Volume 9, Number 1 January, 2000
1009-1963/2000/09(01)/0042-07 CHINESE PHYSICS © 2000 Chin. Phys. Soc.

STUDY ON ONE-DIMENSIONAL CI PHASE TRANSITION WITH TRIPLE-WELL INTERACTIONS*

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(Received 7 July 1999)

To study modulated structures and commensurate-incommensurate (CI) transitions, we generalize the Frenkel-Kontorova model to the Frenkel-Kontorova-Devonshire model where the interparticle interactions are the triple-well potential. By use of the so called effective potential method, numerical solutions of the eigenvalue problem are used to work out the exact phase diagrams of W, a triple-well potential. According to the winding number ω and the rotation number Ω, we analyze the periodicity of the phase diagram and find some complex but regular phase structures. These new structures result from the triple-well interatomic interactions. A series of new transition behaviors enrich the traditional understanding on the periodicity of CI transitions.

PACC: 6470R; 6460; 0570

I. INTRODUCTION

Commensurate-incommensurate(CI) phase transitions pose a number of interesting and challenging theoretical problems. One difficulty in studing them is the scarcity of exactly solvable models. The Frenkel-Kontorova(FK) model describes a one-dimensional chain of particles connected by harmonic springs subjected to an external sinusoidal potential.[1] The FK-type models are defined by the following potential energy,

$$H = \sum_{n=-\infty}^{\infty} [W(x_{n+1} - x_n) + V(x_n)] . \qquad (1)$$

They have been studied by Aubry[2], Copersmith and Fisher[3], Biham and Mukamel[4], and Hu *et al*[5]., when the interparticle interactions are convex. Griffiths and Chou[6] presented the effective potential method that can be used to the study of the FK-type models with nonconvex interparticle interactions. Such models are studied by Banejea and Taylor[7], Marchand[8], Yokoi[9], Xu[10] and Braun *et al*.[11] In recent years, Little and Zangwill[12] also introduced a Frenkel-Kontorova-Devonshire model where the usual quadratic spring potential is replaced by a phenomenological potential identical in form to a sixth-degree Landau free-energy functional introduced by Devonshire[13] in connection with a study of ferroelectricity. As a function of a single parameter (which is regarded as the temperature), the interparticle potential changes smoothly from a quadratic single well to a symmetric triple well and finally to a symmetric double well. Up to now, we only know very little about the models with the multi-well potentials, though Griffiths and Chou[6], Marchand[8] and Little and Zangwill[12] have done some attempts. In this parper, we devote to this kind of study through two microscopic models with triple-well interactions. According to the winding number ω and the rotation number Ω, we analyze the periodicity of the phase diagram and find some complex but regular phase structures. These new structures result from the triple-well interatomic interactions. A series of new transition behaviors enrich the traditional understanding on the periodicity of CI transitions.

An outline of the rest of the paper is as follows. The models are given in Sec. Ⅱ. Determining the ground states and recovering the chain of particles using the effective potential method are discussed in Sec. Ⅲ. In Sec. Ⅳ, we obtain the phase diagram as a function of K and γ. Finally, the main results are discussed and summarized in Sec. V. We can find that they yield phase diagrams with transitions between states with the same rotation number but different symmetry.

* Project supported by the National Natural Science Foundation of China (Grant No. 19774049) and Science Foundation of China Academy of Engineering Physics (Grant Nos. 970116 and 980112).

Ⅱ. THE MODELS

The Frenkel-Kontorova-Devonshire (FKD) model considered in this paper is defined by the potential energy

$$H=\sum_{n=-\infty}^{\infty}\Big[\frac{1}{2}a_2(x_{n+1}-x_n-\gamma)^2 + \frac{1}{4}a_4(x_{n+1}-x_n-\gamma)^4+\frac{1}{6}a_6(x_{n+1}-x_n-\gamma)^6 + K(1-\cos 2\pi x_n)\Big]. \quad (2)$$

Here, x_n is the position of the nth atom and γ is the lattice constant of the film material. Both are measured in units of the substrate lattice constant. The energy parameter K is the strength of the substrate potential, the coefficients a_2, a_4 and a_6 are linear functions of temperature. The generalized FK model is called one-dimensional FKD model.[12]

The first derivative of $W(x_{n+1}-x_n)$ with respect to $x_{n+1}-x_n$ is give by

$$W'(x_{n+1}-x_n)=a_2(x_{n+1}-x_n-\gamma) + a_4(x_{n+1}-x_n-\gamma)^3+a_6(x_{n+1}-x_n-\gamma)^5. \quad (3)$$

The simplest case occurs when all the coefficients are positive and W will have only a minimum value (i.e., single-well potential). However, if some of the other coefficients are negative, then the potential may take a more complicated form. Suppose that a_4 is negative and a_6 is positive. We will find that W have two minimum values when $a_2 \le 0$ and have three minimum values (i.e., triple-well potential) when $a_2 > 0$ and $|a_4| \ge 4a_2a_6$. With the increase of a_2, W will not have only a minimum value until $a_2 \ge |a_4|/4a_6$. That is to say, as a function of temperature, the potential changes from a quadratic single well to a symmetric triple-well and finally to a symmetric double-well. The generalized CI transition models with single-well interactions and double-well interactions discussed before are simply extreme cases in high-temperature and low-temperature of the triple-well interactions. In this paper, we focus on the case that three minimum values are equal. Then we have

$$a_2+a_4(x_{n+1}-x_n-\gamma)^2+a_6(x_{n+1}-x_n-\gamma)^4=0\,, \quad (4)$$

$$\frac{1}{2}a_2(x_{n+1}-x_n-\gamma)^2+\frac{1}{4}a_4(x_{n+1}-x_n-\gamma)^4 + \frac{1}{6}a_6(x_{n+1}-x_n-\gamma)^6=0\,, \quad (5)$$

and from Eqs.(4) and (5) we find

$$x_{n+1}-x_n-\gamma=\pm\sqrt{-\frac{3a_4}{4a_6}}\,, \quad (6)$$

$$a_2=\frac{3a_4^2}{16a_6}\,. \quad (7)$$

If we take $a_4=-4$, $a_6=3$, then we find $x_{n+1}-x_n-\gamma=\pm\gamma_1=\pm1.0$, $a_2=1$, so that $W(x_{n+1}-x_n)$ is given by

$$W(x_{n+1}-x_n)=\frac{1}{2}(x_{n+1}-x_n-\gamma)^2-(x_{n+1}-x_n-\gamma)^4 + \frac{1}{2}(x_{n+1}-x_n-\gamma)^6. \quad \text{(model 1)} \quad (8)$$

If we take $a_4=-3$, $a_6=1$, then we find $x_{n+1}-x_n-\gamma=\pm\gamma_2=\pm1.5$, $a_2=27/16$, so that $W(x_{n+1}-x_n)$ is given by

$$W(x_{n+1}-x_n)=\frac{27}{32}(x_{n+1}-x_n-\gamma)^2-\frac{3}{4}(x_{n+1}-x_n-\gamma)^4 + \frac{1}{6}(x_{n+1}-x_n-\gamma)^6. \quad \text{(model 2)} \quad (9)$$

The curves of $W(x)$ for the two models are shown in Fig.1. Figure 1(a) denotes $W(x)$ for model 1 and Fig.1(b) denotes that for model 2. $W(x)$ has three equal minima located at $x_{n+1}-x_n-\gamma=0,\pm1.0$ for model 1, and it also has three equal minima located at $x_{n+1}-x_n-\gamma=0,\pm1.5$ for model 2.

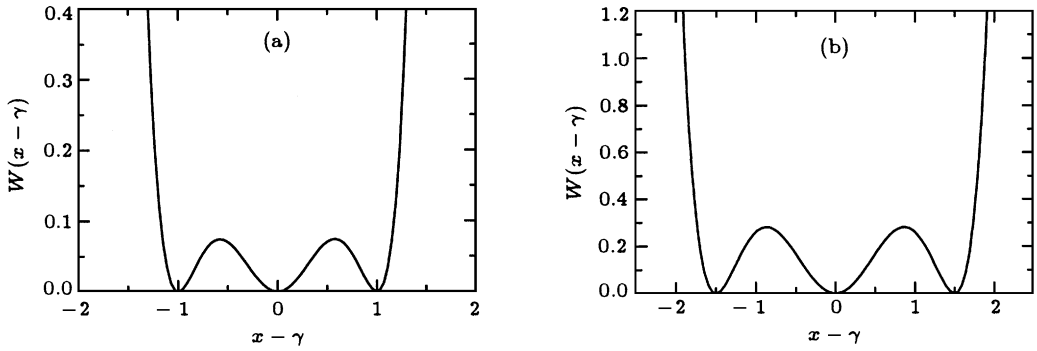


Fig.1. The curves of $W(x)$, Fig.1(a) for model 1 and Fig.1(b) for model 2.

Ⅲ. EFFECTIVE POTENTIAL AND GROUND STATES

The interparticle interactions is nonconvex, we need to make use of the effective potential method[6] with the numerical implementation suggested by Floria and Griffiths[14], in order that the ground states and the phase diagram can be obtained. One way to proceed is to discretize the unit cell. We replace the continuous set of possible particle positions x_n by a discrete u_n of G points uniformly spaced on an interval D which is the period of the external potential, where u_n denotes the displacement of the nth particle with respect to the substrate minimum,

$$u_n = -\frac{D}{2} + n\frac{D}{G} \qquad (n = 1, 2, \cdots, G)\,. \tag{10}$$

The relation between x_n and u_n is given by

$$u_n = x_n + m_n D\,, \tag{11}$$

where m_n is a certain integer. Typicaly we choose $G = 400$, $\epsilon = 10^{-5}$, although at the selected spots much larger values have to be used to confirm the ground states. Such checks occasionally produced minor cycle length changes although the ground state configurations are always qualitatively unchanged. As noted by Floria and Griffiths, convergence is generally slower when the ground state cycle length increases or there are nearly degenerate states near the ground state.

Under the minimum-enthalpy condition, W can be replaced by W^*, where $W^* = \min_m W(x+mD)$, m is an arbitary integer which satisfies a certain condition. Hence W^* is periodic in a certain direction and the period is just that of the external potential.

To characterize the modulted phase more precisely, we define two parameters as follows: the winding number is defined as

$$\omega = P/Q\,, \tag{12}$$

where Q is the period of the ground state and P is the period number of the external potential between the 1st and the $(Q+1)$th particles. One can find that when W is a convex function everywhere, this definition is equivalent to the tradition one of the winding number. Next define the rotation number

$$\Omega = \frac{1}{Q}\sum_{n=1}^{Q} \Theta(u_{n-1} - u_n)\,, \tag{13}$$

where Q is the period of the ground state, $u_Q = u_0$, and $\Theta(x) = +1$ (if $x \geq 0$) and $\Theta(x) = 0$ (if $x < 0$). In the following sections, one can find that $\omega = \Omega$ in some cases and $\omega \neq \Omega$ in other cases. The coorperation of the two parameters can yield more information about the ground states.

When we use the effective potential method to study the ground states, all the u_n contained in the interval $[-D/2, D/2]$ do not denote the real positions of the particles in the chain. We can recover the chain of particles in the following way. Once we have obtained the effective potential, then in the process of calculating the ground state, for a given $x_n = u_n$, we should record the period number of the external potential, say m_{n-1}, which should be moved to left from u_{n-1} to obtain x_{n-1}. Thus for a ground state of the period Q, assume $x_Q = u_Q$, then $x_{Q-1} = u_{Q-1} - m_{Q-1}D$, $x_{Q-2} = u_{Q-2} - (m_{Q-1} + m_{Q-2})D, \cdots, x_1 = u_1 - (m_{Q-1} + m_{Q-2} + \cdots + m_1)D$, $x_0 = u_0 - (m_{Q-1} + m_{Q-2} + \cdots + m_1 + m_0)D$, where $u_0 = u_Q$ and $\omega = P/Q \equiv (m_{Q-1} + m_{Q-2} + \cdots + m_1 + m_0)/Q$. In the following sections one can find that different ground states may correspond to the same unrecovered chain.

The examples of an effective potential $F(u)$ for a particular choice of K and γ are shown in Fig.2(a) for model 1 where $K = 0.03$, $\gamma = 1.75$, $\Omega = 4/5$, $\omega = 9/5$, and Fig.2(b) for model 2 where $K = 0.02$, $\gamma = 1.90$, $\Omega = 5/6$, $\omega = 13/6$. It is clear that $F(u)$ generally has many absolute minima of equal energy. These absolute minima are located at the possible atomic positions of the ground state.

In general, the periodic potential will tend to "lock" the system in a commensurate configuration. As a function of γ at fixed K, one expects the winding number ω to show a "devil's staircase" behavior.[15]

It is more interesting to examine the behavior of the effective potential $F(u)$. It is clear from Fig.3 that $F(u)$ generally has many absolute minima of equal energy, which are localized at the possible atomic positions of the ground state. Nevertheless, in the vicinity of the boundary between $\Omega = 1/2$ and $\Omega = 2/3$ phase field, the secondary minima are visible to be located at metastable atomic positions with higher energy. Starting from one of these secondary minima, the iteration will lead us to other secondary minima and ultimately to the ground-state periodic cycle. This sequence of atomic positions represents an elementary defect which we call a soliton. The soliton creation energy can be obtained by calculating the difference between the $F(u)$ evaluated at the atomic positions of the defect and that at the atomic positions of the ground state. However, because of discretization, the result obtained in this manner may not be very accurate.[8]

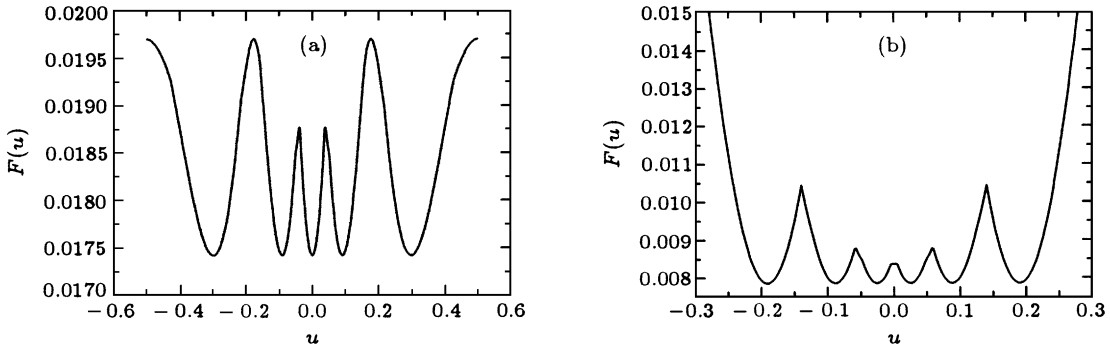


Fig.2. Examples of effective potential $F(u)$; Fig.2(a) shows $F(u)$ for model 1, where $K = 0.03$, $\gamma = 1.75$, $\Omega = 4/5$, $\omega = 9/5$, Fig.2(b) shows $F(u)$ for model 2, where $K = 0.02$, $\gamma = 1.90$, $\Omega = 5/6$, $\omega = 13/6$.

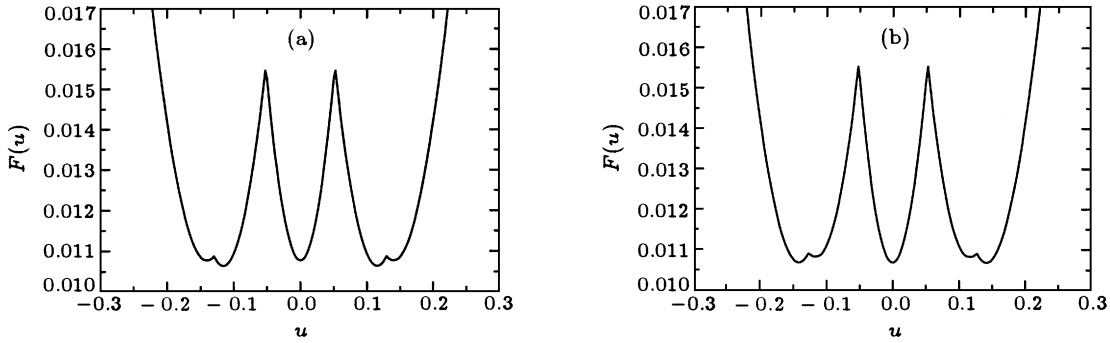


Fig.3. Effective potential $F(u)$ in the vicinity of $\Omega = 1/2$ and $\Omega = 2/3$ for model 1, where $K = 0.08$ (a) $\gamma = 1.6047$, $\Omega = 1/2$, (b) $\gamma = 1.6048$, $\Omega = 2/3$.

In the dimerized phase, if γ is changed such that the $\Omega = 2/3$ phase is approached [Fig.3(a)] then the three secondary minima, suggesting the proximity to the trimerized phase, appear. If γ is changed a little more [Fig.3(b)], then we move into the trimerized phase, where the three secondary minima of Fig.3(a) become the absolute minima. Clearly, the competition between the 1/2 and 2/3 phases is reflected in the competition between the two minima of the 1/2 phase and the three minima of the 2/3 phase. From Figs.3(a) and 3(b), the secondary minima and absolute minima are interchanged. In this range of γ values, the iteration has two periodic cycles: one cycle of period three located at the absolute minima of Fig.3(b) and another cycle of period two located at the absolute minima of Fig.3(a). The iteration then leads us to one of these two attractors depending on the starting position. The transition where the two different periodic cycles have been observed simultaneously is the first-order transition.

Figure 4 shows an example of ground state for model 1, where every black dot denotes a particle; Fig.4(a) shows the ground state $\{u_n\}$ where $K = 0.03$, $\gamma = 1.75$, $\Omega = 4/5$, $\omega = 9/5$. All the particles in one period of the ground state have been plotted in one well of the external potential, which do not denote the real positions of the particles; Fig.4(b) shows the recovered chain from Fig.4(a) in

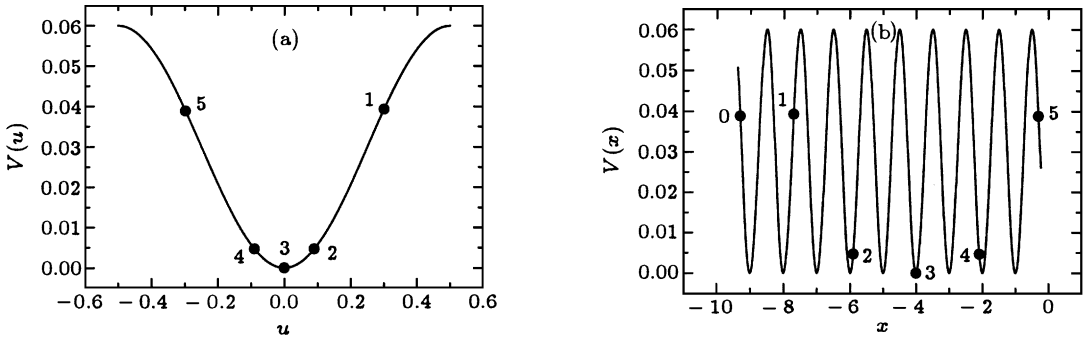


Fig.4. An example of the ground state for model 1; Fig.4(a) shows the ground state $\{u_n\}$, where $K = 0.03$, $\gamma = 1.75$, $\Omega = 4/5$, $\omega = 9/5$; Fig.4(b) shows the recovered chain from Fig.4(a) in one period.

one period. Figure 5 shows an example of ground state for model 2, where $K = 0.02$, $\gamma = 1.90$, $\Omega = 5/6$, $\omega = 13/6$. It is noted that different ground states may correspond to the same unrecovered chain, so we have numerically prove that the energies of the two phases are unequal.

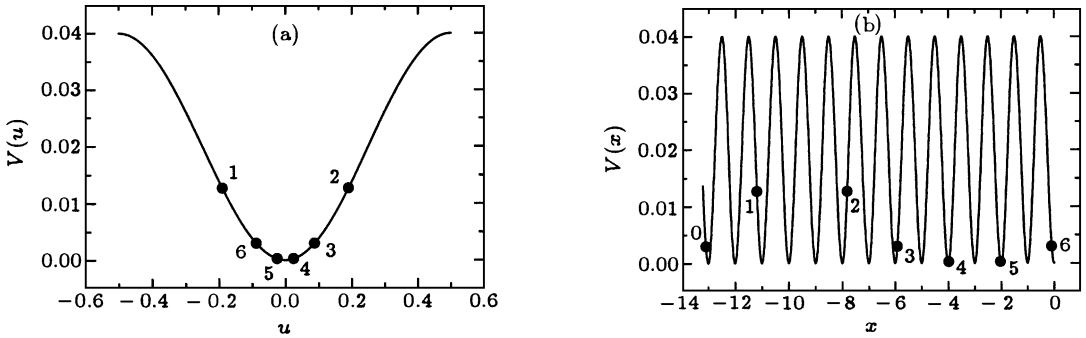


Fig.5. An example of the ground state for model 2; Fig.5(a) shows the ground state $\{u_n\}$, where $K = 0.02$, $\gamma = 1.90$, $\Omega = 5/6$, $\omega = 13/6$; Fig.5(b) shows the recovered chain from Fig.5(a) in one period.

IV. THE PHASE DIAGRAMS

For the present model 1 (or model 2), when $\gamma \geq \gamma_1$ (or $\gamma \geq \gamma_2$), $W(x)$ can take any one of the three equal minima and $W^*(x)$ is periodic in a certain direction. So if we only use the rotation number Ω to describe phases, the phase diagram is periodic and the period is just the same as that of the external potential. When $\gamma < \gamma_1$ (or $\gamma < \gamma_2$), $W(x)$ cannot take its left minimum, and the phase diagram may be greatly different.

From the above analysis, one can easily find that the modulated phases with the same rotation number may have different winding numbers, which may correspond to different phase structures. If $W(x)$ is convex function everywhere, then $\omega = m + \Omega$, where m is an appropriate non-negative integer. If $W(x)$ is nonconvex, the relation between ω and Ω is much more complex, though there are rules to obey. The numerical results support our analysis, as shown in the following examples.

We use the Farey tree structure to study the phase diagram.[10] Figure 6 shows the example of the phase diagram of model 1 in the case of $\gamma_1 \leq \gamma \leq \gamma_1 + D$. Here, only the phases with $Q \leq 5$ are shown. The rotation numbers are $\Omega = 1/1, 1/5, 1/4, 1/3, 2/5, 1/2, 3/5, 2/3, 3/4, 4/5, 1/1$, respectively. It is clear that the phase diagram is similar to that of the standard FK model in appearance, which is composed of commensurate and incommensurate ground states in the (K, γ) parameter space. For any given rotation number Ω, there is a corresponding commensurate area (Arnold's tongue), in which Ω is a constant. Between any two "tongues" there is a gap which contains incommensurate states as well as higher order commensurate states. The phase structures are similar to that of the standard FK model, with the increase of γ, the values of Ω occur periodically and conform to the structure of Farey tree except for the case of $Q = 1$, the values of ω increase monotonically. In Fig.6, in the far left regions of uniform phase, $\Omega = \omega = 1/1$, within the other "tongues" $\omega = \Omega + 1$. But it is noticed that $\Omega = 1/1$ and $\omega = 3/1$ when $\gamma = 1$; $\Omega = 1/1$ and $\omega = 6/1$ when $\gamma = 2$. The period of the phase diagram is just the same as that of the external potential. If $\Omega = \Omega_0$ and $\omega = \omega_0$ when $\gamma = \gamma_0$, then $\Omega = \Omega_0$ and $\omega = m + \omega_0$ when $\gamma = mD + \gamma_0$, where m is an appropriate non-negative integer. When $0 \leq \gamma \leq \gamma_1$, the phase diagram is similar to that of the case of $\gamma_1 \leq \gamma \leq \gamma_1 + D$ in appearance.

There are some new and complex properties which are different from the standard FK model. In the regions limited by the dashed lines in Fig.6, one can find some typical phases with $\Omega = 2/4$, the corresponding winding numbers are $\omega = 5/4$ in the region limited by the left dashed line (see the inset of Fig.6) and $\omega = 7/4$ in the region limited by the right dashed line. In the region of $\Omega = 1/2$, we also find some typical phases with $\Omega = 2/4$, $\omega = 6/4$. Our numerical results show that the appearance of the typical phases does not influence the values of ω which increase monotonically. The typical phases with the numerator and the denominator having a common divisor depend on whether or not the particles in the ground state experience the nonconvex part of the interaction. When some of the particles in the ground state experience the nonconvex part of the interaction potential, the phases with the rotation number and the winding number not uniquely defined are found in the phase diagram. So, we called the typical phases "nonconvex" phases.

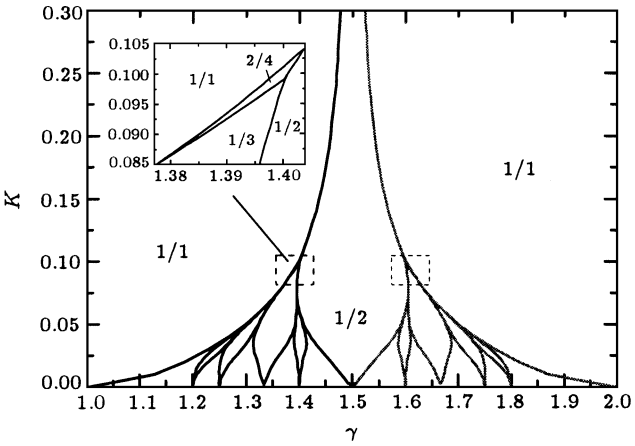


Fig.6. Phase diagram of model 1 in the case of $\gamma_1 \le \gamma \le \gamma_1 + D$, where only the phases with period $Q \le 5$ are shown. The fraction numbers labelled in the figures are the rotation numbers of the corresponding tongues.

Figure 7 shows the example of phase diagram of model 2 in the case of $\gamma_2 \le \gamma \le \gamma_2 + D$. Here, only the phases with $Q \le 5$ are shown. One can find that among the commensurate "tongues", the structure of Farey tree occurs twice within one period of the external potential. We also find the two parts are symmetric and the corresponding winding numbers decrease monotonically in this case. From the left to the right, the corresponding winding numbers are ω=3/1, 14/5, 11/4, 8/3, 13/5, 5/2, 12/5, 7/3, 9/4, 11/5, 2/1, 9/5, 7/4, 5/3, 8/5, 3/2, 7/5, 4/3, 5/4, 6/5, 1/1, respectively. But it is noticed that $\Omega = 1/1$ and $\omega = 5/1$ when $\gamma = 2.50$. When $\gamma_2 - D \le \gamma < \gamma_2$, the phase diagram is just the same as that of the case of $\gamma_2 \le \gamma \le \gamma_2 + D$ in appearance.

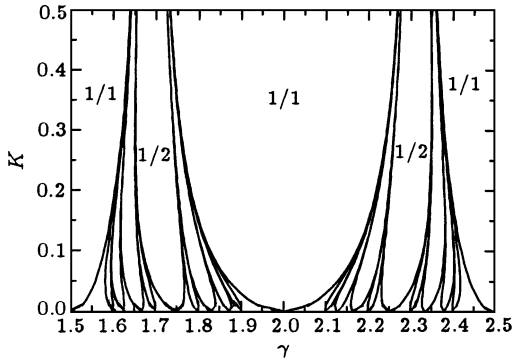


Fig.7. Phase diagram of model 2 in the case of $\gamma_2 \le \gamma \le \gamma_2 + D$, where only the phases with $Q \le 5$ are shown. The fraction numbers labelled in the figures are the rotation numbers of the corresponding tongues.

V. CONCLUSION

In this paper, we have presented and investigated a detailed analysis of two models with the triple-well interparticle interactions. The ground state $\{u_1, u_2, \cdots, u_Q\}$ is obtained by using the effective potential method, where $\{u_1, u_2, \cdots, u_Q\}$ do not denote the real positions $\{x_1, x_2, \cdots, x_Q\}$ of particles in the chain. The chain of particles can be recoverd using the relation between x_n and $u_n : u_n = x_n + m_n D$.

A series of new and interesting phase structures such as the "nonconvex" phase and multiphase points are found. The typical phases with the numerator and the denominator having a common divisor depend on whether or not the particles in the ground state experience the nonconvex part of the interaction. When some of the particles in the ground state experience the nonconvex part of the interaction potential, the phases with the rotation number and the winding number not uniquely defined are found in the phase diagram. Because of the symmetry of the triple-well interactions in our models, the phase diagrams and the properties of the phase structures are similar to the standard FK model. For model 1, with the increase of γ, the values of Ω occur periodically and conform to the structure of Farey tree except for the case of $Q = 1$, the values of ω increase monotonically. For the two models, the phase diagrams whether $\gamma \ge \gamma_1$ for model 1 (or $\gamma \ge \gamma_2$ for model 2) or $\gamma \le \gamma_1$ for model 1 (or $\gamma \le \gamma_2$ for model 2) are similar. These appearance are different from the double-well interactions.[10]

In subsequent papers, we plan to investigate the evolutive and critical behaviors from the triple-well to single-well interactions and from the triple-well to double-well interactions. These studies are currently in progress.

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