The theory of two-dimensional incommensurate crystals

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The ground state and the thermodynamics of a two-dimensional lattice of atoms placed in a periodic one-dimensional field is investigated. It is shown that at zero temperature there is produced in the incommensurate state a one-dimensional superstructure (periodic solitons) whose direction is determined by the elastic properties of the initial lattice, and whose period depends also on the potential and on the initial incommensurability. The transition from the commensurate to the incommensurate structure is continuous. The solution and, in particular, the critical behavior change substantially if the crystal tends to occupy, under the influence of the potential, an area larger than the substrate area. The spectrum of small oscillations and questions involving the stability of various phases are investigated. At temperatures greatly exceeding the characteristic value of the potential, the periodicity and the asymmetry in the soliton direction vanish, but the average incommensurability remains. The thermodynamics of the system is considered by the renormalization-group method. At a definite relation between the parameters, the problem is solved exactly by a transition to the equivalent Hamiltonian of Fermi particles (solitons). The phase diagram of the system is obtained. The diffraction pattern is analyzed. The applications of the theory to submonolayers of atoms adsorbed by an ideal crystal surface and to a lattice of Abrikosov vortices in a corrugated superconducting film are considered.

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INTRODUCTION

Recently, in connection with the progress in the experimental capabilities, interest has increased in two-dimensional crystal systems. The simplest realization of such a system is a submonolayer of atoms adsorbed by a sufficiently perfect surface of a crystal. Such monolayers were investigated experimentally on tungsten and molybdenum surfaces and on various graphite substrates. Both thermodynamic methods and structural methods were used (diffraction of slow electrons or neutrons, x-ray structure analysis). The experimental situation is described in detail in the reviews of Bolśhov *et al.*,[1] Nielssen *et al.*,[2] and Dash.[3]

In many cases the observed crystalline phases of the adsorbed-atom film were not commensurate with the substrate (for example, for Cs layers on molybdenum and tungsten,[1] of Ne and H_2 on graphite, etc.). The purpose of the present paper is a theoretical study of the conditions for the onset of two-dimensional incommensurate structure and of its physical properties.

Another two-dimensional, or more accurately quasi-two-dimensional object in which incommensurate structures were observed are chalcogenides of transition metals (for example, $TaSe_2$), in which charge-density waves appear.[4] Our theory does not provide a complete description of these structures, since we did not concern ourselves with the properties of the electron subsystem. Nonetheless, many statements concerning the lattice properties and the phase diagram are valid also for these systems, especially near phase-transition points.

One more object in which incommensurate crystal lattices seem to appear are thin corrugated films of superconducting aluminum placed in a magnetic field perpendicular to their surfaces (Daldini *et al.*[5]). The film thickness is of the order of 2500 Å and the depth of corrugation is ~50 Å, the corrugation is one-dimensional, periodic, with a period 2000 Å. In the smooth film there is produced a triangular lattice of Abrikosov vortices, whose period is determined by the magnetic field, the result being a flux quantum ϕ_0 per unit cell. On the other hand, it is more convenient for the vortices to be located in places where the film is thinner, since the vortex energy is proportional to its length. A competition arises between the period imposed by the magnetic field and the period imposed by the corrugation. Experiment[5] has revealed maxima of the critical field at magnetic-field values corresponding to a prime ratio of these two periods. At the present time, a complete phase diagram of such a system is under construction and new effects are being predicted.

The simplest theoretical model of an incommensurate structure was proposed by Ying.[6] By regarding the substrate as a periodic potential field in which adsorbed atoms connected by springs are located, he has shown within the framework of perturbation theory that the incommensurate structure is favored. He has also found that in such a structure there are decaying (acoustic) oscillation modes. The applicability of perturbation theory can be debated, inasmuch as in sufficiently high order one can have arbitrarily exact commensurability, i.e., arbitrarily small denominators. This question was analyzed in the papers by one of us and Uĭmin,[7,8] where the spectrum likewise turned out to be complicated (discontinuous at each point!). Similar results in somewhat different form were obtained by Aubrey.[9] Novaco and McTague[10] have noted that within the framework of the same approximation the energy depends on the angle between the axes of the sublattices of the substrate and the adsorbed atoms. As a result, orientational epitaxy appears—rotation of the lattice of the adsorbed atoms when their concentration is changed. Uimin and Shchur[11] have shown that orientational phase transitions of first order are possible. Burkov[12] has observed the

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possibility of orientational second-order phase transitions.

An approach that does not employ perturbation theory was proposed for the one-dimensional problem by Bulaevskiĭ and Khomskiĭ,[13] by the authors of the present paper,[14] and by Theodorou and Rice.[15] All have demonstrated the existence of super-structures (of periodic solitons) in the commensurate phase. A similar approach is developed in the present paper for the two-dimensional problem. Luther and one of us[16] solved the problem of the phase transition from a commensurate to an incommensurate crystal for a one-dimensional quantum system. Another variant of the same problem is that of charge-density waves in a two-dimensional system at finite temperature. The methods of Ref. 16 are generalized in the present paper to include a description of a more complicated situation, the temperature behavior of a two-dimensional elastic system on a periodic substrate. The latter problem has many features in common with the problem of two-dimensional crystals, considered by Mermin,[17] Jancovici,[18] Berezinskii,[19] Kosterlitz and Thouless,[20] and Halperin and Nelson.[21]

Methods of investigating incommensurate structures in the immediate vicinity of the transition point were developed by Bak *et al.*[22-25] These studies dealt with a system of weakly overlapping solitons in one or two dimensions at zero temperatures. We shall discuss later on some of the results of these papers and their bearing on our results (see Secs. 10 and 11). We present a brief plan of the article. In Secs. 1 and 2 we discuss the formulation of the problem and its solution at zero temperature, first on an unbounded substrate (Sec. 2) and then on a bounded area (Sec. 3). In Sec. 4 we determine the spectrum of the acoustic modes and discuss the stability of the obtained solutions. In Secs. 5–9 we investigate the behavior of the system at various temperatures. Section 10 is devoted to the diffraction pattern produced when slow electrons, neutrons, or x rays are scattered. In Sec. 11 we present a qualitative picture of the phenomena near a phase transition. Section 12 is a systematic exposition of the new experimental consequences of the theory and contains indications of the conditions for their observations.

We use the abbreviations C and I for the commensurate and incommensurate phase, respectively, C–I for the phase transition from the commensurate to the incommensurate phase, and adatoms for adsorbed atoms. The results of the present paper were reported in a brief communication earlier.[26]

1. RESONANCE APPROXIMATION

The influence of the substrate on the adatoms will be described by a periodic potential $V(\mathbf{r})$ which we expand in a Fourier series:

$$V(r)=\sum_{\mathbf{q}} V_{\mathbf{q}} e^{i\mathbf{q}\mathbf{r}}, \tag{1}$$

where $\mathbf{q}$ are the reciprocal-lattice vectors of the substrate. The potential $V(\mathbf{r})$ is assumed to be weak. We assume that on an absolutely smooth substrate ($V(\mathbf{r})=0$) the adatoms have a regular lattice. The vectors of this lattice will be designated by the letter $\mathbf{R}$, and the reciprocal-lattice vectors by the letter $\mathbf{b}$. The potential energy of the lattice is written in the harmonic approximation in the form

$$H_0=\sum_{\mathbf{k}} s_\alpha(\mathbf{k})\varepsilon_{\alpha\beta}(\mathbf{k})s_\beta(\mathbf{k}), \tag{2}$$

where $s_\alpha(\mathbf{k})$ are the Fourier components of the displacements of the adatoms and $\varepsilon_{\alpha\beta}(\mathbf{k})$ is the dynamic matrix. The dynamic matrix has the following properties: it is periodic with periods $\mathbf{b}$ and its eigenvalues tend quadratically to zero as $k\to 0$. Minimizing the total potential energy of the adatoms, we obtain the equilibrium displacements $s^0_\alpha(\mathbf{k})$. In the lowest-order approximation in V we have

$$s_\alpha^0(\mathbf{k})=-i\sum_{\mathbf{q}}\varepsilon^{-1}_{\alpha\beta}(\mathbf{q})q_\beta V_{\mathbf{q}}\delta_{\mathbf{k},\mathbf{q}}. \tag{3}$$

It is obvious that the largest values are possessed by those Fourier components $s_\alpha(\mathbf{k})$ for which $\mathbf{k}$ are close to the reciprocal-lattice vectors $\mathbf{b}$. We assume that this condition is satisfied for only one pair of vectors, $\mathbf{k}$ and $\mathbf{b}$. This situation is typical in the case when the substrate and the adsorbed atoms have lattices that differ in form.[1)] The case of lattices having the same form will be considered separately. Of course, sufficiently large reciprocal-lattice vectors can be made arbitrarily close for incommensurate periods. We shall assume, however, that V_q decreases with increasing q so rapidly that these effects are insignificant. In the situation described above it is natural to neglect all the V_q in (1), with the exception of those for which $\mathbf{q}$ are close to $\mathbf{b}$. Of course, if $\mathbf{q}$ is close to $\mathbf{b}$, then $2\mathbf{q}$ is close to $2\mathbf{b}$, etc. All the corresponding Fourier components V_{nq} should be considered together with V_q. This will be called the resonance approximation.

It is natural also to consider in the resonance approximation those vectors $\mathbf{k}$ in (2) and (3) which are close to $\mathbf{b}$. We write the vector $\mathbf{q}$ in the form $\mathbf{q}=\mathbf{b}+\mathbf{p}$, where $\mathbf{p}$ is a small vector. The radius vector of the adatom with vector number R is written in the form $\mathbf{R}+\mathbf{s}_R$. Then the energy of the interaction with the substrate takes the form

$$V_i=\sum_{\mathbf{R}} f(\mathbf{pR}+\mathbf{bs}_R), \tag{4}$$

where the periodic function $f(\varphi)$ is defined as

$$f(\varphi)=\sum_{n=-\infty}^{+\infty} b^n V_{n(\mathbf{b}+\mathbf{p})}e^{in\varphi}. \tag{5}$$

In (4) we have neglected the term $\mathbf{p}\cdot\mathbf{s}_R$ in the argument of the cosine. In view of the smallness of $\mathbf{p}$ we can assume $\mathbf{R}$ to be a continuous argument. A similar approximation for the one-dimensional model was proposed in Refs. 13–15.

The dynamic matrix $\varepsilon_{\alpha\beta}(k)$ determines at small $\mathbf{k}$ the elastic properties of the crystal, and can therefore be described by a set of elastic moduli. In all the experimentally investigated cases, the adatoms in the incommensurate phase crystalized to form a simple triangular lattice. We shall henceforther consider only this case.

It is known that a triangular lattice is equivalent in its elastic properties to an isotropic elastic medium described by the Lamé coefficients λ and μ.

We direct the x axis along the vector b and denote by u/b and v/b respectively the components of the displacements along x and y. The potential energy of the adatoms in the resonance approximation takes the form

$$U=\int\int\left\{\frac{\lambda+\mu}{2}\left(\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}\right)^2+\frac{\mu}{2}\left[\left(\frac{\partial u}{\partial x}-\frac{\partial v}{\partial y}\right)^2+\left(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right)^2\right]+f(\varphi)\right\}\frac{dx\,dy}{b^2}, \tag{6}$$

where $\varphi=\mathbf{u}+\mathbf{p}\cdot\mathbf{R}$.

2. QUASI-ONE-DIMENSIONAL SOLUTIONS

The equilibrium condition for the potential (6) is of the form

$$\begin{aligned}(\lambda+\mu)\left(\frac{\partial^2\varphi}{\partial x^2}+\frac{\partial^2 v}{\partial x\,\partial y}\right)+\mu\Delta\varphi-f'(\varphi)=0,\\ (\lambda+\mu)\left(\frac{\partial^2\varphi}{\partial x\,\partial y}+\frac{\partial^2 v}{\partial y^2}\right)+\mu\Delta v=0.\end{aligned} \tag{7}$$

We seek the solution of the system (7) in the form

$$\varphi=\varphi(\xi),\quad v=w(\xi)+rx+sy,\quad \xi=x\cos\theta+y\sin\theta. \tag{8}$$

From the second equation of (7) we obtain the connection between the functions φ and w:

$$w=-\frac{(\lambda+\mu)\sin\theta\cos\theta}{\mu+(\lambda+\mu)\sin^2\theta}\varphi. \tag{9}$$

The solution of Eqs. (7) takes the form

$$\int_{\varphi_0}^{\varphi}\frac{d\varphi}{[2(f(\varphi)+\mathscr{E})]^{1/2}}=\xi\left[\frac{\mu+(\lambda+\mu)\sin^2\theta}{\mu(\lambda+2\mu)}\right]^{1/2}, \tag{10}$$

where $\mathscr{E}$ and φ_0 are integration constants. The solution (10) is meaningful if $\mathscr{E}\geq\mathscr{E}_c=-\min f(\varphi)$.

We have found a solution that depends on four parameters: r, s, θ, and $\mathscr{E}$. We note that the vector p can be regarded as directive along the x axis, since the energy depends only on the difference p_y-r.

Substituting the solution (8)–(10) in (6), we obtain the potential energy per unit area:

$$\bar{U}\equiv b^2\frac{U}{l^2}=\frac{E}{K}-\frac{2\pi h}{K}-\mathscr{E}+\frac{1}{2}[(\lambda+\mu)(p-s)^2+\mu(p+s)^2+\mu r^2], \tag{11}$$

where the functions $K(\mathscr{E})$ and $E(\mathscr{E})$ are defined in analogy with the complete elliptic integrals:

$$\begin{aligned}K(\mathscr{E})&=\int_0^{2\pi}\frac{d\varphi}{[2(f(\varphi)+\mathscr{E})]^{1/2}},\\ E(\mathscr{E})&=\int_0^{2\pi}[2(f(\varphi)+\mathscr{E})]^{1/2}d\varphi\end{aligned} \tag{12}$$

and the quantity h is connected with the parameters, p, r, s, and θ by the relation

$$\begin{aligned}h=\left[\frac{\mu}{(\lambda+2\mu)(\mu+(\lambda+\mu)\sin^2\theta)}\right]^{1/2}\{(\lambda+\mu)(p-s)\cos\theta\\ +(p+s)\cos\theta[\lambda+2\mu-(\lambda+\mu)\cos 2\theta]-r\sin\theta[(\lambda+2\mu)-(\lambda+\mu)\cos^2\theta]\}.\end{aligned} \tag{13}$$

The problem now is to minimize the energy $\bar{U}$ with respect to the parameters $\mathscr{E}$, r, s, and θ. Minimization with respect to $\mathscr{E}$ is carried out exactly as in the one-dimensional case, and leads to an analogous equation:

$$h=E/2\pi. \tag{14}$$

Minimization with respect to the remaining three parameters is elementary, although somewhat cumbersome. Leaving out the intermediate steps, we present the results: at $\sigma>0$ we get $\tan^2\theta=\sigma$,

$$p=\frac{E}{2\pi(1-\sigma^2)^{1/2}}\frac{1}{(\lambda+2\mu)^{1/2}},\quad s=\sigma p,\quad r=0, \tag{15}$$

$$\bar{U}_1=-\mathscr{E}+{}^1/_2p^2(1-\sigma^2)(\lambda+2\mu). \tag{16}$$

There exists one other solution of Eq. (7): $\varphi=\varphi_0$, $v=\sigma py$, where φ_0 is the value of φ at the minimum of the function $f(\varphi)$. This solution corresponds to a phase that is commensurate in one direction with the substrate (along the x axis). Its energy U_2 is connected with p by the relation

$$\bar{U}_2=f_{min}+{}^1/_2p^2(1-\sigma^2)(\lambda+2\mu). \tag{17}$$

We explain now the physical meaning of the solution (8)–(16). The different turns in the Hamiltonian (6) correspond to opposing tendencies in the arrangement of the atoms. The interaction of the substrate $f(\varphi)$ tends to place the adatoms at the minima of the periodic potential of the substrate. On the other hand, the interaction between the adatoms tends to place them in their own regular lattice, which differs from that of the substrate. The system of adatoms at equilibrium assumes some compromise arrangement: there are long sections with the periodicity of the substrate, alternating with short sections on which the distances between the atoms differ greatly from the lattice. The foregoing pertains to the case of sufficiently small commensurability. In the general case periodic modulation takes place of the density of the adatom lattice.

Thus, a superstructure is produced in the incommensurate phase and has a period that is a continuous function of the parameters V and p. The modulation of the density is directed at an angle $\theta=\tan^{-1}\sqrt{\sigma}$ to the almost coinciding reciprocal vectors, and its period in terms of the initial units of length is $(2\mu)^{1/2}K(\mathscr{E})$. The lattice is slightly deformed in the perpendicular direction, with a tension coefficient $s=\sigma p$.

The incommensurate phase exists at $p\geq p_c$, where the critical value p_c is connected with the minimal value of E by the relation

$$p_c=\frac{E_{min}}{2\pi}\left(\frac{\lambda+2\mu}{4\mu(\lambda+\mu)}\right)^{1/2}. \tag{18}$$

The minimum of E corresponds to $\mathscr{E}_c=-f_{min}$. At $p<p_c$ the minimum of the potential energy is realized by the commensurate phase. The energy $\bar{U}_1$ goes over continuously into $\bar{U}_2$ at $p=p_c$. As usual, when p approaches p_c from above the period of the supersubstructure increases logarithmically, and the boundaries between the "domains" (static solitons) acquire the standard form and length.[13–15]

Within the framework of the approximation assumed here, the considered transition is a second-order phase transition with respect to p. We note some important

singularities of the incommensurate phase. The first is that in the two stress components of the incommensurate phase, σ_{xy} and σ_{yy}, are equal to zero at any point of space. The initial expression (6) for the potential energy is invariant with respect to the reflections $X(x \to -x, u \to -u)$ and $Y(y \to -y, v \to -v)$. The commensurate state is in fact also invariant with respect to these transformations (accurate to a common phase shift 2π). In the incommensurate state, however, these symmetries are violated, since the mean values $\langle \partial u/\partial y \rangle$ and $\langle \partial v/\partial x \rangle$ differ from zero.

The ground state of the incommensurate crystal is doubly degenerate with respect to the angle θ. The choice of one of the two roots of the equation $\tan^2\theta = \sigma$ violates the initial symmetry. At the same time, the symmetry with respect to the total inversion XY is preserved. We note that for the dipole interaction, which apparently predominates in lattices of alkali and alkaline-earth adatoms on the surfaces of tungsten and molybdenum, we have $\sigma = 5/11$ and $\theta \approx 24°$. For a lattice of Abrikosov vortices $\lambda = \infty$ and $\theta = 45°$.

3. LATTICE UNDER CONDITIONS OF BOUNDED AREA

So far we have assumed that no limitations are imposed on the values of φ and v. Actually the quantities $x(1 - p/b) + \varphi/b$ and $y + v/b$ are coordinates of the adatoms in a real configuration, and x and y are the numbers of these atoms or their coordinates on an absolutely smooth substrate. In our problem the role of the conserved number (the number of adatoms) is played by $S_0 = \int dx\, dy$, which can also be interpreted as the area occupied by the lattice of the adatoms on an absolutely smooth substrate. If the area S_0 is smaller than the area of the substrate S, then a small change in it (of the order of p/b) is immaterial, and no limitations arise on φ and on v, and the solution obtained by us is realized. This is precisely the situation if the adatoms attract each other at large distances and form on a smooth substrate their own lattice, while their number is sufficient for this lattice to fill the entire substrate.

The situation is entirely different if the adatoms repel each other as is apparently the case for adatoms of alkali and alkaline-earth on tungsten and molybdenum.[1] In the case the atoms are constrained only by the boundaries of the substrate, so that on the absolutely smooth substrate they fill its entire area ($S_0 = S$). Exactly the same situation arises if the adatoms are attracted at large distances but their number is sufficiently large to make $S_0 = S$. With further increase of the concentration of the adatoms, they begin to repel each other effectively.

If $S_0 = S$, then the solution to the problem depends substantially on the sign of the incommensurability p. We shall show that at positive p, i.e., in the case when the substrate tends to decrease the constant of the adatom lattice, the solution obtained by us is realized. In the opposite case $p < 0$ the solution must be modified somewhat.

Neglecting boundary effects (a procedure valid if $p \gg S^{-1/2}$), we consider only the area occupied by the adatoms. Its change δS can be written in the form

$$\delta S = S_0 \left(\frac{1}{b}\right)\left(\left\langle \frac{\partial u}{\partial x}\right\rangle + \left\langle \frac{\partial v}{\partial y}\right\rangle\right). \tag{19}$$

At $p < 0$ we must impose on the solution the additional condition $\delta S = 0$. This condition obviously does not change the Lagrange variational equations (7). Therefore we shall seek their solution likewise in the earlier form (8). However, the parameters θ, s, r and $\mathscr{E}$ must in this case be determined by minimizing the quantity

$$U = \bar{U} + \nu b \delta S / S_0, \tag{20}$$

where $\bar{U}$ is defined by Eq. (11) and ν is a Lagrangian multiplier. The quantity $\delta S/S_0$ can be written in the form

$$b\frac{\delta S}{S_0} = -\frac{2\pi}{K}\cos\theta\left[\frac{\mu}{(\lambda+2\mu)(\mu+(\lambda+\mu)\sin^2\theta)}\right]^{1/2} + s - p. \tag{21}$$

After minimization it is necessary to put $\delta S/S_0 = 0$. From the obtained system of equations we were able to determine all the parameters:

$$\begin{aligned} \theta &= \operatorname{arctg}\sqrt{\sigma}, \\ p &= -\frac{1}{2(\lambda+2\mu)^{1/2}}\left[\left(\frac{\lambda+\mu}{\mu}\right)^{1/2}\frac{E}{2\pi} + \left(\frac{\mu}{\lambda+\mu}\right)^{1/2}\frac{2\pi}{K}\right], \\ s &= -\frac{1}{2(\lambda+2\mu)^{1/2}}\left[\left(\frac{\lambda+\mu}{\mu}\right)^{1/2}\frac{E}{2\pi} - \left(\frac{\mu}{\lambda+\mu}\right)^{1/2}\frac{2\pi}{K}\right], \\ \bar{U}_1 &= -\mathscr{E} + 2\mu p^2 - \frac{\mu}{2(\lambda+\mu)}\left(\frac{2\pi}{K}\right)^2. \end{aligned} \tag{22}$$

In the case of a bounded area, the commensurate phase is also different. Actually, putting $\varphi = \text{const}$ and stipulating constancy of the area, we find that $\langle \partial v/\partial y \rangle = p$. The energy of the commensurate state is

$$\bar{U}_2 = f_{\min} + 2\mu p^2. \tag{23}$$

A second-order phase transition takes place at the critical value

$$|p_c| = \frac{1}{2}\left[\frac{\lambda+\mu}{\mu(\lambda+2\mu)}\right]^{1/2}\frac{E_c}{2\pi}. \tag{24}$$

It is easily seen that this value of $|p_c|$ is less than the corresponding value (18) for the unbounded area.

Thus, limiting the area leads to a certain asymmetry of the phase diagram with respect to the point $p = 0$.

4. SPECTRUM OF SMALL OSCILLATIONS AND STABILITY

The total Hamiltonian of the system includes the kinetic energy and can be written in the form

$$H = \int \frac{\rho}{2}\left[\left(\frac{\partial\varphi}{\partial t}\right)^2 + \left(\frac{\partial v}{\partial t}\right)^2\right]\frac{dx\,dy}{b^2} + U, \tag{25}$$

where U is defined by Eq. (6). We put $\varphi = \varphi_0(x) + \varphi_1(x, t)$ and $v = v_0(x) + v_1(x, t)$, where φ_0 and v_0 are defined by Eqs. (8)–(10), while φ_1 and v_1 are assumed to be small. Then, confining ourselves to terms quadratic in φ_1 and v_1, we obtain the Hamiltonian of the harmonic system, the spectrum of which we shall now investigate.

It is convenient to change over to a coordinate frame ξ, η obtained from x, y by rotation through an angle θ, and to consider the displacement vector φ, v in the same frame ξ, η. In other words, it is necessary to

change over to new unknown functions Φ and Ψ, connected with φ_1 and v_1 by the relations

$$\Phi=\varphi_1\cos\theta+v_1\sin\theta,\quad \Psi=-\varphi_1\sin\theta+v_1\cos\theta\quad (\operatorname{tg}\theta=\sqrt{\sigma}). \tag{26}$$

In the new variables, the Hamiltonian becomes

$$H=\int\Big\{\frac{\rho}{2}\Big[\Big(\frac{\partial\Phi}{\partial t}\Big)^2+\Big(\frac{\partial\Psi}{\partial t}\Big)^2\Big]+\frac{\lambda+\mu}{2}\Big(\frac{\partial\Phi}{\partial\xi}+\frac{\partial\Psi}{\partial\eta}\Big)^2 +\frac{\mu}{2}\Big[\Big(\frac{\partial\Phi}{\partial\xi}-\frac{\partial\Psi}{\partial\eta}\Big)^2+\Big(\frac{\partial\Phi}{\partial\eta}+\frac{\partial\Psi}{\partial\xi}\Big)^2\Big] +\frac{1}{2}f''(\varphi_0)[\Phi\cos\theta-\Psi\sin\theta)^2\Big\}\frac{d\xi\,d\eta}{b^2}. \tag{27}$$

This Hamiltonian leads to the following dispersion equation which is valid at small k, q, and ω:

$$\Big\{(k+q\sqrt{\sigma})^2+4q^2\frac{\mu}{\lambda+2\mu}-\frac{2\mu}{\lambda+2\mu}\Omega^2\Big\}\Big\{c^2(k-q\sqrt{\sigma})^2 +\frac{4\lambda}{\lambda+2\mu}q^2+\frac{1}{R}\frac{(\mu-\lambda)^2}{\mu(\lambda+2\mu)}q^2-\Omega^2\frac{\lambda+\mu}{\lambda+2\mu}\Big\} -\frac{1}{R}\frac{\lambda}{\mu}\Big[\Omega^2\frac{\mu}{\lambda+2\mu}-\frac{\lambda+3\mu}{\lambda+2\mu}q^2+kq\frac{\mu-\lambda}{(\lambda(\lambda+2\mu))^{1/2}}\Big]^2=0. \tag{28}$$

Here $\Omega^2=\rho\omega^2/\mu$, ω is the frequency, k and q are respectively the ξ and η components of the wave vector,

$$R=\frac{EK}{4\pi^2},\qquad c^2=-\frac{K^2}{E\,dK/d\mathscr{E}}.$$

Equation (28) is quadratic in Ω^2 and determines two acoustic branches of the oscillations. Near the transition point, when R is large enough, Eq. (28) breaks up approximately into two independent equations, which were given in our previous communication.[26] Near the transition point, one of the velocity components of the first branch vanishes like $\sqrt{p-p_c}$[2]. Simultaneously the region of admissable values of k tends to zero like $|1/\ln(p-p_c)|$. Thus, the first branch is "crowded out" of the spectrum, whereas the second tends to a finite limit. It can be verified that the squares of the frequencies, determined by the dispersion equation (28), are strictly positive at $k\neq 0$ and $q\neq 0$. This proves that the obtained solution is at least metastable.

The spectrum of the commensurate phase can be obtained in trivial fashion. It is sensible to return to the initial coordinate system x and y. The dispersion equation for the oscillations in this phase is of the form

$$(\rho\omega^2)^2-\rho\omega^2[f_0''+(\lambda+2\mu)(k^2+q^2)] +f_0''[(\lambda+\mu)q^2+\mu(k^2+q^2)]+\mu(\lambda+2\mu)(q^2+k^2)^2=0, \tag{29}$$

where f_0'' is the value of the second derivative of $f(\varphi)$ at the minimum point, and k and q are the components of the wave vector along the axes x and y. It is easy to verify that Eq. (29) has only positive roots. At small k and q, one of the solutions tends to a constant limit $(f_0''/\rho)^{1/2}$ (optical band), and the other to zero (acoustic band). The existence of the acoustic branch in the commensurate phase is attributed to the fact that the commensurability is attained only in one direction. Obviously, neither the optical band nor the acoustic band that exists in the commensurate phase is subjected to significant changes on going to the incommensurate phase.

The behavior of the soft acoustic mode that vanishes in the commensurate phase is similar to the behavior of the analogous soft mode in the one-dimensional case.[13,14]

Our investigations shows that although the transition from the commensurate to the incommensurate crystal is of second order, the commensurate phase continues to remain metastable in the entire region of existence of the incommensurate phase. This possibility of "superheating" in a second-order phase transition is apparently a unique phenomenon. On the other hand, it is impossible to "supercool" an incommensurate phase.

For a lattice of adatoms lying on a metal surface, the small-oscillation spectrum obtained by us is suitable only at not too low a frequency. At low frequencies the ohmic losses play the decisive role and cause the lattice motions to acquire a relaxation character: $\omega\sim iq^2$. We estimate now the frequency region $\omega\leqslant\omega_0$ in which the ohmic losses prevail. It can be assumed that the ions, as they glide over the surface, produce an electric current in a layer whose thickness is of the order of the lattice constant. Equating the ohmic losses during the period of the oscillations in this layer to the stored energy, we obtain for ω_0 in the case of molybdenum and tungsten the estimate

$$\omega_0\sim 10^9\frac{\sigma(T)}{\sigma_0}\ [\sec^{-1}],$$

where σ_0 is the room-temperature conductivity and $\sigma(T)$ is the conductivity at the given temperature.

For an Abrikosov vortex lattice in a superconducting film, ohmic losses prevail under the following condition

$$\omega<\omega_0=\sigma H^2/n_e m_e c^2, \tag{30}$$

where σ is the conductivity, H is the magnetic field, n_e is the volume density of the electron, m_e is the mass of the electron, and c is the speed of light. For fields $H\sim 100$ G the estimate (30) yields $\omega_0\sim 10^7\ \sec^{-1}$. Lattice vibrations of adatoms on tungsten and molybdenum in the high frequency region could possibly be observed by using Mandel'shtam-Brillouin scattering of visible light. Estimates made by Veshchunov[27] show that such observations are feasible in experiment. The existence of acoustic branches of the spectrum was confirmed only indirectly, although quite convincingly in our opinion, in the experiments of Naumovets and Fedorus,[28] who measured the intensity of Bragg reflections.

5. MONOLAYER AT FINITE TEMPERATURE

The symmetry of the Hamiltonian is violated in the ground state of an incommensurate crystal in two ways. First, the produced superstructure destroys the translational symmetry. Second, the deviation of the modulation direction ($\theta\neq 0$) from the x axis violates the reflection symmetry (see Sec. 2). Therefore at zero temperature the system is characterized by two long-range order parameters, which we shall call translational and orientational.[3)] At nonzero temperature, the orientational long-range order is preserved, and the translational one is violated. The reason is that the orientational symmetry group is discrete, whereas the

group of quasitranslations is continuous[6,7,14] and it corresponds to the Goldstone branches of the spectrum. The incommensurate phase forms at $T \neq 0$ a two-dimensional crystal without long-range order but with nonzero static shear modulus, and is thus an object which, with certain stipulations, one can apply the two-dimensional-crystals theory of Mermin *et al.*[17-21]

In the commensurate phase there remains in this case one Goldstone branch, so that the translational long-range order along the y axis vanishes at $T \neq 0$, but long-range order along the x axis remains. The superstructure is commensurate in the ground state, but the two-dimensionality of the system manifests itself in the fact that this one-dimensional order is not upset by quantum fluctuations. Our first task is to establish the appearance of the phase diagram on the (p, T) plane. We use for this purpose the Wilson renormalization-group method, first applied to two-dimensional systems with similar symmetry by Kosterlitz and Thouless[20] and by Kosterlitz.[29] The problem closest to it in formulation is that of a field that satisfies the sine-Gordon equation. The renormalization method for this field was developed by Wigman.[30] We have only slightly modified his method to allow for the pecularities of our problem.

We first performed the calculations for a special form of the function $f(\varphi) = b^4 V \cos\varphi$. We shall show subsequently that the higher harmonics $f(\varphi)$ are insignificant at nonzero temperature. We change from the variables φ and v to the variables $\varphi\sqrt{\mu}/b\sqrt{T}$ and $v\sqrt{\mu}/b\sqrt{T}$, and introduce also the symbol $\gamma = V/T$. The temperature is then formally eliminated from the argument of the Boltzmann exponential, but does enter into the argument of the cosine. In place of U/T we can now write in the argument of the Boltzmann exponential formally the quantity

$$\mathcal{L} = \int\int \Big\{ \frac{1}{2}\frac{\lambda+\mu}{\mu}\Big(\frac{\partial\varphi}{\partial x}+\frac{\partial v}{\partial y}-\frac{p}{\beta}\Big)^2 + \frac{1}{2}\Big(\frac{\partial\varphi}{\partial x}-\frac{\partial v}{\partial y}-\frac{p}{\beta}\Big)^2 + \frac{1}{2}\Big(\frac{\partial\varphi}{\partial y}+\frac{\partial v}{\partial x}\Big)^2 + b^2\gamma\cos\beta\varphi\Big\}\,dx\,dy, \tag{31}$$

where $\beta = b\sqrt{T}/\sqrt{\mu}$, $2\pi/b = a$ is the lattice constant.

The dimensionless quantity γ will henceforth be regarded as small. This means that calculations by the method of the renormalization group are valid at not too low temperatures $T \gg V$. The equation for the renormalized quantity γ takes the form

$$d\gamma_R/d\xi = 2(1 - T_R/T_1)\gamma_R, \tag{32}$$

where R labels renormalized quantities and

$$T_1 = 16\pi \frac{\mu}{\lambda+3\mu}\frac{\lambda+2\mu}{b^2}. \tag{33}$$

We see that at $T_R > T_1$ the quantity γ decreases with increasing ξ. The straight line $\gamma = 0$ is a line of fixed points, but these points are stable only at $T_R > T_1$. The point T_1 is critical. At $T_R < T_1$ the field of the large-scale displacements becomes free, and consequently the long-range order (along the x axis) vanishes. At $T_R < T_1$ the coefficient γ of $\cos\beta\varphi$ increases asymptotically.

To justify our conclusions we must analyze the behavior of the renormalized temperature T_R (or of the coefficient β). The renormalization-group equation for the temperature takes the form

$$dT_R/d\xi = -\text{const}\cdot\gamma_R^2 T_R^2. \tag{34}$$

The system (32) and (34) must be solved with the initial conditions

$$T_R|_{\xi=0} = T, \quad \gamma_R|_{\xi=0} = \gamma.$$

It is important that at $T > T_1$ and $(T - T_1)/T_1 \gg \gamma^2$ the renormalized temperature coincides with the initial T accurate to small quantities of order γ^2. Equation (32) can therefore be solved by assuming $T_R = T$ to be a constant quantity.

It should also be noted that, strictly speaking, renormalization gives rise to anisotropy of the elastic properties, since, for example, the coefficients of $(\partial\varphi/\partial x)^2$ and $(\partial\varphi/\partial y)^2$ vary differently. However, the resultant anisotropy is also of order γ^2 and can be neglected at $(T - T_1)/T_1 \gg \gamma^2$.

The general character of the phase portrait of the system remains the same as in the renormalization-group equations of Anderson and Yuval[31] and of Kosterlitz.[29] At $T < T_1$ the solutions of (32) increase as $\xi \to \infty$. The growth, however, can stop when the nonlinear terms not accounted for in (32) become substantial. This takes place at $\gamma_R \sim 1$.

Let a_R be the characteristic scale over which a constant value γ_R is established. The reciprocal of a_R is usually denoted m_R. This quantity satisfies the equation

$$m_R a_0 = (m_0 a_0)^{1/2\tau} F(T) = \gamma^{1/2\tau} F(T), \quad \tau = 1 - \frac{T}{T_1}, \tag{35}$$

where $m_0 = \gamma/a_0$ and $F(T)$ is a slowly varying function of the temperature. In its physical meaning, m_R agrees, within a constant factor, with the gap in the energy spectrum of the commensurate phase.

We examine now the renormalization of the higher harmonics $(n \neq 1)$ of the periodic function $f(\varphi)$. In (32) the coefficient $2(1 - T/T_1)$ for the n-th harmonic must be replaced by $2(1 - n^2 T/T_1)$. Therefore in the incommensurate phase the higher harmonics decrease as $\xi \to \infty$ more rapidly than the first harmonic, and can be neglected.

We proceed now to consider a nonzero incommensurability parameter p. The scale dimensionality of p, and consequently of p_c coincides with that of m. The equation for the transition curve then takes the form

$$p_c = (V/T)^{1/2\tau}\mathcal{F}(T). \tag{36}$$

6. THE TRANSITION-MATRIX METHOD

To calculate the partition function we use the known transition-matrix method. We distinguish one of the coordinates, for the sake of argument y, treat it from now on as the time, and follow the development of the system with variation of this coordinate. To emphasize this distinction, following the established tradition, we designate differentiation with respect to y by a superior dot and differentiation with respect to x by a prime. We break up the entire interval of variation of y from 0

to l into N small segments of dimension Δ and represent the partition function in the form

$$Z=\mathrm{Sp}\,(\hat{T})^N, \tag{37}$$

where the operator $\hat{T}$ is expressed in terms of the Hamiltonian $\hat{H}$ in the following manner:

$$\hat{T}=1-\Delta\hat{H}, \tag{38}$$

and the Hamiltonian $\hat{H}$ is obtained from the Lagrangian in the usual manner (apart from the sign):

$$\hat{H}=\int(-\dot{\varphi}P-\dot{v}Q+\mathscr{L})\,dx. \tag{39}$$

The field momenta $P=\partial\mathscr{L}/\partial\dot{\varphi}$, $Q=\partial\mathscr{L}/\partial\dot{v}$ should be replaced in the final expression for $\hat{H}$ by the variational derivatives $P=\delta/\delta\varphi(x)$, $Q=\delta/\delta v(x)$. The explicit expression for $\hat{H}$ is

$$\hat{H}=\int\left\{-\frac{P^2}{2\mu}-\frac{Q^2}{2(\lambda+2\mu)}+v'P+\frac{\lambda}{\lambda+2\mu}(\varphi'-p)Q+\frac{2(\lambda+\mu)\mu}{\lambda+2\mu}(\varphi'-p)^2+\gamma b^2\cos\beta\varphi\right\}dx. \tag{40}$$

The problem reduces to calculation of the minimal eigenvalue E_0 of the Hamiltonian $\hat{H}$, and of the corresponding state vector $\Psi_0\{\mathbf{u}\}$. We note that in the initial form (40) the Hamiltonian $\hat{H}$ is not Hermitian, since P and Q are anti-Hermitian operators.

The non-Hermitian Hamiltonian (40) can be reduced to Hermitian in the following manner. We note that the integrals with respect to v following functional integration of $E^{-\mathscr{L}}$ are Gaussian. Therefore integration with respect to v reduces to finding the extremum of the functional $\mathscr{L}(\varphi,v)$ with respect to v at fixed φ. It is clear that this extremum does not change if we change from the real variable to the pure imaginary $v=iw$. If we simultaneously replace the variable y by it, then the Lagrangian $\mathscr{L}$ remains real, but Δ must be regarded as imaginary. As a result the field momentum P becomes a Hermitian operator, Q is anti-Hermitian, and the Hamiltonian H becomes Hermitian.

The transition to the imaginary v is natural, since v is the "temporal" components of the displacement vector. The ground-state vector of the Hermitian Hamiltonian can be chosen real (even in the case of discrete degeneracy).

The mean value of the arbitrary quantity $A\{\mathbf{u},\dot{\mathbf{u}}\}$ is calculated by the formula

$$\langle\hat{A}\rangle=\langle\Psi_0|\hat{A}|\Psi_0\rangle=\int\Psi_0\{\mathbf{u}\}\hat{A}\Psi_0\{\mathbf{u}\}D\mathbf{u}, \tag{41}$$

where Ψ_0 is the ground-state vector.

We calculate now the mean values of the operators

$$P=\frac{\delta}{\delta\varphi(x)},\quad Q=\frac{\delta}{\delta v(x)}.$$

Since $\Psi_0\{\mathbf{u}\}$ is real (see above), we have

$$\langle P\rangle=\langle Q\rangle=0. \tag{42}$$

Returning to the initial problem, we can easily verify that the quantities P and Q are components of the stress tensor. Namely, $P=\sigma_{xy}$ and $Q=\sigma_{yy}$. The equality (42) therefore means that the mean values $\langle\sigma_{xy}\rangle$ and $\langle\sigma_{yy}\rangle$ are equal to zero at each point of the plane also at nonzero temperatures (cf. the end of Sec. 2).

7. SOLITON REPRESENTATION

The classical ground state of the incommensurate phase (see Secs. 2 and 3) can be treated as static periodically repeating solitons. At nonzero temperature, the solitons begin to move in both directions, and consequently the periodicity is lost. In addition, a thermodynamic-equilibrium number of antisolitons appears—inflections in the opposite side (see Fig. 1). The physical picture is similar to that considered by Luther and one of us[16] (see also Ref. 14), who dealt mainly with quantum fluctuations of a one-dimensional system. They have noted that in the simplest cases the two-dimensional statistical system can be reduced to a one-dimensional quantum system, so that the temperature of the statistical system is proportional to Planck's constant of the one-dimensional quantum problem.

Solitons in the one-dimensional problem can be treated as particles subject to Fermi statistics. The incommensurability p plays the role of the chemical potential of these particles. A certain advantage, say, arises for particles over antiparticles. The difference between the numbers n_s and n_a of the solitons and antisolitons is equal, apart from a constant factor, to the gradient of the phase φ. A phase transition from this point of view takes place when the chemical potential reaches the values of the renormalized mass of the solitons. At lower values of p the difference n_s-n_a is equal to zero, and this corresponds to the commensurate phase.

Let us show how to apply these concepts to our problem. Since our problem involves two boson fields, φ and v, we introduce two different types of fermions, described by the spinor operators ψ_a and χ_a in accordance with the following equations

$$\psi_1=\frac{1}{(2\pi a)^{1/2}}\exp\left\{-\frac{2\pi}{\beta}\int_{-\infty}^{x}P\,dx-\frac{\beta i}{2}\varphi\right\}\exp\left\{-\frac{2\pi i}{\alpha}\int_{-\infty}^{+\infty}Q\,dx\right\},$$
$$\psi_2=\frac{-i}{(2\pi a)^{1/2}}\exp\left\{-\frac{2\pi}{\beta}\int_{-\infty}^{x}P\,dx+\frac{\beta i}{2}\varphi\right\}\exp\left\{-\frac{2\pi i}{\alpha}\int_{-\infty}^{+\infty}Q\,dx\right\}; \tag{43}$$

$$\chi_1=-\frac{i}{(2\pi a)^{1/2}}\exp\left\{-\frac{2\pi i}{\alpha}\int_{-\infty}^{x}Q\,dx-\frac{\alpha}{2}v\right\},$$
$$\chi_2=\frac{1}{(2\pi a)^{1/2}}\exp\left\{-\frac{2\pi i}{\alpha}\int_{-\infty}^{x}Q\,dx+\frac{\alpha}{2}v\right\}. \tag{44}$$

Here α is an arbitrary real constant. The operators φ and Q are assumed Hermitian and v and p anti-Hermitian; this corresponds to the imaginary "time" (see the

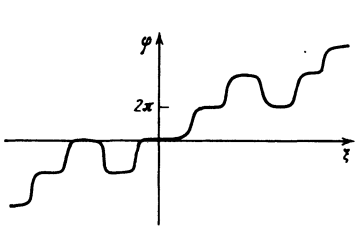

FIG. 1.

preceding section).

By virtue of the commutation relations between P and φ and between Q and v, the operators $\psi_\alpha, \psi_\alpha^+, \chi_\alpha, \chi_\alpha^+$, taken at different values of x anticommute with each other. Equations (43) and (44) are a modification of the Mandelstam representations[32] of fermion operators that generate solitons and antisolitons. In a somewhat different form it was obtained by Luther and Emery.[33]

The boson operators are expressed in terms of the fermion operators in the following manner:

$$\varphi' = \frac{2\pi}{\beta}(\psi_1^+\psi_1 + \psi_2^+\psi_2), \quad v' = -\frac{2\pi i}{\alpha}(\chi_1^+\chi_1 + \chi_2^+\chi_2), \tag{45}$$

and

$$P = \frac{\beta i}{2}(\psi_1^+\psi_1 - \psi_2^+\psi_2), \quad Q = \frac{\alpha}{2}(\chi_2^+\chi_2 - \chi_1^+\chi_1). \tag{46}$$

Substituting (45) and (46) in the Hamiltonian (40) and replacing $\cos\beta\varphi$ by $\pi a\bar{\psi}\psi$, we obtain the Hamiltonian for the fermions

$$H = H_\psi + H_\chi + H_{\psi\chi}, \tag{47}$$

where

$$H_\psi = \int \{ic_\psi\psi^+\sigma_z\psi' + g_{\psi\psi}\psi_1^+\psi_1\psi_2^+\psi_2 - \xi(\psi_1^+\psi_1 + \psi_2^+\psi_2) + m\bar{\psi}\psi\}\,dx, \tag{48}$$

$$H_\chi = \int \left\{ ic_\chi\chi^+\sigma_z\chi' + g_{\chi\chi}\chi_1^+\chi_1\chi_2^+\chi_2 + p\frac{\alpha}{2\beta}\sigma(\chi_1^+\chi_1 - \chi_2^+\chi_2)\right\} dx, \tag{49}$$

$$H_{\psi\chi} = \int \left\{ \pi\left[\frac{\beta}{\alpha} + \frac{\alpha}{\beta}\sigma\right](\psi_1^+\psi_1\chi_2^+\chi_2 - \psi_2^+\psi_2\chi_1^+\chi_1) + \pi\left[\frac{\beta}{\alpha} - \frac{\alpha}{\beta}\sigma\right](\psi_1^+\psi_1\chi_1^+\chi_1 - \psi_2^+\psi_2\chi_2^+\chi_2)\right\} dx. \tag{50}$$

The constants $c_\psi, c_\chi, g_{\psi\psi}, g_{\chi\chi}, \xi$ are connected with the parameters of the boson problem by the relations

$$c_\psi = \frac{\beta^2}{8\pi} + \frac{8\pi}{\beta^2}\frac{\lambda+\mu}{\lambda+2\mu}, \tag{51}$$

$$g_{\psi\psi} = \frac{16\pi^2}{\beta^2}\frac{\lambda+\mu}{\lambda+2\mu} - \frac{\beta^2}{4}, \tag{52}$$

$$c_\chi = \frac{g_{\chi\chi}}{2\pi} = \frac{\alpha^2}{8\pi}\frac{\mu}{\lambda+2\mu}, \quad \xi = p\frac{8\pi}{\beta^2}\frac{\lambda+\mu}{\lambda+2\mu}. \tag{53}$$

Finally, $m = 2\pi^2\gamma b$. We put henceforth $\alpha = \beta/\sqrt{\sigma}$.

The fermion field ψ has a bare mass that becomes renormalized by the interaction. The renormalized mass was determined in Sec. 5 [see Eq. (35)]. The fermions χ remain massless also when the interaction is turned on.

8. EXACT SOLUTIONS

At certain values of the parameters, the fermion problem admits of an exact solution. Namely, we impose on parameters σ and β the condition that the velocities c_ψ and c_χ coincide [(see (51) and (53)]:

$$\left(\frac{\beta^2}{8\pi}\right)^2 = \frac{\lambda}{\mu-\lambda}\frac{\lambda+\mu}{\lambda+2\mu}. \tag{54}$$

In addition, we stipulate that the coupling constant $g_{\psi\psi}$ vanish [see Eq. (52)]. Then β and σ are determined uniquely:

$$\sigma = 1/5, \quad \beta^2 = 8\pi\sqrt{3/5}. \tag{55}$$

The interaction in this model reduces to scattering processes of the type $\psi-\chi$ and $\chi-\chi$. We consider first the processes of the first type. The energy and momentum conservation laws can be satisfied only if the momentum of each particle is conserved in the scattering. It is easily seen in the case of unequal velocities c_ψ and c_χ scattering with change of the value of the momentum becomes possible, and this makes for an extremely complicated problem. A problem with this scattering cannot be solved exactly. In the case $c_\psi = c_\chi$ the scattering can lead only to a multiplication of the wave function by a certain phase factor. A simple calculation shows that this factor is equal to $e^{gi/2}$, where $g = \pi/\sqrt{3}$. The fact that the change of the phase does not depend on the momenta of the colliding particles greatly simplifies the solution of the problem. The scattering of particles χ_1 by χ_2 leads to multiplication of the wave function by (-1).

Let the number of the χ fermions be $N_{\chi 1}$ and $N_{\chi 2}$. Then transport of the particle ψ from left to right along the x axis causes the phases of the wave function to change by an amount

$$kl + (N_{\chi_1} + N_{\chi_2})\,g/2,$$

where k is the momentum of the ψ particle.

We stipulate satisfaction of the cyclic boundary conditions

$$kl + (N_{\chi_1} + N_{\chi_2})\,g/2 = 2\pi n \tag{56}$$

(n is an arbitrary integer). Since g does not depend on the momentum k, we can assume with arbitrarily high accuracy that the number $(N_{\chi 1} + N_{\chi 2})g/2$ is a mutliple of 2π. Then the cyclic boundary conditions (56) take the form

$$kl = 2\pi n.$$

But this is precisely the form that they have also for the free particles ψ. Consequently the $\psi-\chi$ scattering does not change the energy of the fermion system. Obviously, the same can be said also of the $\chi-\chi$ scattering.

Thus, in our case the fermions ψ and χ can be regarded in a certain sense to be non-interacting. Their energies are given by

$$E_\psi = \pm(c^2k^2 + m^2)^{1/2}, \quad E_\chi = \pm ck,$$

where $c = 2\sqrt{3/5}$. All the ψ-fermion states with energies less than $\xi = \sqrt{3/5}\,p$, are occupied, as are also all the χ-fermion states with energy less than zero. If p exceeds the critical value $p_c = \sqrt{5/3}\,m$, then

$$\langle n_\psi\rangle = \frac{\beta}{2\pi}\left\langle\frac{\partial\varphi}{\partial x}\right\rangle$$

differs from zero (incommensurate phase).

The quantity $\langle\partial\varphi/\partial x\rangle$, which characterizes the incommensurability, is of the form

$$\left\langle\frac{\partial\varphi}{\partial x}\right\rangle = \frac{(p^2-p_c^2)^{1/2}}{(8\pi)^{1/2}}\left(\frac{5}{3}\right)^{1/4}. \tag{57}$$

In accordance with the general considerations (see Sec. 6), the quantities

$$\langle P\rangle\sim\langle n_{\psi_1}\rangle-\langle n_{\psi_2}\rangle,\quad \langle Q\rangle\sim\langle n_{\chi_1}\rangle-\langle n_{\chi_2}\rangle$$

are equal to zero. In the exact solution, however, it is seen that

$$\langle \partial v/\partial x\rangle=\langle n_{\chi_1}\rangle+\langle n_{\chi_2}\rangle=0$$

from which and from the fact that $\langle P\rangle=0$ it follows also that $\langle \partial\varphi/\partial y\rangle=0$.

We consider now a more general situation, when Eq. (54), which guarantees equality of the velocities c_ψ and c_χ, is satisfied but β is arbitrary. In this case, just as in the one considered earlier, the $\psi-\chi$ collisions lead only to multiplication of the wave function by an inessential phase factor. The ψ fermions, however, interact with one another. The spectrum of the ψ-particle system is the same as in the Thirring massive model. The model was investigated by Berkgnoff and Thacker,[34] who found the exact ground state and the excitation spectrum for a zero chemical potential. The case of interest to us differs from that considered by them in that the chemical potential

$$\xi=p\frac{8\pi}{\beta^2}\frac{\lambda+\mu}{\lambda+2\mu}$$

differs from zero. Obviously, in the case $\xi<m_R$, where m_R is the renormalized fermion mass, the ground state of the system does not change. At $\xi>m_R$ there arises, as previously, a nonzero quantity $\langle n_\psi\rangle$, which is proportional to $\langle \partial\varphi/\partial x\rangle$. Since the χ particles do not interact in fact with ψ, we have in the ground state $\langle n_\chi\rangle=0$.

We are unable to write down for $\langle \partial\varphi/\partial x\rangle$ an exact formula similar to (57), since the presence of a nonzero $\langle n_\chi\rangle$ changes the spectrum of the particles. At ξ close to m_R (p close to p_c), however, when $\langle n_\psi\rangle$ is small and the change of the spectrum can be neglected, we obtain again

$$\langle \partial\varphi/\partial x\rangle\sim(p-p_c)^{1/8}.$$

Just as in the case considered above,

$$\langle P\rangle=\langle Q\rangle=\left\langle\frac{\partial v}{\partial x}\right\rangle=\left\langle\frac{\partial\varphi}{\partial y}\right\rangle=0.$$

An exact solution can be obtained also in the limit $\lambda=\infty$. This is precisely the limit realized in the vortex lattice in a superconducting film (see the introduction). In this case $c_\chi=g_{\chi\chi}=0$ [see Eq. (53)]. Therefore the χ fermions are immobile. Their energy does not depend on the momentum. Using this, we construct a vacuum state such that the χ fermions are at the sites of a one-dimensional periodic lattice with period a, but there are two on each site. The wave function ψ at the collision point is multiplied by the phase factor $\exp(ig_{\psi\chi}/c_\psi)$, where $g_{\psi\chi}=2\pi\sqrt{\sigma}$. Just as in the preceding case, the ψ and χ fermions do not interact in fact. Therefore the problem was reduced to the solution of the same Thirring model as in the preceding case. The only difference lies in the correlation properties of the χ fermions.

We note that the double degeneracy that occurs at $T=0$ does not appear at finite T. The transition temperature can lie only in that region where neither the classical nor the renormalization-group approaches are applicable, i.e., at $T\sim V$. We thus arrive at the conclusion that at a certain temperature $T_0\sim V$ there occurs an orientational phase transition that causes vanishing of the symmetry breaking due to the deviation of the direction of the modulation in this superstructure from the x axis.

9. BRAGG REFLECTIONS

The form factor $S(\mathbf{k})$ measured in experiments on the scattering of neutrons, x rays, and electrons is the Fourier component of a correlation function of the form

$$G_{\mathbf{k}}(\mathbf{x},\mathbf{x}')=\langle\exp[i\mathbf{k}(\mathbf{u}_{\mathbf{x}}-\mathbf{u}_{\mathbf{x}'})]\rangle, \tag{58}$$

where $\mathbf{u}_{\mathbf{x}}$ is the vector of the displacement at the point x. We are interested in momentum transfers $\mathbf{k}$ close to the reciprocal-lattice vectors of the adsorbed atoms $\mathbf{k}=\mathbf{b}+\boldsymbol{\varkappa}$, and in distances $|\mathbf{x}-\mathbf{x}'|$, considerably exceeding the lattice constant.

In the C phase (we recall that it is commensurate only in one direction) the x coordinates of the atoms are ordered and fluctuations cause only a Debye-Waller decrease of the peaks, inasmuch as there is a gap in the spectrum of the fluctuations. Oscillations along the y axis lead to the vanishing of the long-range order along this coordinate at finite temperatures.

In the I phase, the long-range order vanishes also along the x axis. However, at sufficiently low temperatures $T\ll V$ the fluctuations of $\mathbf{u}$ can be neglected and we can substitute in (58) the solution obtained in Secs. 2 and 3. In the commensurate phase in this temperature region we have $u_x=-px/b$, $u_y=\sigma py/b$. It is also legitimate to neglect the fluctuations in the C phase at $T\ll\mu a^2$.

In the region $T\gg V$, the mean value (58) can be reduced in the I phase to a certain fermion mean values. The form factor $S(\mathbf{k})$ is connected with $G_{\mathbf{k}}(\mathbf{x})$ by the relation

$$S(\mathbf{k})=\sum_{\mathbf{x},\mathbf{x}'}\exp\{i\mathbf{k}(\mathbf{x}-\mathbf{x}')\}G_{\mathbf{k}}(\mathbf{x},\mathbf{x}'), \tag{59}$$

where the summation is over the sites of the adsorbed-atom lattice, and $\mathbf{x}$ is the vector number of the lattice site.

We consider first the classical case $T\ll V$, when the fluctuations can be neglected. In this case the correlator $\langle\exp\{i\mathbf{ku}(\mathbf{x})\}\exp\{-i\mathbf{ku}\cdot(\mathbf{x}')\}\rangle$ depends on the two coordinates $\mathbf{x}$ and $\mathbf{x}'$, and not merely on their difference. We can substitute in (58) and in (59) the solution $\mathbf{u}(\mathbf{x})$ obtained in Secs. 2 and 3. We can then represent $S(k)$ in the form

$$S(\mathbf{k})=\left|\sum_{\mathbf{x}}\exp\{i\mathbf{kx}+i\mathbf{ku}(\mathbf{x})\}\right|^2=|\Sigma(\mathbf{k})|^2. \tag{60}$$

We assume $\mathbf{k}$ to be close to some reciprocal-lattice vector $\mathbf{b}=n_1\mathbf{b}_1+n_2\mathbf{b}_2$, where $\mathbf{b}_1$ is directed along the x axis. The basis vector $\mathbf{a}_2$ of the crystal lattice has only a y component, whereas both components of $\mathbf{a}_1$ are in general different from zero. Calculation of the sum $\Sigma(\mathbf{k})$ for specified n_1 and n_2 yields

$$\Sigma(\mathbf{k})=\frac{1}{2\pi}\sum_{m}F_{m_1m_2}\delta\left(\mathbf{ka}_1'-2\pi n_1-\frac{2\pi(\mathbf{va}_1)}{(2\mu)^{1/2}K}m\right)$$
$$\times\delta\left(\mathbf{ka}_2'-2\pi n_2-\frac{2\pi(\mathbf{va}_2)}{(2\mu)^{1/2}K}m\right). \quad (61)$$

Here $F_{m_1m_2}$ are the Fourier components of the periodic function $\exp\{(ik_x\tilde{\varphi}+ik_y\tilde{v})/b\}$ ($\tilde{\varphi},\tilde{v}$ are the periodic parts of φ and v), and $\mathbf{a}_i'$ are the basis vectors of the deformed lattice, whose coordinates a_{ik}' are connected with the coordinates a_{ik} of the initial basis vectors by the relations

$$a_{11}'=a_{11}\left(1-\frac{p}{b}+\frac{1}{b}\left\langle\frac{\partial\varphi}{\partial x}\right\rangle\right),$$
$$a_{12}'=a_{12}\left(1+\frac{\sigma p}{b}\right), \quad (62)$$

with $a_{11}=a$, $a_{21}=0$; the vector $\mathbf{v}$ is a unit vector of the direction of modulation with coordinates $\cos\theta$ and $\sin\theta$, where $\tan^2\theta=\sigma$.

Thus, the diffraction pattern is represented by an aggregate of principal Bragg extrema, which are determined by vectors a_i' and by a linear set of satellites which are determined by the period of the superstructure $(2\mu)^{1/2}K$. We note that at large p the values of a_{i1}' coincide with the components of the basis vectors of the adatom lattice on a smooth substrate a_{i1}, whereas at p close to the critical value a_{i1}' go over into the components of the basis vectors of the substrate lattice.

We proceed now to the temperature region $T\gg V$. Putting $\mathbf{k}=\mathbf{b}+\boldsymbol{\varkappa}$ and assuming $\boldsymbol{\varkappa}$ to be small enough, we obtain approximately

$$S(\mathbf{k})=\frac{A}{A_0}\int\exp(i\boldsymbol{\varkappa}\mathbf{x})G_b(x)d^2x, \quad (63)$$

where A_0 is the unit-cell area and A is the adatom area; it was assumed that $G_k(\mathbf{x},\mathbf{x}')$ depends only on the difference $\mathbf{x}-\mathbf{x}'$. Let $\mathbf{k}=n\mathbf{b}_1$, where $\mathbf{b}_1$ is the basis vector of the reciprocal lattice along the x axis. We obtain

$$\exp(ik\mathbf{u}_x)=e^{-inpx}e^{in\beta\varphi}=e^{-inpx}(\psi_1+\psi_2)^n(2\pi a)^n.$$

Consequently at $T\gg V$, for $\mathbf{k}$ directed along the x axis, only two Bragg reflections with $n=\pm1$ "survive." All others are small by virtue of the smallness of the smallness of the parameter V/T.

This conclusion is equally valid for the C and I phases. The only difference lies in the behavior of $G_k(\mathbf{x}-\mathbf{x}')$ at large $|\mathbf{x}-\mathbf{x}'|$. For the C phase ($n=1$) we get

$$G_k(\mathbf{x}-\mathbf{x}')\approx\exp\{-\beta^2\langle\varphi^2\rangle\}\exp\{-ip(x-x')\}\approx m_Ra\exp\{-ip(x-x')\}. \quad (64)$$

Equation (64) can be obtained by assuming φ to be a quantity with a Gaussian distribution up to a certain distance of the order m_R^{-1}. It is of interest, from this point of view, to estimate the reflections with $n\neq1$ in the C phase. Their intensity turns out to be proportional to $(m_Ra)^{n^2}$. This is in fact the accuracy of the fermion (and renormalization-group) approximation. The result means that in the C phase in Bragg reflections of the substrate are replaced by a quantity $\sim m_Ra$ which is assumed in our approximation to be small.

In the I phase at $n=1$, $\sigma=1/5$ and $\beta^2=8\pi\sqrt{3/5}$, the neutrons are scattered by the ψ fermions as on free

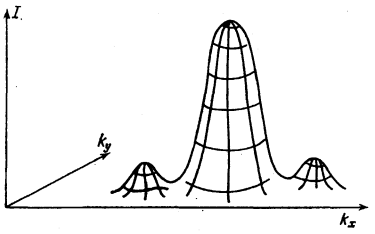

FIG. 2.

fermions. Under the condition $p_F=(\xi^2-m^2)^{1/2}/c\ll m$, and $|\varkappa_x|\ll m$, the Fourier component of the correlator $G_k(\mathbf{x}-\mathbf{x}')$ takes the form

$$\frac{m}{8\pi c\varkappa_x}\ln\left[\frac{(p_F+\varkappa_x/2)^2+(m\varkappa_y/c\varkappa_x)^2}{(p_F-\varkappa_x/2)^2+(m\varkappa_y/c\varkappa_x)^2}\right]+\frac{1}{2\pi}\left(1+\frac{2m^2}{c^2\varkappa_y^2}\right)$$
$$\times\left(1+\frac{4m^2}{c^2\varkappa_y^2}\right)^{-1/2}\ln\left[\frac{(1+4m^2/c^2\varkappa_y^2)^{1/2}+1}{(1-4m^2/c^2\varkappa_y^2)^{1/2}-1}\right]$$
$$+\frac{1}{\pi}\ln\frac{2}{ma}-\frac{2m}{(2m)^2+c^2\varkappa_y^2}\frac{cp_F}{2\pi}. \quad (65)$$

The diffraction pattern is the following. The principal Bragg peaks decreased rapidly [like $(ma)^{n^2}$] with increasing number. Near the first principal peak there are two weak satellites at $\varkappa_x=\pm2p_F$. Their intensity decreases and their width increases with decreasing $\varkappa_y^{-1}$. The diffraction pattern is shown schematically in Fig. 2. We note the logarithmically large background intensity.

10. GENERAL CHARACTER OF THE PHASE DIAGRAM

The phase diagram in the (p, T) plane consists of alternating regions of commensurate and incommensurate crystalline phases, as shown in Fig. 3. It is known that the widths of the sections of the commensurate phase at $T=0$ are proportional to $(V/\mu a^2)^{N/2}$, where N is the commensurability order (by definition, the commensurability order N is the denominator of the ratio d/a, where d is the period of the substrate and a is the period of the lattice of adatoms on a smooth substrate). Therefore high commensurability orders correspond to very narrow strips on the phase diagrams. It was shown in Refs. 14 and 15 that in the case of the N-th commensurability order the interaction with the substrate is described by a potential of the type $V^N\cos N\varphi$, where φ is the coordinate of the center of the unit cell. Repeating the renormalization procedure (see Sec. 5) for such a potential, we find that the critical temperature T_N of a commensurate phase of N-th order is equal to T_1/N^2, where T_1 is the critical temperature of the commensurate phase of the

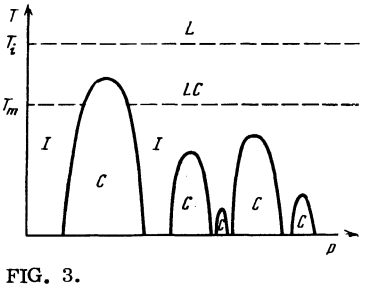

FIG. 3.

lowest order [Eq. (33)]. Obviously the substrate defects which violate the coherence at distances of the order of Na destroy the commensurate phases with large commensurability order. Another reason why commensurate phases of high orders cannot be observed is the finite value of $V/\mu a^2$. In fact, in the region of existence of commensurate phases of low orders one cannot observe commensurate phases of high orders, which are formally located inside this region. With increasing $V/\mu a^2$, the widths of the commensurable phases increase. A situation is therefore possible, for example, wherein there is only one region of commensurate phase and there are no incommensurate phases at all, or else, say, there exists only a single region of incommensurate phase.

As shown by Halperin and Nelson,[21] above the melting temperature T_m of the incommensurate phase the two-dimensional system acquires the properties of a liquid crystal, and at a still higher temperature T_i it goes over into an isotropic liquid. The general form of the phase diagram is shown schematically in Fig. 3. The anisotropy of the substrate causes the orientational order in the film to be preserved also at high temperatures. Therefore the phase transition at the temperature T_i becomes smeared out, with ΔT proportional to $V^2/\mu a^2$.

The "bare" incommensurability is an inconvenient quantity for use as a thermodynamic characteristic. This raises the question of the conversion from the quantity p to experimentally obtainable parameters. This is simplest to do in the case of a corrugated superconducting film in a magnetic field (Ref. 5; see also the Introduction). In this case the reciprocal-lattice vector of the "substrate," whose role is assumed by the corrugation, is fixed while the vector of the reciprocal lattice of the vortices in the smooth film is proportional to $\sqrt{H}$. We can therefore plot H instead of the ratio of the reciprocal vectors. The points corresponding to initially commensurable lattices are

$$H=H_{MN}=\frac{2}{\sqrt{3}}\frac{\phi_0}{a^2}\frac{M^2}{N^2},$$

where M and N are relatively prime integers. Near each of these points, according to our theory, there should occur an incommensurability region whose width ΔH relative to the field is proportional at $T=0$ to $\delta^{N/2}$, where δ is the depth of the corrugation.

The melting temperature and the critical temperature of the commensurate phases are determined by Eq. (33), in which we must put $\lambda=\infty$, $a^2=2\phi_0/H\sqrt{3}$. In addition, it must be recognized that $\mu \sim H^2 a \sim H^{3/2}\phi_0^{1/2}$. Therefore the critical temperature dependence on the magnetic field like $T_1(H)\propto H^{1/2}\phi_0^{3/2}$, i.e., $T_1(H)\sim 2\cdot 10^5 H^{1/2}$ [K].

The obtained estimate shows that the vortex lattice is extremely rigid and its melting is not determined at all by the dislocations, but simply by the vanishing of the superconductivity. This means that at practically at any $H<H_{c2}$ the lattice vanishes at the superconducting-transition temperature. Consequently, the state of the vortex lattice is practically independent of the temperature up to T_c, and depends only on the magnetic field. The phase diagram is shown schematically in Fig. 4. At $\lambda=\infty$ the regions of the existence of the commensurate phases are symmetrical about the straight lines $H=H_{MN}$.

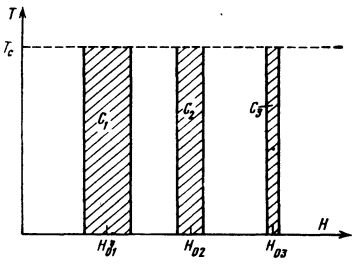

FIG. 4.

Daldini *et al.* investigated in their experiments the critical current as a function of the magnetic field. If corrugation and film are ideal the critical current should vanish in the incommensurate crystal. A schematic plot of the critical current as a function of H at a fixed temperature T is shown in Fig. 5 (the dashed curve). In a real situation the defects of the crystal under the corrugation produce additional pinning centers for the vortices, so that the critical current is not zero even in the incommensurate phase (solid curve of Fig. 5). Experiments on diffusion in submonolayers of adsorbed atoms yield for motion over the surface potential barriers of the order of 0.1–0.3 eV (Refs. 35, 36).[4)] Since incommensurate phases have been observed in many cases, the characteristic values λa^2 and μa^2 at sufficiently high concentrations c of the adatoms turn out to be of the same order of magnitude or larger. Therefore the commensurate phases with small concentrations go over directly into liquid with increasing temperature.

The melting of the commensurate phase is, generally speaking, a first-order phase transition if there are no special causes that lead to continuous melting (Alexander,[37] Domany, Schick, and Walker,[38] and Domany and Ridel[39]). So far, experiments with submonolayers have revealed only one phase-diagram region corresponding to an incommensurate crystal.[40] The boundary of the region of the incommensurate phase is, with high accuracy, the straight line $c=\text{const}$.[5)] We regard this as natural, inasmuch as the temperature T in the entire region of the existence of the crystal is low compared with V, λa^2, and μa^2. Melting of the incommensurate phase takes place at the temperature

$$T_m=\frac{\mu_R}{4\pi}\frac{\lambda_R+\mu_R}{\lambda_R+2\mu_R}a^2$$

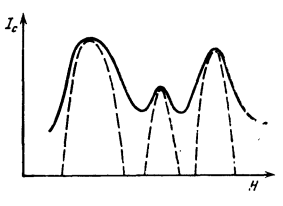

FIG. 5.

(Halperin and Nelson[21]). Therefore the melting curve in the plane (T, c) determines the dependence of the elastic moduli on the concentration. Naturally, T_m increases with increasing concentration, while the ratio $V/\mu a^2$ decreases. For C phases of higher order, the role of the effective interaction is assumed by the quantity $V(V/\mu a^2)^{N-1}$, where N is the commensurability order (i.e., the number of adatoms in the unit cell). Therefore the theory predicts the appearance of narrow sections of complicated C phases inside the region of the I phase. The search for these phases is an interesting experimental problem.

Usually the experimental situation becomes more complicated, since the restructuring of one phase into another proceeds via diffusion, which is greatly slowed down in dense phases. In the region of the existence of the C crystal, however, the I phase is absolutely unstable. In this case, therefore, the restructuring will occur rapidly enough. The observation of small commensurate sections in an incommensurate phase seems to us feasible in principle. Our theory should yield a quantitatively correct description of such transitions.

11. QUALITATIVE APPROACH TO THE PHASE-TRANSITION PROBLEM

In a small vicinity of the phase transition in the I phase, the distances between the solitons become large and it is this in fact which makes it possible to speak of isolated solitons. In this situation we can describe the entire picture of the phase transition qualitatively by introducting certain phenomenological parameters in the spirit of the Landau theory. The approach described in the present section was used by Bak *et al.*[25] to describe phase transitions on graphite substrates at $T=0$.

We denote by ε the energy of the individual soliton. We assume ε to be a variable quantity that depends on the concentration and on the temperature. In the region of negative ε, the solitons appear spontaneously, i.e., this is the region of the existence of the I phase. We identify similarly the region of positive ε with the region of existence of the C phase. The quantity ε plays the same role as $p-p_c$ in our theory. We consider first the one-dimensional case and a zero temperature. Let n denote the number of solitons per unit length (the density of the number of solitons). The energy density of the system of solitons is written in the form

$$E(n)=\varepsilon n+Ae^{-B/n}, \tag{66}$$

where A and B are certain constants. The first term in the right-hand side of (66) is the energy of the individual solitons, the second is the energy of interaction of the neighboring solitons. The exponential describes the effects of the weak overlap of the solitons. The minimum of the energy $E(n)$ corresponds to nonzero n only at $\varepsilon<0$, and the equilibrium value n_0 is determined by the equation

$$n_0=-B/\ln(-\varepsilon). \tag{67}$$

This result agrees with the classical results of Sec. 2 near p_c.

The considered simple phenomenological approach, however, yields utterly incorrect results in the case of a bounded area. An analysis of the exact solution (22) shows that in this case $n\sim p-p_c$ and $\bar{U}\sim(p-p_c)^2$. This result can be obtained by assuming that the energy of the system of solitons is

$$E=\varepsilon n+Dn^2, \tag{68}$$

where, as before, $\varepsilon\sim p-p_c$ is the soliton energy. The term quadratic in n characterizes the soliton-interaction energy. It can be interpreted as a result of long-range repulsion with an energy proportional to l^{-3}, where l is the distance between the solitons. It appears that this interaction is connected with the nonzero components σ_{xy} and σ_{yy} of the elastic-stress tensor, which arise under conditions of bounded area.

To obtain the answer for the one-dimensional quantum problem, we allow the solitons to move.[16,14] It is then necessary to add to the energy (66) the kinetic energy of the solitons. We regard the solitons as Fermi particles. That this can be done has been proved by Luther and Emery,[33] Coleman[42] and Mandelstam.[32] The Fermi momentum p_F of the solitons is connected with the density by the relation $p_F=\pi n$, and the kinetic-energy density is

$$E_{\text{kin}}=\frac{p_F^3}{6\pi m}=\frac{\pi^2 n^3}{6m},$$

where m is the soliton mass.

Thus, the total energy density takes the form

$$E(n)=\varepsilon n+Ane^{-B/n}+{}^1/_3Cn^3. \tag{69}$$

In the immediate vicinity of the transition point (small n) the exponential can be neglected compared with the power function $Cn^3/3$. In this case minimization yields $n_0\propto(-\varepsilon)^{1/2}$.[16] If the quantum effects are small, then at relatively small n the classical potential term becomes the principal one and we again obtain for n_0 the classical result (67). We can interpret Eq. (69) as an interpolation formula that connects the classical and quantum regions.

In the two-dimensional problem the quantum fluctuations do not disturb the order given in an incommensurate crystal, but thermal fluctuations do disturb the order. We have considered the one-dimensional potential of the interaction with the substrate. At zero temperature this interaction leads to the appearance of linear periodic soliton superstructures whose energy, just as in the one-dimensional case, is determined by expression (66).

The transition to a finite temperature can be effected by using the known connection between the quantum mechanics of a one-dimensional system and the statistical mechanics of the two-dimensional problem. One of the coordinates plays here the role of the time (for example, y). The motion of the soliton in time in a one-dimensional quantum system corresponds to bending of the solitons in the two-dimensional statistical system (see Fig. 6). The fermion behavior of the solitons means that we can disregard soliton intersections, since such configurations have a small statisti-

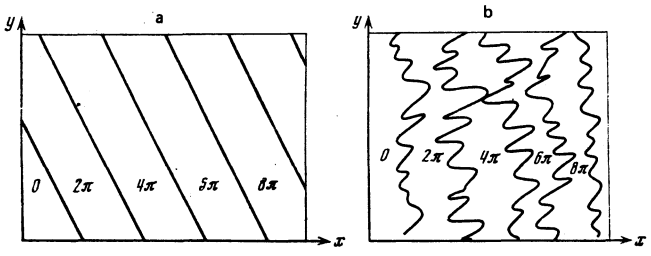

FIG. 6. a) Soliton superstructure at $T=0$; b) the same at $T \gg V$.

cal weight. This means that at finite temperatures the energy of the two-dimensional system is described by expression (69), where C is proportional to the temperature and ε is proportional to $p-p_c(T)$ or $T-T_c(p)$. Therefore near the line of the transition we have $n \sim [p-p_c(T)]^{1/2}$ or $n \sim [T-T_c(p)]^{1/2}$ (cf. Ref. 26). A more careful analysis (see Sec. 7 of the present paper) shows that the energy of the solitons can be regarded as local only when one introduces their interaction with the displacement field v or with the massless fermions χ, but this does not change the earlier results.

Recently Bak *et al.*[25] have found that in a certain vicinity of the phase-transition point (if this is a second-order transition) quasi-one-dimensional superstructures are energywise favored over two-dimensional ones. The reason is that in two-dimensional classical superstructures the principal interaction of the solitons is connected with their intersection. If we denote by the latter n the number of solitons that cross a segment of unit length, then the energy density of the two-dimensional system of solitons is equal to

$$E_2(n)=\varepsilon n+\tilde{D}n^2. \tag{70}$$

For the system to be stable, the constant $\tilde{D}$ in (70) must be positive. Minimizing (70) with respect to n and comparing the result with the energy of one-dimensional, superstructure (66) at the minimum (67), Bak *et al.*[25] reached the conclusion that near a second-order phase transition the one-dimensional superstructure is energywise favored.

This conclusion patently contradicts the existing experimental data. Chinn and Fain[43] used the method of diffraction of slow electrons to investigate krypton adsorbed on a graphite substrate, in equilibrium with krypton gas. The $C-I$ transition for this system proceeded continuously. No disturbance of the symmetry of the substrate was observed. Recently Stephens *et al.*[44] observed by x-ray structure analysis, in the same system, a superstructure having a hexagonal substrate symmetry. We can attribute this result to the fact that the transition took place under bounded-area conditions. Comparing (68) with (70) we find that the symmetrical superstructure is favored if $D > \tilde{D}$.

The coefficients D and $\tilde{D}$ depend strongly on the details of the interaction with the substrate. In principle, the case $D < \tilde{D}$ is also possible, wherein a one-dimensional superstructure is realized near the transition. Observation of one-dimensional CO superstructures on the (111) surface of cobalt, palladium and platinum close to a concentration $c=1/3$ is reported in Ref. 45. Similar phenomena were observed in cesium lattices on tungsten and molybdenum.[1] More detailed investigations are needed, however, before agreement between theory and experiment can be asserted with assurance.

12. CONCLUSIONS

In this section we present a brief summary of the experimental consequences of our theory and of the conditions under which the appearance of new effects can be expected.

1. Commensurate structures exist on an ideal surface in small vicinities (relative to the number of adatoms) of all the commensurability points. These vicinities become narrower with increasing temperature and vanish at $T_N = T_1/N^2$. At low temperatures the width of the region of existence of the commensurate phase decreases exponentially with increasing number of adatoms per unit cell.

2. In the incommensurate phase, at low temperatures, there is a superstructure whose period depends continuously on the temperature and pressure. Near the $C-I$ transition point this superstructure is a periodic sequence of one-dimensional standing solitons, the normal to which makes an angle $\theta = \pm \tan^{-1}\sqrt{\sigma}$ with the coinciding reciprocal-lattice vectors.

3. The diffraction pattern at low temperatures constitutes an assembly of principal extrema shifted relative to the extrema of the substrate (see Sec. 10), and linear series of satellites whose position makes it possible to determine the direction of the wave vector and the period of the superstructure.

4. At sufficiently high temperatures, the direction of the superstructure in the incommensurate phase coincides with the direction of the nearby reciprocal vectors. At a certain intermediate temperature $T \sim V$, where V is the characteristic energy of the interaction with the substrate, an orientational phase transition takes place with a change in the orientation of the superstructure. The higher harmonics of the periodic potential of the interaction with the substrate do not play any role at $T > V$.

5. At a finite temperature, the solitons begin to bend, and this leads to a destruction of a long-range order. In the temperature region $T > V$ the diffraction pattern, in both the commensurate and incommensurate phases, differ from the diffraction structure of the substrate in that the intensities of the principal Bragg extrema are changed. The difference of the intensities of the substrate with the adatoms in a pure substrate has a maximum for the diffraction peaks with $n=1$ and decreases sharply with increasing n. In the incommensurate phase, two satellites are located along the x axis near the principal peak.

The $C-I$ phase transition is of second order. Near the transition line, the incommensurability (i.e., the distance from the principal Bragg peak to the satellites) increases like $[T-T_c(p)]^{1/2}$ or $[p-p_c(T)]^{1/2}$ at $(T-T_c)/T_c$, $(p-p_c)/p_c \ll (T/T_1)^2$ and like $|\ln(T-T_c)|^{-1}$, $|\ln(p-p_c)|^{-1}$ on an unbounded area and like $T-T_c$,

$p-p_c$ on a bounded area at $(T-T_c)/T_c$, $(p-p_c)/p_c \gg (T/T_1)^2$.

At sufficiently large incommensurabilities, orientational phase transitions of first or second order can occur. The peculiarity of the $C-I$ transition is that the C phase can be superheated but the A phase cannot be supercooled.

7. In the I phase there exists a zero-gap (Goldstone) mode of small vibrations of the adatom lattice relative to the substrate. The component of the velocity of this sound along the x axis tends to zero near the $C-I$ transition. In principal, the existence of this mode can be observed by means of Mandel'shtam-Brillouin scattering.

8. Another possible type of experiment for the observation of the "supermobility" of a film of adatoms relative to a substrate is similar to the experiment of Bishop and Reppy[46] with helium films. Observation of the singularities of the response of a system that executes small oscillations in the region of low frequencies would be proof that the adatom lattice slides relative to the substrate.

9. We have assumed the interaction with the substrate to be weak compared with interatomic interaction of the adatoms. This does not seem to be very valid for most known systems of atoms adsorbed on graphite or on molybdenum and tungsten. Therefore the phase diagrams of the $C-I$ transition for the lowest orders of commensurability are determined in practice by the equation $c=\text{const}$, where c is the concentration of the adatoms. In this case there simply is no region $T>V$, and the commensurate phases melt directly into liquids at sufficiently high temperatures. It is possible, however, to expect the discovery of new commensurate phases in the region where at present there is only one incommensurate phase. For this hypothetical commensurate phases, the phase diagram takes the theoretically predicted form shown in Fig. 3, where p should be taken to mean the concentration and T_N should generally speaking be regarded as dependent on p.

Another possibility is to study the properties of adatoms on the surface of solidified noble gases. In this case the interaction with the substrate is weaker than the interaction between the adatoms even at relatively low concentrations.

10. For a lattice of Abrikosov vortices in a corrugated superconducting films placed in a magnetic field, the melting temperature turns out to be much higher than the critical temperature than the superconductor T_c. In this case the $C-I$ transition is determined only by the magnitude of the magnetic field. The theory predicts the appearance of commensurate phases and a growth of the critical current in the vicinities of the values of the magnetic field H_{MN}. The dimension of the region $|(H-H_{MN})/H_{MN}|$, in which the C phase exists equals, accurate to a numerical factor of the order of unity, $(\delta/d)^{N/2}$, where δ is the depth of the corrugation and d is the thickness of the film. The critical current at the maximum is $I_{MN} \sim (\delta/d)^{N/2}$.

We thank J. Villain and P. Bak for preprints of their articles and lectures.

[1)]It is important to have the moduli of the corresponding vectors close to one another, since rotation of one of the sublattices can always bring the directions of these vectors close together.

[2)]In the case of a bounded area we have $c \sim \exp[-\text{const}/(p-p_c)]$.

[3)]Our definition of these parameters does not agree with the customary one,[17,21] although it has many features in common.

[4)]The potential is much lower for noble gases on graphite.

[5)]Similar results were obtained for cesium on tungsten.[41]

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Three-dimensional Wigner crystal in a magnetic field

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We solve the quantum problem of the oscillations of a Wigner lattice in a strong magnetic field in the harmonic approximation, taking into account the transverse radiation field. We calculate the energy of the zero-point oscillations of the lattice and the dependence of the mean squared displacement of the particles from the lattice sites on the temperature and on the magnetic field. We consider the specific heat, the magnetic moment, and the dielectric constant of the lattice in a strong magnetic field, and discuss the stability of the lattice as a function of the particle density in the limit of a strong magnetic field.

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1. INTRODUCTION

The question of the ground state of an electron–hole plasma in a semi-conductor or semimetal in the limit of a strong magnetic field ($\hbar\omega_c \gg \mathrm{Ry}$, ω_c is the cyclotron frequency of the carriers and Ry is the exciton ionization potential) has attracted considerable interest recently. Babichenko and Onishchenko[1] have shown that if the carriers of different type have comparable mass, the homogeneous state of the system in a strong magnetic field is unstable to formation of a charge-density wave (CDW). Rakhmanov[2] has analyzed the case of carriers with strongly differing masses (for example, electrons and holes in bismuth) and determined the conditions under which the heavier particles (holes) form a Wigner lattice (WL) against an approximately homogeneous compensating background of lighter particles (electrons). The possibility of formation of a WL in a magnetic field was investigated earlier in Refs. 3 and 4, where it was shown that in a strong magnetic field the WL (CDW in the case of high density[5]) is energywise favored over a homogeneous ground state. We note, however, that the cited references are qualitative and variational in character, whereas the problems connected with the stability of a lattice and with the calculation of its equilibrium characteristics must be solved on the basis of quantitative analysis of the spectrum of the crystal-structure oscillations. We report here in this connection a detailed quantitative investigation of the vibrational properties of a WL in a magnetic field. We confine ourselves to the case of an immobile compensating background. In Sec. 2 we obtain the spectrum of the eigenvalues of the Hamiltonian of the WL oscillations in an arbitrary magnetic field[1)]; we calculate the energy of the ground state of the system, which turns out to depend on the orientation of the magnetic field relative to the crystallographic axes. In Sec. 3 we determine the dependence of the mean squared displacement of the particle from the WL site on the temperature and on the magnetic field, and find that the "soft mode" $\nu_1 \sim 1/\omega_c$ that appears in a strong magnetic field, just as in the two-dimensional case,[6] does not cause lattice instability. It is shown in Sec. 4 that the low-temperature heat capacity depends substantially on the magnetic field and is proportional to $T^{3/2}$ (T is the temperature), as against T^3 for ordinary phonons; we calculate also the temperature dependence of the magnetic moment of a WL and the dielectric constant of a WL, the latter being strongly anisotropic in a strong magnetic field.

In Sec. 5 we solve the problem of the coupling of the electromagnetic and vibrational modes of a WL in a magnetic field. An exact dispersion equation is obtained and the spectrum of the eigenvalues of the system is briefly investigated with account taken of the transverse radiation field. It is shown that in the limit of a strong magnetic field allowance for the transverse field does not change qualitatively the results of the preceding sections.

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