retain only the large logarithms. With logarithmic accuracy, we obtain

$$D_c \approx \frac{(1+\sqrt{3})\pi^2\hbar}{3\sqrt{3}\, m \varkappa_D u_2} - \frac{4\pi^2 T}{9 m \varkappa_D^2 u_2^2} \ln\left(\frac{\hbar u_3 k_{zD}}{2T} \right). \qquad (3.14)$$

Equation (3.14) determines D_c (see (3.2), (3.7), (3.8)) in the entire region where D_a exists (see (2.14) and (2.15)).

Analogous calculations yield $\langle \rho(\mathbf{q}) \rangle / N$ for the reciprocal-lattice vectors $\mathbf{q}$ lying in the XOY plane:

$$\frac{\langle \rho(\mathbf{q}) \rangle}{N} \approx \exp\left[-\frac{(1+\sqrt{3})\hbar q \Delta^{1/2}}{2(2mT)^{1/2}} \right] \left[\frac{\pi\hbar (g''(0))^{1/2}}{mT} \right]^{\Delta}. \qquad (3.15)$$

Just as in the preceding case, $\langle \rho(\mathbf{q}) \rangle / N$ vanishes together with $g''(0)$.

Thus, an arbitrarily weak three-dimensionalization of the system leads to the appearance of long-range order in it; the degree of this order is given by expressions (3.12) and (3.15).

Mikeska [13] considered inelastic scattering of thermal neutrons by a two-dimensional lattice, and showed that the resonant frequency is a branch point of the dynamic structure factor (see also [14,15]):

$$S(\mathbf{q}+\boldsymbol{\varkappa}, \omega) \sim \left[\frac{(u\varkappa)^2}{\omega^2 - (u\varkappa)^2} \right]^{1-2\Delta}. \qquad (3.16)$$

Here $\mathbf{q}$ is the reciprocal-lattice vector and $\boldsymbol{\varkappa} \cdot \mathbf{a} \ll 1$. Expression (3.16) can be used also for a layered crystal, if it is noted that the time of establishment of the three-dimensional order is $\tau \sim c/u_3$, and the frequencies are $\omega \sim u_{1,2}\varkappa$. Consequently, when the condition $\omega\tau \gg 1$ is satisfied, i.e., $u_{1,2} c\varkappa / u_3 \gg 1$, relation (3.16) holds. The last inequality is perfectly feasible, for although $\varkappa a \ll 1$, on the other hand $u_{1,2} \gg u_3$ and $c \gg a$.

In conclusion, I wish to note that the topic of this paper was proposed by V. L. Prokovskiĭ and discussed with him many times, for which I am most grateful to him. I am also indebted to G. V. Uĭmin, D. E. Khmel'nitskiĭ, and A. P. Mineev for interest in the work.

[1)] We disregard throughout the possible precence of dislocations and vacancies in crystal, since their production calls for a finite energy, and consequently, their concentration is negligible at sufficiently low temperatures.

[2)] The terms "flat crystal structure" and "two-dimensional crystal" are used throughout in accordance with Berezinskiĭ's definition, i.e., there is a shear modulus but there is no long-range order.

[3)] The system (2.4) was solved in order to ascertain the conditions for the stability of the anharmonic crystal in the one-dimensional case in [8] and in the three-dimensional case in [9]. Allowance for the anharmonicities with the aid of the self-consistency method, as used in [9], makes it possible to calculate the temperature dependence of the frequencies, of the force constants, and of the mean-squared displacements far enough from the melting temperature, but there is no justification whatever for calculating the singularities of the thermodynamic functions at the transition point itself with the aid of this method (see [9]).

[4)] If the atom mass is large enough, then this "classical" region can include also arbitrarily low temperatures.

[5)] The simplest of the layered crystals, graphite, has a much more complicated structure (see, e.g., [11]), but since we are interested in the establishment of the order in the plane, it suffices to consider such a simple model in order to obtain qualitatively correct results.

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