

Correlation function of large-period adatom lattices

I. F. Lyuksyutov

Institute of Physics, Academy of Sciences of the Ukrainian SSR, Kiev

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An investigation is made of the correlation properties of large-period structures. It is shown that a Berezinskii phase, which is characterized by power-law decay of the correlations, can exist in such structures at temperatures $T > T_p$. Transition to this phase from one with an ordinary long-range order is isomorphous with a phase transition in a two-dimensional plasma. Therefore, in the static limit, in spite of the potential relief of the substrate which is considerably greater than the interaction between adatoms, the behavior of large-period structures at temperatures $T > T_p$ is equivalent to the behavior of a crystal on a smooth substrate.

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1. Many adatom structures are known in which the period along one or two directions represents several (up to nine) substrate periods (see Refs. 1 and 2 and the literature cited there). The physical reason for the existence of such structures is, for example, the dipole-dipole interaction of adatoms (for other mechanisms see Refs. 3–5). Clearly, in the case of large-period structures the potential relief of the substrate is considerably greater than the interaction between adatoms. However, adatoms may be displaced over distances (substrate period) which are small compared with the structure period. Therefore, we can expect that in the static limit and at finite temperatures these structures behave as a two-dimensional elastic crystal. This behavior of two-dimensional systems (the appearance of properties typical of systems with a continuous symmetry in a system which has a discrete symmetry) was first predicted in the case of the Z_p model in Ref. 6. The model has been investigated subsequently by many authors (for a review see Ref. 7).

Halperin and Nelson⁸ demonstrated that a continuous translation group can appear at finite temperatures in the case of commensurate structures subject to a weak potential relief. Ostlund⁹ obtained the same result for adatom sublattices subject to a strong potential relief and this was done by selecting a special interaction potential. We shall show that in the case of large-period structures with a practically arbitrary potential of the interaction of adatoms with one another and with the substrate there is a possibility of the existence of a phase with the correlation properties of a two-dimensional crystal on a smooth substrate (Berezinskii phase¹⁰). The results obtained can be applied to a large number of real experimental systems.

2. Linear structures are the simplest example of large-period structures. These structures are observed on faces with a strongly anisotropic atomic relief. The atomic and, clearly, the potential relief of the W(112), Ma(112), Re(10 $\bar{1}$ 0), etc. faces is in the form of deep grooves along which the amplitude of the relief is considerably less than in the transverse direction. Linear structures are rows of adatoms (for example, Sr, Li, Mg, and La) oriented across the grooves. The structure period along a row is equal to the corresponding substrate period (Fig. 1) and across a row it amounts to several (up to nine) lattice periods; these are structures of the

($1 \times p$) type. A detailed description and elementary estimates of the parameters of such systems can be found in Ref. 2.

Adatoms in their ground state are located at minima of the potential relief with the coordinates $(r_x pa, r_y b)$ where p is the linear-structure period, and r_x and r_y are integers. Since the structure period is large, the interaction between rows should be significantly less than the potential relief (or the binding energy in a row) and adatoms are always located at the minima of the relief. In this case the displacements of adatoms between lattice positions $\mathbf{r} = (r_x, r_y)$ can only have a discrete set of values $u_r = n_r a$. We shall discuss a model in which an increase in the energy as a result of displacement of adatoms from their equilibrium positions is of the form

$$H = \frac{1}{2} \sum_{\mathbf{r}, \mathbf{r}'} V(\mathbf{r} - \mathbf{r}') (n_{\mathbf{r}} - n_{\mathbf{r}'})^2. \quad (1)$$

Here, the sum over \mathbf{r} and \mathbf{r}' is taken over all the adatoms in a linear structure. A set of values of $V(\mathbf{r})$ is determined by the actual form of the interaction between adatoms.

It should be noted that the proposed model differs from that discussed in Ref. 2. In the latter, only one excited state was considered. Therefore, the dependences of the melting point and of the depinning temperature on the interaction constants obtained below differ from those found in Ref. 2. The two models represent different limiting cases. The model of Ref. 2 should describe best the structures in which the number of excited states is small, i.e., when the structure period is not too large. The model discussed in the present paper should describe the case of very long periods ($p \gg 1$).

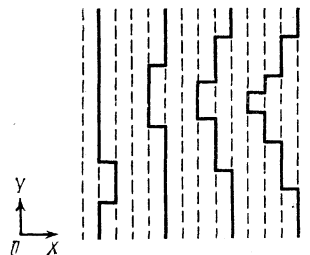


FIG. 1. Schematic representation of a (1×4) linear structure. The thick lines are the row of adatoms and the dashes are the minima of the potential relief along the X axis of the substrate.

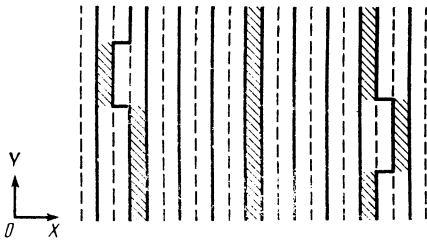


FIG. 2. Schematic representation of a superstructure formed as a result of mixing of linear structures with periods 2 and 1. The notation is the same as in Fig. 1. The superstructure is identified by shading.

The case of very long periods may be encountered as a result of mixing of linear structures with different periods. For example, in the Mg-Re(1010) system there are linear structures² with periods $3a$ and $2a$, respectively, when the coverage is $\theta = 1/3$ and $1/2$. The diffraction reflections obtained for intermediate coverages can be explained if we assume that a uniform mixing of structures with periods 2 and 3 takes place. The resultant superstructure is shown in Fig. 2. Finally, the third class of systems which can be described by the model adopted in the present paper are lattices of solitons in incommensurate crystals under conditions of pinning by the substrate¹¹ (this is discussed below).

3. It is most convenient to consider the model of Eq. (1) in the case of linear adatom structures. We shall be interested in the range of temperatures in which the condition $\langle n_r^2 \rangle \ll p^2$ is obeyed. In this case the contribution of states with large values of n_r is small (an estimate is obtained below) and in the partition function we can sum over all the values of n_r . The set of variables n_r can be converted conveniently by a dual transformation to a different set N_r . The variables N_r appear as a result of a change from the summation over n_r to integration with respect to a continuous variable φ_r using the Poisson summation formula. Consequently, the partition function of a system described by the Hamiltonian (1) is

$$Z = \prod_{\mathbf{r}} \sum_{N_r = -\infty}^{\infty} \int d\varphi_r \exp \left\{ -\frac{1}{2T} \sum_{\mathbf{r}, \mathbf{r}'} V(\mathbf{r}-\mathbf{r}') (\varphi_r - \varphi_{\mathbf{r}'})^2 \right\} \times \exp(2\pi i \varphi_r N_r). \quad (2)$$

In the partition function of Eq. (2) the integral with respect to φ_r is Gaussian and integration can be carried out exactly. As a result, we obtain (to within a normalization factor)

$$Z \propto \prod_{\mathbf{r}} \sum_{N_r = -\infty}^{\infty} \delta \left(\sum_{\mathbf{r}} N_r \right) \exp \left(\pi T \sum_{\mathbf{r}, \mathbf{r}'} v(\mathbf{r}-\mathbf{r}') N_r N_{\mathbf{r}'} \right), \quad (3)$$

$$v(\mathbf{r}) = \int_0^{2\pi} \frac{dq_x}{2\pi} \int_0^{2\pi} dq_y \frac{1 - e^{i\mathbf{q}\mathbf{r}}}{V(\mathbf{q})}, \quad V(\mathbf{q}) = \sum_{\mathbf{r}} 2V(\mathbf{r}) (1 - \cos \mathbf{q}\mathbf{r}). \quad (4)$$

The quantity $V(\mathbf{q})$ is simply a Fourier transform of the interaction energy in Eq. (1). In the long-wavelength approximation the form of $V(\mathbf{q})$ is governed by the theory of elasticity. The symmetry of linear structures yields unambiguously

$$V(\mathbf{q}) = \varepsilon_1 q_x^2 + \varepsilon_2 q_y^2. \quad (5)$$

The dependence (5) means that the interaction between var-

iables (charges) N_r increases logarithmically at large distances. Therefore, the energy required for the creation of one charge N_r diverges logarithmically on increase in the dimensions of the system. Consequently, the charges N_r can appear only in pairs with opposite signs, which makes Eq. (3) subject to the condition $\sum_{\mathbf{r}} N_r = 0$. We thus find that the problem of fluctuations in linear structures is isomorphous with the problem of a two-dimensional Coulomb plasma.^{12,13} A two-dimensional plasma has two phases: in one of them the charges of opposite sign combine into molecules and the plasma is an insulator, whereas in the other the molecules split into separate unbounded charges and the plasma is conducting. The conducting plasma phase corresponds to a low-temperature phase of linear structures (the phase with large values of N_r), whereas the insulating plasma phase corresponds to a high-temperature phase of linear structures (N_r become bound to form neutral pairs). The temperature of the transition between these two phases^{12,13} is governed by the quantities ε_1 and ε_2 :

$$T_p = (2/\pi) (\varepsilon_1 \varepsilon_2)^{1/2}. \quad (6)$$

The correlation function of displacements in a linear structure can be expressed directly in terms of the variables N_r . In fact, by definition, we have

$$G(\mathbf{r}_1 - \mathbf{r}_2) = \left\langle \exp \left[\frac{2\pi i}{pa} (u_{\mathbf{r}_1} - u_{\mathbf{r}_2}) \right] \right\rangle / Z. \quad (7)$$

Here, the angular brackets denote averaging over the states of the Hamiltonian (1) and pa is the linear structure period. Comparing Eqs. (7) and (2), we can readily see that the expression in the angular brackets differs from the partition function of Eq. (2) only by additional fractional charges $+1/p$ and $-1/p$, respectively, located at lattice sites \mathbf{r}_1 and \mathbf{r}_2 . Therefore, at high temperatures when the phase we are dealing with is characterized by the fact that N_r become bound into pairs and the number of pairs is small, we can simply ignore N_r ; then, the correlation function (7) becomes

$$G(\mathbf{r}) = \exp \left[- (2\pi T/p^2) v(\mathbf{r}) \right]. \quad (8)$$

This means that over long distances the correlation function decreases in accordance with a power law; for example, along the X axis (i.e., along the grooves) it decreases as

$$G(x, 0) \propto |x|^{-\Delta}, \quad \Delta = 2\pi T p^{-2} (\varepsilon_1 \varepsilon_2)^{-1/2}. \quad (9)$$

In the low-temperature phase the quantities N_r are large and can be regarded as continuous variables. The addition of $1/p$ simply represents an unimportant shift of the variable N_r . Therefore, the correlation function of Eq. (7) is simply equal to unity. We can see that the low-temperature phase is characterized by the usual long-range order, whereas the high-temperature phase exhibits the Berezinskii order.¹⁰

The Berezinskii ordering is typical of a two-dimensional crystal on a smooth substrate. Therefore, in the static limit at temperatures $T > T_p$ we can regard a linear structure as an elastic anisotropic (with one component of the strain tensor) crystal with the elastic moduli K_1 and K_2 . These elastic moduli are proportional to the constants ε_1 and ε_2 , respectively. The relationships between them can easily be obtained by the scaling transformation:

$$K_1 = \varepsilon_1 p / ab, \quad K_2 = \varepsilon_2 b / a^3 p, \quad (10)$$

and hence we obtain directly

$$T_p = (2a^2/\pi) (K_1 K_2)^{1/2}. \quad (11)$$

We shall now consider the physical picture of the transition in terms of the displacements u_r . We shall do this by estimating the mean-square value of displacements in one row at temperatures $T \gtrsim T_p$:

$$\langle u^2 \rangle \propto T_p / (K_1 K_2)^{1/2} \sim a^2. \quad (12)$$

Thus, at $T = T_p$ a row is "smeared out" between the neighboring minima of the potential relief. It should be noted that the temperature T_p is much less than the melting point T_m of a two-dimensional anisotropic crystal, which is given by (see, for example, Ref. 14):

$$T_m = (p^2 a^2 / 8\pi) (K_1 K_2)^{1/2} = (p/4)^2 T_p \gg T_p. \quad (13)$$

4. We shall now consider a situation when a displacement u_r of a row can assume a continuous range of values, i.e., when the substrate potential has a finite amplitude. This potential can be selected in the form suggested by Villain¹⁵:

$$w(u_r) = -2T \ln \left\{ \sum_{m_r=-\infty}^{\infty} \exp \left[-\frac{1}{2} \frac{w_0}{T} \left(m_r - \frac{u_r}{a} \right)^2 \right] \right\}. \quad (14)$$

The potential (14) is periodic, the period being a , and at low temperatures characterized by $T \ll w_0$, this potential becomes

$$w(u_r) = w_0 (u_r/a)^2. \quad (15)$$

We shall now adopt a new variable M_r in Eq. (14) using the Poisson summation formula

$$\begin{aligned} & \sum_{m_r=-\infty}^{\infty} \exp \left[-\frac{1}{2} \frac{w_0}{T} \left(m_r - \frac{u_r}{a} \right)^2 \right] \\ &= \left(\frac{2\pi T}{w_0} \right)^{1/2} \sum_{M_r=-\infty}^{\infty} \exp \left[-\frac{1}{2} \frac{T}{w_0} (2\pi M_r)^2 \right] \exp \left(\frac{2\pi i}{a} u_r M_r \right). \end{aligned} \quad (16)$$

In the case under consideration the partition function can be written in the form (apart from a normalization factor)

$$\begin{aligned} Z \propto \prod_r \sum_{M_r=-\infty}^{\infty} \int_{-\infty}^{\infty} du_r \exp \left\{ -\frac{1}{2T} \sum_{r,r'} V(r-r') (u_r - u_{r'})^2 \right\} \\ \times \exp \left[-\frac{1}{2} \frac{T}{w_0} (2\pi M_r)^2 \right] \exp \left(\frac{2\pi i}{a} u_r M_r \right). \end{aligned} \quad (17)$$

In the partition function (17), exactly as in the case of the partition function (2), integration is carried out over all the values of u_r , since large values of u_r such that $u_r/a \sim p$ make only a small contribution. We can easily see that the partition function (17) differs from that given by Eq. (2) simply by a larger chemical potential of the formation of pairs of charges M_r . The phase transition occurs at a point at which dissociation of the charge pairs begins. The first to dissociate are the pairs of the largest size. Therefore, the transition temperature is determined by the interaction between charges over large distances and not by the concentration of pairs. This means that the transition temperature T_p of linear structures is governed solely by the interaction of rows

with one another and not by the magnitude of the potential relief. It is natural to assume that the expression for T_p is independent of the potential relief also in the case when its form differs from Eq. (14).

We shall use these results to investigate depinning of a soliton lattice in a two-dimensional incommensurate crystal (see Ref. 11). In an incommensurate crystal a soliton lattice should form near the commensurate point when the difference between the film and substrate periods is compensated (for details see Ref. 16). When an incommensurate crystal is formed from a commensurate one by compression along one of the crystallographic directions of the substrate, the resultant soliton superstructure has a one-dimensional periodicity. In the case of large periods a soliton lattice can be represented by a system of lines oriented along one direction of the substrate and displaced in the perpendicular direction. The energy of a single soliton depends periodically, with the lattice period, on its position (this is known as the pinning of solitons by the substrates¹¹). The amplitude of the corresponding potential relief differs from the potential relief of the substrate in the case of single adatoms. We can easily see that the problem of the correlation properties of a soliton lattice in the case of pinning by the substrate is physically analogous to the above problem of linear structures. The elastic moduli of a soliton lattice K_1 and K_2 governing the transition temperature T_p in the case when the soliton collisions are ignored is given by¹⁷:

$$K_1 = A (\varepsilon_0/l) e^{-1/l_0} + B (\lambda a^3/l^3), \quad K_2 = \varepsilon_0/l. \quad (18)$$

Here l is the soliton lattice period; $l_0 \sim a(\lambda/w_0)^{1/2}$, where λ is the elastic modulus of an adatom lattice, is the soliton width; w_0 is the substrate potential; $\varepsilon_0 \sim a(\lambda/w_0)^{1/2}$ is the energy density per unit length of a soliton; $A \sim 1$ and B are of the order of the ratios of the elastic constants of the filament substrate. The temperature T_p is described by

$$T_p = \frac{2}{\pi} \frac{a^4}{l^2} \left\{ A \frac{\varepsilon_0^2 l^2}{a^4} \exp \left(-\frac{l}{l_0} \right) + B \frac{\lambda \varepsilon_0}{a} \right\}^{1/2}. \quad (19)$$

At finite temperatures the collisions of solitons begin to play an important role in their thermodynamics.¹⁶ We shall estimate a contribution to the temperature T_p . According to Ref. 14, such collisions make a contribution ΔK_1 only to the elastic modulus K_1 :

$$\Delta K_1 = \pi^2 T^2 / \varepsilon_0 l^3. \quad (20)$$

It follows from Eqs. (18) and (20) that at $T = T_p$, we have

$$\Delta K_1 = 2\pi K_1 (a/l)^4 \ll K_1. \quad (21)$$

Our analysis shows that soliton collisions make no significant contribution to the value of T_p . It is clear that a similar conclusion can also be drawn for large-period adatom sublattices.

The approach developed above makes it possible to investigate also the case when both adatom lattice periods are large compared with the substrate periods. This corresponds to a problem of a two-dimensional plasma with two kinds of charges, exactly as in the problem of melting of a two-dimensional crystal.⁸ A detailed investigation of this topic is outside the scope of the present paper but we may point out that

once again a transition is possible to a phase with power-law decay of correlations.

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