Hierarchical description of phonon dynamics on finite Fibonacci superlattices

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We study the phonon dynamics of Fibonacci heterostructures where two kinds of order (namely, periodic and quasiperiodic) coexist in the same sample at different length scales. We derive analytical expressions describing the dispersion relation of finite Fibonacci superlattices in terms of nested Chebyshev polynomials of the first and second kinds. In this way, we introduce a unified description of the phonon dynamics of Fibonacci heterostructures, able to exploit their characteristic hierarchical structure in a natural way.

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I. INTRODUCTION

During the last decades the notion of aperiodic order has progressively evolved in order to properly describe an increasing number of complex systems of physical interest.[1] This notion applies to systems which are well ordered, albeit lacking long-range periodicity. Thus, the order present in the system can be described in terms of suitable mathematical expressions other than the usual periodic functions. Typical examples are provided by quasiperiodic functions, describing the atomic arrangement of quasicrystals,[2–4] or the Fibonacci numbers sequence $F_n=\{1,1,2,3,5,8,13,21,\ldots\}$, describing the arrangement of certain botanical elements, like leaves and flowers, in plants.[5–7] The terms in this sequence are obtained by simply adding the preceding two, starting with $F_1=F_2=1$. Hence, the sequence is perfectly ordered, but its generating rule has nothing to do with periodicity. The symbolical analog of the Fibonacci sequence, constructed by using two types of building blocks—say, A and B—can be obtained from the substitution rule $A\to AB$ and $B\to A$, whose successive application generates the sequence of letters $A,AB,ABA,ABAAB,ABAABABA$, … and so on. This iteration scheme has been fruitfully exploited in the design of novel structures with potential practical applications. For instance, one can grow layered structures consisting of a large number of aperiodically arranged films. The simplest example of such nanostructured materials is a two-component Fibonacci heterostructure, where layers of two different materials (metallic, semiconductor, superconductor, dielectric, ferroelectric, ceramics) are arranged according to the Fibonacci sequence.[8,9] In this way, *two kinds of order* are introduced in the same sample *at different length scales*. At the atomic level we have the usual crystalline order determined by the periodic arrangement of atoms in each layer, whereas at longer scales we have the quasiperiodic order determined by the sequential deposition of the different layers. This long-range aperiodic order is artificially imposed during the growth process and can be precisely controlled. Since different physical phenomena have their own relevant physical scales, by properly matching the characteristic length scales we can efficiently exploit the aperiodic order we have introduced in the system, hence opening new avenues for technological innovation.

In fact, the possibility of designing novel devices, based on the construction of hybrid multilayers where both periodic and quasiperiodic orderings coexist in the same structure, has been proposed for optical applications.[10,11] Following this line of reasoning, recent numerical studies have analyzed the possible use of hybrid order heterostructures in order to control thermal transport in thermoelectric devices of technological interest.[12,13] In the light of these results, the introduction of an analytical treatment, able to fully encompass the physical implications of quasiperiodic order in the study of the transport properties of multilayered systems, is very appealing.

The theory of wave propagation in one dimension through an aperiodic medium has experienced considerable progress during the last decades.[14–28] Nonetheless, a general theory describing the relationship between the atomic topological order and the physical properties stemming from it is still missing. In this work we focus on the dynamics of phonons propagating through heterostructures arranged according to the Fibonacci sequence and derive *analytical* expressions describing the dispersion relation of finite Fibonacci superlattices (FSL's). The obtained expressions are based on a systematic use of Chebyshev polynomials of the first and second kinds, and we take advantage of some of their useful properties to gain additional physical insight. In fact, it is well known that Chebyshev polynomials are very convenient to perform numerical calculations in a broad collection of one-dimensional finite systems, ranging from disordered Bethe lattices[29] to deterministic self-similar lattices, like Fibonacci or Thue-Morse chains. In this regard, we have based this work on previous works by us where several issues related to the dynamics of electrons and phonons in Fibonacci lattices,[30–33] the propagation of light through Fibonacci dielectric multilayers,[10,34] the charge transfer efficiency of DNA chains,[35–37] or the thermoelectric properties of short oligonucleobases[38,39] were discussed, and closed analytical expressions for several magnitudes of interest, like the transmission coefficient or the Lyapunov exponent, were derived in terms of Chebyshev polynomials. On the other hand, in a series of works devoted to the study of *periodic* superlattices it was reported that Chebyshev polynomials play, for *finite* systems, a similar role to the one played by the Bloch functions in the description of transport properties of infinite periodic systems.[40–42] In addition, the ability of these polynomials to properly describe the propagation of both quantum and classical waves in *locally periodic* media (namely, systems having only a relatively small number of repeating elements) in a compact way has been recently illustrated,[43] as

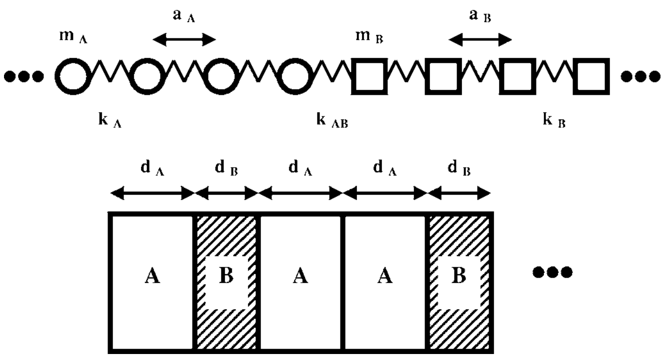

FIG. 1. Sketch illustrating the hierarchical arrangement of a Fibonacci heterostructure. At the atomic scale (top frame) the system can be modeled as a lattice chain composed of two kinds of atoms m_A and m_B coupled via force constants k_A (layer A), k_B (layer B), and k_{AB} (interfaces). At a larger scale (bottom frame) the system is described in terms of a sequence of layers of different composition and width $d_A = n_A a_A$ and $d_B = n_B a_B$, respectively, where n_ν is the number of atoms composing the layer and a_ν is its lattice constant.

well as their convenience when describing the presence of extended states in *correlated random* systems.[44,45]

II. MODEL

A FSL is based on two distinct building blocks—say, A and B—arranged according to the Fibonacci sequence. This sequence is obtained by successive application of the concatenation rule

$$S_{n+1} = S_n S_{n-1} \quad (n \geqslant 1), \tag{1}$$

starting with $S_0 = \{B\}$ and $S_1 = \{A\}$. In our model each building block is composed of a layer of a given material of thickness $d_{A(B)}$, respectively. The sequence S_n comprises F_n layers of type A and F_{n-1} layers of type B, where F_n is the nth Fibonacci number given by the recurrent law $F_{n+1} = F_n + F_{n-1}$ with $F_0 = F_1 = 1$. The key feature of this aperiodic structure is the coexistence of two kinds of order in the same sample at different length scales as is illustrated in Fig. 1. Thus, we have the usual periodic order in the crystalline arrangement of atoms in each layer, along with the quasiperiodic order given by the sequential deposition of the different layers. Consequently, when studying aperiodic heterostructures we should consider different description levels. At the atomic level we consider a lattice model characterized by the atomic masses $m_{A(B)}$ and the force constants $k_{A(B)}$. At a larger scale (given by the layers thickness) we should consider a multilayered system, whose physical properties are determined by the size and sequence distribution of the different layers as well as by the presence of an interface between them. In this way, the heterostructure dynamic behavior can significantly differ from that corresponding to the bulk materials present in their constituting layers.

In this work we are mainly interested in the dynamic effects stemming from the quasiperiodic arrangement of layers in the FSL. Accordingly, in Sec. III we will restrict ourselves to the study of the on-site model, focusing on the aperiodic distribution of masses through the heterostructure. Afterwards, in Sec. IV we will further work out our mathematical approach in order to properly account for the presence of interfaces between the different layers.

III. ANALYTICAL EXPRESSIONS

A. Generalization of the trace map formalism

As a first approximation, following previous works,[46] we will simplify the physical description by assuming all the force constants to be equal—i.e., $k_A = k_B = k_{AB} \equiv k$. Within the transfer matrix formalism the dynamic response of the FSL can be then expressed in terms of the global transfer matrix

$$\mathcal{M} = \ldots L_B L_A L_A L_B L_A, \tag{2}$$

where we have introduced the *layer matrices*

$$L_A \equiv Q_A^{n_A} = \begin{pmatrix} 2-\lambda & -1 \\ 1 & 0 \end{pmatrix}^{n_A}, \quad L_B \equiv Q_B^{n_B} = \begin{pmatrix} 2-\alpha\lambda & -1 \\ 1 & 0 \end{pmatrix}^{n_B} \tag{3}$$

describing the phonon propagation through layers A and B as a product of *atomic matrices* Q_A and Q_B, respectively. These matrices are characterized by the normalized frequency $\lambda \equiv m_A \omega^2/k$, where ω is the phonon frequency, the mass ratio $\alpha \equiv m_B/m_A$, and the number of atoms in each layer $n_{A(B)}$, respectively. In a FSL the layers are arranged according to the Fibonacci sequence $ABAAB\ldots$, which determines their order of appearance in the matrix product given by Eq. (2). Making use of the Cayley-Hamilton theorem for unimodular matrices the power matrices given by Eq. (3) can be readily expressed as[47]

$$L_r = \begin{pmatrix} U_{n_r}(x_r) & -U_{n_r-1}(x_r) \\ U_{n_r-1}(x_r) & -U_{n_r-2}(x_r) \end{pmatrix}, \quad r = \{A,B\}, \tag{4}$$

where $U_{n_r}(x_r) = \sin[(n_r+1)\varphi_r]/\sin\varphi_r$, with $x_A \equiv 1-\lambda/2 \equiv \cos\varphi_A$ and $x_B \equiv 1-\alpha\lambda/2 \equiv \cos\varphi_B$, are Chebyshev polynomials of the second kind, and we have explicitly used Eq. (A1) given in the Appendix. Making use of Eq. (4) in Eq. (2) the global transfer matrix can be numerically calculated in a straightforward way. Nonetheless, since L_r is a product of $SL(2,\mathbb{R})$ group elements, the layer matrices are unimodular themselves, and we will exploit this fact in order to obtain closed analytical results.[48] To this end, we will extend the so-called trace map formalism, originally introduced to describe a Fibonacci lattice of atoms (one-dimensional quasicrystal) to the FSL case. This approach is based on the following theorem. Consider a set of matrices M_n belonging to the $SL(2,\mathbb{R})$ group and satisfying the concatenation rule $M_{n+1} = M_{n-1} M_n$; then,[49,50]

$$\mathrm{tr} M_{n+1} = \mathrm{tr} M_n tr M_{n-1} - \mathrm{tr} M_{n-2}, \tag{5}$$

where tr$A$ stands for the trace of matrix A. By defining $z_n \equiv \mathrm{tr} M_n/2$, Eq. (5) is rewritten as the dynamical map

$$z_{n+1} = 2 z_n z_{n-1} - z_{n-2}, \tag{6}$$

usually referred to as the trace map. This map has the constant of motion[49,50]

$$I = z_{-1}^2 + z_0^2 + z_1^2 - 2z_{-1}z_0z_1 - 1, \quad (7)$$

determined by the initial conditions $z_{-1}=\mathrm{tr}M_0/2$, $z_0=\mathrm{tr}M_1/2$, and $z_1=\mathrm{tr}M_2/2$. Now, we recall that $L_r \in \mathrm{SL}(2,\mathbb{R})$ and, according to Eq. (1), the FSL global transfer matrix can be expressed as

$$\mathcal{M}(F_n) = \mathcal{M}(F_{n-2})\mathcal{M}(F_{n-1}), \quad n \geqslant 2. \quad (8)$$

Therefore, the set of *superlattice transfer matrices* $\mathcal{M}(F_n)$ satisfies the conditions of the theorem as well. Accordingly, the dynamical map given by Eq. (6) can be properly applied to the FSL system,[51] provided the initial conditions

$$z_{-1} = \frac{1}{2}\mathrm{tr}L_B = T_{n_B}(x_B), \quad (9)$$

$$z_0 = \frac{1}{2}\mathrm{tr}L_A = T_{n_A}(x_A), \quad (10)$$

$$z_1 = \frac{1}{2}\mathrm{tr}(L_BL_A) = T_{n_A}(x_A)T_{n_B}(x_B) + (x_Ax_B - 1)U_{n_A-1}(x_A)U_{n_B-1}(x_B), \quad (11)$$

where $T_{n_r}(x_r)=\cos(n_r\varphi_r)$ are Chebyshev polynomials of the first kind. To obtain Eqs. (9) and (10) we made use of Eq. (A2),[52] and Eq. (11) is derived in the Appendix. In this way, the trace map formalism can be extended to discuss the phonon propagation through a Fibonacci superlattice characterized by the presence of two relevant physical scales.

B. Physical meaning of the generalized trace map

The dynamical map given by Eqs. (6) and (9)–(11) can be physically interpreted as follows. By equating $z_{-1}=T_{n_B}(x_B)\equiv\cos(qd_B)$ and $z_0=T_{n_A}(x_A)\equiv\cos(qd_A)$, where q is the wave vector, we readily obtain the dispersion relation corresponding to the A or B layer,

$$\omega^2 = \frac{4k}{m_{A(B)}}\sin^2\left(\frac{qa_{A(B)}}{2}\right), \quad (12)$$

respectively. Analogously, the equation $z_1\equiv\cos[q(d_A+d_B)]$ leads to the dispersion relation corresponding to the binary periodic superlattice with unit cell $S_1=AB$,[46,53]

$$\cos[q(d_A + d_B)] = \cos(n_A\varphi_A)\cos(n_B\varphi_B) + (\cos\varphi_A\cos\varphi_B - 1)\frac{\sin(n_A\varphi_A)\sin(n_B\varphi_B)}{\sin\varphi_A\sin\varphi_B}. \quad (13)$$

Accordingly, the initial conditions implementing the generalized trace map are directly related to the phonon dispersion relations corresponding to the constituent layers (z_{-1} and z_0) and the lowest-order periodic approximant to the FSL (z_1). Consequently, the expression

$$z_n \equiv \cos(qD) \quad (n \geqslant 2), \quad (14)$$

with $D=F_nd_A+F_{n-1}d_B$, can be properly regarded as the dispersion relation corresponding to successive FSL approximants obtained from a continued iteration of the trace map.[54] In this way, the trace map given by Eq. (6) directly relates the dispersion relation of a given length FSL approximant to the dispersion relations corresponding to shorter ones. This nested structure of the resulting trace map is a natural consequence of the characteristic topological self-similarity of Fibonacci sequences, which is thus reflected in their dispersion relations.

C. Phonon dispersion relation for low-order approximants

The phonon spectrum of the FSL can then be obtained as the asymptotic limit of a series of approximants whose dispersion relations are determined by the successive application of the trace map recursion relation given by Eq. (6). Making use of the initial conditions given by Eqs. (9)–(11) we get (for simplicity hereafter we do not explicitly show the arguments of the Chebyshev polynomials)

$$z_2 = T_{2n_A}T_{n_B} + (x_Ax_B - 1)U_{2n_A-1}U_{n_B-1}, \quad (15)$$

where we have used Eqs. (A3) and (A4) given in the Appendix. Note that Eq. (15) can be obtained from Eq. (11) by simply replacing $n_A\to 2n_A$ in the latter one. Physically, this transformation is a natural consequence of interpreting the equation $z_2=\cos[q(2d_A+d_B)]$ as the dispersion relation corresponding to a periodic superlattice whose unit cell contains two A layers and one B layer, irrespectively of their particular order of appearance—namely, AAB, ABA, or BAA. This symmetry property can be formally proved by deriving the dispersion relation of the ternary periodic lattice ABC and realizing that the resulting expression is invariant under cyclic permutations of the layers.[55]

The next approximant superlattice is based on the unit cell $S_3=ABAAB$. In this case, the presence of the double layer AA breaks the trivial alternating pattern of layers A and B characteristic of the previously considered unit cells S_1 and S_2. Accordingly, one may now expect the presence of some new features in the corresponding dispersion relation. By plugging Eqs. (10), (11), and (15) into Eq. (6) we obtain

$$z_3 = T_{3n_A}T_{2n_B} + (x_Ax_B - 1)U_{3n_A-1}U_{2n_B-1} + \tilde{z}_3, \quad (16)$$

where

$$\tilde{z}_3 \equiv 4(x_A - x_B)^2T_{n_A}U_{n_A-1}^2U_{n_B-1}^2. \quad (17)$$

The details of the derivation are given in the Appendix. The first and second terms in Eq. (16) can be obtained from Eq. (11) by replacing $n_A\to 3n_A$ and $n_B\to 2n_B$, hence generalizing the previously discussed transformation leading to z_2. By introducing the notation $z_1^P\equiv\mathrm{tr}(L_BL_A)/2=z_1$, $z_2^P\equiv\mathrm{tr}(L_AL_BL_A)/2=z_2$, and $z_3^P\equiv\mathrm{tr}(L_AL_BL_AL_BL_A)/2$ we can express Eq. (16) as the sum of two contributions—namely, $z_3=z_3^P+\tilde{z}_3$, where z_3^P can be interpreted as the dispersion relation corresponding to a periodic superlattice with unit cell $ABABA$, whereas $\tilde{z}_3$ is a characteristic feature stemming from the presence of the AA double layer in the FSL approximant unit cell. To gain additional insight into the physical meaning of Eq. (17), we will explicitly evaluate the constant of motion given by Eq. (7). Making use of Eqs. (9)–(11) we get (see the Appendix)

$$I=(x_A-x_B)^2U^2_{n_A-1}U^2_{n_B-1}. \tag{18}$$

Thus, Eq. (16) can be written in the closed form

$$z_3=z_3^P+4IT_{n_A}, \tag{19}$$

which explicitly depends on the dynamical trace map invariant I. This constant of motion determines a noncompact, two-dimensional manifold for quasiperiodic chains, which becomes compact in the periodic case corresponding to the value $I=0$.[50] In agreement with these previous results, the dispersion relation given by Eq. (19) properly reduces to that corresponding to a periodic superlattice—i.e., $z_3=z_3^P$—when I vanishes.

This result indicates that the dispersion relation of a FSL approximant can be generally split into two complementary contributions. The first one describes a periodic binary lattice, where the layers alternate in the form $ABABABA\ldots$. The other one includes effects related to the emergence of quasiperiodic order in the system. A similar splitting has been previously discussed in order to describe the general structure of Fibonacci quasicrystals, where it was shown that their quasilattice can be seen as an average periodic structure plus quasiperiodic fluctuations.[56] In this sense, Eq. (19) represents a natural extension of this topological result to the study of dynamical effects in quasiperiodic heterostructures.

The next approximant unit cell is given by the sequence $S_4=ABAABABA$, and the corresponding trace map can be expressed as

$$z_4\equiv 2z_3z_2-z_1=2(z_3^P+4IT_{n_A})z_2^P-z_1^P=2z_3^Pz_2^P-z_1^P+8IT_{n_A}z_2^P. \tag{20}$$

The expression $2z_3^Pz_2^P-z_1^P$ in Eq. (20) is formally analogous to the trace map equation given by Eq. (6) so that it is tempting to explore its recursive properties. By defining

$$z_\nu^P=T_{F_\nu n_A}T_{F_{\nu-1}n_B}+(x_Ax_B-1)U_{F_\nu n_A-1}U_{F_{\nu-1}n_B-1}, \tag{21}$$

the following relationship is obtained by induction after some algebra:

$$2z_\nu^Pz_{\nu-1}^P-z_{\nu-2}^P=z_{\nu+1}^P+2(x_A-x_B)^2U_{F_\nu n_A-1}\times U_{F_{\nu-1}n_A-1}U_{F_{\nu-1}n_B-1}U_{F_{\nu-2}n_B-1},\quad \nu\geqslant 3. \tag{22}$$

Accordingly, the expression $2z_\nu^Pz_{\nu-1}^P-z_{\nu-2}^P$ only reduces to the canonical trace map structure given by Eq. (6) in the trivial periodic case $x_A=x_B$. On the other hand, plugging Eq. (22) into Eq. (20) we get

$$z_4=z_4^P+2(x_A-x_B)^2U_{3n_A-1}U_{2n_A-1}U_{2n_B-1}U_{n_B-1}+8IT_{n_A}z_2^P. \tag{23}$$

Therefore, Eq. (23) fits the proposed splitting in terms of a periodic plus a quasiperiodic contribution. Nevertheless, as the recursive process proceeds, the quasiperiodic contribution gets more and more involved, containing an increasing number of additional crossed terms which cannot be easily grouped together.

D. Scale transformation in terms of nested Chebyshev polynomials

In order to improve our understanding of the underlying physics, it is convenient to make use of the functional equations

$$T_{pq}(x)=T_q[T_p(x)],$$

$$U_{pq-1}(x)=U_{p-1}[T_q(x)]U_{q-1}(x), \tag{24}$$

to rewrite Eq. (19) in the explicit form

$$z_3=T_3[T_{n_A}(x_A)]T_2[T_{n_B}(x_B)]+(x_Ax_B-1)U_{n_A-1}(x_A)U_{n_B-1}(x_B)U_2[T_{n_A}(x_A)]U_1[T_{n_B}(x_B)]+4IT_1[T_{n_A}(x_A)]. \tag{25}$$

By inspecting Eq. (25) we realize that the dynamics of the system is described at three different scale lengths in this expression, ranging from the atomic level, to the layer level, and ending up at the heterostructure level. The atomic-scale length is described in terms of the variables x_r. The layer scale is described in terms of the Chebyshev polynomials $T_{n_r}(x_r)$ and $U_{n_r-1}(x_r)$, which contain the atomic-scale variables x_r as their natural arguments. Finally, the heterostructure scale is described by means of the nested Chebyshev polynomials $T_{F_\nu}[T_{n_r}]$ and $U_{F_\nu-1}[T_{n_r}]$, which contain the layer-scale variables $T_{n_r}(x_r)$ as their natural arguments in turn. We note that the subscripts of the nested Chebyshev polynomials explicitly depend on the Fibonacci numbers F_ν, measuring the number of layers composing the heterostructure at a given iteration step. Accordingly, recourse to Chebyshev polynomials allows us to introduce a *unified description* of the dynamics of FSL's able to encompass their characteristic aperiodic hierarchical structure in a natural way.

In fact, within this framework the functional relationships given by Eq. (24) can be regarded as describing a *scale transformation*, which can be formally expressed as

$$T_{n_r}(x_r)\to X_r. \tag{26}$$

By applying this transformation to Eqs. (9)–(11) the trace map initial conditions now read

$$z_{-1}=X_B,$$

$$z_0=X_A,$$

$$z_1=X_AX_B+\sqrt{I+Y_A^2Y_B^2}, \tag{27}$$

where we have introduced the auxiliary variables $Y_r=\sqrt{1-X_r^2}$. On the other hand, we can express the constant of motion I given by Eq. (7) in the form

$$I=(x_Ax_B-1)^2U^2_{n_A-1}U^2_{n_B-1}-Y_A^2Y_B^2. \tag{28}$$

By inspecting Eq. (28) we realize that the trace map invariant couples the atomic-scale and layer-scale variables among them. Therefore, we can use Eq. (28) to eliminate any explicit dependence of the variables x_r and $U_{n_r-1}(x_r)$ in Eqs.

(15) and (25) to obtain [for the sake of simplicity hereafter we will introduce the notation $T_n(X_r) \equiv T_{nr}$ for the nested Chebyshev polynomials]

$$z_2 = T_{2A}T_{1B} + 2T_{1A}\sqrt{I + Y_A^2Y_B^2}, \tag{29}$$

$$z_3 = T_{3A}T_{2B} + 2T_{1B}(2T_{2A} + 1)\sqrt{I + Y_A^2Y_B^2} + 4IT_{1A}, \tag{30}$$

where we have used the relationships $U_2(X_r) = 4X_r^2 - 1 = 2T_2(X_r) + 1$, $U_1(X_r) = 2X_r = 2T_1(X_r)$, and $U_0(X_r) = 1$. In this way, the z_n terms only depend on Chebyshev polynomials of the first kind. Analogously, Eq. (22) can be expressed in the form

$$2z_\upsilon^P z_{\upsilon-1}^P - z_{\upsilon-2}^P = z_{\upsilon+1}^P + \frac{I}{2Y_A^2Y_B^2}(T_{F_{\upsilon-2}A} - T_{F_{\upsilon+1}A})(T_{F_{\upsilon-3}B} - T_{F_\upsilon B}). \tag{31}$$

Making use of Eqs. (27) and (31) we can recursively obtain the dispersion relation for any FSL approximant of arbitrary length in terms of T_{nr} polynomials only, a recourse which provides us with a convenient framework to perform numerical calculations as well.

IV. INCLUSION OF INTERFACE EFFECTS

In this section we will explicitly consider the physical effects related to the presence of an interface separating each layer in the superlattice, so that the force constants k_{AB}, k_A, and k_B take on different values. In this general case the global transfer matrix can be expressed as

$$\mathcal{M} = \ldots \Lambda_B\Lambda_A\Lambda_A\Lambda_B\Lambda_A, \tag{32}$$

where the auxiliary layer matrices $\Lambda_A \equiv FL_A'\bar{F}$ and $\Lambda_B \equiv \bar{G}L_B'G$ describe the effects of the interface matrices

$$F \equiv \begin{pmatrix} 1+\gamma(1-\lambda) & -\gamma \\ 1 & 0 \end{pmatrix}, \quad \bar{F} \equiv \begin{pmatrix} 1-\lambda+\gamma^{-1} & -\gamma^{-1} \\ 1 & 0 \end{pmatrix}$$

$$G = \begin{pmatrix} 1+\dfrac{1}{\gamma'}(1-\gamma\alpha\lambda) & -\dfrac{1}{\gamma'} \\ 1 & 0 \end{pmatrix},$$

$$\bar{G} \equiv \begin{pmatrix} 1+\gamma'(1-\alpha\beta\lambda) & -\gamma' \\ 1 & 0 \end{pmatrix}, \tag{33}$$

where $\gamma \equiv k_A/k_{AB}$, $\gamma' \equiv k_B/k_{AB}$, and $\beta \equiv k_A/k_B$, on the modified layer matrices

$$L_A' \equiv \begin{pmatrix} 2-\lambda & -1 \\ 1 & 0 \end{pmatrix}^{n_A-2}, \quad L_B' \equiv \begin{pmatrix} 2-\alpha\beta\lambda & -1 \\ 1 & 0 \end{pmatrix}^{n_B-2}. \tag{34}$$

The dynamical coupling between the layers A and B is described by the force constant k_{AB}, while the factor β appearing in Eqs. (33) and (34) accounts for unhomogeneity effects. Then, for the sake of simplicity we will assume $k_A = k_B \equiv k$, so that $\gamma' = \gamma$ and $\beta = 1$. Making use of Eqs. (33) and (34) the auxiliary layer matrices can then be expressed as

$$\Lambda_r = \gamma^{-1}\begin{pmatrix} \gamma^2U_{n_r}(x_r) + 2\gamma\delta U_{n_r-1}(x_r) + \delta^2U_{n_r-2}(x_r) & -\gamma U_{n_r-1}(x_r) - \delta U_{n_r-2}(x_r) \\ \gamma U_{n_r-1}(x_r) + \delta U_{n_r-2}(x_r) & -U_{n_r-2}(x_r) \end{pmatrix}, \quad r = \{A,B\}, \tag{35}$$

where $\delta \equiv 1-\gamma$ measures the relative variation of the force constant at the interface. By comparing Eqs. (4) and (35) we realize that the inclusion of interface effects leads to significantly more involved algebra. In particular, we note that the interface matrices given by Eq. (33) are no longer unimodular, so that the unimodularity of the Λ_r matrices must be explicitly checked in this case. From Eq. (35) we obtain $\det(\Lambda_r) = U_{n_r-1}^2(x_r) - U_{n_r}(x_r)U_{n_r-2}(x_r) = 1$, so that Λ_r belong to $SL(2,\mathbb{R})$ group albeit the interface matrices F, $\bar{F}$, G, and $\bar{G}$ do not. This remarkable property allows us to generalize the extension of the trace map formalism introduced in Sec. III A to account for interface effects as well. In particular, we can make use of the dynamical map given by Eq. (6) provided the new set of initial conditions

$$z_{-1}' \equiv \frac{1}{2}\mathrm{tr}\Lambda_B = z_{-1} + \delta(1-x_B)U_{n_B-1}(x_B), \tag{36}$$

$$z_0' \equiv \frac{1}{2}\mathrm{tr}\Lambda_A = z_0 + \delta(1-x_A)U_{n_A-1}(x_A), \tag{37}$$

$$z_1' \equiv \frac{1}{2}\mathrm{tr}(\Lambda_B\Lambda_A) = z_1 + 2[\Delta_0U_{n_B}(x_B) + \Delta_{-1}U_{n_A}(x_A) + \Delta_0\Delta_{-1} + qU_{n_A-1}(x_A)U_{n_B-1}(x_B)], \tag{38}$$

where $q \equiv \delta(2x_Ax_B - x_A - x_B)$, $\Delta_{-1} \equiv z_{-1}' - z_1$ and $\Delta_0 \equiv z_0' - z_0$. As we can see, this set of initial conditions properly reduces to those given by Eqs. (9)–(11) when the value of the force constant at the interfaces reduces to the corresponding layer's value (i.e., $\delta = 0$). Accordingly, all the results derived in the previous sections can be extended to the more general case $k_{AB} \neq k$ in a straightforward way, although in that case the obtained analytical expressions become much more involved.

V. CONCLUSIONS

In this work the trace-map analysis, which was originally introduced to describe one-dimensional quasicrystals, has been extended to describe the phonon dynamics in finite Fibonacci heterostructures where two kinds of order (periodic at the atomic scale and quasiperiodic beyond the layer scale) are present in the same sample at different scale lengths. To this end, the trace map is cast in terms of nested Chebyshev polynomials of the form $T_{F_\nu}[T_{n_r}(x_r)]$ and $U_{F_\nu-1}[T_{n_r}(x_r)]$, where the variable x_r describes the atomic-scale physics and the function $T_{n_r}(x_r)$ describes the dynamics at the layer scale. Since the trace map itself can be interpreted as giving the dispersion relation of a given FSL realization in terms of the dispersion relations corresponding to lower-order approximants, this nested structure provides a suitable unified description for the dynamics of FSL's, able to encompass their characteristic hierarchical structure in a natural way. This interesting result provides a direct link between the topological self-similarity of these quasiperiodic heterostructures and the dynamics of the elementary excitations propagating through them. In this regard, the emergence of specific features related to the quasiperiodic order imposed to the heterostructure can be properly described in terms of the scale transformation given by Eq. (26). The inclusion of interface effects renders a much more involved mathematical description, although does not significantly affect the underlying physical basis of the approach. In this way, the mathematical framework introduced in this work could be a first step towards a more general analytical treatment of the transport properties in aperiodic systems.

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APPENDIX

We list some useful relations involving Chebyshev polynomials. For simplicity we express $U_n(x) \equiv U_n$ and $U_m(x') \equiv U'_m$. Similarly, $T_n(x) \equiv T_n$ and $T_m(x') \equiv T'_m$. Recurrence relations:

$$U_n - 2xU_{n-1} + U_{n-2} = 0, \quad \text{(A1)}$$

$$U_n - U_{n-2} = 2T_n. \quad \text{(A2)}$$

Multiplication formulas:

$$T_{2n} = 2T_n^2 - 1, \quad \text{(A3)}$$

$$U_{2n-1} = 2T_nU_{n-1}, \quad \text{(A4)}$$

$$2T_nT_m = T_{m+n} + T_{m-n}, \quad \text{(A5)}$$

$$2T_nU_{m-1} = U_{m+n-1} + U_{m-n-1}, \quad \text{(A6)}$$

$$2y^2U_{n-1}U_{m-1} = T_{m-n} - T_{m+n}, \quad \text{(A7)}$$

$$2y^2U_{n-1}^2 = 1 - T_{2n}, \quad \text{(A8)}$$

where $y = \sqrt{1-x^2}$.

Derivation of z_1

According to Eq. (4) we have

$$\frac{1}{2}\text{tr}(L_BL_A) = \frac{1}{2}(U_nU'_m - 2U_{n-1}U'_{m-1} + U_{n-2}U'_{m-2}), \quad \text{(A9)}$$

making use of Eq. (A1) we get

$$4xx'U_{n-1}U'_{m-1} = U_nU'_m + U_nU'_{m-2} + U_{n-2}U'_m + U_{n-2}U'_{m-2}, \quad \text{(A10)}$$

and analogously, from Eq. (A2), we get

$$4T_nT'_m = U_nU'_m - U_nU'_{m-2} - U_{n-2}U'_m + U_{n-2}U'_{m-2}, \quad \text{(A11)}$$

by adding Eqs. (A10) and (A11) and plugging the obtained result into Eq. (A9) we finally obtain Eq. (11).

Derivation of z_3

Making use of Eqs.(10), (11), and (15) in Eq. (6) we obtain

$$z_3 = T_n(2T_{2n}T_m'^2 - 1) + (xx' - 1)2T'_mU'_{m-1}(T_{2n}U_{n-1} + T_nU_{2n-1}) + 2(xx'-1)^2U_{2n-1}U_{n-1}U_{m-1}'^2, \quad \text{(A12)}$$

Making use of Eqs. (A3) and (A4) the first term of Eq. (A12) can be expressed as

$$\frac{1}{2}(T_{3n} + T_n)(T'_{2m} + 1) - T_n = \frac{1}{2}(T_{3n}T'_{2m} + T_{3n} + T_nT'_{2m} - T_n),$$

adding and subtracting $\frac{1}{2}T_{3n}T'_{2m}$ we get

$$T_{3n}T'_{2m} + \frac{1}{2}(T_{3n} - T_n)(1 - T'_{2m}).$$

From the definitions of the Chebyshev polynomials of the first and second kinds we have

$$T_n - T_{3n} = \cos n\varphi - \cos 3n\varphi = 4\cos n\varphi \sin^2 n\varphi \equiv 4y^2T_nU_{n-1}^2. \quad \text{(A13)}$$

On the other hand, making use of Eq. (A8) the first term of Eq. (A12) finally adopts the form

$$T_{3n}T'_{2m} - 4y^2y'^2T_nU_{n-1}^2U_{m-1}'^2. \quad \text{(A14)}$$

Let us now consider the second term in Eq. (A12). Taking into account Eq. (A6) we can express

$$T_{2n}U_{n-1} + T_nU_{2n-1} = \frac{1}{2}(2U_{3n-1} + U_{n-1} + U_{-n-1}) = U_{3n-1}, \quad \text{(A15)}$$

$$2T'_mU'_{m-1} = U'_{2m-1} + U'_{-1} = U'_{2m-1}, \quad \text{(A16)}$$

where we have made use of the relationships $U_{-1}=0$ and $U_{-n-1}=-U_{n-1}$. Then, the second term of Eq. (A12) reduces to

$$(xx'-1)U_{3n-1}U'_{2m-1}. \tag{A17}$$

Finally, making use of Eq. (A4) the third term of Eq. (A12) reads

$$4(xx'-1)^2 T_n U_{n-1}^2 {U'_{m-1}}^2. \tag{A18}$$

By plugging Eqs. (A14), (A17), and (A18) into Eq. (A12) and grouping terms, we finally obtain Eq. (16).

Derivation of *I*

By plugging Eqs. (9)–(11) into Eq. (7), after some simplification we get

$$I=(1-T_n^2)({T'_m}^2-1)+(xx'-1)^2U_{n-1}^2{U'_{m-1}}^2. \tag{A19}$$

Making use of Eqs. (A3) and (A8) the first term of Eq. (A19) can be expressed as

$$-\frac{1}{4}(1-T_{2n})(1-T'_{2m})=-y^2y'^2U_{n-1}^2{U'_{m-1}}^2. \tag{A20}$$

Then, by substituting Eq. (A20) into Eq. (A19) and grouping terms, we finally obtain Eq. (18).

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