Renormalization transformation of periodic and aperiodic lattices

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In this work we introduce a similarity transformation acting on transfer matrices describing the propagation of elementary excitations through either periodic or Fibonacci lattices. The proposed transformation can act at two different scale lengths. At the atomic scale the transformation allows one to express the systems' global transfer matrix in terms of an equivalent on-site model one. Correlation effects among different hopping terms are described by a series of local phase factors in that case. When acting on larger scale lengths, corresponding to short segments of the original lattice, the similarity transformation can be properly regarded as describing an effective renormalization of the chain. The nature of the resulting renormalized lattice significantly depends on the kind of order (i.e., periodic or quasiperiodic) of the original lattice, expressing a delicate balance between chemical complexity and topological order as a consequence of the renormalization process.

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I. INTRODUCTION

Many problems of physical interest are described by linear ordinary second-order differential equations for which different types of transfer matrices can be introduced.[1] In this way, the description of elementary excitations in low-dimensional systems can be reduced to the study of one-dimensional lattice models defined by the following general equation:[2–5]

$$\alpha_n \phi_n = t_{n,n-1}\phi_{n-1} + t_{n,n+1}\phi_{n+1}, \tag{1}$$

along with an appropriate set of boundary conditions. In Eq. (1), ϕ_n is the amplitude of the elementary excitation at the nth lattice position, and α_n depends on the excitation energy (or frequency) E (or ω), as well as on other characteristic physical magnitudes of the system, like atomic masses m_n, elastic constants $k_{n,n\pm1}$, or electronic binding energies ε_n, as illustrated in Table I. The hopping integrals $t_{n,n\pm1}$ describe the excitation transfer from site n to its neighboring sites $n\pm1$ (hence $t_{n,n\pm1}=t_{n\pm1,n}$), and will generally depend on the excitation energy. It is customary to cast Eq. (1) in the following matrix form:

$$\begin{pmatrix} \phi_{n+1} \\ \phi_n \end{pmatrix} \equiv \mathbf{T}_n \begin{pmatrix} \phi_n \\ \phi_{n-1} \end{pmatrix}, \tag{2}$$

where

$$\mathbf{T}_n(E) \equiv \begin{pmatrix} \dfrac{\alpha_n}{t_{n,n+1}} & -\dfrac{t_{n,n-1}}{t_{n,n+1}} \\ 1 & 0 \end{pmatrix} \tag{3}$$

is the so-called transfer matrix at site n. By iterating Eq. (2) one obtains the global transfer matrix, defined by the product

$$\mathcal{M}_N(E) = \prod_{n=N}^{1} \mathbf{T}_n(E), \tag{4}$$

and, from the knowledge of the $\mathcal{M}_N(E)$ matrix elements, several magnitudes of physical interest, like the transmission coefficient, the dispersion relation, the density of states, or the localization length, can be readily evaluated.[2–5] In this way, the transfer matrix formalism provides a simple mathematical tool allowing for a unified treatment of such diverse problems as electron or phonon dynamics in both periodic and aperiodic lattices,[6–16] optical properties of dielectric multilayers,[17–21] the propagation of acoustic waves in semiconductor heterostructures and metallic superlattices,[22–24] localization of elastic waves in heterogeneous media,[25] or charge transport through DNA chains.[26–30]

A significant number of works have focused on the study of systems based on two simple kinds of transfer matrices, namely, the so-called on-site and transfer models. In the on-site model one assumes all the hopping integrals to be equal, so that $\mathbf{T}_n$ becomes unimodular [i.e., $\det(\mathbf{T}_n)=1$] at every site of the chain. In the transfer model, all the on-site energies are assumed to be identical (and usually set to zero), so that we have $\det(\mathbf{T}_n)=t_{n,n-1}/t_{n,n+1}\neq 1$, in this case. From a physical point of view, one expects that the value of the hopping integral, coupling two neighbor atoms in the lattice, will be determined by the chemical nature of these atoms which, in turn, define a certain distribution of on-site energies along the chain. Therefore, in most physical situations of interest, one must consider the so-called mixed models, where both the on-site energies and the hopping integrals explicitly appear in Eq. (3). In that case, one must deal with nonunimodular transfer matrices at every lattice site, as well.

Now, it is well known that unimodular matrices [belonging to the Sl$(2,\mathbb{C})$ group] have a number of appealing mathematical properties, rendering the study of on-site models much easier than the study of mixed ones. This fact has spurred the interest in searching for a suitable transformation, able to reduce the general motion equation (1) to the on-site form

TABLE I. Values adopted by the different coefficients appearing in the general Eq. (1) depending on the considered elementary excitation.

Parameters	Electrons	Phonons
ϕ_n	ψ_n	u_n
α_n	$E-\varepsilon_n$	$k_{n,n-1}+k_{n,n+1}-m_n\omega^2$
$t_{n,n\pm1}$	$t_{n,n\pm1}$	$-k_{n,n\pm1}$

$$u_n\varphi_n + t\varphi_{n-1} + t\varphi_{n+1} = 0, \tag{5}$$

where φ_n, u_n, and t are determined by the transformation rule. In this way, the dynamics of elementary excitations in the original mixed system could be described in terms of an effective on-site model, while still preserving its generality. Aiming at this goal, Flores introduced the local transformation $\phi_n \rightarrow \varphi_n/\lambda_n$ into Eq. (1).[31] This transformation can be physically interpreted as a rescaling of the elementary excitation amplitude at each lattice site, where the parameter $\lambda_n \in \mathbb{C}$ plays the role of a local scale factor, which is determined from the relationship $\lambda_{n,n\pm1}\lambda_n^* \equiv t_{n,n\pm1}^{-1}$. Making use of this transformation in Eq. (1) we obtain $\alpha_n|\lambda_n|^2\varphi_n + \varphi_{n-1} + \varphi_{n+1} = 0$, which has the form of Eq. (5) with $t=1$ and $u_n \equiv \alpha_n|\lambda_n|^2$. Accordingly, both the the original on-site energies ε_n and the excitation energies E (included in the u_n coefficients) are affected by the transformation.[31] Following a different approach Lindquist and Riklund introduced a unitary transformation satisfying the condition $\mathbf{H}=\mathbf{U}\mathbf{H}_0\mathbf{U}$, where $\mathbf{H}$ and $\mathbf{H}_0$ are tridiagonal Hamiltonian matrices related to Eqs. (1) and (5), respectively, and $\mathbf{U}$ is a unitary diagonal matrix.[32] In this case, the energies of the eigenstates are not affected by the transformation and the elements of the transformation matrix are recursively obtained from the knowledge of the original hopping integrals.[32]

Inspired by these previous results, in this work we will introduce a local similarity transformation which can act at two different scale lengths. At the atomic scale the transformation adopts the form $\mathbf{M}_n\mathbf{T}_n\mathbf{M}_n^{-1} = \widetilde{\mathbf{T}}_n$, transforming a nonunimodular transfer matrix $\mathbf{T}_n$ into a unimodular one $\widetilde{\mathbf{T}}_n$. Making use of this transformation, the global transfer matrix given by Eq. (4) can be expressed as a product of unimodular matrices, so that it becomes unimodular itself. When acting on larger scale lengths, corresponding to short segments of the original lattice, the main effect of this transformation is to map the original mixed lattice into an effective on-site lattice which is related to the original one by means of a renormalization process. Accordingly, the similarity transformation can be properly regarded as a renormalization operator acting on one-dimensional lattice models in this case.

II. INTRODUCING THE SIMILARITY TRANSFORMATION

Our mathematical approach is based on the following general result.

Theorem 1. Let $\mathbf{Q}$ be an arbitrary matrix belonging to the $\mathrm{Sl}(2,\mathbb{C})$ group. This matrix can be transformed according to the expression

$$\mathbf{M}\mathbf{Q}\mathbf{M}^{-1} = \mathbf{P} \equiv \begin{pmatrix} A & -e^{-\lambda} \\ e^{\lambda} & 0 \end{pmatrix}, \tag{6}$$

where $\mathbf{M}$ is a 2×2 matrix, $A \equiv \mathrm{tr}\mathbf{Q}$ is the trace of matrix $\mathbf{Q}$, and $e^{\lambda} \in \mathbb{C}$ satisfies the relationship

$$\mathbf{Q}^t\begin{pmatrix} m_{21} \\ m_{22} \end{pmatrix} = e^{\lambda}\begin{pmatrix} m_{11} \\ m_{12} \end{pmatrix}, \tag{7}$$

involving the transformation matrix coefficients $m_{ij} \in \mathbf{M}$.

The proof of this result is given in the Appendix. The transformed $\mathbf{P}$ matrix can be rewritten in the standard transfer matrix form

$$\mathbf{P} = e^{\lambda}\begin{pmatrix} \frac{A}{e^{\lambda}} & -\frac{e^{-\lambda}}{e^{\lambda}} \\ 1 & 0 \end{pmatrix} \equiv e^{\lambda}\widetilde{\mathbf{T}}, \tag{8}$$

so that Eq. (6) can be expressed as

$$\mathbf{M}\mathbf{Q}\mathbf{M}^{-1} = e^{\lambda}\widetilde{\mathbf{T}}. \tag{9}$$

This expression can be physically interpreted as a similarity transformation rendering any arbitrary unimodular matrix into a transferlike one $\widetilde{\mathbf{T}}$, where the phase factor e^{λ} plays the role of an effective hopping term. Accordingly, Eq. (9) allows one to relate any arbitrary element of the $\mathrm{Sl}(2,\mathbb{C})$ group to a transfer matrix describing the propagation of some elementary excitations through a certain lattice. To this end, it is convenient to guarantee that the transfer matrix form is preserved when general products involving $\mathbf{M}$ and $\mathbf{T}$ matrices are considered, that is, $\mathbf{M}\mathbf{T} = e^{\lambda'}\mathbf{T}'$ (closure relation). This requirement is naturally satisfied by simply imposing that $\mathbf{M}$ belongs to the upper triangular matrix group (i.e., $m_{21} \equiv 0$), as can be readily seen from the general relationship

$$\begin{pmatrix} m_{11} & m_{12} \\ 0 & m_{22} \end{pmatrix}\begin{pmatrix} \alpha & -\beta \\ 1 & 0 \end{pmatrix} = m_{22}\begin{pmatrix} \frac{m_{12}+m_{11}\alpha}{m_{22}} & -\frac{m_{11}\beta}{m_{22}} \\ 1 & 0 \end{pmatrix}. \tag{10}$$

Then, making use of Eq. (7), we can explicitly express the matrix $\mathbf{M}$ in terms of the $\mathbf{Q}$ matrix coefficients q_{ij} as follows:

$$\mathbf{M} = m_{22}\begin{pmatrix} e^{-\lambda}q_{21} & e^{-\lambda}q_{22} \\ 0 & 1 \end{pmatrix}. \tag{11}$$

Finally, the free parameter m_{22} will be determined by imposing the condition $\det\mathbf{M}=1$, so that we obtain

$$\mathbf{M} = \pm\frac{e^{-\lambda/2}}{\sqrt{q_{21}}}\begin{pmatrix} q_{21} & q_{22} \\ 0 & e^{\lambda} \end{pmatrix}. \tag{12}$$

We note that, in order to obtain the explicit transformation matrix form given by Eq. (12), we have introduced some restrictions onto the transformation matrix $\mathbf{M}$. These particular choices have been motivated by the physical goal we have in mind and could be relaxed in other instances, as we will discuss in the concluding section.

III. GLOBAL TRANSFER MATRIX FOR GENERAL MIXED LATTICES

Let us consider a general one-dimensional lattice composed of N atoms which can be periodically, aperiodically, or even randomly distributed along the chain. In that case, the local transfer matrices are given by Eq. (3), so that $\det(\mathbf{T}_n) \neq 1$ in general. In order to be able to apply Theorem 1 we will make use of the decomposition property[33,34]

$$\mathbf{T}_n \equiv \begin{pmatrix} \dfrac{\alpha_n}{t_{n,n+1}} & -\dfrac{t_{n,n-1}}{t_{n,n+1}} \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} t_{n,n+1}^{-1} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \alpha_n & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & t_{n,n-1} \end{pmatrix}, \tag{13}$$

so that, by properly rearranging the product given in Eq. (4), the global transfer matrix can be expressed as

$$\mathcal{M}_N(E) = \mathbf{\Lambda}_{N+1} \left(\prod_{n=N}^{1} \mathbf{Q}_n \right) \mathbf{\Lambda}_0^{-1}, \tag{14}$$

where

$$\mathbf{Q}_n \equiv \begin{pmatrix} \alpha_n t_{n,n-1}^{-1} & -t_{n,n-1} \\ t_{n,n-1}^{-1} & 0 \end{pmatrix} \tag{15}$$

are unimodular matrices and the boundary conditions are given by the nonunimodular matrices

$$\mathbf{\Lambda}_{N+1} \equiv \begin{pmatrix} t_{N,N+1}^{-1} & 0 \\ 0 & 1 \end{pmatrix}, \quad \mathbf{\Lambda}_0 \equiv \begin{pmatrix} t_{0,1}^{-1} & 0 \\ 0 & 1 \end{pmatrix}. \tag{16}$$

Then, according to Theorem 1 one can introduce a similarity transformation which acts locally in order to express every $\mathbf{Q}_n$ matrix in the form

$$\mathbf{Q}_n = \mathbf{M}_n^{-1} \mathbf{P}_n \mathbf{M}_n, \tag{17}$$

where

$$\mathbf{P}_n = \begin{pmatrix} \alpha_n t_{n,n-1}^{-1} & -e^{-\lambda_n} \\ e^{\lambda_n} & 0 \end{pmatrix}. \tag{18}$$

By inspecting Eq. (15) we realize that $q_{22}=0$ and $q_{21}=t_{n,n-1}^{-1}$, so that Eq. (12) adopts the diagonal form

$$\mathbf{M}_n = \pm \begin{pmatrix} e^{-\lambda_n/2} t_{n,n-1}^{-1/2} & 0 \\ 0 & e^{\lambda_n/2} t_{n,n-1}^{1/2} \end{pmatrix}. \tag{19}$$

By plugging Eq. (17) into Eq. (14) we get

$$\mathcal{M}_N(E) = \mathbf{\Lambda}_{N+1} \mathbf{M}_N^{-1} \left(\prod_{n=N}^{1} \mathbf{P}_n \mathbf{D}_n \right) \mathbf{M}_0 \mathbf{\Lambda}_0^{-1}, \tag{20}$$

where we have introduced the auxiliary diagonal matrices

$$\mathbf{D}_n \equiv \mathbf{M}_n \mathbf{M}_{n-1}^{-1} = \begin{pmatrix} e^{(\lambda_{n-1}-\lambda_n)/2} t_{n,n-1}^{-1/2} t_{n-1,n-2}^{1/2} & 0 \\ 0 & e^{-(\lambda_{n-1}-\lambda_n)/2} t_{n,n-1}^{1/2} t_{n-1,n-2}^{-1/2} \end{pmatrix}. \tag{21}$$

Now we will exploit the degrees of freedom associated with the local phase factor λ_n in order to further simplify Eq. (20). To this end, we explicitly calculate the product

$$\mathbf{P}_n \mathbf{D}_n = e^{(\lambda_{n-1}+\lambda_n)/2} \sqrt{\frac{t_{n-1,n-2}}{t_{n,n-1}}} \begin{pmatrix} \dfrac{\alpha_n}{t_{n,n-1}} e^{-\lambda_n} & -\dfrac{t_{n,n-1}}{t_{n-1,n-2}} e^{-\lambda_n-\lambda_{n-1}} \\ 1 & 0 \end{pmatrix}, \tag{22}$$

and impose the condition

$$e^{\lambda_n+\lambda_{n-1}} \equiv t_{n,n-1}/t_{n-1,n-2}, \tag{23}$$

so that Eq. (22) reduces to

$$\mathbf{P}_n \mathbf{D}_n = \begin{pmatrix} u_n & -1 \\ 1 & 0 \end{pmatrix} \equiv \mathbf{B}_n, \tag{24}$$

where $\mathbf{B}_n$ is a unimodular matrix adopting the standard on-site model form with

$$u_n \equiv \alpha_n e^{-\lambda_n} t_{n,n-1}^{-1}. \tag{25}$$

Finally, making use of Eq. (24) in Eq. (20) the global transfer matrix can be expressed as

$$\mathcal{M}_N(E) = \mathbf{L}_{N+1} \left(\prod_{n=N}^{1} \mathbf{B}_n \right) \mathbf{L}_0, \tag{26}$$

where the boundary matrices are given by

$$\mathbf{L}_{N+1} \equiv \mathbf{\Lambda}_{N+1} \mathbf{M}_N^{-1} = \pm e^{-\lambda_N/2} t_{N,N-1}^{-1/2} \begin{pmatrix} e^{-\lambda_{N+1}} & 0 \\ 0 & 1 \end{pmatrix} \tag{27}$$

and

$$\mathbf{L}_0 \equiv \mathbf{M}_0 \mathbf{\Lambda}_0^{-1} = \pm e^{\lambda_0/2} t_{0,-1}^{1/2} \begin{pmatrix} e^{\lambda_1} & 0 \\ 0 & 1 \end{pmatrix}, \tag{28}$$

where we have made explicit use of Eq. (23). By adopting periodic boundary conditions we have $t_{0,-1}=t_{N,N-1}$, $\lambda_{N+1}=\lambda_1$, and $\lambda_0=\lambda_N$, so that Eq. (26) adopts the simple form

$$\mathcal{M}_N(E) = \mathbf{L}_1^{-1} \left(\prod_{n=N}^{1} \mathbf{B}_n \right) \mathbf{L}_1, \tag{29}$$

where

$$\mathbf{L}_1 \equiv \begin{pmatrix} e^{\lambda_1} & 0 \\ 0 & 1 \end{pmatrix}. \tag{30}$$

By introducing $\tilde{\mathcal{M}}_N(E) \equiv \Pi_{n=N}^{1} \mathbf{B}_n \in \mathrm{SI}(2,\mathbb{C})$, Eq. (29) can be finally rewritten as

$$\tilde{\mathcal{M}}_N(E) = \mathbf{L}_1 \mathcal{M}_N(E) \mathbf{L}_1^{-1}. \tag{31}$$

Accordingly, the original global transfer matrix of the system, $\mathcal{M}_N \notin \mathrm{SI}(2,\mathbb{C})$, can be transformed into the unimodular global transfer matrix $\tilde{\mathcal{M}}_N$ by means of a similarity transformation involving a boundary phase λ_1 only. From a physical viewpoint, Eq. (29) shows that the dynamics of elementary excitations in any arbitrary system, originally described by means of transfer matrices of the form given by Eq. (1), can be properly expressed in terms of an equivalent on-site model given by the transfer matrix set $\{\mathbf{B}_n\}$.

At this point, some words about the physical meaning of Eq. (25) are in order. By comparing our expression obtained for u_n with that previously derived by Flores,[31] we realize that they share a similar mathematical form, though in our case the $t_{n,n\pm1}$ hopping integrals explicitly appear in Eq. (25). In addition, the local phase factors $e^{-\lambda_n}$ appearing in Eq. (25) exhibit a very remarkable feature, namely, their value at a given lattice site is determined by the values of all the hopping integrals which precede them along the chain. In fact,

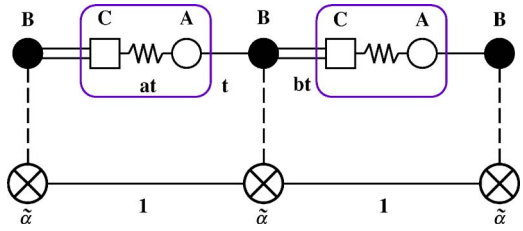

FIG. 1. (Color online) A mixed ternary lattice is mapped into an equivalent renormalized monatomic chain by decimating the AC dimers.

by taking logarithms in Eq. (23) and substituting successive terms into each other, one obtains

$$\lambda_n = (-1)^n \left[\ln\left(t_{N,N-1} \prod_{k=1}^{n-1} t_{k,k-1}^{2(-1)^k} \right) + \lambda_N \right] + \ln t_{n,n-1}, \quad n \geqslant 2, \tag{32}$$

along with the boundary relation

$$\lambda_1 = \ln t_{1,N} - \ln t_{N,N-1} - \lambda_N. \tag{33}$$

According to Eq. (32), the value of the phase at a given site is a cumulative magnitude expressing the correlations among different hopping terms in an explicit form. Therefore, λ_n values will generally depend on the possible presence of long-range correlations in the system.

IV. PERIODIC LATTICES WITH ARBITRARY UNIT CELL

The general treatment introduced in the previous section is valid for any arbitrary topological order of the lattice, as determined by the sequence of appearance of the different transfer matrices in Eq. (4). In this section we will consider the simplest case, corresponding to periodic arrangements of atoms. In order to illustrate the main features of our approach we must go beyond the binary chain composed of two types of atoms A and B periodically arranged in the form $ABABAB\ldots$. In fact, in this case we have $t_{n,n\pm1}=t_{AB}\equiv t$, so that we are dealing with an on-site model from the very beginning. Therefore, we will explicitly consider the ternary mixed model corresponding to the unit cell ABC, which is illustrated in Fig. 1. Taking $t_{AB}\equiv t$ as a reference value we can express $t_{BC}=bt$ and $t_{CA}=at$, without loss of generality. Accordingly, the boundary conditions read $t_{N,N-1}=t_{BC}=bt$ and $t_{N,1}\equiv t_{1,0}=t_{AC}=at$ in this case. First, we will obtain the global transfer matrix as given by Eq. (26), and from its knowledge, we will obtain the ternary chain dispersion relation by means of the expression

$$\cos(qL) = \frac{1}{2}\mathrm{tr}[\mathcal{M}_N(E)], \tag{34}$$

where q is the wave vector, $L\equiv Na_0$, and a_0 measures the interatomic distance. The translation symmetry ensures we have just three kinds of sites α_A, α_B, and α_C, periodically arranged along the chain, satisfying $\lambda_A=\lambda_{1\pm3k}, \lambda_B=\lambda_{2\pm3k}$, and $\lambda_C=\lambda_{3\pm3k}$, with $k=0,1,\ldots$. Making use of the condition $\lambda_4=\lambda_1\equiv\lambda_A$ in Eqs. (32) and (33) we obtain $\lambda_A=-\ln b$, $\lambda_B=\ln(b/a)$ and $\lambda_C=\ln a$, so that the transformed on-site energies given by Eq. (25) read

$$u_A = \alpha_A \frac{b}{at}, \quad u_B = \alpha_B \frac{a}{bt}, \quad u_C = \alpha_C \frac{1}{abt}. \tag{35}$$

On the other hand, making use of the Cayley-Hamilton theorem for unimodular matrices, we obtain the power matrix

$$(\mathbf{B}_C\mathbf{B}_B\mathbf{B}_A)^m = \begin{pmatrix} U_m + u_B U_{m-1} & (1-u_B u_C)U_{m-1} \\ (u_A u_B - 1)U_{m-1} & -u_B U_{m-1} - U_{m-2} \end{pmatrix}, \tag{36}$$

where $m\equiv N/3$, and $U_m(z)=\sin[(m+1)\phi]/\sin\phi$, with

$$z \equiv \frac{\alpha_A\alpha_B\alpha_C - t^2(b^2\alpha_A + a^2\alpha_B + \alpha_C)}{2abt^3} \equiv \cos\phi, \tag{37}$$

are Chebyshev polynomials of the second kind satisfying the recursion relationship $U_m-2zU_{m-1}+U_{m-2}=0$. Plugging Eq. (36) into Eq. (29) we obtain

$$\mathcal{M}_N(E) = \begin{pmatrix} U_m + u_B U_{m-1} & e^{-\lambda_1}(1-u_B u_C)U_{m-1} \\ e^{\lambda_1}(u_A u_B - 1)U_{m-1} & -u_B U_{m-1} - U_{m-2} \end{pmatrix}, \tag{38}$$

so that we get $\mathrm{tr}[\mathcal{M}_N(E)]/2=(U_m-U_{m-2})/2=T_m(z)$, where $T_m(z)=\cos(m\phi)$ is a Chebyshev polynomial of the first kind. Then, making use of Eq. (34), we finally obtain the dispersion relation

$$2t_{AB}t_{BC}t_{CA}\cos(3qa_0) = \alpha_A\alpha_B\alpha_C - \alpha_A t_{BC}^2 - \alpha_B t_{CA}^2 - \alpha_C t_{AB}^2, \tag{39}$$

which is invariant under cyclic permutations of the atoms in the unit cell, a property that has been recently discussed in the study of light propagation through optical multilayers.[35] It is then clear that the outlined procedure can be straightforwardly extended to obtain the dispersion relation of periodic lattices with arbitrary unit cells.

Now, we will provide some physical insight into the expression (9) by the light of the results just obtained. To start with, we note that the mixed ternary lattice is characterized by three local transfer matrices, namely,

$$\mathbf{T}_A = \begin{pmatrix} \frac{\alpha_A}{t} & -a \\ 1 & 0 \end{pmatrix}, \quad \mathbf{T}_B = \begin{pmatrix} \frac{\alpha_B}{bt} & -b^{-1} \\ 1 & 0 \end{pmatrix}, \quad \mathbf{T}_C = \begin{pmatrix} \frac{\alpha_C}{at} & -\frac{b}{a} \\ 1 & 0 \end{pmatrix}, \tag{40}$$

none of which is unimodular. Quite remarkably, however, the product

$$\mathbf{Q} \equiv \mathbf{T}_C\mathbf{T}_B\mathbf{T}_A = \frac{1}{bt^2}\begin{pmatrix} \frac{1}{at}(\alpha_A\alpha_B\alpha_C - b^2t^2\alpha_A - t^2\alpha_C) & b^2t^2 - \alpha_B\alpha_C \\ \alpha_A\alpha_B - t^2 & -at\alpha_B \end{pmatrix} \tag{41}$$

belongs to the $\mathrm{Sl}(2,\mathbb{C})$ group, for any choice of the system

parameters and for any value of the elementary excitation energy. Accordingly, we can apply Theorem 1 to transform $\mathbf{Q}$ to the form $\mathbf{MQM}^{-1}=e^{\lambda}\tilde{\mathbf{T}}$, where

$$\tilde{\mathbf{T}}=\begin{pmatrix}\frac{\mathrm{tr}\mathbf{Q}}{e^{\lambda}} & -\frac{e^{-\lambda}}{e^{\lambda}}\\ 1 & 0\end{pmatrix}. \tag{42}$$

At this point we note that by defining $\mathrm{tr}\,\mathbf{Q}\equiv E-\tilde{\alpha}$, the matrix $\tilde{\mathbf{T}}$ can be properly regarded as a transfer matrix describing the elementary excitation propagation through a monatomic lattice, composed of atoms of on-site energy $\tilde{\alpha}$ coupled to their neighbors through hopping integrals $\tilde{t}_{k,k\pm1}=e^{\pm\lambda}$. Then, it is tempting to think of Eq. (9) as describing an effective renormalization of the original mixed ternary lattice leading to the monatomic one. To confirm this physical scenario we shall consider the lattice pentamers $ACBAC$ in the ternary chain and decimate the AC sites, as illustrated in Fig. 1. In so doing, we obtain $\tilde{t}_{n,n\pm1}=1$, and

$$E-\tilde{\alpha}=\frac{\alpha_A\alpha_B\alpha_C-t^2(b^2\alpha_A+a^2\alpha_B+\alpha_C)}{abt^3}, \tag{43}$$

which coincides with $\mathrm{tr}\,\mathbf{Q}$, as given by Eq. (41). Therefore, we conclude that the similarity transformation given by Eq. (9) describes a *local renormalization* transformation, acting on certain segments of the original ternary lattice in order to transform it to an effective monatomic lattice. Since the renormalized hopping integrals trivially reduce to unity, all the relevant physical information is now contained in the renormalized on-site energies $\tilde{\alpha}$. In fact, by comparing Eqs. (37) and (43), we get the relation $E=\tilde{\alpha}+\cos\phi$, which is closely related to the ternary chain dispersion relation given by Eq. (39). On the basis of the obtained results, a question naturally arises regarding the possibility of extending this approach to lattices exhibiting aperiodic arrangements of atoms as well. This issue will be addressed in the next section.

V. GENERAL FIBONACCI LATTICES

In this section we will consider the electron dynamics (a completely analogous procedure applies to the study of the phonon problem[10,36]) in Fibonacci lattices composed of two types of atoms A and B arranged according to the substitution rule $A\rightarrow AB$ and $B\rightarrow A$, whose successive application generates the sequences A, AB, ABA, $ABAAB$, $ABAABABA$,… and so on. The total number of atoms in the chain is $N=F_k$, where F_k is a Fibonacci number obtained from the recursion relation $F_k=F_{k-1}+F_{k-2}$, starting with $F_1=1$ and $F_2=1$.

Earlier models focused on either diagonal models, where hopping integrals are constant over the lattice and the aperiodicity relies on the on-site potential energies, or off-diagonal models, where the on-site energies are usually set to zero while hopping integrals are aperiodically arranged. Some exact results, based on renormalization-group transformations exploiting the self-similar, hierarchical structure of the underlying lattice were reported.[37,38] Less attention was paid to the class of models for which both diagonal and off-diagonal terms are simultaneously present in the Hamiltonian.[39,40] These mixed models turn out to be more appropriate in order to describe realistic aperiodic systems, in which one expects that the hopping terms should take on different values depending upon the chemical nature of neighboring atomic species. Nevertheless, in this general case the self-similarity property adopts a more complex structure, so that previously considered renormalization schemes are no longer applicable.

In fact, in the mixed model the Hamiltonian describing the electron dynamics can be cast in terms of the following matrices:[41,42]

$$\mathbf{X}\equiv\begin{pmatrix}\frac{E-\varepsilon_B}{t_{AB}} & -1\\ 1 & 0\end{pmatrix},\quad \mathbf{Y}\equiv\begin{pmatrix}\gamma^{-1}\frac{E-\varepsilon_A}{t_{AB}} & -\gamma^{-1}\\ 1 & 0\end{pmatrix},$$

$$\mathbf{Z}\equiv\begin{pmatrix}\frac{E-\varepsilon_A}{t_{AB}} & -\gamma\\ 1 & 0\end{pmatrix},\quad \mathbf{W}\equiv\begin{pmatrix}\frac{E-\varepsilon_A}{t_{AB}} & -1\\ 1 & 0\end{pmatrix}, \tag{44}$$

where E is the electron energy, $t_{AB}=t_{BA}$ and t_{AA} are the corresponding hopping integrals, and $\gamma\equiv t_{AA}/t_{AB}>0$. For the sake of simplicity we will set the origin of energies in such a way that $\varepsilon_B=-\varepsilon_A$, and will fix the energy scale so that $t_{AB}\equiv1$ without loss of generality. In previous works we have shown that we can translate the atomic sequence $ABAAB$… describing the topological order of the Fibonacci lattice to the transfer matrix sequence …**XZYXZYXWXZYXW** describing the behavior of electrons moving through it.[42] In spite of its greater apparent complexity, we realize that by renormalizing this transfer matrix sequence according to the blocking scheme $\mathbf{R}_A\equiv\mathbf{ZYX}$ and $\mathbf{R}_B\equiv\mathbf{WX}$, we get the considerably simplified sequence …$\mathbf{R}_B\mathbf{R}_A\mathbf{R}_A\mathbf{R}_B\mathbf{R}_A$. The subscripts in the $\mathbf{R}$ matrices are introduced to emphasize the fact that the renormalized transfer matrix sequence is also arranged according to the Fibonacci one and, consequently, the topological order present in the original lattice is preserved by the renormalization process. Making use of Eq. (44) we explicitly obtain

$$\mathbf{R}_A=\gamma^{-1}\begin{pmatrix}qy-x\gamma^2 & \gamma^2-y^2\\ q & -y\end{pmatrix},\quad \mathbf{R}_B=\begin{pmatrix}q & -y\\ x & -1\end{pmatrix}, \tag{45}$$

where $x\equiv E+\varepsilon_A$, $y\equiv E-\varepsilon_A$, and $q\equiv xy-1$. It is readily checked that both the $\mathbf{R}_A$ and $\mathbf{R}_B$ matrices are unimodular for any choice of the system parameters and for any value of the electron energy. Accordingly, they satisfy the conditions of Theorem 1 and, according to Eq. (9), we can transform them to the form $\mathbf{M}_A\mathbf{R}_A\mathbf{M}_A^{-1}=e^{\lambda_A}\tilde{\mathbf{T}}_A$ and $\mathbf{M}_B\mathbf{R}_B\mathbf{M}_B^{-1}=e^{\lambda_B}\tilde{\mathbf{T}}_B$, respectively, where

$$\tilde{\mathbf{T}}_A=\begin{pmatrix}\frac{\mathrm{tr}\mathbf{R}_A}{e^{\lambda_A}} & -\frac{e^{-\lambda_A}}{e^{\lambda_A}}\\ 1 & 0\end{pmatrix},\quad \tilde{\mathbf{T}}_B=\begin{pmatrix}\frac{\mathrm{tr}\mathbf{R}_B}{e^{\lambda_B}} & -\frac{e^{-\lambda_B}}{e^{\lambda_B}}\\ 1 & 0\end{pmatrix}. \tag{46}$$

Now, by analogy with the treatment introduced in the study of periodic lattices, we note that by defining $\mathrm{tr}\,\mathbf{R}_A\equiv E-\tilde{\alpha}$ and $\mathrm{tr}\,\mathbf{R}_B\equiv E-\tilde{\beta}$ the matrices $\tilde{\mathbf{T}}_A$ and $\tilde{\mathbf{T}}_B$ can be

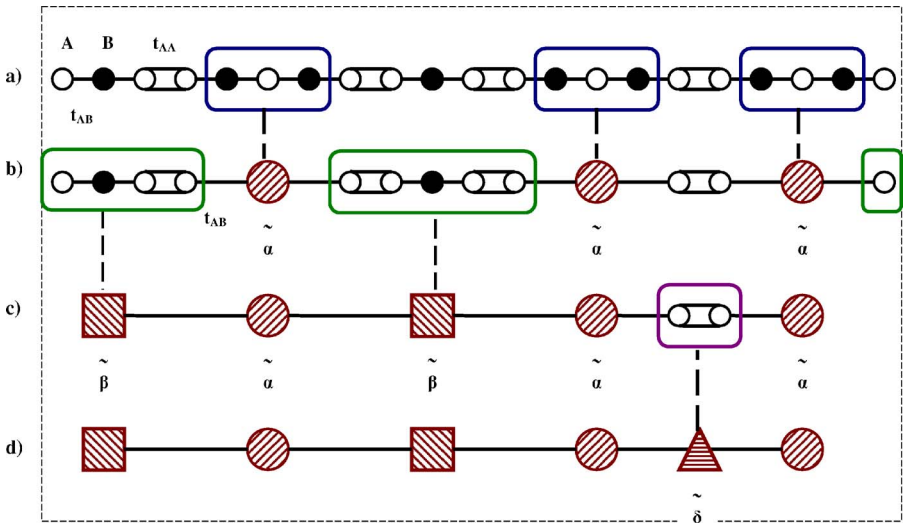

FIG. 2. (Color online) Renormalization scheme mapping a mixed Fibonacci lattice model into an effective on-site model, which proceeds according to the following steps: (a) decimation of the *B* sites in the *BAB* trimers to obtain the renormalized on-site energy sites $\tilde{\alpha}$; (b) decimation of the *AA* dimers belonging to the *AABAA* pentamers to obtain the renormalized on-site energy sites $\tilde{\beta}$; and (c) decimation of the remaining *AA* dimers to obtain the on-site energy sites $\tilde{\delta}$. The resulting aperiodic ternary lattice is shown in (d).

properly regarded as transfer matrices describing the electron propagation through a lattice composed by atoms of on-site energy $\tilde{\alpha}$ (alternatively $\tilde{\beta}$) coupled to their neighbors through hopping integrals $\tilde{t}_{k,k\pm1}=e^{\pm\lambda_A}$ (alternatively $\tilde{t}_{k,k\pm1}=e^{\pm\lambda_B}$). To confirm this physical picture we shall consider the lattice trimers *BAB* in the Fibonacci chain and decimate the *B* sites, as illustrated in Fig. 2(a). In so doing, we obtain $E-\tilde{\alpha}=xy-2$, which coincides with $\mathrm{tr}\,\mathbf{R}_B=q-1$, as given by Eq. (45). In a similar way, we consider the lattice pentamers *AABAA* and decimate the *AA* dimers, as indicated in Fig. 2(b), to obtain $E-\tilde{\beta}=\gamma^{-1}[x(y^2-\gamma^2)-2y]$, which coincides with $\mathrm{tr}\mathbf{R}_A=\gamma^{-1}[y(q-1)-x\gamma^2]$ as given by Eq. (45). Therefore, we conclude that the similarity transformation given by Eq. (9) also describes a *renormalization transformation* in the quasiperiodic lattice case. By simultaneously applying the renormalization transformations shown in Figs. 2(a) and 2(b) the original Fibonacci chain is mapped into the lattice shown in Fig. 2(c), where some *AA* dimers, connected via γ hopping terms, still remain. In order to complete the renormalization of the original chain, we decimate these dimers, obtaining the fully renormalized lattice shown in Fig. 2(d), where $E-\tilde{\delta}=y-\gamma$. As we can see, the resulting lattice is now composed of three different atoms, and all the hopping integrals coupling them have the same value, $\tilde{t}=t_{AB}\equiv1$. Therefore, the original binary Fibonacci chain has been transformed in an equivalent ternary lattice which can be properly described in terms of an on-site model. Broadly speaking we can say that the reduction of the mixed model to an on-site one is obtained at the cost of increasing the system's chemical complexity (i.e., we now have three different atomic flavors, rather than the original two). In addition, the topological order present in the renormalized lattice is no longer described by the Fibonacci sequence, although it is still an aperiodic one.

To gain some physical insight into this interesting feature in Fig. 3 we show the renormalized lattices corresponding to two Fibonacci lattices of different size. By inspecting these chains we observe that the renormalized on-site energies sequence characterizing them, $\tilde{\alpha}\tilde{\delta}\tilde{\alpha}\tilde{\beta}\tilde{\alpha}\tilde{\delta}\tilde{\alpha}\tilde{\beta}\tilde{\alpha}\tilde{\beta}\ldots$, can be obtained from the substitution rule

$$\tilde{\alpha}\to\tilde{\beta},$$

$$\tilde{\beta}\to\tilde{\alpha}\tilde{\delta}\tilde{\alpha},$$

$$\tilde{\delta}\to\tilde{\alpha}, \tag{47}$$

starting with the initial word $\tilde{\alpha}\tilde{\delta}$. The corresponding substitution matrix reads[43]

$$\mathbf{F}_0=\begin{pmatrix}0&2&1\\1&0&0\\0&1&0\end{pmatrix}. \tag{48}$$

Therefore, the renormalized aperiodic sequence we have obtained does not correspond to any of the ternary Fibonacci lattices which have been previously considered in the literature, which are characterized by the substitution rules $A\to B$, $B\to C$, and $C\to A^pB^qC$, where p and q are positive integers,[44,45] with

$$\mathbf{F}_1=\begin{pmatrix}0&0&p\\1&0&q\\0&1&1\end{pmatrix}, \tag{49}$$

or $A\to A^pC^q$, $B\to A$, and $C\to B$[46–48] with

$$\mathbf{F}_2=\begin{pmatrix}p&1&0\\0&0&1\\q&0&0\end{pmatrix}. \tag{50}$$

Thus, we will pay some attention to the main properties of the sequence given by Eq. (47). To this end, we focus on the spectrum of the matrix $\mathbf{F}_0$.[44] In fact, the roots of its characteristic polynomial $P(\mu)=(\mu+1)(\mu^2-\mu-1)$ are $\mu_1=\tau$, $\mu_2=-\tau^{-1}$, and $\mu_3=-1$, where $\tau=(1+\sqrt{5})/2$ is the golden mean. Then, although the leading eigenvalue $\mu_1>1$, we have $|\mu_3|=1$, so that the substitution rule does not satisfy the Pisot property.[49] In that case, the Bombieri-Taylor theorem indicates that the renormalized lattice is not quasiperiodic.[50] Physically this means that the Fourier spectrum of the renormalized lattice cannot further be expressed as a finite sum of

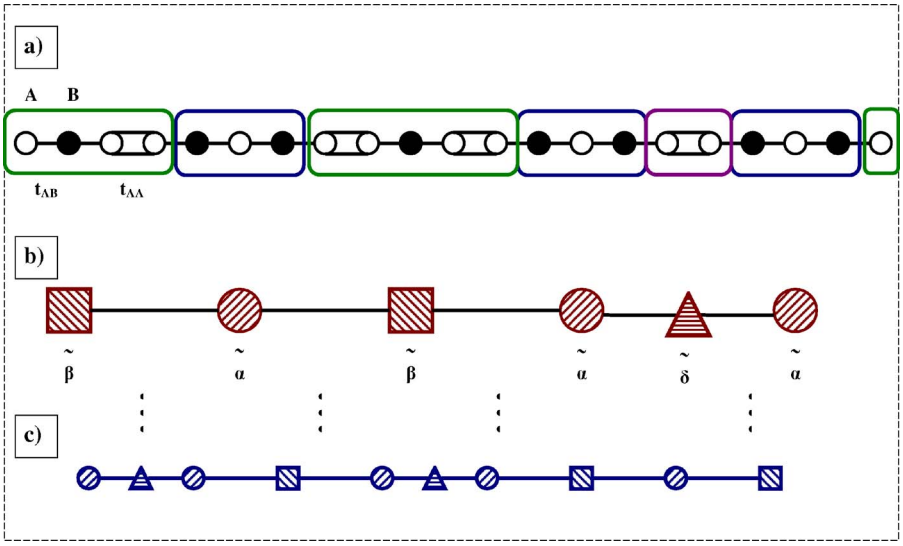

FIG. 3. (Color online) The Fibonacci mixed lattice with $N=21$ shown in (a) is mapped into the aperiodic on-site model shown in (b). By considering a Fibonacci mixed chain with $N=34$ we obtain the renormalized on-site lattice shown in (c). By inspecting (b) and (c) we can obtain by induction the substitution rule given by Eq. (47).

weighted Dirac δ functions.[43] Nevertheless, the renormalized chain is self-similar. In fact, the normalized eigenvector corresponding to the leading eigenvalue $\mu_1=\tau$ is $(1/2, \tau^{-1}/2, \tau^{-2}/2)$, whose components give the relative frequencies of the renormalized sites $\tilde{\alpha}$, $\tilde{\beta}$, and $\tilde{\delta}$, respectively. In turn, these sites are related, through Eq. (47), to words of sizes $l_{\tilde{\alpha}}\equiv 1$, $l_{\tilde{\beta}}=3$, and $l_{\tilde{\delta}}=1$. Therefore, any finite part of the original sequence will be deflated by the factor $\xi\equiv(l_{\tilde{\alpha}}+l_{\tilde{\beta}}\tau^{-1}+l_{\tilde{\delta}}\tau^{-2})/2=\tau$. Therefore, the aperiodic ternary sequence we are considering obeys the Conway theorem, stating that for any finite word in the sequence of length, say, l_W, an identical word can be found within a distance $d\leqslant 2l_W$.[51,52] Accordingly, one reasonably expects that its finite realizations would exhibit well-defined diffraction spectra, probably supported on singular continuous spectra, as has been previously discussed in the literature for other lattices exhibiting the singular feature $|\mu_i|=1$ in the substitution matrix spectrum.[43,53]

VI. CONCLUSIONS

In this paper we report on two main results based on the application of Theorem 1. In the first place, we have shown that the global transfer matrix of any arbitrary system originally described in terms of a general mixed model can be expressed in terms of an equivalent on-site one. The global transfer matrices describing both systems are related through the similarity transformation given by Eq. (31). To this end, we have applied Theorem 1 to the original transfer matrices (properly rearranged) in order to obtain Eq. (29) in terms of the new transfer matrix set given by Eq. (24). The corresponding on-site terms in these matrices describe a transformation that acts at the atomic scale on every lattice site, according to Eq. (25). This expression involves the presence of a series of local phase factors λ_n, including correlation effects among different hopping terms in the original lattice.

In the second place, we have applied Theorem 1 to certain products of local transfer matrices, describing the propagation of elementary excitations through short segments of either periodic or Fibonacci lattices. In this case, the similarity transformation associated with Eq. (9) acts on a larger scale length, and we have shown that it can be properly regarded as describing an effective renormalization of the original lattice. In the periodic lattice case, all the relevant physics of the original chain is encoded in the renormalized on-site energy values of the resulting monatomic chain, hence trivially preserving its periodic order. This interesting result allows us to readily obtain the dispersion relation of any periodic lattice with an arbitrary unit cell. On the contrary, the original Fibonacci lattice significantly changes its original topology as a result of the renormalization process, so that only its self-similar property remains in the renormalized chain. In addition, the chemical complexity of renormalized chain is increased in this case (three different on-site energies instead of the two kinds of atoms originally present in the Fibonacci chain), while the chemical complexity of the periodic lattice is reduced as a consequence of the renormalization process. These differences illustrate the richness of quasiperiodic order as compared to the periodic one and suggest that the balance between chemical complexity and lattice topology deserves a closer scrutiny.

Finally, we will comment on some possible extensions of this work. In this sense, we note that Eq. (23) is just a convenient choice, aimed to guarantee that $\mathbf{B}_n$ matrices adopt the proper on-site transfer matrix form. Nevertheless, other possible choices may be also possible if one has other purposes in mind. Thus, for example, one may think of transforming different kinds of aperiodic systems (like Thue-Morse or Rudin-Shapiro chains, for instance) among them, or even to transform an aperiodic lattice into a periodic one instead. Such transformations may be accomplished by imposing the conditions

$$\frac{\alpha_n}{t_{n,n-1}}e^{-\lambda_n}\equiv\frac{\tilde{\alpha}_n}{\tilde{t}_{n,n+1}},\quad \frac{t_{n,n-1}}{t_{n-1,n-2}}e^{-\lambda_n-\lambda_{n-1}}\equiv\frac{\tilde{t}_{n,n-1}}{\tilde{t}_{n,n+1}} \tag{51}$$

in Eq. (22), which allow us to transform a given aperiodic mixed lattice into another one. In the same vein, we could also relax the condition $\det \mathbf{M}=1$, adopted to obtain the explicit form for the transforming matrix given by Eq. (12),

and consider a different set of transforming matrices satisfying the condition $\det \mathbf{M} \equiv e^{-\lambda}$, instead. According to Eqs. (3) and (8), this condition can be physically interpreted as $t_{n,n\pm1} = (\det \mathbf{M})^{\mp 1}$. In this way, the determinant of the transformation matrix would be related to the hopping integral values, and the nonunimodular character of $\mathbf{M}$ would appear as a natural consequence of the fact we are considering a mixed lattice, where the values of hopping terms are different for different kinds of neighboring atoms.

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APPENDIX: PROOF OF THEOREM 1

For convenience we define

$$\mathbf{Q} \equiv \begin{pmatrix} q_{11} & q_{12} \\ q_{21} & q_{22} \end{pmatrix}, \quad \mathbf{M} \equiv \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \quad \mathbf{M}^{-1} \equiv \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix},$$

where

$$\alpha = \frac{d}{\det \mathbf{M}}, \quad \beta = -\frac{b}{\det \mathbf{M}}, \quad \gamma = -\frac{c}{\det \mathbf{M}}, \quad \delta = \frac{a}{\det \mathbf{M}}. \tag{A1}$$

Now, we introduce the auxiliary matrix

$$\mathbf{S} \equiv \mathbf{MQ} = \begin{pmatrix} s_{11} & s_{12} \\ s_{21} & s_{22} \end{pmatrix} = \begin{pmatrix} aq_{11} + bq_{21} & aq_{12} + bq_{22} \\ cq_{11} + dq_{21} & cq_{12} + dq_{22} \end{pmatrix} \tag{A2}$$

satisfying $\det \mathbf{S} = \det \mathbf{M}$. Then, the transformation $\mathbf{MQM}^{-1} \equiv \mathbf{SM}^{-1} = \mathbf{P}$, can be expressed in the form

$$\begin{pmatrix} s_{11} & 0 & s_{12} & 0 \\ 0 & s_{11} & 0 & s_{12} \\ s_{21} & 0 & s_{22} & 0 \\ 0 & s_{21} & 0 & s_{22} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \\ \gamma \\ \delta \end{pmatrix} = \begin{pmatrix} A \\ -e^{-\lambda} \\ e^{\lambda} \\ 0 \end{pmatrix}, \tag{A3}$$

whose solution is given by

$$\alpha = \frac{As_{22} - e^{\lambda} s_{12}}{\det \mathbf{S}}, \quad \beta = -e^{-\lambda} \frac{s_{22}}{\det \mathbf{S}},$$

$$\gamma = \frac{e^{\lambda} s_{11} - As_{21}}{\det \mathbf{S}}, \quad \delta = e^{-\lambda} \frac{s_{21}}{\det \mathbf{S}}. \tag{A4}$$

By equating Eqs. (A1) and (A4), taking into account Eq. (A2), we obtain the homogeneous system

$$\begin{pmatrix} e^{\lambda}\mathbf{I} & -\mathbf{Q}^t \\ e^{\lambda}\mathbf{Q}^t & \mathbf{I} - A\mathbf{Q}^t \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} \equiv \mathbf{BX} = \mathbf{0}, \tag{A5}$$

where $\mathbf{u} = (a,b)^t$, $\mathbf{v} = (c,d)^t$, and $\mathbf{I}$ is the identity matrix. Making explicit use of the unimodular property of the $\mathbf{Q}$ matrix it is readily seen that $\mathrm{rank}(\mathbf{B}) = 2$, so that the system given by Eq. (A5) finally reduces to $\mathbf{u} = e^{-\lambda}\mathbf{Q}^t\mathbf{v}$ [alternatively, $\mathbf{v} = e^{\lambda}(\mathbf{Q}^t)^{-1}\mathbf{u}$]. ■

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