Sliding mode and breaking of analyticity in the double-chain model of incommensurate composites

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The double chain model (DCM) generalizes the Frenkel-Kontorova model for composite systems, coping with situations when both subsystems are deformable. We show how the shape and amplitude of the intermodulation of subsystems depend on the intersubsystem interaction potential, elastic constants, and average repeat distances of the subsystems. We characterize and study the behavior of the sliding mode, that is a pseudo-Goldstone mode of the system. DCM undergoes an analyticity breaking transition that leads to intrinsic pinning of the sliding mode, when the strength of the intersubsystem coupling is increased above a threshold value. [S0163-1829(99)02042-1]

I. INTRODUCTION

Incommensurate composites belong to the class of quasiperiodic crystals, and are defined by the presence in their structure of at least two interpenetrating modulated crystalline subsystems, that have incommensurate average repeat distances along one or several common crystallographic directions. The most studied composites are the intergrowth or inclusion compounds,[1,2] for which the connectivity of at least one of the subsystems is linear, and the misfit layer or intercalation compounds,[3] whose subsystems form alternating parallel layers with planar connectivity.

Because the irrational ratio of average repeat distances cannot be easily modified (unless the chemical nature of one of the subsystems is altered) composites remind of quasicrystals. The fact that one or both subsystems are modulated by their mutual interaction reminds of modulated incommensurate crystals. In this sense incommensurate composites represent an intermediate case. As usual for quasiperiodic crystals, the structure of incommensurate composites can be usefully described by superspace analysis. The general principles of the superspace embedding as well as the application of this method to the description of the structure of intergrowth compounds like $Hg_{3-\delta}AsF_6$ were introduced by Janner and Janssen.[4] Using this approach van Smallen[5] analyzed the structure of several incommensurate misfit layer and intergrowth compounds. In the case of incommensurate composites at least two sets of atomic surfaces are needed, one for each subsystem. The dimension of the superspace lattice is $3+d$ where d is the number of independent incommensurate length ratios in the structure, and it seems that the intermodulation does not introduce new incommensurate ratios (does not change d).

Hydrodynamic modes of the intergrowth compound $Hg_{3-\delta}AsF_6$ were computed in Ref. 6. Elasticity theory of composites was discussed in Ref. 7. The Frenkel-Kontorova model (FK) (Refs. 8 and 9) consisting of a harmonic chain of atoms under the influence of a rigid periodic substrate would describe a special composite system, when one of the subsystems is infinitely rigid. Double Frenkel-Kontorova models[10,11] allowed some understanding of solitons involving deformation of both subsystems. None of the previous models are able to explain correctly static properties like the intermodulation, or to give a full account of the lattice dynamics by taking into account the discrete nature of the composite. In order to provide a more accurate description of the static and dynamic properties of composites, we have recently introduced[12] the double-chain model (DCM), consisting of two harmonic chains of atoms that interact with each other via pair potentials. DCM generalizes the FK model by replacing the rigid periodic substrate of the latter by a second, deformable chain. Unlike the double FK model[10] that represents the action of one chain on the other by an average periodic potential, the DCM deals with the mutual deformation of the chains in a more realistic way.

Recent experimental work focused on structural and dynamic properties of urea-alkane inclusion compounds and motivated our theoretical approach. X-ray and neutron-scattering experiments showed the presence of satellite reflections, due to the intermodulation of both subsystems.[13,14] The positions in the reciprocal space of the main reflections and satellites are linear combinations of two wave vectors corresponding to the inverse average periods of the subsystems.[13] This implies that the modulation function of each subsystem has the period of the other subsystem. Measuring the intensities of different x-ray reflections allowed the structure refinement of the $C_{17}H_{36}$/urea inclusion compound, taking into account atomic displacements associated with the modulation.[14] Lattice dynamics has been studied via Brillouin light scattering and inelastic neutron scattering. Special attention has been given to the detection of the controversial phason mode, that for composites should involve the relative displacement of the subsystems and therefore is also called sliding mode. Optical measurements on C_nH_{2n+2}/urea compounds ($n=12$, 14, 17, 19) are compatible with the existence of a sliding mode[15] that may be pinned.[16]

In this paper we intend to discuss some general features of the statics and dynamics of composites. For simplicity we make a rather special choice of the interchain pair potential that is considered to be Gaussian. We shall present elsewhere[17] a methodology for determining the shape and the amplitude of the interchain pair potential for specific inclu-

sion compounds. This uses the model developed here and allows direct confrontation of the theory with experimental data on intermodulation and dynamics.

Another purpose of this work is the study of the analyticity breaking transition (ABT) for the DCM. The FK model develops a zero-temperature transition when the amplitude of the substrate potential increases above a threshold value. The signature of the transition is the loss of analyticity of the modulation function of the chain, accompanied by the pinning of the phason mode. Aubry[18] provided a rigorous analysis of the FK model, emphasizing that ABT corresponds to breaking invariant tori of a two-dimensional (2D) dynamical system. We show that DCM also undergoes ABT when a critical line in the plane of the coupling constants is crossed. This result shows that this type of transition is very general and that the presence of a rigid periodic substrate is not really necessary in order for this to happen.

This paper is structured as follows. The next section describes the DCM. The ground states of the DCM and their superspace embedding are described in Sec. III A. In Sec. III B we discuss symmetry breaking and the two Goldstone modes of the model: the acoustical phonon and the phason (sliding) mode. The analyticity breaking transition is discussed in Sec. III C. In Sec. III D we use Poisson sum formula and perturbation theory in order to calculate the modulation amplitudes. Section III E contains an analysis of the relation between the average repeat distances ratio and the relative modulation amplitudes of the subsystems. A special effect is emphasized that we call enhanced rigidity of the longer period subsystem.

II. DOUBLE-CHAIN MODEL

The double-chain model (DCM) consists of two parallel chains of atoms. The atoms interact via pair potentials and move only longitudinally along the common direction of the chains.

A configuration of the DCM is defined by the 1D positions of the atoms along the two chains $\mathcal{C}:=\{x_n^{(1)},x_m^{(2)}\}_{m,n\in Z}$. The potential energy of a configuration is

$$\mathcal{E}(\mathcal{C})=\sum_{n,n'}\mathcal{V}^{(1,1)}(x_n^{(1)}-x_{n'}^{(1)})+\sum_{m,m'}\mathcal{V}^{(2,2)}(x_m^{(2)}-x_{m'}^{(2)})+\sum_{n,m}\mathcal{V}^{(1,2)}(x_n^{(1)}-x_m^{(2)}). \tag{2.1}$$

Here we restrict the range of intrachain interactions to successive neighboring atoms, and use convex harmonic intrachain potentials $\mathcal{V}^{(1,1)},\mathcal{V}^{(2,2)}$. In other words, successive atoms on the chains 1 and 2 are connected by springs of elastic constants $k^{(1)}$, and $k^{(2)}$, and undeformed lengths a_1,a_2, respectively. We also consider that the interchain potential $\mathcal{V}^{(1,2)}$ has a finite range ρ. In this paper $\mathcal{V}^{(1,2)}$ is a Gaussian potential $\mathcal{V}^{(1,2)}(x)=(k^{(1,2)}\rho^2/2)V(x/\rho)$ where $V=-\exp(-x^2)$. In a previous paper[12] we have considered the case of a truncated harmonic potential that leads to analytic results. As we show elsewhere[17] the shape of the interchain potential may be adapted to the particular composite system that is studied.

After several rescalings the energy becomes

$$E=\frac{1}{2\chi^{(1)}}\sum\,(y_n^{(1)}-y_{n-1}^{(1)}-1)^2+\frac{1}{2\chi^{(2)}}\sum\,(y_m^{(2)}-y_{m-1}^{(2)}-\alpha)^2+\frac{r^2}{2}\sum\,V\left(\frac{y_n^{(1)}-y_m^{(2)}}{r}\right), \tag{2.2}$$

where $E=\mathcal{E}/(k^{(1,2)}a_1^2)$, $y_n^{(1)}=x_n^{(1)}/a_1$, $y_m^{(2)}=x_m^{(2)}/a_1$, $\alpha=a_2/a_1, r=\rho/a_1$, $\chi^{(1)}=k^{(1,2)}/k^{(1)}$, $\chi^{(2)}=k^{(1,2)}/k^{(2)}$.

A stationary (equilibrium) configuration obeys

$$(\partial^{(1)}E)_n=(2y_n^{(1)}-y_{n+1}^{(1)}-y_{n-1}^{(1)})/\chi^{(1)}+\frac{r}{2}\sum_m V'\left(\frac{y_n^{(1)}-y_m^{(2)}}{r}\right)=0,$$

$$(\partial^{(2)}E)_m=(2y_m^{(2)}-y_{m+1}^{(2)}-y_{m-1}^{(2)})/\chi^{(2)}-\frac{r}{2}\sum_n V'\left(\frac{y_n^{(1)}-y_m^{(2)}}{r}\right)=0. \tag{2.3}$$

The frequencies of phonon excitations, and the corresponding atomic displacements in reduced coordinates $\zeta_n^{(i)}=\sqrt{m_i}y_n^{(i)}$ are the square roots of eigenvalues, and the eigenvectors of the infinite dimensional dynamical matrix D, respectively:

$$D=\begin{bmatrix}\frac{1}{m_1}\partial^{(1,1)}E & \frac{1}{\sqrt{m_1m_2}}\partial^{(1,2)}E\\ \frac{1}{\sqrt{m_1m_2}}\partial^{(2,1)}E & \frac{1}{m_2}\partial^{(2,2)}E\end{bmatrix}, \tag{2.4}$$

where $\partial^{(i,j)}E$ are the four blocks of the Hessian of E (two for intrachain and two for interchain interaction).

For commensurate ground states, the Bloch theorem may be used to decompose D into a family of finite dimensional dynamical matrices.[12] In order to find commensurate ground states we have used a conjugate-gradient method to minimize the configuration energy [Eq. (2.2)] with periodic boundary conditions ($y_{n+p}^{(1)}=y_n^{(1)}+p, y_{m+q}^{(2)}=y_m^{(2)}+wq, p,q\in\mathbb{Z}$), at fixed winding number $w=\lim_{r\to\infty}(y_{m+r}^{(2)}-y_m^{(2)}/y_{n+r}^{(1)}-y_n^{(1)})=p/q=\alpha$. Series of rational winding numbers converging to an irrational α allowed examining incommensurate ground states.

III. INTERMODULATION AND PHASON MODE

A. Circle map and superspace representation

A ground-state configuration corresponding to the winding number α can be described by giving the displacements of each atom with respect to equidistant positions. Similarly to the case of the Frenkel-Kontorova (FK) model, the complete information describing these displacements can be encapsulated in two modulation functions (one for FK model) defined each one on the circle. Provided that ground states exist with the imposed winding number (as valid for the FK

model[19]), it is always possible to define modulation functions for each subsystem having the periodicity of the other subsystem, as follows:

$$y_n^{(1)} = n + f^{(1)}(n), \quad f^{(1)}(y+\alpha) = f^{(1)}(y),$$

$$y_m^{(2)} = m\alpha + \delta + f^{(2)}(m\alpha+\delta), \quad f^{(2)}(y+1) = f^{(2)}(y). \tag{3.1}$$

The relation (3.1) between displacements and modulation functions can be rewritten by using the circle map $C_\alpha : \mathbb{R}/\mathbb{Z} \to \mathbb{R}/\mathbb{Z}, C_\alpha(x) = x + \alpha (\mathrm{mod}\, 1)$:

$$f^{(1)}(\alpha C_{1/\alpha}^n(0)) = y_n^{(1)} - n,$$

$$f^{(2)}(C_\alpha^m(\delta)) = y_m^{(2)} - m\alpha - \delta. \tag{3.2}$$

For arbitrary β the orbit of any point x under the circle map is $\cup_n \{C_\beta^n(x)\} = \{x + n\beta (\mathrm{mod}\, 1) | n \in \mathbb{Z}\}$. This orbit fills densely the circle for irrational $\beta = \alpha, \alpha^{-1}$. If $\alpha \notin \mathbb{Q}$ then Eqs. (3.2) define the values of the modulation functions on sets that are dense in the circle. For the FK model any ground state has a well defined winding number and when this number is irrational the modulation function can always be extended to left or right continuous functions on the entire circle.[19] Furthermore, the modulation function is analytic if the substrate potential is weak enough. We expect the same to be true for DCM. It is actually at this point that we get the full meaning of the property that each subsystem is modulated with the period of the other. The modulation functions are analytic or at least left or right continuous when they are defined for each subsystem with the period of the other subsystem. In more general situations[20] when more than two periods are involved the convenient periodicity of the modulation function is dictated by the Diophantine relations between the periods of the system; this may lead to quasiperiodic modulation functions as well. For $\alpha = p/q,\ p,q \in \mathbb{Z}$ the circle map orbits are finite and Eqs. (3.1) and (3.2) define the values of the modulation functions on finite sets of points equidistantly distributed on the circle, and the successive values $f^{(1)}(r/q), r = 0, \ldots, p-1$, $f^{(2)}(\delta + s/q), s = 0, \ldots, q-1$, are the relabeled values of the displacements $y_n^{(1)} - n$, $y_m^{(2)} - m\alpha - \delta$ via the permutations $r = n * q (\mathrm{mod}\, p)$, $s = m * p (\mathrm{mod}\, q)$. We have used this property to construct the modulation functions for ground states calculated with periodic boundary conditions.

The above constructions find a simple geometrical interpretation in the 2D superspace formalism.[4] Positions of atoms in the two chains are the intersections of the 1D physical line (Fig. 1, horizontal) with two families of parallel atomic lines (one for each chain). If no intermodulation is present the atomic lines are straight and cut the physical line at equidistant positions n and $m\alpha + \delta$. The superlattice is defined by the intersections between the two families of straight lines. As shown in Fig. 1 the geometry of the 2D superlattice is not entirely fixed by the winding number. Two angles have to be specified, giving the inclination of the two families of lattice lines with respect to the physical line. One of these two angles is usually chosen $\pi/2$ for simplicity, and thus one family of atomic lines is perpendicular to the physical line, while the second angle (γ) is arbitrary. This, however,

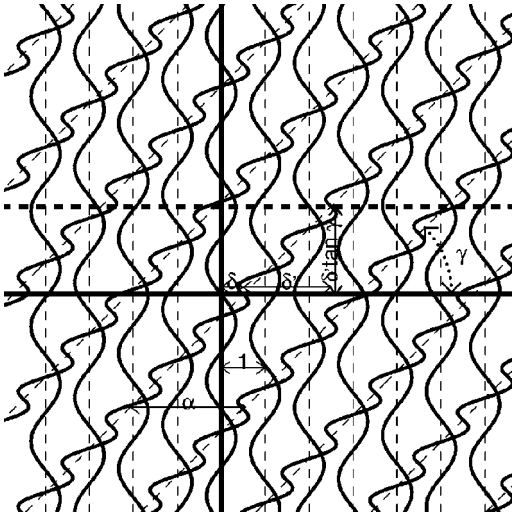

FIG. 1. Atomic lines for an incommensurate composite. Atoms are at the intersections of these lines with the physical line (x axis). A phason shift is a translation of the x axis.

masks in a way the symmetry between the two subsystems, but it is in general convenient. As true in general, the Fourier transform of the intersection of the superspace distribution with the physical line is the projection of the Fourier transform of this distribution onto the physical line. One can check that for any value of γ, the projection of the reciprocal superlattice onto the physical line is the dense Fourier module $\{2\pi(n + m/\alpha)\}_{n,m \in \mathbb{Z}}$ that contains the positions of all Bragg peaks of the composite. In the general (modulated) case, it can be shown that the two families of undulating atomic lines are uniquely defined by: (i) the intersections of the two families of atomic lines with the physical line are $x_n^{(1)}, x_m^{(2)}$, respectively; (ii) the set of atomic lines have the periodicity of the superlattice. The equations of the two families of atomic lines are

$$x = f^{(1)}[-y/\tan(\gamma) + n] + n,$$

$$x = f^{(2)}[y/\tan(\gamma) + m\alpha + \delta] + y/\tan(\gamma) + m\alpha + \delta. \tag{3.3}$$

B. Phason (sliding) mode and Goldstone theorem

Not counting space inversion, there are two types of symmetry elements of the configuration energy of the DCM. Some of these symmetry elements form the group of continuous translations T_λ:

$$T_\lambda(\{y_n^{(1)}, y_m^{(2)}\}) = \{y_n^{(1)} + \lambda, y_m^{(2)} + \lambda\}. \tag{3.4}$$

Other symmetry elements form a countable group, consisting in shifts of atomic indices, that preserve sequential order inside each chain.

$$S_{r,s}(\{y_n^{(1)}, y_m^{(2)}\}) = \{y_{n+r}^{(1)}, y_{m+s}^{(2)}\}. \tag{3.5}$$

Let $\mathcal{G} = \{n + f^{(1)}(n), m\alpha + \delta + f^{(2)}(m\alpha + \delta)\}$ be a ground state corresponding to the irrational winding number α. We call group of phason translations the subgroup $\{P_{r,s}\} := \{T_{-r} S_{r,s}\}_{r,s \in \mathbb{Z}}$ of the direct product $T_\lambda \times S_{r,s}$. $P_{r,s}$ acts on $\mathcal{G}$ in the following way:

$$P_{r,s}(\{n+f^{(1)}(n),\quad m\alpha+\delta+f^{(2)}(m\alpha+\delta)\})$$
$$=\{n+f^{(1)}(n-\delta'),\quad m\alpha+\delta+\delta'+f^{(2)}(m\alpha+\delta+\delta')\},\tag{3.6}$$

where $\delta'=s\alpha-r$. Using Eqs. (3.3) we may show that this transformation corresponds exactly to a shift of the physical line (horizontal) in the vertical direction by a distance $\delta'\tan(\gamma)$ (Fig. 1). Equation (3.6) shows the ''sliding'' character of the phason translation: this induces an average relative displacement δ' of one chain with respect to the other (the modulation functions have zero mean, hence the shifts of the arguments produce displacements that compensate on the average).

If $f^{(1)},f^{(2)}$ are differentiable, the countable set $P_{r,s}\mathcal{G}$ is densely embedded in the differentiable manifold of ground states $P_{\delta'}\mathcal{G}:=[n+f^{(1)}(n-\delta'),m\alpha+\delta+\delta'+f^{(2)}(m\alpha+\delta+\delta')]$, with δ' now a continuous parameter. The action of the translation group T_λ extends the manifold $P_{\delta'}I$ to the 2D differentiable manifold $T_\lambda P_{\delta'}\mathcal{G}$. This is typically the kind of situation ensuring the existence of two hydrodynamic Goldstone modes. Precisely, all vectors in the 2D tangent bundle of the manifold of ground states are in the kernel of the second derivative of the energy, therefore they are zero-energy modes. In order to prove this one has to differentiate the stationarity equation for a ground state $\partial E(T_\lambda P_{\delta'}\mathcal{G})=0$ with respect to either λ or δ' and find thus $\partial^2 E(T_\lambda P_{\delta'}\mathcal{G})v_i=0,i=1,2$.

The acoustical phonon corresponding to the rigid displacement of both chains is $v_1=\partial T_\lambda P_{\delta'}\mathcal{G}/\partial\lambda=\{1,1\}$.

The phason (sliding) mode is

$$v_2=\frac{\partial T_\lambda P_{\delta'}\mathcal{G}}{\partial\delta'}=\left\{-\frac{df^{(1)}}{dx}(n),1+\frac{df^{(2)}}{dx}(m\alpha+\delta)\right\}.\tag{3.7}$$

It corresponds to the rigid displacement of one chain with respect to the other, on which zero mean, oscillating components, equal to the derivatives of the modulation functions, are superimposed. In the superspace image the phason mode is polarized perpendicularly to the physical line.

There is a fundamental difference between the acoustical phonon and the phason. The first one is a true Goldstone mode, because it breaks the continuous translation symmetry, and therefore remains hydrodynamic even if the modulation functions are not continuous. The latter is a pseudo-Goldstone mode because it breaks only a countable (although dense) subgroup of translations, therefore loses its hydrodynamic character in the case of discontinuous modulation functions, when the countable set of degenerated ground states can no longer be embedded in a differentiable manifold. One important difference between the DCM and the FK model is the absence of continuous translational symmetry and of the acoustical phonon for the latter, when only the pseudo-Goldstone mode exists (the phason).

C. Analyticity breaking transition

For the FK model the stationarity Eqs. (2.3) lead to a dynamical system[18,19] in $\mathbb{R}^2$. For zero coupling the system is integrable and the orbits corresponding to irrational winding numbers fill densely invariant 2D tori. The Kolmogorov-Arnold-Moser theorem[19] ensures that tori corresponding to sufficiently irrational winding numbers are preserved and only deformed for sufficiently small coupling. DCM does not provide such low dimensional dynamical systems, except for zero coupling ($k^{(1,2)}=0$, integrable case when DCM becomes a system of two uncoupled harmonic chains). For finite coupling, each atom of one chain interacts with each atom of the other chain, hence the interchain coupling is not rigorously a local perturbation and the Kolmogorov-Arnold-Moser theorem can not be applied in its standard form. In spite of this complexity, numerical simulation shows that orbits having as coordinates displacements of successive atoms $\{y^{(1)}_{n-1}-(n-1),y^{(1)}_n-n\}=\{f^{(1)}(n-1),f^{(1)}(n)\}$ and $\{y^{(2)}_{n-1}-(n-1)\alpha-\delta,y^{(2)}_n-n\alpha-\delta\}=\{f^{(2)}[(n-1)\alpha+\delta],f^{(2)}(n\alpha+\delta)\}$ fill densely 2D smooth closed curves (Fig. 2). These smooth curves exist for weak interchain coupling. The

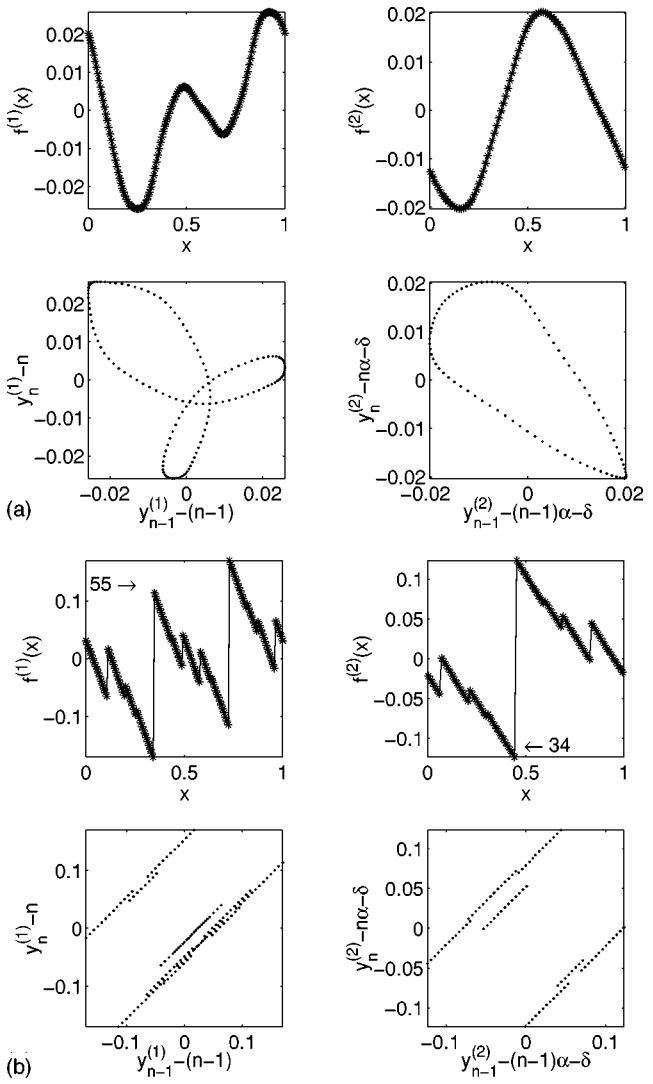

FIG. 2. Modulation functions and corresponding 1+1-dimensional manifolds: (a) analytic [$\chi^{(1)}=\chi^{(2)}=0.5$, $r=1/3$, $\alpha=144/89\approx\tau=(1+\sqrt{5})/2$, approximant of the golden mean] and (b) discontinuous ($\chi^{(1)}=\chi^{(2)}=1.5$, $r=1/3$, $\alpha=144/89$). The atoms No. 55 and 34 are nearest neighbors and correspond to edges of the largest discontinuities of the modulation functions of the first and second chain, respectively.

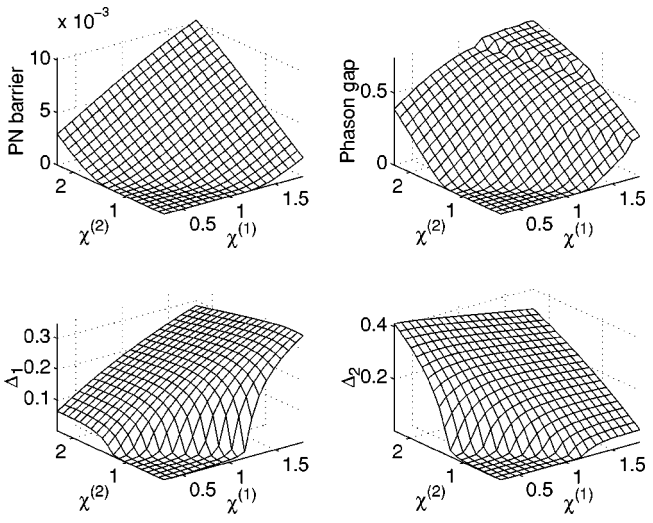

FIG. 3. Behaviour of the Peierls-Nabarro barrier, phason gap, largest discontinuity jumps in the modulation functions (Δ_1,Δ_2), at the analyticity breaking transition. The calculation was made for $r=1/3,\alpha=89/55\approx\tau$.

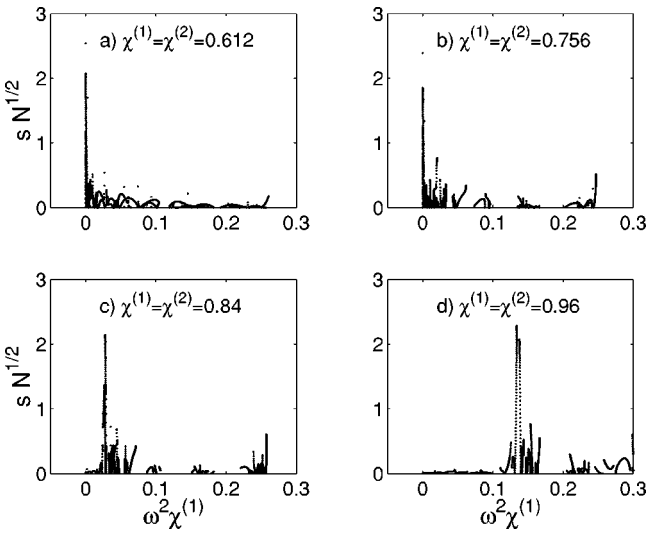

FIG. 4. Sliding parameter s for different modes, as a function of frequency $(r=1/3,\ \alpha=144/89\approx\tau)$. (a) In the analytic regime; (b) at the analyticity breaking transition; (c) and (d) in the nonanalytic regime. The phason corresponds to the maximum of the sliding parameter. s was rescaled by $\sqrt{N}$ where $N=233$ is the number of atoms in the unit cell, in order to ensure convergence when $N\to\infty,\ \alpha\to\tau$.

dense confinement of a configuration inside a pair of smooth 2D closed curves is equivalent to the smoothness of the modulation functions and atomic lines. If the interchain coupling is strengthened, or if the chains are softened, i.e., if $\chi^{(1)}$ and $\chi^{(2)}$ are increased the modulation functions $f^{(1)}$ and $f^{(2)}$ become discontinuous in an infinite number of points. The analyticity of the modulation functions is broken simultaneously for the two chains, when a critical transition line in the plane $\chi^{(1)},\chi^{(2)}$ is crossed. The physics changes across the transition line: the phason becomes pinned, phason translations no longer involve continuous displacements and produce atomic jumps, neighboring ground states are isolated by Peierls-Nabarro barriers, and an infinite hierarchy of metastable states can be produced by atomic jumps over barriers with various energetic heights. In order to study the analyticity breaking transition we have determined the dependence on $\chi^{(1)},\chi^{(2)}$ of several quantities.

Order parameters. The normalized widths of the largest discontinuity jumps of the modulation functions, defined as $\Delta_{1,2}=\max[f^{(1,2)}(x+)-f^{(1,2)}(x-)]/[\max f(x)-\min f(x)]$, can be chosen as order parameters for the ABT. In the analytical regime, $\Delta_{1,2}$ are zero (they scale like $\Delta_1\sim 1/p$, $\Delta_2\sim 1/q$ for periodic boundary conditions). In the nonanalytic regime $\Delta_{1,2}$ become simultaneously finite, the transition occurring simultaneously in the two chains (Fig. 3).

Phason gap. For the FK model the phason gap is defined as the lowest frequency in the phonon spectrum. This is zero for analytic modulation functions and increases in the nonanalytic regime according to a power law.[21] For the DCM the lowest frequency in the phonon spectrum is always zero because of the continuous translational symmetry. In the analytical regime the zero frequency has twofold degeneracy and the phason mode is rigorously defined by Eq. (3.7). In the nonanalytic regime it is difficult to identify the phason mode because this is no longer described by Eq. (3.7) and the phason frequency is not the lowest in the spectrum. We have chosen to call phason the mode corresponding to the highest value of the sliding parameter $s=|\langle u^{(1)}\rangle-\langle u^{(2)}\rangle|$ representing the relative displacement between the centers of mass of the two chains in a normalized eigenvector and we defined the phason gap as the energy of the phason mode. This definition agrees with Eq. (3.7) in the analytic regime and is motivated by our expectation that the ''sliding'' character of the phason should be preserved also in the nonanalytic regime. Figure 4 shows that our expectation is fulfilled and that a cluster of modes with high values of s is moving towards higher frequencies when the coupling parameters $\chi^{(1)},\chi^{(2)}$ are increased in the nonanalytic regime. Interestingly enough, the phason mode defined as above corresponds to either a real gap in the spectrum or to a discontinuity in the density of states (discontinuity of the slope of IDOS in Fig. 5). The dependence of the phason energy as a function of $\chi^{(1)},\chi^{(2)}$ is rather complex, showing discontinuity jumps

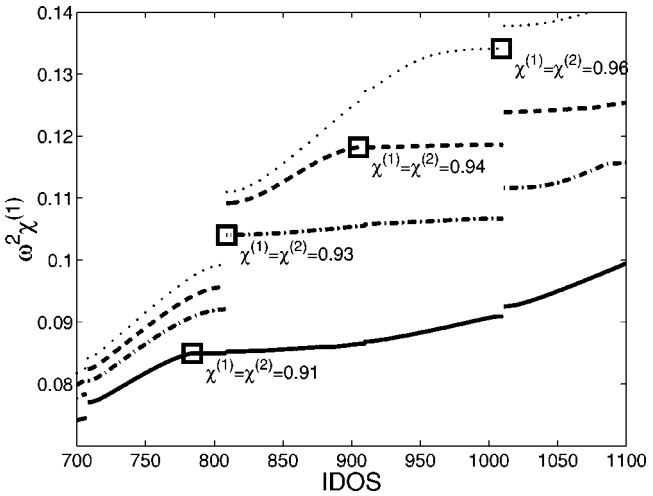

FIG. 5. Integrated density of states for different values of the coupling parameters $(r=1/3,\ \alpha=144/89\approx\tau)$. The squares mark the position of the phason which is either a gap edge, or a discontinuity of the density of states (slope of IDOS).

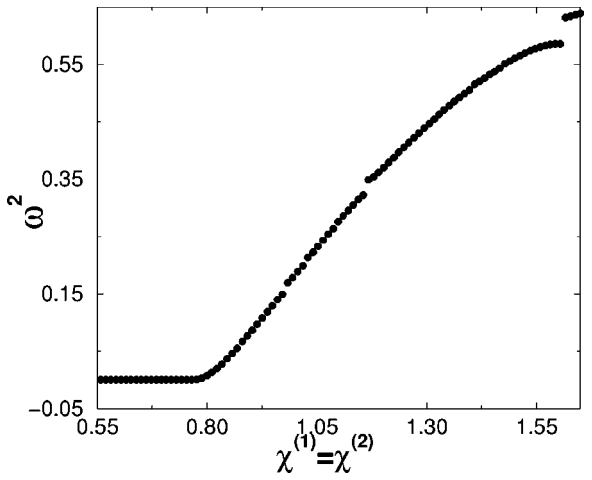

FIG. 6. Phason energy as a function of the coupling, at equal rigidity of the subsystems ($r=1/3$, $\alpha=89/55\approx\tau$).

(Figs. 3 and 6). Nevertheless, the jumps in the phason energy are large only far away from the critical line and become vanishingly small close to it. We should mention that the parameter s defining the phason is neither a topological invariant nor a symmetry property of this mode, therefore the continuity of the phason energy as a function of the coupling parameters is not guaranteed. For the 1D DCM and in the analytical regime the zero frequency phason and phonon belong both to the antisymmetric representation of the point symmetry group $\mathbb{Z}_2$. For 2D or 3D structures with more symmetry the situation may change and the phason may have a different symmetry from that of the phonon. In this case one might be able to choose a symmetry definition of the phason that would ensure the continuity of the phason energy even in the nonanalytic regime.

Peierls-Nabarro (PN) barrier. The PN barrier is defined as the maximum energy height of an optimal path between two contiguous ground states in the configuration space, i.e., states whose modulation functions are one left and the other right continuous, respectively. For continuous modulation functions contiguous states coincide and the PN barrier is zero. In the FK model, the physical meaning of a path between contiguous ground states is the jump of an atom from one valley of the substrate potential to a neighboring one over a potential maximum, accompanied by smaller displacements (that do not jump over potential maxima) of all other atoms.[21] The choice of the atom that jumps is not arbitrary: its position relabeled via the circle map should be on the edge of the largest discontinuity of the modulation function. Similarly, for the DCM one has to move the atom on the edge of the largest discontinuity of the modulation function of one chain, while keeping fixed the atom on the second chain closest to it in the direction of movement (this second atom is on the edge of the largest discontinuity of the modulation function of the second chain, Fig. 2). The result is the jump of the first atom from the left (or right) side to the right (or left) side of the second atom. As for the FK model, this position permuting jump is accompanied by smaller displacements of all other atoms that preserve positional order; each atom move corresponds to crossing a discontinuity of the modulation functions. This special local deformation of the system was called ''effective discommensuration.''[22]

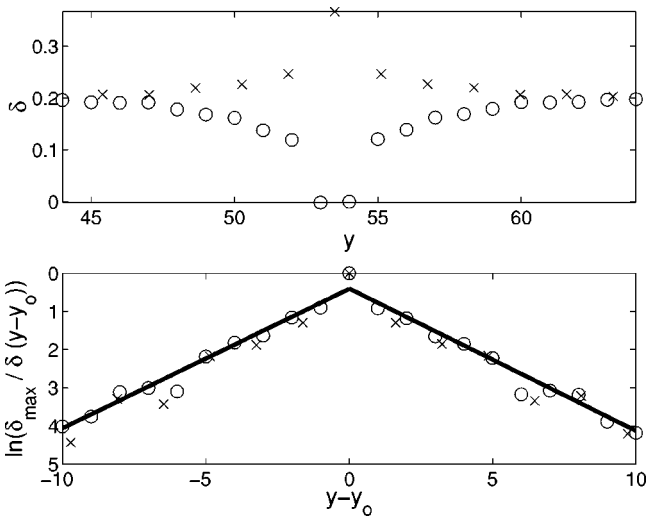

FIG. 7. The displacements δ of atoms on the first ($\times$) and on the second ($\bigcirc$) chain, corresponding to an effective discommensuration (positioned at y_o) ($\chi^{(1)}=\chi^{(2)}=1.0, r=1/3, \alpha=144/89\approx\tau$). The correlation length (the same for both chains) is the inverse slope of the interpolated straight lines.

The displacements decay exponentially with the distance to the selected atom and the corresponding characteristic lengths (correlation lengths) are equal along the two chains (Fig. 7). Like the FK model, DCM predicts that the height of the PN barrier decreases with the correlation length (width of the discommensuration). The correlation length diverges and the PN barrier vanishes at the ABT. In the superspace representation an ''effective discommensuration'' corresponds to an infinitesimal phason translation of the physical line and is analog to the phason flip in quasicrystals.[23,24] The difference between DCM and a cut and projection model of a quasicrystal is that the number of unequivalent discontinuities of the atomic lines and therefore the number of atoms that move are infinitely many for the first model and in finite number for the latter.

D. Perturbation theory estimates of the modulation amplitudes

Let $f^{(1)}(y)=\Sigma_m \tilde{f}_m^{(1)} \exp(2\pi m i y/\alpha)$, and $f^{(2)}(y)=\Sigma_n \tilde{f}_n^{(2)} \exp(2\pi i n y)$ be the Fourier series expansions of the modulation functions, and let $\tilde{V}(k)=\int \exp(-ikx)V(x)dx$ be the Fourier transform of the interchain interaction potential. For absolutely summable potentials V and bounded periodic functions f of period b, the following generalized Poisson sum formulas are valid (see Appendix), for any a:

$$\sum_n V(x-na)f(na+y)$$

$$=\frac{1}{a}\sum_{r,p}\tilde{V}\left[2\pi\left(\frac{p}{b}+\frac{r}{a}\right)\right]\tilde{f}_p \exp\left[2\pi i x\left(\frac{p}{b}+\frac{r}{a}\right)\right]$$

$$\times\exp\left(2\pi i y\frac{p}{b}\right) \tag{3.8a}$$

$$\sum_n V(x-na)=\frac{1}{a}\sum_r \tilde{V}\left(\frac{2\pi r}{a}\right)\exp\left(2\pi i x\frac{r}{a}\right). \quad (3.8b)$$

Using the stationarity Eq. (2.3), the above identities, and a first order Taylor expansion of the interchain potential in the modulation amplitudes, we obtain the following system of equations:

$$\frac{4}{\chi^{(1)}}\sin^2\left(\frac{\pi m}{\alpha}\right)\tilde{f}^{(1)}_{\delta,m} = -\frac{\pi r^3 i m}{\alpha^2}\tilde{V}\left(\frac{2\pi m r}{\alpha}\right) + \frac{2\pi^2 r^4}{\alpha}\left\{\sum_s \left(\frac{m-s}{\alpha}\right)^2 \tilde{V}\left(\frac{2\pi(m-s)r}{\alpha}\right)\tilde{f}^{(1)}_{\delta,s} - \sum_p \left(p+\frac{m}{\alpha}\right)^2 \tilde{V}\left[2\pi\left(p+\frac{m}{\alpha}\right)\right]\tilde{f}^{(2)}_p\right\}, \quad (3.9a)$$

$$\frac{4}{\chi^{(2)}}\sin^2(\pi n\alpha)\tilde{f}^{(2)}_n = -\pi r^3 i n\tilde{V}(-2\pi n r)+2\pi^2 r^4 \times\left\{\sum_s (n-s)^2\tilde{V}[-2\pi r(n-s)]\tilde{f}^{(2)}_s - \sum_p \left(\frac{p}{\alpha}+n\right)^2\tilde{V}\left[2\pi r\left(\frac{p}{\alpha}+n\right)\right]\tilde{f}^{(1)}_{\delta,p}\right\}, \quad (3.9b)$$

where $\tilde{f}^{(1)}_{\delta,m}:=\tilde{f}^{(1)}_m\exp(2\pi i\delta m/\alpha)$.

Equations (3.9) allow us to find the expansions of the harmonics of the modulation functions up to second order in the coupling parameters $\tilde{f}^{(1)}_{\delta,m}=\tilde{f}^{(1,1)}_{\delta,m}+\tilde{f}^{(1,2)}_{\delta,m}$, $\tilde{f}^{(2)}_n=\tilde{f}^{(2,1)}_n+\tilde{f}^{(2,2)}_n$ where

$$\tilde{f}^{(1,1)}_{\delta,m}=-\frac{\pi r^3 i m\chi^{(1)}}{4\alpha^2\sin^2(\pi m/\alpha)}\tilde{V}\left(\frac{2\pi m r}{\alpha}\right), \quad (3.10a)$$

$$\tilde{f}^{(2,1)}_n=\frac{-\pi r^3 i n\chi^{(2)}}{4\sin^2(\pi n\alpha)}\tilde{V}(-2\pi n r), \quad (3.10b)$$

$$\tilde{f}^{(1,2)}_{\delta,m}=\frac{\pi^2 r^4\chi^{(1)}}{2\alpha\sin^2(\pi m/\alpha)}\left\{\sum_s\left(\frac{m-s}{\alpha}\right)^2\tilde{V}\left(\frac{2\pi(m-s)r}{\alpha}\right)\tilde{f}^{(1,1)}_{\delta,s} - \sum_p\left(p+\frac{m}{\alpha}\right)^2\tilde{V}\left[2\pi\left(p+\frac{m}{\alpha}\right)\right]\tilde{f}^{(2,1)}_p\right\}, \quad (3.10c)$$

$$\tilde{f}^{(2,2)}_n=\frac{\pi^2 r^4\chi^{(2)}}{2\sin^2(\pi n\alpha)}\left\{\sum_s (n-s)^2\tilde{V}[-2\pi r(n-s)]\tilde{f}^{(2,1)}_s - \sum_p\left(\frac{p}{\alpha}+n\right)^2\tilde{V}\left[2\pi r\left(\frac{p}{\alpha}+n\right)\right]\tilde{f}^{(1,1)}_{\delta,p}\right\}. \quad (3.10d)$$

For $\alpha\in\mathbb{Q}$, different harmonics diverge in any order of the perturbation series in Eqs. (3.10), because of the small denominators $\sin^2(\pi m/\alpha)$, $\sin^2(\pi n\alpha)$, while for $\alpha\notin\mathbb{Q}$ sufficiently irrational the perturbation series is convergent, and Eqs. (3.10) provide approximations of the shapes and amplitudes of the modulation functions. In Fig. 8 we have compared the modulation amplitudes resulting from the perturbation theory calculation [using a limited number of harmonics in Eqs. (3.10), $|m|,|n|\leqslant 4$] and from the numerical determination of the ground state. We can notice that for winding numbers that are large denominator rationals the second-order perturbation theory gives amplitudes in good agreement with the numerical values. Deviations correspond to winding numbers with small denominators.

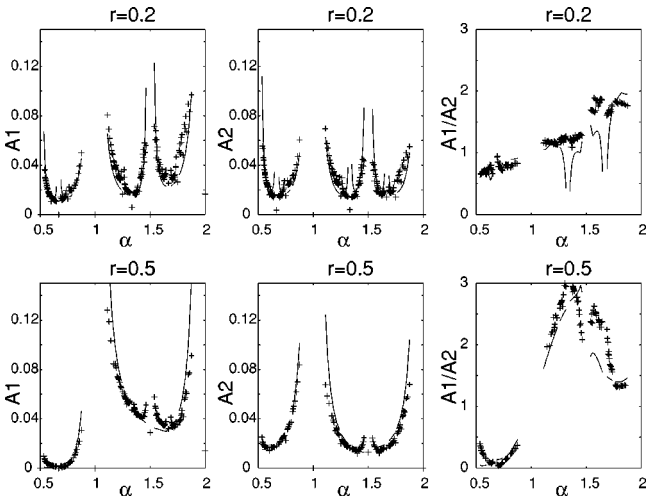

FIG. 8. Amplitudes of the modulation functions for $\chi^{(1)}=\chi^{(2)}=0.5$ as found numerically (+) compared with the result of the perturbation theory calculation (solid lines). The enhanced rigidity of the longer period subsystem, meaning that $A_1/A_2>1$ when $\alpha>1$ and vice versa, is more accentuated for the longer range of the interchain interaction ($r=0.5$).

From Eqs. (3.10) $f^{(1)}_n\sim\chi^{(1)}$, $f^{(2)}_m\sim\chi^{(2)}$, and using Eqs. (2.2), (3.1), and (3.8) we can write the energy of the DCM in the limit $\chi^{(1)}\to 0$ that means infinitely rigid subsystem 1, or $\chi^{(2)}\to 0$, i.e., infinitely rigid subsystem 2:

$$E_{\infty,1}\sim\frac{1}{2}\sum_m (y^{(2)}_m-y^{(2)}_{m-1}-\alpha)^2+\frac{\chi^{(2)}r^3}{2} \times\sum_n \tilde{V}(-2\pi n r)\exp(2\pi i n y^{(2)}_m), \quad (3.11a)$$

$$E_{\infty,2}\sim\frac{1}{2}\sum_n\left(z^{(1)}_n-z^{(1)}_{n-1}-\frac{1}{\alpha}\right)^2 + \frac{\chi^{(1)}}{2}\left(\frac{r}{\alpha}\right)^3\sum_m\tilde{V}\left(\frac{2\pi m r}{\alpha}\right)\exp\left[2\pi i m\left(z^{(1)}_n-\frac{\delta}{\alpha}\right)\right], \quad (3.11b)$$

where $z^{(1)}_n=y^{(1)}_n/\alpha$.

The DCM with one of the subsystems infinitely rigid becomes the FK model with periodic, but not necessarily sinusoidal substrate potential. For sufficiently smooth and rapidly decreasing interchain potential the following property is valid: (P) The ratio ζ between the amplitudes of the second and of the first harmonic of the substrate potential resulting

in the limit when one of the subsystems becomes infinitely rigid goes to zero when the range $r \to \infty$.[25] For this type of potentials DCM becomes the FK model with sinusoidal potential. In the limit $\chi^{(1)} \to 0$, $r \to \infty$, provided that $2\chi^{(2)} r^3 \tilde{V}(-2\pi r) \to \chi_{FK}$, or in the limit $\chi^{(2)} \to 0$, $r \to \infty$, provided that $2\chi^{(1)}(r/\alpha)^3 \tilde{V}(2\pi r/\alpha) \to \chi_{FK}$, the configuration energy becomes $E_{FK}^{\infty,1} \sim \frac{1}{2}\Sigma_m (y_m^{(2)} - y_{m-1}^{(2)} - \alpha)^2 + (\chi_{FK}/2)\Sigma_n \cos(2\pi y_m^{(2)})$, or $E_{FK}^{\infty,2} \sim \frac{1}{2}\Sigma_m (z_m^{(1)} - z_{m-1}^{(1)} - 1/\alpha)^2 + (\chi_{FK}/2)\Sigma_n \cos(2\pi z_m^{(1)})$, respectively. A Gaussian potential belongs to this class because $\tilde{V}(k) = -\sqrt{\pi}\exp(-k^2/2)$ and therefore $\zeta = \tilde{V}(-4\pi r)/\tilde{V}(-2\pi r) = \exp(-6\pi^2 r^2)$ or $\zeta = \tilde{V}(-4\pi r/\alpha)/\tilde{V}(-2\pi r/\alpha) = \exp(-6\pi^2 r^2/\alpha^2)$ if the first or the second chain are rigid, respectively. In order to obtain the FK model with a sinusoidal potential we must consider the limits $\chi^{(1)} \to 0$, $\chi^{(2)} \to \infty$, $r \to \infty$, provided that $2\sqrt{\pi}\chi^{(2)} r^3 \exp(-2\pi^2 r^2) \to \chi_{FK}$, or $\chi^{(2)} \to 0$, $\chi^{(1)} \to \infty$, $r \to \infty$, provided that $2\sqrt{\pi}\chi^{(1)}(r/\alpha)^3 \exp(-2\pi^2 r^2/\alpha^2) \to \chi_{FK}$.

E. Enhanced rigidity of the longer period subsystem

At equal rigidities of the chains $\chi^{(1)} = \chi^{(2)}$, the dependence of the ratio A_1/A_2 of the modulation amplitudes on the winding number α and the range r of the interchain interaction shows (Fig. 8) that as soon as r becomes large enough, $A_1 < A_2$ for $\alpha < 1$ and $A_1 > A_2$ for $\alpha > 1$. We call this phenomenon ''enhanced rigidity of the longer period subsystem,'' that means that for $\chi^{(1)} = \chi^{(2)}$ the longer period subsystem is less deformed. We believe this to be rather general for composite systems as shown by the following argument. An atom of the longer period subsystem feels on the average interactions with more atoms than an atom of the shorter period subsystem is able to do, hence it feels a smaller amplitude effective potential. This is no longer true for a very short range intersubsystem potential, as one can understand from the extreme case when each atom on each subsystem interacts with at most one atom of the other subsystem. Let us now leave the situation of equal rigidities and soften one of the subsystems. This will induce an increase of the modulation amplitude of the softened subsystem and also as a secondary effect a weaker increase of the modulation amplitude of the other subsystem. If the softened subsystem is the long period one the inequality of the modulation amplitudes will be weakened, otherwise this inequality will be reinforced. In the alkane/urea intergrowth compounds the urea subsystem has shorter period but higher rigidity than the alkane subsystem. It is thus possible that the combined effect of the difference in rigidity and periodicity produces comparable modulation amplitudes of the two subsystems as shown by x-ray-diffraction measurements of urea/nonadecane compounds.[14] In order to compare experimental results and theoretical predictions of the model one needs information on the intersubsystem potential, as well on the elastic constants. A method for obtaining and using this information will be presented elsewhere.[17] As shown by Fig. 3, softening of any of the two subsystems increases pinning (increases the PN barrier $\mathcal{E}_{PN}$). Nevertheless, in the nonanalytic regime $\partial\mathcal{E}_{PN}/\partial\chi^{(2)} < \partial\mathcal{E}_{PN}/\partial\chi^{(1)}$ when $\alpha > 1$, i.e., pinning is more sensitive to the softening of the shorter period subsystem. This is again the effect of the enhanced rigidity of the longer period subsystem tending to compensate its softening.

IV. CONCLUSIONS

The double-chain model can be used to understand static and dynamic properties of composite incommensurate and commensurate compounds. Due to its 1D character this model is suitable for the study of inclusion compounds with one set of parallel channels (urea, thiourea or selenourea inclusion compounds[2]).

DCM predicts intermodulation effects, each subsystem being modulated with the period of the other. The shapes and the amplitudes of the modulation functions can be calculated using numerical methods or perturbation theory. An interesting property is the enhanced rigidity of the longer period subsystem that can be softer, but still not much more deformed than the shorter period subsystem.

A genuine feature of the dynamics of the DCM is the existence of a phason (sliding) mode. We have overcome the difficulties in defining the phason in a system with continuous translation symmetry, for which acoustic phonons and the phason mix together, by showing the existence of a mode with pronounced ''sliding'' character, measured by the average relative shift of the subsystems in a normalized eigenvector. This property of the phason could be particularly important for optical experimental studies of lattice dynamics. The sliding mode produces large nonzero average relative displacements of one subsystem with respect to the other and has a greater chance to induce variations of dipolar momenta which couple to light radiation. As a counterpart, dissipation processes, not studied here, may affect rather strongly the detection of this mode. We showed that for strong intersubsystems coupling the phason is pinned. Furthermore, pinning increases with softening of subsystems and is more sensitive to the rigidity of the shorter period subsystem.

These general results provide tools for analysing specific compounds.[17] It is particularly interesting to compare properties of homologous inclusion compounds that differ only by the length of the guest molecule, therefore by the period of the guest subsystem.

Of a certain interest for statistical mechanics is the occurrence of the analyticity breaking transition in this rather complex model, in the absence of a rigid substrate that imposes its periodicity as in the case of the FK model. For the DCM it is not generally possible to write a finite dimensional dynamical system describing stationary configurations, therefore our conclusions rely entirely on numerical results. Nevertheless, the DCM is not isolated in the realm of FK-type models. Because each chain feels the effective quasiperiodic potential produced by its companion, the DCM is related to the FK model with a quasiperiodic substrate.[20] In the limit when the rigidity of one of the chains becomes infinite we obtain the FK model with a multiharmonic potential substrate. Numerical studies[26] suggest that this type of model has nonuniversal critical behavior. We shall report elsewhere on the comparison between DCM and the above models.

ACKNOWLEDGMENTS

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APPENDIX: GENERALIZED POISSON SUM FORMULAS

Let us consider the version of the Poisson sum formula that is most familiar to physicists:

$$\sum_{n=-\infty}^{\infty} \exp(inay) = \frac{2\pi}{a} \sum_{n=-\infty}^{\infty} \delta\left(y - \frac{2n\pi}{a}\right). \tag{A1}$$

From Eq. (A1) it follows that

$$\begin{aligned}\sum_n v(x+na) &= \frac{1}{2\pi} \sum_n \int dk \tilde{v}(k) \exp[ik(x+na)] \\ &= \frac{1}{a} \sum_r \int dk \tilde{v}(k) \exp(ikx) \delta\left(k - \frac{2\pi r}{a}\right) \\ &= \frac{1}{a} \sum_r \tilde{v}\left(\frac{2\pi r}{a}\right) \exp\frac{2\pi i r x}{a}\end{aligned} \tag{A2}$$

and

$$\begin{aligned}&\sum_n v(x-na) f(na+y) \\ &= \frac{1}{2\pi} \sum_{n,p} \int dk \tilde{v}(k) \tilde{f}_p \exp\left[i\left(kx + \frac{2\pi p y}{b}\right)\right] \\ &\quad \times \exp\left[ina\left(\frac{2\pi p}{b} - k\right)\right] \\ &= \frac{1}{a} \sum_{p,r} \int dk \tilde{v}(k) \tilde{f}_p \exp\left[i\left(kx + \frac{2\pi p y}{b}\right)\right] \delta \\ &\quad \times \left(\frac{2\pi p}{b} - k - \frac{2\pi r}{a}\right) = \frac{1}{a} \sum_{r,p} \tilde{v}\left[2\pi\left(\frac{p}{b} + \frac{r}{a}\right)\right] \\ &\quad \times \tilde{f}_p \exp\left[2\pi i x\left(\frac{p}{b} + \frac{r}{a}\right)\right] \exp\left(2\pi i y \frac{p}{b}\right).\end{aligned} \tag{A3}$$

Equations (A2) and (A3) are the two Poisson formulas used in this paper.

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