Phason hierarchy and electronic stability of quasicrystals

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We show that under a random phasonic field, there is a hierarchy in the probability of making a phason in real space. This effect divides the quasicrystal in a stable backbone plus an unstable part. The stable backbone and the unstable sites are obtained by the deflation rules of the corresponding quasicrystalline lattice, and thus analytical formulas to find the stable and unstable parts are provided. A discussion is made about how the electronic stabilization of a quasicrystal is affected by phason jumps in unstable sites. As a result, it is shown that phasons in unstable sites do not compromise the electronic stabilization of the structure, since they only affect low-amplitude diffraction spots of the quasicrystal.

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I. INTRODUCTION

Quasicrystals are materials that have long-range orientational order but without periodicity.[1] This particularity means that they are considered as a different kind of matter agglomeration, and after two decades of intensive research that followed the discovery of quasicrystals, many features are now understood in a general fashion,[2] such as the nature of the structure, or the electronic stabilization of the structure via the Hume-Rothery mechanism.[2] Other physical properties still are not completely well understood,[3] as for example, the behavior of the elementary excitations, such as electrons or phonons. Both excitations are important in order to explain the thermal and electronic conductivities. Experiments show that although quasicrystals are made from metals, their conductivity is similar to that observed among amorphous semiconductors.[3] However, theoretical studies[4,5] and numerical simulations[6] predict a marginal metallic regimen due to the Conway theorem, since from a theoretical point of view, the wave function resonates in a self-similar way.[6] In spite of this, when the effects of frustration of antibonding states around the Fermi level are considered, the conductivity can be reduced by a considerable amount by localizing the wave function.[7] In fact, frustration produces a kind of mobility edge in two dimensions,[7] which has been confirmed in many numerical simulations.[8–10] Another question that up to now is not completely solved is how do quasicrystals grow. There are many clues that this happens by an agglomeration of clusters,[11] but it is clear that any attempt to solve this question completely must be related to the fact that quasicrystals are stabilized via the Hume-Rothery mechanism, i.e., the structure has to produce a pseudogap of the density of states around the Fermi level in order to reduce the energy per electron. Another particularity of quasicrystals is the extra degrees of freedom that are present in the elastic properties[12] and that are related to the behavior of the elementary excitations and stability.[13] In a crystal, any function of the density (and the density itself) is described as a superposition of reciprocal wave vectors. Then the Fourier transform (FT) of the density is just a series of sharp spots in the reciprocal space. A perturbation on the Fourier transform (FT) phases of the atomic positions induces a displacement of the atoms. Associated with such a perturbation, there are three hydrodynamic modes: two transverse and one longitudinal acoustic *phonons*.[12] These are the Goldstone modes associated with the breaking of a continuous symmetry, in this case the translational invariance of the Hamiltonian. A quasicrystalline structure is obtained by projecting a hyperlattice in D dimensions into a real d dimensional space, and the FT contains more reciprocal basis vectors than the dimension of the space.[2] There are $D-d$ of such degrees of freedom for the phases of the FT. A change in d of these phases produces phonons, while a change in the remaining phases produces local rearrangements of some atomic sites.[12] The corresponding hydrodynamic Goldstone modes associated with these changing phases are called *phasons*. Phason modes are diffusive, with very large diffusive times.[14] Phason jumps have been seen by time-of-flight experiments.[15]

Phasons are considered as low-energy excitations, but on the other hand, a phason corresponds to a rearrangement of sites that requires jumps over local energy barriers, which are of the order of the energy for creating a vacancy in the lattice (E_v). This seems to be contradictory, but, in fact, the picture depends on the scale. At small scales, phasons are local jumps, but at macroscopic scales, symmetry and conservation laws determine the dynamics.[12] From the atomic point of view, phasons in real space should be considered as local defects with only short-distance correlations. The hydrodynamic picture suggests long-distance correlations.[16] In this paper, we show that a random phason field produced in a hyperlattice leads to a certain spatial correlation in the probability for making a phason because some parts of the QC are more unstable against phason disorder. These sites happen to be obtained from the deflation rules, and thus there is a hierarchy in the probability for making phason jumps. As a result, there is a well-correlated distribution for phason jumps, with a length scale bigger than the original lattice. In fact, there are some direct experimental observations using an atomic-resolution annular dark-field scattering transmission electron microscope of localized atomic jumps that are well correlated in a superlattice of the quasicrystal that is deflated with respect to the original one.[17] Here we will also discuss some consequences of this fact, especially in the stability and dynamics of the lattice, since we expect that the structure must remain stable against phason jumps in the

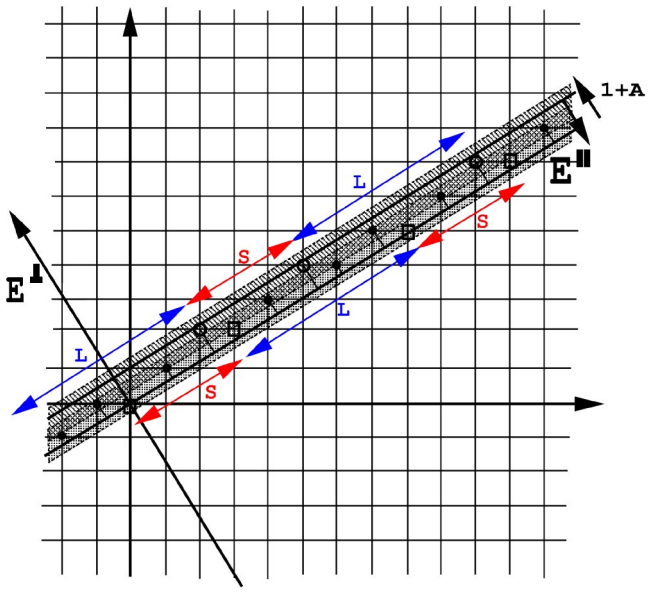

FIG. 1. Schematic illustration of the cut and projection method. The band (space delimited between the two solid inclined dark lines) is displaced $+A$ and $-A$ along $E^{\parallel}$, as indicated by the arrows. The corresponding bands are denoted by two different filling patterns. The effective bandwidth corresponds to the intersection of these two patterns. Stable sites are represented by dark-filled circles. Unstable sites that result from the displacement by $-A(+A)$ are shown as open circles (open square). The resulting deflated lattices are indicated by arrows along $E^{\parallel}$.

unstable sites and thus the effects of phasons will depend strongly on the atomic site, as has been found in numerical investigations of the Penrose tiling.[18]

The structure of this paper is the following. In Sec. II we explain how this phason hierarchy in deflated lattices arises. Section III is devoted to finding the positions for phason jumps in two-dimensional (2D) and three-dimensional (3D) lattices. In Sec. IV, we discuss the relationship between electronic stability and phason jumps; and finally, in Sec. V we give the conclusions of the work.

II. PHASON HIERARCHY AND DEFLATION RULES

The phason hierarchy for the probability of making a phason and its relation with the deflation rules can be explained in a simple way by using the Fibonacci lattice (FL). In Fig. 1, the usual cut-and-projection scheme is shown:[19] a line $E^{\parallel}$ with an inclination $\alpha=(\sqrt{5}-1)/2$ crosses a 2D square lattice, that we denote by $\mathcal{L}$. The FL is obtained by projecting, onto $E^{\parallel}$, the points falling inside a band of width L. The high dimensional space is subdivided into $E^{\parallel}$ and its orthogonal complement $E^{\perp}$. Using this subspaces, any point $\mathbf{r}$ can be written as $\mathbf{r}=\mathbf{r}^{\parallel}+\mathbf{r}^{\perp}$. The coordinates of the FL are $x=\mathbf{r}^{\parallel}W(\mathbf{r})$, where $W(\mathbf{r})$ is the window function, which is one when $\mathbf{r}$ falls inside the band and zero in any other case.

For higher dimensions, the scheme is exactly the same: $\mathcal{L}$ is a hypercubic lattice of N dimensions. The dimension of the space to be tiled can be $d=2$ or $d=3$, and $E^{\perp}$ has $N-d$ dimensions. The coordinates $\mathbf{x}$ of the lattice in the tiling subspace are,[19]

$$\mathbf{x}=\sum_{\mathbf{r}\in\mathcal{L}}\mathbf{r}^{\parallel}W(\mathbf{r})=\sum_{l=1}^{N}\sum_{n_l=-\infty}^{n_l=\infty}n_l\mathbf{e}_l W\left(\sum_{l=1}^{N}n_l\mathbf{q}_l\right),$$

where $\mathbf{e}_l$ (with $l=1,\ldots,N$) are the projections of the hypercubic basis vectors ($\mathbf{q}_l$) onto the parallel subspace.

A phason field can be introduced just by moving the band in $E^{\perp}$ at each point $\mathbf{r}$. As the window is moved, some points leave the band and some others are included in it. When this happens, a phason is produced in the "real space" of the quasicrystal. Points near the edges of the band fall very easily outside the band because, in such points, even a small movement of the window can throw them out of the lattice, whereas points at the center are very difficult to move. Clearly, the points near the center are very stable against window movements; they constitute what we will call the *stable backbone*. The main property of this set of stable points is that $\|\mathbf{r}^{\perp}\|$ is very small.

To be more precise, the effect a phason field in the coordinates of the FL can be written as $x=\mathbf{r}^{\parallel}W[\mathbf{r}+\boldsymbol{\eta}^{\perp}(\mathbf{r})]$, where $\boldsymbol{\eta}^{\perp}(\mathbf{r})$ is the displacement of the band in $E^{\perp}$. Using that $W[\mathbf{r}+\boldsymbol{\eta}^{\perp}(\mathbf{r})]=W[\mathbf{r}^{\parallel}+\mathbf{r}^{\perp}+\boldsymbol{\eta}^{\perp}(\mathbf{r})]$, points where $\mathbf{r}^{\perp}\approx\pm L/2$ are very close to the edge of the band. This situation makes them "unstable" against phason disorder since, even for a very small $\boldsymbol{\eta}^{\perp}(\mathbf{r})$, they can be dropped out. This observation holds for any phason field, whatever the shape of the function $\boldsymbol{\eta}^{\perp}(\mathbf{r})$, that can be a periodic modulation or even a random function. In the case of a random field, we can model the field by $\boldsymbol{\eta}^{\perp}(\mathbf{r})=A\chi(\mathbf{r})$, where A is the amplitude of the field, and $\chi(\mathbf{r})$ is a random variable with the most simple distribution: a uniform distribution between $[-1/2,1/2]$, although the results for other distributions are similar. To avoid vacancies in the lattice, we will assume that $A<1/2$, which still is a large amount of disorder compared to the average distances in the lattice. For the particular case of a random field with a uniform distribution, it is clear that the probability of producing a phason $[p_{ph}(\mathbf{r})]$ in an unstable region is $p_{ph}(\mathbf{r})=[\|\mathbf{r}^{\perp}\|-(L/2-A)]/2A$, i.e., $p_{ph}\propto\|\mathbf{r}^{\perp}\|/2A$ (note that the 2 in the denominator is due to the fact that only half of the movements of the window are in the direction where the points leave the band).

A way to generate the stable lattice is to use two displaced quasilattices in $E^{\perp}$, one displaced by A and the other one by $-A$ in the direction of $E^{\perp}$. The points that are stable against the perturbation are those that remain inside the three bands, since even a displacement of size A of the band can not throw them away, as explained in Fig. 1. However, finding the points that fall in the intersection of the three bands is equivalent to obtain a quasiperiodic sequence with a different narrow effective band width of size $\delta\equiv L-2A$. Thus, the set of stable points is given by $\mathbf{r}^{\parallel}W^{\text{stable}}(\mathbf{r})$, where

$$W^{\text{stable}}(\mathbf{r})=\begin{cases}1, & \text{if } \|\mathbf{r}^{\perp}\|\leqslant\delta\\ 0, & \text{in any other case}\end{cases}.$$

As can be observed from a direct inspection of Fig. 1, the effect of shrinking the bandwidth is just equivalent to create

a deflated lattice with some vacancies (if the band is moved in only one direction along $E^{\perp}$, the deflated lattice has no vacancies; vacancies appear when the movement along the other direction is considered). Figure 1 also shows that unstable points are in two deflated lattices.

This also suggests that p_{ph} has a hierarchy determined by the deflation rules in the following sense. We say that two vertices of a quasiperiodic tiling, say $\mathbf{r}_1$ and $\mathbf{r}_2$ belong to the same probability hierarchy if they satisfy the following inequality for a chosen degree of precision given by a small quantity ϵ bigger than zero,

$$\|p_{ph}(\mathbf{r}_1^{\perp}) - p_{ph}(\mathbf{r}_2^{\perp})\| < \epsilon, \tag{1}$$

and since $p_{ph}(\mathbf{r}^{\perp}) \propto \|\mathbf{r}^{\perp}\|/2A$, we get,

$$\|\mathbf{r}_1^{\perp} - \mathbf{r}_2^{\perp}\| < 2A\epsilon. \tag{2}$$

The last equation means that for small ϵ, all of the points that differ by ϵ in their probabilities also have a distance in perpendicular space given by $2A\epsilon$. But again, all of these points fall inside a band determined by a window of width $2A\epsilon$. Thus, the set of points that satisfy Eq. (2), when projected to real space also form a quasiperiodic lattice where the vertex positions are at $\mathbf{r}^{\parallel} W^{eff}(\mathbf{r})$, and the effective window is

$$W^{eff}(\mathbf{r}) = \begin{cases} 1, & \text{if } \|\mathbf{r}^{\perp}\| \leqslant 2A\epsilon \\ 0, & \text{in any other case} \end{cases}.$$

We know that this is just a deflation of the original lattice because the orientation of the band has not been changed; only the density of points has been lessened as a result of the narrower band. Note that due to the different possible directions of the band displacement, one gets more than one deflated lattice. These lattices only differ by a translation in real space, as can be seen in Fig. 1. In the Appendix, the case of the FL is worked out with analytical formulas. As a result, the probability of making a phason in the nth site of the lattice is given by

$$p_{ph}(n) = (|\{n\alpha\} - 1/2| - 1 + A)/2A, \tag{3}$$

where $\{z\}$ denotes the fractional part of z. The points with maximal probability are the ones that have $\{n\alpha\} \simeq 0, 1$.

III. STABLE BACKBONE AND UNSTABLE SITES IN 2D AND 3D QUASICRYSTALS

In this section, we obtain an analytical expression for the stable and unstable parts of a quasiperiodic tiling, using some formulas for the QC vertex coordinates that we obtained in a previous work.[20] Using the generalized grid method,[12] the QC is built from N star vectors e_l, where $l = 1, \ldots, N$. To detect the stable regions, we apply a shift $\pm A$ to the window function. We can apply different shifts A_l for each of the directions in $E^{\perp}$. To simplify the expressions we will consider the same uniform shift in all directions. The corresponding expressions for a 3D QC with a shift in the window function is given by

$$\mathbf{x}' = \sum_{k<j<s}^{N} \left\{ \sum_{\gamma,\delta,\epsilon=0}^{1} \sum_{n_s,n_j,n_k}^{\infty} \left[(n_s + \gamma)\mathbf{e}_s + (n_j + \delta)\mathbf{e}_j + (n_k + \epsilon)\mathbf{e}_k + \sum_{l\neq j\neq k\neq s}^{N} (\lceil R(n_s,n_j,n_k) \mp A \rceil)\mathbf{e}_l \right] \right\}, \tag{4}$$

where $\lceil z \rceil = \lfloor z \rfloor + 1$, $\lfloor z \rfloor$ is the floor function of z, and $R(n_s, n_j, n_k)$ is a function defined by

$$R(n_s,n_j,n_k) = x_{n_s}\frac{V_{lsj}}{V_{sjk}} + x_{n_j}\frac{V_{ljk}}{V_{sjk}} + x_{n_k}\frac{V_{slk}}{V_{sjk}} - \alpha_l$$

and n_s, n_j, n_k are integers that run from $-\infty$ to ∞, l, k, j, and s are integers that run from 1 to N, V_{lsj} is the volume defined by $V_{sjk} = \mathbf{e}_s \cdot (\mathbf{e}_j \times \mathbf{e}_k)$, α_l are real numbers for $l = 1, \ldots, N$ that define a phase in each direction of the star vectors.[20] x_{n_s} is an abbreviation for $x_{n_s} = n_s - \alpha_s \pm A$. Note that the last sum over l in Eq. (4) is carried only for $l \neq j \neq k \neq s$. The condition for the unstable points is similar to the one obtained for the FC and consists of an analysis of the floor function of Eq. (4). After some algebra, using the identity $z = \lfloor z \rfloor + \{z\}$, the condition for the unstable regions is

$$\{R(n_s,n_j,n_k) \mp A\} = \{R(n_s,n_j,n_k)\} \mp A \pm 1. \tag{5}$$

Thus, the probability of making a phason in site $\mathbf{x}$ is given by the condition,

$$p_{ph}(\mathbf{x}) = [\{R(n_s,n_j,n_k)\} - 1/2 - (1 - A)]/A. \tag{6}$$

The unstable points are those for which

$$n_s\frac{V_{lsj}}{V_{sjk}} + n_j\frac{V_{ljk}}{V_{sjk}} + n_k\frac{V_{slk}}{V_{sjk}} \approx \alpha_s\frac{V_{lsj}}{V_{sjk}} + \alpha_j\frac{V_{ljk}}{V_{sjk}} + \alpha_k\frac{V_{slk}}{V_{sjk}} + M,$$

for the directions defined by the star vectors $\mathbf{e}_s, \mathbf{e}_j$, with respect to the direction $\mathbf{e}_l$. The integer M can take the values 0 or 1. These equations correspond to regions that define worm planes. A similar calculation for a 2D tiling shows that in fact the unstable regions coincide with lines that are called worms.[21] Here we showed that there is a hierarchy in the probabilities for creating worms in different parts of the lattice.

IV. ELECTRONIC STABILITY AND PHASON DISORDER

We may wonder if all of the previous properties have some physical consequences. Suppose for example that thermal noise produces random fluctuations of the band. If this is true, at a certain temperature there will be always sites of the lattice that are more stable than others. In fact, we expect that A should be of order $\bar{\lambda}\exp(-E_v/kT)$, where $\bar{\lambda}$ is the average separation of atoms. As a result, when the temperature of the quasicrystal is changed, some sites will show more jumps than others, and these sites are going to form a deflated sublattice. Very recently, a similar effect has been observed[17] in the imaging of the thermal vibration of decagonal $Al_{72}Ni_{20}Co_8$, which suggests that there is some degree of hierarchy in the lattice. A second question that arises from the previous scenario is the following: since quasicrystals are stabilized by the electronic structure that produces a

pseudogap around the Fermi level, should one expect a robust electronic density of states with respect to sites where there is a high probability of making a jump? It is natural to think that points in the stable backbone are the ones that mainly determine the electronic structure.

To answer this question, let us consider the most simple Hamiltonian to model the electronic structure: an *s*-band tight-binding Hamiltonian defined on a chain of n sites, with a potential V_n at site n, and hopping integral t_{n+1} between sites n and $n+1$. The corresponding Schrödinger equation is $t_n\psi_{n-1}+t_{n+1}\psi_{n+1}+V_n\psi_n=E\psi_n$, where ψ_n is the value of the wave function at site n. This equation can be rewritten in terms of a transfer matrix T_n,

$$T_n = \begin{bmatrix} (E-V_n)/t_{n+1} & t_n/t_{n+1} \\ 1 & 0 \end{bmatrix},$$

and a vector $\mathbf{\Psi}_n$ with components (ψ_n, ψ_{n-1}), such that $\mathbf{\Psi}_{n+1} \equiv T_n \mathbf{\Psi}_n$. The wave function at site n is given by a successive application of the transfer matrix,

$$\mathbf{\Psi}_n = T_n T_{n-1} \ldots T_1 \Psi_1 \equiv M_n \mathbf{\Psi}_1. \tag{7}$$

The spectrum is the set of energies for which the trace norm $\tau_n(E) \equiv trM_n$ is <2.[4] The FL is made with two kinds of atoms, L and S, arranged following the Fibonacci sequence, i.e., if one defines the first generation $F_{ch}(1) \equiv L$ and the second one $F_{ch}(2) \equiv LS$, the subsequent generations are given by $F_{ch}(l) = F_{ch}(l-1) \oplus F_{ch}(l-2)$. For instance, $F_{ch}(3) = LSL$. To each kind of site we assign a potential V_L or V_S. For simplicity we will suppose that all the hopping integrals are equal $t_n = t$. The total transfer matrix for a FL can be written using a recursion rule for the matrices of previous FL generations,[4]

$$M_{F(l)} = M_{F(l-1)} M_{F(l-2)}, \tag{8}$$

where $F(l)$ is a Fibonacci number of generation l, defined as $F(l) = F(l-1) + F(l-2)$, with initial conditions $F(0) = 1$ and $F(1) = 1$.

A simple way to perform a single-phason flip in a FL of generation $F(l)$ for l even, is obtained by reversing the recursion rule only for the last step of the construction,

$$M^p_{F(l)} = M_{F(l-2)} M_{F(l-1)}, \tag{9}$$

where $M^p_{F(l)}$ is the resulting matrix with a phason flip. For example, the FL of generation 4 is the sequence: *LSLLS* made by joining a chain of generation 3 (sequence *LSL*) and generation 2 (sequence *LS*). If this chains are joined in reverse order in the last step of recursion, we get *LSLSL*, which is the original chain plus a phason flip at the end. To prove that the energy spectrum remains invariant under this flip, consider the trace of $M^p_{F(l)}$. Using the recursion for the transfer matrices we get

$$trM^p_{F(l)} = tr[M_{F(l-2)} M_{F(l-1)}] = tr[M_{F(l-2)} M_{F(l-2)} M_{F(l-3)}],$$

but using the cyclic property of a matrix product trace

$$tr[M_{F(l-2)} M_{F(l-2)} M_{F(l-3)}] = tr[M_{F(l-2)} M_{F(l-3)} M_{F(l-2)}]$$
$$= trM_{F(l)}.$$

Thus, $trM^p_{F(l)} = trM_{F(l)}$, which shows that a phason in this special site leaves the electronic spectrum unchanged. Another important relation can be obtained from the previous sequence of cyclic permutations

$$tr[M^p_{F(l-1)} M_{F(l-2)}] = tr[M_{F(l-3)} M_{F(l-2)} M_{F(l-2)}] = trM_{F(l)}. \tag{10}$$

Since $M^p_{F(l-1)}$ is a sequence with a phason flip at site $F(l-1)$, then $M^p_{F(l-1)} M_{F(l-2)}$ is a sequence with a phason flip at a the site where two Fibonacci sequences of previous generations are joined. For example, for generation 5, we take generation 4 with a phason flip at the end, *LSLSL*, and we join it with the sequence of generation 3, *LSL*. If we join both sequences following Eq. (10), we get the sequence *LSLSLLSL*, which has a phason flip between sites 4 and 5, since the original sequence is *LSLLSLSL*. In the Appendix, it is shown that this site is the one with the greatest phason probability. We can conclude that at least for this special site, there is a clear relationship between phason and electronic stability. Phasons in some other sites of the FL can change in a dramatic way the spectrum and induce a localization transition[22] because of the self-similar properties of the FL Green's function.[22] The method presented here, i.e., the decomposition in products of lower generations and then the application of the cyclic permutations, allows the construction of chains with the same spectrum but different degrees of phason disorder. Although the previous demonstration is very clear, it does not provide an explanation of what is behind this remarkable property. To have a better understanding, let us study the structure of the potential in reciprocal space. For a Fibonacci sequence, the potential at site n can be written as

$$V(n) = \overline{V} + \Delta V f(n), \tag{11}$$

where $f(n)$ is the hull function defined as

$$f(n) = \{n\alpha\} - \{(n+1)\alpha\}, \tag{12}$$

α is an irrational number [in this case $(\sqrt{5}-1)/2$], $\overline{V}$ is the average potential energy, given by $\alpha V_A + \alpha^2 V_B$, and $\Delta V \equiv |V_A - V_B|$ is a fluctuation part. The fractional part of a number is a periodic function with the shape of a sawtooth and can be Fourier expanded to get

$$V(n) = \overline{V} + \sum_{s=1}^{\infty} \tilde{V}(s) \cos[\pi s \alpha (2n+1)], \tag{13}$$

where $\tilde{V}(s)$ is the s harmonic of the Fourier series,

$$\tilde{V}(s) = 2\Delta V \frac{\sin(\pi s \alpha)}{\pi s}. \tag{14}$$

Note that each harmonic of the series is in the form of a Harper potential, for which a lot of properties are known.[23,24] In other words, a Fibonacci potential is just a superposition of Harper potentials with an appropriate weight plus an over-

all shift given by the average potential energy $\overline{V}$. As explained in the Appendix, phasons are obtained by changing the fractional part with a random function. The corresponding potential can be written as,

$$V^{ph}(n) = \overline{V} + \Delta V\{[(n-1)\alpha + A\chi(n-1)] - [n\alpha + A\chi(n)]\},$$

where $\chi(n)$ is a random variable with uniform distribution between $-1/2$ and $1/2$. Sites in the stable backbone are not affected by disorder, while the most unstable points are those where $\{n\alpha\} \approx 0,1$. These points are the ones that are in the edges of the sawtooth function $\{z\}$. An heuristic explanation of the stability of the spectrum is the following: to define the edges of $\{z\}$ in a sharp way, $\tilde{V}(s)$ coefficients of very high frequency are needed in the Fourier expansion. For high frequencies, these coefficients are very small, and albeit the reciprocal space of quasicrystal is a countable dense set, it has been shown that only very few of the reciprocal-lattice vectors are of importance in altering the overall electronic structure.[25] To further develop this idea, consider the case of just one phason between sites m and $m-1$. The potential energy with such a phason can be written as

$$V^{ph}(n) = V(n) + [V(n-1) - V(n)] \times [\delta(n-m) - \delta(n-m+1)], \quad (15)$$

where $\delta(n-m)$ is a δ function at site m. Using Eq. (13), and that $\sin(2\pi s\alpha n) = \sin[2\pi s(\lfloor \alpha n \rfloor + \{\alpha n\})] = \sin(2\pi s\{\alpha n\})$, the previous equation is converted into

$$V^{ph}(n) = V(n) + \sum_{s=1}^{\infty} 2\tilde{V}(s)\sin(\pi s\alpha)\sin(2\pi s\{\alpha n\}) \times [\delta(n-m) - \delta(n-m+1)].$$

The second term in the last equation can be considered as a perturbation of the original potential $V(n)$. However, the term $\sin(2\pi s\{\alpha n\})$ in the perturbation is nearly zero whenever $\{\alpha n\} \simeq 0$ or 1. The fraction $\{\alpha n\}$ is never 0 or 1 due to the irrationality of α (except of course $n=0$), but for a site n where $\{\alpha n\} \ll 1$, the perturbation part potential can be expressed as

$$8\{\alpha n\}\Delta V \sum_{s=1}^{s_c} \sin^2(\pi s\alpha)[\delta(n-m) - \delta(n-m+1)],$$

for any s lower than a cutoff determined by the condition $s_c \approx 1/2\pi\{\alpha n\}$. Terms with $s > s_c$ have a higher contribution to $\sin(2\pi s\{\alpha n\})$, but the coefficients $\tilde{V}(s)$ are already very small. This proves that for the first harmonics, the perturbation is proportional to $\{\alpha n\}$ where $\{\alpha n\} \ll 1$ (for $\{\alpha n\} \simeq 1$, the proof is similar). Furthermore, since $\{n\alpha\} \propto A[1-2p_{ph}(\mathbf{r}^{\perp})] - (1/2)$, the perturbation decreases linearly with the probability of making a phason. For higher harmonics, the perturbation has more weight with respect to $V(n)$, but this only affects Fourier coefficients of high frequencies, which have a lower amplitude. In fact, for a rational approximant, the spectral gaps (Δ_q) are produced by each diffraction spot of the potential in reciprocal space $[V(\mathbf{q})]$, due to the relation[26] $\Delta_q \simeq \|V(\mathbf{q})\|$, where $\mathbf{q}$ is a reciprocal wave vector. According to our result, a phason in an unstable site alters mainly low-amplitude diffraction spots, and thus the spectrum remains similar since only small gaps are affected.

A similar argument can be invoked for a higher-dimensional system. For simplicity, consider a δ-function potential of magnitude V_0 centered at each point of the lattice. In that case, the Fourier transform of the potential can be written as

$$\tilde{V}(\mathbf{q}) = V_0 \sum_{\mathbf{x}} e^{i\mathbf{q}\cdot\mathbf{x}}. \quad (16)$$

As is well known, Eq. (16) with or without phasons can be evaluated using the convolution theorem, and many years ago the scaling of the peaks in terms of $\mathbf{q}^{\perp}$ was the source of a debate between the random tiling model and perfect quasiperiodic tilings.[12] Here we will concentrate on the electronic stability of phasons. For sites inside the stable backbone, Eq. (16) remains equal, while for points where a phason is made, we add a bounded extra term $\mathbf{\Delta}(\mathbf{x})$ that produces a phason flip at position $\mathbf{x}$. We obtain

$$\tilde{V}^{ph}(\mathbf{q}) = V_0 \sum_{\mathbf{x}\in\mathcal{L}_{st}} e^{i\mathbf{q}\cdot\mathbf{x}} + V_0 \sum_{\mathbf{x}\in\mathcal{L}_{ph}} e^{i\mathbf{q}\cdot[\mathbf{x}+\mathbf{\Delta}(\mathbf{x})]}.$$

$\mathcal{L}_{st}$ denotes the set of points that belong to the stable lattice, and $\mathcal{L}_{ph}$ is the set of vertices in the unstable part. In some previous works,[20,27] we showed that a quasiperiodic structure can be described as an average structure plus a fluctuation part, i.e., a vertex in a position $\mathbf{x}$ can be obtained as an average $\langle\mathbf{x}\rangle$ plus a fluctuation part $\mathbf{f}(\mathbf{x})$, which is bounded.[20] From Sec. III, it is easy to see that this fluctuating part is given by

$$\mathbf{f}(\mathbf{x}) = \sum_{l\neq j\neq k\neq s}^{N} \{R(n_s, n_j, n_k)\}\mathbf{e}_l. \quad (17)$$

As explained in Sec. III, points in the unstable part have the property that $\mathbf{f}(\mathbf{x})$ is very small. Using this piece of information, and expanding the exponential for the bounded fluctuating part, Eq. (16) can be written as

$$\tilde{V}^{ph}(\mathbf{q}) = \tilde{V}(\mathbf{q}) + V_0 \sum_{t=1}^{\infty}\sum_{r=0}^{\infty}\sum_{\mathbf{x}\in\mathcal{L}_{ph}} \frac{[i\mathbf{q}\cdot\mathbf{\Delta}(\mathbf{x})]^t}{t!}\frac{[i\mathbf{q}\cdot\mathbf{f}(\mathbf{x})]^r}{r!}e^{i\mathbf{q}\cdot\langle\mathbf{x}\rangle}.$$

Since $\mathbf{\Delta}(\mathbf{x})$ and $\mathbf{f}(\mathbf{x})$ are smaller than the average atomic separation, only for high values of $\mathbf{q}$ the last term has an important contribution. According to Eq. (6), $p_{ph}(\mathbf{x}) = [\{R(n_s, n_j, n_k)\} - 1/2 - (1-A)]/A$, which shows that the perturbation decreases with the probability of making a phason. In fact, in a previous work we showed that the average structure contains a very important fraction of the scattered amplitude.[28] This average structure remains the same when a small phason field is applied, and as a result, phasons in unstable sites affect mainly higher harmonics, which have less amplitude, with a small impact in the density of states. It is worthwhile mentioning that in quasicrystals, the Hume-Rothery argument is invoked in connection with the most intense peaks in the diffraction pattern, which defines the so-called Jones zone.[2] In that sense, phasons at unstable sites do not compromise the Jones zones and the Hume-Rothery

mechanism. Also, the previous approach shows that very different effects on the density of states are expected, depending on the site where the phason is performed. There is some numerical evidence that this is the case,[18] since the effects in the electronic density of states of the Penrose strongly depends on the type of flips in the lattice,[18] as has been seen in the analysis of the first spectral moments.[29]

V. CONCLUSIONS

In this paper, we have studied the probabilities of making a phason in quasiperiodic lattices. In particular, we have shown that the lattice can be divided into a stable backbone plus sites where the probability of making a phason is bigger. Furthermore, sites with a similar probability are in deflated structures of the original lattice. The possibility of having sites with high probabilities of phason jumps raises the question of how the electronic stability of a quasicrystal depends on such jumps. In a simple one-dimensional model, phason jumps in unstable sites do not change the electronic spectrum. These unstable sites seem to affect less the electronic spectrum due to the property of only changing reciprocal vectors with a high moment. A similar argument in two and three dimensions can be responsible for the robust electronic density of states against phason disorder in unstable sites. Note that very probably, there are some connections between how quasicrystals grow and the creation of a stable backbone with a hierarchical structure via some kind of self-similar Peierls instability.

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APPENDIX

For the FL, the unstable and stable sites are easy to obtain. Using the cut and projection technique, the coordinates of the n point of the FL are given by[27]

$$x_n = nL + (L - S)\lfloor n\alpha \rfloor = n\overline{\lambda} - (L - S)\{n\alpha\}, \qquad \text{(A1)}$$

where n is an integer, $\overline{\lambda} = (1+\alpha)L - \alpha S$ is the average lattice parameter,[27] L and S are the two possible separations of the quasilattice points, $\lfloor z \rfloor$ is the integer part of z, and $\{z\}$ is the fractional part of z. If we apply a phason field into this expression, a sequence x_n' is obtained. Phasons are produced when both sequences differ,

$$x_n' - x_n = (L - S)(\{n\alpha \pm A_\chi[(n,\lfloor n\alpha \rfloor)]\} \mp A - \{n\alpha\}) = \pm (L - S),$$

since $\{n\alpha\}$ has period one. The stable points satisfy $\{n\alpha \pm A\} = \{n\alpha\} \pm A$, and unstable points are those for which $\{n\alpha \pm A\} = \{n\alpha\} \pm A \pm 1$. Stable points correspond to n such that $A < \{n\alpha\} < 1 - A$, and unstable points satisfy $0 \leqslant \{n\alpha\} \leqslant A$ and $1 - A \leqslant \{n\alpha\} \leqslant 1$. If $A \to 0$ the most unstable points are those where $\{n\alpha\} \approx 0$ or 1, which means that $n\alpha \approx \lfloor n\alpha \rfloor$. When α is approximated by the rational approximant $F(l-1)/F(l)$, these points have the form $n = mF(l)$, where m is any integer. Then, unstable points are separated by Fibonacci numbers. For a uniform distribution of the random field with $A \neq 0$, the probability of making a phason in the unstable region is given by

$$p_{ph}(n) = (|\{n\alpha\} - 1/2| - 1 + A)/2A, \qquad \text{(A2)}$$

since $\|\mathbf{r}^{\perp}\|$ is the distance between the point $(n,\lfloor n\alpha \rfloor)$ in $\mathcal{L}$, and the subspace $E^{\parallel}$ defined by the line $y = \alpha x$.

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