

## A Surface Effect on a One-Dimensional Competitive System: Free Domain-Wall Structures Induced by a Free-Surface

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Some one-dimensional classical systems with competitive interactions show quite complex ground-state phase-diagrams, in which infinitely many phases exist. A free-surface effect on the ground-state structures of one of such systems is discussed. A direct numerical method is applied to evaluate the ground-state structure of the semi-infinite system. We pay attention to the area near the phase boundary between a non-uniform modulated phase and a uniform phase. The free-surface induces domain-wall structures. The domain-wall may be free from the free surface in some parameter region although it is usually bound near the surface.

KEYWORDS: one-dimensional classical system, competitive interaction, free surface, ground state, numerical calculation, domain-wall

### §1. Introduction

To analyze properties of systems independent of the boundary conditions, we usually regard the size of the systems as infinite. However, of course, to obtain properties near the boundaries, effect of the boundary conditions must be correctly treated. Free surface is one of the simplest boundary conditions.

Semi-infinite systems with a free surface for classical spins or particles have been discussed by many authors to analyze behaviors of the systems near the surface. For example, LePage and Camley<sup>1)</sup> have analyzed surface spin-wave modes of a semi-infinite Fe/Gd superlattice and showed that a surface mode is softened, indicating a surface phase transition. The possibility of a first-order surface transition in a semi-infinite Blume-Capel model was shown by Buzano and Pelizzola.<sup>2)</sup>

As for the ordering or disordering phenomena which are related to the surface of alloys, some works have recently been performed. Extensive Monte-Carlo simulations<sup>3)</sup> have dealt with the surface-induced ordering or disordering in fcc Cu-Au type alloys. Seok and Oxtoby<sup>4)</sup> have studied the order-disorder transition in Cu<sub>3</sub>Au using a density functional approach. They obtained surface transition and segregation phenomena similar to experimental results. Ritschel and Czerner<sup>5)</sup> have studied the spatial dependence of the order parameter near surface, which is related to the experimentally observed long-range order near the surface of Fe<sub>3</sub>Al.

Surface effects on the phase transitions of uniaxial antiferromagnets have been discussed by de Moraes and Figueiredo.<sup>6)</sup> In connection with the uniaxial antiferromagnets, the ground state of a semi-infinite system with a field along the easy axis has been formerly discussed concerning the surface spin-flop state.<sup>7, 8)</sup> Recently, Tralori *et al.*<sup>9)</sup> have shown that the so-called surface spin-

flop state does not exist in the system in contradiction to the results of the previous studies.<sup>7, 8)</sup> On the other hand, Chung<sup>10)</sup> has claimed that the surface spin-flop state does exist and the transition from the surface spin-flop to bulk spin-flop is first-order-like. These studies show that even the ground state cannot so easily be obtained for semi-infinite systems.

The ground state of one-dimensional classical systems with competitive interactions has long been discussed by many authors. The reason is that the systems show very many commensurate phases with short-period or long-period leading to very complex ground-state phase-diagrams in spite of the simplicity of the system. The model proposed by Marchand, Hood and Caillé (MHC)<sup>11-13)</sup> is the simplest one of those systems. The Hamiltonian of the model is given by

$$H_{\text{MHC}} = \sum_{n=-\infty}^{\infty} [V(u_n) + W(u_{n+1} - u_n)], \quad (1.1)$$

where  $u_n$  is the displacement of the  $n$ -th particle from the reference position where the one-particle potential  $V(u_n)$  is minimized. The one-particle potential and the interaction potential  $W$  are respectively given by

$$V(x) = \frac{1}{2}Kx^2, \quad (1.2)$$

$$W(x) = -\frac{1}{2}(x - \gamma)^2 + \frac{1}{4}(x - \gamma)^4, \quad (1.3)$$

where  $K$  is a positive constant and  $\gamma$  is a parameter expressing the competition between the one-particle potential and the interaction-potential. The properties of the model have been studied in detail and a complete ground-state phase-diagram has been obtained. Many (infinitely many) modulated phases exist in the ground-state phase-diagram and between those phases both the first-order and the second-order phase transitions are caused. The non-convexity of the interaction potential induces this complexity of the phase diagram.

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Most of the studies for the competitive systems including that by MHC have been focused mainly on systems of infinite length, namely systems with translational symmetry. The effect of a free surface or any other boundary conditions on the system has not so often been discussed,<sup>14)</sup> though the free surface or any other boundary conditions may cause interesting phenomena as shown now for other semi-infinite systems. The boundaries are expected to add a new competition to the competitive systems.

In the present paper, we discuss the free surface-effect by means of the semi-infinite version of the MHC model. The Hamiltonian is given by

$$H = \sum_{n=1}^{\infty} [V(u_n) + W(u_{n+1} - u_n)]. \quad (1.4)$$

Note that  $u_1$  stands for the displacement of the “surface particle”.

We observe some new phenomena unexpected before, especially near the phase boundary between the two phases of the infinite system. Since near the phase boundaries, the energies of the neighboring two phases are quite close, near the surface the ground-state structures of the two phases are expected to be blended. So we concentrate our attention on parameter regions near the phase boundaries of the infinite system. Near the phase boundaries, there appear “domain-wall” structures connecting the two types of ground state structure. The free surface makes the translational symmetry of the system disappear and induces the domain-wall. The domain-wall is usually bound near the surface. However, it can be at any position inside the bulk in some parameter region. Thus, the “free” domain-wall structure appears.

To investigate the ground state, we introduce a numerical method. This “sweep-down method” is simple and direct, and is applicable to various types of systems. The method is explained in the next section.

The ground state of the competitive system obtained by numerical calculation will be given in §3. The free domain-wall appears if the displacement of the particles near the surface is not smaller than that of the particles in the bulk. In the modulated phase region near the phase boundary, the displacement of the surface particles is larger than that in the bulk. Away from the phase boundary, it is smaller than that in the bulk. Then, the free domain-wall appears near the phase boundary. In addition to this region, at a special point in the parameter space, the free domain-wall appears. At this point, the displacement of the particles near the surface is just equal to that of the particles in the bulk though it is smaller around the point. Therefore, this “free domain-wall” point is isolated in the parameter space.

The wall structure is induced by the surface. Therefore, presence of the free domain-wall means that the surface effect is not limited near the free surface but penetrates deep into the system.

The last section is devoted to summary and discussions.

## §2. The Numerical Method: The Multi-Channel Sweep-Down Method

It is not easy to obtain the ground state and the ground-state energy of competitive systems. However, the effective potential method by Griffiths and Chou<sup>15,16)</sup> is a very powerful method for one-dimensional systems and has been used by many authors to discuss the ground state.<sup>17)</sup> Unfortunately, this method is not applicable to the semi-infinite system such as (1.4). Trallori *et al.*<sup>9)</sup> have introduced a two-dimensional area preserving mapping method to investigate the existence of the surface spin-flop state in the semi-infinite and the finite uniaxial-antiferromagnetic systems. However, this method, also, cannot be used to the system (1.4).

We propose a direct numerical method to obtain the ground state of any one-dimensional classical system with semi-infinite or finite length. The method, we call as the “sweep-down method”, is as follows.

At first we convert the problem for the semi-infinite system into that of the finite system. Sufficiently deep inside the semi-infinite system, the ground state must be the same as the ground state of the corresponding infinite system. The state of the semi-infinite system must be different from the infinite system only near the free surface. Let the displacement  $u_n$  for  $n \geq N_B$  be equal to that in the infinite-length system  $u_n^*$  which are obtained by the effective potential method.<sup>11-13)</sup> Thus, the energy of the system is expressed in terms of the displacement in the “surface region”;

$$H(\{u_n\}_{n=1}^{N_B-1}) = H_S(\{u_n\}_{n=1}^{N_B-1}, u_{N_B}^*) + E_B, \quad (2.1)$$

where  $H_S$  is the “surface” Hamiltonian given by

$$\begin{aligned} H_S(\{u_n\}_{n=1}^{N_B-1}, u_{N_B}^*) \\ = \sum_{n=1}^{N_B-2} [V(u_n) + W(u_{n+1} - u_n)] \\ + V(u_{N_B-1}) + W(u_{N_B}^* - u_{N_B-1}), \end{aligned} \quad (2.2)$$

and  $E_B$  is the energy of the bulk part. Hence, it is sufficient to analyze the finite-length system  $H_S$  instead of the semi-infinite system (1.2) and find the appropriate number  $N_B$ . In the finite-length system, one end ( $u_1$ ) of the two ends is free and the other ( $u_{N_B} = u_{N_B}^*$ ) is fixed.

We then arrange on the finite system an initial particle-configuration. We sweep the particles one by one from the fixed end ( $n = N_B - 1$ ) to the free boundary end ( $n = 1$ ). At each particle we search the minimum energy position and put the particle on the position, keeping the position of the two particles on both sides of that particle. Then, we sweep from the free boundary end to the fixed end searching the minimum energy position of the particle. We repeat the sweep until all particles in the system attain to its energy minimum position. Let this type of method to search the minimum-energy be called the one-particle sweep-down method.

A more valid method is available to reach surely the true ground state or nearly degenerate states. Instead of searching the energy minimum position of only one

particle at once, we may seek the minimum energy position of the two neighboring particles at once, keeping the position of the two particles on both sides of those particles (the two-particle sweep-down method). For the two-particle, the configuration for the minimum energy obtained by the one-particle search is chosen as the initial configuration. Furthermore, we seek the minimum energy positions of the three neighboring particles at once, keeping the position of the two particles on both sides of the three particles (the three-particle sweep-down method). In this case, the configuration for the minimum energy obtained by the two-particle search is chosen as the initial configuration. In the same way, we can introduce the larger-number particle sweep-down method. Note that the minimum energy configuration obtained by the  $n$ -particle sweep down method is chosen as the initial configuration for the  $(n + 1)$ -particle sweep-down method.

To avoid straying into local minimum states, we must improve the sweep-down method. For the one-particle sweep-down we provide many initial configurations instead of only one, in which we set randomly the initial configurations for the particles in the surface region and sweep the particles at random instead of sweeping successively from one end to the other end. We, then, sweep successively from the fixed end to the free end. We sweep the particles at random. Then we sweep successively from the free end to the fixed end. We repeat the process until all particles in the system attain to its energy minimum position. We perform the process for all the provided initial configurations. We obtain consequently many candidates for the ground state. We expect that the lowest energy state is the ground state. Let us call this type of sweep down method the one-particle "multi-channel" sweep-down method (the one-particle MCSW method). Using the minimum energy configurations obtained by the one-particle MCSW method as the initial configuration, we can perform the two-particle and the three-particle MCSW methods.

In our experience, rather large portion of the candidates get to the true ground state. Furthermore, the many candidates, although they are not the true ground state, give physically meaningful results. Information about the system can be extracted from them.

### §3. Numerical Analysis of the Free-Surface Effect

The ground-state phase-diagram of the infinite system (1.1) was obtained by MHC.<sup>13)</sup> The complete phase diagram is shown in Fig. 7 of their paper.

We consider the semi-infinite system (1.4) in the parameter region near the phase boundary between the uniform phase and the modulated phase with period two (the dimerized phase). At the phase boundary, the "second-order" phase transition is caused. The phase diagram near the boundary is shown in Fig. 1.

We pay attention to the free-surface effect along the broken line in Fig. 1. Fixing the parameter  $\gamma$  to be 0.3, we investigate the particle configurations near the surface for  $2.47 \leq K \leq 3.0$ , where the phase transition of the infinite system is caused at  $K = 2.920$ .

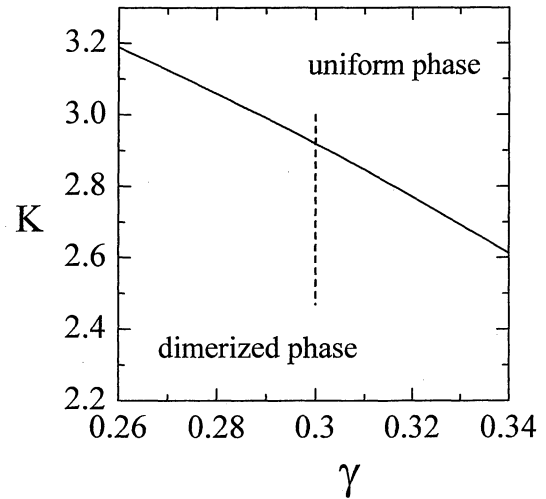


Fig. 1. The ground state phase diagram near the phase boundary between the uniform phase and the dimerized phase. We investigate the surface effect along the broken line.

For the infinite system with period  $p$ , there are  $p$  different positions of the particles. Let us image that we cut the infinite system with period  $p$  into two parts to obtain the semi-infinite system. There are  $p$  different cutting positions; there are  $p$  different "original" positions of the surface particle. Thus, for the system with period  $p$ , there are  $p$  different surfaces. For the dimerized system discussed in the present paper, we have two kinds of free surface. For one of the two types, the "original position" of the surface particle takes a positive value  $u^+$  and for the other, that takes a negative value  $u^-$ . Let us call the two surfaces the  $u^+$ -surface and the  $u^-$ -surface respectively.

Of course, the surface particle remains no longer at the original position after the cutting; the surface is relaxed. The particle on the free surface feels only the two-body interaction potential from the inner particle. The surface particle will be shifted from the equilibrium position of the infinite system. The outward move and the inward move of the surface particle respectively stand for expansion and contraction of the system.

The "size"  $N_B$  in the sweep-down method was chosen as  $N_B = 100$  or  $N_B = 200$  depending on the parameter  $K$ . The range of the variable  $u_n$  was adequately chosen, usually from  $-0.2$  to  $0.2$ . The range was divided at 10,000 or 20,000 intervals.

We take up, at first, the  $u^-$ -surface in the dimerized phase. There is no inconsistency between the particle configurations near the surface and in the bulk. The particle configuration near the surface connects smoothly with that in the bulk. The results of numerical calculation are shown in Fig. 2. The change in the configuration is smooth and reasonable, as we cross the phase boundary.

However, two characteristic phenomena must be indicated. At  $K = 2.560$ , the configuration near the surface is the same as that in the bulk. The surface is not relaxed at all. At this point, the semi-infinite system is not conscious of the free surface. Contrastively to the above, the free-surface effect penetrates, though exponentially

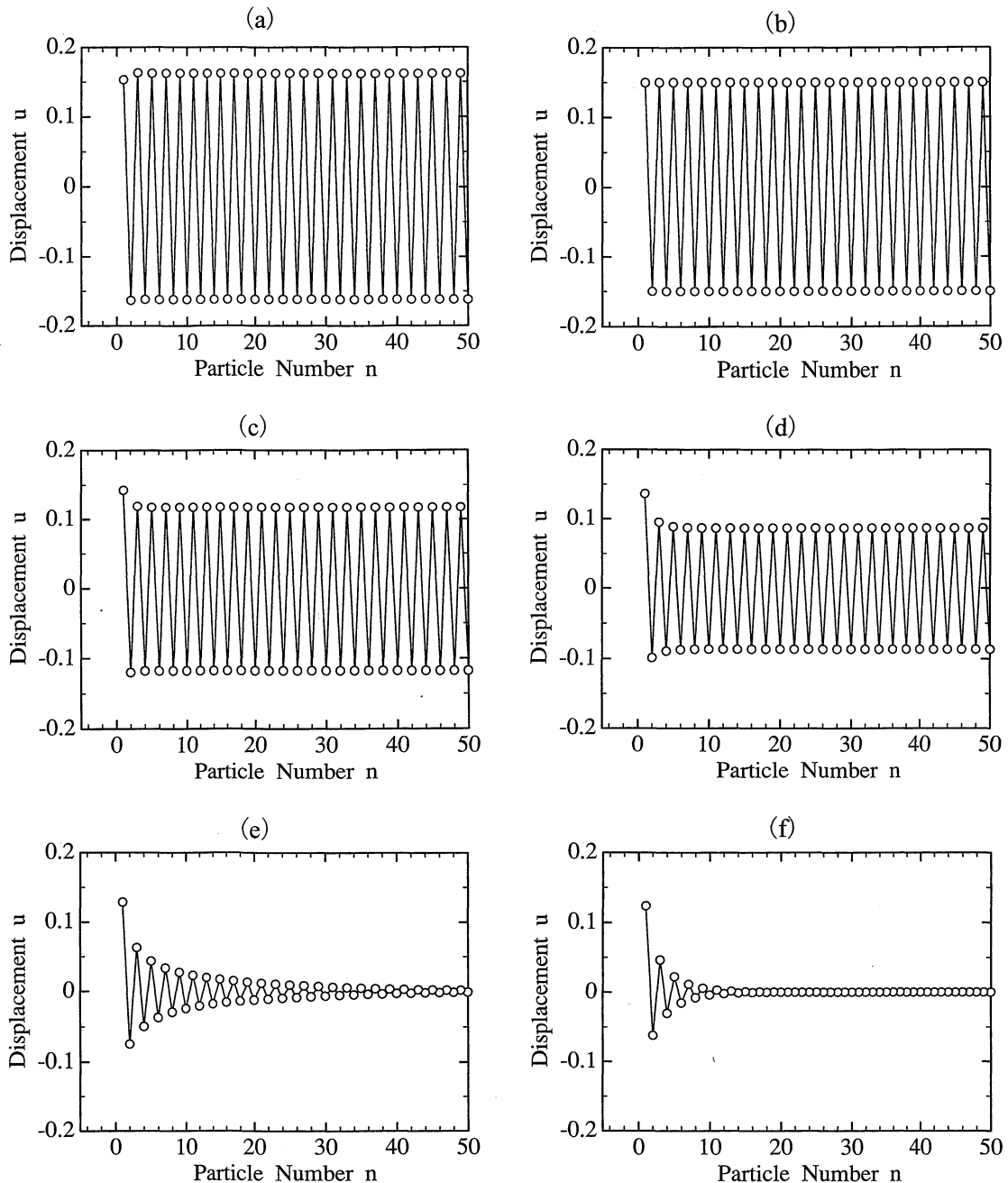


Fig. 2. Particle configurations near the  $u^-$ -surface. (a)  $K = 2.50$ . (b)  $K = 2.56$ . (c)  $K = 2.70$ . (d)  $K = 2.80$ . (e)  $K = 2.92$ . (f)  $K = 3.00$ . The surface particle moves outward for  $K < 2.56$  and moves inward for  $K > 2.56$ . The surface particle does not move at all at  $K = 2.56$ . The effect of a free surface penetrates deep into the bulk at  $K = 2.92$ .

decaying, deep into the bulk at  $K = 2.920$ ; i.e. at the phase boundary. This phenomenon is due to the second order phase transition at the boundary.

Next, we take up the  $u^+$ -surface. As we vary the parameter  $K$ , the particle configuration does change considerably. This is because that near the  $u^+$ -surface, the particle configuration does not connect smoothly with that in the bulk configuration. There must appear a "domain-wall" between the two configurations. The results of numerical calculation at some values of  $K$  less than 2.560 are shown in Fig. 3. If the parameter  $K$  is less than 2.502, the surface effect is limited near the surface. In the range  $2.503 \leq K < 2.560$ , we can see a "twist" in the configuration, which expresses relaxation

of the inconsistency between the particle configuration near the surface and that in the bulk. The area in which the twist particle-configuration appears is regarded as the domain-wall connecting the two types of configuration. This domain-wall stays near the surface in this parameter region. The center of the twist (or the center of the domain-wall), which is defined by the value of  $n$  with  $u_n \simeq 0.0$ , is at  $n = 6$ .

However, when the value of the parameter  $K$  is 2.560, the configuration changes drastically. The result of numerical calculation at  $K = 2.560$  is shown in Fig. 4. The center of the domain-wall may situate at any even site  $n$ , where  $n$  is any even integer larger than or equal to 8. This means that the domain-wall can hop freely with-

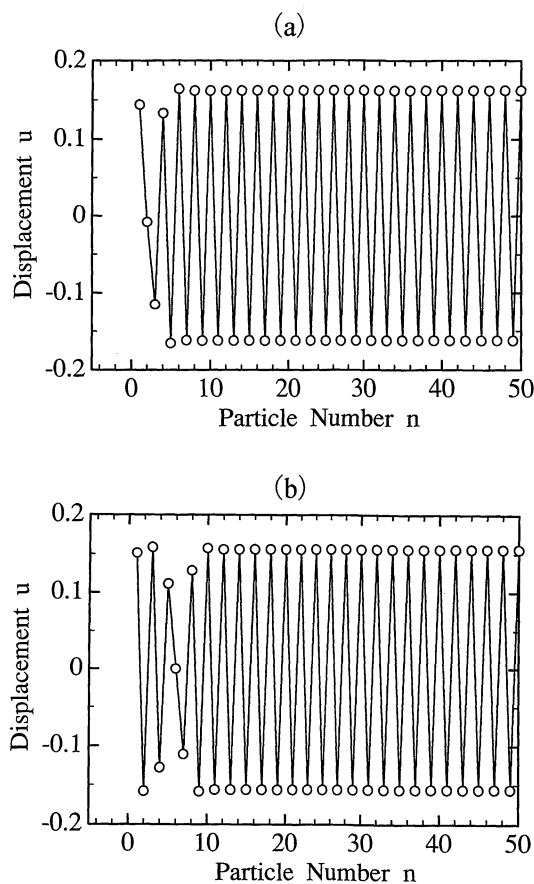


Fig. 3. Particle configurations near the  $u^+$ -surface. (a)  $K = 2.50$ . (b)  $K = 2.53$ . The center of the domain wall, which means  $u_n \approx 0$ , is at  $n = 2$  if  $K = 2.50$  and is at  $n = 6$  if  $K = 2.53$ .

out energy loss; the “free” domain-wall appears at this value of the parameter. This phenomenon could not be expected before the calculation.

In the range  $2.560 < K \leq 2.623$ , the domain-wall can not hop freely again. The results of numerical calculation at some values of  $K$  in that range are shown in Fig. 5. In the range  $2.560 < K \leq 2.5613$ , the domain-wall is at  $n = 8$ . But, in the range  $2.5614 \leq K \leq 2.576$ , it is at  $n = 4$ . The domain-wall comes closer to the surface. In the range  $2.577 \leq K \leq 2.621$ , it is at  $n = 6$ . In the range  $2.622 \leq K \leq 2.623$ , it is again at  $n = 8$ . The domain-wall goes away from the surface. In this parameter region, the relation between the value of the parameter  $K$  and the position of the wall is not monotonous but rather complex.

When the parameter  $K$  becomes larger, the free domain-wall structure again appears. The results of numerical calculation at some values of  $K$  larger than or equal to 2.624 are shown in Fig. 6. For larger  $K$ , the domain-wall hops freely in the region more away from the surface. For an example, at  $K = 2.624$ , the domain-wall may situate at any even  $n$  larger than or equal to 8, whereas, at  $K = 2.700$ , it may situate at any even  $n$  larger than or equal to 18. Furthermore, at  $K = 2.800$ , domain-wall may situate at any even  $n$  larger than or equal to 28. The width of the domain-wall in the larger  $K$  region is wider than that in the smaller  $K$ . However, it does not diverge and remains a few lattice spaces.

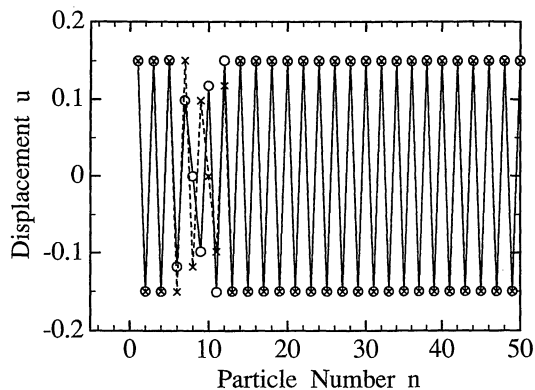


Fig. 4. Particle configurations near the  $u^+$ -surface. The parameter  $K$  is chosen as  $K = 2.56$ . The center of the domain wall may situate at any even site  $n$ , where  $n$  is any even integer greater than or equal to 8. In the figure, only the first two configurations, in which the domain wall is at  $n = 8$  or  $n = 10$ , are shown. The configuration nearest to the surface ( $n = 8$ ) is shown by circles connected by solid lines, and configuration next nearest to the surface ( $n = 10$ ) is shown by crosses connected by dotted lines.

For  $K \geq 2.624$ , there appears effectively “a repulsive force” between the domain-wall and the surface. As  $K$  becomes large, the displacement of the particles becomes small. The cause of “the repulsive force” is that the displacement of the particles near the surface becomes large compared to that in the bulk, whereas the displacement of particles near the domain-wall remains small. If the domain-wall with small particle-displacement approaches the surface, the interaction potential energy  $W$  increases. The increase of the interaction potential induces the repulsive force. The range of the repulsive force is short. The domain-wall hops freely outside the range. This is the cause of the appearance of the free domain-wall in the region  $K \geq 2.624$ .

In general, the displacement of the particles in the bulk decreases with increasing  $K$ , since the strong one-particle potential  $V(u_n) = (1/2)Ku_n^2$  suppresses the displacement. At the free surface, the lack of the outer-side interaction-potential induces the particle displacement. Therefore, in the large  $K$  region ( $K > 2.560$ ), the displacement of the particle at the surface is larger than that in the bulk. This suggests that the free domain-wall appears in regions near the phase boundary of the dimerized phase.

The position of the domain-wall is summarized in Fig. 7, where the region  $K \geq 2.84$  is omitted. If the parameter  $K$  is larger than 2.84 and gets close to 2.920, the range of the repulsive force from the surface becomes large and the domain-wall is pushed away deep into the bulk. The domain-wall hops freely in the area far from the surface. Near the phase boundary, the displacement of the dimerized particles in the bulk part gets small and fades out at the phase boundary. But, even quite near the phase boundary, the width of the free domain-wall remains finite.

We may say that there is effectively “an attractive force” between the domain-wall and the surface in the region  $K \leq 2.623$ . In this region, the displacement of the second particle ( $n = 2$ ) is smaller than that in the bulk, though the displacement of the first particle on the

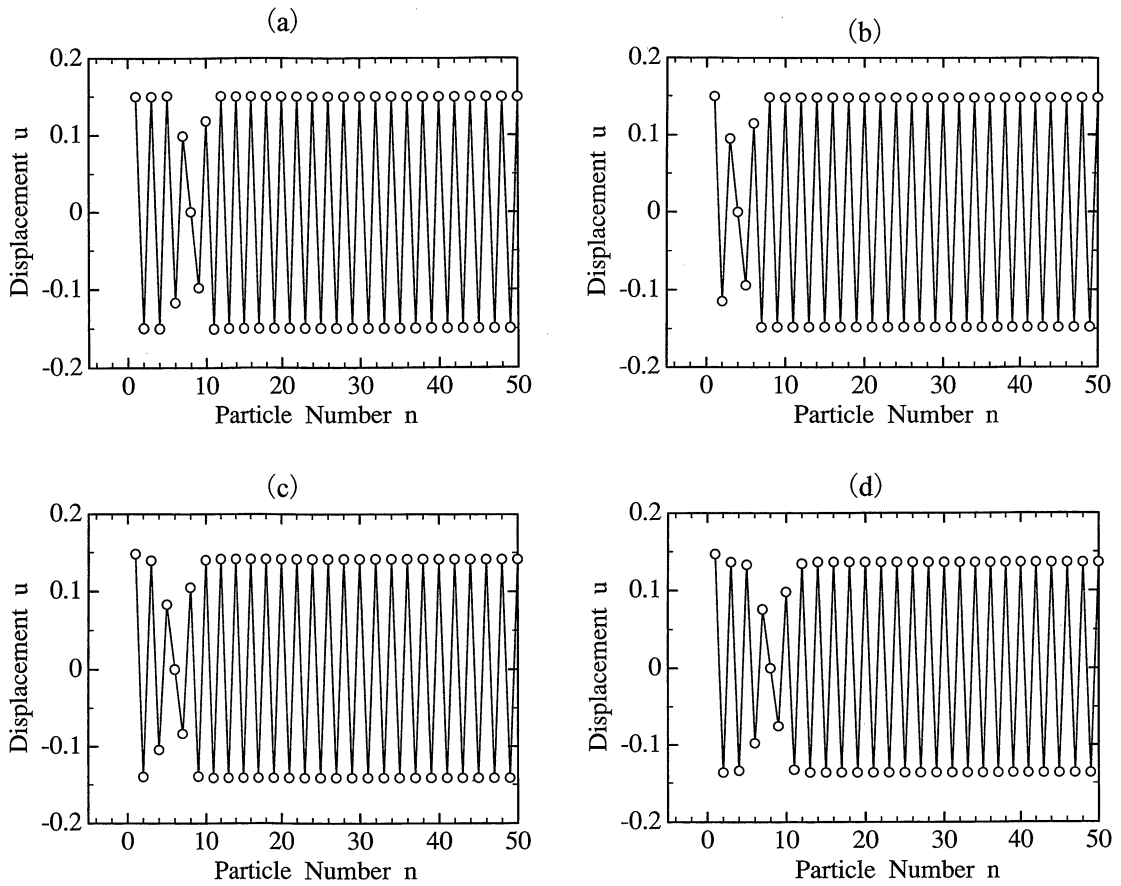


Fig. 5. Particle configurations near the  $u^+$ -surface. (a)  $K = 2.561$ . (b)  $K = 2.57$ . (c)  $K = 2.60$ . (d)  $K = 2.622$ . The center of the domain wall comes closer to the surface and goes away from the surface with increasing  $K$ .

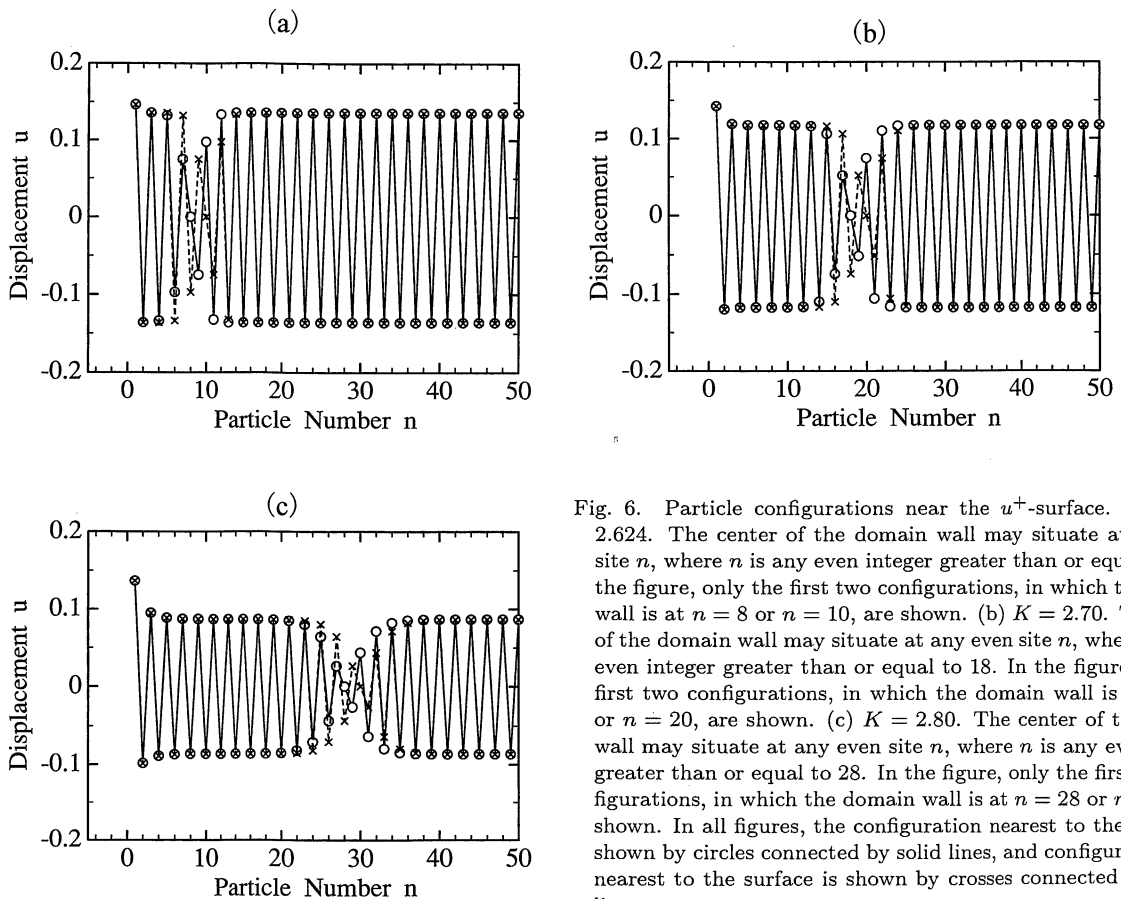


Fig. 6. Particle configurations near the  $u^+$ -surface. (a)  $K = 2.624$ . The center of the domain wall may situate at any even site  $n$ , where  $n$  is any even integer greater than or equal to 8. In the figure, only the first two configurations, in which the domain wall is at  $n = 8$  or  $n = 10$ , are shown. (b)  $K = 2.70$ . The center of the domain wall may situate at any even site  $n$ , where  $n$  is any even integer greater than or equal to 18. In the figure, only the first two configurations, in which the domain wall is at  $n = 18$  or  $n = 20$ , are shown. (c)  $K = 2.80$ . The center of the domain wall may situate at any even site  $n$ , where  $n$  is any even integer greater than or equal to 28. In the figure, only the first two configurations, in which the domain wall is at  $n = 28$  or  $n = 30$ , are shown. In all figures, the configuration nearest to the surface is shown by circles connected by solid lines, and configuration next nearest to the surface is shown by crosses connected by dotted lines.

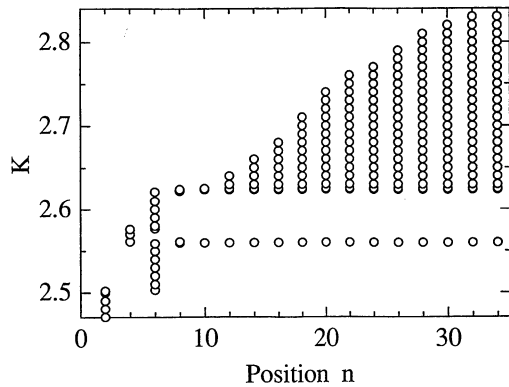


Fig. 7. The position  $n$  of the center of the domain wall. The region  $K \geq 2.84$  is omitted. If the parameter  $K$  is greater than 2.84 and gets closer to 2.920, the domain wall moves deeper into the bulk and penetrates infinitely deep into the system at  $K = 2.92$ .

surface ( $n = 1$ ) is larger ( $2.560 < K \leq 2.623$ ) or smaller ( $2.470 \leq K < 2.560$ ) compared to that in the bulk. In this connection, the displacement of the second particle ( $n = 2$ ) is just equal to that in the bulk at  $K = 2.560$  and  $K = 2.624$ . The particles in the domain-wall do not interact directly with the first particle on the surface, but interact with the second particle or the particles near the surface. Therefore, in the region  $K \leq 2.623$ , the interaction potential energy between the particles near the surface and the particles in the domain-wall is smaller than that between the particles in the bulk and the particles in the domain-wall. This induces the attractive force. However, the domain-wall cannot locate quite near the surface because the domain-wall too close to the surface breaks the surface structure. This induces quite-short-range repulsive force. The domain-wall locates at the position where the attractive and the repulsive forces balance.

As mentioned in the previous paragraph, at  $K = 2.560$ , the free domain-wall happens to appear. At  $K = 2.560$ , the displacement of particles near the surface is just equal to that in the bulk, as we mentioned in the statement about the  $u^-$ -surface. The displacement of the first particle or the second particle on the surface is the same as that in the bulk. Then, the attractive force disappears and the domain-wall becomes free.

Now, we can understand the non-monotonous change of the position of the domain-wall for the region  $K \leq 2.623$ , which is shown in Fig. 7. It is caused by the position of the second particle, which is, needless to say, influenced by the first particle on the surface. The displacement of the second particle is small compared to that in the bulk in the region  $K \leq 2.623$  but is just the same as that in the bulk when  $K = 2.560$  or  $K = 2.624$ . It becomes larger than that in the bulk for  $K > 2.624$ .

If the parameter  $K$  is slightly less than 2.560, the displacement of the second particle is small but near that in the bulk. As the parameter  $K$  becomes smaller, the displacement of the second particle becomes smaller compared to that in the bulk, which means that the attractive force between the surface and the domain-wall becomes stronger. The position of the domain-wall comes

closer to the surface.

If the parameter  $K$  is slightly larger than 2.560, the displacement of the second particle is small but near that in the bulk. As the parameter  $K$  becomes larger, the displacement of the second particle becomes smaller compared to that in the bulk, which means that the attractive force between the surface and the domain-wall becomes stronger. The position of the domain-wall comes closer to the surface. However, as  $K$  becomes large still more and approaches to 2.624, the displacement of the second particle becomes large and approaches to that in the bulk, which means that the attractive force between the surface and the domain-wall becomes weaker. The position of the domain-wall goes away from the surface.

#### §4. Summary and Discussions

We paid attention to the surface effect on the ground state of one-dimensional competitive systems. To investigate the surface effect, we must analyze the system with “semi-infinite” length. The ground-state structure of the system with infinite length can be obtained by the effective potential method. However, the method is not applicable to the semi-infinite system. Therefore, we introduced a numerical calculation method called the multi-channel sweep-down method. This method is applicable not only to semi-infinite systems but also to finite systems.

We chose the competitive model introduced by Marchand, Hood and Caillé (MHC).<sup>13</sup> The model is composed of particles in the one-particle potential connected by the two-particle potential. The competition of the two potentials induces various modulated structures in the ground state. By means of the multi-channel sweep-down method, we investigated the free surface effect near the phase boundary between the uniform phase and the dimerized phase in the ground-state phase-diagram of the infinite system.

In general, for the ground-state structure with period  $p$ , there are  $p$  types of surface. Then, in the dimerized phase, there are two types of surface. One of them (called the  $u^-$  surface in the previous section) induces no attractive surface phenomena.

There is no inconsistency between the surface configuration and the bulk configuration. The surface configuration connects smoothly with the bulk configuration. At the phase boundary, however, we obtain the penetration behavior of the surface effect.

For the other type of surface (the  $u^+$  surface), the surface effect induces an unexpected characteristic behavior. In the dimerized phase, the direction of the particle displacement from the reference place changes alternately. In a parameter region, the “phases” of the alternation near the surface and in the bulk become different. Thus, the system is composed from two domains with different-type particle-configurations. In the area where the two types of configuration connect, the particle nearly remains at the reference place. This type of the particle configuration is called as “twist” and this area in the system is called as domain-wall. Near the phase boundary, the ground state energy is independent of the position of the domain-wall. This means that the domain-wall

hops freely. In addition to the parameter region, the free domain-wall appears at an isolated point in the parameter space. In other regions, the domain-wall is bound near the surface.

The cause of the different “types” of domain-wall is understood as follows. Near the phase boundary ( $K \geq 2.624$ ), the displacement of the surface particles is larger than that of the particles in the bulk. The displacement of the particles in the domain-wall is small. If the domain-wall of particles with small displacement approaches to the surface, the interaction potential energy between the surface particles and the particles in the domain-wall increases. This means existence of an “effective repulsive force” between the surface and the domain-wall. The range of the repulsive force is short. The domain-wall hops freely in the bulk region, outside of the range.

In the parameter region far from the phase boundary, the displacement of the surface particles (especially the second particle) is smaller than that of the bulk. Therefore, an “attractive force” exists effectively between the surface and the domain-wall. The attractive force binds the domain-wall to the surface. But at an isolated parameter point ( $K = 2.560$ ), the displacement of the surface particles is just equal to that of the bulk. The domain-wall hops freely in the bulk region. Around the parameter point, however, the displacement of the second particle is smaller than that in the bulk. The domain-wall is attracted to the surface and cannot hop freely in the bulk region.

In this scenario for the behaviors of the domain-wall, the competition between the one-particle potential  $V$  and the inter-particle potential  $W$  of the MHC model plays an important role. The competition changes the relative magnitude of the displacements of the surface particle and the bulk particle.

We have also performed the numerical calculation near the phase boundary between the uniform phase and the phase of period four. The phase transition is of first order. In the region, new surface effects different from those presented in the present paper are expected. The results will be published in other paper.

Systems of finite-length have recently been investigated by many authors,<sup>18-22)</sup> because the competition between walls on both sides shows interesting phenomena. Thin film of Ising ferromagnets with competing surface fields, which are directed in opposite direction on the surfaces, are discussed by Binder *et al.*<sup>20)</sup> They observe the interface localization-delocalization transition using Monte Carlo method. On the other hand, thin film of Heisenberg ferromagnets with competing surface fields are discussed by Jang and Grimson<sup>21)</sup> using Monte Carlo method. No spontaneous magnetization is observed in the Heisenberg system.

We can add a prediction to finite-length systems with

free surface on both sides. A finite-length system of the same type discussed in this paper will have two very different ground states as the number of the particles in the system is even or odd. For a system with even particles, we may not expect an interesting phenomenon except at the phase boundary. But for a system with odd particles, there must be a domain-wall in the system. The domain-wall, depending on the parameter, may stay near one of the two surfaces or may wander about inside the system.

The phenomena shown in this paper seem to be universal for other semi-infinite system with competitive interactions. We have a plan to investigate other semi-infinite systems. Those results will be published in near future.

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