Periodic metastable structures in the discrete φ^4 model

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(Received 25 September 2000; published 14 August 2001)

For the discrete φ^4 model a class of metastable periodic solutions is given in the form of Fourier series. From the symmetry consideration, we eliminate the harmonics with zero amplitudes and thus, reduce the number of degrees of freedom. For the rest of harmonics we establish the hierarchy of their significance. For solutions with a small period we give the exact expression of energy density in terms of amplitudes of harmonics. Conditions of existence and stability of the solutions are discussed. For some limiting cases the approximate solutions of different kinds are given. The analytical results are compared with the results of numerical study. We also discuss a mechanism of transition from a metastable periodic structure into the ground state and apply the results to the lock-in transition in dielectric crystals supporting incommensurate phase.

DOI: 10.1103/PhysRevE.64.036202 PACS number(s): 05.45.−a, 45.05.+x, 64.60.−i

I. INTRODUCTION

Recently there has been growing interest in incommensurate phases in dielectric crystals [1,2]. The incommensurate phase usually appears on cooling as a result of second-order phase transition from a high-symmetry phase. Just below the transition point the modulation has sinusoidal form. On further cooling the amplitude of modulation increases, therefore the role of anharmonicity also increases and the sinusoidal modulation gradually transforms into a low-symmetry commensurate phase with periodically arranged domain walls. As a rule, on cooling down below the domain wall regime, there is another phase transition, of the first order, at which the modulation disappears from the low-symmetry commensurate phase (lock-in transition). The phenomenological theory of the lock-in transition has been developed [3] but the microscopic features of this transition are not clear.

We have reported one possible mechanism of lock-in transition [4] according to which the transition occurs in the domain wall subsystem. Above the transition point, the domain walls are mutually repulsive that is why they are equally spaced. Below the transition point domain walls become mutually attractive, their equidistant arrangement becomes unstable and they start to move, collide, and annihilate by pairs. Each domain wall carries some energy that is why their annihilation is a phase transition of the first order. However, there are some crystals, for example, $NaNO_2$, where the modulation keeps the sinusoidal form until the lock-in transition [5]. In this case the mechanism described above cannot work.

In the present study, in frame of the φ^4 model, we consider the modulated phases near the lock-in transition. It is well known, that the φ^4 model does not show the effect of modulational instability due to the absence of the second-neighbor interactions [6]. However, modulated phases with sufficiently large amplitude of displacements can be stable or, more precisely, metastable. We estimate the stability limits for the metastable periodic structures and consider the transition from metastable state into the ground state as another possible mechanism of the lock-in transition, which can work for the case of $NaNO_2$ as well. We also show that the presence of imperfections like domain walls can reduce the range of stability of the metastable phase.

There exists a vast literature on the discrete φ^4 and Frenkel-Kontorova (FK) [7] models [8–14]. The periodic solutions to these models can be found by, for example, map technique [13,14].

The φ^4 model with the next-nearest interactions, rewritten in several mathematically equivalent forms, like the discrete frustrated φ^4 (DIFFOUR) model and the elastically-hinged molecule (EHM) model, has been used in the incommensurate phase studies [4,6,15–21]. Analytic expressions for some periodic metastable solutions were given, e.g., by Janssen and Tjon [16] and by Ishibashi [17]. An approximate seven-periodic solution has been given by Hlinka, Orihara, and Ishibashi [19].

In the present paper we give a class of periodic solutions to the φ^4 model. This class is a subset of all possible periodic solutions, but it contains all the solutions that can appear as a result of modulational instability in the φ^4 model with the next-nearest interaction.

The Hamiltonian of the φ^4 and FK models can be written in the form

$$H=\sum_n \left[\frac{1}{2}\dot{u}_n^2+\frac{C}{2}(u_{n+1}-u_n)^2+V_n\right], \tag{1}$$

where u_n is the displacement of the nth particle. The first term in the right-hand side of Eq. (1) is the kinetic energy of nth particle, the second term gives the energy of the elastic bond between nth and $(n+1)$th particles. The bond has the unit length and the elastic constant C. The third term is the energy of nth particle due to the on-site potential, which is often taken in one of the two following forms:

$$V_n=\frac{1}{4}(1-u_n^2)^2 \quad \text{for} \quad \varphi^4, \tag{2}$$

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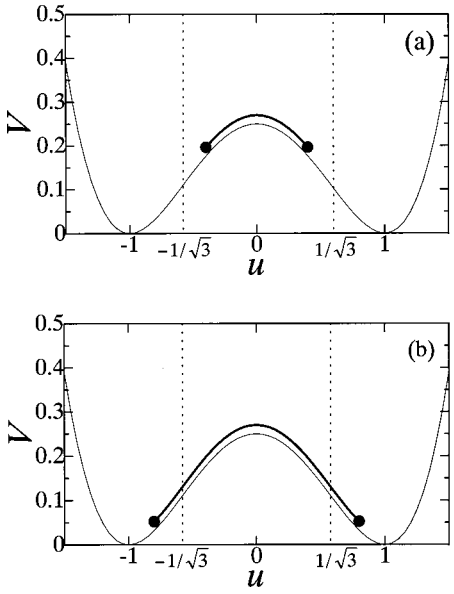

FIG. 1. The two elastically bound particles in the double-well potential. (a) A case of a strong elastic bond. Equilibrium is unstable. (b) For a weak elastic bond, when particles are below the inflection point of the potential, equilibrium is stable.

$$V_n = 1 - \cos(u_n), \quad \text{for FK.} \tag{3}$$

The equations of motion corresponding to Eq. (1) are

$$\ddot{u}_n - C(u_{n-1} - 2u_n + u_{n+1}) + V_n' = 0. \tag{4}$$

We consider, as the starting point, the two elastically bound particles placed into the potential $V(u) = \frac{1}{4}(1-u^2)^2$ as is shown in Fig. 1. In (a) and (b), the equilibrium states are presented for the cases of a strong and a weak elastic bond, respectively. It is easily seen that the equilibrium in (a) is unstable. Indeed, let us consider a small displacement of both particles, say, to the right and assume, for the sake of simplicity, that the length of the bond does not change. Then, the increase of the potential energy for the left particle will be smaller than the decrease of the energy for the right particle, so the total energy will decrease. However, in (b), the equilibrium is stable because a similar displacement of the particles causes an increase of the potential energy. This simple consideration suggests that, for bonds weak enough, the metastable structures can exist in the φ^4 model. The particles in a stable configuration are below the inflection point of the potential which is at $u = \pm 1/\sqrt{3}$.

The paper is organized as follows. In Sec. II, a class of the periodic solutions to the φ^4 model is described. The solutions are divided into four groups with the periods 2, $4l$, $4l+2$, and $2l+1$, where l is a positive integer. In Secs. III and IV, we give some exact and approximate analytical solutions, respectively. In Sec. IV D, we apply the obtained results to the discussion of the lock-in transition. In Sec. V, the existence and stability of the solutions are discussed. In Sec. VI, which concludes the paper, we briefly discuss the FK model.

II. PERIODIC SOLUTIONS

Obviously, Eq. (4) with the φ^4 on-site potential Eq. (2) has the unstable trivial solution, $u_n = 0$, and the two stable solutions, $u_n = \pm 1$. Besides, the model admits the stability of the N-periodic structures ($u_n = u_{n+N}$) given below.

We study the structures with a rational wave number

$$\kappa = \frac{M}{N}, \quad 2M \leqslant N, \tag{5}$$

where M and N are coprime positive integers.

A two-periodic structure ($N=2$, $\kappa = 1/2$) is given by

$$u_n = A\cos[2\pi\kappa(n+m)] = \pm(-1)^n A. \tag{6}$$

Other even-periodic structures are divided into two subsets, one with the period $N = 4l$ (l is a positive integer)

$$u_n = \sum_{j=1}^{N/4} A_j \cos\left[(2j-1)\left\{2\pi\kappa(n+m) + \frac{\pi}{N}\right\}\right], \tag{7}$$

and another one with the period $N = 4l+2$

$$u_n = \sum_{j=1}^{(N/2+1)/2} A_j \cos[2\pi\kappa(2j-1)(n+m)]. \tag{8}$$

Odd-periodic structures with $N = 2l+1$ can be written as

$$u_n = \pm A_{(N+1)/2} \pm \sum_{j=1}^{(N-1)/2} A_j \cos[2\pi\kappa(2j-1)(n+m)]. \tag{9}$$

In Eqs. (6)–(9), m can take any value from the set $m = \{0,1,\ldots,N-1\}$ and amplitudes A_j are the unknown functions of the parameter C.

Equations (6), (7), and (8) each describe N different domains of N-periodic structure, each domain being defined by m. Equation (9) describes $2N$ different domains of N-periodic structure with an odd N, each domain being defined by m and by a specific choice of the sign.

The way of numbering of the harmonics in Eqs. (7)–(9) differs from the conventional way of numbering of the Fourier harmonics. The advantage of the numbering used here is that $|A_1| > |A_2| > \ldots$. The Fourier representation for the periodic structures given above takes into account the symmetry of the structures and thus, reduces the number of degrees of freedom.

Even-periodic structures Eqs. (6)–(8) have concentration 1/2 (fraction of particles lying in, say, left well of the on-site potential). An odd-periodic structure Eq. (9) with period N has concentration $(N-1)/2N$ that approaches 1/2 with increase in N.

As it is well known, the φ^4 model with $C \to 0$ supports an infinite number of structures, periodic and chaotic. For a small C the periodic structures with concentrations different from 1/2 are possible. For example, one can easily imagine the $1/(N-1)$ concentration structure with all particles, except each Nth particle, lying in the same well of the on-site potential. Thus, the solutions Eqs. (6)–(9) do not give an

exhaustive list of periodic solutions, but, as mentioned above, they give an exhaustive list of solutions that can appear as a result of modulational instability in the φ^4 model with the next-nearest interaction.

To describe an arbitrary periodic structure one has to consider the Fourier series in a general form. For example, for an arbitrary odd-periodic structure, Eq. (9) can be written in the form

$$u_n = \pm A_{(N+1)/2} \pm \sum_{j=1}^{(N-1)/2} A_j \cos[2\pi\kappa(2j-1)(n+m)+\varphi_j], \tag{10}$$

where the $(N+1)/2$ amplitudes A_j and $(N-1)/2$ phases φ_j are the N parameters of the Fourier decomposition. In the present paper we restrict ourselves by the structures with $\varphi_j=0$ so it is important to demonstrate that energy of the structure always has a local minimum at all $\varphi_j=0$. To prove it, we substitute Eq. (10) into the Hamiltonian Eq. (1) with the on-site potential Eq. (2) and average the energy over one period (N particles). It turns out that the energy contributions from the harmonic terms $\Sigma(u_{n+1}-u_n)^2$ and Σu_n^2 do not depend on the phase φ_j. The phase-sensitive term is the anharmonic term Σu_n^4. This term has a local extremum at $\varphi_j=0$ because it is an even function of φ_j. It is not difficult to show that the extremum is a local minimum. For the even-periodic structures the analysis is similar.

III. EXACT SOLUTIONS

In this and in the two following sections we consider the φ^4 model.

A. Two-periodic structure

Substituting Eq. (6) into Eq. (1) one can express the energy density of the two-periodic structure as

$$U_2 = 2CA^2 + \frac{1}{4}(1-A^2)^2. \tag{11}$$

From the condition $dU_2/dA=0$ the following nontrivial solution for amplitude can be found

$$A^2 = 1-4C, \tag{12}$$

and hence, $U_2=2C-4C^2$. The solution exists for $C\leqslant 1/4$ and it is stable for $C<1/6$. At $C=1/6$, the absolute value of displacement $|u_n|=A=1/\sqrt{3}$, which is the abscissa of the inflection point of the double well potential.

B. Structures with period 4*l*

For the displacements u_n given by Eq. (7) we calculate the terms of the Hamiltonian Eq. (1) averaged within one period

$$\frac{1}{N}\sum_{n=1}^{N} u_n^2 = \frac{1}{2}\sum_{j=1}^{N/4} A_j^2, \tag{13}$$

$$\frac{1}{N}\sum_{n=1}^{N} (u_{n+1}-u_n)^2 = \sum_{j=1}^{N/4} A_j^2\{1-\cos[(2j-1)2\pi\kappa]\}. \tag{14}$$

The averaged anharmonic term of Eq. (1) for a given N can be written in the form

$$\frac{1}{N}\sum_{n=1}^{N} u_n^4 = X_N, \tag{15}$$

where X_N is a function of the amplitudes A_j. Let us write the function X_N in an explicit form for $N=4,8,12$:

$$X_4 = \frac{1}{4}A_1^4, \tag{16}$$

$$X_8 = \frac{3}{8}(A_1^2+A_2^2)^2 + \frac{1}{2}(A_1^3A_2 - A_1A_2^3), \tag{17}$$

$$X_{12} = \frac{3}{8}(A_1^2+A_3^2)^2 + \frac{1}{4}A_2^4 + \frac{3}{2}(A_1^2A_2^2 + A_2^2A_3^2 + A_1^2A_2A_3 - A_1A_2A_3^2) + \frac{1}{2}(A_1^3A_2 - A_2A_3^3). \tag{18}$$

Note that the anharmonic term is not a function of M. This means that it is same for different structures with the same period, for example, it is same for eight-periodic structures with $\kappa=1/8$ and $\kappa=3/8$. This will be also true for the anharmonic terms of structures with periods $4l+2$ and $2l+1$.

Particularly, for the four-periodic structure ($M=1,N=4$) the energy density, in view of Eqs. (13)–(16), has the form

$$U_4 = \frac{C}{2}A_1^2 + \frac{1}{4}\left(1-\frac{1}{2}A_1^2\right)^2. \tag{19}$$

The minimum energy condition is satisfied at

$$A_1^2 = 2-4C, \tag{20}$$

which is possible for $C\leqslant 1/2$. In view of Eq. (20), the energy density of the four-periodic structure can be written as $U_4=C-C^2$. The four-periodic structure is stable when $C<1/3$. At $C=1/3$, the absolute value of the displacement is equal to $|u_n|=1/\sqrt{3}$, which is the abscissa of the inflection point of the double well potential.

C. Structures with period 4*l*+2

For the displacements u_n given by Eq. (8) we calculate the terms of the Hamiltonian Eq. (1) averaged within one period

$$\frac{1}{N}\sum_{n=1}^{N} u_n^2 = A_{(N/2+1)/2}^2 + \frac{1}{2}\sum_{j=1}^{(N/2-1)/2} A_j^2, \tag{21}$$

$$\frac{1}{N}\sum_{n=1}^{N}(u_{n+1}-u_n)^2 = 4A_{(N/2+1)/2}^2 + \sum_{j=1}^{(N/2-1)/2} A_j^2\{1-\cos[(2j-1)2\pi\kappa]\}, \tag{22}$$

$$\frac{1}{N}\sum_{n=1}^{N} u_n^4 = X_N, \tag{23}$$

where X_N is a function of the amplitudes A_j. Particularly, for $N=6,10,14$,

$$X_6 = \frac{3}{8}A_1^4 + A_2^4 + A_1^3A_2 + 3A_1^2A_2^2, \tag{24}$$

$$X_{10} = \frac{3}{8}(A_1^4+A_2^4) + A_3^4 + \frac{3}{2}A_1^2A_2^2 + \frac{1}{2}(A_1^3A_2 + A_1A_2^3) + 3A_3^2(A_1^2+A_2^2) + 3A_3(A_1^2A_2 + A_1A_2^2), \tag{25}$$

$$X_{14} = \frac{3}{8}(A_1^4+A_2^4+A_3^4) + A_4^4 + \frac{3}{2}(A_1^2A_2^2 + A_1^2A_3^2 + A_2^2A_3^2) + \frac{1}{2}(A_1^3A_2 + A_1A_3^3 + A_2^3A_3) + \frac{3}{2}(A_1^2A_2A_3 + A_1A_2^2A_3 + A_1A_2A_3^2) + 3A_4(A_1A_2^2 + A_1^2A_3 + A_2A_3^2 + 2A_1A_2A_3) + 3A_4^2(A_1^2+A_2^2+A_3^2). \tag{26}$$

In view of Eqs. (21)–(24), the energy density of the six-periodic structure ($M=1$, $N=6$) is

$$U_6 = \frac{1}{4} + \frac{C}{4}(A_1^2+8A_2^2) - \frac{1}{4}A_1^2 - \frac{1}{2}A_2^2 + \frac{1}{4}\left(\frac{3}{8}A_1^4 + A_2^4 + A_1^3A_2 + 3A_1^2A_2^2\right). \tag{27}$$

The minimum energy conditions are satisfied at

$$A_1 = \gamma A_2, \quad A_2^2 = \frac{4(1-C)}{3\gamma^2+6\gamma+12}, \tag{28}$$

where $\gamma<-1$ is a real root of

$$(1-C)\gamma^3 + 3(1+2C)\gamma^2 - 6(1-4C)\gamma - 4(2-11C) = 0. \tag{29}$$

From Eq. (28) it follows that the six-periodic solution does not exist for $C>1$.

D. Structures with period $2l+1$

For the displacements u_n given by Eq. (9) we calculate the terms of the Hamiltonian Eq. (1) averaged within one period

$$\frac{1}{N}\sum_{n=1}^{N} u_n^2 = A_{(N+1)/2}^2 + \frac{1}{2}\sum_{j=1}^{(N-1)/2} A_j^2, \tag{30}$$

$$\frac{1}{N}\sum_{n=1}^{N}(u_{n+1}-u_n)^2 = \sum_{j=1}^{(N+1)/2} A_j^2\{1-\cos[(2j-1)2\pi\kappa]\}, \tag{31}$$

$$\frac{1}{N}\sum_{n=1}^{N} u_n^4 = X_N, \tag{32}$$

with

$$X_3 = X_6, \quad X_5 = X_{10}, \quad X_7 = X_{14}, \tag{33}$$

where X_6, X_{10}, X_{14} are given by Eqs. (24)–(26). Note that the averaged terms u_n^2 and u_n^4 for the $(2l+1)$-periodic structure coincide with that for the $(4l+2)$-periodic structure. This is not surprising because these structures can be obtained one from another by changing the sign of displacements for each odd (or even) node [17].

Density of potential energy of the three-periodic structure ($M=1$, $N=3$) is

$$U_3 = \frac{1}{4} + \left(\frac{3C}{4} - \frac{1}{4}\right)A_1^2 - \frac{1}{2}A_2^2 + \frac{1}{4}\left(\frac{3}{8}A_1^4 + A_2^4 + A_1^3A_2 + 3A_1^2A_2^2\right). \tag{34}$$

The energy has minimum at

$$A_1 = \gamma A_2, \quad A_2^2 = \frac{4-12C}{3\gamma^2+6\gamma+12}, \tag{35}$$

where $\gamma<-1$ is a real root of

$$(1-3C)\gamma^3 + 3(1-6C)\gamma^2 - 6\gamma - 4(2+3C) = 0. \tag{36}$$

It can be seen from Eq. (35) that the three-periodic structure does not exist for $C>1/3$. Actually, the solution exists for $C<C^*$, where $C^*\approx 0.135$ is such that the discriminant of the cubic Eq. (36) equals to zero and the two real roots merge together.

IV. APPROXIMATE SOLUTIONS

A. Limit of $C\to 0$

At $C\to 0$ the displacements of particles $u_n \to \pm 1$ and the amplitudes of harmonics in Eqs. (6)–(9) approach the values A_j^0 given below.

For the two-periodic structure

$$A^0 = 1. \tag{37}$$

For the even-periodic structures with the period $N=4l$ (l is a positive integer)

$$A_j^0=(-1)^j\frac{4}{N}\sqrt{1+S_j^2},\quad j=1,\ldots,N/4, \tag{38}$$

where

$$S_j=\sum_{k=1}^{N/2}\sin\left[\frac{(2j-1)2\pi k}{N}\right]. \tag{39}$$

For the even-periodic structures with the period $N=4l+2$

$$A_j^0=(-1)^j\rho_j\frac{4}{N}\sqrt{1+S_j^2},\quad j=1,\ldots,(N/2+1)/2, \tag{40}$$

where S_j is given by Eq. (39) and

$$\rho_j=1\quad\text{for}\quad j\neq(N/2+1)/2,$$
$$\rho_j=\frac{1}{2}\quad\text{for}\quad j=(N/2+1)/2. \tag{41}$$

For the odd-periodic structures with $N=2l+1$ the amplitudes are

$$A_j^0=(-1)^j\rho_j\frac{4}{N}\sqrt{\frac{1}{4}+S_j^2},\quad j=1,\ldots,(N+1)/2, \tag{42}$$

where

$$S_j=\sum_{k=1}^{(N-1)/2}\sin\left[\frac{(2j-1)2\pi k}{N}\right], \tag{43}$$

and

$$\rho_j=1\quad\text{for}\quad j\neq(N+1)/2,$$
$$\rho_j=\frac{1}{2}\quad\text{for}\quad j=(N+1)/2. \tag{44}$$

The amplitudes A_j^0 given above can be used as a zero approximation for the construction of the approximate solutions at a small C. For example, for the six-periodic structure ($\kappa=1/6$), from Eq. (40) one finds $A_1^0=4/3$ and $A_2^0=-1/3$. Then, for a small C, one can find the following estimation

$$A_1=4/3+a_1,\quad A_2=-1/3-a_1/2+a_2,$$
$$a_1=\frac{-b+\sqrt{b^2-4ac}}{2a},\quad a_2=\frac{21a_1^2+24a_1C+12a_1+16C}{60a_1+48C+24}, \tag{45}$$

where $a=33C+24$, $b=12C^2+42C+12$, $c=16C^2+8C$, and we assumed $a_1\ll 1$ and $a_2\ll a_1$.

For the case of a large C the exact solution given by Eq. (28) can be simplified assuming that $A_1\ll 1$ and $A_2\ll A_1$. The result reads

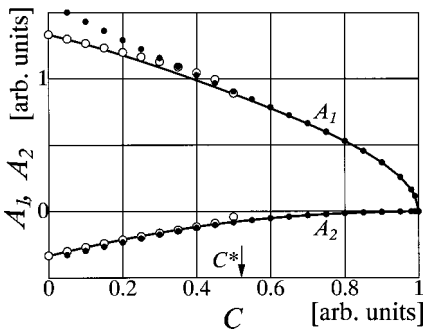

FIG. 2. Amplitudes of Fourier harmonics for the six-periodic structure as a function of C. The exact solution is shown by the thick solid lines. Small C approximation Eq. (45) is shown by the open circles and the solid circles show the small amplitude approximation Eq. (46). The solution does not exist for $C>1$. The six-periodic solution is unstable for $C>C^*=0.520$. The stability criteria Eqs. (59) and (60) give the estimations $C^*=0.567$ and $C^*=0.550$, respectively.

$$A_1=\sqrt{-\frac{3}{2}(2C-1)+\sqrt{\frac{11}{3}C^2-\frac{7}{3}C+\frac{11}{12}}},$$
$$A_2=\frac{-A_1^3}{16C-4+6A_1^2}. \tag{46}$$

In the succeeding section a similar two-harmonic approximation will be given for structures with any κ except $\kappa=0,1/2,1/3,1/4,1/6$.

In Fig. 2 we compare the exact solution for the six-periodic structure Eq. (28) with the approximate solutions. The exact result is shown by the solid lines, small C approximation Eq. (45) is shown by the open circles and the solid circles show the small amplitude approximation Eq. (46). The solution does not exist for $C>1$, which is consistent with Eq. (57). We found numerically the stability limit for the six-periodic solution as $C^*=0.520$. The approximate stability criterion Eq. (59) gives an estimation $C^*=0.567$ and Eq. (60) gives $C^*=0.550$.

B. Two-harmonic approximation

If the displacements are small, the higher order harmonics can be neglected in Eqs. (7)–(9). Under the assumption $A_1\ll 1$ and $A_2\ll A_1$, the following two-harmonic approximation can be easily determined

$$u_n=A_1\cos(2\pi n\kappa+\varphi)+A_2\cos(6\pi n\kappa+3\varphi). \tag{47}$$

Substituting Eq. (47) into the Hamiltonian Eq. (1) and averaging over a period (N nodes), gives the energy density

$$U=\frac{1}{4}+\alpha A_1^2+\beta A_2^2+\frac{3A_1^4}{32}+\frac{A_1^3A_2}{8}+\frac{3A_1^2A_2^2}{8},$$
$$\text{for}\quad \kappa\neq 0,\frac{1}{2},\frac{1}{3},\frac{1}{4},\frac{1}{6}, \tag{48}$$

with

$$\alpha = C\sin^2(\pi\kappa) - \frac{1}{4}, \quad \beta = C\sin^2(3\pi\kappa) - \frac{1}{4}. \tag{49}$$

The energy Eq. (48) has minimum at

$$A_1 = \sqrt{-\frac{8}{5}(2\alpha+\beta) + \frac{8}{5}\sqrt{(2\alpha+\beta)^2 - \frac{20}{3}\alpha\beta}},$$

$$A_2 = \frac{-A_1^3}{16\beta + 6A_1^2}. \tag{50}$$

The phase of the solution Eq. (47) cannot be determined without taking into account the higher harmonics. To make the approximation Eq. (47) consistent with Eqs. (7)–(9), we put

$$\varphi = \frac{\pi}{N}, \quad \text{for } N = 4l,$$

$$\varphi = 0, \quad \text{for other } N. \tag{51}$$

Note that Eqs. (48)–(50) are valid for any κ except $\kappa = 0,1/2,1/3,1/4,1/6$. For these exceptional cases the exact solutions were given in Sec. III. An approximate two-harmonic solution for the structure with $\kappa = 1/6$ is given by Eq. (46).

Equation (47) is accurate only for small amplitudes. However, this solution will be used for rough estimations in the numerical investigation. We will also use this solution for discussion of the existence condition for various periodic structures.

C. Kink at a small *C*

Let us consider the kink, which is the transition of particles from one well of the on-site potential to another one, as it is shown in Fig. 3(a). For C small enough, one can assume that only two particles from each side of the kink have displacements different from ± 1. Taking into account the symmetry, there are two unknown displacements, u_0 and u_1. Under the assumption $1-u_0 \ll 1$ and $1-u_1 \ll 1-u_0$, we find

$$u_0 = 1 - b + \sqrt{b^2 - \frac{2C}{3}}, \quad u_1 = 1 - \frac{C}{2+C}(1-u_0), \tag{52}$$

where $b = (2+4C+C^2)/(6+3C)$.

The energy of the kink is

$$U_K = \frac{1}{2}(1-u_0^2)^2 + \frac{1}{2}(1-u_1^2)^2 + C(3u_0^2 + 2u_1^2 - 2u_0u_1 - 2u_1 + 1). \tag{53}$$

In Fig. 3(b), the numerically obtained magnitudes for u_0 and u_1 (solid lines) are compared with the approximate solution Eq. (52) (dashed lines).

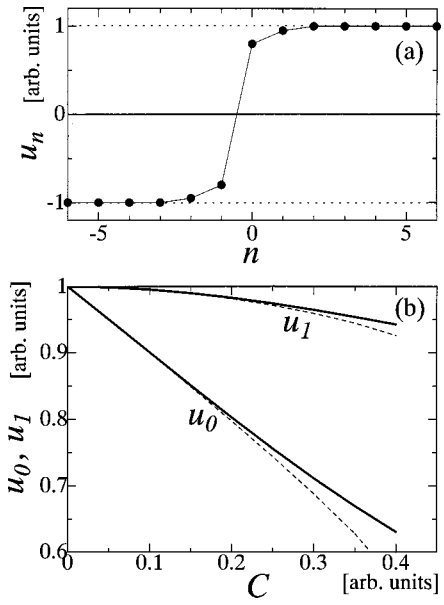

FIG. 3. (a) Kink at a small C. We assume that only two particles from each side of the kink have displacements different from ± 1. (b) Numerically obtained u_0 and u_1 as functions of C are shown by the solid lines. Approximate solution Eq. (52) is shown by the dashed lines.

D. Domain wall in two-periodic structure—Autowaves

There are two different domains of the two-periodic structure. In one domain the even nodes have positive displacements and in another domain so do the odd nodes. In Fig. 4(a), the domain wall separating two domains is presented. Assuming that only two particles from each side of the domain wall have displacements different from $\pm A$, where A is given by Eq. (12), and taking into account the symmetry, one can find for u_0 and u_1 the following approximation:

$$u_0 = A + \frac{-b + \sqrt{b^2 + 24A^2C}}{6A},$$

$$u_1 = -A + \frac{C}{2-10C}(u_0 - A), \tag{54}$$

where $b = (4-42C+109C^2)/(2-10C)$ and we assumed $u_0 - A \ll 1$ and $u_1 + A \ll u_0 - A$. The energy of the domain wall is

$$U_{DW} = \frac{1}{2}(1-u_0^2)^2 + \frac{1}{2}(1-u_1^2)^2 + C(u_1-u_0)^2 + C(u_1-A)^2 - 10CA^2 - (1-A^2)^2, \tag{55}$$

which is the difference between energy of the structure having a domain wall and the energy of the ideal two-periodic structure.

Domain wall in the two-periodic structure is stable if

$$3u_1^2 + 2C - 1 > 0. \tag{56}$$

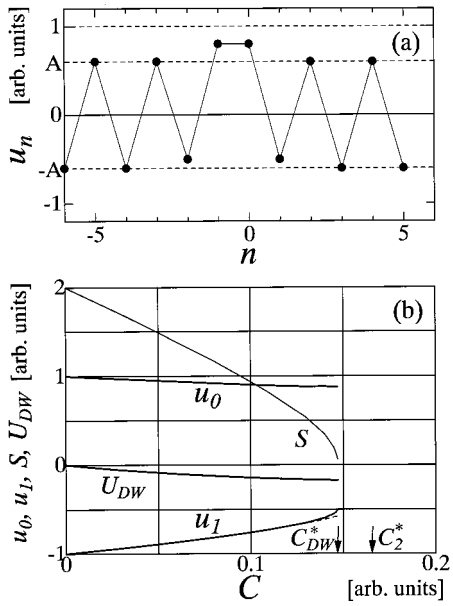

FIG. 4. (a) The domain wall in the two-periodic structure. We assume that only two particles from each side of the domain wall have displacements different from $\pm A$. (b) Numerically found displacements u_0 and u_1 are plotted by the solid lines and the approximate solution Eq. (54) is shown by the dashed lines. For the displacement u_0 curves overlap each other. For u_1 the deviation is noticeable only at the stability limit of the domain wall, which is at $C^*_{DW}=0.147$. The stability limit for two-periodic structure is $C^*_2=1/6\approx 0.167$. Line S shows the left-hand side of Eq. (56), which is the stability criterion for the domain wall. U_{DW} is the energy of the domain wall.

This approximate stability criterion can be derived considering the change in the energy of domain wall due to a small perturbation of u_0 and u_1.

The results of numerical study of the domain wall are presented in Fig. 4(b). Numerically found displacements u_0 and u_1 are plotted by the solid lines and the approximate solution Eq. (54) is shown by the dashed lines. For the displacement u_0 curves overlap each other. For u_1 the deviation is noticeable only at the stability limit of the domain wall, which is at $C^*_{DW}=0.147$. Note that the stability limit for two-periodic structure is $C^*_2=1/6\approx 0.167$. The line labeled S shows the left-hand side of Eq. (56), which is the stability criterion for the domain wall. One can see that S approaches zero when C approaches C^*_{DW}. We also plot the energy of the domain wall U_{DW}. Note that U_{DW} is always negative therefore, the domain wall can be viewed as a nucleus of the lowest energy phase.

The two-periodic structure with a domain wall shows an interesting behavior at C lying between C^*_{DW} and C^*_2. In this case the two-periodic structure is stable but the domain wall is unstable. The unstable domain wall initializes the two autowaves moving in the opposite directions and transforming the two-periodic structure into the ground state $u_n=1$. This process is presented in Fig. 5 at $C=0.15$. For this simulation, we added the dissipative term with the coefficient equal to unity to the equation of motion Eq. (4). In spite of the dissipation, the autowaves move with a constant velocity. The

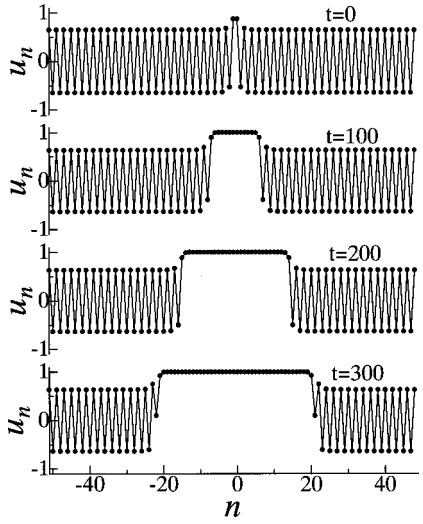

FIG. 5. The unstable domain wall initializes the two autowaves moving in the opposite directions and transforming the two-periodic structure into the ground state $u_n=1$ ($C=0.15$). We introduced a strong dissipation in the system. In spite of the dissipation, the autowaves move with a constant velocity. The driving force for this motion comes from the energy delivered in the structure transformation.

driving force for this motion comes from the energy delivered in the structure transformation.

In the above example, the transformation of the two-periodic structure into the ground state was studied. However, the same effect can be observed for other metastable periodic structures. Domain walls in any structure, except the two-periodic one, are of two types. One type of domain wall is formed by removal of a node of the chain and another type is formed by adding of a node. The critical conditions for the domain walls of different types are different.

In our opinion, the loss of stability by a modulated metastable structure described above and illustrated in Fig. 5, can be regarded as a mechanism of the lock-in transition. By contrast to the mechanism described in [4], the mechanism proposed here can work for the case of $NaNO_2$ as well.

V. EXISTENCE AND STABILITY

Let us determine the existence region for a structure with any κ. At the existence limit, the displacements are nearly zero and even single-harmonic approximation is valid. Putting $A_2=0$ in Eq. (48), one finds that the energy has minimum at $A_1=4\sqrt{-\alpha/3}$, which is correct for any κ except $\kappa=0,1/2,1/4$. Thus, the solution with the wave number κ exists when $\alpha<0$, or

$$C<\frac{1}{4\sin^2(\pi\kappa)}. \tag{57}$$

In spite of the fact that the estimation for A_1 is not valid for $\kappa=0,1/2,1/4$, Eq. (57) is correct even for these exceptional cases.

Equation (57) suggests that the structures with a small κ exist in a wide range of parameter C, while the short periodic structures exist only in a highly discrete chain (small C).

Let u_n^0 be a known N-periodic equilibrium solution to Eq. (4). To examine it for stability one can study the time evolution of a small perturbation $u_n(t)=u_n^0+\varepsilon_n(t)$. The solution u_n^0 is stable if the dispersion relation of the linearized equation of motion for the function $\varepsilon_n(t)$ has no imaginary frequencies. However, this approach allows to check for stability only the simplest structures.

To simplify the problem, let us assume that perturbation is a constant. Substituting $u_n=u_n^0+\varepsilon$ into the Hamiltonian Eq. (1), we calculate the variation of energy due to the perturbation and average the energy over one period (N nodes)

$$\Delta U=\frac{\varepsilon}{2N}\sum_{n=1}^{N}\left[3\varepsilon(u_n^0)^2-\varepsilon+2(u_n^0)^2-u_n^0\right], \qquad (58)$$

where we omitted the higher order terms in ε. The stability condition is $d^2(\Delta U)/d\varepsilon^2>0$. However, assuming a constant perturbation we overestimated the stability of the system. Thus, we can claim that a structure with the wave number κ cannot be stable if

$$\frac{1}{N}\sum_{n=1}^{N}(u_n^0)^2<\frac{1}{3}. \qquad (59)$$

Obviously, the found stability condition is accurate for the structures with $\kappa=1/2$ and 1/4.

The stability criterion Eq. (59) suggests that the displacements in a stable structure are large.

A more precise stability criterion can be obtained under the assumption that the perturbation is proportional to the shape of the on-site potential $u_n=u_n^0+[1-(u_n^0)^2]^2\varepsilon$. Similar calculations show that the structure cannot be stable if

$$\frac{1}{N}\sum_{n=1}^{N}\left[C(V_{n+1}^0-V_n^0)^2+(V_n^0)^2[3(u_n^0)^2-1]\right]<0, \qquad (60)$$

where $V_n^0=[1-(u_n^0)^2]^2$. This criterion is accurate for the structures with $\kappa=1/2$, 1/3, and 1/4.

VI. CONCLUSION

In the present paper the φ^4 model was discussed. The FK model also supports the periodic metastable solutions given by Eqs. (6)–(9). The properties of the solutions are very similar for both of these models. The only important difference between them is that in the FK model the particles can occupy more than two wells of the on-site potential. However, here we will not discuss this general case.

The curvature of the FK on-site potential at the top of the potential barrier coincides with that for the φ^4 potential. That is why the existence condition Eq. (57) is true for either model.

Let $u_n^0+\pi$ is a periodic equilibrium solution to the FK model. The shift by π means that we consider the displacements with respect to the top of the potential. Considering the perturbation in the form of a constant, $u_n=u_n^0+\pi+\varepsilon$, we find that the solution cannot be stable if

$$\frac{1}{N}\sum_{n=1}^{N}\cos(u_n^0)>0. \qquad (61)$$

Thus, we have described a class of periodic equilibrium solutions to the φ^4 and FK models. They are also the solutions to the φ^4 model with the next-nearest interactions and, sequentially, to the DIFFOUR and EHM models. In the φ^4 model the amplitude of a stable solution is large, while in the φ^4 model with the next-nearest interaction the solutions with vanishingly small amplitude can be stable. The described class of solutions is an exhaustive list of periodic structures that can appear as a result of modulational instability in the φ^4 model with the next-nearest interaction.

The solutions with a small wave number are stable in a wide range of the parameter C, while the solutions with a large wave number can be stable only in a highly discrete chains (small C). The described solutions are metastable, except for the case of $C=0$. A mechanism of transformation of a metastable structure into a ground state was discussed. The transformation occurs by means of motion of a pair of autowaves. The autowaves can be initialized, for instance, by an unstable domain wall.

The effect of instability of a metastable periodic structure gives a qualitative description of the lock-in transition when modulated phase in a dielectric crystal transforms to a low-symmetry commensurate phase.

ACKNOWLEDGMENTS

We thank Yu. S. Kivshar and O. Braun for valuable discussions. One of us, S.V.D., wishes to thank the Japan Society for the Promotion of Science for its financial support.

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