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ENERGY DYNAMICS IN A ONE-DIMENSIONAL APERIODIC ANHARMONIC LATTICE

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We study the nature of collective excitations in classical anharmonic lattices with aperiodic and pseudo-random harmonic spring constants. The aperiodicity was introduced in the harmonic potential by using a sinusoidal function whose phase varies as a power-law, $\phi \propto n^{\nu}$, where n labels the positions along the chain. In the absence of anharmonicity, we numerically demonstrate the existence of extended states and energy propagation for a sufficiently large degree of aperiodicity. Calculations were done by using the transfer matrix formalism (TMF), exact diagonalization and numerical solution of the Hamilton's equations. When nonlinearity is switched on, we numerically obtain a rich framework involving stable and unstable solitons.

Keywords: Nonlinearity; localization; solitons.

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1. Introduction

The localization of vibrational modes in random low-dimensional lattices is a quite general well-known issue with direct connections with Anderson localization theory for electrons.[1] Within the context of disordered harmonic chains, it was shown that there are about $\sqrt{N}$ low-frequency nonlocalized modes, where N is the number of masses in the chain.[1–3] Besides these low-frequency extended modes, short- or long-range correlations in the disorder distribution (spring constants or masses) lead to a new set of nonscattered modes.[4–8] Another interesting class of low-dimensional classical systems that displays high-frequency extended modes is composed by aperiodic harmonic systems. The role played by a specific aperiodic structure on the localization properties and/or energy transport in harmonic chains was studied in Refs. 9−11. In Ref. 11, two-dimensional harmonic lattices with masses following a distribution similar to that used in Refs. 12, 13 were studied using the transfer matrix method and direct solution of Hamilton's equations. It was numerically demonstrated that, due to the aperiodicity of the mass array, low-frequency extended vibrational modes can exist. The dynamics of an initially localized excitation has shown that, associated with the emergence of a phase of delocalized modes, a ballistic regime takes place. One of the properties of harmonic chains is the possibility to decompose the heat flux into the sum of independent contributions associated to the various eigenmodes.[14]

Although the degree of nonperiodicity is a key ingredient to understand the behavior of the thermal conductivity in classical lattices, the presence of nonlinearity also plays an important role on the energy flux.[15–30] In fact, the heat flux in low-dimensional classical anharmonic systems has been targeted by recent intense investigations.[15–27] The main issue here is whether these systems display finite thermal conductivity in the thermodynamic limit, a question that remains controversial.[17–23] One of the most known properties of nonlinear chains is the presence of kink-soliton solutions. It is well-known that the solitonic effect is damped by the presence of disorder. In fact, the scattering of solitons by disorder can be measured through the reduction of localized energy within the localization region, the time dependent acceleration of energy flux and long-time behavior of the diffusion coefficient. The competition between disorder and anharmonicity was studied in detail in Ref. 29. It was numerically demonstrated that, while anharmonicity promotes energy transport through ultrasonic solitons, disorder decreases the propagation due to the well-known Anderson localization.[29] The soliton dynamics in a Toda lattice with randomly distributed masses was studied in Ref. 30. The disordered Toda's model consists of a one-dimensional chain of disordered masses where each mass interacts with the others through a nearest-neighbor exponential potential. By using the inverse scattering transform, it was derived the effective equations for the decay of the soliton amplitude that take into account radiative losses. It was shown that the soliton energy decays as $\propto N^{3/2}$ for small-amplitude solitons and $\propto \exp(2N)$ for large-amplitude solitons.[30] Moreover, in a more general context, the presence of nonlinearity in nonperiodic solids represents a general challenge with a rich framework of nonintuitive phenomena.

In this work, we focus on the effect of anharmonicity on nonperiodic classical lattices. We study numerically the competition between aperiodic harmonic spring constants and nonlinear quartic potentials. To produce an aperiodic distribution of spring constants, it was used a sinusoidal function whose phase varies as a power-law, $\phi \propto n^{\nu}$, where n labels the positions along the chain. In the absence of anharmonic couplings, we numerically demonstrate the existence of extended states and energy propagation for a sufficiently large degree of aperiodicity. Calculations were done by using the transfer matrix formalism (TMF), exact diagonalization and numerical solution of the Hamilton's equations. By using numerical solutions of Hamilton's equations, we consider the effect of nonlinear terms in the Hamiltonian. Our results indicate the presence of stable soliton solutions when $\nu < 1$. In the pseudo-random limit $\nu > 1$, our calculations indicated the presence of unstable solitonic behavior. The energy flux in both regimes are considered.

2. Model and Formalism

We consider a one-dimensional anharmonic lattice of N masses, for which the classical Hamiltonian can be written as $H = \sum_n h_n(t)$, where the energy $h_n(t)$ of the mass at site (n) is given by

$$h_n(t) = \frac{P_n^2}{2m_n} + \frac{1}{4}[\beta_n(Q_{n+1} - Q_n)^2 + \beta_{n-1}(Q_n - Q_{n-1})^2] + \frac{\eta}{8}[(Q_{n+1} - Q_n)^4 + (Q_n - Q_{n-1})^4]. \tag{1}$$

Here P_n and Q_n define the momentum and displacement of the mass at site (n). Here we will consider all masses identical with $m_n = 1$. The harmonic elastic constants β_n will be considered to follow a deterministic rule given by

$$\beta_n = V_0 + [\cos(\alpha n^\nu)], \tag{2}$$

with α being an arbitrary rational number ($\alpha = 0.1$ here) and ν being a tunable parameter.[12,13] From this sinusoidal form, one can control the degree of aperiodicity in the sequence of hopping couplings. In what follows, $V_0 = 2$ will be taken in order to avoid negative or null elastic constants. The main motivation for considering this specific model we study in this manuscript is that from the sinusoidal form we can control the degree of aperiodicity in the harmonic forces. Within the context of on-site diagonal terms, the regime $\nu > 1$ was called “pseudo-random” at reference.[31] It was shown that one electron eigenstates become localized in the presence of an aperiodic potential on this regime. In our calculations, we assume there is no disorder in the anharmonic contribution. Following Wagner and co-workers[29] $\eta \approx 10$ may be physically reasonable to simulate realistic nonlinear effects. For $\beta_n = \text{const.}$ the Eq. (1) is the Fermi–Pasta–Ulam (FPU) β model.[32] The Hamilton's equations were solved by using the exact eigenmodes of the harmonic system as the initial condition. The dynamics of energy was studied in detail and the manifestation of solitons was pointed out. Besides having shown the complexity of nonlinear systems, the (FPU) β model also emphasized the value of computer simulations in the context of theoretical physics.[29,32]

3. Numerical Calculation: Harmonic Limit ($\eta = 0$)

In the absence of nonlinearity ($\eta = 0$), we inserted a solution of the form $Q_n = q_n \exp(i\omega t)$ and the displacement of the masses is written as[29]

$$\beta_n q_{n+1} + \beta_{n-1} q_{n-1} = (\beta_n + \beta_{n-1} - \omega^2) q_n. \tag{3}$$

Equation (3) can be solved using the (TMF) that is obtained by using a matrix recursive reformulation of the displacement equation. The matricial equation is

$$\begin{pmatrix} q_{n+1} \\ q_n \end{pmatrix} = \begin{pmatrix} \dfrac{-\omega^2 + \beta_n + \beta_{n-1}}{\beta_n} & -\dfrac{\beta_{n-1}}{\beta_n} \\ 1 & 0 \end{pmatrix} \begin{pmatrix} q_n \\ q_{n-1} \end{pmatrix} = T_n \begin{pmatrix} q_n \\ q_{n-1} \end{pmatrix}. \tag{4}$$

The wave amplitude of the complete one-dimensional system is given by the product of the transfer matrices $M_N = \prod_{n=1}^{N} T_n$. The logarithm of the smallest eigenvalue of the limiting matrix $\Gamma = \lim_{N\to\infty}(M_N^\dagger Q_N)^{1/2N}$ defines the Lyapunov exponent (inverse of localization length $\lambda = 1/\Gamma$). Further details about the computation of this parameter can be found in Refs. 33, 34.[a] The nature of the vibrational modes can also be investigated by computing the participation ratio ξ, since it displays a linear dependence on the chain size for extended states and is finite for exponentially localized ones. ξ is defined as[6,8,10] $\xi(\omega) = (\sum_{n=1}^{N} q_n^2)/(\sum_{n=1}^{N} q_n^4)$, where the displacements q_n are those associated with an eigenmodes ω of a chain of N masses and are obtained by direct diagonalization of the $N \times N$ secular matrix A defined by $A_{n,n} = (\beta_n + \beta_{n-1})$, $A_{n,n+1} = A_{n+1,n} = \beta_n$, and all other $A_{n,m} = 0$.[6,8,10] In our calculations we compute the average participation ratio defined as $\langle\xi\rangle = \frac{1}{N_f}\sum_{\omega=0.5}^{\omega=1.5}\xi(\omega)$ where N_f is the number of acoustic modes within the interval $[0.5, 1.5]$. Let us stress that the bottom of the band was avoided in this sum because the participation ratio of a low-frequency acoustic wave is large even in the presence of strong uncorrelated disorder.[28,29] We are interested in the existence of extended states apart the bottom of the band. Therefore, $\langle\xi\rangle/N$ does not depend on N for extended modes and goes to zero for localized ones. In addition, we study the dynamics of an initially localized energy pulse by solving numerically the Hamilton's equations.[6,8,10]

$$\begin{aligned} \dot{P}_n(t) &= -\frac{\partial H}{\partial Q_n} = \beta_n(Q_{n+1} - Q_n) - \beta_{n-1}(Q_n - Q_{n-1}), \\ \dot{Q}_n(t) &= \frac{\partial H}{\partial P_n} = P_n(t). \end{aligned} \tag{5}$$

By considering an initial excitation at the site n_0 at $t = 0$, we solve the differential equations for $P_n(t)$ and $Q_n(t)$ and compute the fraction of the total energy H at the site n $(f_n = h_n(t)/H)$. Therefore, we can define the following time dependent quantity $\Xi(t) = 1/(\sum_n^N f_n^2)$. The function Ξ measures the number of masses that participate of the energy transport. This function is similar to the participation number for electrons.[8] By considering a uniform energy packet spread on a pure harmonic chain with N masses, we have $f_n \approx 1/N$, it means, $\Xi \propto N$. Therefore we conclude that $\Xi(t) \propto t$ for the energy transport in a periodic harmonic chain.[6,10] Moreover, we can extract information about the range of eigenmodes that participate of the energy dynamics through the spectral analysis of the momentum around

[a] For a review see, e.g. Ref. 35.

the chain end. We compute the Fourier transform of the displacement of the mass at position nf ($A(\omega) = Q_{nf}(\omega)$). In our calculations $nf \approx 0.9N$. For transmitted vibrational modes, $A(\omega) > 0$ and goes to zero for filtered ones. We can obtain a similar trend through the numerical calculation of the Fourier transform of the fraction of the energy or momentum at mass nf ($f_{nf}(\omega)$ or $P_{nf}(\omega)$). When nonlinearity is turned on ($\eta \neq 0$), our goal is to understand the time evolution of originally localized excitations. Therefore, in the anharmonic limit, we will consider an initially localized impulse excitation (i.e. $P_n = \delta_{n,n_0}$ and $Q_n = 0$) and compute the spatial and temporal evolution of the energy inside the lattice. We will basically compute the amount of the total energy H at the site n ($h_n(t)$).

4. Numerical Calculation: Anharmonic Limit ($\eta \neq 0$)

In the presence of nonlinear terms (i.e. $\eta \neq 0$), our numerical formalism shall be based on the numerical solution of the nonlinear Hamilton's equation:

$$\begin{aligned} \dot{P}_n(t) &= \beta_n(Q_{n+1} - Q_n) - \beta_{n-1}(Q_n - Q_{n-1}) \\ &\quad + \eta[(Q_{n+1} - Q_n)^3 + (Q_n - Q_{n-1})^3], \\ \dot{Q}_n(t) &= P_n(t). \end{aligned} \tag{6}$$

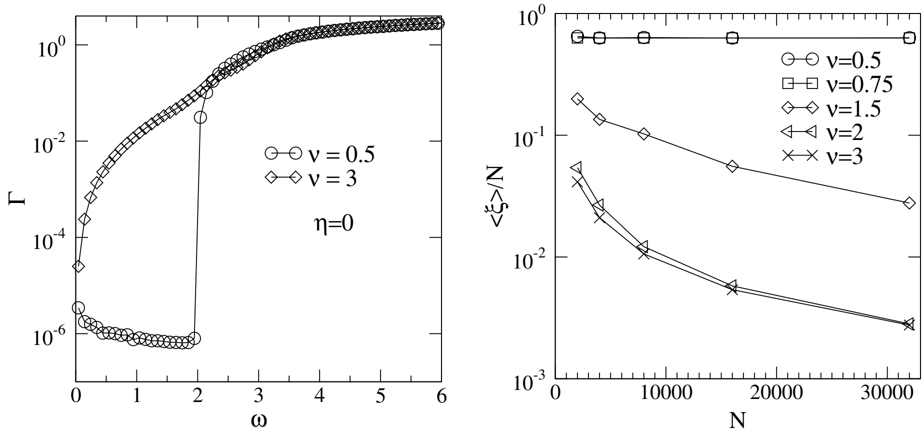
The spatial and temporal evolution of the energy of lattice vibrations will be described by the energy $h_n(t)$ of the mass at site (n). The spatio-temporal shape of $h_n(t)$ was previously used, both from the analytical and numerical point of view, to detect the presence of solitonic waves in anharmonic periodic and disordered systems.[28,29]

5. Results

Lyapunov exponents of the eigenmodes were computed by using the transfer-matrix technique for a long chain with $N \approx 5 \times 10^6$. In this method, the self-averaging effect automatically takes care of statistical fluctuations. We estimate and control these fluctuations following the deviation of the calculated eigenvalues of two adjacent iterations. The finally obtained data have statistical errors less than 5%. Eigenmodes and eigenfrequencies were obtained by direct diagonalization of the $N \times N$ secular matrix A with N up to 32 000. In addition we solved the Hamilton's equations for Q_n and P_n by using a standard fourth-order Runge−Kutta method[36,37] with time step $dt \approx 10^{-3}$. Energy conservation was used to check the numerical accuracy at every time step.

5.1. *Harmonic limit*

In Fig. 1 we plot the Lyapunov exponent γ as a function of frequency ω for $\nu = 0.5$, $\nu = 3$ and $\eta = 0$. For $\nu = 3$ the Lyapunov exponent vanishes close to the low-frequency region ($\omega \rightarrow 0$) and it is finite in the high-frequency region, as expected for low-dimensional nonperiodic harmonic systems. For $\nu = 0.5$ the Lyapunov is of the



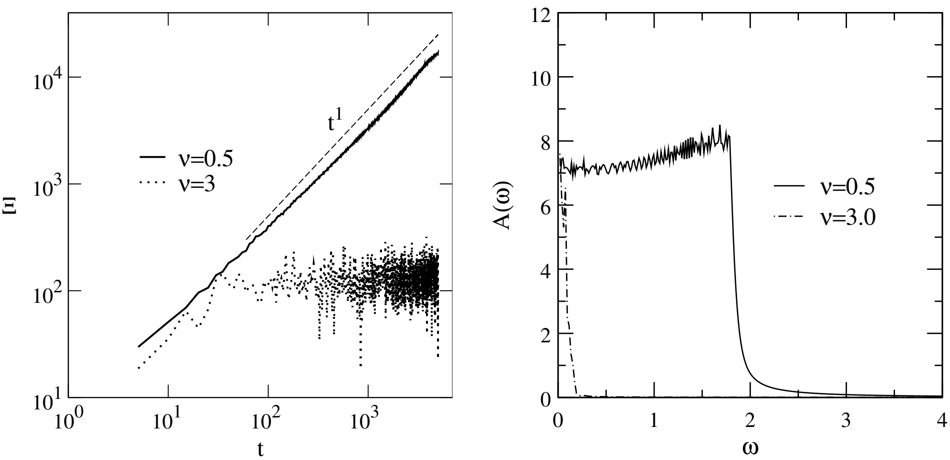
(a) (b)

Fig. 1. (a) Lyapunov exponent γ as a function of frequency ω for $\nu = 0.5$, $\nu = 3$ and $\eta = 0$. For $\nu = 3$ the Lyapunov exponent vanishes close to the low-frequency region ($\omega \to 0$) and it is finite in the high-frequency region, as expected for low-dimensional nonperiodic harmonic systems. For $\nu = 0.5$ the Lyapunov exponent is about $1/N$ for $\omega < \omega_c \approx 2$. Therefore, our calculations indicate that in the absence of anharmonic terms, this aperiodic lattice can support extended vibrational modes. (b) Scaled average participation number $\langle \xi \rangle / N$ versus the number of masses N. As it can be noticed, we obtain extended states with $\langle \xi \rangle \propto N$ for $\nu < 1$.

order of $1/N$ for $\omega < \omega_c \approx 2$. Therefore, our calculations indicate that in the absence of anharmonic terms, this aperiodic lattice can support extended vibrational modes. In Fig. 1(b) we show, in the absence of nonlinearity, the scaled average participation number $\langle \xi \rangle / N$ versus the number of masses N for $\nu = 0.5$ up to $\nu = 3$. We numerically demonstrate that there are extended vibrational modes with a divergent participation number ($\xi \propto N$) for $\nu < 1$. In Fig. 2(a) we plot the time-dependent participation function $\Xi(t)$ as a function of time for an aperiodic harmonic lattice with $\nu = 0.5$ (solid line), and $\nu = 3.0$ (dotted). The initial excitation was $P_n = \delta_{n,n_0}$ with $n_0 = N/2$ and $Q_n = 0$. For ν smaller than 1, a ballistic energy spread $\Xi \propto t^2$ was obtained. However, when the degree of aperiodicity exceeds 1 a localized energy transport takes place. In Fig. 2(b) we collect data from the spectral intensity of the mass displacement nf $(A(\omega) = Q_{nf}(\omega))$ as a function of frequency ω for $\nu = 0.5$, $\nu = 3$ and $\eta = 0$. For $\nu = 0.5$ all vibrational modes with $\omega > \omega_c$ decay, and the medium behaves as a filter to transmit only the modes below frequency $\omega_c \approx 2$. For $\nu = 3$, only the modes close to the low-frequency region ($\omega \to 0$) propagate along the chain.

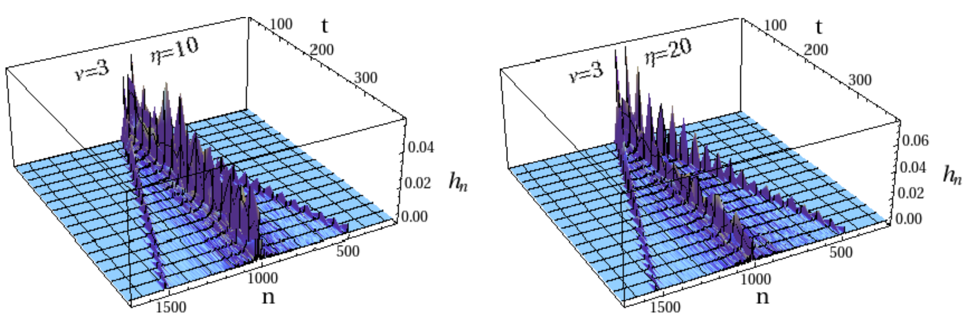
5.2. *Anharmonic regime*

We start considering the case of pseudo-random harmonic spring constants ($\nu > 1$) and anharmonic interaction $\eta = 10$ and 20 (see Fig. 3). The initial excitation was $P_n = \delta_{n,n_0}$ with $n_0 = N/2$ and $Q_n = 0$. We can see that both Anderson localization



(a) (b)

Fig. 2. (a) Time-dependent participation function $\Xi(t)$ as a function of time for an aperiodic harmonic lattice with $\nu = 0.5$ (solid line), and $\nu_y = 3.0$ (dotted line). For $\nu < 1$, a ballistic energy spread $\Xi \propto t^2$ was obtained. However, when the degree of aperiodicity exceeds 1 a localized energy transport takes place. (b) Spectral intensity of the displacement of the mass nf ($A(\omega) = Q_{nf}(\omega)$) as a function of frequency ω for $\nu = 0.5$, $\nu = 3$ and $\eta = 0$. For $\nu = 0.5$ all vibrational modes with $\omega > \omega_c$ decay, and the medium behaves as a filter to transmit only the modes below frequency $\omega_c \approx 2$. For $\nu = 3$, only the modes close to the low-frequency region ($\omega \to 0$) propagates along the chain.



(a) (b)

Fig. 3. (Color online) The amount of the total energy H at the site n ($h_n(t)$) for a pseudo-random anharmonic chain with $\nu = 3$ and $\eta = 10$ and 20. The initial excitation was $P_n = \delta_{n,n_0}$ with $n_0 = N/2$ and $Q_n = 0$. We can see that both Anderson localization and soliton-like solution for short times are present. For long time, a finite fraction of initial energy pulse remains trapped at the initial site n_0. The soliton-like modes that appear for initial times are not stable and disappear at long times.

and soliton-like solution for short times are present. For long times, a finite fraction of initial energy pulse remains trapped at the initial site n_0. We observe that the soliton-like modes appearing for initial times are not stable and disappear at long time. We can also see that the anharmonicity reduces the intensity of the energy

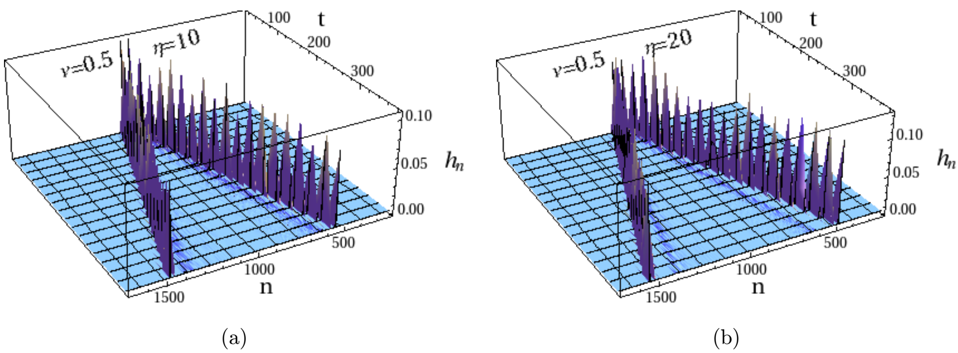


Fig. 4. (Color online) $h_n(t)$ times t and n for an aperiodic anharmonic chain with $\nu = 0.5$ and $\eta = 10$ and 20. The initial excitation was $P_n = \delta_{n,n_0}$ with $n_0 = N/2$ and $Q_n = 0$. Our results have shown that the initial excitation splits in two stable soliton modes that propagates along the chain.

trapped on the initial site. The results obtained for $\nu > 1$ are in perfect agreement with those obtained for disordered anharmonic chains.[29] In Fig. 4 we collect data of $h_n(t)$ times t and n for an aperiodic anharmonic chain with $\nu = 0.5$ and $\eta = 10$ and 20. We have used an initial impulse excitation located at site $n_0 = N/2$. Our results have shown that the initial excitation splits in two soliton-like modes that propagates along the chain. Within our numerical precision, the energy intensity of both soliton-like modes seems to remain constant. These results indicate that the energy dynamics found on this aperiodic chain signals the presence of stable soliton solutions. In addition we compute numerically the distance d_s between the solitons (see Fig. 5). Calculations were done for the same chain of Fig. 4. Our results indicate that the solitons display a ballistic dynamics with $d_s \propto t$. Due to the finite fraction of

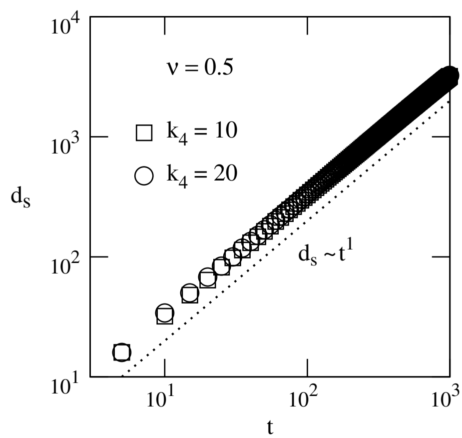
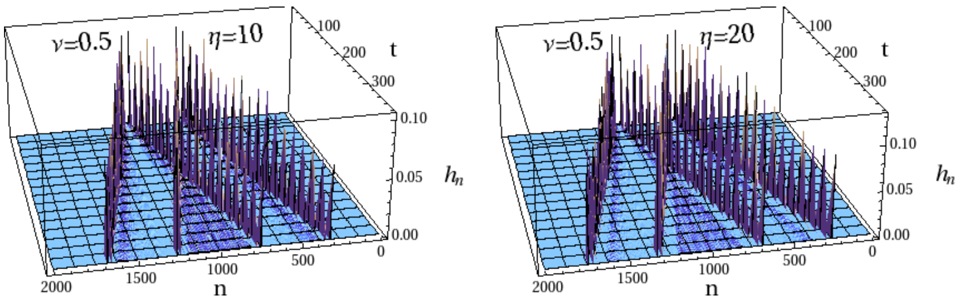


Fig. 5. The distance d_s between the solitons reveals the ballistic energy flux inside the anharmonic chain ($d_s \propto t$). Calculations were done for the same chain of Fig. 4.



(a) (b)

Fig. 6. (Color online) Numerical experiment of soliton collision. We solve the Hamilton equation with an initial excitation such that $P_n(t = 0)$ and $Q_n(t = 0)$ are null except $P_{N/4}(t = 0) = 1$ and $P_{3N/4}(t = 0) = 1$. The solitonic forms propagate from the initial points $N/4$ and $3N/4$ and collide without changing their shape, a clear signature of stable solitonic solutions.

energy that both solitons carry, the linear behavior of d_s indicate a ballistic flux of energy along the chain. Within the main literature of solitons it is well-known that solitary waves do not obey the principle of superposition, and instead of interacting through interference and simple addition, they collide in a nonlinear and complex manner.[29,32,38] In general lines, solitons collide with each other without change in their shapes. In Fig. 6 we analyze this specificity for the solitary waves found here. To promote the collision, we started with an initial excitation such that P_n and Q_n are null except $P_{N/4} = 1$ and $P_{3N/4} = 1$. Therefore we obtain the solitonic propagations from the initial points $N/4$ and $3N/4$ (see Fig. 6). We can see that the solitary waves found in our aperiodic FPU model displays also the most famous signature of stable soliton solution: collision without deformation.

6. Summary and Conclusions

In summary, we studied the effect of anharmonicity on nonperiodic classical lattices. We considered numerically a classical chain with aperiodic harmonic spring constants and nonlinear quartic potentials. To produce an aperiodic distribution of spring constants, it was used as sinusoidal function whose phase varies as a power-law, $\phi \propto n^\nu$, where n labels the positions along the chain. In the absence of anharmonic couplings, we numerically demonstrated the existence of extended states and energy propagation for large degrees of aperiodicity $\nu < 1$. For $\nu < 1$ the extended vibrational phase and also the ballistic energy dynamics can be understood following simple heuristic arguments. For large n, β_n is very slowly varying and can be regarded as a constant β' locally. In this case, the eigenmode equation becomes $q_{n+1} + q_{n-1} = (2 - \omega^2/\beta')q_n$. Therefore, for $\nu < 1$ and in the absence of anharmonic couplings the system shall behave as an ordered harmonic chain with extended vibrational modes and ballistic transport. We also considered the effect of nonlinear terms in the Hamiltonian. Our results indicated the presence of stable soliton solutions in the aperiodicity regime with $\nu < 1$. The stability of solitary waves found here was studied numerically following the amount of energy trapped and also considering the soliton−soliton collision behavior. Within our numerical precision, we found that the soliton waves found here can ballistically transport a finite fraction of the total energy and also collide without deterioration of their shape. In the pseudo-random limit $\nu > 1$, our calculations indicated the presence of unstable solitonic behavior. Our results on the existence of extended states and soliton like waves for $\nu < 1$, despite having been obtained here for the specific value of $\alpha = 0.1$, are also valid for other rational values of α.

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