Exactly solved Frenkel-Kontorova model with multiple subwells

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We exactly solve a class of Frenkel-Kontorova models with a periodic potential composed of piecewise convex parabolas having the same curvature. All rotationally ordered stable configurations can be depicted with appropriate phase parameters. The elements of a phase parameter are grouped into subcommensurate clusters. Phase transitions, manifested in the gap structure changes previously seen in numerical simulations, correspond to the splitting and merging of subcommensurate clusters with the appearance of incommensurate nonrecurrent rotationally ordered stable configurations. Through the notion of elementary phase shifts, all the possibilities for the existence of configurations degenerate with the ground state are scrutinized and the domains of stability in the phase diagram are characterized. At the boundaries of a domain of stability, nonrecurrent minimum energy configurations are degenerate with the ground state configurations and phase transitions occur.

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I. INTRODUCTION

Spatially modulated structures have been experimentally observed in many condensed matter physical systems.[1] The wave-vector characterizing the modulation varies with external parameters sometimes in a continuous manner but often remains constant, equal to a certain rational locking value, through some range of the external parameters. The physical origin of this complicated behavior is understood in terms of competing interactions in the free energy of the system. The Frenkel-Kontorova (FK) class of models is one of the simplest among those models displaying such interesting behavior.[2] In this work, we will investigate a generalization of the ''locking'' behavior in a specific FK model and show that as the external parameters are adjusted to the boundary of the ''locking'' region, some ''nonrecurrent'' configuration becomes degenerate with a recurrent one.

The FK model describes a one-dimensional chain of coupled atoms subject to a periodic potential $V(u)$. The Hamiltonian of the system is given by

$$H(\{u_n\})=\sum_n \left[\frac{1}{2}(u_n-u_{n-1})^2+\lambda V(u_n)\right], \tag{1.1}$$

where u_n denotes the position of the nth atom. In the limit of shallow potential $(\lambda\to 0)$, the atoms are kept at an equilibrium distance by a tensile force σ. Such models are also widely studied in the context of two-dimensional area-preserving twist maps.[3] The period of the potential can be set to 1 by choosing a suitable spatial scale. The amplitude of the external potential λ can be regarded as a measure of the nonlinearity.

For a stationary configuration one has $\partial H/\partial u_n=0$ and thus

$$u_{n+1}-2u_n+u_{n-1}=\lambda V'(u_n). \tag{1.2}$$

This equation can be recast as coupled first order difference equations, which provides the correspondence between stationary configurations in an FK model and orbits in a twist map.[4] In this paper, we will use these two sets of language interchangeably.

In the study of FK models, one is particularly concerned with minimum energy configurations[5] (or minimizing orbits[3]), in which H cannot be decreased by altering a finite number of u_n's. In the case where the potential $V(u)$ satisfies some criteria,[6] there is a well-defined winding number for these configurations

$$\omega\equiv \lim_{N,N'\to\infty}\frac{u_N-u_{-N'}}{N+N'}, \tag{1.3}$$

the inverse of which $1/\omega$ gives the average number of atoms per period of the potential. A ground state configuration is, by definition, a recurrent minimum energy one, and can be depicted by[5]

$$u_n=f_\omega(n\omega+\alpha), \tag{1.4}$$

where the hull function $f_\omega(x)$ is an increasing function of x and satisfies

$$f_\omega(x+1)=f_\omega(x)+1. \tag{1.5}$$

α is a phase variable to determine the relative position of the atomic chain with respect to the periodic potential. As λ increases, the plot of the orbit (defined on a cylinder) for an incommensurate ground state undergoes a transition from a KAM invariant curve, corresponding to an unpinned phase, to a Cantor-Aubry-Mather (CAM) set[7] or a cantorus, corresponding to a pinned phase. In the latter case $f_\omega(x)$ fails to be a continuous function and the positions of the atoms can be depicted by choosing either the right-hand side limit $f^r_\omega(x)$ or the left-hand side one $f^l_\omega(x)$ when a discontinuity is encountered. The transition, featured by the breaking of the KAM invariant curve, is termed ''the transition by breaking of analyticity'' (TBA).[2,4,5] On the other hand, for a rational ω, the hull function is piecewise constant[8] unless there is a zero-frequency phonon mode.[5] More specifically, for $\omega=p/q$ (assumed to be irreducible throughout this paper) and

without distinct (stated explicitly later) degenerate ground state configurations, the hull function is composed of plateaux, each with width $1/q$. The incommensurate hull function can be obtained as a limit of commensurate hull functions.[8]

In the study of the area-preserving twist map (always considered to be defined on the cylinder), the invariant set is of fundamental importance. In the incommensurate case, depending on whether it is a KAM curve or a cantorus, the invariant set plays the role of a total or a partial barrier, respectively, for the transport in the phase space.[9,10] Even if the invariant KAM curve is broken, its remnants, the rotationally ordered (RO) invariant set still satisfies Eq. (1.2) and is semiconjugate to a rotation by a continuous mapping which is one-to-one but defined on a countable set.[11]

The first analytical study on FK models was conducted by Aubry,[4,12] where TBA was proposed and a devil's staircase was explicitly derived to exhibit the locking of winding numbers to rationals. The potential is the simplest nonlinear one in that the nonlinearity only occurs at one point in each period. Simple as the model may seem, it captures the essence of the ''cantorus'' phase and features a lot of unstable regular structures generically found in typical twist maps for large nonlinearity parameters.[13]

In this paper, we will exactly solve an extension of the Aubry model, where the potential has d subwells in a period. This model was first proposed by Griffiths *et al.*[14] Several interesting new phenomena such as the nonrecurrent minimum energy (NRME) configuration in the incommensurate case, discontinuous cantorus-cantorus phase transitions (i.e., phase transitions in the gap structure), and independent orbits of gaps composing the complement of the CAM set (i.e., a gap structure with multiple discontinuity classes or holes[15]) were found in the $d=2$ case. Recent work on this model[16,17] concentrated on acquiring ground state configurations through studying directional derivatives of the energy function, giving the average energy per atom, with respect to the elements in the phase parameter (defined later). However, as we shall see, for a given set of winding number and phase parameter, the depicted RO configurations may not be unique up to shift operations (defined later). Thus the correspondence between RO configurations and phase parameters is not quite clear, and the meanings of the energy function as well as its derivatives for an arbitrary phase parameter are obsessed with ambiguity. Moreover, the above mentioned new phenomena found in the $d=2$ case have not been analyzed in the general case.

To resolve the ambiguity, we will provide two approaches. We first introduce the notion of subcommensurate clusters for the elements of a phase parameter. A phase parameter with multiple subcommensurate clusters builds up a composite hull function to describe a mixed phase. The meaning of the energy function on the whole space of phase parameters is thus clarified and the procedures adopted in Refs. 16 and 17 can be justified. Instead of studying the average energy per atom, another approach to determine if a given RO configuration is a ground state one is conducted through studying the energy differences resulting from moving some of the atoms across the potential tips (defined later). To keep the resultant configurations RO, we find that only a limited number (at most 2^d-2 for the case with d subwells in each period of potential) of such operations need be investigated. The evaluation of these energy differences is further reduced to solving a set of linear relations among some atomic positions.

The presence of multiple subcommensurate clusters in the phase parameter, as we shall see, naturally leads to multiple compatible configurations (the mixed phase, see Sec. IV) in the commensurate case. To carry the notion of compatible configurations to the incommensurate case, we have to introduce the notion of extended numbers[18] as the elements in the phase parameter and then the nonrecurrent RO (NRO) structure automatically emerges.

The paper is organized as follows. In Sec. II, we define the FK model to be investigated and establish a one-to-one correspondence between stable configurations and coding sequences. RO configurations and the corresponding phase parameters are introduced in Sec. III. An associated energy function, giving the average energy per atom, is also derived. In Sec. IV, composite hull functions are introduced to depict multiple compatible configurations. As the notion of compatible configurations is carried over to the incommensurate case, the NRO configuration emerges. Two approaches to determine minimum energy configurations are provided in Sec. V. In Sec. VI, we build up the phase diagram and characterize the domain of stability. In Sec. VII, incommensurate NRME configurations are investigated. It is found that the NRME configuration naturally emerges at the boundary of the domain of stability. Though some of the results concerning the gap structure in the incommensurate case have been briefly reported in Ref. 18, we provide all the details to make this paper reasonably self-contained.

II. THE MODEL

The potential of period 1, with d pieces of parabolas in each period, is given by

$$V(u)=\min_i\{V_i(u)\}, \tag{2.1}$$

where

$$V_i(u)=\frac{1}{2}(u-b_i)^2+h_i \tag{2.2}$$

with $h_{d+i}=h_i$ and $b_{d+i}=1+b_i$ for every integer i. Here, h_i's and b_i's are independent parameters, arranged in the order

$$b_1<b_2<\cdots<b_d<1+b_1. \tag{2.3}$$

Requiring $V(u)$ to be continuous, the positions of the tips are given by

$$t_i=\frac{b_i+b_{i+1}}{2}+\frac{\Delta h_i}{\Delta b_i} \tag{2.4}$$

with $\Delta h_i\equiv h_{i+1}-h_i$ and $\Delta b_i\equiv b_{i+1}-b_i$. We set

$$t_0=0<t_1<\cdots<t_d=1, \tag{2.5}$$

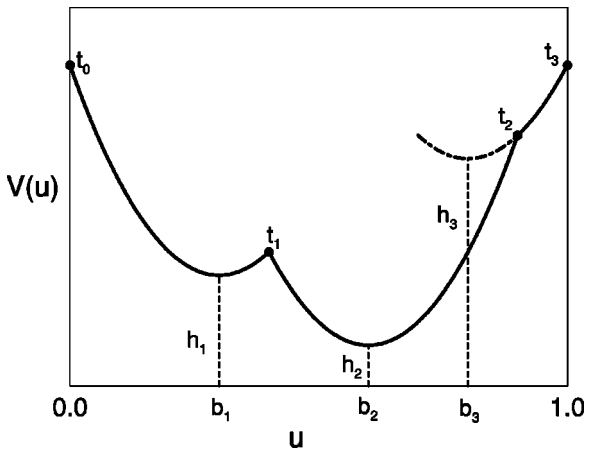

FIG. 1. Periodic potential V in Eq. (2.1) for $d=3$.

where the condition $t_0=0$ is chosen to fix the translational degree of freedom, leading to

$$h_1+b_1^2/2=h_0+b_0^2/2. \tag{2.6}$$

An example for $d=3$ is shown in Fig. 1. Particularly for $t_{j-1}<u<t_j$, $V_j(u)$ should be the one picked up to minimize $V(u)$ in Eq. (2.1). This potential branch is named the jth subwell (or branch) and the collection of all those ith subwell with $i=j \pmod d$ are named the jth type of subwells. The tips at the right ends of those subwells are called the jth tip and the jth type of tips, correspondingly. Since only the relative value of the potential height is relevant and $t_0=0$, there are $2d-2$ degrees of freedom in defining the potential. For convenience, we will choose $\mathbf{t}\equiv\{t_0=0,t_1,t_2,\ldots,t_{d-1}\}$ and $\mathbf{b}\equiv\{b_1,b_2,\ldots,b_d\}$ as the potential parameters. $\mathcal{T}$ and $\mathcal{B}$ are employed to denote the sets of $\mathbf{t}$ and $\mathbf{b}$, respectively, satisfying Eqs. (2.5) and (2.3). The constraint

$$b_0=\sum_{i=1}^{d-1} t_i\Delta b_i-\frac{1}{2}, \tag{2.7}$$

implied in Eqs. (2.4) and (2.6), reduces a degree of freedom in the set of $2d-1$ variables.

The force-balance equation is given by

$$u_{n+1}+u_{n-1}-(2+\lambda)u_n=-\lambda b(u_n), \tag{2.8}$$

with $b(u_n)$ equal to either b_i, if $t_{i-1}<u_n<t_i$, or $b(t_i)\equiv(b_i+b_{i+1})/2$, if $u_n=t_i$. The latter assignment is the average of $b(t_i^+)$ and $b(t_i^-)$, which is not compulsory. However, it is irrelevant as long as only the stable configurations are concerned, for which no atoms can be located at the tips. The reason is as follows. The derivatives of the system energy with respect to the position of the atom right at t_i are $\lambda[b(t_i)-b(t_i^-)]$ and $\lambda[b(t_i)-b(t_i^+)]$ for infinitesimal negative and positive displacements, respectively. No matter how $b(t_i)$ is assigned, there must be either $b(t_i^-)-b(t_i)<0$ or $b(t_i^+)-b(t_i)>0$. Thus such a configuration cannot be a stable one and, needless to say, a minimum energy one. This fact implies that the fundamental lemma in Ref. 5 applies for minimum energy configurations in this FK model and, accordingly, minimum energy configurations must be RO.[15,19–21] The exact values of $b(t_i)$'s are relevant for minimax orbits.[3] Throughout this paper only *stable* configurations are of our concern. In fact, as we will show in Sec. V, there is some depletion region around each tip, where no atom could visit in minimum energy configurations.

In the terminology of dynamical systems, the FK model under investigation satisfies the criterion for a twist homeomorphism[22,23] and the stable configurations correspond to solutions of the Euler-Lagrange equation due to Percival.[24] All the properties derived there without involving the smoothness of the homeomorphism apply here. In particular, the winding number is a continuous function of the hull function in the Hausdorff topology, which guarantees that the property of the incommensurate case can be derived as a limit of that of the commensurate cases and vice versa.[25] In the following, we will adopt the strategy to discuss the commensurate case first and then take the incommensurate case as a limit of commensurate cases.

The formal solution for a stable configuration is given by

$$u_n=d_0\sum_{k=-\infty}^{\infty} e^{-|k|\chi}b_{\langle n+k\rangle}, \tag{2.9}$$

where $e^{-\chi}\equiv[1+\lambda/2-\sqrt{\lambda(1+\lambda/4)}]$ and $d_0\equiv\tanh(\chi/2)$. Here, $\{b_{\langle n\rangle}\}$ or $\{\langle n\rangle\}$ (Ref. 26) is the coding sequence. They must satisfy

$$b_{\langle n\rangle}=b(u_n) \quad \text{or, equivalently,} \quad t_{\langle n\rangle-1}<u_n<t_{\langle n\rangle} \tag{2.10}$$

in order to consist with Eq. (2.8) so that $\{u_n\}$ denotes a *stable* configuration. In other words, the $\langle n\rangle$ designates the potential branch picked up by u_n in Eq. (2.1) for every n. In this manner, we provide a one-to-one correspondence between a stable configuration of the FK model and an allowed coding sequence $\{\langle n\rangle\}$ or $\{b_{\langle n\rangle}\}$ of the symbolic dynamics[27] with Eq. (2.10) employed to prune unallowable sequences.

One should note that, for a stable configuration in our FK model, the phonon gap[28] is $\sqrt{\lambda/m}$ with m denoting the atomic mass and the gap parameter[7,28] is given by $\lambda/(4+\lambda)$. Consequently, all these configurations are uniformly hyperbolic[28] and have nonvanishing phonon gaps for $\lambda>0$. All the theorems and corollaries in Appendix B of Ref. 15 apply here. Losing the phonon gap happens as some continuous variations in the potential parameters force u_n to touch $t_{\langle n\rangle-1}$ or $t_{\langle n\rangle}$ for a certain n when the configuration ceases to be stable. As a result, this configuration loses its uniform hyperbolicity and disappear through bifurcation.[29]

III. ROTATIONALLY ORDERED CONFIGURATIONS

Two configurations $\{u_n\}$ and $\{v_n\}$ are said to intersect if there are $u_n\geqslant v_n$ and $u_m\leqslant v_m$ for some n and m. While, they are said to *coincide* if $u_n=v_n$ for every n. $\{u_n\}$ and $\{u_{n+m}+l\}$ with arbitrary integers m and l, will not be regarded as *distinct* since they can be made coincident by the shift operation, including shifts in the u axis by integers (periods of the potential) and in the numbering of the atoms. An incommensurate RO configuration should not self-intersect, i.e., not to intersect its own shifts (by applying the shift operation

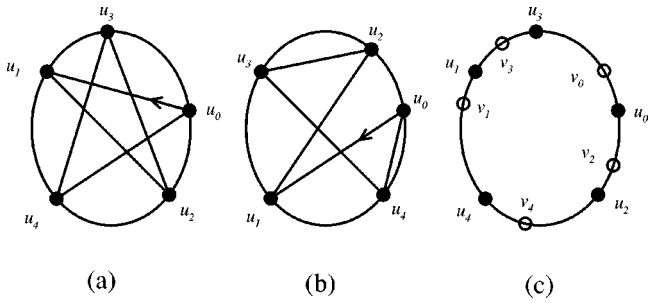

FIG. 2. (a) The cyclic order (counterclockwise) of an RRO configuration $\{u_n\}$ with $\omega=2/5$. (b) The cyclic order of a configuration with the same ω but not RRO. (c) The cyclic order of two compatible configurations $\{u_n\}$ (solid circles) and $\{v_m\}$ (open circles) with $\omega=2/5$.

to itself),[15,19] while for the commensurate case, an RO configuration should not intersects, unless coincides with, its own shifts. According to the fundamental lemma in Ref. 5, all minimum energy configurations in our model must be RO (an FK model allowing of minimum energy configurations not RO, even without a well-defined winding number was discussed in Ref. 30).

A related concept called compatibility (after Katok in Ref. 25) will be employed in later discussions for degenerate ground state configurations. Two distinct configurations are said to be compatible if they cannot be made to intersect through any shift operation (and, therefore, it is apparent that each compatible configuration must itself be RO). The criterion for $\{u_n\}$ and $\{v_n\}$ to be compatible can be recast as, for any n and m, $\mathrm{Frac}[u_n]>\mathrm{Frac}[v_m]$ implies $u_{n\pm1}-\mathrm{Int}[u_n]>v_{m\pm1}-\mathrm{Int}[v_m]$ and vice versa. If we exclude the possibility of discommensurations (which is not of concern in this paper, one may refer to Refs. 5 and 18 for details), two phase variables α and β can be found such that the order of the union of two sequences $\{\mathrm{Frac}[n\omega+\alpha]|-\infty<n<\infty\}$ and $\{\mathrm{Frac}[m\omega+\beta]|-\infty<n<\infty\}$, arranged according to the magnitude, is kept in the union of sequences $\{\mathrm{Frac}[u_n]|-\infty<n<\infty\}$ and $\{\mathrm{Frac}[v_m]|-\infty<m<\infty\}$. An illustration for RO and compatible configurations is shown in Fig. 2. These properties are closely related to the fact that two compatible configuration can be depicted by a single hull function, as will be shown in the next section.

Next, we would like to depict a given RO stable configuration with a hull function. Consider the commensurate case with $\omega=p/q$ at first. To avoid variations due to shift operations, we demand $0\leqslant u_0<1$ and $n=0$ to be the one minimizing $\mathrm{Frac}[u_n]$ in $\{u_n\}$ (termed the fixing condition), which leads to $\mathrm{Int}[u_n]=\mathrm{Int}[n\omega]$ for all n. We further introduce a set of integers n_i's such that $n=n_i$ is the one minimizing $\mathrm{Frac}[u_n-t_i]$ in $\{u_n\}$ for $0<i<d$. Define the phase parameter $\boldsymbol{\beta}\equiv\{\beta_0=0,\beta_1,\ldots,\beta_{d-1}\}$ by

$$\beta_i\equiv\mathrm{Frac}[n_i\omega] \tag{3.1}$$

for $0\leqslant i<d$ and use $\beta_{i+d}=1+\beta_i$ to extend the definition of β_i for arbitrary integer i. The $\{n_{ij}\}$, satisfying

$$\mathrm{Frac}[n_{ij}\omega]=\mathrm{Frac}[\beta_i-\beta_j] \tag{3.2}$$

for $0\leqslant i,j<d$, is also introduced for later use. The values of n_i and n_{ij} are required to be within $(-q/2,q/2]$ in order to be uniquely determined.

For an RO stable configuration $\{u_n\}$, there must be $t_i<u_n<t_{i+1}$ for $\beta_i\leqslant n\omega<\beta_{i+1}$. Introduce $\boldsymbol{\nu}\equiv\{\nu_1,\nu_2,\ldots,\nu_d\}$, given by $\nu_i\equiv\beta_i-\beta_{i-1}$ for each i, with the physical meaning as follows. Consider the model as a twist map defined on a cylinder $[0,1)\times\mathbf{R}$ with u_n replaced by $\mathrm{Frac}[u_n]$. All atomic positions for $\{u_n\}$ form a set of q points, called the periodic cycle. ν_i denotes the atomic fraction located inside the ith type of subwells. $\boldsymbol{\nu}$ must be a partition of unity, i.e., $\nu_i\geqslant0$ and $\nu_1+\nu_2+\cdots+\nu_d=1$.

The hull function to depict $\{u_n\}$ through Eq. (1.4) will be denoted by $f_{\boldsymbol{\omega}}(x)$, where the parameter $\boldsymbol{\omega}\equiv(\omega,\boldsymbol{\beta})$ explicitly reveals the dependence on $\boldsymbol{\beta}$. The restriction $f^l_{\boldsymbol{\omega}}(0)<0\leqslant f^r_{\boldsymbol{\omega}}(0)$, is adopted to pin down the translational degree of freedom in the origin of the x axis. Define a coding function $\tilde{b}_{\boldsymbol{\beta}}(x)$ by $\tilde{b}_{\boldsymbol{\beta}}(x)\equiv b_i$, as well as $\tilde{h}_{\boldsymbol{\beta}}(x)\equiv h_i$ (for later use), for $\beta_{i-1}\leqslant x<\beta_i$. One can introduce the hull function, given by

$$\begin{aligned}
f_{\boldsymbol{\omega}}(x)&=d_0\sum_{n=-\infty}^{\infty}e^{-|n|\chi}\tilde{b}_{\boldsymbol{\beta}}(x+n\omega)\\
&=d_0\sum_{n=-\infty}^{\infty}e^{-|n|\chi}\mathrm{Int}[x+n\omega]\\
&\quad+d_0\sum_{i=1}^{d}b_i\sum_{n=-\infty}^{\infty}e^{-|n|\chi}(\mathrm{Int}[x+n\omega-\beta_{i-1}]\\
&\quad-\mathrm{Int}[x+n\omega-\beta_i])\\
&=1+b_j+d_0\sum_{i=j}^{j+d-1}\Delta b_i\sum_{n=-\infty}^{\infty}e^{-|n|\chi}\\
&\quad\times\mathrm{Int}[x+n\omega-\beta_i]
\end{aligned}\tag{3.3}$$

with any integer j. This hull function satisfies the equation of motion

$$f_{\boldsymbol{\omega}}(x+\omega)+f_{\boldsymbol{\omega}}(x-\omega)-(2+\lambda)f_{\boldsymbol{\omega}}(x)=-\lambda\tilde{b}_{\boldsymbol{\beta}}(x). \tag{3.4}$$

Both $\tilde{b}_{\boldsymbol{\beta}}(x)$ and $f_{\boldsymbol{\omega}}(x)$ are increasing in x. The consistency condition for stable configurations is given by

$$f^l_{\boldsymbol{\omega}}(\beta_i)<t_i<f^r_{\boldsymbol{\omega}}(\beta_i) \tag{3.5}$$

for each i. As will be shown in Sec. VI, Eq. (3.5) can always be respected, for any prescribed set of $\boldsymbol{\omega}$ and $\boldsymbol{\Delta b}\equiv\{\Delta b_1,\Delta b_2,\ldots,\Delta b_{d-1}\}$, by choosing an appropriate set of $\mathbf{t}$.

Particularly, for $\omega=p/q$, every element β_i in $\boldsymbol{\beta}$ should be restricted in the form of l_i/q with integers $0=l_0\leqslant l_1\leqslant\cdots\leqslant l_{d-1}\leqslant q$ so that with any choice of phase variable α, the hull function will depict a specific RO configuration and all its shifts through Eq. (1.4).

The coding function and hull function, introduced above, apply as well for the incommensurate case, with $\boldsymbol{\nu}$ denoting

limiting values (since an infinitely long, but not repetitious, atomic chain is considered) of atomic fractions. The details will be given elsewhere.[31]

A crucial point is that, for given **t** and $\mathbf{\Delta b}$, there are generically $d-1$ degrees of freedom in choosing the $\boldsymbol{\beta}$ to satisfy Eq. (3.5). Consequently, for a given ω, there is a $(d-1)$-parameter family of RO stable configurations, as compared to the uniqueness of the RO stable configuration in the case with a single-well potential in each period.[18] Such a difference will lead to the existence of multiple compatible RO stable configurations, as will be discussed in the next section. Particularly, the existence of the $(d-1)$-parameter family of RO solutions to the corresponding Euler-Lagrange equation of Percival, instead of being an artifact due to the specific choice of the nonanalytical potential, was also observed numerically in a model with smooth potential.[32] Thus, the phenomena described afterwards that result from the existence of additional parameters to characterize RO stable configurations must be applicable to quite a general class of FK models.

To the atom u_n, one can assign the amount of energy

$$E(u_n)=\frac{1}{4}(u_{n+1}-u_n)^2+\frac{1}{4}(u_n-u_{n-1})^2+\frac{\lambda}{2}[u_n-b(u_n)]^2+\lambda h(u_n), \tag{3.6}$$

where $h(u_n)=h_i$ if $b(u_n)=b_i$. The average energy per atom for $\{u_n\}$ is given by

$$E_{av}=\lim_{N,N'\to\infty}\frac{1}{N+N'+1}\sum_{n=-N'}^{N}E(u_n) \tag{3.7}$$

if the limit exists. For an RO configuration, this limit always exists and Eqs. (3.6) and (3.7) can be replaced by

$$\mathcal{E}_{\boldsymbol{\omega}}(x)=\frac{1}{4}[f_{\boldsymbol{\omega}}(x+\omega)-f_{\boldsymbol{\omega}}(x)]^2+\frac{1}{4}[f_{\boldsymbol{\omega}}(x)-f_{\boldsymbol{\omega}}(x-\omega)]^2+\frac{\lambda}{2}[f_{\boldsymbol{\omega}}(x)-\tilde{b}_{\boldsymbol{\beta}}(x)]^2+\lambda\tilde{h}_{\boldsymbol{\beta}}(x) \tag{3.8}$$

as well as

$$E_{\rm av}=\lim_{N,N'\to\infty}\frac{1}{N+N'+1}\sum_{n=-N'}^{N}\mathcal{E}_{\boldsymbol{\omega}}(\alpha+n\omega), \tag{3.9}$$

with the phase variable α corresponding to u_0. $\mathcal{E}_{\boldsymbol{\omega}}(x)$ is periodic in x with period 1.

Once the hull function is obtained, a useful quantity, called the energy function, can be derived straightforwardly,[16,18] given by

$$\begin{aligned}\Psi(\boldsymbol{\omega})&\equiv\int_0^1\mathcal{E}_{\boldsymbol{\omega}}(x)\,dx\\&=\frac{\omega^2}{2}+\lambda\sum_{i=1}^{d}h_i\nu_i+\frac{\lambda}{2}\sum_{0\le i<j\le d-1}[(b_i-b_j)\\&\quad\times(1+b_i-b_j)\,\nu_i\nu_j]-\frac{\lambda\,d_0}{4}\sum_{n=-\infty}^{\infty}e^{-|n|\chi}\\&\quad\times\left[\sum_{i,j=0}^{d-1}\Delta b_i\Delta b_j\,S(n\omega+\beta_j-\beta_i)\right]\end{aligned} \tag{3.10}$$

with $S(x)\equiv\mathrm{Frac}[x](1-\mathrm{Frac}[x])$. The energy function gives the energy averaging, with uniform weight, over the phase variable α since the integration over x is conducted. In the incommensurate case, $\Psi(\boldsymbol{\omega})$ and $E_{\rm av}$ are equivalent no matter which α is chosen in Eq. (3.9) according to the Weyl's criterion[33] since $\mathcal{E}_{\boldsymbol{\omega}}(x)$ is Riemann integrable.[34] In the commensurate case, different RO configurations may be depicted with different choices of α in Eq. (1.4), as will be discussed in the following section.

IV. COMPATIBLE CONFIGURATIONS

In the phase diagram, the boundary between two neighboring domains of stability is where these two phases coexist (become degenerate). As we will see in the next section, degenerate ground state (minimum energy) configurations must be compatible. Therefore, to built up the phase diagram, we should identify the compatible configurations at first. Here we will begin with the compatible configurations in the commensurate case.

As shown in the last section, with every element β_i in $\boldsymbol{\beta}$ restricted in the form of l_i/q for integers $0=l_0\le l_1\le\cdots\le l_{d-1}\le q$, the depicted configurations are a specific RRO (recurrent or repetitious RO) configuration with $\omega=p/q$ and all its shifts. Thus a $\boldsymbol{\beta}$, with all elements in $\mathcal{S}_\omega\equiv\{\mathrm{Frac}[n\omega]\,|-\infty<n<\infty\}$, as well as its accompanying coding function and hull function are termed elementary and denote a pure phase. The union of all pure phases constitutes a set of finite points (countably infinite many points but with null measure in the incommensurate case) of the the phase parameter space $\Omega\equiv\{\boldsymbol{\beta}|0=\beta_0\le\beta_1\le\cdots\le\beta_{d-1}\le\beta_d=1\}$.

In Refs. 16 and 17, the ground state configurations are found through studying directional derivatives of the energy function with respect to the elements in the phase parameter. In this approach, the values of the energy function as $\boldsymbol{\beta}$ varies continuously are of concern. Thus the contents of the energy function evaluated at a nonelementary $\boldsymbol{\beta}$ should also be examined in order to justify such an approach. As a result, the composite phase parameter, consisting of more than one subcommensurate clusters and thus depicting more than one distinct compatible RO stable configurations, is introduced. The composite phase parameter is proposed to denote a *mixed phase*, with the abundance associated with each pure phase specified by $\boldsymbol{\beta}$ in a proper way described below.

Consider the pure phase first. For a given RRO stable configuration $\{u_n\}$ with $\omega=p/q$, we introduce the coding

function satisfying $\tilde{b}_{\boldsymbol{\beta}}(x)=b(u_n)$ for $n\omega\leqslant x<n\omega+1/q$ and $1\leqslant n\leqslant q$. In this way, the associated $\boldsymbol{\beta}$ is automatically elementary. On the other hand, for each elementary phase parameter $\boldsymbol{\beta}$ with respect to the winding number p/q, one can define an increasing coding function $\tilde{b}_{\boldsymbol{\beta}}(x)$. If the accompanying hull function satisfies Eq. (3.5), there exists an RRO stable configuration with winding number p/q depicted by it. In this manner, we build up a one-to-one correspondence between an RRO stable configuration with all its shifts and an elementary phase parameter $\boldsymbol{\beta}$ with the accompanying hull function consistent with Eq. (3.5).

Now let us look into the gap (the discontinuity in the hull function) structure for the pure phase. The invariant set $\{\mathrm{Frac}[f_{\boldsymbol{\omega}}(x+n\omega)]|-\infty<n<\infty\}$, defined on the circle $[0,1)$, will be denoted by $\Sigma_{\boldsymbol{\omega}}(x)$ and $\Sigma_{\boldsymbol{\omega}}\equiv\cup_{0\leqslant x<1}\Sigma_{\boldsymbol{\omega}}(x)$. For an elementary $\boldsymbol{\beta}$, the value of x is irrelevant and $\Sigma_{\boldsymbol{\omega}}=\Sigma_{\boldsymbol{\omega}}(x)$. In $\Sigma_{\boldsymbol{\omega}}$, there is one hole (discontinuity class) composed of q gaps, which come in orbits cyclically[15] and are the discontinuities of $f_{\boldsymbol{\omega}}(x)$ located at $x=i/q$ for every $0\leqslant i<q$. For all the other x, one has $df_{\boldsymbol{\omega}}(x)/dx=0$.

The gap structure can be analyzed according to the amount of discontinuity resulting from a certain Δb_i in Eq. (3.3). Associated with each Δb_i for $0\leqslant i<d$, there is a principle opening (referring to a certain amount of discontinuity in the gap) at $x=\beta_i$ (positioned around $u=t_i$ and this very i will be employed to characterize the specific type of openings). The principal opening has width $d_0\Delta b_i$ and carries a sequence of derived openings, at $x=\mathrm{Frac}[\beta_i+n\omega]$ for all n, having widths $e^{-|n|\chi}d_0\Delta b_i$. The width of the gap in $f_{\boldsymbol{\omega}}(x)$ at $x=j/q\equiv\mathrm{Frac}[m_j\omega]$ with some $0\leqslant j<q$ is given by $\Sigma_{i=0}^{d-1}\chi_q(m_j-n_i)d_0\Delta b_i$, where the n_i's are given in Eq. (3.1) and $\chi_q(n)\equiv\Sigma_{m=-\infty}^{\infty}e^{-|n+mq|\chi}$. Every gap contains d types of openings (referring to the summation over i), each from a certain Δb_i, due to the *resonance* among d types of openings. Particularly, for a given integer $0\leqslant l<q$, there exists an integer $0\leqslant k_i<q$ such that $\mathrm{Frac}[\beta_i+k_i\omega]=l/q$ for each β_i; therefore, d types of openings merge to form a gap and we say that openings of d types are in resonance.

In fact, there is another kind of resonance among openings for repetitious configurations. The factor $\chi_q(n)=\Sigma_{m=-\infty}^{\infty}e^{-|n+mq|\chi}$, instead of a single term $e^{-|n|\chi}$ as appeared in Eq. (3.3), is employed to take account of the resonance among openings of the same type. Specifically, $\beta_{i+mpd}=\beta_i+mp$ for every integer m so that each opening, resulting from Δb_i, merges with one of the openings, from Δb_{i+mpd}. Such resonance occurs only in the commensurate case and it allows the emergence of commensurate NRO configurations.[18]

The connecting points of neighboring gaps compose the periodic cycle $\Sigma_{\boldsymbol{\omega}}$. This $\Sigma_{\boldsymbol{\omega}}$ is an invariant set[19] in the sense that it is invariant under the twist map and it is also a minimal set[35] in the sense that it has no invariant proper subset.

Next, let us turn to the mixed phase with a composite phase parameter. We shall find that the range of the composite hull function carries a gap structure with multiple holes, which provides a valuable example for us to inspect such a gap structure in an analytical way. As we proceed to implement the phase parameter to depict multiple compatible RO stable configurations, one will find that all the restrictions imposed on $\boldsymbol{\beta}$ could, indeed, be loosened except the one with $\boldsymbol{\beta}\in\Omega$.

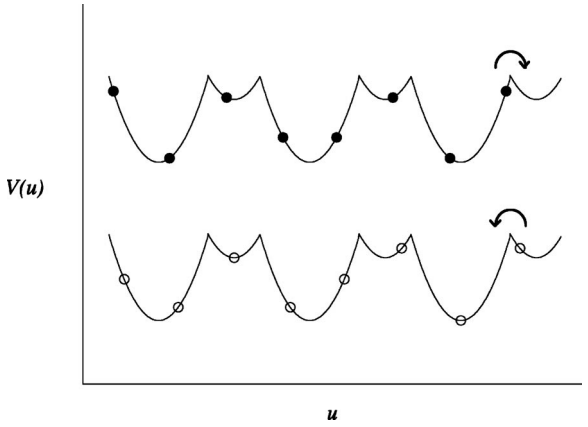

FIG. 3. An example of compatible configurations $\{u_n\}$ (solid circles) and $\{u'_n\}$ (open circles), with $d=2$, $\omega=3/8$, $\beta_1=6/8$, and $\beta'_1=5/8$. By moving the atoms closet to the tip across it (illustrated by the arrows in the figure), corresponding to an elementary phase shift, either of these two configurations is transformed to the other. Compatible configurations are generated by elementary phase shifts.

Consider two compatible stable configurations $\{u_n\}$ and $\{u'_n\}$ both observing the fixing condition. They must have the same winding number $\omega=p/q$. Without loss of generality, assume $u_n\leqslant u'_n$ and these two compatible configurations must be related in such a way that

$$\begin{cases} u'_{n+m}>u_{n+m}>u'_n+l>u_n+l, & \text{for } l<m\omega, \\ u_{n+m}<u'_{n+m}<u_n+l<u'_n+1, & \text{for } l>m\omega, \end{cases} \tag{4.1}$$

for all n, to guarantee $\{u_n\}$ and $\{u'_n\}$ not to intersect through any shift operation. These relations hold among all compatible configurations, even in the incommensurate case.

Using elementary $\boldsymbol{\beta}$ and $\boldsymbol{\beta}'$ to denote the phase parameters respectively for $\{u_n\}$ and $\{u'_n\}$, there must be $\beta_0=\beta'_0=0$ and $\beta_i-\beta'_i=0$ or $1/q$, with the value $1/q$ taken at least once for $1\leqslant i\leqslant d-1$. Two phase parameters related in such a way are said to be related by an elementary phase shift. The physical picture is that, to transform the configuration $\{u_n\}$ to $\{u'_n\}$, one in every period of q atoms must be moved across one of the ith type of tip from the left to the right for those i's with $\beta_i-\beta'_i=1/q$. See Fig. 3 for an example.

Now we will construct a phase parameter to depict both configurations. Let $\beta_i(\gamma)\equiv\gamma\beta_i+(1-\gamma)\beta'_i$ for every integer i with some $0<\gamma<1$. One can derive the corresponding $\tilde{b}_{\boldsymbol{\beta}(\gamma)}(x)$ and $f_{\boldsymbol{\omega}(\gamma)}(x)$. Consider the RO stable configurations depicted by $u_n^{r,l}(\xi)=f^{r,l}_{\boldsymbol{\omega}(\gamma)}(n\omega+\alpha)$ with $\xi\equiv\mathrm{Frac}[q\alpha]$. The configurations $\{u_n^r(\xi)\}$ with $0\leqslant\xi<\gamma$, as well as $\{u_n^l(\xi)\}$ with $0<\xi\leqslant\gamma$, are the same as the one depicted by $\boldsymbol{\beta}(1)=\boldsymbol{\beta}$. The configurations for all the other ξ are

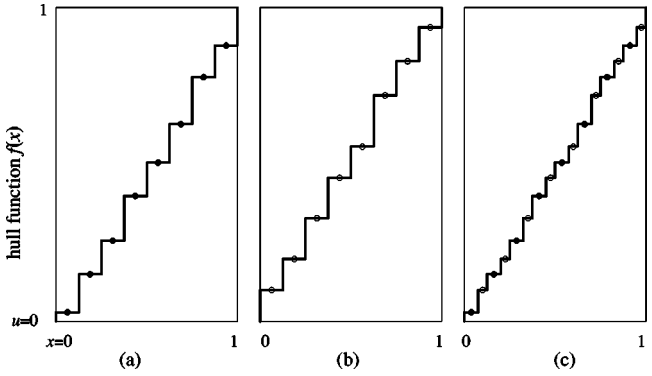

FIG. 4. The hull functions for the compatible configurations in Fig. 3. (a) Is the hull function for $\{u_n\}$, (b) is the hull function for $\{u'_n\}$, and (c) is the composite hull function for both with $\gamma=0.6$.

the same as the one depicted by $\boldsymbol{\beta}(0)=\boldsymbol{\beta}'$. See Fig. 4 for an example.

Such a $\boldsymbol{\beta}(\gamma)$ can be decomposed into two disjoint nonempty subsets: one with elements in the form of k/q and the other, of $(k+\gamma)/q$, with integer k. Within each subset, any two elements β_i and β_j observe the subcommensurate condition,[36] defined by $\mathrm{Frac}[\beta_i-\beta_j]\in\mathcal{S}_\omega$. These two subsets are called subcommensurate clusters. $\boldsymbol{\beta}(\gamma)$, as well as $\tilde{b}_{\boldsymbol{\beta}(\gamma)}(x)$ and $f_{\boldsymbol{\omega}(\gamma)}(x)$, will be termed composite. $\boldsymbol{\beta}$ and $\boldsymbol{\beta}'$ are called the constitutional elementary phase parameters of $\boldsymbol{\beta}(\gamma)$. Furthermore, $\Sigma_{\boldsymbol{\omega}(\gamma)}=\Sigma_{\boldsymbol{\omega}}\cup\Sigma_{\boldsymbol{\omega}'}$. In Ω, $\boldsymbol{\beta}$ and $\boldsymbol{\beta}'$ are two points and the set of $\boldsymbol{\beta}(\gamma)$ with $0<\gamma<1$ forms a one simplex (a straight line) with $\boldsymbol{\beta}$ and $\boldsymbol{\beta}'$ as its vertexes. This $\boldsymbol{\beta}(\gamma)$ is taken to depict a mixed phase, with the ratio of the abundance of the two pure phases $\boldsymbol{\beta}$ and $\boldsymbol{\beta}'$ given by $\gamma:(1-\gamma)$ because any associated physical quantity (e.g., the energy function) with its value evaluated through an integration over x, is attributed to these two pure phases with their corresponding weights in such a ratio.

The extension to the case of more than two compatible stable configurations is straightforward. In fact, the relation between $\{u_n\}$ and $\{u'_n\}$, as discussed above, should be respected by any two among all simultaneously compatible configurations. If there are l distinct RO stable configurations compatible simultaneously, one can arrange their corresponding elementary phase parameters $\boldsymbol{\beta}^{I_1}$, $\boldsymbol{\beta}^{I_2}$, . . . , and $\boldsymbol{\beta}^{I_l}$ such that $\beta_i^{I_1}-\beta_i^{I_j}=k_i^{I_j}/q$ for all $1\leqslant j\leqslant l$ and $0\leqslant i<d$, where $k_i^{I_j}$ are either zero or one with $k_0^{I_j}=0$ for all j and $0=k_i^{I_1}\leqslant k_i^{I_2}\leqslant\cdots\leqslant k_i^{I_l}\leqslant 1$ for each $0<i<d$. We use I_j to denote the positive integers whose binary representation is $k_1^{I_j}k_2^{I_j}\cdots k_{d-1}^{I_j}$ and it follows that $0=I_1<I_2<\cdots<I_l<2^{d-1}$. In this setting, it is clear that $\boldsymbol{\beta}^{I_j}$'s are independent vectors in a d-dimensional space so that $1\leqslant l\leqslant d$. Define the phase parameter $\beta_i(\boldsymbol{\gamma})\equiv(\gamma_1-\gamma_0)\beta_i^{I_1}+(\gamma_2-\gamma_1)\beta_i^{I_2}+\cdots+(\gamma_l-\gamma_{l-1})\beta_i^{I_l}$ for each i with $\boldsymbol{\gamma}\equiv\{\gamma_0=0<\gamma_1<\cdots<\gamma_l=1\}$. One can derive the accompanying $\tilde{b}_{\boldsymbol{\beta}(\gamma)}(x)$ and $f_{\boldsymbol{\omega}(\gamma)}(x)$. Consider the RO configuration depicted by $u_n^{r,l}(\xi)=f^{r,l}_{\boldsymbol{\omega}(\gamma)}(\alpha+n\omega)$ with $\xi\equiv\mathrm{Frac}[q\alpha]$. The configurations $\{u_n^r(\xi)\}$ with $\gamma_{j-1}\leqslant\xi<\gamma_j$, as well as $\{u_n^l(\xi)\}$ with $\gamma_{j-1}<\xi\leqslant\gamma_j$ are the same as the one depicted by $\boldsymbol{\beta}^{I_j}$ for each j. In the phase parameter $\boldsymbol{\beta}(\boldsymbol{\gamma})$ there are l subcommensurate clusters, each having elements in the form of $(k+\gamma_j)/q$ with k integer. Equivalently, there are l constitutional (elementary) phase parameters $\boldsymbol{\beta}^{I_1}$, $\boldsymbol{\beta}^{I_2}$, . . . , and $\boldsymbol{\beta}^{I_l}$, for the composite $\boldsymbol{\beta}(\boldsymbol{\gamma})$. The invariant set $\Sigma_{\boldsymbol{\omega}(\boldsymbol{\gamma})}$ has l distinct minimal proper subsets (periodic cycles). In addition, the set of all the $\boldsymbol{\beta}(\boldsymbol{\gamma})$ with admissible $\boldsymbol{\gamma}$ forms an $(l-1)$ simplex in Ω with these l constitutional phase parameters as its vertexes. The weight of the pure phase, depicted by $\boldsymbol{\beta}^{I_j}$, in the mixed phase, depicted by $\boldsymbol{\beta}(\boldsymbol{\gamma})$, is given by $\gamma_j-\gamma_{j-1}$ for each j.

For the potential with d subwells in a period, there can be at most d subcommensurate clusters in a phase parameter $\boldsymbol{\beta}$. Thus there are at most d compatible distinct RO stable configurations. The classification by the number of subcommensurate clusters, from 1 to d, exhaustes all the possibilities for the phase parameters in Ω and we have successfully attached the physical meaning to the phases (pure or mixed) associated with *any* $\boldsymbol{\beta}\in\Omega$ in order to be consistent for the value of the physical quantities like the energy at such a $\boldsymbol{\beta}$.

Now let us inspect the gap structure of a composite phase parameter. The openings are classified into d types according to the index i in Δb_i (or β_i). Each subcommensurate cluster carries a corresponding hole. In $[0,1)$, gaps resulting from the cluster containing β_i are the discontinuities of the hull function $f_{\boldsymbol{\omega}(\gamma)}(x)$, located at $x=\mathrm{Frac}[n\omega+\beta_i]$ for all n. Inside each of these gaps, there is an opening from every element in the very cluster. For the case with l subcommensurate clusters, there are l holes and lq gaps in $\Sigma_{\boldsymbol{\omega}(\boldsymbol{\gamma})}$. Here and thereafter, the coalescence of opening of the same type in the commensurate case is understood and will not be addressed explicitly.

One can use the γ_j to characterize the hole and its accompanying gaps (to avoid confusion, recall that the openings are characterized by the index i in Δb_i or β_i). In the description below, we will identify γ_i with γ_j for $j=i(\mathrm{mod}\,l)$. In the interval $[0,1)$, each gap of the γ_i type [associated with a cluster with elements in the form of $(k+\gamma_i)/q$] contacts one of the γ_{i-1} type in the left and one of the γ_{i+1} type in the right. They come in orbits side by side. Thus the holes are arranged in a cyclic order according to the magnitude of γ_i. The connecting points, between gaps of the adjacent type, γ_{i-1} and γ_i, also come in orbits and compose the $\Sigma_{\boldsymbol{\omega}I_i}$ for $0<i\leqslant l$. These l distinct periodic cycles form l compatible RRO stable configurations.

Now let us look into how the resonance among openings of different types affects the gap structure. For $l=d$, each gap contains a single type of opening. Assume that the gaps from β_i and β_j are of adjacent types; i.e., they are of the γ_k and γ_{k+1} types, respectively, for some k. Consider the process to adjust the values of the elements in $\boldsymbol{\gamma}$ (or $\boldsymbol{\beta}$) continuously until Eq. (3.2) holds for β_i and β_j with some integer n_{ij}; i.e., the value of $\gamma_{k+1}-\gamma_k$ decreases to zero and their corresponding openings become in resonance. Just before the resonance happened, every gap consisting of the opening of the ith type neighbors one consisting of the opening of the jth type. All the pairs of such neighboring gaps and their connecting points come in orbits and the latter form a

periodic cycle. After the resonance occurs, every pair of two neighboring gaps coalesce into one and the periodic cycle consisting of joint points of these two types of gaps disappears. The number of subcommensurate clusters is, accordingly, decreased by one. With β_i and β_j bound together in one cluster, one can continue the process of adjusting the values of the elements in $\boldsymbol{\gamma}$ (or $\boldsymbol{\beta}$) to make more gaps get in resonance in a similar way. This process is the commensurate version of an l to $(l-1)$-hole transition.[20] Vice versa, the decomposition of one subcommensurate cluster of multiple elements into two, the reverse process, involves the splitting of the corresponding hole and gaps, as well as the emergence of a new periodic cycle between them. This is the commensurate version of an l to $(l+1)$-hole transition. On the other hand, if the above process referring to the joining of β_i and β_j conducts in such a way that $(\beta_j-\beta_i)$ continues to vary in the same trend after getting in resonance, they will break resonance again. After breaking resonance, every gap consisting of the opening of the ith type still neighbors one of the jth type but their relative positions with respect to their connecting points are interchanged.

To carry the above discussion for the compatible configurations in the commensurate case over to the incommensurate case, difficulty will be encountered due to the absence of a well-defined $1/q$. The scrutiny through $\boldsymbol{\gamma}$ is no longer feasible. Nevertheless, with the set $\mathcal{S}_\omega$ still employed to classify subcommensurate clusters and n_{ij} to determine *the* ''degree'' of resonance between the gaps associated with t_i and t_j (to be more specific, the opening due to t_i with width $d_0\Delta b_i e^{-|n|\chi}$ at $x=\mathrm{Frac}[\beta_i+n\omega]$ is merged with an opening due to t_j with width $d_0\Delta b_i e^{-|n+n_{ij}|\chi}$), we will explicitly show the existence of distinct compatible RO stable configurations and an invariant set with a gap structure of multiple holes.

In the incommensurate case an infinitely long atomic chain is taken into account, so the β_i's, being the phase of the atom closest to the ith type of tips, are defined to be limiting values of sequences and the set $\mathcal{S}_\omega$ is dense in $[0,1]$. The way to find out the phase parameter in order to depict a given incommensurate RO stable configuration is described in detail in Ref. 31. Here, let us see what new results will come out in this limiting process.

For an incommensurate RO stable configuration characterized by the phase parameter $\boldsymbol{\beta}$, one may not be able to find the atom, closest to the ith type of tips from above (below) among all the atoms in an infinitely long chain, in a finite spatial extent. However, one can always locate it at u_0^r (u_0^l) by renumbering the atoms with $u_n^r=f_{\boldsymbol{\omega}}^r(n\omega+\beta_i)$ $[u_n^l=f_{\boldsymbol{\omega}}^l(n\omega+\beta_i)]$.[37] Once this is done, it is then impossible to pin down the atom closest to the ith type of tips from below (above) in the finite spatial extent of the configuration $\{u_n^r\}$ $(\{u_n^l\})$.

More generally, for any $0\leqslant i<j<d$, let us introduce $n_{ji}(N)$ and $-n_{ij}(N)$ to be the integers n, respectively, minimizing and maximizing $\mathrm{Frac}[n\omega+\beta_i-\beta_j]$ (maximizing and minimizing $\mathrm{Frac}[\beta_j-\beta_i-n\omega]$) with $-N\leqslant n\leqslant N$ for some positive integer N to simulate the effect due to cutoff in the limiting process (driving $N\to\infty$). In other words, $u^r_{n_{ji}(N)}$ $(u^l_{n_{ji}(N)})$ and $u^r_{-n_{ij}(N)}$ $(u^l_{-n_{ij}(N)})$ are, respectively, the atoms closest to the jth type of tips from above and from below in $\{u_n^r\}$ $(\{u_n^l\})$ for $-N\leqslant n\leqslant N$. As $N\to\infty$, $\mathrm{Frac}[n_{ji}(N)\omega]$ and $\mathrm{Frac}[-n_{ij}(N)\omega]$ converge to $\beta_j-\beta_i$. Two different cases, according to whether $\beta_j-\beta_i$ is in $\mathcal{S}_\omega$ or not, will be scrutinized below.

If $\beta_j-\beta_i\notin\mathcal{S}_\omega$, both $n_{ij}(N)$ and $n_{ji}(N)$ diverge as $N\to\infty$. $e^{-|n_{ij}(N)|\chi}$ and $e^{-|n_{ji}(N)|\chi}$ go to zero as $N\to\infty$ and openings of the ith type and of the jth type are not in resonance. In particular, if none of the other elements in $\boldsymbol{\beta}$ are subcommensurate to β_i, then in $\Sigma_{\boldsymbol{\omega}}$ the gap at the left-hand (right-hand) side of $\mathrm{Frac}[u_n^r]$ $(\mathrm{Frac}[u_n^l])$ has the width $d_0\Delta b_i e^{-|n|\chi}$ and there are infinitely many gaps of infinitesimal widths at its right-hand (left-hand) side. The configuration $\{u_n\}$ $(\{u_n^l\})$ is thus *recurrent* and the closure of $\Sigma_{\boldsymbol{\omega}}(\beta_i)$ is a cantorus.

For the case with $\beta_j-\beta_i=\mathrm{Frac}[n_{ji}\omega]\in\mathcal{S}_\omega$, there are again two possibilities. The first is when $n_{ji}(N)=n_{ji}$ $(n_{ij}(N)=-n_{ji})$ for all $N\geqslant|n_{ji}|$, while the value of $n_{ij}(N)$ $[n_{ji}(N)]$ diverges for $N\to\infty$. That is, in $\{u_n^r\}$ $(\{u_n^l\})$ the 0th atom and the n_{ji}th atom are, respectively, the atoms closest to the ith and to the jth types of tips from above (below), while the atom closest to the jth type of tips from below (above) cannot be found in the finite spatial extent. In $\Sigma_{\boldsymbol{\omega}}$, the gap at the left-hand (right-hand) side of $\mathrm{Frac}[u_n^r]$ $(\mathrm{Frac}[u_n^l])$ contains two openings with widths $d_0\Delta b_i e^{-|n|\chi}$ and $d_0\Delta b_j e^{-|n+n_{ij}|\chi}$. At the right-hand (left-hand) side of $\mathrm{Frac}[u_n^r]$ $(\mathrm{Frac}[u_n^l])$ are infinitely many gaps with infinitesimal widths; therefore, $\{u_n^r\}$ and $\{u_n^l\}$ are recurrent.

The other possibility is when $n_{ij}(N)=-n_{ji}$ $[n_{ji}(N)=n_{ji}]$ for all $N\geqslant|n_{ji}|$, while the value of $n_{ji}(N)$ $[n_{ij}(N)]$ diverges for $N\to\infty$. That is, in $\{u_n^r\}$ $(\{u_n^l\})$ the 0th atom and the n_{ji}th atom are, respectively, the atoms closest to the ith type of tips from above (below) and to the jth type of tips from below (above), while the atom closest to the jth type of tips from above (below) cannot be found in the finite spatial extent. In $\Sigma_{\boldsymbol{\omega}}$, the gap at the left-hand (right-hand) side of $\mathrm{Frac}[u_n^r]$ $(\mathrm{Frac}[u_n^l])$ contains an opening with width $d_0\Delta b_i e^{-|n|\chi}$ and the gap at the right-hand (left-hand) side of $\mathrm{Frac}[u_n^r]$ $(\mathrm{Frac}[u_n^l])$ contains an opening with width $d_0\Delta b_j e^{-|n+n_{ij}|\chi}$. Therefore, $\{u_n^r\}$ and $\{u_n^l\}$ are not recurrent. In this case, $\beta_j-\beta_i$ would rather be identified with an extended number β^+ (β^-), denoting the (equivalent class of) strictly increasing (decreasing) sequences with elements in $\mathcal{S}_\omega$ and the limiting value $\beta\equiv\mathrm{Frac}[n_{ji}\omega]$.

Now let us see how to employ extended numbers as elements of the phase parameter in the above example. Let $\boldsymbol{\beta}$, $\boldsymbol{\beta}'$, and $\boldsymbol{\beta}''$, respectively, denote $\{\beta_0,\ldots,\beta_j,\ldots,\beta_i,\ldots\}$, $\{\beta_0,\ldots,\beta_{j-1},\beta_j',\beta_{j+1},\ldots,\beta_i,\ldots\}$, and $\{\beta_0,\ldots,\beta_{j-1},\beta_j'',\beta_{j+1},\ldots,\beta_i,\ldots\}$, where $\beta_j=\beta_i+\beta$, $\beta_j'=\beta_i+\beta^+$, $\beta_j''=\beta_i+\beta^-$, and $\beta=\mathrm{Frac}[n_{ji}\omega]$. Assume that none of the other elements in $\boldsymbol{\beta}$ are subcommensurate to β_i or β_j. Use $u_n^r=f_{\boldsymbol{\omega}}^r(n\omega+\beta_i)$ and $u_n^l=f_{\boldsymbol{\omega}}^l(n\omega+\beta_i)$ for the recurrent configurations as well as $v_n=f_{\boldsymbol{\omega}'}(n\omega+\beta_i)$ and $w_n=f_{\boldsymbol{\omega}''}^l(n\omega+\beta_i)$ for the nonrecurrent ones. It is straightforward to show that

$$
\begin{aligned}
v_n &= f_{\boldsymbol{\omega}'}(n\omega+\beta_i) \\
&= f_{\boldsymbol{\omega}}(n\omega+\beta_i) + d_0\Delta b_j \sum_{m=-\infty}^{\infty} e^{-|m|\chi} \\
&\quad \times \{\mathrm{Int}[(n+m)\omega-\beta^+] \\
&\quad - \mathrm{Int}[(n+m)\omega-\beta]\} \\
&= u_n^r - d_0\Delta b_j e^{-|n-n_{ji}|\chi}
\end{aligned} \tag{4.2}
$$

and

$$
\begin{aligned}
w_n &= f^l_{\boldsymbol{\omega}''}(n\omega+\beta_i) \\
&= f^l_{\boldsymbol{\omega}}(n\omega+\beta_i) + d_0\Delta b_j \sum_{m=-\infty}^{\infty} e^{-|m|\chi} \\
&\quad \times \{\mathrm{Int}^-[(n+m)\omega-\beta^-] \\
&\quad - \mathrm{Int}^-[(n+m)\omega-\beta]\} \\
&= u_n^l + d_0\Delta b_j e^{-|n-n_{ji}|\chi}.
\end{aligned} \tag{4.3}
$$

The difference between $\boldsymbol{\beta}$ and $\boldsymbol{\beta}'$ (or $\boldsymbol{\beta}''$) captures the essence of an elementary phase shift for the incommensurate case and these phase parameters indeed depict compatible configurations. In other words, the notion of extended numbers naturally comes out as the concept of elementary phase shifts is carried over from the commensurate case to the incommensurate case.

In particular, $v_n = u_n^l + d_0\Delta b_i e^{-|n|\chi} = u_n^r - d_0\Delta b_j e^{-|n-n_{ji}|\chi}$ ($w_n = u_n^r - d_0\Delta b_i e^{-|n|\chi} = u_n^l + d_0\Delta b_j e^{-|n-n_{ji}|\chi}$). Consequently, v_n (w_n) is inside the gap between u_n^r and u_n^l, and $\{v_n\}$ ($\{w_n\}$) is RO and compatible with $\{u_n^r\}$ and $\{u_n^l\}$. Moreover, the orbits of $\{v_n\}$ and $\{w_n\}$ are homoclinic to those of $\{u_n^r\}$ and $\{u_n^l\}$. All of them are not discernible to any prescribed accuracy as $|n|\to\infty$. To be more specific, the difference between the configurations, depicted, respectively, by $f_{\boldsymbol{\omega}'}(n\omega+\alpha)$ [$f^l_{\boldsymbol{\omega}''}(n\omega+\alpha]$ and by $f_{\boldsymbol{\omega}}(n\omega+\alpha)$ [$f^l_{\boldsymbol{\omega}}(n\omega+\alpha]$ with α not subcommensurate to β_i, is not discernible for any finite n. Namely, by choosing a phase variable α not subcommensurate to β_i, the discernible part between the two configurations due to the difference between β_j' (β_j'') and β_j is driven to the spatial infinity. To bring the discernible part of the difference to the finite spatial extent in an infinitely long chain, an appropriate choice of the phase variable α is indispensable (in our example, $\alpha - \beta_i \in \mathcal{S}_\omega$).

Though the values of extended numbers β^+, β^-, and their limit β are not discernible to any accuracy, they can be employed to denote distinct configurations. The openings, respectively, of the ith type and jth type, will be considered to be about to break their resonance for both phase parameters $\boldsymbol{\beta}'$ and $\boldsymbol{\beta}''$.

The multiple-hole structure is discernible only as the resonant openings are just about to split. Namely, one can decompose the elements in a subcommensurate cluster into two groups and, for every gap associated with this cluster, find the dividing point with the openings from one of the group at the right-hand side and those from the other at the left-hand side. The set of these dividing points will form a new minimal invariant set $\Sigma_{\boldsymbol{\omega}'}$. The orbit composed of the dividing points is not recurrent and the closure of $\Sigma_{\boldsymbol{\omega}'}$ is not a cantorus. However, the set of limiting points in $\Sigma_{\boldsymbol{\omega}'}$ is still in the closure of the original invariant set $\Sigma_{\boldsymbol{\omega}}$, so $\Sigma_{\boldsymbol{\omega}'}$ is a Denjoy set.[38] This splitting process and its reverse, the coalescing process, dictate the hole transition in the incommensurate case.

V. MINIMUM ENERGY CONFIGURATIONS

In the FK model under discussion, minimum energy configurations must be RO.[39] Here, two approaches to determine minimum energy and ground state configurations from the collection of all RO stable configurations will be devised. One is based on the investigation of the energy differences resulting from some atomic movements conducted in a given RO stable configuration. The other is based on studying the directional derivatives of the energy function.

A. Elementary phase shifts

Consider a stable configuration $\{u_n\}$, accompanied with the coding sequence $\{\langle n\rangle\}$, given in Eq. (2.9). Assuming that $\langle 0\rangle < \langle 1\rangle = i+1$, one can construct another formal configuration $\{u_n'\}$ with $\langle n\rangle$ replaced by $\langle n\rangle' = \langle n\rangle - \delta_{n,1}$ in Eq. (2.9). Here, $\delta_{n,m}$ denotes the Kronecker delta function. The energy difference between $\{u_n'\}$ and $\{u_n\}$ is given by

$$
\begin{aligned}
&H(\{u_n'\}) - H(\{u_n\}) \\
&\quad = \sum_n \left\{ \frac{1}{2}(u_n' - u_{n-1}')^2 + \frac{\lambda}{2}[u_n' - b_{\langle n\rangle} + \delta_{n,1}(b_{i+1}-b_i)\right]^2 \\
&\qquad - \sum_n \left[\frac{1}{2}(u_n - u_{n-1})^2 + \frac{\lambda}{2}(u_n - b_{\langle n\rangle}\right)^2 + \lambda(h_i - h_{i+1}) \\
&\quad = \lambda\Delta b_i \left(u_1 - t_i - \frac{d_0}{2}\Delta b_i \right) = \lambda\Delta b_i \left(u_1' - t_i + \frac{d_0}{2}\Delta b_i \right).
\end{aligned} \tag{5.1}
$$

Note that $H(\{u_n'\}) < H(\{u_n\})$ if $u_1 - t_i < d_0\Delta b_i/2$. In this case, $\{u_n\}$ cannot be a minimum energy configuration. We deliberately called $\{u_n'\}$ a formal configuration because it may happen that $t_{\langle n\rangle'-1} < u_n' < t_{\langle n\rangle'}$ fails for some $n=m$; namely, $\{u_n'\}$ may not be stable. Say $t_{j-1} < u_m' < t_j$ for some $j \neq \langle m\rangle'$, the energy of $\{u_n'\}$ is overestimated in Eq. (5.1) by the amount $\lambda[V_{\langle m\rangle}(u_m') - V_j(u_m')]$ because $V_j(u)$ should be the one picked up to minimize $V(u)$ in Eq. (2.1) for $u = u_m'$. On the other hand, if $u_m' = t_j$ for some j, then $\{u_n'\}$ is unstable. Under a small perturbation it will relax to one with lower energy. Therefore, the statement, that $\{u_n\}$ cannot be a minimum energy configuration if $u_1 - t_i < d_0\Delta b_i/2$, still holds.

Vice versa, one can also consider the case that $\{u_n'\}$ is stable and $\{u_n\}$ is a formal configuration resulting from moving the atom positioned at u_1' across the potential tip t_i at its

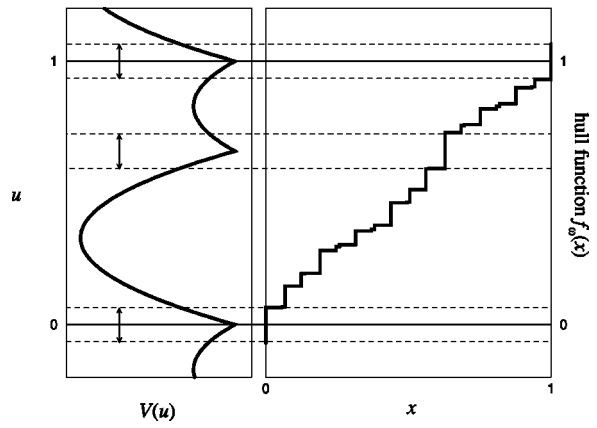

FIG. 5. The potential with $d=2$ and the hull function for the minimum energy configuration with $\omega=50/89$. Inside the dashed lines are the depletion regions.

right-hand side. Eq. (5.1) gives $H(\{u_n'\})>H(\{u_n\})$ if $u_1'>t_i-d_0\Delta b_i/2$. As a result, we have the following theorem.

Theorem 1. For the FK model with potential given by Eq. (2.1), there cannot be any atom within $d_0\Delta b_i/2$ reach of the ith tip for every i in a minimum energy configuration.

Theorem 1 provides a necessary condition for minimum energy configurations. The region within $d_0\Delta b_i/2$ reach of the ith tip for every i is called the depletion region for minimum energy configurations. An example is shown in Fig. 5, where every depletion region is indeed inside a gap of the hull function for the minimum energy configuration.

It is interesting to note that for $t_i-t_{i-1}<d_0(b_{i+1}-b_{i-1})/2$, no atom is allowed in the ith type of subwells for minimum energy configurations. In this case, it makes no difference whether in Eq. (2.1) all the ith type of potential branches are removed or not as long as only minimum energy configurations are concerned. Say $t_2-t_1<d_0(b_3-b_1)/2$ (as shown in Fig. 6), let t' be the tip supposed to be between the first and the third potential branches, if the branch $V_2(u)$ is removed. One has $(b_3-b_1)t'=\Delta b_1 t_1+\Delta b_2 t_2$ with $t'=(b_1+b_3)/2+(h_3-h_1)/(b_3-b_1)$. For minimum energy configurations, no atoms are allowed

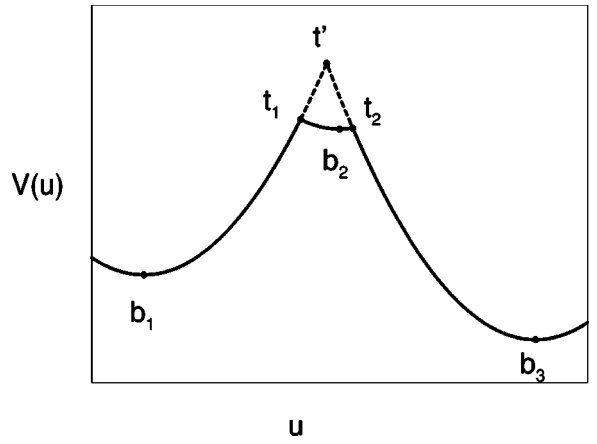

FIG. 6. A segment of $V(u)$ showing that the second type of potential branches can be deleted without affecting the minimum energy configurations.

within $d_0(b_3-b_1)/2$ reach of the tip located at t', which is more stringent than that proposed in theorem 1 since $[t'+d_0(b_3-b_1)/2]-(t_2+d_0\Delta b_2/2)=[\Delta b_1/(b_3-b_1)][d_0(b_3-b_1)/2-(t_2-t_1)]>0$ and $[t'-d_0(b_3-b_1)/2]-(t_1-d_0\Delta b_1/2)=[\Delta b_2/(b_3-b_1)][(t_2-t_1)-d_0(b_3-b_1)/2]<0$. Hence, all the second type potential branches can be removed without affecting minimum energy configurations. This process can be regarded as the coalescence of the depletion regions belonging to two adjacent tips and the subwell in-between is depleted. The coalescing process can be applied repeatedly; namely, for $t_j-t_i<d_0(b_{j+1}-b_i)/2$ with $j>i+1$, all the kth types of potential branches with $j>k>i$ can be removed without affecting minimum energy configurations.

Now let us turn to ground state configurations and investigate the commensurate case first. From theorem 5 in Ref. 39, only repetitious configurations need be considered. For $\omega=p/q$, an RRO stable configuration satisfies $u_{m+nq}=f_{\boldsymbol{\omega}}(x+nq\omega)=np+f_{\boldsymbol{\omega}}(x)=np+u_m$ and $b_{\langle n+q\rangle}=b_{\langle n\rangle}+p$. Given the coding sequence, $\{u_n\}$ can be expressed as

$$u_n=d_0\sum_{m=1}^{q} b_{\langle m\rangle}\chi_q(m-n)+\frac{d_0 p[e^{n\chi}-e^{(q+1-n)\chi}]}{(e^{\chi}-1)(e^{q\chi}-1)} \tag{5.2}$$

$$=d_0\sum_{m=1}^{q} b_{\langle n+m\rangle}\chi_q(m)-\frac{d_0 p[e^{(q+1)\chi}-1]}{(e^{\chi}-1)(e^{q\chi}-1)}, \tag{5.3}$$

where $\chi_q(n)\equiv\{\exp(-l\chi)+\exp[-(q-l)\chi]\}/[1-\exp(-q\chi)]$ with $l\equiv n(\mathrm{mod}\,q)$ for $0\leqslant l<q$. Note that Eq. (5.2) is valid for $0\leqslant n\leqslant q+1$, while Eq. (5.3) is valid for arbitrary n. Such a configuration is specified by q codes $\langle 1\rangle\leqslant\langle 2\rangle\leqslant\cdots\leqslant\langle q\rangle\leqslant\langle 1\rangle+pd$.

Assume that $\langle q\rangle-pd<\langle 1\rangle=i+1$, and consider another repetitious configuration $\{u_n'\}$ (associated with the coding sequence $\{\langle n\rangle'\}$), constructed from $\{u_n\}$ by moving the $(nq+1)$th atom, for every n, to the neighboring subwell at its left-hand side, i.e., from an $(i+1)$th type of subwell to the neighboring ith type of subwell. One can show that the energy difference per period of q atoms between $\{u_n'\}$ and $\{u_n\}$ is given by

$$H_q(\{\langle n\rangle'\})-H_q(\{\langle n\rangle\})=\lambda\Delta b_i\left(u_1-t_i-\frac{d_0}{2}\Delta b_i\chi_q\right), \tag{5.4}$$

where $\chi_q\equiv\chi_q(0)$. Similarly, we have the following lemma.

Lemma 2. For the FK model with potential given by Eq. (2.1), there cannot be any atom within $\chi_q d_0\Delta b_i/2$ reach of the ith tip for every i in a commensurate ground state configuration with winding number p/q.

Theorem 1 is for minimum energy configurations and lemma 2 is for ground state configurations. Taking the irrational numbers as the limits of rational numbers with $q\to\infty$, the same depletion regions as those for minimum energy configurations will be obtained for the incommensurate ground state.

To determine the commensurate ground state configuration, one must compare the energy of a given RRO stable

configuration with those of all the other RRO configurations with the same winding number. Let $\{\langle n\rangle'\}$ denote any other repetitious configuration with the same winding number and $\{u_n'\}$ is specified by Eq. (5.3) with $b_{\langle n\rangle}$ replaced by $b_{\langle n\rangle'}$. The energy difference per period of q atoms between $\{\langle n\rangle'\}$ and $\{\langle n\rangle\}$ is given by

$$\begin{aligned}\Delta H_q(\{\delta\langle n\rangle\}) &\equiv H_q(\{\langle n\rangle'\}) - H_q(\{\langle n\rangle\}) \\ &= -\lambda \sum_{n=1}^{q} \delta b_{\langle n\rangle}\Bigg[u_n - t'_{\langle n\rangle} \\ &\quad + \frac{d_0}{2}\sum_{m=1}^{q} \delta b_{\langle m\rangle}\ \chi_q(n-m)\Bigg] \\ &= -\lambda \sum_{n=1}^{q} \delta b_{\langle n\rangle}\left(\frac{u_n+u_n'}{2} - t'_{\langle n\rangle}\right), \quad (5.5)\end{aligned}$$

where $\delta\langle n\rangle \equiv \langle n\rangle' - \langle n\rangle$ and $\delta b_{\langle n\rangle} \equiv b_{\langle n\rangle'} - b_{\langle n\rangle}$. For a nonzero $\delta\langle n\rangle$, $t'_{\langle n\rangle}$ denotes the position of the tip supposed to be between the $\langle n\rangle'$th and the $\langle n\rangle$th potential branches, if all the in-between potential branches are removed, i.e., $h_{\langle n\rangle} + (b_{\langle n\rangle} - t'_{\langle n\rangle})^2/2 = h_{\langle n\rangle'} + (b_{\langle n\rangle}' - t'_{\langle n\rangle})^2/2$. While for a null $\delta\langle n\rangle$, the value of $t'_{\langle n\rangle}$ is irrelevant.

For $\{\langle n\rangle\}$ specifying a ground state configuration $\{u_n\}$, there must be

$$\Delta H_q(\{\delta\langle n\rangle\}) \geqslant 0 \quad (5.6)$$

for every $\{\delta\langle n\rangle\}$. However, only a subclass of $\{\delta\langle n\rangle\}$, namely, the set of directional movements with all $\delta\langle n\rangle \geqslant 0$ or all $\delta\langle n\rangle \leqslant 0$, need be considered, as will be shown below.

For an arbitrary movement $\{\delta\langle n\rangle\}$, one can introduce two directional movements, $\{\delta\langle n\rangle^+\}$ and $\{\delta\langle n\rangle^-\}$, defined by $\delta\langle n\rangle^+ = \max(\delta\langle n\rangle, 0)$ and $\delta\langle n\rangle^- = \min(\delta\langle n\rangle, 0)$ for every n. They are accompanied with $\{\delta b^+_{\langle n\rangle}\}$ and $\{\delta b^-_{\langle n\rangle}\}$, respectively. It follows that

$$\begin{aligned}\Delta H_q(\{\delta\langle n\rangle\}) &= \Delta H_q(\{\delta\langle n\rangle^+\}) + \Delta H_q(\{\delta\langle n\rangle^-\}) \\ &\quad - \lambda d_0 \sum_{n=1}^{q}\sum_{m=1}^{q} \delta b^+_{\langle n\rangle}\delta b^-_{\langle m\rangle}\chi_q(n-m),\end{aligned} \quad (5.7)$$

where the last term on the right-hand side is definitely positive unless either $\{\delta\langle n\rangle^+\}$ or $\{\delta\langle n\rangle^-\}$ is null. If Eq. (5.6) fails for some $\{\delta\langle n\rangle\}$, then it must fail for either $\{\delta\langle n\rangle^+\}$ or $\{\delta\langle n\rangle^-\}$. Thus only those $\{\langle n\rangle'\}$ having no intersections with $\{\langle n\rangle\}$ needs be compared. Combined with the shift operations, only configurations compatible with $\{u_n\}$ need be considered. Recall that, in our model, the incommensurate case can be regarded as a limit of the commensurate cases, so the derivation applies for the incommensurate case as well.

Now assume that there are two degenerate ground state configurations (in the commensurate case, or minimum energy configurations in the incommensurate case) with the same winding number but not compatible (i.e., not related by any elementary phase shift), one can apply a certain shift operation to make them intersect (i.e., to make the $\{\delta\langle n\rangle\}$ between them consisting of both positive and negative elements). From Eq. (5.7), there must exist some other configuration with the same winding number but having lower system energy, which contradicts the original assumption. We summarize these crucial results as follows.

Theorem 3. For the FK model with potential given by Eq. (2.1), a given RO stable configuration, depicted by an elementary phase parameter $\boldsymbol{\beta}$, is a ground state if and only if the differences in the system energy induced by all the elementary phase shifts are non-negative.

Corollary 4. For the FK model with potential given by Eq. (2.1), if there exist more than one distinct degenerate minimum energy configurations with the same winding number, these configurations must be compatible.

This corollary is deliberately stated in a way to be also applicable for NRME configurations with discommensurations.[18]

The above properties are closely related to the fundamental lemma in Ref. 39, which holds for quite general classes of FK models. The new ingredient in our case is that the cyclic ordering of atoms in RO stable configurations is faithfully encoded in the coding sequences. With multiple codes assigned in each period of potential, extra parameters are required to characterize RO stable configurations in addition to the winding number, which provides the possibility for the analytical investigation of multiple compatible RO stable configurations. Therefore, we conjecture that these theorems should also hold, in some suitable form, for other FK models above TBA, where the hull functions for RO stable configurations is not uniquely determined by the winding number (in other words, when the winding number and the phase variable α is not sufficient to characterize an RO stable configuration).

Theorem 3 allows us to determine if an elementary $\boldsymbol{\beta}$ depicts a ground state configuration by checking the energy differences induced by 2^d-2 distinct elementary phase shifts only. Furthermore, Eq. (5.5) simplifies the determination to examining a set of inequality relations linear in the atomic positions, each of which is nearest to a certain type of tips from below or above. Hence, all we need are the values of $f^{r,l}_{\boldsymbol{\omega}}(\beta_i)$ for $0 \leqslant i < d$. The relations in Eq. (5.5) amounts to giving 2^d-2 restrictions for depletion regions.

In the commensurate case, the elementary phase shifts can be characterized by $\Delta\boldsymbol{\beta}^I = \{0 = k_0^I, k_1^I/q, \ldots, k_{d-1}^I/q\}$. For $0 < I < 2^{d-1}$, $k_1^I k_2^I \cdots k_{d-1}^I$ is the binary representation of I. For $-2^{d-1} < I < 0$, every k_i^I is equal to $-k_i^{|I|}$. The resultant phase parameter is $\boldsymbol{\beta}^I \equiv \boldsymbol{\beta} - \Delta\boldsymbol{\beta}^I$ with $\beta_i^I = \beta_i - k_i^I/q$ for $0 < i < d$. $-2^{d-1} < I < 2^{d-1}$ can thus be employed to represent 2^d-2 distinct elementary phase shifts except for the null one. For the case with some atomic fraction $\nu_i \equiv \beta_i - \beta_{i-1} = 0$, those elementary phase shifts leading to some $\boldsymbol{\beta}^I \notin \Omega$ should be excluded.

Now let us see how to conduct these elementary phase shifts in an RO stable configuration given by $u_n^r = f_{\boldsymbol{\omega}}(n\omega)$ with $\mathrm{Frac}[u^r_{n_i}] = f_{\boldsymbol{\omega}}(\beta_i)$. Only the movement of atoms in a period of q atoms is described and the corresponding movements should also be conducted in all the other periods. One can choose to move the n_ith atom, for each $0 \leqslant i < d$, across

the tip at its left-hand side or not, resulting in 2^d configurations. However, the two, with either all or none of the d atoms moved, are equivalent, up to the shift operation, to the original one. The remaining 2^d-2 choices correspond to the 2^d-2 distinct elementary phase shifts.

To carry the above discussions over to the incommensurate case, H_q should be replaced by H, $\chi_q(n)$ by $e^{-|n|\chi}$ (no more resonance among the same type of tips), the range of the summations Σ_1^q by $\Sigma_{-\infty}^{\infty}$, and the other terms (e.g., the elementary phase shift) by their corresponding ones defined in a limiting sense for the incommensurate case. Such replacement amounts to taking the whole chain of infinitely many atoms as within a single period (i.e., $q\to\infty$). Some comments for the incommensurate case will be made further on.

Consider the ground state characterized by an elementary phase parameter ($\beta_i\in\mathcal{S}_\omega\equiv\{\mathrm{Frac}[n\omega]|\infty<n<\infty\}$ for all $0\leqslant i<d$). For the configuration given by $u_n^r=f_{\boldsymbol{\omega}}(n\omega)$, each of these 2^d-2 distinct elementary phase shifts comprises some of the movements of the n_ith atoms across the tips at their left-hand side for $0\leqslant i<d$. The phase parameter $\boldsymbol{\beta}'$ of the resultant configuration is defined as follows. For the 0th atom staying in the original potential branch $\beta_i'=\beta_i^+$ if the movement of the n_ith atom across the tip is conducted, and $\beta_i'=\beta_i$, if not. On the other hand, for the 0th atom moved across the 0th tip $\beta_i'=\beta_i$ if the movement of the n_ith atom across the tip is conducted and $\beta_i'=\beta_i^-$, if not. Here β^+ and β^- are the extended numbers with respect to ω. The statement, that distinct RO configurations that are not compatible cannot be degenerate with the ground state, remains true. However, the elements of $\boldsymbol{\beta}'$ are decomposed into two groups, with the differences between any pair of elements belonging to different groups being extended numbers. Thus, it turns out that, in the incommensurate case under consideration, at most one of the compatible configurations is recurrent and all the others are, in fact, NRO configurations. Hence, they should be termed, more precisely, *degenerate minimum energy configurations* (as we did in corollary 4).

In general, there may be multiple subcommensurate clusters in the phase parameter to characterize the ground state. Consider a phase parameter $\boldsymbol{\beta}$ composed of l subcommensurate clusters with d_i elements in the ith cluster such that $d_1+d_2+\cdots+d_l=d$. Particularly, for β_i and β_j not in the same cluster, the difference between them is assumed to be neither a number in $\mathcal{S}_\omega$ nor an extended number, to assure that the depicted configuration is recurrent. For the configuration given by $u_n^r=f_{\boldsymbol{\omega}}(n\omega+\beta_i)$, if the n_{ji}th atom is moved across the $(d\ \mathrm{Int}[n_{ji}\omega]+j)$th tip, the displacement of the n_{ji}th atom will be $-d_0\Delta b_j$, while that of the 0th atom will be $-e^{-|n_{ji}|\chi}d_0\Delta b_j$. If β_j is not in the same cluster as β_i, then the limiting value of n_{ji} will diverge as the whole of the infinitely long atomic chain is taken into account. In this case, the 0th atom is indifferent to whether the n_{ji}th atom is moved or not because $e^{-|n_{ji}|\chi}\to 0$ and the atom closest to the jth type of tips moves to infinity in this limit. Such behavior explains the meaning of two types of openings not in resonance in the incommensurate case. Consequently, we need only consider the elementary phase shifts cluster by cluster. The 2^d-2 inequality relations for the depletion regions, in the commensurate case, to be fulfilled in order to determine if the $\boldsymbol{\beta}$ characterizes the ground state are now reduced to $\Sigma_{k=1}^{l}(2^{d_k}-2)$ inequality relations and $l-1$ equality relations. Each term under the summation over k comes from one of the subcommensurate clusters. The $2^{d_k}-2$ elementary phase shifts for the kth cluster come from the two choices, with each of the d_k atoms corresponding to the elements in the very cluster moved across its corresponding tip or not, excluding the two with either none or all of the d_k atoms moved. The condition that each of the elementary phase shifts must involve non-negative energy change gives one of the inequality relations.

An additional equality relation [in the form of Eq. (6.9)] for each cluster arises from the case when all of the d_k atoms are moved in the kth cluster. Namely, the total energy of the system must be the same for $u_n^r=f_{\boldsymbol{\omega}}^r(n\omega+\beta_i)$ and $u_n^l=f_{\boldsymbol{\omega}}^l(n\omega+\beta_i)$. Both configurations are depictable by the same phase parameter and they must have the same energy if the given phase parameter defines the ground state. In this sense, the very phase parameter are thought of to denote a mixed phase. This equality relation will reduce the dimension of the domain of stability by one, to conform to the Gibbs' phase rule[40] [some related discussion from another aspect is given around Eq. (5.9)]. Since we can use the left-hand and right-hand side limits of β_i (or any value subcommensurate to β_i), respectively, as the phase variables to depict these two configurations, we may as well think of them as related by different choices of phase variables and refer the elementary phase shifts for the kth cluster only to the $2^{d_k}-2$ ones mentioned above.

The last "-1" in "$l-1$" equality relations is from the redundant relation corresponding to the case where all of the d corresponding atoms are moved. Specifically, the above l equalities are not all independent because the equality

$$\sum_{i=0}^{d-1}\Delta b_i[f_{\boldsymbol{\omega}}^l(\beta_i)+f_{\boldsymbol{\omega}}^r(\beta_i)]=2\sum_{i=0}^{d-1}\Delta b_i t_i, \tag{5.8}$$

is guaranteed in the formulation for the hull function [in particular, see Eq. (6.1)]. To be more precise, assign the cluster containing $\beta_0=0$ to be the lth cluster. One can obtain $l-1$ independent equalities to equate the system energies of $\{f_{\boldsymbol{\omega}}^l(\beta_i+n\omega)\}$ and $\{f_{\boldsymbol{\omega}}^r(\beta_i+n\omega)\}$ for a certain β_i in each of the first $l-1$ clusters. Then the equivalence of the system energies of $\{f_{\boldsymbol{\omega}}^l(n\omega)\}$ and $\{f_{\boldsymbol{\omega}}^r(n\omega)\}$ will be assured by Eq. (5.8).

B. The energy function

The determination of ground state configurations through studying directional derivatives of the energy function has been conducted in Refs. 16 and 17. However, without properly introducing the notion of mixed phase and extended numbers, the domain of stability is difficult, if not impossible, to scrutinize. Here we will put emphasis on the new ingredients that we have built. Specifically, now we have a better grasp of the phase represented by a general phase pa-

rameter so that the physical meaning of taking directional derivatives in the phase parameter space Ω becomes clearer. It will turn out that all results, obtained from the notion of elementary phase shifts, can, in principle, be achieved through studying the energy function.

For a given $\boldsymbol{\omega}$, the energy function, given in Eq. (3.10), is continuous and convex over the space $\bar{\Omega}\equiv\{\omega\}\otimes\Omega$ (see Appendix A). More specifically, the curvature of the energy function is null almost everywhere (occupying the whole measure).[41] The nontrivial cases happen in a dense set with null measure, where either the commensurate condition (with ω rational) or some subcommensurate condition (e.g., $\mathrm{Frac}[n\omega+\beta_i-\beta_j]=0$ for certain $0\leqslant i<j<d$ and $-\infty<n<\infty$) holds. For this case, the curvature at any point on the hyperplane, specified by the commensurate or subcommensurate condition, along a direction transverse to the hyperplane becomes singular and positive.

In the commensurate case, a composite phase parameter $\boldsymbol{\beta}(\gamma)$ with two subcommensurate clusters is related to its two constitutional phase parameters $\boldsymbol{\beta}'$ and $\boldsymbol{\beta}''$ by $\beta_i(\gamma)=\gamma\beta_i'+(1-\gamma)\beta_i''$ for a suitable $0<\gamma<1$ and every $0<i<d$. It is obvious that $\Psi[\omega,\boldsymbol{\beta}(\gamma)]=\gamma\Psi(\omega,\boldsymbol{\beta}')+(1-\gamma)\Psi(\omega,\boldsymbol{\beta}'')$, so the derivative of the energy function at $\boldsymbol{\beta}(\gamma)$ along the direction of varying γ is a constant and the curvature is null.

In the incommensurate case one can also regard the elementary phase parameter to denote the pure phase, while all the others can be thought of to denote mixed phases, in the sense given below. For a given $\boldsymbol{\beta}$ composed of two subcommensurate clusters, one can keep the cluster containing $\beta_0=0$ fixed and add a number x to every element of the other cluster, with $\mathcal{Z}$ denoting the set of subscripts (i) of all its elements (β_i), to form a family of phase parameters $\boldsymbol{\beta}(x)$ with $\boldsymbol{\beta}=\boldsymbol{\beta}(0)$. The curvature of the energy function along the direction of varying x at $x=0$ is null since none of the $\mathrm{Frac}[n\omega+\beta_i-\beta_j]=0$ is satisfied for β_i and β_j not in the same cluster [see Eq. (A1)]. The two neighboring elementary phase parameters to constitute $\boldsymbol{\beta}(x=0)$ are not well defined. More specifically, there are $x_1>0$ and $x_2<0$ in any neighborhood of 0 such that $\boldsymbol{\beta}(x_1)$ and $\boldsymbol{\beta}(x_2)$ are elementary. Nevertheless, the domain of stability (in the space of potential parameters) for $\boldsymbol{\beta}(x=0)$ has the dimensionality lowered by one, than that of an elementary phase parameter, because the null-curvature condition $\partial^2\Psi[\omega,\boldsymbol{\beta}(x)]/\partial x^2|_{x=0}=0$ leads to the equality

$$
\begin{aligned}
&\partial_x^+\Psi[\omega,\boldsymbol{\beta}(x)]|_{x=0}\\
&\quad\equiv\lim_{\epsilon\to 0,\epsilon>0}\frac{\Psi[\omega,\boldsymbol{\beta}(\epsilon)]-\Psi[\omega,\boldsymbol{\beta}(0)]}{\epsilon}\\
&\quad=\lim_{\epsilon\to 0,\epsilon>0}\lambda\sum_{i\in\mathcal{Z}}\Bigg[(h_i-h_{i+1})+\frac{\Delta b_i}{2}(1+2b_0-b_i-b_{i+1})\\
&\qquad-\frac{d_0}{2}\Delta b_i\sum_{n=-\infty}^{\infty}e^{-|n|\chi}\sum_{j=0}^{d-1}\Delta b_j(\mathrm{Int}[n\omega\\
&\qquad+\beta_j-\beta_i-\epsilon\delta_{j\notin\mathcal{Z}}]-\mathrm{Int}[n\omega+\beta_i-\beta_j+\epsilon\delta_{j\notin\mathcal{Z}}])\Bigg]\\
&\quad=\lambda\sum_{i\in\mathcal{Z}}\Delta b_i\left[f^r_{\boldsymbol{\omega}}(\beta_i)-\frac{d_0}{2}\sum_{j\in\mathcal{Z}}\Delta b_j e^{-|n_{ij}|\chi}-t_i\right]\\
&\quad=\lambda\sum_{i\in\mathcal{Z}}\Delta b_i\left[f^l_{\boldsymbol{\omega}}(\beta_i)+\frac{d_0}{2}\sum_{j\in\mathcal{Z}}\Delta b_j e^{-|n_{ij}|\chi}-t_i\right]\\
&\quad=\partial_x^-\Psi[\omega,\boldsymbol{\beta}(x)]|_{x=0}\\
&\quad\equiv\lim_{\epsilon\to 0,\epsilon>0}\frac{\Psi[\omega,\boldsymbol{\beta}(0)]-\Psi[\omega,\boldsymbol{\beta}(-\epsilon)]}{\epsilon}.
\end{aligned}
\tag{5.9}
$$

As compared with the incommensurate version of Eq. (5.5), Eq. (5.9) gives, in fact, the energy difference between $\{f^r_{\boldsymbol{\omega}}(\beta_i+n\omega)\}$ and $\{f^l_{\boldsymbol{\omega}}(\beta_i+n\omega)\}$ for any $i\in\mathcal{Z}$. To determine the domain of stability for $\boldsymbol{\beta}(x=0)$, two inequality relations $\partial_x^-\Psi[\omega,\boldsymbol{\beta}(x)]|_{x=0}\leqslant 0$ and $\partial_x^+\Psi[\omega,\boldsymbol{\beta}(x)]|_{x=0}\geqslant 0$, are now replaced by the equality $\partial_x\Psi[\omega,\boldsymbol{\beta}(x)]|_{x=0}=0$. Note the resemblance to the case with potential composed of a single subwell in each period.[12] In that case, the energy function $\Psi(\omega)$ is a function of the winding number only. For rational ω, one has $\partial_\omega^+\Psi(\omega)>\partial_\omega^-\Psi(\omega)$ and $\partial_\omega^-\Psi(\omega)\leqslant\sigma\leqslant\partial_\omega^+\Psi(\omega)$ defines the plateau in the phase diagram for ω vs σ. One has $\partial_\omega^+\Psi(\omega)=\partial_\omega^-\Psi(\omega)$ for ω irrational and this equivalence condition defines a single point in the phase diagram. Similarly, the equality Eq. (5.9) defines a hyperplane in the space of potential parameters. In this sense, the very composite $\boldsymbol{\beta}$ consisting of two subcommensurate clusters is considered to denote a mixed phase with two pure components.

It is straightforward to extend the above consideration to the phase parameters with l subcommensurate clusters for any $0<l\leqslant d$. One can add $x_1, x_2, \ldots,$ and x_{l-1} to each cluster except the one containing $\beta_0=0$. The curvature of the energy function along any direction lying on the hyperplane spanned by the respective axes of varying $x_1, x_2, \ldots,$ and x_{l-1} at the point given by $x_1=x_2=\cdots=x_{l-1}=0$ is null, which will give $l-1$ equalities to determine the corresponding domain of stability. This domain of stability has the dimensionality lowered by $l-1$, than that of an elementary phase parameter. Hence, it is thought of to denote a mixed phase of l distinct pure components with these $l-1$ equalities to assure that these l distinct pure phases have the same system energy.

In general, for a given ω, only denumerable many points in Ω denote pure phases. Since the curvature of the energy function is null almost everywhere, one only needs to compare the energy function of the pure phases (with positive-definite curvature) to pick out the ground state configuration(s) for a given set of potential parameters. A mixed phase can be the ground state only if certain fields (determined by the potential parameters) conjugate to the β_i's accidentally match the derivatives of the energy function along the directions with null curvature [such as Eq. (5.9)].

Also due to the fact that the curvature of the energy function is positive-definite only at elementary phase parameters,

to determine if an elementary phase parameter $\boldsymbol{\beta}$ depicts the ground state, only the directional derivatives directing to its neighboring pure phases need be investigated. In the commensurate case with $\omega=p/q$, the neighboring pure phases are those with β_i' equal to β_i+1/q, β_i, or β_i-1/q for $0<i<d$. In the incommensurate case, the neighboring pure phases can be considered to be those differing with the original one depicted by $\boldsymbol{\beta}$ by at most one atom moved across each type of tips. Hence, one only needs to replace the above β_i+1/q and β_i-1/q, for the commensurate case, by extended numbers β_i^+ and β_i^-.

From Eq. (A1), the $\partial^2\Psi/\partial\beta_i\partial\beta_j$ with $i\neq j$ is negative definite for any elementary $\boldsymbol{\beta}$. The cases with $\beta_i'=\beta_i^+$ and $\beta_j'=\beta_j^-$ for some $i\neq j$ should be excluded accordingly. In fact, those excluded in this way are not even compatible with $\boldsymbol{\beta}$. As a result, the remaining $2(2^{d-1}-1)$ directional derivatives to be inspected turn out to correspond to the elementary phase shifts, which is consistent with theorem 3.

The analysis of the commensurate case is straightforward, so we will only describe how the directional derivative is conducted for the incommensurate case. For an elementary $\boldsymbol{\beta}$, one has

$$\begin{aligned}\partial^+_{\beta_i}\Psi &\equiv \lim_{\epsilon\to 0,\epsilon>0}\frac{\Psi(\beta_i+\epsilon)-\Psi(\beta_i)}{\epsilon}\\ &=\lambda(h_i-h_{i+1})+\frac{\lambda}{2}\Delta b_i(1+2b_0-b_i-b_{i+1})\\ &\quad-\frac{\lambda d_0}{2}\Delta b_i\sum_{n=-\infty}^{\infty}e^{-|n|\chi}\sum_{j=0}^{d-1}\Delta b_j(\mathrm{Int}[n\omega\\ &\quad+\beta_j+\delta_{j,i}\epsilon-\beta_i-\epsilon]-\mathrm{Int}[n\omega+\beta_i-\beta_j])\\ &=\lambda\Delta b_i\left[f^r_{\boldsymbol{\omega}}(\beta_i)-\frac{d_0}{2}\Delta b_i-t_i\right]\\ &=\lambda\Delta b_i\left[\frac{f^r_{\boldsymbol{\omega}}(\beta_i)+f^r_{\boldsymbol{\omega}'}(\beta_i)}{2}-t_i\right],\end{aligned}\tag{5.10}$$

in comparison with

$$\begin{aligned}\partial^-_{\beta_i}\Psi &\equiv \lim_{\epsilon\to 0,\epsilon>0}\frac{\Psi(\beta_i)-\Psi(\beta_i-\epsilon)}{\epsilon}\\ &=\lambda(h_i-h_{i+1})+\frac{\lambda}{2}\Delta b_i(1+2b_0-b_i-b_{i+1})\\ &\quad-\frac{\lambda d_0}{2}\Delta b_i\sum_{n=-\infty}^{\infty}e^{-|n|\chi}\sum_{j=0}^{d-1}\Delta b_j(\mathrm{Int}[n\omega\\ &\quad+\beta_j-\delta_{j,i}\epsilon-\beta_i+\epsilon]-\mathrm{Int}[n\omega+\beta_i-\beta_j])\\ &=\lambda\Delta b_i\left[f^l_{\boldsymbol{\omega}}(\beta_i)+\frac{d_0}{2}\Delta b_i-t_i\right]\\ &=\lambda\Delta b_i\left[\frac{f^l_{\boldsymbol{\omega}}(\beta_i)+f^l_{\boldsymbol{\omega}''}(\beta_i)}{2}-t_i\right],\end{aligned}\tag{5.11}$$

where $\boldsymbol{\beta}'$ and $\boldsymbol{\beta}''$ are almost the same as $\boldsymbol{\beta}$ except $\beta_i'=\beta_i^+$ and $\beta_i''=\beta_i^-$. All the elements in $\boldsymbol{\omega}$, except β_i, are kept fixed in taking the directional derivative. The above two equations respectively, give the energy needed to move the atom closest to the ith type of tips from above, of $\{u_n=f_{\boldsymbol{\omega}}(n\omega)\}$, to its left neighboring subwell and the energy needed to move the atom closest to the ith type of tips from below, of $\{u_n^l=f^l_{\boldsymbol{\omega}}(n\omega)\}$, to its right neighboring subwell. They are special cases of Eq. (5.1) for RO stable configurations.

In this way, one can build up a one-to-one correspondence between the elementary phase shifts and the directional derivatives of the energy function, evaluated at a certain elementary phase parameter and directing to a compatible one. Thus the same results, as those derived from studying the elementary phase shifts, are also obtainable from studying these directional derivatives, once the physical meaning of the phases associated with all phase parameters in Ω is clarified and the notion of extended numbers is appropriately employed.

VI. THE PHASE DIAGRAM

In determining the ground state configuration, one can regard $\boldsymbol{\beta}$ as dependent variables while $\mathbf{b}\equiv(b_1,b_2,\ldots,b_{d-1})$ and $\mathbf{h}\equiv(h_1,h_2,\ldots,h_{d-1})$ as independent variables, and ω as a controlling parameter for a fixed $\lambda>0$. In fact, any faithful transformations can be conducted on those independent variables. For example, one can choose the set $\Delta\mathbf{b}\equiv(\Delta b_1,\Delta b_2,\ldots,\Delta b_{d-1})$ and $\mathbf{t}\equiv(t_1,t_2,\ldots,t_{d-1})$ instead, with $\Delta b_0=1-\Delta b_1-\Delta b_2-\cdots-\Delta b_{d-1}$ and $t_0=0$ implied. The transformations can be conducted through Eqs. (2.4) and (2.7). In terms of this new choice, Eq. (3.3) can be recast as

$$f_{\boldsymbol{\omega}}(x)=\frac{1}{2}+\sum_{i=0}^{d-1}\Delta b_i\left(t_i+d_0\sum_{n=-\infty}^{\infty}\mathrm{e}^{-|n|\chi}\mathrm{Int}[x+n\omega-\beta_i]\right).\tag{6.1}$$

$\Delta\mathbf{b}$ and $\mathbf{t}$ will be promoted, in preference to $\mathbf{b}$ and $\mathbf{h}$, as the independent variables because the formulation of Eq. (5.6) is simpler in terms of the former. The boundary of $\mathcal{T}$, i.e., the region in $\mathcal{T}$ with $t_i=t_{i+1}$ for some i, will be denoted by $\partial\mathcal{T}$.

To minimize the system energy, only $d-1$ dependent variables $\boldsymbol{\beta}$ are to be determined for a given point in a $(2d-2)$-dimensional space $(\Delta\mathbf{b}\oplus\mathbf{t})$. In the following, we would like to regard $\mathbf{t}$ as independent variables and $\Delta\mathbf{b}$ as parameters. This choice is just for convenience (as we have seen, the relations to determine the domain of stability can be expressed as linear relations in t_i's; in addition, $\boldsymbol{\beta}$ and $\mathbf{t}$ can sort of be regarded as conjugate variables). Our goal is to study the domain of stability $D[\boldsymbol{\beta}]$, i.e., the set of $\mathbf{t}$ in $\mathcal{T}$, in which the configurations depicted by the given $\boldsymbol{\beta}$ have the lowest energy (either a ground state or a minimum energy configuration), for a given set of ω and $\Delta\mathbf{b}$. As we shall see, any point in $\mathcal{T}$ is generically (with probability 1) locked in some $D[\boldsymbol{\beta}]$ with the $\boldsymbol{\beta}$ containing a single subcommensurate cluster.

A. The domain of stability

Now let us find out the (Lebesque's) dimensionality of the domain of stability for a given phase parameter in Ω. Consider the commensurate case with winding number p/q at first. For an elementary $\boldsymbol{\beta}$ and a given $\Delta\mathbf{b}$, one can derive the relation

$$f^{r,l}_{\boldsymbol{\omega}}(\beta_i)=f^{c}_{\boldsymbol{\omega}}(\beta_i)\pm\frac{d_0}{2}\sum_{j=0}^{d-1}\Delta b_j\chi_q(n_i-n_j) \tag{6.2}$$

with $f^{c}_{\boldsymbol{\omega}}(\beta_i)\equiv[f^{r}_{\boldsymbol{\omega}}(\beta_i)+f^{l}_{\boldsymbol{\omega}}(\beta_i)]/2$ for later use.

The domain $D[\boldsymbol{\beta}]$ is closed, in the sense that it contains all its boundary points, because the inequality in Eq. (5.6) is not strict (distinct degenerate ground state configurations are thus allowed). In addition, the union of all $D[\boldsymbol{\beta}]$ with elementary $\boldsymbol{\beta}$'s is the whole $\mathcal{T}$. As a result, the boundary of each $D[\boldsymbol{\beta}]$ with an elementary $\boldsymbol{\beta}$ is composed of pieces given either by $\partial\mathcal{T}\cap D[\boldsymbol{\beta}]$ or by $D[\boldsymbol{\beta}^I]\cap D[\boldsymbol{\beta}]$ for some $1\leqslant|I|\leqslant 2^{d-1}$ to specify the elementary phase shift.

The energy difference per period of q atoms induced by an elementary phase shift specified by a nonzero I is, from Eq. (5.5), given by

$$\begin{aligned}\Delta H^I_q(\boldsymbol{\beta})|_{\Delta\mathbf{b}}&=-\lambda\sum_{i=1}^{d-1}k^I_i\Delta b_i\left[\frac{\hat f_{\boldsymbol{\omega}}(\beta_i)|_{\Delta\mathbf{b}}+\hat f_{\boldsymbol{\omega}^I}(\beta_i)|_{\Delta\mathbf{b}}}{2}-t_i\right]\\&=-\lambda\sum_{i=1}^{d-1}k^I_i\Delta b_i\left[\hat f_{\boldsymbol{\omega}}(\beta_i)|_{\Delta\mathbf{b}}\right.\\&\quad\left.+\frac{d_0}{2}\sum_{j=1}^{d-1}k^I_j\Delta b_j\chi_q(n_i-n_j)-t_i\right],\end{aligned} \tag{6.3}$$

where the hull function $\hat f\equiv f^r$ for $I<0$ and $\hat f\equiv f^l$ for $I>0$. The condition $\Delta H^I_q(\boldsymbol{\beta})|_{\Delta\mathbf{b}}=0$ specifies a $(d-2)$-dimensional hyperplane in $\mathcal{T}$.[42] In this hyperplane, $H_q(\boldsymbol{\beta})=H_q(\boldsymbol{\beta}^I)$. On one side of it, $H_q(\boldsymbol{\beta})>H_q(\boldsymbol{\beta}^I)$ while, on the other side, $H_q(\boldsymbol{\beta})<H_q(\boldsymbol{\beta}^I)$. Consequently, their intersection $D[\boldsymbol{\beta}]\cap D[\boldsymbol{\beta}^I]$ is contained in this hyperplane and plays as the boundary between $D[\boldsymbol{\beta}]$ and $D[\boldsymbol{\beta}^I]$.

Define $\overline{\mathbf{t}}(\boldsymbol{\beta})\equiv\{\overline{t}_1,\overline{t}_2,\ldots,\overline{t}_{d-1}\}$, with $\mathbf{t}=\overline{\mathbf{t}}(\boldsymbol{\beta})$ to be the solution of $t_i\equiv f^c_{\boldsymbol{\omega}}(\beta_i)$ for $1\leqslant i\leqslant d-1$. From the fact that Eq. (6.3) is continuous in $\mathbf{t}$, one knows that $\overline{\mathbf{t}}(\boldsymbol{\beta})$ is inside $D[\boldsymbol{\beta}]$ (not a boundary point) for an elementary $\boldsymbol{\beta}$ with all $\nu_i>0$ because $f^r_{\boldsymbol{\omega}^I}(\beta_i)>f^l_{\boldsymbol{\omega}}(\beta_i)$ for $I<0$ and $f^l_{\boldsymbol{\omega}^I}(\beta_i)<f^r_{\boldsymbol{\omega}}(\beta_i)$ for $I>0$. Hence, $D[\boldsymbol{\beta}]$ occupies a finite $(d-1)$-dimensional Lebesgue measure in $\mathcal{T}$. This domain is bounded by the hyperplanes $\Delta H^I_q(\boldsymbol{\beta})=0$ for 2^d-2 distinct elementary phase shifts I and is, therefore, a convex hyperpolygon. Such a domain is called a $d-1$ domain.

For an elementary $\boldsymbol{\beta}$ with some atomic fraction $\nu_i=0$, one has $\overline{t}_i=\overline{t}_{i-1}$ and, therefore, $\overline{\mathbf{t}}(\boldsymbol{\beta})\in\partial\mathcal{T}$. Such a $D[\boldsymbol{\beta}]$ still extends to the bulk of $\mathcal{T}$ since a subwell with sufficiently small t_i-t_{i-1} is allowed, which will be depleted as suggested in lemma 2. This $D[\boldsymbol{\beta}]$ is still a convex hyperpolygon, bounded by $\partial\mathcal{T}$ and $\Delta H^I_q(\boldsymbol{\beta})=0$ for the elementary phase shifts I leading to $\boldsymbol{\beta}^I\in\Omega$, and is still a $d-1$ domain.

The intersection $D[\boldsymbol{\beta}]\cap D[\boldsymbol{\beta}^I]$ for a certain I is constrained in a $(d-2)$-dimensional hyperplane, given by $\Delta H^I_q(\boldsymbol{\beta})=-\Delta H^{-I}_q(\boldsymbol{\beta}^I)=0$, and accordingly occupies a null $(d-1)$-dimensional Lebesgue measure in $\mathcal{T}$, but occupies a finite $(d-2)$-dimensional Lebesgue measure on the hyperplane. Such a domain is called a $d-2$ domain. In general, if the intersection of l distinct $d-1$ domains is not empty, these l elementary phase parameters must be *compatible* and there is a unique way to arrange them as $\{\boldsymbol{\beta}^{I_1},\boldsymbol{\beta}^{I_2},\ldots,\boldsymbol{\beta}^{I_l}\}$ with $0=I_1<I_2<\cdots<I_l<2^{d-1}$. Their intersection occupies a finite Lebesgue measure on a $(d-l)$-dimensional hyperplane, given by relations $\Delta H^{I_j}_q(\boldsymbol{\beta})=0$ for $1<j\leqslant l$, and is thus a $d-l$ domain.

Next, let us turn to the case with a composite phase parameter, which can be decomposed into l nonempty subcommensurate clusters for some $1\leqslant l\leqslant d$. One can arrange its l constitutional phase parameters as $\{\boldsymbol{\beta}^{I_1},\boldsymbol{\beta}^{I_2},\ldots,\boldsymbol{\beta}^{I_l}\}$ with $0=I_1<I_2<\cdots<I_l<2^{d-1}$ and a certain $\boldsymbol{\gamma}$, so that the composite elementary parameter can be denoted by $\boldsymbol{\beta}(\boldsymbol{\gamma})$. In $D[\boldsymbol{\beta}(\boldsymbol{\gamma})]$, every constitutional phase parameter can be used to depict a ground state configuration, so that $D[\boldsymbol{\beta}(\boldsymbol{\gamma})]=D[\boldsymbol{\beta}^{I_1}]\cap D[\boldsymbol{\beta}^{I_2}]\cap\cdots\cap D[\boldsymbol{\beta}^{I_l}]$. In fact, for all the $\boldsymbol{\beta}(\boldsymbol{\gamma}')$ inside the $(l-1)$ simplex of Ω with the constitutional phase parameters of $\boldsymbol{\beta}(\boldsymbol{\gamma})$ as its vertices, $D[\boldsymbol{\beta}(\boldsymbol{\gamma}')]$ coincides with $D[\boldsymbol{\beta}(\boldsymbol{\gamma})]$. Such results conform to the Gibb's phase rule to consider the composite $\boldsymbol{\beta}(\boldsymbol{\gamma})$ to denote a mixed phase composed of l distinct pure phases. For there to be one more coexistent pure phase (in our case, one more constitutional elementary phase parameter to represent an additional pure phase), an additional equality must be imposed on the set of field variables (in our case, the degree of freedom for the domain of stability in the phase diagram is decreased by 1).

Particularly, the set of all the points in $\mathcal{T}$, allowing composite phase parameters to depict ground state configurations is a union of denumerable many sets with null $(d-1)$-dimensional Lebesgue measure. Accordingly, an arbitrarily chosen point in $\mathcal{T}$ is generically (with probability 1) inside some $d-1$ domain specified by a single elementary phase parameter. The other cases happen only accidentally (with probability 0). As a result, the allowable phase parameter to depict ground state configurations is generically locked into an elementary one, which meets all the subcommensurate conditions.

In the incommensurate case, $\chi_q(n)$ should be replaced by $e^{-|n|\chi}$ to take away the resonance among openings of the same type. Even with such a replacement conducted upon Eq. (6.2), it is obvious that the point $\overline{\mathbf{t}}(\boldsymbol{\beta})$, with $\mathbf{t}=\overline{\mathbf{t}}(\boldsymbol{\beta})$ to be the solution of $t_i\equiv f^c_{\boldsymbol{\omega}}(\beta_i)$ for $1\leqslant i\leqslant d-1$, is still inside $D[\boldsymbol{\beta}]$ for every elementary $\boldsymbol{\beta}$. Most features of $D[\boldsymbol{\beta}]$ with an elementary $\boldsymbol{\beta}$, derived from Eq. (6.3), for the commensurate case can thus be carried over to the incommensurate case. $D[\boldsymbol{\beta}]$ is still a $d-1$ domain for an elementary $\boldsymbol{\beta}$. The elementary phase shift with $k^I_i=1$ ($k^I_i=-1$) will take β_i to β_i^- (β_i^+), and the subcommensurate cluster in the resultant $\boldsymbol{\beta}^I$ is about to break into two groups. We shall use $\Delta H^I(\boldsymbol{\beta})$ to denote the energy required to conduct such a phase shift. Thus $\Delta H^I(\boldsymbol{\beta})=0$ gives the hyperplane, overlapping part of the boundary of $D[\boldsymbol{\beta}]$.

As we learned in the last section, this $\boldsymbol{\beta}^I$ does not depict a recurrent configuration. One must be careful in counting the dimensionality of the domain $D[\boldsymbol{\beta}^I]$. Here we describe the case with $I<0$ and the other case can be treated similarly. Consider the configuration $u_n=f_{\boldsymbol{\omega}}(n\omega)$ with $\beta_i=\mathrm{Frac}[n_i\omega]$ for $0<i<d$. Moving $\mathbf{t}$ beyond the boundary of $D[\boldsymbol{\beta}]$, given by $\Delta H^I(\boldsymbol{\beta})=0$, will make $\Delta H^I(\boldsymbol{\beta})<0$. That is, at this $\mathbf{t}$, moving all the n_ith atoms with $k_i^I<0$, respectively, to their left neighboring subwells (called the operation I), resulting in the configuration $\{u_n'\}$, will reduce system energy. However, we shall show below that $\{u_n'\}$ is not the minimum energy configuration.

Since $\{u_n\}$ is recurrent, one can always find some integer $M\neq 0$ such that $\mathrm{Frac}[u_{n_i+M}-t_i]$ are close to $\mathrm{Frac}[u_{n_i}-t_i]$ within any prescribed accuracy for every $0\leqslant i<d$. Thus no matter how close the given $\mathbf{t}$ is to the hyperplane specified by $\Delta H^I(\boldsymbol{\beta})=0$, the integer $M\neq 0$ can always be found such that moving all the (n_i+M)th atoms with $k_i^I<0$, respectively, to their left neighboring subwells (regarded as conducting the operation I in another part of $\{u_n\}$ shifted by M) will reduce the energy of $\{u_n\}$. From the fact that $\mathrm{Frac}[u_n']$ should be inside the gap at the left-hand side of $\mathrm{Frac}[u_n]$ in the invariant set $\Sigma_{\boldsymbol{\omega}}$ for all n, we have $\mathrm{Frac}[u_{n_i}-t_i]<\mathrm{Frac}[u'_{n_i+M}-t_i]<\mathrm{Frac}[u_{n_i+M}-t_i]$. As a result, moving all the (n_i+M)th atoms with $k_i^I<0$, in $\{u_n'\}$, respectively, to their left neighboring subwells (i.e., conducting the operation I in the part of $\{u_n\}$ shifted by M after the operation I in the part of $\{u_n\}$ shifted by $M=0$ has been conducted) will still reduce the system energy at the given $\mathbf{t}$. That is to say, $\{u_n'\}$ is no longer a minimum energy configuration as $\mathbf{t}$ is moved beyond the the hyperplane specified by $\Delta H^I(\boldsymbol{\beta})=0$. We thus come to the conclusion that $D[\boldsymbol{\beta}^I]$ is restricted to the $(d-2)$-dimensional hyperplane given by $\Delta H^I(\boldsymbol{\beta})=0$ and is a $d-2$ domain coincident with part of the boundary of $D[\boldsymbol{\beta}]$. In words, for any given atomic segment of any finite length in $\{u_n\}$, one can always find infinitely many segments of atoms that are close to the given one (after the shifts by integers) within any prescribed precision because $\{u_n\}$ is recurrent. Thus the fact that conducting the operation I, thought of as adding a defect, in some place of $\{u_n\}$ will reduce the system energy implies that adding such defects in infinitely many suitable places of this atomic chain can still reduce the system energy. As a result, the NRO configuration $\{u_n'\}$, with a single defect, cannot be the minimum energy configuration.

Crossing the boundary $D[\boldsymbol{\beta}^I]$ of the elementary $D[\boldsymbol{\beta}]$, infinitely many $d-2$ domains with infinitesimal thickness along the direction orthogonal to the hyperplane given by $\Delta H^I(\boldsymbol{\beta})=0$ will be encountered. These $d-2$ domains are associated with phase parameters composed of two subcommensurate clusters, corresponding to the two groups with their resonance broken by the elementary phase shift I.

With the applications of different kinds of elementary phase shifts, one by one, on an elementary phase parameter, the subcommensurate cluster can be decomposed into l nonempty groups for some $1<l\leqslant d$. Each step produces a new NRO configuration compatible to the background RRO one and all the resultant NRO configurations are compatible with one another. The domain of stability for the resultant phase parameter is restricted to a $(d-l)$-dimensional hyperplane and is a $d-l$ domain on the boundary of $D[\boldsymbol{\beta}]$.

B. The geometry of domains

Here, we would like to recognize the shape of the domain of stability from the interaction (splitting or merging) among different types of openings. In the commensurate case, an arbitrarily chosen $\boldsymbol{\beta}$ in Ω generically (with probability 1) has d subcommensurate clusters and can be expressed by a $\boldsymbol{\beta}(\boldsymbol{\gamma})$ with $0=\gamma_0<\gamma_1<\cdots<\gamma_d=1$. We shall show that in this case the domain of stability $D[\boldsymbol{\beta}]$ is a single point.

Consider the configuration $\{u_n^{r,l}(\xi)\}$, associated with a coding sequence $\{\langle n^{r,l}(\xi)\rangle\}$, defined by

$$u_n^{r,l}(\xi)\equiv f_{\boldsymbol{\omega}}^{r,l}\left(\frac{\xi}{q}+n\omega\right) \tag{6.4}$$

with $0\leqslant\xi<1$. For each j with $0<j<d$, $\{\langle n^r(\gamma_j)\rangle\}$ and $\{\langle n^l(\gamma_j)\rangle\}$ differ only by one code in their corresponding q consecutive codes. In $D[\boldsymbol{\beta}]$, these two configuration, $\{u_n^r(\gamma_j)\}$ and $\{u_n^l(\gamma_j)\}$, are degenerate. An equality, in the form of

$$t_j=f_{\boldsymbol{\omega}}^c(\beta_j), \tag{6.5}$$

is thus imposed on $\mathbf{t}\in D[\boldsymbol{\beta}]$ from lemma 2 because $f_{\boldsymbol{\omega}}^r(\beta_j)-f_{\boldsymbol{\omega}}^l(\beta_j)$ is exactly equal to the width of the depletion region associated with the tip t_j. As ξ is increased from 0 to 1, d distinct minimal periodic cycles are explored and the positions of $d-1$ tips are uniquely determined [recall the redundant relation due to Eq. (5.8)] with the solution of $\mathbf{t}$ denoted by $\overline{\mathbf{t}}$ (therefore, theorem 1 and lemma 2 are also sufficient conditions if no resonance occurs among gaps). Since the right-hand side of Eq. (6.5) is still dependent on $\mathbf{t}$ from Eq. (6.1), we would rather choose another set of coordinate system $\mathbf{t}^*\equiv\{t_1^*,t_2^*,\ldots,t_{d-1}^*\}$ to describe the points in $\mathcal{T}$, which is related to $\mathbf{t}$ through the linear transformation

$$t_i^*=t_i-b_0=t_i+\frac{1}{2}-\sum_{j=1}^{d-1}\Delta b_j t_j, \tag{6.6}$$

for $0<i<d$. Now the phase space $\mathcal{T}$ is constrained, in the coordinate $\mathbf{t}^*$, by $1/2-\Sigma_{j=1}^{d-1}\Delta b_j t_j\equiv t_0^*\leqslant t_1^*\leqslant\cdots\leqslant t_{d-1}^*\leqslant t_d^*\equiv 1+t_0^*$. Particularly, the coordinates $\mathbf{t}$ and $\mathbf{t}^*$ are faithfully (with a constant non-zero Jacobian Δb_0) linearly related and thus the reference to the geometry (shape) of a domain is the same for both coordinate systems. We also introduce

$$\overline{t_i^*}\equiv\overline{t_i}-b_0=f_{\boldsymbol{\omega}}^c(\beta_i)-b_0 \tag{6.7}$$

for $0<i<d$, which is a function of $\Delta\mathbf{b}$ and $\boldsymbol{\beta}$ but independent of $\mathbf{t}$ or $\mathbf{t}^*$, from Eqs. (2.7) and (6.1). Hence, Eq. (6.5) can be written as

$$t_i^*=\overline{t_i^*}\quad(0<i<d), \tag{6.8}$$

which specifies a single point in $\mathcal{T}$. As a result, $D[\boldsymbol{\beta}]$ is a single point in $\mathcal{T}$.

Turn to the case that one of the subcommensurate cluster, with elements in the form of $(k+\gamma_j)/q$ with integer k, contains multiple elements, say, m elements $\{\beta_{1'},\beta_{2'},\ldots,\beta_{m'}\}$. As ξ is increased from below γ_j to above γ_j, m atoms in each period of q atoms should be moved across their corresponding tips, *together*. Namely, inside such a $D[\boldsymbol{\beta}]$, only these m atoms all or none moved across corresponding tips are allowed for ground state configurations. In this case, m openings, corresponding to the m elements in the very cluster, coalesce to form a single gap. The previous m separate conditions in the form of Eq. (6.8) are now replaced by a single one $H_q[\{\langle n^r(\gamma_j)\rangle\}]=H_q[\{\langle n^l(\gamma_j)\rangle\}]$ or, from Eq. (5.5),

$$\sum_{i=1}^{m}\Delta b_{i'}t_{i'}^{*}=\sum_{i=1}^{m}\Delta b_{i'}\overline{t_{i'}^{*}}, \tag{6.9}$$

where the term at the right-hand side is independent of $\mathbf{t}^*$. In the $(t_{1'}^*,t_{2'}^*,\ldots,t_{m'}^*)$ space (a m'-dimensional projected subspace of $\mathcal{T}$), a single point, previously specified by m equations in the form of Eq. (6.8), is now replaced by an $m-1$ dimensional hyperplane, specified by Eq. (6.9). This reveals how the resonance (subcommensurate condition) dictates the domain of stability.

Specifically, consider a subcommensurate cluster containing two elements β_i and β_j. The domain of stability in the (t_i^*,t_j^*) subspace (a projected 2 dimensional space in $\mathcal{T}$) is now given by, instead of $t_i^*=\overline{t_i^*}$ and $t_j^*=\overline{t_j^*}$, a single relation

$$\Delta b_i(t_i^*-\overline{t_i^*})+\Delta b_j(t_j^*-\overline{t_j^*})=0, \tag{6.10}$$

with the constraint (see afterwards),

$$\Delta b_i|t_i^*-\overline{t_i^*}|\leqslant d_{ij}(\text{or }\ \Delta b_j|t_j^*-\overline{t_j^*}|\leqslant d_{ji}) \tag{6.11}$$

where $d_{ij}\equiv d_0\chi_q(n_{ij})\Delta b_i\Delta b_j/2$. It describes a straight line segment with endpoints (t_i^*,t_j^*) given by $\mathbf{t}_{i,j}^*\equiv(\overline{t_i^*}-d_{ij}/\Delta b_i,\overline{t_j^*}+d_{ji}/\Delta b_j)$ and $\mathbf{t}_{j,i}^*\equiv(\overline{t_i^*}+d_{ij}/\Delta b_i,\overline{t_j^*}-d_{ji}/\Delta b_j)$. In the interior of this line segment, the phase parameter for the ground state must have openings of ith and jth types in resonance. At the endpoint $\mathbf{t}_{i,j}^*$, these two types of openings are allowed to break resonance with openings of the ith type on the left and those of the jth type on the right, whereas the other way around for the endpoint $\mathbf{t}_{j,i}^*$. Beyond the endpoints, along the line given by Eq. (6.10), are the domains with β_i and β_j subcommensurate with other values of n_{ij}.

Let us come back to the constraint. Consider the configuration depicted by $u_n=f_{\boldsymbol{\omega}}(n\omega+\beta_j)$. $n=0$ and $n=n_{ij}$ designate the atoms respectively closest to the jth and the ith types of tips from above. Eq. (6.10) amounts to the statement that simultaneous moving the 0th and the n_{ij}th atoms, respectively, across the tips at their left-hand side does not cost energy, while the two relations in Eq. (6.11) amount to the statement that moving either one of the two atoms across the corresponding tip cost energy. The latter two relations correspond to the elementary phase shifts allowed to be conducted on the very subcommensurate cluster. In general, for there to be k elements in a subcommensurate cluster, there will be 2^k-2 relations, in the form of Eq. (6.11), and one equality, in the form of Eq. (6.10), to equalize the energies of $\{u_n^r\}$ and $\{u_n^l\}$ [recall the redundant relation in Eq. (5.8)].

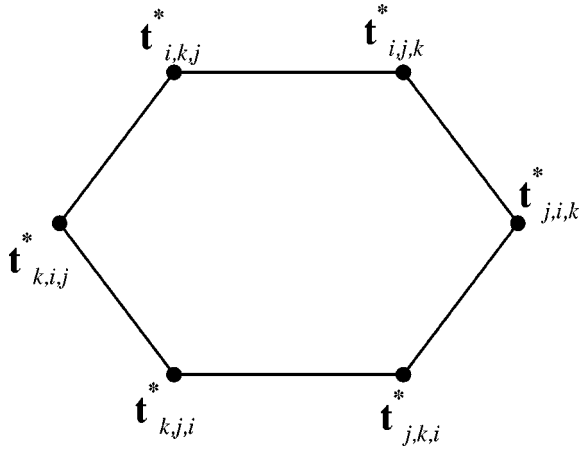

FIG. 7. The domain of stability with β_i, β_j, and β_k subcommensurate on the plane, given by Eq. (6.12), in the (t_i^*,t_j^*,t_k^*) subspace. The point $(\overline{t_i^*},\overline{t_j^*},\overline{t_k^*})$ is at the center of the domain.

For a subcommensurate cluster composed of three elements β_i, β_j, and β_k, the domain of stability in the (t_i^*,t_j^*,t_k^*) subspace is given by

$$\Delta b_i(t_i^*-\overline{t_i^*})+\Delta b_j(t_j^*-\overline{t_j^*})+\Delta b_k(t_k^*-\overline{t_k^*})=0, \tag{6.12}$$

with the constraint

$$\Delta b_i|t_i^*-\overline{t_i^*}|\leqslant d_{ij}+d_{ik} \tag{6.13}$$

and the other two combinatorial partners (over i, j, and k). These six conditions (each equation contains two relations) are equivalent to

$$|\Delta b_i(t_i^*-\overline{t_i^*})+\Delta b_j(t_j^*-\overline{t_j^*})|\leqslant d_{ik}+d_{jk}, \tag{6.14}$$

and the other two combinatorial partners. The set of points conforming to the above constraint forms a hexagon in the plane, given by Eq. (6.12), as shown in Fig. 7. The coordinates of the six vertices (t_i^*,t_j^*,t_k^*) are, respectively, given by $\mathbf{t}_{i,j,k}^*\equiv(\overline{t_i^*}-d_{ij}/\Delta b_i-d_{ik}/\Delta b_i,\overline{t_j^*}+d_{ji}/\Delta b_j-d_{jk}/\Delta b_j,\overline{t_k^*}+d_{ki}/\Delta b_k+d_{kj}/\Delta b_k)$ and the other five permutation partners ($\mathbf{t}_{j,k,i}^*$, $\mathbf{t}_{k,i,j}^*$, $\mathbf{t}_{k,j,i}^*$, $\mathbf{t}_{i,k,j}^*$, and $\mathbf{t}_{j,i,k}^*$). Inside the hexagon, the phase parameters for the ground state must have openings of the ith, jth, and kth types in resonance. On the line segment between $\mathbf{t}_{i,j,k}^*$ and $\mathbf{t}_{i,k,j}^*$, the resonant openings are allowed to split into two groups, with opening of the ith type on the left and the resonant openings of jth and kth on the right. Right at the vertex $\mathbf{t}_{i,j,k}^*$, the resonant openings are allowed to split into three, with openings of the ith, jth, and kth types arranged from left to right.

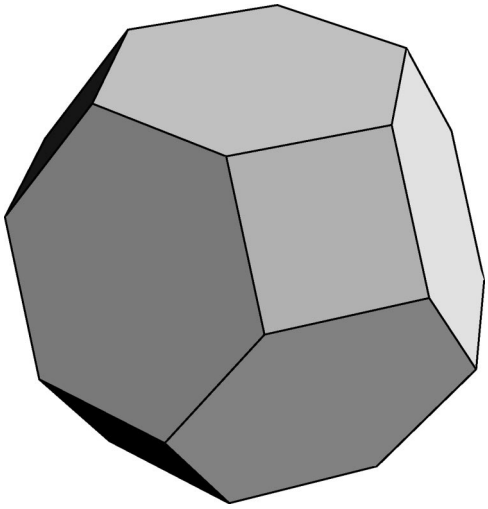

FIG. 8. The domain of stability with four elements of $\boldsymbol{\beta}$ subcommensurate on the three-dimensional hyperplane, given by Eq. (6.15), in the $(t_i^*, t_j^*, t_k^*, t_l^*)$ subspace.

For a subcommensurate cluster composed of four elements β_i, β_j, β_k, and β_l, the domain of stability in the $(t_i^*, t_j^*, t_k^*, t_l^*)$ subspace is given by

$$\Delta b_i(t_i^* - \overline{t_i^*}) + \Delta b_j(t_j^* - \overline{t_j^*}) + \Delta b_k(t_k^* - \overline{t_k^*}) + \Delta b_l(t_l^* - \overline{t_l^*}) = 0. \tag{6.15}$$

With appropriate constraint, it gives rise to a three-dimensional polyhedron (see Fig. 8) with 24 vertices $(t_i^*, t_j^*, t_k^*, t_l^*)$, respectively, given by $\mathbf{t}^*_{i,j,k,l} = (\overline{t_i^*} - d_{ij}/\Delta b_i - d_{ik}/\Delta b_i - d_{il}/\Delta b_i, \overline{t_j^*} + d_{ji}/\Delta b_j - d_{jk}/\Delta b_j d_{jl}/\Delta b_j, \overline{t_k^*} + d_{ki}/\Delta b_k + d_{kj}/\Delta b_k - d_{kl}/\Delta b_k, \overline{t_l^*} + d_{li}/\Delta b_l + d_{lj}/\Delta b_l + d_{lk}/\Delta b_l)$ and its 23 permutation partners (over i, j, k, and l). It has eight faces with six vertices and six faces with four vertices. There are $2^4 - 2 = 14$ faces in total. The eight faces is similar to that shown in Fig. 7 and each of them has vertices such as $\mathbf{t}^*_{\{i,j,k\},l}$ or $\mathbf{t}^*_{l,\{i,j,k\}}$, where the $\{i,j,k\}$ in the subscript means that the six vertices are specified by the six permutations over i, j, k. Specifically, the face given by $\mathbf{t}^*_{\{i,j,k\},l}$ is on the plane given by $t_l^* = \overline{t_l} + (d_{li} + d_{lj} + d_{lk})/\Delta b_l$ in the three-dimensional hyperplane given by Eq. (6.15). It amounts to a direct product of a point in the t_l^* subspace and a hexagon in the (t_i^*, t_j^*, t_k^*) subspace. In this face, the resonant opening are allowed to split into two groups, the resonant opening of the ith, jth, and kth types on the left and that of the lth type on the right. One can continue to analyze the boundaries of the very face (e.g., line segments or vertices) in the same way as the above case for a subcommensurate cluster with three elements. The other six faces are direct products of two line segments. One of them has vertices given by $\mathbf{t}^*_{\{i,j\},\{k,l\}}$. It is on the plane given by $\Delta b_i(t_i^* - \overline{t_i^*}) + \Delta b_j(t_j^* - \overline{t_j^*}) = -d_{ik} - d_{il} - d_{jk} - d_{jl}$ and amounts to the direct product of a line segment from $\mathbf{t}^*_{i,j,k,l}$ to $\mathbf{t}^*_{j,i,k,l}$ in the (t_i^*, t_j^*) subspace and the other from $\mathbf{t}^*_{i,j,k,l}$ to $\mathbf{t}^*_{i,j,l,k}$ in the (t_k^*, t_l^*) subspace. Again, the resonant openings are allowed to break into two groups, each with two types of openings, in this face.

The domain of stability $D[\boldsymbol{\beta}]$ in $\mathcal{T}$ is a direct product of convex hyperpolygons, each corresponding to a subcommensurate cluster and being constructed in the way described above, with the parts outside $\mathcal{T}$, if any, truncated.[43] Descriptions of the hyperpolygon for a general subcommensurate cluster and of the surroundings for a given domain of stability are given in Appendix B.

Next, turn to the incommensurate case. In every subcommensurate cluster of a general phase parameter in Ω, the domain of stability in the corresponding projected subspace in $\mathcal{T}$ is determined by relations similar to Eqs. (6.10) and (6.11). Hence, the subcommensurate clusters dictate the domains of stability in the same way as in the commensurate case. That is, using the description of resonance between openings in counting the dimensionality and determining the shape of the domains of stability can be carried over from the commensurate case to the incommensurate case. However, there is still one important different feature, as we shall describe below.

The domain of stability for a phase parameter $\boldsymbol{\beta}$ with l (>1) subcommensurate clusters has the same shape as that in the commensurate case and is a $d-l$ domain. Recall that though the very $\boldsymbol{\beta}$ represents a mixed phase, its constitutional pure phases are not well defined (can only be defined as limits). Thus it is not on the boundary of any $d-l+1$ domain. On the other hand, the boundary of $D[\boldsymbol{\beta}]$ is composed of the hyperplanes ($d-l-1$ domains) which are domains of the stability for the phase parameters, resulting from conducting elementary phase shifts on a certain subcommensurate cluster of $\boldsymbol{\beta}$ and denoting NRO configurations. Crossing the boundary (along the direction to tear the subcommensurate cluster into two), layers of infinitely many $d-l-1$ domains (with infinitesimal thickness) will be met, just as in the case at the endpoint of the plateau in the devil's staircase.

The number of all the elementary phase parameters in the incommensurate case is infinite but still denumerable, and the set of all the corresponding 0 simplexes is dense (having a $d-1$ fractal dimension) in Ω but has a null n dimensional Lebesgue measure for any $1 \leqslant n \leqslant d-1$. Nevertheless, their domains of stability are $d-1$ domains and the union of all these domains occupy the whole measure of $\mathcal{T}$. On the contrary, though the phase parameters with multiple subcommensurate clusters occupy the whole measure in Ω, they have null curvature in one or another direction. Thus they have null Jacobians for the mapping from Ω to $\mathcal{T}$. Consequently, an arbitrary chosen $\mathbf{t}$ is generically (with probability 1) inside some $d-1$ domain with the corresponding phase parameter elementary. We then propose that the phase diagram is a *complete* $(d-1)$-dimensional devil's staircase.

VII. INCOMMENSURATE NONRECURRENT MINIMUM ENERGY CONFIGURATION

The existence of incommensurate NRME configurations was first proposed in Ref. 14. Here, we would like to show

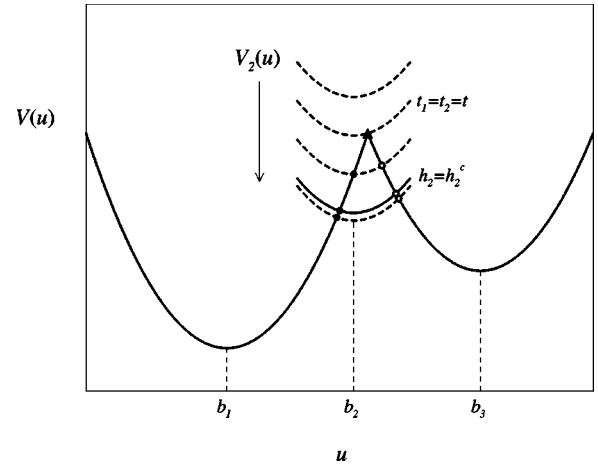

FIG. 9. The variation of the potential as h_2 is lowered. t_1 is denoted by the solid circles and t_2, by the open circles. An NRME configuration is allowed at $h_2=h_2^c$.

how they can be implemented in the general case. Consider the FK model with potential given by Eq. (2.1) having an incommensurate ground state configurations with winding number ω and phase parameter $\boldsymbol{\beta}$. Assume h_2 is so high that t_1 and t_2 are close enough to make the second type of subwells depleted by the coalescence of depletion regions (see Fig. 9). Then, one has $\beta_1=\beta_2$ with $f^l_{\boldsymbol{\omega}}(\beta_1)<t_1\leqslant t_2<f^r_{\boldsymbol{\omega}}(\beta_1)$ to depict the ground state configuration. That is to say, β_2 and β_1 are subcommensurate with $n_{21}=0$. Now let us see what happens as h_2 is decreased.

As h_2 is varied, t_1 and t_2 vary accordingly. Define $\Delta b=b_3-b_1$ and t to be the tip, supposed to be between the first and third potential branches if the second branch is neglected. For h_2 decreased gradually from a sufficiently large value, the second potential branch becomes observable at $t=t_1=t_2$. However, according to theorem 1, the minimum energy configuration (including ground state) is not affected until h_2 reaches the value h_2^c such that either $t_2=f_{\boldsymbol{\omega}}(\beta_1)-d_0\Delta b_2/2$ or $t_1=f^l_{\boldsymbol{\omega}}(\beta_1)+d_0\Delta b_1/2$ is satisfied, which occurs at

$$h_2^c=h_3-\lambda\Delta b_2\left[f_{\boldsymbol{\omega}}(\beta_1)-\frac{d_0}{2}\Delta b_2-\frac{1}{2}(b_2+b_3)\right] \quad (7.1)$$

or

$$h_2^c=h_1+\lambda\Delta b_1\left[f^l_{\boldsymbol{\omega}}(\beta_1)+\frac{d_0}{2}\Delta b_1-\frac{1}{2}(b_1+b_2)\right], \quad (7.2)$$

respectively. These two cases happen simultaneous only when β_1 and β_2 are not subcommensurate to any other elements in $\boldsymbol{\beta}$. Now we will describe the case when Eq. (7.1) is reached first and the other case can be treated similarly.

As Eq. (7.1) is reached, the ground state configuration at this point is still depicted by $u_n=f_{\boldsymbol{\omega}}(n\omega+\beta_1)$ and the NRME configuration, given by $u'_n=u_n-d_0\Delta b_2 e^{-|n-n_1|\chi}$, emerges. There are two facts to demonstrate that $\{u'_n\}$ is nonrecurrent. The zeroth atom is the only atom sitting at the second type of subwells. In addition, the limiting value of n'_{21} (taking the limit of an infinitely long chain for the incommensurate case[31]) diverges but the limiting value of Frac$[n'_{21}\omega]$ is still 0. In this case, we identify β'_2 with β_1^+ (an extended number), to reveal the fact that the openings of the first and second types are about to break their resonance.

As h_2 is lowered further, the configurations continued from $\{u'_n\}$ or $\{u_n\}$ are no longer minimum energy configurations, since moving certain (in fact, infinitely many) atoms from the third types of subwells into the second type of subwells will lower the system energy. There must be a finite fraction of the infinite many atoms in this atomic chain moved across the second types of tips from above in order to achieve a ground state configuration again. Therefore, one may well say that the defects produced by the elementary phase shifts mediate the subcommensurate-subincommensurate phase transition relating to β_1 and β_2, which differentiates the fraction $(\beta_2-\beta_1)$ of atoms in the second type of subwells, for the ground state configuration, to be locked in $\mathcal{S}_\omega$ or not.

The above implementation can be regarded as to break the resonance (with $n_{21}=0$) between β_1 and β_2. It can be easily generalized to the case for any β_i and β_j with n_{ij} finite, as described in Appendix C. The shift of h_2 amounts to moving **t** from a $d-l$ domain to its boundary, a $d-l-1$ domain. Such implementation can also be generalized to break the resonance between two groups of elements in a subcommensurate cluster. This is indeed what occurs at the transition point for an l to $(l+1)$-hole transition.[15]

One can imagine how to use different elementary phase shifts to implement more compatible NRO configuration from an RRO background, and these NRO configurations are allowed to become NRME ones as **t** is driven to appropriate place (in a $d-l-k$ domain on the boundary of a $d-l$ domain if k distinct NRME configurations are allowed). That is to say, any NRO stable configuration can be made to be an NRME configuration by choosing an appropriate set of **t**. Therefore, the properties of the NRO configurations can be carried over to the NRME configurations. In particular, the NRME configuration is homoclinic to its background RRO configuration and no net phase shift is introduced. In this sense, the emergence of the NRME configuration signals a phase transition in the gap structure (occurring in the Ω space) instead of the commensurate-incommensurate phase transition[2] (occurring in the ω space).

VIII. CONCLUSIONS

In this paper, we exactly solve a class of FK models, whose potential has d subwells in a period. The RO stable configuration is characterized by a winding number and a phase parameter in Ω, with elements $0=\beta_0\leqslant\beta_1\leqslant\beta_2\leqslant\cdots\leqslant\beta_{d-1}\leqslant 1$.

To depict all RO stable configurations with hull functions, phase parameters expressed in terms of extended numbers must be included for the incommensurate case. The depicted configurations in such cases are shown to be nonrecurrent. The existence of these NRO configurations assures the existence of incommensurate NRME configurations for a suitable choice of potential parameters.

The notions of subcommensurate clusters, and resonance between different types of openings are introduced to fully characterize the gap structure. These notions are helpful in visualizing phase transitions in the gap structures.

We provided an approach to determine the ground state configurations through the information about the relative positions of tips for the potential and gaps for the RO configurations. All the possibilities of degenerate ground state configurations are explored. Using these results, we are able to study the phase diagram. In the incommensurate case, we show that the phase diagram in $\mathcal{T}$ is an extension of the complete devil's staircase to $(d-1)$ dimensions. It will be interesting to see if the conclusion is still valid in the $d \to \infty$ limit.

We also provided a general method to implement an incommensurate NRME configuration. For any FK model beyond TBA, which allows more than one discontinuity classes, it appears that such incommensurate NRME configurations should also exist at the transition points for any l to $(l+1)$-hole transitions. In general, NRME configurations emerge as long as a certain locking condition (either the subcommensurate condition in our case or the commensurate condition) of the parameters to characterize the configuration (including the phase parameters in our case and the winding number) is allowed to break down, which are expected to occur at boundaries of the domains of stability, where some locking conditions prevail.

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APPENDIX A

From Eq. (3.10), it is straightforward to show that

$$\frac{\partial^2 \Psi}{\partial \beta_i \partial \beta_j} = -\lambda \Delta b_i \Delta b_j \sum_{n=-\infty}^{\infty} e^{-|n|\chi} \times \delta(\mathrm{Frac}[n\omega+\beta_i-\beta_j]), \quad \text{for } 0<i<j<d, \tag{A1}$$

$$\frac{\partial^2 \Psi}{\partial \beta_i^2} = \lambda \Delta b_i \sum_{j=1, j\neq i}^{d-1} \Delta b_j \sum_{n=-\infty}^{\infty} e^{-|n|\chi} \times \delta(\mathrm{Frac}[n\omega+\beta_i-\beta_j]), \quad \text{for } 0<i<d, \tag{A2}$$

$$\frac{\partial^2 \Psi}{\partial \beta_i \partial \omega} = -\lambda \frac{d_0}{2} \Delta b_i \sum_{j=1, j\neq i}^{d-1} \Delta b_j \sum_{n=-\infty}^{\infty} n\, e^{-|n|\chi} \times \delta(\mathrm{Frac}[n\omega+\beta_i-\beta_j]), \quad \text{for } 0<i<d, \tag{A3}$$

and

$$\frac{\partial^2 \Psi}{\partial \omega^2} = \lambda \frac{d_0}{2} \sum_{i,j=1}^{d-1} \Delta b_i \Delta b_j \sum_{n=-\infty}^{\infty} n^2 e^{-|n|\chi} \times \delta(\mathrm{Frac}[n\omega+\beta_i-\beta_j]), \tag{A4}$$

where $\delta(\cdots)$ denotes the Dirac delta function. For every point $(\zeta_0, \zeta_1, \zeta_2, \ldots, \zeta_{d-1}) \equiv (\omega, \beta_1, \beta_2, \ldots, \beta_{d-1})$ in $\overline{\Omega} \equiv \{\omega \in [0,1)\} \oplus \Omega$, define the curvature matrix $\mathbf{M}$, with elements given by

$$\mathbf{M}_{k,l} = \frac{\partial^2 \Psi}{\partial \zeta_k \partial \zeta_l}. \tag{A5}$$

This matrix can be decomposed into

$$\mathbf{M} = \lambda \sum_{n=-\infty}^{\infty} e^{-|n|\chi} \left[\sum_{i=0}^{d-1} \Delta b_i^2 \delta(\mathrm{Frac}[n\omega]) \mathbf{M}^{n,0} + 2 \sum_{0<i<j<d} \Delta b_i \Delta b_j \delta(\mathrm{Frac}[n\omega+\beta_i-\beta_j]) \mathbf{M}^{n,i,j} \right] \tag{A6}$$

with

$$\mathbf{M}^{n,0}_{k,l} \equiv n^2 \frac{d_0}{2} \delta_{k,0} \delta_{l,0} \tag{A7}$$

and

$$\mathbf{M}^{n,i,j}_{k,l} \equiv \delta_{k,i}\delta_{l,i} + \delta_{k,j}\delta_{l,j} - \delta_{k,i}\delta_{l,j} - \delta_{k,j}\delta_{l,i} + n\frac{d_0}{2}(\delta_{k,0}\delta_{l,i} + \delta_{k,i}\delta_{l,0} - \delta_{k,0}\delta_{l,j} - \delta_{k,j}\delta_{l,0}) + n^2 \frac{d_0}{2} \delta_{k,0}\delta_{l,0}. \tag{A8}$$

It is easy to check that every matrix $\mathbf{M}^{n,i,j}$ is positive semidefinite, where the fact that $0<d_0<1$ should be employed. As a result, the energy function is convex in $\overline{\Omega}$.

APPENDIX B

In general, for a subcommensurate cluster composed of $1 \leq k \leq d$ elements, the domain of stability is an $(k-1)$-dimensional convex hyperpolygon with $k!$ vertices in the projected phase subspace. All pieces of the hypersurfaces on its boundary are flat (hyperplanes) and are the direct product of two convex hyperpolygons of lower dimensions. On the boundary hypersurface, the subcommensurate cluster is allowed to split into two groups. Each of the lower dimensional hyperpolygons can still be decomposed in the same way until the vertices (with dimensionalities 0) are reached, where the subcommensurate cluster is allowed to decompose into k one-element groups.

Let us inspect the circumstances of each domain of stability. For a phase parameter $\boldsymbol{\beta}$ containing l subcommensurate clusters, with d_1, d_2, ..., and d_l elements, respectively. The corresponding $D[\boldsymbol{\beta}]$ is a $d-l$ domain and the hypersurfaces on its boundary are $d-l-1$ domains. Each of these

$d-l-1$ domains is also the overlapping region of $D[\boldsymbol{\beta}]$ with its adjacent $d-l$ domain. Hence, the number of ways to split the l holes (subcommensurate clusters) into $l+1$ through continuously varying the elements in $\boldsymbol{\beta}$ gives the number of $d-l-1$ domains surrounding $D[\boldsymbol{\beta}]$. For $D[\boldsymbol{\beta}]\cap\partial\mathcal{T}=\varnothing$ (i.e., $\nu_i>0$ for all i), the number is given by $\Sigma_{j=1}^{l}(2^{d_j}-2)$. Similar procedure to count the number of ways to split the l holes into k holes, for any $l<k\leqslant d$, will give the number of $d-k$ domains on the boundary of $D[\boldsymbol{\beta}]$. In particular, the number of vertices (0 domains) of this domain is given by $\Pi_{j=1}^{l}(d_j!)$.

On the other hand, a $d-l$ domain can play as the boundary (overlapping region) of $l!/[k!(l-k)!]$ distinct $d-k$ domains for $l>k\geqslant 1$. The number of $d-k$ domains is from counting the ways to coalesce adjacent holes $l-k$ times among the l cyclic holes.

Care should be taken in counting the number of $d-l$ domains adjacent to a given $d-l$ domain $D[\boldsymbol{\beta}]$. The overlapping part of two adjacent $d-l$ domains can be a $d-l-1$ domain or a domain with lower dimensionality. Here, we only consider the cases with the overlapping parts being $d-l-1$ domains. The number is given by $l\Sigma_{j=1}^{l}(2^{d_j}-2)$ if $D[\boldsymbol{\beta}]\cap\partial\mathcal{T}=\varnothing$.

APPENDIX C

Consider a ground state configurations $u_n^{l,r}=f_{\boldsymbol{\omega}}^{l,r}(\beta_i+n\omega)$ with the winding number ω irrational and the phase parameter $\boldsymbol{\beta}$ with two of the elements β_i and β_j subcommensurate with a finite n_{ij}. Adjust the potential parameter **t** to the boundary of $D[\boldsymbol{\beta}]$ where moving the n_{ji}th atom in the $\{u_n^r\}$ configuration across the $(d\,\mathrm{Int}[n_{ji}\omega]+j)$th tip does not cost energy. Such a movement can be conducted via an elementary phase shift characterized by $k_l^I=-\delta_{jl}$ for $0<l<d$. The resultant configuration $\{u_n'\}$ has a segment, with one atom (say, the nth one) located at the $(i+1)$-th type of subwells [say, the $(md+i+1)$-th subwell] and the $(n+n_{ji})$-th atom located at the $(md+d\,\mathrm{Int}[n_{ji}\omega]+j)$th subwell, occurring only at $n=0$ and $m=0$. There is no other place to find such a segment in $\{u_n'\}$. Therefore, $\{u_n'\}$ is an incommensurate NRME configuration. It emerges where the two types of openings, associated with β_i and β_j respectively, are just about to break their resonance. Namely, n_{ji} has a finite limiting value but the limiting value of n_{ji}' diverges as the infinitely long atomic chain is taken into account even though the limiting values of $\mathrm{Frac}[n_{ji}\omega]$ and $\mathrm{Frac}[n_{ji}'\omega]$ are the same.

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[37] Two limiting processes are involved in this formulation. One is related to take the incommensurate case as a limit of commensurate cases, while the other is relate to take the right-hand or left-hand side limits of the hull function. Throughout this paper, the latter limit is always taken before the former one.
[38] See, for example, B. A. Dubrovin, A. T. Fomenko, and S. P. Novikov, *Modern Geometry-Methods and Applications* (Springer-Verlag, New York, 1985), Vol. II, Chap. 7.
[39] S. Aubry and P. Le Daeron, Physica D **8**, 381 (1983).
[40] See, for example, E. M. Lifshitz and L. P. Pitaevskii, *Statistical Physics*, 3rd ed. (Pergamon Press, Oxford, 1980), pt. 1.
[41] As a comparison, in Ref. 17 the energy function was thought to be strictly convex.
[42] A piece of hypersurface on the boundary of $D[\boldsymbol{\beta}]$ is in fact a hyperplane since $\Delta H_q^I(\boldsymbol{\beta})|_{\Delta \mathbf{b}} = 0$ is a linear equation in $\mathbf{t}$. However, if one chooses another set of $d-1$ variables from $\Delta \mathbf{b} \otimes \mathbf{t}$ as parameters, the corresponding equation is in general nonlinear as a function of the remaining $d-1$ independent variables. It will give a hypersurface in the phase space of the $d-1$ independent variables.
[43] For example, if $\nu_i = \beta_i - \beta_{i-1} = 0$, a small negative value of $t_i - t_{i-1}$ will be allowed by the constraint. But it is not allowed for the potential in our consideration.