Coherency of phason dynamics in Fibonacci chains

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The effects of phason disorder on the dynamical structure factor of Fibonacci chains are studied, and the existence of a coherent phason field in real quasicrystals is addressed. The neutron-scattering response is modeled for coherent and random phasons. The results show that coherent and random phasons can be distinguished for high values of the momentum transfer. However, for both sorts of phasons the response in the acoustic-mode region is quite similar, since the only important quantity is the average length between atoms. In particular, it is shown that a random phason produced in the quasicrystal's hyperspace leads to a coherent phason field in real space. [S0163-1829(99)00622-0]

I. INTRODUCTION

Quasicrystals (QC's) (see, for instance Refs. 1 and 2) present a peculiar kind of order. Despite lacking translational order, the positions of the atoms are not arbitrary, as in an amorphous solid, but are precisely determined, and spots in the diffraction patterns are observed. The issue of determining the positions of the atoms in real QC's is not resolved yet, although there are currently some structural models for certain alloys that are able to reproduce the available data from x rays and electron-diffraction experiments.[3,4]

Some simple theoretical models retaining the basic features of quasicrystalline order have been proposed, such as the one-dimensional Fibonacci chain (FC), or the family of Penrose lattices in two and three dimensions.[5–7] These models are useful to study the peculiarities of QC's and to predict the effects of the quasicrystalline order on their physical properties. In particular, an exclusive kind of local defect, called phason, could be investigated in detail by means of these theoretical models.

A phason can be obtained from the cut-and-projection method for QC's,[8] which consists in projecting a D-dimensional hyperspace periodic lattice onto a d-dimensional space where a quasiperiodic lattice is obtained. The Fourier transform (FT) of a QC is made by linear combinations of the D reciprocal basis vectors, which project onto the real space. This explains why the diffraction pattern of a QC is made of sharp diffraction spots, since the square modulus of the Fourier transform is proportional to the diffraction pattern.

In a crystal, a uniform change of the phases on the FT induces a uniform displacement of the atomic positions in real space. The hydrodynamic modes associated with such a perturbation in a crystal are called acoustic phonons. In a quasicrystal there are D degrees of freedom for changing the phases of the FT. A change in d of them produces a translation in real space, or phonons. A change in the other $(D-d)$ phases produces local rearrangements of some atomic sites.[9] The hydrodynamic modes associated with changing $(D-d)$ phases are the phasons.

According to Lubensky *et al.*,[10] the phason modes in a QC are diffusive, with very large diffusion times. Observe that, as hydrodynamic modes, phasons are low-energy excitations. On the other hand, a phason corresponds to a rearrangement of sites that requires atoms to jump over local energy barriers,[9] which can be large (this energy is nearly the energy for creating a vacancy in the lattice). Then, the picture depends upon the scale; at macroscopic scales, symmetries and conservation laws determine the dynamics of the phasons.[11]

During solidification of a QC, phason and phonon strains could be present, but phonon strain relaxes quickly leaving only phason strain. This strain produces a widening of the characteristic peaks in experimental diffraction patterns of QC's by x rays, electrons, or neutrons.[12] In particular, the time of jump of atomic species in QC's with phason disorder was recently obtained using time-of-flight quasielastic neutron scattering.[13]

However, it is not clear yet if phasons should be coherent modes in real space, as the hydrodynamic picture implies. From the atomic point of view, phasons should be considered as local defects with only short-distance correlations. If this is the case, then the use of a hyperlattice description of phasons is controversial.

In this paper we examine both points of view and study the peculiarities of phasons produced in either a coherent or an incoherent way. In order to do so, we concentrate our attention on the simplest QC, the Fibonacci chain, with the

simplest possible dynamical Hamiltonian, a harmonic one with nearest-neighbor springs of constant strength and equal masses. This choice allows us to investigate the role of the atomic positions exclusively, which can be probed with neutron-scattering experiments, leaving aside all the complications due to other dynamical details of the problem. In real experiments it is difficult to disentangle the effects due to phason disorder or substitutional disorder,[14] or other kinds of imperfections (see, for instance, Refs. 15 and 16); therefore, models that treat separately these effects should be useful for a full understanding of experimental data. Our simple model could be criticized because only one type of these sites is considered. However, these sites could be thought of as molecules following a quasicrystalline array, or something more complicated. In any case, the possibility of having real one-component quasicrystals has been put forward.[17] The quantity to obtain is the dynamical structure factor $S(q,\omega^2)$ as a function of the variables that define phason disorder in the chains.

In Sec. II we define the dynamical structure factor $S(q,\omega^2)$ for the model used and find general expressions to calculate it. In Sec. III we describe in detail the procedure to calculate $S(q,\omega^2)$ in a Fibonacci chain. In Sec. IV we explain how to obtain expressions for different kinds of phason disorder, and calculate the dynamical structure factor for coherent phasons (CP's), phasons generated by randomly disturbing the hyperspace, or random window phasons (RWP's) and phasons regarded as local defects produced randomly by exchanging neighbor bonds in a FC, or real-space random phasons (RP's). Finally, in Sec. V we discuss the results of the model and point out the peculiarities of the spectra obtained with the various sorts of phasons, and we draw some general conclusions from this work and also comment on possible extensions of this theory to more realistic situations.

II. DYNAMICAL STRUCTURE FACTOR

In an inelastic neutron-scattering experiment, most measurable quantities are related to the response of the system in frequency (ω) and momentum (q) space, which is characterized[18] by the *dynamical structure factor* $[S(q,\omega^2)]$.[19] For a chain of N sites, this is written as,[20]

$$S(q,\omega^2)=-\frac{1}{N}\sum_{x,x'} e^{iq(x-x')}\mathrm{Im}\,G_{x,x'}(\omega^2), \tag{1}$$

where $G_{x,x'}(\omega^2)$ is the retarded Green's function,[20] describing the excitations that couple to the neutrons, as phonons or magnons. In this work we discuss only the phonon case, since structural defects modify mainly the vibrational modes. Therefore, $G_{x,x'}(\omega^2)$ represents the displacement-displacement (u,u') correlations between sites x and x'.

We shall consider a simple Hamiltonian of springs of equal strength (J) in a chain of equal unitary masses,

$$H=\sum_x \left[\frac{1}{2}\left(\frac{du_x}{dt}\right)^2+\frac{J}{2}\sum_{x'}(u_x-u_{x'})^2\right],$$

since we are interested on the effects of structural disorder more than in the specific dynamics.

This model is particularly suitable to isolate the effects of the quasiperiodicity from the dynamics, since the vibrational density of states $[\eta(\omega^2)]$ is insensitive to changes in the bond lengths, and it is the same as for a perfect linear chain, but the neutron response should sense bond-length disorder. In a linear chain, $x=m$ in units of the lattice parameter, where m is any integer. The Green's function correlating sites m and m' can be written[21]

$$G_{m,m'}(\omega^2)=-i\frac{1}{\sqrt{(2J)^2-(\omega^2-2J)^2}}e^{i\theta(\omega^2)|m-m'|}$$
$$=-i\pi\eta(\omega^2)e^{i\theta(\omega^2)|m-m'|}, \tag{2}$$

where $\theta(\omega^2)$ satisfies

$$\theta(\omega^2)=\arctan\left(-\frac{\sqrt{(2J)^2-(\omega^2-2J)^2}}{\omega^2-2J}\right), \tag{3}$$

or, $\omega^2(\theta)=2J(1-\cos\theta)$, which is the well-known dispersion relation of a linear chain. A useful expression for $S(q,\omega^2)$ is obtained by plugging Eq. (2) into Eq. (1), that is,

$$S(q,\omega^2)=\frac{\pi\eta(\omega^2)}{N}\sum_{m,m'}^{N}\exp(i[q(x_m-x_{m'})$$
$$-\theta(\omega^2)(m-m')]). \tag{4}$$

This is the basic result of the model and shall be used for all the chains with disorder. The only ingredient needed is an expression for x_m. Once one has an expression for the coordinates, one could in principle calculate Eq. (4) in a computer. However, as in all interference phenomena, the contribution from distant sites in the summations do not converge rapidly, and one has to spend large amounts of effort to approximate the result. Therefore, it is more than convenient to derive more analytical expressions.

In particular, the response of the linear chain is

$$S(q,\omega^2)=\pi\eta(\omega^2)\delta[q-\theta(\omega^2)]=\delta[\omega^2-\omega^2(q)],$$

which is the correct limit. In the next section we shall examine the perfect FC.

III. THE FIBONACCI CHAIN

For the FC it is convenient to use the cut and projection method.[8,11] One uses a two-dimensional (2D) rectangular lattice, and projects on a straight line with incommensurate slope, $\tan(\phi)=b/\tau a$, where $\tau=(\sqrt{5}+1)/2$ is the Golden mean, and a (b) is the lattice parameter in the x (y) direction.

The points (m,n) of the 2D lattice are projected into the straight line, giving a position $(ma\cos\phi+nb\sin\phi)$. Then, the coordinate of the mth point in the FC is expressed as

$$x_m=\sum_n (ma\cos\phi+nb\sin\phi)W(m,n), \tag{5}$$

where the window function $W(m,n)$ selects the points in the hyperspace to be projected.

The form of this window function can be obtained analytically,[22] by defining a band of constant width, parallel to the straight line given by $y=x\tan\phi+y_0$. The ordinate at the origin y_0 determines a unique point of the lattice that precisely intersects the straight line. In particular, if $y_0=0$,

this point is the origin. The distance from any other point in the lattice to this line is different from zero, since $\tan\phi$ is irrational. For a given width $W_0 \leqslant b\cos(\phi)$ only one point n is chosen for each m. The slightest change in the slope causes another point to intersect, defining a period, and consequently a crystal, which is known as a rational approximant of a FC. Considering $y_0 \neq 0$ can be regarded as a horizontal translation of the origin.

If $W_0 = b\cos(\phi)$ and $y_0 = 0$, it is clear that

$$W(m,n) = \delta\left(n - \left\lfloor \frac{ma\tan\phi}{b} \right\rfloor\right), \tag{6}$$

where $\lfloor z \rfloor$ denotes the integer part of z, and δ is the Kronecker function. Then, by using Eq. (5) one obtains

$$x_m = mS + \left\lfloor \frac{m}{\tau} \right\rfloor (L-S). \tag{7}$$

Therefore, the distance between two consecutive points in the FC can be either $S = a\cos\phi$ or $L = b\sin\phi + S$. Observe that a and b give the lengths of the short (S) and long (L) distances that alternate following the Fibonacci sequence.[11] Using the identity $z = \lfloor z \rfloor + \{z\}$, where $\{z\}$ is the fractional part of z, Eq. (7) can be recasted as

$$x_m = m\bar{\lambda} - \left\{ \frac{m}{\tau} \right\} (L-S), \tag{8}$$

where $\bar{\lambda} = L/\tau + S/\tau^2$ is the average lattice parameter, since in a FC the ratio between the number of L and S intervals is τ. As it will be shown later, this quantity dominates the behavior of the dynamic structure factor for long-wavelength modes. The other term in Eq. (8) gives the fluctuations around $\bar{\lambda}$.

The corresponding dynamical structure factor for the FC is obtained by substituting Eq. (8) into Eq. (4). The double sum over sites can be performed separately. One of these summations can be written as

$$\sum_{m=-\infty}^{\infty} e^{im\gamma} e^{-iq(L-S)\{m/\tau\}}, \tag{9}$$

where $\gamma = q\bar{\lambda} - \theta(\omega^2)$. This can be calculated exactly by using the convolution theorem for Fourier transforms ($\tilde{f}$), which reads

$$\widetilde{f_1 f_2}(\gamma) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{f_1}(\Omega)\tilde{f_2}(\gamma - \Omega)\, d\Omega. \tag{10}$$

Let us define $f_1 = e^{-iq(L-S)\{m/\tau\}}$ and $f_2 = 1$. Using the fact that $\{z\}$ is periodic, with period one, and that $\{z\} = z$ in the interval $[0,1)$, the Fourier expansion of f_1 is[23]

$$e^{iC\{z/\tau\}} = \sum_{n=-\infty}^{\infty} \frac{(e^{iC}-1)}{i(C-2\pi n)} \exp\left[\frac{i2\pi zn}{\tau}\right], \tag{11}$$

where $C = -q(L-S)$. One can easily identify that $\Omega = 2\pi n/\tau$. Therefore, Eq. (9) becomes

$$\sum_{n=-\infty}^{\infty} \frac{e^{-iq(L-S)} - 1}{i[-q(L-S) - 2\pi n]} \delta(\gamma - 2\pi n/\tau). \tag{12}$$

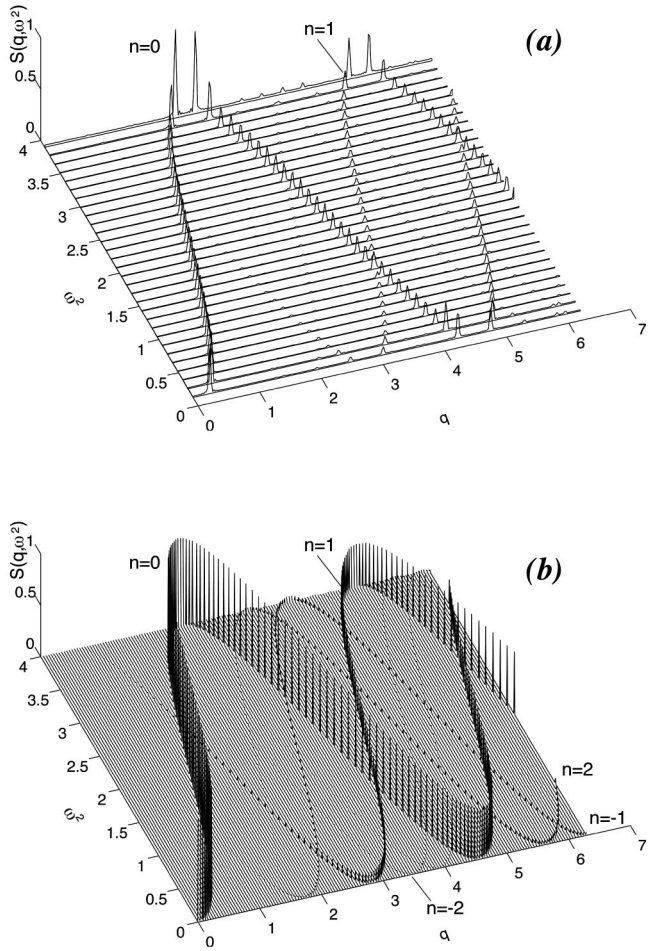

FIG. 1. (a) Dynamical structure factor $S(q,\omega^2)$ for a perfect Fibonacci chain of 200 atoms, calculated with Eq. (4). (b) The same calculated with Eq. (13) and up to 20 branches n.

The same procedure can be done for the summation over m' in Eq. (4), and the final result is

$$S(q,\omega^2) = 4\sin^2\left(\frac{q(L-S)}{2}\right) \sum_{n=-\infty}^{\infty} \frac{\delta[\omega^2 - \omega^2(q\bar{\lambda} + 2\pi n/\tau)]}{[q(L-S) - 2\pi n]^2}. \tag{13}$$

This equation shows that $S(q,\omega^2)$ covers densely the (q,ω^2) plane with a set of functions of the form $2J[1 - \cos(q\bar{\lambda} + 2\pi n/\tau)]$. The main contributions arise when $n \sim (L-S)q/2\pi$, since in Eq. (13) the denominator becomes small. Therefore, only a few of the n branches should have appreciable amplitude in a given region of q.

Equation (13) satisfies two important limits, when $L = S$ the response is that of a linear chain, as expected. When L/S is a rational number, $S(q,\omega^2)$ is periodic. When $L = \tau$ and $S = 1$, and knowing that $\{\tau\} = 1/\tau$, we recover the expression found by Ashraff and Stinchcombe.[23]

In order to test the validity of computer simulations against the results of Eq. (13), we calculated $S(q,\omega^2)$ for the FC by a direct simulation using the fundamental definition of it [Eq. (4)]. In Fig. 1(a) we show the result for a chain of 200 sites, with $S = 1$ and $L = \tau$, and for a mesh of 200×400 in the (q,ω^2) space. Notice that in spite of the huge calculation ($\approx 10^{10}$ steps), the amplitudes of the different branches are

completely wrong, and the shape given by the $\eta(\omega^2)$ factor is not removed, due to the finite summation. In Fig. 1(b) we show the result from Eq. (13) with only 20 terms in the single summation. Considering more terms does not change the results noticeably.

Observe that in the interval $q \in [0,2\pi]$, although there is a dense spectrum, only few branches of small n are visible and indicated in the figure. All branches have a period of 4.55, which agrees with the value $2\pi/\overline{\lambda} = 4.546$, calculated from Eq. (8). The amplitudes of the branches are modulated by the condition $q(L-S) \sim 2\pi n$, and the phase between branches $n=0$ and $n=1$ is 2.8, as predicted by $2\pi/\tau\overline{\lambda} = 2.8099$.

An interesting question is the behavior of the FC in the acoustic region $(q \to 0)$. If one calculates the second moment of $S(q,\omega^2)$,

$$\langle \omega^2(q) \rangle = \int \omega^2 S(q,\omega^2) d\omega^2, \tag{14}$$

by using Eq. (A8) in Appendix A, one finds that the second moment in the limit $q \to 0$ is given by

$$\langle \omega^2(q) \rangle = Jq^2 \left(\frac{L^2}{\tau} + \frac{S^2}{\tau^2} \right) = Jq^2 \overline{\lambda^2}. \tag{15}$$

This number is always higher than the square of the velocity of sound $J(\overline{\lambda})^2$, which is the same for the FC as for a periodic or random chain with an average lattice parameter, provided that the proportion of L and S bonds remains constant. This is due to the model, which separates the dynamics of vibrations from the scattering processes. The velocity of sound is dictated only by the dynamics, while the second moment of the scattering response has contributions of the various branches for a single q in the dynamical spectra.

Another distinctive feature of the spectrum is the finite width of the spectrum at $q=0$. The width is given by

$$\Delta = \frac{\langle \omega^4 \rangle - \langle \omega^2 \rangle^2}{\langle \omega^2 \rangle},$$

which depends only on the distribution of pairs of bonds with different length. In Appendix A we show that for a FC, Δ is always finite, and only in the limit $q=0$ the result is the same as the one obtained for a chain with a random distribution of bonds L and S.

IV. DYNAMICAL STRUCTURE FACTOR FOR PHASON DISORDER

In this section we examine the effects of having structural disorder, in the form of phasons, as deviations from the perfect FC. As mentioned before, it is not clear yet if phasons are coherent modes in real space, or if they should be considered as local random defects, with only short-distance correlations. Let us consider first the case of a coherent phason field.

Coherent phasons can be produced in various ways using the cut and projection method. One needs fluctuations in the window of acceptance that result in a rearrangement of the atomic positions in real space. In a FC, a local phason corresponds to changing the sequence $LS \to SL$ (or $SL \to LS$). This operation of interchanging contiguous intervals is called a flip-flop. For example, the sequence LSL can be converted into LLS by making a flip-flop.

The simplest coherent phason field that can be produced is a periodic fluctuation of the window in the y direction. We shall consider a sinusoidal modulation of the acceptance window of the form $W = W_0 + bA \sin(Q_p x + \alpha)$ where W_0 and A are constants. Q_p is the wave vector of the phason and α is a phase that fixes the point in the chain that coincides exactly with the origin of the hyperspace. This results in a kind of coherent modulation in the perpendicular space. If in Eq. (7) one substitutes m/τ by $m/\tau + A \sin(mQ_p a + \alpha)$, the Fibonacci sequence is converted into

$$x_m(A) = mS + \left\lfloor \frac{m}{\tau} + A \sin(mQ_p a + \alpha) \right\rfloor (L-S). \tag{16}$$

The chain generated by Eq. (16) is an example of a FC with *coherent phasons*. The effect of the oscillating term is the introduction of flips-flops in the original chain. The density of flips-flops (ρ) with respect to the perfect FC as a function of A, Q_p, and α is calculated in Appendix B. A flip-flop is introduced for a given m if the difference $\Delta(m)$ between the chains defined by Eqs. (7) and (16) is not null,

$$\Delta(m) = x_m(A) - x_m(0) = (L-S) \times \left(\left\lfloor \frac{m}{\tau} + A \sin(mQ_p a + \alpha) \right\rfloor - \left\lfloor \frac{m}{\tau} \right\rfloor \right), \tag{17}$$

so the positions in the chain with CP's are given by

$$x_m = m\overline{\lambda} - \left\{ \frac{m}{\tau} \right\} (L-S) + \Delta(m). \tag{18}$$

When one considers phasons as a random process, this can be done by altering the window function at random, or directly choosing sites in real space to make flip-flops. We shall obtain RWP's in the former case and real-space RP's in the latter.

These three cases can be treated with the same formalism, once the quantity $\Delta(m)$, which gives the deviations with respect to the perfect FC, is specified.

A. Coherent phasons

We substitute in Eq. (4) the positions of the sites in the chain, which now are given by Eqs. (18) and (17). For the sake of clarity, we shall set $\alpha = 0$, since this only means a uniform translation of all coordinates, and its effect is only important when comparing a disordered chain with a perfect chain in order to count the number of defects, or calculating the density of phasons, that we shall treat below. If we set $a=1$, we need to perform the following summation:

$$\sum_{m=-\infty}^{\infty} e^{im\gamma + iq(L-S)[A \sin(Q_p m) - \{m/\tau + A \sin(Q_p m)\}]}. \tag{19}$$

As with Eq. (10), we use the convolution theorem, but this time we define f_1 as

$$f_1 = e^{iq(L-S)[A \sin(Q_p m) - \{(m/\tau) + A \sin(Q_p m)\}]}. \tag{20}$$

Again, the decimal part of $\{m/\tau + A \sin(Q_p m)\}$ is periodic, and we use the following Fourier series:

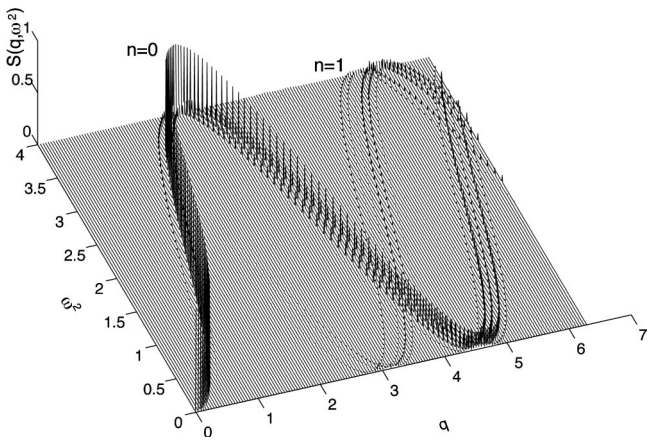

FIG. 2. Dynamical structure factor $S(q,\omega^2)$ for a FC with coherent phasons, produced using $A/b=0.5$, $\alpha=0$, and $Q_p=0.05\pi$, giving $\rho\approx 25\%$.

$$e^{iC\{m/\tau+A\sin(Q_p m)\}}=\sum_{n=-\infty}^{\infty}\frac{e^{iC}-1}{i(C-2\pi n)}e^{i2\pi n[(m/\tau)+A\sin(Q_p m)]}. \tag{21}$$

In order to perform the summation over m, we observe again that the function $e^{iB\sin(Q_p m)}$ is also periodic, and write the following Fourier expansion:[24]

$$e^{iB\sin(Q_p m)}=\sum_{s=-\infty}^{\infty}J_s(B)e^{iQ_p s m}, \tag{22}$$

where $B=A|q(L-S)-2\pi n|$ and $J_s(B)$ is its corresponding Bessel function.

Therefore, using Eq. (10), and $f_2=1$, Eq. (19) becomes

$$\sum_{n,s=-\infty}^{\infty}\frac{e^{-iq(L-S)}-1}{i[-q(L-S)-2\pi n]}J_s(B)\,\delta[q\bar{\lambda}-\theta(\omega^2) -2\pi n/\tau-Q_p s]. \tag{23}$$

The final expression for the dynamical structure factor is

$$S(q,\omega^2)=4\sin^2\left(\frac{q(L-S)}{2}\right)\times\sum_{n,s=-\infty}^{\infty}\frac{J_s^2(B)\,\delta[\omega^2-\omega^2(q\bar{\lambda}+2\pi n/\tau+Q_p s)]}{[q(L-S)-2\pi n]^2}. \tag{24}$$

Thus, $S(q,\omega^2)$ conserves the structure of the FC, except that the intensity of each peak of the FC ($s=0$), given by the condition $n\approx q(L-S)/2\pi$, is diminished by the factor $J_0^2(q)\leqslant 1$. Furthermore, there are satellites around each peak, given by the terms $s\neq 0$, all of which are less intense, the peaks with $s=\pm 1$ being the most pronounced ones.

Figure 2 shows the dynamical structure factor calculated, with Eq. (24) for $Q_p=0.05\pi$, $A=0.5$, $L=\tau$, and $S=1$, which results in a density of CP $\rho=25\%$. Notice that the first two branches of the perfect FC are still present but with less intensity, giving a modified overall appearance of the structure factor, as compared with the perfect case of Fig. 1(b). Furthermore, new satellite branches, due to $s=\pm 1$ and ± 2, appear as predicted. Observe that the separation of the satellite peaks is constant and equal to $Q_p/\bar{\lambda}=0.1137$. When Q_p is of the order of π, the appearance of the spectrum is not like the FC anymore, since satellites from different branches may overlap. When the wavelength of the phason is commensurate with the period of the FC branches, the response is identical to the FC spectrum, except that the amplitudes of the branches are changed by the satellites, whose responses always coincide with some branch. Equation (24) also shows that there is coupling between the neutron momentum (q), and the wave vector of the phason (Q_p). Equation (23) gives the following condition for generalized momentum conservation:

$$q\bar{\lambda}=\theta(\omega^2)+\frac{2\pi n}{\tau}+Q_p s, \tag{25}$$

which shows that this coupling is mediated by phonons.

B. Random window phasons

The second way of producing phasons is to move the acceptance window in a random fashion in each site m. For this RWP, the deduction is similar to the CP case, except that instead of having a sine function inside the window function, we must consider a random one. Therefore,

$$\Delta(m)=x_m(A)-x_m(0)=(L-S)\left(\left\lfloor\frac{m}{\tau}+R_m\right\rfloor-\left\lfloor\frac{m}{\tau}\right\rfloor\right), \tag{26}$$

where R_m is a random variable with a flat distribution between 0 and some amplitude A, related to the phason density ρ in a complicated way. For simplicity, from now on we shall take $A=1$.

We need to evaluate the average response over an ensemble of realizations of disorder. Thus, the analog of Eq. (19) is

$$\langle S(q,\omega^2)\rangle=\frac{\pi\eta(\omega^2)}{N}\sum_{m,m'}^{N}e^{i\gamma(m-m')}F_1(m,m')\times\langle F_2(m,m')\rangle, \tag{27}$$

where

$$F_1(m,m')=e^{-iq(L-S)(\{m/\tau\}-\{m'/\tau\})}$$

and

$$\langle F_2(m,m')\rangle=\sum_{\Delta(m)-\Delta(m')}e^{iq\{[\Delta(m)-\Delta(m')]\}}P(\Delta(m),\Delta(m')).$$

where $\langle\cdots\rangle$ denotes the average using a two-particle probability distribution function $P(\Delta(m),\Delta(m'))$. If the density of phasons is small, the statistical fluctuations are bounded and uncorrelated, since $\Delta(m)$ represents a local flip-flop (see Appendix B). In that case, $P(\Delta(m),\Delta(m'))=P(\Delta(m))P(\Delta(m'))$, and thus the two summations in Eq. (27) can be performed separately.

The manner in which disorder is produced in the hyperspace window can be written as

$$\Delta(m)=(L-S)[R_m+\{m/\tau\}-\{m/\tau+R_m\}]. \tag{28}$$

Observe that $\{m/\tau+R_m\}$ is $\{m/\tau\}+R_m$ if $R_m<1-\{m/\tau\}$, and it is $\{m/\tau\}+R_m-1$ otherwise. Therefore,

$$f_2(m)=e^{iq\Delta(m)}=\begin{cases}1 & \text{if} \quad R_m<1-\{m/\tau\}\\ e^{-iC} & \text{if} \quad R_m\geqslant 1-\{m/\tau\}.\end{cases} \tag{29}$$

This can be written as $\langle f_2\rangle=P(m)+e^{-iC}[1-P(m)]$. Since R_m obeys a flat distribution, $P(m)=1-\{m/\tau\}$ is the probability that on site m the random number does not exceed $1-\{m/\tau\}$. Then,

$$\langle f_2(m)\rangle=1+[e^{-iC}-1]\{m/\tau\}. \tag{30}$$

In Eq. (30), the first term will give a response similar to Fibonacci and the second term is periodic and can be Fourier expanded. The summation over m turns out to be

$$\sum_{n=-\infty}^{\infty}\left[\frac{1}{C-2\pi n}\right]\Bigg[(\sin C)\,\delta(\gamma-2\pi n/\tau)+(1-\cos C)\times\sum_{s=1}^{\infty}\frac{\delta[\gamma-2\pi(n+s)/\tau]-\delta[\gamma+2\pi(n-s)/\tau]}{\pi s}\Bigg]. \tag{31}$$

The summation over m' reads exactly the same, with proper conjugated factors. Finally,

$$\langle S(q,\omega^2)\rangle=\cos^2\left(\frac{C}{2}\right)S_{Fib}(q,\omega^2)+\sin^2\left(\frac{C}{2}\right)S_{Sat}(q,\omega^2), \tag{32}$$

where $S_{Fib}(q,\omega^2)$ is the response of the FC, given by Eq. (13), and the rest of the oscillator strength is added to satellites whose response is

$$S_{Sat}(q,\omega^2)=\sum_{s=1}^{\infty}4\sin^2\left(\frac{C}{2}\right)\frac{\delta[\omega^2-\omega^2(q\bar{\lambda}-2\pi(n+s)/\tau)]+\delta[\omega^2-\omega^2(q\bar{\lambda}-2\pi(n-s)/\tau)]}{[\pi s(C-2\pi n)]^2}. \tag{33}$$

This result shows that the effect of disorder in the RWP is to modify the intensity of different branches without any broadening. Observe that the satellites correspond to constructive interference of coherent phasons with $Q_p=2\pi s/\tau$. We can conclude that if phason disorder is small, the response is coherent as explained in Appendix B. Figure 3 is the graphical representation of Eq. (33). Observe that the FC branches are still present, but with different intensity. This is due to the fact that the satellites of a given branch coincide exactly with the positions of other branches. This fact has the effect of diminishing the amplitude difference between consecutive n branches. If one compares Fig. 1(b) with Fig. 3, one notices that the latter is the FC spectrum, but the branches with higher n are more visible.

C. Real-space random phason

Finally, one can introduce phason disorder in the FC by choosing randomly a bond and exchanging it with the next one (flip-flop). The equations to solve are the same as those of the last section, except that R_m in Eq. (28) can be either zero or one, instead of having a flat distribution. For a given pair of sites m and m' the phase in $F_2(m,m')$ could be either 0, $\pm(L-S)$, or $\pm 2(L-S)$, depending on the nature of the pair of sites. These phases can be found for all the possible situations, and are shown in Table I.

For example, there is a probability $(1-\rho)^2$ that none of the extreme sites m and m' are chosen for a flip, where ρ is the density of phasons (see Appendix B). The situation in which only one of the extreme sites is chosen for a flip with probability $\rho(1-\rho)$ could result in a phase change of C, or in no phase change at all, if the chosen site produces no

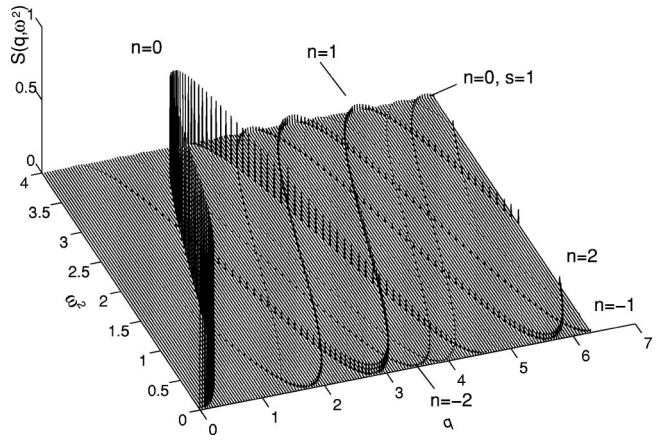

FIG. 3. Dynamical structure factor $S(q,\omega^2)$ for a FC with random window phasons, when the amplitude of the random variable is one, which corresponds to a maximum density ρ_{max}.

TABLE I. Possible phase factors for the RP. The blanks in the m and m' columns mean either LL, LS, or SL indistinctly.

R_m	$R_{m'}$	m	m'	$\Delta(m)-\Delta(m')$
1	1	LL	LL	0
		LS	LS	
		SL	SL	
		LL	SL	$+(L-S)$
		LS	LL	
		LL	LS	$-(L-S)$
		SL	LL	
		LS	SL	$+2(L-S)$
		SL	LS	$-2(L-S)$
0	1		LL	0
			SL	$+(L-S)$
			LS	$-(L-S)$
1	0	LL		0
		SL		$+(L-S)$
		LS		$-(L-S)$
0	0			0

difference with the exchange. Following this procedure and collecting terms, one finally gets

$$F_2(m,m')=(1-\rho)^2+2\rho(1-\rho)[P_{LL}+(P_{LS}+P_{SL})\cos C] + \rho^2[w(LS,SL)+w(SL,SL)+w(LL,LL) + 2\{w(LL,SL)+w(LS,LL)\}\cos C + 2w(LS,SL)\cos 2C], \quad (34)$$

where $P_{LL}=1/\tau^2$ and $P_{SL}=P_{LS}=1/\tau^3$ are the bond pair probabilities in the FC. This expression depends on m and m' only via the terms multiplying ρ^2 through the factors $w(m=A,m'=B)$, where $A,B=LL,LS,SL$. These factors should be understood as conditioned probabilities in chains of length $l=|m-m'|$.

If ρ is small, the fluctuations are bounded, and the pair distribution can be written as $w(A,B)=P_AP_B$. Observe that the expression in this approximation is separable on the variables m and m', and if one continues the convolution procedure, as in the previous cases, one finds a Fibonacci response reduced by a factor $(1-\rho)^2$, together with satellites responses with intensities depending on ρ, without broadening. This is due to the fact that we have neglected correlations, and single isolated phasons cannot modify the distances between sites by more than $2(L-S)$ at any distance.

It is certainly true, although highly improbable, that one can obtain large sequences of L bonds by just performing flip-flops. This would represent a high-density problem, in which our approximation breaks down. Therefore, we should study the high-density limit, when the fluctuations are unbounded.

Let us start by remembering the expression for the structure factor in the case when each atomic position is modified by random variables R_m and R'_m. For fixed values of the random variables (a given realization of disorder), one has

$$S(q,\omega^2)=\frac{\pi\eta(\omega^2)}{N}\sum_{m,m'=-\infty}^{\infty}e^{i\gamma(m-m')}e^{-iC(R_m-R'_m)} \times e^{iC(\{m/\tau+R_m\}-\{m/\tau+R'_m\})}. \quad (35)$$

Observe that $\{m/\tau+R_m\}$ is still periodic and that Eq. (35) only depends on $l=m-m'$ and the random variable $\chi_l=R_m-R'_m$. Therefore, one can perform the summations as in the FC case, and perform an average over the realizations of disorder,

$$S(q,\omega^2)=4\pi\eta(\omega^2)\sin^2\left(\frac{q(L-S)}{2}\right) \times\sum_{l,n=-\infty}^{\infty}\left[\frac{1}{[q(L-S)-2\pi n]^2}\right] \times e^{i(\gamma-2\pi n/\tau)l}\langle e^{-i[q(L-S)-2\pi n]\chi_l}\rangle. \quad (36)$$

In the high-density limit one should find the probability distribution for χ_l considering the probability of having a displacement χ_l in a random walk with two kinds of steps, L or S, and a fixed number of steps l. This is a binomial distribution, and the central limit theorem asserts that this tends to a Gaussian distribution $\Omega(\chi_l)$ with a zero mean,

$$\Omega(\chi_l)=\frac{1}{\sqrt{2\pi lp(1-p)}}\int_{-\infty}^{\infty}e^{-\chi_l^2/2lp(1-p)}d\chi_l. \quad (37)$$

Therefore,

$$\langle e^{-i[q(L-S)-2\pi n]\chi_l}\rangle=\int_{-\infty}^{\infty}e^{i[q(L-S)-2\pi n]\chi_l}\Omega(\chi_l)d\chi_l =e^{-[q(L-S)-2\pi n]^2/2\tau^3 l}. \quad (38)$$

The last step in Eq. (38) follows because the probability of performing a step of length S is $p=1/\tau^2$.

Thus, the final result is obtained by convoluting again, which means that each peak of the perfect FC presents a Lorentzian broadening due to disorder,

$$\langle S(q,\omega^2)\rangle=4\sin^2\left(\frac{q(L-S)}{2}\right)\sum_{n=-\infty}^{\infty}\left[\frac{1}{[q(L-S)-2\pi n]^2}\right]\frac{[q(L-S)-2\pi n]^2/2\tau^3}{\{[q(L-S)-2\pi n]^2/2\tau^3\}^2+[\omega^2-\omega^2(q\overline{\lambda}+2\pi n/\tau)]^2}. \quad (39)$$

The spectrum is very much broadened, since the width depends on $[q(L-S)-2\pi n]^2$, as measured in some experiments,[25] and suggested theoretically before.[26] Obviously, a reasonable case of random phason disorder should be a combination of the two limits, that is, a spectrum with δ functions centered in the FC lines, without broadening, and a small broadened part due to diffused scattering from the large fluctuations. A good model for this situation should be obtained by starting with Eq. (34), where ρ should be understood as the density of phasons, and introducing expressions like Eq. (37) for the conditioned probabilities multiplying the factor ρ^2. The result for this combined effect is

$$\langle S(q,\omega^2)\rangle_T=\left[(1-\rho)^2+\frac{2\rho(1-\rho)}{\tau^3}(\tau+2\cos C)\right] \times S_{Fib}(q,\omega^2)+\left[\frac{\rho}{\tau^3}(\tau+2\cos C)\right]^2 \times S_{diff}(q,\omega^2), \quad (40)$$

where $S_{diff}(q,\omega^2)$ is given by Eq. (39). Figure 4 shows only this broadened part of $S(q,\omega^2)_T$, calculated from Eq. (39). The reason to show only this part is because the unbroadened part dominates and it would be difficult to illustrate the

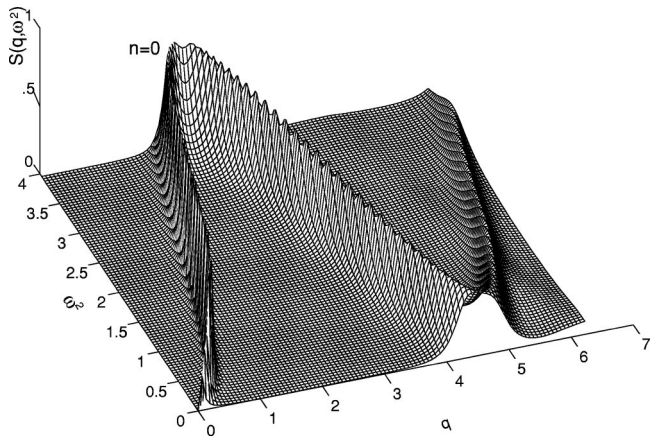

FIG. 4. Diffused part of the dynamical structure factor $S(q,\omega^2)$ for a FC with randomization in real space. The phason density has been taken to be $\rho=0.3\approx\rho_{max}=1/\tau^3$.

marked dependence of the broadening with q. For acoustic modes, the response of the $n=0$ branch is similar to the FC, with an increasing broadening as q grows. However, the other branches are faint in this region of q, because their centers of minimal broadening occur at very large values of q. This result could be used to compare with the spectra obtained from real quasicrystals with phason disorder, since this is the only case in which coherency is lost. It is worthwhile pointing out that the broadening is Lorentzian, despite the fact that the disorder follows a Gaussian distribution.

V. DISCUSSION AND CONCLUSIONS

In Fig. 5 we show a comparison for fixed $\omega^2=2$, between the FC and the three different types of phasons. The FC branch $n=0$ crosses the axis three times in the interval $q\in[0,2\pi]$. This feature is preserved in all cases for low q.

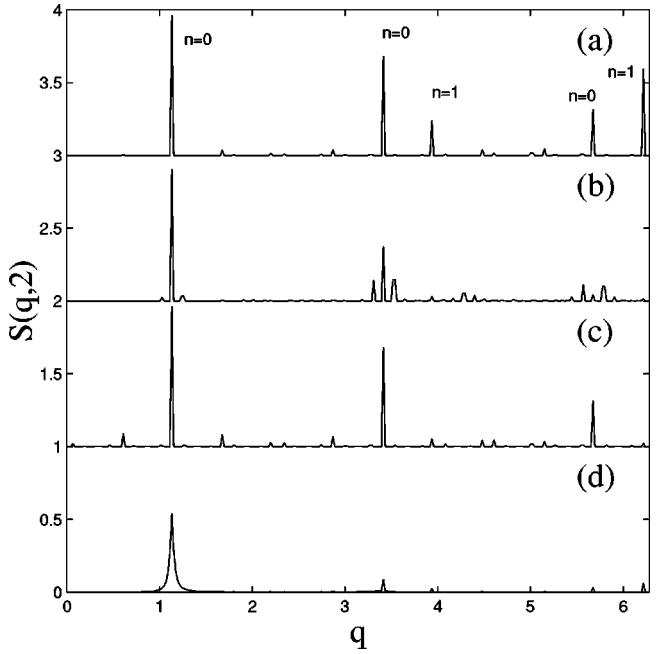

FIG. 5. Comparison of $S(q,\omega^2)$ between the FC and chains with the three sorts of phasons at a constant frequency $\omega^2=2$. (a) Perfect FC, (b) FC with CP, (c) FC with RWP, (d) FC with RP.

However, for larger q there are noticeable differences. The coherent phasons [Fig. 5(b)] present satellites associated with each FC peak. Their oscillator strength is taken from the main branches, for instance, in the figure it is clear that the intensity of branch $n=0$ decreases more rapidly with q. The RWP [Fig. 5(c)] can be considered as a special case of CP, when the satellites coincide with the main branches; as a result the spectrum presents the same FC peaks, but with very much modified intensities. The RP [Fig. 5(d)] was calculated with Eq. (40) for a density of phasons of $\sim 30\%$. Observe that in this case, the broadening for high q washes out all the FC branches. Of all the three cases of phason disorder, the only one that produces new peaks is the CP, since one is introducing a further periodicity in the chain. Strictly speaking none of the peaks are new; because the spectrum is dense they merely become more apparent with disorder.

An important conclusion of this work is that broadening is impossible to be produced with coherent phasons. It can be said that coherent phasons do not produce broadening because the structure of the FC in the hyperspace is somewhat preserved, the changes due to a coherent phason field are only in the relative intensities of the FC lines. The only way to produce broadening is to allow for unbounded fluctuations, when there is a Lorentzian q dependent broadening. Our results agree with physical intuition, since long wavelengths are not sensitive to the microscopical quasicrystalline disorder.

By looking at all our expressions for $S(q,\omega^2)$ we realize that the quantities $2\pi(n/\tau)/\overline{\lambda}=Q^{\parallel}$, and $q(L-S)-2\pi n=Q^{\perp}W_0$ are always appearing where $q=Q^{\parallel}$ because of the δ function. These quantities are known to be the components of the reciprocal lattice vector for the quasicrystal.[27] It is known that the diffraction pattern in quasicrystals[28] presents peaks whose positions are given by $Q^{\parallel}$ and their intensities, or oscillator strengths, depend on $Q^{\perp}$, in agreement with our expressions.

In the case of RP disorder, the dispersion corresponding to $n=0$ is practically the only one that survives, because the difference in $Q^{\perp}$ between the $n=0$ and the $n=1$ branches is large for a q value between zero and 2π. We conclude that the presence of broadening in the experiment, on top of the usual thermal broadening, is proof of the absence of a coherent phason field in real quasicrystals. On the other hand, the presence of satellites seems to be a signature of some coherency of phason disorder.[29]

Summarizing, we have found expressions for $S(q,\omega^2)$ for a simple dynamical model in which all the restoring forces and masses are the same. This allows us to isolate the effect of the defects in the structure from other complexities and also allows us to obtain simple expressions for $S(q,\omega^2)$ in a FC and a FC with phason disorder. In the perfect FC, $S(q,\omega^2)$ consists of a dense set of cosine branches with different phases, modulated by a q-dependent factor. For acoustic modes it was predicted that the FC looks similar to a simple linear chain with an average spacing between sites.

The FC with phasons was produced in three different ways, either by varying the window acceptance function $[W(m,n)]$ in the hyperspace construction, with a periodic function, or with a random variable, or by randomly producing exchange of sites in real space. The results show that

even a random-bounded displacement of a window function in the hyperspace produces coherency in real space.

The effect of a coherent phason is always reflected in $S(q,\omega^2)$ by giving well-defined satellites of the FC's most prominent branches when Q_p is small. The positions of the satellites depend on the period of the coherent phason. Even in the case of randomly varying the acceptance function (RWP), this coherency is preserved because mistakes are made only in certain sites of the chain. However, a RP is distinguishable from the other cases because the response is washed out for large values of $Q^{\perp}W_0 = q(L-S) - 2\pi n$.

Despite the extreme simplicity of the model, we have showed some fundamental features of the dynamics of a QP lattice. Our results agree with physical intuition, although they are not expected to be quantitatively correct when regarding a real system. However, we still expect our conclusions to be valid when considering lattices of higher dimension and more realistic Hamiltonians.

ACKNOWLEDGMENTS

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APPENDIX A: THE MOMENTS OF $S(q,\omega^2)$ IN A FC

The moments of $S(q,\omega^2)$ for the FC can be calculated in two ways: either by a direct application of the analytical expression for the dynamical structure factor [cf. Eq. (13)], or by obtaining the statistical distribution of bond configurations in the FC. In this appendix, we use both methods in order to verify the results obtained with Eq. (13).

We start with the latter method, which consists of a direct application of the general formula for $S(q,\omega^2)$ [cf. Eq. (4)], and thus, is valid for any kind of chain. By definition, the nth moment is

$$\begin{aligned}\langle \omega^{2n}(q)\rangle &= \frac{1}{N}\sum_{m,m'} e^{iq(x_m - x'_m)} \sum_k e^{ik(m-m')} \\ &\quad \times \int \omega^{2n}\delta(\omega^2-\omega_k^2)\,d\omega^2 \\ &= \frac{1}{N}\sum_{m,m'} e^{iq(x_m-x'_m)} I_n ,\end{aligned} \tag{A1}$$

where the first integrals (I_0, I_1, and I_2) are

$$I_0 = \sum_k e^{ik(x_m - x'_m)} = \delta_{m,m'} , \tag{A2}$$

$$\begin{aligned}I_1 &= 2J\sum_k e^{ik(x_m-x'_m)}(1-\cos k) \\ &= 2J\left(\delta_{m,m'} - \frac{1}{2}(\delta_{m,m'+1}+\delta_{m,m'-1})\right),\end{aligned} \tag{A3}$$

$$\begin{aligned}I_2 &= 4J^2\sum_k e^{ik(x_m-x'_m)}(1-2\cos k+\cos^2 k) \\ &= 4J^2\left(\frac{3}{2}\delta_{m,m'} - (\delta_{m,m'+1}+\delta_{m,m'-1}) \right. \\ &\quad \left. + \frac{1}{4}(\delta_{m,m'+2}+\delta_{m,m'-2})\right).\end{aligned} \tag{A4}$$

Now, the moments are given by the statistics of each bond configuration in the lattice. The zeroth moment only gives the correct normalization condition,

$$\langle \omega^0(q)\rangle = 1. \tag{A5}$$

The first moment depends on the statistical distribution of the distance between first neighbors, since

$$\begin{aligned}\langle \omega^2(q)\rangle &= 2J\left(1 - \frac{1}{N}\sum_m (1-\cos qL_m)\right) \\ &= 2J(1-\langle \cos qL_m\rangle),\end{aligned} \tag{A6}$$

where L_m is the distance between two contiguous sites in the lattice. In a FC, L_m can take the values L or S, with probabilities $1/\tau$ and $1/\tau^2$, respectively. Thus,

$$\langle \omega^2(q)\rangle = 2J\left(1 - \frac{1}{\tau}\cos qL - \frac{1}{\tau^2}\cos qS\right). \tag{A7}$$

In the acoustic limit ($q \approx 0$), we obtain

$$\langle \omega^2(q)\rangle = Jq^2\left(\frac{L^2}{\tau} + \frac{S^2}{\tau^2}\right). \tag{A8}$$

This value is always higher than $\overline{\lambda^2}$. As we show below, the difference between the coefficient of q^2 and $\overline{\lambda^2}$ arises from the contribution of all the modes with n different from zero in Eq. (13).

The width of the spectrum is

$$\Delta = \frac{\langle \omega^4\rangle - \langle \omega^2\rangle^2}{\langle \omega^2\rangle}, \tag{A9}$$

where the second moment is

$$\langle \omega^4(q)\rangle = 4J^2\left(\frac{3}{2} - 2\langle \cos(qL_m)\rangle - \frac{1}{2}\langle \cos q(L_1+L_2)\rangle\right), \tag{A10}$$

and L_1+L_2 is the distance between second neighbors. In the FC, L_1+L_2 is either $S+L$ or $L+L$, with probabilities $2/\tau^2$ and $1/\tau^3$, respectively. For acoustic modes,

$$\langle \omega^4(q)\rangle = \frac{2J^2q^2}{\tau^2}(L-S)^2. \tag{A11}$$

Thus, we obtain in the limit $q \to 0$,

$$\Delta = \frac{2J(L-S)^2}{\tau L^2 + S^2}, \tag{A12}$$

which is *not* zero, unless $L = S$.

Another method to obtain the moments is by taking the analytical expression for $S(q,\omega^2)$ [Eq. (13)]. The first moment is calculated with Eq. (14), resulting in

$$\langle\omega^2(q)\rangle = 4\sin^2\left(\frac{q(L-S)}{2}\right) \times \sum_{n=-\infty}^{\infty} \frac{2J[1-\cos(q\bar{\lambda}-2\pi n/\tau)]}{[q(L-S)+2\pi n]^2}. \quad \text{(A13)}$$

Using a Taylor expansion for small q,

$$\langle\omega^2(q)\rangle \approx Jq^2\left(\bar{\lambda^2}+\frac{(L-S)^2}{\pi^2}\sum_{n=1}^{\infty}\left[\frac{1}{n^2}-\frac{\cos(2\pi n/\tau)}{n^2}\right]\right), \quad \text{(A14)}$$

and summing up over n, the final expression is

$$\langle\omega^2(q)\rangle = Jq^2\left(\bar{\lambda^2}+\frac{(L-S)^2}{\tau^3}\right) = Jq^2\left(\frac{L^2}{\tau}+\frac{S^2}{\tau^2}\right), \quad \text{(A15)}$$

which agrees with the result obtained before using the first equation. We clearly see that the $n=0$ mode contributes as a periodic lattice with a velocity of sound given by $\sqrt{J\bar{\lambda}}$. However, there is a finite contribution for all the other modes with $n\neq 0$. The sum of all these contributions is exactly $(L-S)^2/\tau^3$.

APPENDIX B: DENSITY OF PHASONS

Now we discuss how to define the density of phasons (ρ) in each of the cases that are treated in the paper. It could be thought that this quantity is a measure of disorder, but it is not clear yet how ρ depends on the way the defects are produced. We begin by studying the CP case, where Eq. (17) states that the non-flip-flop condition at a given site m $[\Delta(m)=0]$ implies that

$$\left\{\frac{m}{\tau}+A\sin(mQ_pa+\alpha)\right\} = \left\{\frac{m}{\tau}\right\}+A\sin(mQ_pa+\alpha). \quad \text{(B1)}$$

By taking the integer part of the last equation and using that $\lfloor\{z\}\rfloor=0$, the condition for not having a defect is reduced to

$$\left\lfloor\left\{\frac{m}{\tau}\right\}+A\sin(mQ_pa+\alpha)\right\rfloor = 0, \quad \text{(B2)}$$

and analogously, the condition for obtaining a flip-flop at site m is

$$\left\lfloor\left\{\frac{m}{\tau}\right\}+\sin(mQ_pa+\alpha)\right\rfloor = \pm 1, \quad \text{(B3)}$$

which gives $\Delta(m)=\pm(L-S)$.

The density of phasons is defined as the sum over all flip-flops, divided by the total number of sites (N),

$$\rho = \frac{1}{N}\sum_{m=1}^{N}\left|\left\lfloor\left\{\frac{m}{\tau}\right\}+A\sin(mQ_pa+\alpha)\right\rfloor\right|. \quad \text{(B4)}$$

The flip-flops are produced in regions where $\{m/\tau\}\approx 1$. Now, since the function $\{z\}$ covers the interval $[0,1)$ in a dense and uniform way,[11] for long wavelengths ρ grows linearly with A. The phase α can change the average number of phasons, since for some α, the maximum of the sine function can coincide with the point where $\{m/\tau\}\approx 1$.

For the RWP case, the analysis developed for CP density might be applied. Thus,

$$\rho = \frac{1}{N}\sum_{m=1}^{N}\left|\left\lfloor\left\{\frac{m}{\tau}\right\}+R_m\right\rfloor\right|. \quad \text{(B5)}$$

Since R_m is uniformly distributed, the maximum probability for a phason is obtained when $\{m/\tau\}$ is nearly one, i.e., if m is of the form $z\approx\tau s$, where s is an integer. This condition shows that the most probable sites for obtaining phasons are separated by periods proportional to Fibonacci numbers. Then, the distance between flip-flops is given by FC's of lower generations.

In the RP case, despite the fact that the defects are produced at random, the process in the FC is not uncorrelated, as we shall show below. There are sites that do not produce a phason when interchanging sites (for instance, a pair LL). Furthermore, the final configuration depends on the path followed, because a phason could be healed if a site is chosen an even number of times. Therefore, a Monte Carlo-like procedure is correlated and the density of phasons is not necessarily proportional to the number of steps in the randomization process. To be specific, take the sequence $(LSLLSLSLLSLLSL)$, and do all the possible flip-flops in a sequence from left to right. The resulting chain is $(SLLSLSLLSLLSLL)$, which is the same as the original one, except for the ends.

If one repeats the same procedure for an infinite chain, the result is a translation of the original one with no changes, despite the infinite number of steps. Therefore, the number of flips-flops is not necessarily equal to the number of phasons produced. A possible definition for the density is obtained by comparing many times the randomized chain with a FC displaced one site in each comparison. In each of these comparisons, a different number of phasons is obtained. Therefore, we define the number of phasons of a chain as the minimum of these numbers. If x_i^R are the positions of the atoms in the randomized chain and x_i are the positions in the perfect chain, then

$$\rho = \min\left(\sum_{t,i=-\infty}^{\infty}|x_i^R-x_{i-t}|\right), \quad \text{(B6)}$$

where i is a site index and t is a site translation.

An estimation of the number of phasons as a function of the number of steps (n) can be obtained by calculating the probability of making a phason on one site after n steps of randomization, and then multiplying it by the number of sites in which a phason could be made. This number is N/τ, if we assume that in each step of randomization the number of sites in which a phason can be done does not diminish very much. This is an approximation since in each randomization new configurations of SS and LL appear in which a phason cannot be done.

Following this idea, we choose a site to perform a flip-flop in the chain. There are $2N/\tau^2$ sites suitable to do this, since the proportion between the total number of bonds and S bonds is τ^2. Each S bond may be exchanged with either of its

two L neighbors. The probability of choosing this site only one time for making a phason after n steps of randomization is $np(1-p)^{n-1}$, where $p=\tau^2/2N$. If we choose the same site two times, a phason is created the first time and annihilated in the next one. This argument is true for any even number of times. Now, if a site is chosen three times, a phason is obtained with probability $C_3^n p^3(1-p)^{n-3}$, where C_i^n denotes the combinations of n objects in i sites. The process is repeated and it is seen that phasons can be created only if the site is chosen an odd number of times. Then, the density of phasons is

$$\rho(n) \approx \frac{1}{\tau}[np(1-p)^{n-1} + C_3^n p^3(1-p)^{n-3} + C_5^n p^5(1-p)^{n-5} + \cdots] = \frac{1}{\tau^2}\left(1-\left(1-\frac{\tau^2}{N}\right)^n\right). \quad \text{(B7)}$$

A computer simulation of an RP was performed using an ensemble of 100 randomized chains of 100 sites each. In Fig. 6 the calculated $\rho(n)$ is shown, the values of $\rho(n)$ obtained using Eq. (B6), with the minimization process described above, correspond to the lower curve in the figure. Without the minimization process [$t=0$ in Eq. (B6)], the density obtained is always higher, which corresponds to the upper curve in Fig. 6. These results are compared with the analytical prediction given by Eq. (B7). Observe that the theoretical prediction works fine only for small n, because in this case neglecting real-space correlations is a good approximation. Notice that there is an asymptotic behavior for $n\to\infty$, a situation in which the number of created phasons is equal to the number of annihilated ones, the density being $\rho_{max}=1/\tau^3$.

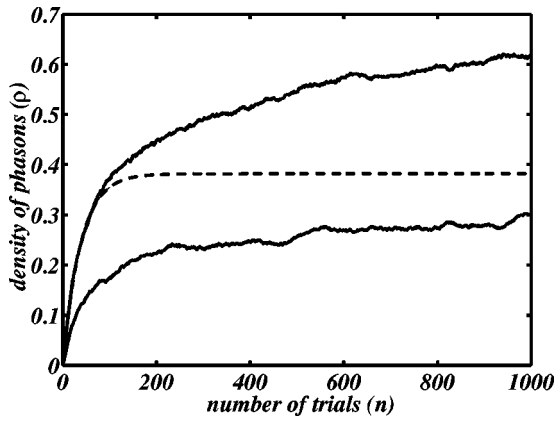

FIG. 6. Calculation of the density (ρ) of real-space random phasons (RP) as a function of the number of Monte Carlo steps in a chain of 100 sites and averaging over an ensemble of 100 chains. The upper and lower continuous lines are the results of comparing the disordered chain with the original FC and with a FC whose origin gives the minimum number of defects, respectively. The dashed line is Eq. (B7), which lies in between these two results, as expected.

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