Exact solutions in the two-dimensional wetting problem

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Wetting transitions in two-dimensional lattice systems are considered. To obtain exact solutions the transfer-matrix method is used. Attention is focused on transitions at proper line defects (domain walls). The effective thickness of the wall increases as the transition point is approached, this being connected with growth of the intermediate (wetting) phase inside the domain wall. Depending on the types of transformations in the system of domain walls, the phase transitions can be first-order, second-order, or infinite-order. The general analysis makes it possible to apply the results obtained to the description of the behavior of the domain walls in the ANNNI model; in particular, the problem of the coexistence of a wetting transition and pinning of domain walls at an external boundary is considered.

1. INTRODUCTION

The wetting transition at the interface of two phases (solid and vapor) is usually attributed to the formation of an intermediate (liquid) phase of macroscopic thickness. Wetting problems have been investigated for a long time, and a recent review of the topic is given in Ref. 1. In recent years serious attention has been paid to systems in which a solid substrate is subjected to partial or complete wetting by a system of adsorbed layers.[2]

In the present paper we consider phase transitions of the wetting type in two-dimensional lattice systems with discrete degeneracy. Among these, transitions in a "domain-wall plus boundary system" (see the pioneering paper Ref. 3), and also the transitions that arise at proper line defects (domain walls) of an adsorbate commensurate with the substrate are of great interest. It is customary to illustrate the latter with the example of an anisotropic commensurate $(p \times 1)$ monolayer with $p \geqslant 3$ (Ref. 4). Here p and 1 denote the periodicity of the structure of the monolayer with respect to the elementary periods of the substrate. The monolayer under consideration can be modeled as a lattice gas with anisotropic interaction; an essential point is that along one of the directions the particles attract each other.

Figure 1a shows possible vacuum states (A, B, and C) of a monolayer with a (3×1) structure, separated by walls of the same type (type b). The different vacua differ by a translation through one period of the substrate, and their energies are assumed to be equal. When the temperature is nonzero the wall migrates along the surface through fluctuational formation of kinks. The probability of such a fluctuation is determined by the Boltzmann factor $\exp(-E_a/T)$, where E_a is the energy loss due to the formation of the kink. One can also cross spatially from vacuum A to vacuum B via the formation of an intermediate region with vacuum state C. For this it is necessary to introduce into the analysis a new type of domain wall (type a). Figure 1b shows the transformation $b \rightarrow a + a$, in which the walls a are arranged in neighboring positions. Fluctuations can either carry walls of type a apart, or collapse them again into state b. Unlike simple wall migration, the transformation of walls of one type into another causes the energy to increase linearly as a function of the length of the "unfavorable" walls. It is convenient to introduce the energies of individual walls (ε) per lattice con-

stant. It is obvious that if the difference $\Delta\varepsilon$ in the energies of walls of different types satisfies $\Delta\varepsilon \gg T$, the unfavorable walls appear extremely rarely in the structure of the monolayer, and are manifested only as point defects. But if their energies become close ($\Delta\varepsilon \lesssim T$), the entropy mechanism comes into play. Thus, in the example given above, for a sufficiently small difference $\Delta\varepsilon = 2\varepsilon_a - \varepsilon_b > 0$ there exists a temperature at which the fluctuation contribution to the free energy from two walls of type a compensates their energy disadvantage $\Delta\varepsilon$. As a result, the transition "$b \rightarrow$ free state of walls a" occurs. It should be noted that we are considering a situation in which the line defect (which has arisen, e.g., as a result of the preparation of the monolayer) is topologically nonremovable. The free energy (per unit length) associated with the defect is $f \gg T$. Therefore, all the possible transformations of the walls (and the formation of new walls) leading to configurations other than the competing b and $a + a$ configurations are unimportant.

The phase that arises between walls of type a plays the role of the third phase (liquid) that appears on the solid-gas boundary in the usual wetting transition, and therefore phase transitions involving the decomposition of domain walls in systems with discrete degeneracy are related to wetting phase transitions.

As mentioned above, the phase transitions under consideration can be described in terms of the anisotropic lattice-gas model, one of the variants of which corresponds to the Hamiltonian
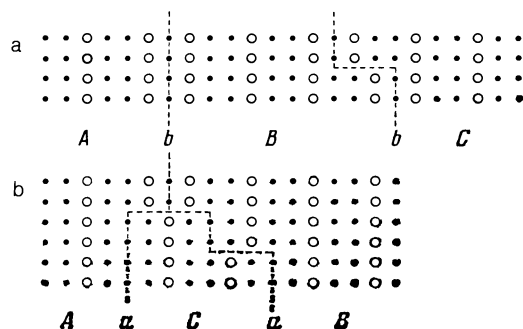

FIG. 1. Possible structures of an anisotropic monolayer with domain walls (O are particles, ● are empty sites): a) two walls of type b (the right wall has a kink); b) transformation of a wall of type b into two walls of type a.

$$H = \frac{1}{2} \sum_{\mathbf{r},\mathbf{r}'} V(\mathbf{r},\mathbf{r}') n_\mathbf{r} n_{\mathbf{r}'} - \mu \sum_\mathbf{r} n_\mathbf{r} \quad (n=0 \text{ or } 1). \quad (1)$$

In this model the particles attract each other along one of the directions [$V(\mathbf{r}, \mathbf{r} + \mathbf{a}_y) < 0$], and repel each other along the other direction [$V(\mathbf{r}, \mathbf{r} + m\mathbf{a}_x) > 0$]. With regard to the repulsion, it is important only that it does not fall off too slowly with distance. In the ground state such a lattice gas forms linear chains, the equilibrium spacings between which are regulated by the chemical potential μ. Their exists a region of values of μ for which the $p \times 1$ structure has the lowest energy. Inside this region, at a certain critical μ, one type of line defect becomes energetically unfavorable and is replaced by another type.

In the analysis of a lattice gas possessing a commensurate 3×1 or 2×1 structure it is convenient to use the ANNNI (axial next-nearest-neighbor Ising) model, which is a particular case of the more general model (1) and is described by the spin Hamiltonian

$$H = -J_0 \sum_\mathbf{r} S_\mathbf{r} S_{\mathbf{r}+\mathbf{a}_y} + J_1 \sum_\mathbf{r} S_\mathbf{r} S_{\mathbf{r}+\mathbf{a}_x} + J_2 \sum_\mathbf{r} S_\mathbf{r} S_{\mathbf{r}+2\mathbf{a}_x} - h \sum_\mathbf{r} S_\mathbf{r}.$$

$$(2)$$

The spin variables S take the value $+1$ or -1. The correspondence between the models (1) and (2) is ensured by the equality $n = \frac{1}{2}(1 - S)$.

A model in which the 3×1 structure arises was proposed in Ref. 5 to describe experiments on the adsorption of oxygen on a Pd(110) face [O/Pd(110)]. The phase diagram in the variables J_1, J_2 for $T = 0$ and fixed h is shown in Fig. 2. The 3×1, 2×1, and 1×1 structures are indicated by $\langle + + - \rangle$, $\langle + - \rangle$, and $\langle + \rangle$, respectively. The walls of type b shown in Fig. 1 correspond to a nucleus of the phase $\langle + - \rangle$ superposed on an ordered $\langle + + - \rangle$ structure, while the walls of type a correspond to a nucleus of the ferromagnetic phase $\langle + \rangle$. Near the line of coexistence of the phases $\langle + + - \rangle$ and $\langle + - \rangle$ the b walls have low energy, being "light," and the a walls are energetically unfavorable ("heavy" walls). In the vicinity of the $\langle + + - \rangle$-$\langle + \rangle$ coexistence line the roles of the walls are reversed.

For the mathematical description of the wetting transition the transfer-matrix method,[6-10] the random walk method,[4] and numerical modeling[11-13] by the Monte Carlo method have been applied. In problems of two-dimensional wetting the method of Müller-Hartmann and Zittartz[19] is extremely popular,[3,14-18] and is equivalent to an analysis of the one-dimensional SOS (solid-on-solid) model. The latter method has been applied mainly to the description of the transition from a bound state of a domain wall near a boundary to a free state. It can be interpreted easily using the example of an ordinary ferromagnetic Ising model in which one of the two vacuum states is surface-active. It should be noted that if transformations are possible near the boundary, i.e., the competition of different types of wall is important, the method of Müller-Hartmann and Zittartz becomes ineffective. In Sec. 7 we give the solution of such a model in the framework of a transfer-matrix method that is unique to the present paper.

In Sec. 2 we present basic information on the transfer-matrix method and demonstrate its application to the problem of the competition of one heavy wall and two light walls.[1] In Secs. 3 and 4 we show in the framework of the lattice model that the transformation of a heavy wall into N light walls ($N \geqslant 3$) is a first-order phase transition. Previously this problem has been considered only with neglect of the discreteness of the possible positions of the walls, in the framework of a continuous random-walk model.[4] In the following section we take into account the effective pair interaction of light walls in the decay $1 \rightleftarrows 3$, which leads to the possibility of the formation of a new (intermediate) type of wall, in the form of a bound complex of two light walls. On the phase diagram an additional line of second-order transitions appears. In the short sixth section we use the results obtained to give a concrete picture of the wetting transitions for the ANNNI model. The seventh section, devoted to an analysis of a system in which the decay of a domain wall competes with its localization the boundary of the sample, ends the paper.

The ANNNI model, which is widely used in the present paper to illustrate different wetting transitions in two-dimensional lattice systems, is of special interest, since it is applicable to the description of such physical systems as oxygen on palladium (already mentioned),[5] and also hydrogen on iron [H/Fe(110)] (Ref. 12).

2. THE TRANSFER-MATRIX FORMALISM; THE 1⇌2 WETTING TRANSITION

The transfer matrix t (from the row with coordinate y to the row with coordinate $y + a_y$) corresponding to the Hamiltonian (1) or (2) has the form

$$t = t_1 t_2, \quad (3)$$

where t_1 is a diagonal matrix acting on the space of all possible states of the row:

$$t_1 = \exp(-H_x/T), \quad (4)$$

and t_2 is an operator that includes the diagonal matrix element and also all possible changes of configuration of the state of one row upon passage to another. The operator H_x contains variables pertaining to only one row.

Thus, in the ANNNI model,

$$t_1 = \exp\left(-\frac{1}{T} \sum_n (J_1 \sigma_n^z \sigma_{n+1}^z + J_2 \sigma_n^z \sigma_{n+2}^z - h \sigma_n^z)\right), \quad (5)$$
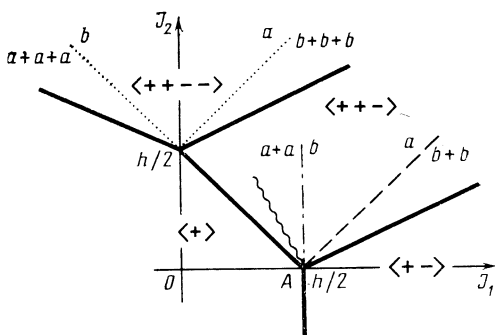
and

FIG. 2. Phase diagram of the ANNNI model in a magnetic field at $T = 0$. For the ferromagnetic phase $\langle + + - \rangle$ the dashed line shows the line of coexistence of walls a and $b + b$, and the dashed-dotted line shows the line of coexistence of walls b and $a + a$. Also shown are the coexistence lines of one heavy and three light walls in the antiferromagnetic phase $\langle + + - - \rangle$.

$$t_2 = \left(2 \operatorname{sh} \frac{2J_0}{T}\right)^{N/2} \exp\left(J_0^* \sum_n \sigma_n^x\right), \qquad (6)$$

where N is the number of sites in a row of the lattice, $J_0^* = \frac{1}{2}\ln\tanh(J_0/T)$, and $\sigma^{x,z}$ are Pauli matrices.

The transfer-matrix formalism and knowledge of the ground state and first excited state of the operator t of lowered dimensionality make it possible to find the following physical quantities[20]: the free energy per unit length,

$$f = \lambda_0 = -T \ln \langle \psi_0 | t | \psi_0 \rangle, \qquad (7)$$

the average spacing between walls

$$\bar{l} = \langle \psi_0 | l | \psi_0 \rangle, \qquad (8)$$

the transverse correlation length

$$\xi_\perp^2 = \langle \psi_0 | (l - \bar{l})^2 | \psi_0 \rangle \qquad (9)$$

and the longitudinal correlation length

$$\xi_\parallel = (\lambda_1 - \lambda_0)^{-1}. \qquad (10)$$

The physical meaning of the latter is related to the longitudinal size of a wetting drop.

In Eqs. (7)–(10) ψ_0 is the normalized wavefunction of the ground state of the operator t, l is the spacing between particles, and λ_1 is the "energy" of the first excited state of the operator t and is defined in analogy with (7).

In the present paper we consider systems composed of one or several domain walls (an example of such systems— the line defects b and $a + a$, is illustrated in Fig. 1). The addition of new domain walls to those already existing involves a large loss in energy. The contribution to the matrix t from all those configurations which differ from the competing ones can be neglected. Since in the given formulation the problem reduces to that of the behavior of one or several walls (or particles, in the language of the transfer-matrix method), the matrix t can be taken into account exactly, by going beyond the framework of the low-temperature Hamiltonian approximation (compare with Ref. 10).

As the first example of the construction of the matrix t we shall consider the ANNNI model with those values of the parameters J_1, J_2, and H that lead to the formation at $T = 0$ of the $\langle + + - \rangle$ structure (3×1 structure, in the language of the lattice-gas model). We shall regard the spin sequence $- + + + -$ (the analog in Fig. 1 is the wall a) as a topologically nonremovable defect. It is obvious that this wall can decay into two walls of the type $- + -$ (walls b in Fig. 1). Comparing the energies of these competing states, we find the $a \rightleftarrows b + b$ coexistence line (see Fig. 2). Our analysis is valid in the vicinity of this line, but not too close to the point where the three phases $\langle + + - \rangle$, $\langle + \rangle$, and $\langle + - \rangle$ coexist (point A in Fig. 2).

The transfer matrix contains diagonal matrix elements corresponding to an unchanged state of the walls upon passage from row to row. The main nondiagonal elements are shown in Fig. 3. They describe kinks induced by two-spin flips; the others are associated with the mutual transformation of walls. The probability of a single flip is proportional to $\gamma = \exp(-2J_0/T)$.

It should be noted that the period of the magnetic structure is three times greater than the period of the original lattice, and all elementary hops of walls occur through ex-
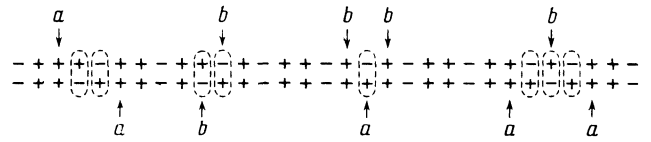

FIG. 3. Spin flips inducing elementary kinks in walls (left) and inducing mutual transformations of kinks (right).

actly one magnetic period. It is convenient to map the sublattices over which the migration of the walls occurs onto a fictitious so-called f-lattice. All hops of particles on this lattice are to neighboring sites, and one of the configurations of the walls b (that shown in Fig. 3) corresponds to an arrangement of particles at one site of the f-lattice. Introducing the wavefunction amplitudes (f_a and f_b) corresponding to different positions of the walls, we obtain the following system of equations:

$$tf_a(n) = (f_a(n) + \gamma^2(f_a(n-1) + f_a(n+1)) + \gamma f_b(n,n))e^{-\varepsilon_a/T}, \qquad (11)$$

$$tf_b(n,m) = f_b(n,m) + \gamma^2(f_b(n-1,m) + f_b(n+1,m) + f_b(n,m-1) + f_b(n,m+1)), \quad m > n. \qquad (12)$$

One further equation corresponds to the arrangement of the particles of b at one site of the f-lattice:

$$tf_b(n,n) = f_b(n,n) + \gamma f_a(n) + \gamma^2(f_b(n-1,n) + f_b(n,n+1)). \qquad (13)$$

In Eq. (11) we have introduced the energy of an a particle, measured from the conventional zero—the energy of two b walls:

$$\varepsilon_a = 4J_1 - 4J_2 - 2h. \qquad (14)$$

We need to know the translationally invariant solutions of the system (11)–(13). Then, if the smallest eigenvalue λ_0 is separated by a gap from the other eigenvalues λ_i corresponding to these solutions, the state of the walls is a bound state. As the gap goes to zero the walls cease to be bound, and the average spacing between them diverges (compare with the result of Sec. 3 for the decay $1 \rightleftarrows 3$). For the translationally invariant solutions the system (11)–(13) should be rewritten in the form

$$tf_a = (f_a(1 + 2\gamma^2) + \gamma f_b(0))e^{-\varepsilon_a/T}, \qquad (11')$$

$$tf_b(m') = f_b(m') + 2\gamma^2(f_b(m'-1) + f_b(m'+1)), \quad m' > 0, \qquad (12')$$

$$tf_b(0) = f_b(0) + \gamma f_a + 2\gamma^2 f_b(1), \qquad (13')$$

where $m' = m - n$.

From Eq. (12') we can immediately find the transfer-matrix eigenvalue t_∞ corresponding to the free state of the particles [$f_b(m) \rightarrow$ const as $m \rightarrow \infty$]:

$$t_\infty = 1 + 4\gamma^2. \qquad (15)$$

From the form of Eqs. (11')–(13') it follows that a solution describing a bound state can be found in the form

$$f_b(n) = f_b e^{-qn}. \qquad (16)$$

Substitution of (16) into Eq. (12') makes it possible to express the eigenvalue t in terms of the parameter q:

$$t = 1 + 4\gamma^2 \operatorname{ch} q. \qquad (17)$$

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The remaining equations (11') and (13), which are linear homogeneous equations in f_a and f_b, give the compatibility condition determining the parameter q:

$$\det\left\|\begin{array}{cc} (1+4\gamma^2\,\mathrm{ch}\,q)\exp(\varepsilon_a/T)-(1+2\gamma^2) & -\gamma \\ -\gamma & 2\gamma^2 e^q \end{array}\right\| = 0. \quad (18)$$

The vanishing of the parameter q determines the temperature shift of the transition line shown in Fig. 3:

$$e^{\varepsilon_a/T}=(1+2\gamma^2)/2(1+4\gamma^2). \quad (19)$$

It is obvious that for $\varepsilon_a < 0$ there exists a wetting transition temperature T_W below which the walls form a bound state.

Solving Eq. (18) for small q, we find that the characteristic lengths defined by Eqs. (8)–(10) diverge as follows as T_W is approached:

$$\bar{l}\sim\xi_\perp\sim q^{-1}\sim(T_W-T)^{-1},\quad \xi_\parallel\sim(t-t_\infty)^{-1}\sim q^{-2}\sim(T_W-T)^{-2}. \quad (20)$$

In the solution demonstrated above it was assumed that the probability of formation of a kink at a wall is small, i.e., $\gamma \ll 1$, or

$$J_0 \gg T_W. \quad (21)$$

The inequality (21) may be substantially weakened, since the problem of the competition of the a and $b+b$ walls can be solved exactly even when kinks of arbitrary size are taken into account. The method of derivation of the equations for the amplitudes f_a and $f_b(n)$, which are a generalization of the system (11')–(13'), is straightforward but cumbersome. We give the result:

$$te^{\varepsilon_a/T}f_a=\left(1+\frac{2\gamma^2}{1-\gamma^2}\right)f_a+\gamma\sum_{p=0}^{\infty}f_b(p)\gamma^{2p}\left(p+\frac{1+\gamma^2}{1-\gamma^2}\right), \quad (22)$$

$$tf_b(n)=\sum_{p=0}^{\infty}f_b(p)\frac{2\gamma^6}{1-\gamma^4}\gamma^{2n+2p}$$

$$+\sum_{p=0}^{\infty}f_b(p)\gamma^{2|p-n|}\left(|p-n|+\frac{1+\gamma^4}{1-\gamma^4}\right)$$

$$+\frac{2\gamma^{2n+1}}{1-\gamma^2}f_a \quad (n\geqslant 0). \quad (23)$$

The simple substitution (16), which gives the solution of Eqs. (11')–(13'), now becomes insufficient—the right-hand side of Eqs. (23) has the following structure:

$$t_z z^n+\gamma_1^n[nA(z)+B(z)], \quad (24)$$

where $\gamma_1 = \gamma^2 = e^{-\alpha}$, $z = e^{-q}$,

$$t_z=\left(\frac{z/\gamma_1}{1-z/\gamma_1}-\frac{z\gamma_1}{1-z\gamma_1}\right)^2=\frac{\mathrm{sh}^2\,\alpha}{(\mathrm{ch}\,q-\mathrm{ch}\,\alpha)^2}, \quad (25)$$

$A(z)=(1-z/\gamma)$, and the expression for $B(z)$ is unwieldy and of no fundamental importance for the subsequent derivations. The form of the expression (24) makes it possible to seek the solution of the system (22), (23) in the form

$$f_b(n)=a_+e^{-q_+n}+a_-e^{-q_-n},$$

where $0\leqslant q_+ < \alpha < q_-$ are the two roots of the equation

$$t_z=t. \quad (26)$$

Then the system of equations (23) turns out to be fully compatible if for any n the equalities

$$n(a_+A(z_+)+a_-A(z_-))+(a_+B(z_+)+a_-B(z_-))=0$$

are fulfilled, this being equivalent to the vanishing of the determinant

$$\det\left\|\begin{array}{cc} A(z_+) & B(z_+) \\ A(z_-) & B(z_-) \end{array}\right\| = 0. \quad (27)$$

The equations (26) and (27) determine the dependence of q_+, q_-, and t on the parameters T and ε_a. The vanishing of q_+ fixes the position of the wetting line $T_W(\varepsilon_a)$.

At the end of this section we shall discuss one further wetting transition, arising as a result of the competition of the b and $a + a$ walls. The position of their coexistence line at $T = 0$ is shown in Fig. 2. Without restricting ourselves to consideration of only the smallest kinks, for the amplitudes $g_a(n)$ and g_b we can obtain equations analogous to the system (22), (23):

$$te^{\varepsilon_b/T}g_b=\left(1+\frac{2\gamma^2}{1-\gamma^2}\right)g_b+\gamma\sum_{p=1}^{\infty}\left(p+\frac{1+\gamma^2}{1-\gamma^2}\right)\gamma^{2p-2}g_a(p), \quad (28)$$

$$tg_a(n)=\sum_{p=1}^{\infty}\left\{2\left(\frac{1}{1-\gamma^2}-\frac{1}{1-\gamma^4}\right)\gamma^{2(n+p-2)}\right.$$

$$+\left.\left(|n-p|+\frac{1+\gamma^4}{1-\gamma^4}\right)\gamma^{2|n-p|}\right\}g_a(p)$$

$$+2\gamma^{2n-1}\left(n-\frac{\gamma^2}{1-\gamma^2}\right)g_b \quad (n\geqslant 1), \quad (29)$$

where $\varepsilon_b = -4J_1 + 2h$.

The substitution (16), as in the case of Eqs. (23), again leads to the structure (24), with the same t_z but different functions $A(z)$ and $B(z)$. The scheme of the exact solution is given above. It should be noted that the critical indices in this case, as in the preceding case, are determined by formulas of the type (20).

In Sec. 7 we shall need the equation describing $g_a(n)$ in the case when the transformation $a + a \to b$ can be neglected. In Fig. 2 this is the region to the left of the dashed-dotted line ($\varepsilon_a \gg T$). The required equations are a consequence of Eqs. (29):

$$tg_a(n)=\sum_{p=1}^{\infty}\left\{2\left(\frac{1}{1-\gamma_4}-\frac{1}{1-\gamma_1^2}\right)\gamma_4^{n+p-2}\right.$$

$$+\left.\left(|n-p|+\frac{1+\gamma_1^2}{1-\gamma_1^2}\right)\gamma_1^{|n-p|}\right\}g_a(p)$$

$$(n\geqslant 1). \quad (30)$$

In the usual ANNNI model, $\gamma_4 = \gamma_1 = \gamma^2$. For reasons that will be clear in the following, we have introduced the independent notation γ_4 for the Boltzmann factor per unit length of the coalesced kink of two walls. Such kinks, of the minimum and doubled length, are depicted in Fig. 4.
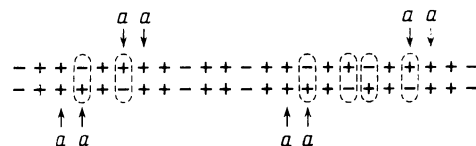

FIG. 4. Parallel "hops" of two walls of type a.

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3. DECAY OF A DOMAIN WALL INTO THREE

We shall consider the general problem of the wetting transition in a system of three equivalent light domain walls, which, when they come together, can be transformed into one heavy wall, and vice versa. Let γ_1 be the Boltzmann factor (statistical weight) corresponding to a kink in a light wall, let γ_2 be that corresponding to a kink in a heavy wall, and let γ_3 be that corresponding to the point of the $1 \rightleftarrows 3$ transformation. The values of γ_i for specific phase transitions in the ANNNI model are given in Sec. 6.

$$tf(n, m) = f(n, m) + \gamma_1[f(n-1, m) + f(n+1, m) + f(n+1, m-1) + f(n-1, m+1) + f(n, m-1) + f(n, m+1)], \quad (31)$$
$$n > 0, \quad m > 0, \quad nm \neq 1,$$

$$tf(1, 1) = f(1, 1) + \gamma_1[f(1, 2) + f(2, 1)] + \gamma_3 g, \quad (32)$$

$$teg = (1 + 2\gamma_2)g + \gamma_3 f(1, 1), \quad (33)$$

where the amplitudes $f(n, m)$ (for the case of three light walls) and g (for a heavy wall) are already taken in translationally invariant form, and

$$\varepsilon = \exp\left(\frac{\varepsilon_g - 3\varepsilon_f}{T}\right).$$

The distances between the light walls (n and m) are assumed to be measured in such a way that their closest approach corresponds to $n = 1$ or $m = 1$, so that in (31) we must set

$$f(n, 0) = f(0, m) = 0. \quad (34)$$

Substitution of (33) into (32) leads to the equation

$$tf(1,1) = (1+U)f(1, 1) + \gamma_1[f(1, 2) + f(2, 1)], \quad (35)$$
$$U = \gamma_3^2/(\varepsilon t - 1 - 2\gamma_2),$$

which can be combined with (31) into a single equation

$$(t - 1 - 6\gamma_1)f(n, m) + \gamma_1\hat{\Delta}_L f$$
$$= U\delta_{n1}\delta_{m1}f(n, m), \quad (36)$$

which is valid for n, $m \geqslant 1$ with the boundary conditions (34). If we regard n and m as the coordinates of a point on a triangular lattice (Fig. 5), the operator $\hat{\Delta}_L$ will be the lattice Laplacian. By completing the right-hand side of (36) in an antisymmetric manner, we can extend this equation to arbitrary integer values of n and m:

$$(t - 1 - 6\gamma_1)f(n, m) + \gamma_1\hat{\Delta}_L f$$
$$= U[\delta_{n, 1}\delta_{m, 1} - \delta_{n, 2}\delta_{m, -1} + \delta_{n, 1}\delta_{m, -2}$$
$$- \delta_{n, -1}\delta_{m, -1} + \delta_{n, -2}\delta_{m, 1} - \delta_{n, -1}\delta_{m, 2}]f(1, 1); \quad (37)$$
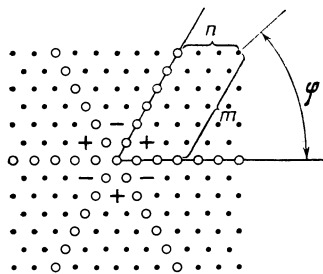

FIG. 5. The sector with positive n and m is physical. The sites at which f vanishes are marked by O. The sources are indicated by plus and minus symbols.

here the boundary conditions (34) will be fulfilled automatically (this follows from symmetry considerations).

The solution of (37) can be found in the form of a linear combination of plane waves:

$$f(n, m) = \int_{-\pi}^{\pi}\int_{-\pi}^{\pi} \frac{dk_1\, dk_2}{(2\pi)^2} \exp i(k_1 n + k_2 m) f_k. \quad (38)$$

Substitution of (38) into (37) leads to

$$(t - t_k)f_k = -2iUS_k f(1, 1), \quad (39)$$

where

$$t_k = 1 + 2\gamma_1[\cos k_1 + \cos k_2 + \cos(k_1 - k_2)], \quad (40)$$

and

$$S_k = \sin(k_1 + k_2) + \sin(k_1 - 2k_2) + \sin(-2k_1 + k_2)$$
$$= -4\sin\frac{k_1 + k_2}{2}\sin\left(\frac{k_1}{2} - k_2\right)\sin\left(k_1 - \frac{k_2}{2}\right).$$

The equations (38) and (39) are mutually consistent only if the condition

$$\frac{2}{3}\int \frac{d^2k}{(2\pi)^2}\frac{US_k^2}{t - t_k} = 1 \quad (41)$$

is fulfilled; this condition is essentially the equation of state specifying the dependence $t(\varepsilon)$ implicitly.

Light walls that have moved apart to infinite distances correspond to the eigenvalue $t_c = 1 + 6\gamma_1$. The equation (41) has a solution $t > t_c$ only for

$$\varepsilon < \varepsilon_c = \frac{1}{1 + 6\gamma_1}\left\{1 + 2\gamma_2\right.$$
$$\left. + \frac{\gamma_3^2}{3\gamma_1}\int\frac{d^2k}{(2\pi)^2}\frac{S_k^2}{3 - \cos k_1 - \cos k_2 - \cos(k_1 - k_2)}\right\}.$$

This inequality determines the region of stability of a heavy domain wall, and, in the terminology of the wetting transition, corresponds to the absence of wetting.

In the neighborhood of the phase-transition point ($\tau \equiv t - t_c \ll \gamma_1$) the equation of state (41) can be rewritten in the form

$$\varepsilon t = \varepsilon_c t_c - a\tau + \frac{b}{2}\tau^2 - O\left(\tau^3 \ln\frac{1}{\tau}\right),$$

and therefore the phase transition occurs as a first-order transition:

$$t - t_c \begin{cases} = 0, & \varepsilon > \varepsilon_c \\ \sim (\varepsilon_c - \varepsilon), & \varepsilon < \varepsilon_c \end{cases},$$

and the leading singular correction to the free energy is proportional to $(\Delta\varepsilon)^3\ln(1/\Delta\varepsilon)$.

We have found the function $f(n, m)$ in the form of a linear combination of "waves" created by six sources, which in Fig. 5 are denoted by plus and minus symbols. It is not difficult to establish (e.g., by going over to the continuous approximation) that for one source $f(n, m)$ behaves as $K_0(qr)$, i.e.,

$$f \sim \begin{cases} \ln\dfrac{1}{rq}, & 1 \ll r \ll q^{-1} \\ \dfrac{1}{r^{1/2}}\exp(-qr), & r \gg q^{-1} \end{cases}$$

where $r^2 = n^2 + nm + m^2$ and $t - t_c = 3\gamma_1 q^2/2$. For the six sources of alternating signs depicted in Fig. 5, $f(n, m)$ falls off as $r^{-3} \sin 3\varphi$ ($1 \ll r \ll q^{-1}$), so that the transverse correlation length (the average spacing between the outer light walls) remains finite as $t \to t_c + 0$.

4. DECAY OF A DOMAIN WALL INTO SEVERAL DOMAIN WALLS (THE GENERAL CASE)

The analysis performed in the preceding section can be generalized to the case of an arbitrary number $N \geqslant 2$ of equivalent light walls, which can be transformed into one heavy wall, and vice versa. In the general case the translationally invariant function $f(n_1, ..., n_{N-1})$ should be regarded as specified at the sites of an $(N-1)$-dimensional Bravais lattice generated by N unit vectors $\mathbf{e}_\alpha$ ($\alpha = 1,...,N; \Sigma_\alpha \mathbf{e}_\alpha = 0$) oriented at equal angles to each other:

$$\mathbf{e}_\alpha \mathbf{e}_\beta = \begin{cases} 1, & \alpha = \beta \\ c < 0, & \alpha \neq \beta \end{cases} .$$

For example, in the case $N = 4$ this will be a bcc lattice in three-dimensional space.

The boundary conditions, analogous to the conditions (34), require the vanishing of f on the $(N-2)$-dimensional planes bounding the sector $n_i > 0$ ($i = 1,..., N-1$). The total number of these planes and also of the planes equivalent to them by symmetry is equal to $N(N-1)/2$ (each of them is defined by a pair of different vectors $\mathbf{e}_\alpha$ ($\alpha = 1, ..., N$), to which the plane is perpendicular). These planes passing through the coordinate origin divide the space into $N!$ equivalent sectors, in each of which a source should be placed. Correct alternation of the signs of the sources makes vanish automatically on $N(N-1)/2$ ($N-2$)-dimensional planes. It follows from this that f for $1 \ll r \ll q^{-1}$ ($q^2 \sim \tau$) falls off like the $[N(N-1)/2]$th spherical harmonic, i.e.,

$$f \sim r^{-[N-3+N(N-1)/2]} = r^{-(N+3)(N-2)/2}. \tag{42}$$

The form of the expression (42) indicates that the average spacing between walls

$$\bar{l} \sim \int d^{N-1} r \, r f^2(r)$$

remains finite right to the transition point for $N^2 > 6$.

The singular term in the equation of state is proportional to

$$\int_{k_{\min}} \frac{d^{N-1}\mathbf{k}}{k^2} \, k^{N(N-1)} \sim \tau^{(N^2-3)/2}$$

(with logarithmic corrections when N^2 is odd), so that the phase transition under consideration is a first-order transition for $N^2 \geqslant 5$.

The results of this section agree with those obtained by Huse and Fisher[4] in the continuous approximation by means of a random-walk analysis.

5. ALLOWANCE FOR THE EFFECTIVE PAIR INTERACTION OF LIGHT WALLS

The technique that we have used makes it possible to elaborate further the problem under consideration. We shall increase the number of nondiagonal transfer-matrix elements included in the analysis, introducing γ_4 (the statistical weight of a kink on a complex of two light walls at the

minimum separation) and γ_5 (the statistical weight of a kink on an analogous complex of N light walls—Fig. 6). The quantity γ_4 determines the effective contact interaction of light walls, while the quantity γ_5 determines the stability of the N-wall complex. Allowance for γ_5 is trivial and reduces to a change of the quantity U that appear in the equation of the form (35):

$$U = \gamma_3^2 / (\varepsilon t - 1 - 2\gamma_2) + 2\gamma_5.$$

However, allowance for a nonzero matrix element γ_4 is a much more complicated problem, since it requires the use of boundary conditions that do not reduce to the simple form (34).

We shall denote the amplitude corresponding to the displacement of N light walls on the sites n_1, $n_2,...,n_N$ by $f_{n_1 n_2 ... n_N}$. It is obvious that the equations for f "in the bulk" (i.e., for $n_{j+1} \geqslant n_j + 2, j = 1,...,N-1$)

$$(t-1) f_{n_1...n_N} = \gamma_1 \sum_{\delta=\pm 1} \sum_{j=1}^{N} f_{n_1...n_j+\delta...n_N}$$

are satisfied as before by an arbitrary plane wave

$$f_{n_1...n_N} = \exp\left(i \sum_{j=1}^{N} k_j n_j \right), \tag{43}$$

where, in order that the amplitude f_N be translationally invariant, we must impose the restriction

$$\sum_{j=1}^{N} k_j = 0.$$

The equation for f with $n_{j+1} = n_j + 1$ will have the form

$$(t-1) f_{...n, n+1...} = ... + \gamma_1 f_{...n-1, n+1...}$$
$$+ \gamma_4 [f_{...n-1, n...} + f_{...n+1, n+2...}] + \gamma_1 f_{...n, n+2...} + ..., \tag{44}$$

where we have omitted the terms corresponding to a shift of the remaining arguments. In order that Eq. (44) hold, it turns out to be necessary to add to the wavefunction (43) the same wavefunction with interchanged values of the momenta k_j and k_{j+1}, i.e., to use the Bethe substitution:

$$f = \exp i [... + k_j n_j + k_{j+1} n_{j+1} + ... - \theta(k_j, k_{j+1})]$$
$$- \exp i [... + k_{j+1} n_j + k_j n_{j+1} + ... + \theta(k_j, k_{j+1})],$$

where

$$\text{tg}\, \theta(k, k') = \frac{\Delta \sin \frac{1}{2}(k-k') \cos (k+k')}{\cos \frac{1}{2}(k+k') - \Delta \cos (k+k') \cos \frac{1}{2}(k-k')},$$

$$\Delta = \frac{\gamma_4}{\gamma_1}. \tag{45}$$

γ_4 γ_5

FIG. 6.

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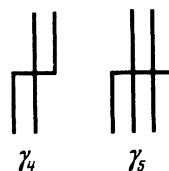
In order that all the $N-1$ boundary conditions of the form (44) be satisfied, we must take a linear combination of $N!$ plane waves with all possible permutations of the momenta k_j. In the case $N = 3$ such a linear combination can be written out (in the notation introduced earlier in Sec. 3, with two independent arguments $n = n_2 - n_1$, $m = n_3 - n_2$) as

$$\psi_k(n, m) = \frac{1}{6^{1/2}}\{\exp i[k_1 n + k_2 m - \theta_1 + \theta_2 + \theta_3]$$

$$-\exp i[k_1 n + (k_1 - k_2)m - \theta_1 - \theta_2 + \theta_3]$$

$$+\exp i[-k_2 n + (k_1 - k_2)m + \theta_1 - \theta_2 + \theta_3]$$

$$-\exp i[-k_2 n - k_1 m + \theta_1 - \theta_2 - \theta_3]$$

$$+\exp i[(-k_1 + k_2)n - k_1 m + \theta_1 + \theta_2 - \theta_3]$$

$$-\exp i[(-k_1 + k_2)n + k_2 m - \theta_1 + \theta_2 - \theta_3]\}, \quad (46)$$

where $\theta_1 = \theta(-k_1, k_2)$, $\theta_2 = \theta(k_2, k_1 - k_2)$, $\theta_3 = \theta(k_1 - k_2, -k_1)$.

Another way of satisfying the boundary conditions (45) is to add imaginary parts to the wave numbers:

$$f_{\ldots n_j n_{j+1} \ldots} = \exp[\ldots + (ip + Q)n_j + (ip - Q)n_{j+1} + \ldots],$$

where $Q > 0$ is connected with p by the relation

$$e^Q \cos p = \Delta \cos 2p,$$

and p belongs to one of the sectors

$$|p| < \frac{1}{2}\arccos\frac{1 + (1 + 8\Delta^2)^{1/2}}{4\Delta^2}, \quad (47a)$$

and

$$\frac{\pi}{2} < |p| < \frac{\pi}{2} + \frac{1}{2}\arccos\frac{2}{1 + (1 + 8\Delta^2)^{1/2}}. \quad (47b)$$

The sector (47a) exists only for $\Delta > 1$.

Thus, for $N = 3$ it turns out to be also necessary to include in the analysis the wavefunction

$$\psi_p(n, m) = A_p\{\exp[(-ip - Q)n + (ip - Q)m]$$
$$-\exp[2ipn + (ip - Q)m + 2i\theta(p - iQ, -2p)]$$
$$-\exp[(-ip - Q)n - 2ipm - 2i\theta(p - iQ, -2p)]\}, \quad (48)$$

where A_p is a normalization factor and p belongs to the regions (47).

The wavefunctions (46) correspond to the eigenvalues t_k determined by formula (40), while the wavefunctions (48) correspond to the eigenvalues

$$t_p = 1 + 2\gamma_1(\cos 2p + 2\cos p \, \mathrm{ch}\, Q)$$

$$= 1 + 2\left[(\gamma_1 + \gamma_4)\cos 2p + \frac{\gamma_1^2}{2\gamma_4}\left(1 + \frac{1}{\cos 2p}\right)\right].$$

The complete system of equations for $f(n, m)$ is finally found to consist of Eqs. (31) (for $n, m \geqslant 2$), two boundary conditions for $m = 1$ and $n = 1$:

$$(t - 1)f(n, 1) = \gamma_1[f(n-1, 2) + f(n, 2)]$$

$$+ (\gamma_1 + \gamma_4)[f(n-1, 1) + f(n+1, 1)], \quad n \geqslant 2$$

$$(t - 1)f(1, m) = \gamma_1[f(2, m-1) + f(2, m)]$$

$$+ (\gamma_1 + \gamma_4)[f(1, m-1) + f(1, m+1)],$$
$$m \geqslant 2,$$

and a special equation for the point $(1, 1)$:

$$(t - 1 - U)f(1, 1) = (\gamma_1 + \gamma_4)[f(1, 2) + f(2, 1)].$$

The solution of this system can be sought in the form

$$f(n, m) = 6\int\frac{d^2k}{(2\pi)^2}f_k\psi_k(n, m) + \int\frac{dp}{2\pi}f_p\psi_p(n, m), \quad (49)$$

where the integration over $\mathbf{k}$ should be limited to one of the six equivalent triangular parts of the hexagonal Brillouin zone, and the integration over p should be limited to the regions (47).

The complete system of equations for $f(n, m)$ can then be rewritten in the form of a single equation

$$(t - 1 - 6\gamma_1)f(n, m) = -\gamma_1\hat{\Delta}_L'f + \delta_{n1}\delta_{m1}[Uf(1, 1) - \gamma_4(f(0, 1) + f(1, 0))], \quad (50)$$

where the operator $\hat{\Delta}_L'$ coincides with the lattice Laplacian $\hat{\Delta}_L$ "in the bulk" (but not on the boundary) and has its own eigenfunctions (46) and (48), and the quantities $f(0, 1)$ and $f(1, 0)$ are assumed to be determined in terms of (46), (48), and (49).

Fourier transformation of Eq. (50) leads to

$$(t - t_k)f_k = \psi_k^*(1, 1)F, \quad (t - t_p)f_p = \psi_p^*(1, 1)F, \quad (51)$$
$$F = Uf(1, 1) - \gamma_4 f(0, 1) - \gamma_4 f(1, 0).$$

Since the quantities $f(1, 1)$, $f(0, 1)$, and $f(1, 0)$ should themselves be expressed in terms of f_k and f_p, Eqs. (51) turn out to be self-consistent only if the condition

$$\int\frac{d^2k}{(2\pi)^2}\frac{\psi_k^*(1, 1)[\psi_k(1, 1)U - \gamma_4(\psi_k(0, 1) + \psi_k(1, 0))]}{t - t_k}$$

$$+ \int\frac{dp}{2\pi}\frac{\psi_p^*(1, 1)[U\psi_p(1, 1) - \gamma_4(\psi_p(0, 1) + \psi_p(1, 0))]}{t - t_p} = 1$$

$$(52)$$

is fulfilled, where the integration over $\mathbf{k}$ is again performed over the complete Brillouin zone. Equation (52) is the generalization of Eq. (41) to the case $\gamma_4 \neq 0$.

For $\gamma_4 \leqslant \gamma_1$ the integration over p is limited to the sectors (47b). For such values of p we have $t_p < 1$, so that the second term in the left-hand side of (52) in this case cannot affect the critical properties. As in Sec. 3, the critical value of ε can be found by substituting $t = t_c \equiv 1 + 6\gamma_1$ into the equation of state (52), and the leading singularities can be found by expanding in $\tau \equiv t - t_c$ about this point.

Since, for $\gamma_4 < \gamma_1$, the quantities $\psi_k(1, 1)$, $\psi_k(1, 0)$, and $\psi_k(0, 1)$ for small k are proportional to k^3, as in the case $\gamma_4 = 0$, the singular term in the free energy has the same character as before.

The behavior of $f(n, m)$ at large distances is determined by the term

$$f(n, m) = \int\frac{d^2k}{(2\pi)^2}\frac{\psi_k(n, m)\psi_k^*(1, 1)}{t - t_k}F.$$

Approximating, for small k and k',

$$\theta(k, k') \approx \frac{b}{2}(k - k'), \quad b = \Delta(1 - \Delta)^{-1},$$

we can represent $\psi_k(n, m)\psi_k^*(1, 1)$ in the form

$$\exp i[k_1(n-1) + k_2(m-1)]$$

$$-\exp i[k_1(n-2-b) + k_2(m+1+2b)]$$

$$+\exp i[k_1(n-1)+k_2(m+2+3b)]$$
$$-\exp i[k_1(n+1+2b)+k_2(m+1+2b)]$$
$$+\exp i[k_1(n+2+3b)+k_2(m-1)]$$
$$-\exp i[k_1(n+1+2b)+k_2(m-2-b)].$$

Thus, at large distances $f(n, m)$ has, as before, the form of a wave created by six sources, and, although their positions are found to be displaced in comparison with the case $\gamma_4 = 0$, they form, as before, a regular hexagon. This implies that no qualitative difference from the case $\gamma_4 = 0$ arises, and, for the region $1 + b \ll r \ll q^{-1}$, f will fall off as the third circular harmonic (i.e., as r^{-3}) and ξ_1 will be finite at the transition point.

For $\gamma_4 = \gamma_1$, both $\psi_k(1, 1)$ and $\psi_k(1, 0)$ and $\psi_k(0, 1)$ have finite limits ($\pm 6^{1/2}$) as $|k| \to 0$, so that a smoothing of the first-order transition occurs:

$$\tau \begin{cases} =0, & \varepsilon > \varepsilon_c \\ \infty \exp(-c/(\varepsilon_c - \varepsilon)), & \varepsilon < \varepsilon_c \end{cases}.$$

As the transition point is approached the region in which $f(n, m)$ behaves as the zeroth cylindrical harmonic (i.e., logarithmically) gets wider and wider, and ξ_1 diverges as $\tau^{-1/2}$. We emphasize that this transition will occur only for $\gamma_5 < \gamma_4$; otherwise, a heavy wall remains stable against decay for all values of ε.

For $\gamma_4 > \gamma_1$ the "high-temperature" (i.e., corresponding to large values of ε) phase is found to consist not of three individual light walls separated from each other by infinite distances but of a light wall and a bound complex of two other light walls. This is due to the fact that the parameter value $\Delta = 1$ is critical for the wetting transition in a system consisting of two light walls. For $\gamma_4 > \gamma_1$ the critical value of t is

$$1+2(\gamma_1+\gamma_4+\gamma_1^2/\gamma_4),$$

and the critical behavior is determined by the second term in the left-hand side of the equation of state (52). As we should expect, the transition belongs to the same universality class as the standard $1 \rightleftarrows 2$ transition (considered in Sec. 2), as does the phase transition on the line $\gamma_1 = \gamma_4$, $\varepsilon > \varepsilon_c$. As in the case $\gamma_4 = \gamma_1$, for $\gamma_4 > \gamma_1$ a phase transition will occur only for not-too-large values of γ_5.

The phase diagram obtained is depicted in Fig. 7 in the variables Δ, ε for the case $\gamma_5 < \gamma_4$.

Thus, we have shown that allowance for the effective pair interaction of light walls leads to a change of the phase diagram of the system, but does not change the critical behavior on the $1 \rightleftarrows 3$ phase-transition line. The scheme of calculations used also makes it possible to include in the analysis the direct interaction of light walls on neighboring sites (which vanishes

in the ANNNI model; see Sec. 6). The analysis of a system with a larger number of light walls leads to considerably greater complexity of the equations.

6. DECAY OF A DOMAIN WALL INTO THREE IN THE ANNNI MODEL

The wetting problem associated with the transformation of domain walls via a $1 \rightleftarrows 3$ scheme was considered in Ref. 13 for the case of an ordered $\langle + + - - \rangle$ phase (see Fig. 2) in the framework of the ANNNI model. In this case, as for the phase $\langle + + - \rangle$, we can distinguish two types of competing walls. The wall which corresponds to the appearance of an extra plus (i.e. $\langle + + + - - \rangle$), will be denoted by a, while the other, corresponding to the disappearance of one of the minuses (i.e. $\langle + + - \rangle$), will be denoted, of course, by b. The position of the lines on which the energy of one of the walls is comparable with the energy of three walls of the other type is also shown in Fig. 2. In Ref. 13 the positions of the $a \rightleftarrows 3b$ and $b \rightleftarrows 3a$ phase-transition lines at finite temperature were analyzed numerically and by the transfer-matrix method without allowance for the possibility of transformation of the walls.

We can now apply the results of Sec. 5 to analyze two of these concrete problems. The statistical weights γ_α ($\alpha = 1, 2, ..., 5$) appearing as parameters can be expressed, in this case, in terms of a single parameter γ (see the table). For $\gamma \ll 1$, in both cases, $\gamma_4 \ll \gamma_1$, and this, according to the results of Sec. 5, guarantees a first-order phase transition.

An analogous problem can be formulated for the same phase $\langle + + - - \rangle$ in the absence of a magnetic field. The difference from the case of a finite field consists in the fact that the domain walls are degenerate with respect to the sign of their magnetization. An elementary kink in this case is found to involve a change of sign of the magnetization of the wall (e.g., in the case of a wall of type a, we have a transition from $\langle + + + - - \rangle$ to $\langle + + - - - \rangle$), while in the decay of one wall into three there appear walls of different signs ($\langle + + + - - \rangle$ undergoes a transition to $\langle + - + - - \rangle$). These differences lead to a change in the values of the parameters γ_α (see the table), but, as before, the condition $\gamma_1 \ll \gamma_4$ will be fulfilled and both phase transitions will be first-order.

7. TWO WALLS AND THE POSSIBILITY OF PINNING AT AN EXTERNAL BOUNDARY

The problem considered in the present section arises in the $\langle + + - \rangle$ phase of the ANNNI model in the case when the system is semi-infinite, i.e., there is an external wall (sample boundary). In this formulation there exist different possibilities, associated with the competition of wetting transitions and pinning of domain walls at the boundary. The boundary conditions on the external wall are specified as the absence of three bonds at two boundary sites of a chain.

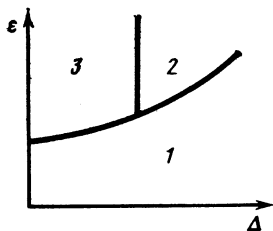There exists a nontrivial example, which is analyzed ex-

FIG. 7. Qualitative form of the phase diagram: 1) region of existence of a single heavy wall; 2) region of existence of a light wall and a bound complex of two light walls; 3) region of existence of three individual light walls.

TABLE I.

		γ_1	γ_2	γ_3	γ_4	γ_5
$h > 0$	$3a \rightleftarrows b$	γ^2	γ^2	γ	γ^4	γ^4
	$3b \rightleftarrows a$	γ^2	γ^2	γ^3	γ^4	γ^6
$h = 0$	$3a \rightleftarrows b$	γ	γ	γ	γ^2	γ^3
	$3b \rightleftarrows a$	γ	γ	γ	γ^2	γ^3

```
+ − + + − + + − + + − + + −  a
+ + + + − + + − + + − + + −  b
+ + − + + + − + + − + + + −  c
+ + − + + − + + − + + + + −  d
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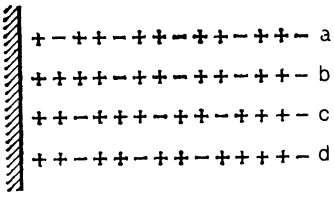
FIG. 8.

actly here. We assume that at infinity there exists a strictly specified sequence (+ + −). In the example under consideration the vacuum state (Fig. 8a) corresponds to the absolute absence of domain walls, and rearrangement of the boundary region induces the appearance of two domain walls of type a (see Secs. 1 and 2). They can be localized near the boundary (Fig. 8b) or can be torn away from it (Figs. 8c, d). Here, in principle, three different states of the system are found to be possible.

I. The vacuum state (Fig. 8a) mixed with a fluctuation-generated pair of domain walls localized on the external boundary.

II. A bound complex of two domain walls, remote from the boundary.

III. Two free domain walls.

If the energy difference

$$\Delta\varepsilon = \varepsilon_{vac} - \varepsilon_2 = -(4J_1 + 2J_2) + 2h$$

is negative and $|\Delta\varepsilon| \gg T$, the system is found to be in state I. For positive values, with $\Delta\varepsilon \gg T$, state II or state III should be realized, depending on the state (bound or free) in which the pair of domain walls is found in the absence of the external boundary.

The statistical weights of kinks of the minimum size on a single domain wall (γ_1) and on a complex of two maximally close walls (γ_4) coincide in the model under consideration, and are equal to γ^2. Thus, to first order in γ^2 a system of two domain walls is found to be exactly on the line of the wetting transition in the bulk (see Sec. 5). This accidental degeneracy is lifted when larger kinks are taken into account.

Now we can return to the end of Sec. 2, where an equation determining the behavior of a pair of walls a was written out. In Eq. (30), parameters γ_1 and γ_4 of kinks of general form were introduced. We shall be interested in the solution of this problem on the transition line, where $z_+ = 1$, and the second solution of Eq. (26):

$$z_- = z_0(\gamma_1) = \exp\left[-\text{Arcch}\,(2\,\text{ch}\,\alpha - 1)\right].$$

The functions $A(z)$ and $B(z)$ appearing in Eq. (27) are as follows:

$$A(z) = -\frac{1}{1 - \gamma_1/z}, \tag{53}$$

$$B(z) = \frac{2z}{\gamma_1(1 - \gamma_1 z)}\left(\frac{1}{1 - \gamma_4} - \frac{1}{1 - \gamma_1^2}\right) - \frac{1}{(1 - \gamma_1/z)^2}. \tag{54}$$

As a result of substituting the values (53) and (54) of these functions at the points z_+ and z_- into Eq. (27) we obtain on the transition line

$$\gamma_4 = 1 - (1 - \gamma_1^2)\left[1 + \frac{\gamma_1^2}{2}\frac{1 - \gamma_1 z_0}{\gamma_1 - z_0}\right]^{-1}. \tag{55}$$

It can be verified that for all possible $0 \leqslant \gamma_1 < 1$ Eq. (55) gives $\gamma_4 > \gamma_1$.

Thus, for $\gamma_4 = \gamma_1$, which corresponds to the usual ANNNI model, the effective attraction of the walls that is expressed through γ_4 turns out to be insufficient for the formation of a "dry" phase—a bound state of the walls a. Of course, the virtual presence of a wall b enhancing the effective attraction makes the existence of such a state possible. But here we assume that the wall b is unimportant, since the line of coexistence of the b and $a + a$ walls (see Fig. 2) turns out to be far from the line $\Delta\varepsilon = 0$ (the wavy line in Fig. 2).

Thus, everything that has been said above makes it possible to conclude that in the system considered by us in this section a phase transition from state I to state III will occur, and all the singularities will have the same form as for $\gamma_4 = 0$.

With neglect of the kinks γ_4 the system of equations for the eigenvalues of the transfer matrix will (in lowest order in γ) have the form

$$(t - 1 - 4\gamma^2)f(n, m) = \delta_{n1}\delta_{m2}Uf(1, 2) + \gamma^2\hat{\Delta}_L f, \quad 1 \leqslant n < m, \tag{56}$$

where $U = \gamma^2(\varepsilon t - 1)^{-1}$, $\varepsilon = \exp(\Delta\varepsilon/T)$, $\hat{\Delta}_L$ is the lattice Laplacian on the square lattice, and

$$f(0, m) = f(n, n) \equiv 0. \tag{57}$$

In order that the boundary conditions (57) be fulfilled automatically, the source appearing in the right-hand side should be supplemented by seven sources of the same intensity but different signs. Their arrangement is shown in Fig. 9. Then Eq. (56), after Fourier transformation, goes over into

$$(t - t_k)f_k = Uf(1, 2)S(k), \tag{58}$$

where

$$t_k = 1 + 2\gamma^2(\cos k_1 + \cos k_2),$$
$$S(k) = 4\sin 2k_1 \sin k_2 - 4\sin k_1 \sin 2k_2$$
$$= 16\sin k_1, \sin k_2 \sin\frac{k_1 + k_2}{2}\sin\frac{k_2 - k_1}{2}.$$

Equation (58) is self-consistent only when the condition

$$\frac{1}{8}\int\frac{d^2k}{(2\pi)^2}\frac{US^2(k)}{t - t_k} = 1$$

is fulfilled. As before, this is the equation of state.

Since for small k we have $S(k) \sim k^4$, the phase transition is found to be first-order and the singular term in the expansion of the free energy in the localized phase is proportional to $(\Delta\varepsilon)^4\ln(1/\Delta\varepsilon)$. At large distances $f(n, m)$ falls off (for $1 \ll r \ll q^{-1}$) as

$$r^{-4}\sin 4\varphi \quad (r^2 = n^2 + m^2),$$

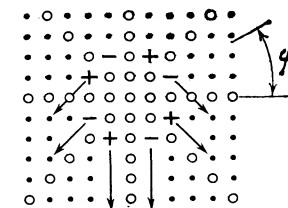and ξ_1 remains finite right to the transition point.

FIG. 9. Arrangement of sources for $\gamma_4 = 0$ and their displacement for $\gamma_4 \neq 0$.

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If, nevertheless, the reader wishes to verify directly that not-too-large values of γ_4 do not lead to a change of the critical behavior, we refer to the scheme of the solution of the problem with $\gamma_4 \neq 0$.

The boundary condition $f(n, n) = 0$ should be replaced by

$$(t-1)f(n, n+1) = \gamma_1[f(n-1, n+1) + f(n, n+2)] + \gamma_4[f(n-1, n) + f(n+1, n+2)],$$

and $f(n, m)$ $(0 < n < m)$ should be sought in the form

$$\int_0^\pi \frac{dk_1}{2\pi} \int_0^{k_1} \frac{dk_2}{2\pi} f_k \psi_k + \int \frac{dp}{2\pi} \psi_p,$$

where

$$\psi_k = 2^{1/2}\{\sin k_1 n \sin [k_2 m - \theta(k_1, k_2) + \theta(k_1, -k_2)]$$
$$-\sin k_2 n \sin [k_1 m + \theta(k_1, k_2) + \theta(k_1, -k_2)]\},$$
$$\psi_p = \sin [p(n+m) + \theta(p+iQ, -p+iQ)] \exp [-Q(m-n)]$$
$$-\sin [p(m-n) + \theta(p+iQ, -p+iQ)] \exp [-Q(m+n)],$$

and $\theta(k, k')$, $Q(p)$, and the region in which p is defined are given in Sec. 5.

Since for $\gamma_4 < \gamma_1$ for small k we have $\psi_k \sim k^4$, a finite value of γ_4 does not have a qualitative effect on the singularity at the transition point. The behavior of $f(n, m)$ at large distances is determined by the term

$$\int \frac{d^2k}{(2\pi)^2} \frac{\psi_k(n, m) \psi_k^*(1, 2)}{t - t_k},$$

where the numerator of the integrand can be approximated for small k as

$$\exp i[k_1(n-1) + k_2(m-2)] - \exp i[k_1(n-2-b) + k_2(m-1+b)]$$
$$+ \exp i[k_1(n-2-b) + k(m+1+b)] - \exp i[k_1(n-1)$$
$$+ k_2(m+2+2b)] + \exp i[k_1(n+1) + k_2(m+2+2b)]$$
$$- \exp i[k_1(n+2+b) + k_2(m+1+b)] + \exp i[k_1(n+2+b)$$
$$+ k_2(m-1+b)] - \exp i[k_1(n+1) + k_2(m-2)].$$

Although the sources do not now form an octagon that is symmetric about the coordinate origin (see Fig. 9), it follows from the symmetry that $f(n, m)$ will nevertheless fall off at large distances as the fourth circular harmonic with center displaced from the point $n = 0$, $m = 0$. The asymptotic behavior remains the same ($\sim r^{-4}$).

We emphasize once again that although here we have given the proof only for $\gamma_4 < \gamma_1$, when kinks of arbitrary size are taken into account it will also be valid on the line $\gamma_4 = \gamma_1$ pertaining to the same phase.

[1] In addition, in Sec. 2 we also give a generalization of the transfer-matrix method to the case of not-too-strong interaction along a line defect. In other words, the proposed procedure makes it possible to take account of kinks of arbitrary size in a system of competing domain walls.

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