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Anharmonic excitations in the FPU and FK models

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Abstract. The properties of vibrational localized (breathers) and traveling (anharmonic phonons) waves are discussed in an infinite, one-dimensional, monoatomic crystal for the Fermi-Pasta-Ulam and Frenkel-Kontorova models. The shooting and finite difference schemes have been implemented to reckon the displacement fields of breathers and anharmonic phonons, respectively. These tools provide localized and traveling waves proving to be indefinitely stable in simulations carried out by solving the equations of motion. The emphasis is laid on the role of the cubic and quartic terms of the anharmonic potential which turn out to oppose and to shore up the restoring force, respectively. The case of vibrational modes arising in an anharmonic crystal subject to a soft phonon induced instability is also addressed.

PACS. 63.20.Pw Localized modes – 63.20.Ry Anharmonic lattice modes

1 Introduction

The dynamics of anharmonic lattices has enjoyed a budding interest for the last decade because of its bearing on heat transport, energy relaxation towards thermal equilibrium and various structural or magnetic instabilities in solid matter including DNA [1–5]. Whereas the dynamics of perfectly periodic, harmonic crystals is completely accounted for by phonons, that of an anharmonic lattice comprises furthermore localized vibrations such as breathers [6] and three kinds of traveling waves, namely moving breathers [7], solitons [8,9] and time-periodic waves [3,10–12] which are the anharmonic counterpart of phonons.

Most of results regarding breathers have been obtained within the quasidiscreteness approach (QDA) [13] including the rotating wave approximation (RWA) [14] as a particular case and the uncoupled oscillator limit (UOL) [15,16]. In QDA and RWA the vibrational field of the breather is worked out from a truncated perturbation expansion. The results are believed to be reliable in case of weak anharmonicity. In UOL they are obtained by switching on continuously the coupling within a finite sequence of initially uncoupled oscillators. The continuation process is likely to break down for strong coupling. As the interatomic potential involves necessarily an on-site contribution, its harmonic limit cannot sustain any acoustic phonon branch due to the lack of continuous translational symmetry. Furthermore as UOL based calculations deal with a finite crystal, conspicuous finite-size effects have been reported [17]. Therefore simulations carried out by solving the equations of motion in large crystals with initial conditions inferred from QDA, RWA or UOL always produce vibrational fields decaying in the long term into phonon-like oscillating tails named as nanopterons [6] so that the existence of such excitations remains questionable.

Time-periodic traveling waves have been studied much less than breathers and solitons in anharmonic lattices. In the continuum limit the Korteweg-de Vries equation was shown [18] to sustain cnoidal waves. Such modes arise also in the integrable Toda model [19]. UOL has been applied to find anharmonic phonons by starting from a sequence of phase-shifted uncoupled oscillators [3,10]. They were seen to produce nanopterons in simulations as in the case of breathers. At last it is worth mentioning an attempt made in the Fermi-Pasta-Ulam and Lennard-Jones lattices that has provided accurate results [11] for nonlinear periodic waves in an infinite crystal.

Breathers and standing waves have been studied in infinite, anharmonic lattices by using the shooting method [12,20]. The successful treatment of the infinite system has been secured by taking advantage of the exact knowledge of the asymptotic behavior of the displacement field at infinite distances. The method will be extended here to the Fermi-Pasta-Ulam (FPU) potential including a cubic term in order to investigate how it conditions the existence of breathers. The shooting method will be applied also to the Frenkel-Kontorova (FK) potential to which a quartic term has been added because the latter shows up a prerequisite for breathers to arise similarly

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to what has already been shown for solitons [21]. The FPU [22] and FK [23] potentials have been extensively studied in various issues connected with non-linear phenomena, regarding in particular energy relaxation [24] in solids, solitons [9,25] and breathers [26]. The calculational scheme devised for solitons [21,27] and consisting of solving a non-linear differential equation involving advanced and retarded terms will be adapted, as already done by previous authors [11], to study the properties of anharmonic phonons in the FK model. The tools developed here have enabled us to investigate breathers and nonlinear periodic waves in presence of a soft phonon. Both localized and propagating modes of this work stand out as generic excitations in infinite, non-linear lattices, as far as they appear to be stable in simulations carried out by solving the equations of motion. Likewise they keep indefinitely the same profile without radiating phonons.

The outline is as follows: Sections 2 and 3 deal with the study of the FPU and FK models, respectively whereas Section 4 is concerned with the unstable crystal case.

2 FPU breathers

An infinite, monoatomic chain is considered. There is a single coordinate per atom u_i designating the displacement at site i with respect to equibrium. The atoms of mass unity are coupled through the FPU pair potential $W_1(u_i - u_{i+1})$ written as

$$W_1(x) = \frac{x^2}{2} + \lambda\frac{x^3}{3} + \frac{x^4}{4},$$

where $x_i = u_i - u_{i+1}$ and $\lambda \in \mathbb{R}$ is taken as a disposable parameter. As stressed elsewhere [21,27], the phonon dispersion associated with the harmonic limit of W_1 conditions strongly the properties of breathers

$$\omega_\phi(k) = \omega_M \sin\left(\frac{k}{2}\right), \tag{1}$$

where ω_ϕ and $k \in [0,\pi]$ stand for the acoustic phonon frequency and wave-vector, respectively, and $\omega_M = 2$ is the largest phonon frequency. The equations of motion read

$$\ddot{u}_i(t) = \frac{\mathrm{d}W_1}{\mathrm{d}x}(x_{i-1}) - \frac{\mathrm{d}W_1}{\mathrm{d}x}(x_i), \quad i \in \mathbb{Z}. \tag{2}$$

A breather-like solution of equation (2) comprises the infinite sequence $\{u_i(t)\}$, characterised by

$$u_i(t+T) = u_i(t), \quad u_{i\to\pm\infty}(t) \to u_{\pm\infty}, \quad \forall t, \tag{3}$$

where T is the vibrational period and $u_{\pm\infty} \in \mathbb{R}$ are constant. The vibrational field decays exponentially [20] at infinite distances

$$\begin{aligned}&(u_{i\to\pm\infty}(t) - u_{\pm\infty}) \propto r^{\pm i}\sin(\omega t), \quad \forall t,\\ &\omega^2 = 2 - r - r^{-1},\end{aligned} \tag{4}$$

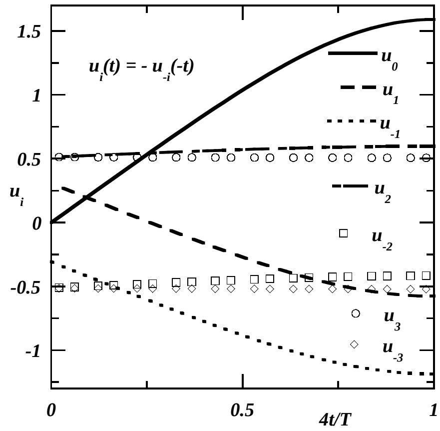

Fig. 1. Plots of $\{u_{i=-3,..3}(t)\}$ for an odd breather sustained by W_1 at $\lambda = 1$ and $\omega = 2\omega_M = 4$.

where $|r| < 1$ and $\omega = \frac{2\pi}{T}$ is the vibrational frequency. It ensues from equation (4) that $\omega > \omega_M$.

We focus on breathers having all atoms vibrating in phase, albeit with different amplitudes, because this is consistent with the time-behavior of $u_{i\to\pm\infty}(t)$ implied by equation (4). Hence all velocities $\dot{u}_i(t)$ should vanish simultaneously. Then as neither t nor $\dot{u}_i$ appear explicitly in equation (2), it comes $u_i(t) = u_i(\frac{T}{2} - t)$, if $\dot{u}_i(\frac{T}{4}) = 0, \forall i$. Therefore it suffices to confine oneself to the range $t \in [-\frac{T}{4}, \frac{T}{4}]$. In an infinite lattice, vibrational patterns such that $u_i(t) = -u_{-i}(\pm t)$ and $u_i(t) = -u_{-i-1}(\pm t)$, referred [14,28] to as odd and even, are consistent with equation (2) for any pair potential being a function of $u_i - u_{i+1}$. Besides the solution of equation (2) depends on a single parameter ω.

The shooting method applied to solve equation (2) has been detailed elsewhere [12,20]. It amounts to solving a system of transcendental equations over $t \in \left[0, \frac{T}{4}\right]$ for the unknown initial displacements and velocities. In the odd case they read $\{u_{i=1,..n=4}(0), \dot{u}_{i=0,..n}(0)\}$ and fulfil the boundary conditions

$$\begin{aligned}&u_0(0) = 0, \quad u_{i>0}(0) = -u_{-i}(0),\\ &\dot{u}_{i>0}(0) = \dot{u}_{-i}(0), \quad \dot{u}_i\left(\tfrac{T}{4}\right) = 0,\\ &\frac{u_{\pm n\pm 1}(t) - u_{\pm\infty}}{u_{\pm n}(t) - u_{\pm\infty}} = r(\omega),\end{aligned} \tag{5}$$

where $n = 4$ proves big enough so that $|u_{\pm n}(t) - u_{\pm\infty}| \ll 1$ and $r(\omega)$ is provided by equations (4). In the even case equation (2) have been solved for the unknowns $\{u_{i=0,..n=4}(0), \dot{u}_{i=0,..n}(0)\}$ under the conditions

$$u_{-1}(0) = -u_0(0), \dot{u}_i\left(\pm\frac{T}{4}\right) = 0, \frac{u_{n+1}(t) - u_\infty}{u_n(t) - u_\infty} = r(\omega).$$

The data pictured in Figures 1, 2 have been obtained by continuation from $\lambda = 0$ while increasing λ stepwise up to the desired $\lambda \neq 0$ value as explained elsewhere [12]. The cubic term $\lambda\frac{x^3}{3}$ in W_1 brings a contribution even *versus* x and thence counteracts the restoring force which is itself odd. Accordingly too strong a cubic term is believed to prevent any breather from arising in Toda's model [29,28].

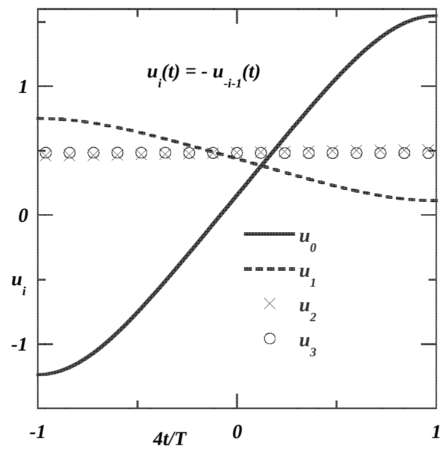

Fig. 2. Plots of $\{u_{i=0,..3}(t)\}$ for an even breather sustained by W_1 at $\lambda = 1$ and $\omega = 2\omega_M = 4$.

This statement has been confirmed here by monitoring the solution $\{u_i(t)\}$ *versus* growing λ at fixed ω. Defining the vibrational amplitude on site i, as $a_i = |u_i(\frac{T}{4}) - u_i(0)|$ and $a_i = |u_i(\frac{T}{4}) - u_i(-\frac{T}{4})|$ for the odd and even cases respectively, the a_i's have been plotted *versus* λ in Figures 3, 4 for two ω values. The breather disappears suddenly for $|\lambda| > \lambda_M$ with $\lambda_M = 2.1, 3.6$ in Figures 3 and 4 respectively, as the Newton method fails to find any solution for the unknowns in the vicinity of the assignment associated with λ_M. Most of realistic pairwise potentials (Toda, Born-Mayer-Coulomb, Lennard-Jones and Morse) display $\lambda < 0$ [29]. Nevertheless there is no difference at all between the $\lambda < 0$ and $\lambda > 0$ data in Figures 3, 4 because the λ dependence of W_1 entails that $u_i(\lambda, t)$ and $-u_i(-\lambda, t)$ are both solutions of equation (2).

As all $u_i(t)$'s have been worked out by solving directly equation (2), they turn out to be exact solutions of the equations of motion valid at any time so that every simulation carried out in an arbitrarily large FPU atomic chain with initial conditions given by $\{u_i(0), \dot{u}_i(0)\}$ remains indefinitely stable. It is then of interest to compare with the results supplied by other methods. It must be noticed first that UOL can by no means deal with the FPU model because it has an acoustic branch. Moreover the vibrational patterns obtained for breathers by QDA [13] and RWA [14,28] read

$$u_i(t) = \xi_i + \phi_i \cos(\omega t), \quad \phi_i \propto r^{|i|}$$

where $|r| < 1$. The QDA and RWA analyses suffer from two shortcomings. First the assumption $\xi_i = -\xi_{-i}, \quad \phi_i = \phi_{-i}$ made for the odd mode appears to be inconsistent with equation (2) for $\lambda \neq 0$. Furthermore there is the relationship [13]

$$\omega^2 = \omega_M^2 \left(1 + \frac{\log(|r|)^2}{8}\right),$$

which agrees with the exact result in equation (4) but for $\omega \to \omega_M^+$. This underscores a basic disagreement with the harmonic limit whenever the displacement becomes vanishingly small, *i.e.* at long distance from the center. It is thence concluded that QDA and RWA provide a useful approximation of an even breather only in a crystal of small size and for ω close to ω_M, which is confirmed by conspicuous nanopterons growing in simulations [14,28].

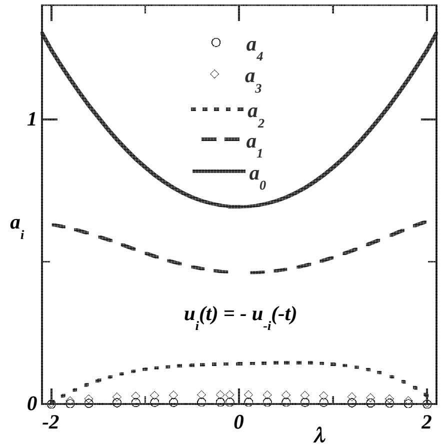

Fig. 3. Plots of $\{a_{i=0,..4}(\lambda)\}$ for an odd FPU breather at $\omega = 2.57$.

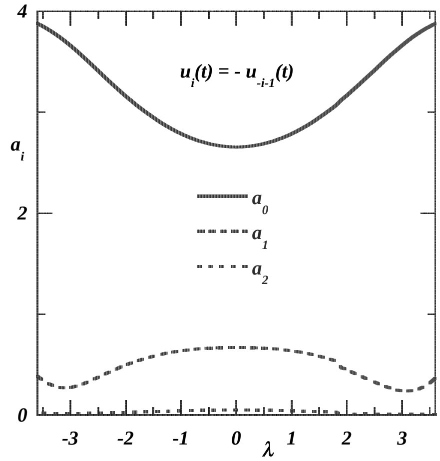

Fig. 4. Plots of $\{a_{i=0,..2}(\lambda)\}$ for an even FPU breather at $\omega = 4$.

3 FK breathers and nonlinear periodic waves

The pair potential has been chosen here to read

$$W_2(u_i, u_{i+1}) = \frac{(u_i - u_{i+1})^2 - \cos(u_i) - \cos(u_{i+1})}{2} + \lambda \frac{(u_i - u_{i+1})^4}{4},$$

where $\lambda \in \mathbb{R}$ is taken as a disposable parameter. Actually all previous authors have assumed $\lambda = 0$ but this case has been confirmed to sustain no soliton in a monoatomic lattice [21]. It will be shown here to sustain no breather and no anharmonic phonon either.

3.1 Breathers

Unlike W_1 the potential W_2 has no continuous translational symmetry. As its optical phonon and breather

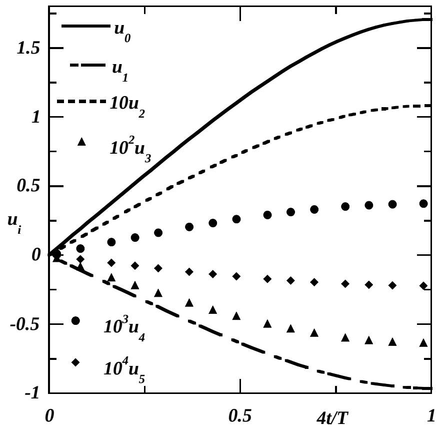

Fig. 5. Plots of $\{u_{i=0,..5}(t)\}$ for a breather sustained by W_2 at $\lambda = 1$ and $\omega = 4.47$.

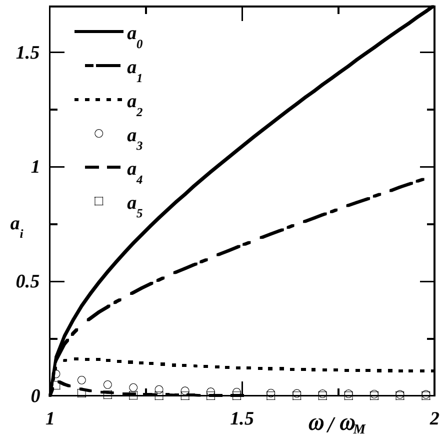

Fig. 6. Plots of $\{a_{i=0,..5} = |u_i(\frac{T}{4})|\}$ *versus* ω for a breather sustained by W_2 at $\lambda = 1$.

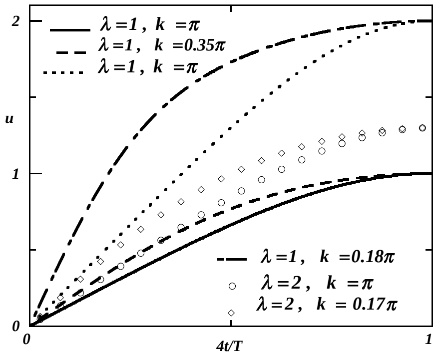

Fig. 7. Plots of $u(t)$ for nonlinear periodic waves sustained by W_2.

dispersion relations stem solely from the harmonic limit of W_2, they are independent of λ and read then

$$\omega_\phi^2(k) = 3 - 2\cos(k), \quad \omega^2 = 3 - r - r^{-1}. \tag{6}$$

Equations (6) imply for the phonon and breather frequencies that $\omega_\phi \in [\omega_m = 1, \omega_M = \sqrt{5}]$, $\omega \notin [\omega_m, \omega_M]$. No breather has been found in the lower gap $\omega < \omega_m$. This seems to stem from the infinite crystal size since breathers have been reported [16,17] to arise in the lower gap in UOL calculations which can cope only with finite lattices. The boundary conditions used in UOL which show up very different from those in equations (3) and UOL taking no account of the dispersion relations in equations (6) are likely to be responsible for the different results in UOL and in this work.

Breathers have then been searched in the upper gap $\omega > \omega_M$ as solutions of

$$\begin{aligned}\ddot{u}_i(t) = u_{i-1} + u_{i+1} - 2u_i - \sin(u_i) \\ +\lambda\left((u_{i-1} - u_i)^3 - (u_i - u_{i+1})^3\right),\end{aligned} \tag{7}$$

under the conditions in equations (3). Due to $W_2(u_i, u_{i+1}) = W_2(-u_i, -u_{i+1})$ a solution such that $u_i(t) = u_{-i}(t)$, $u_i(t) = -u_i(-t)$ is consistent with equations (7). Solving equations (7) while using the same method as for the FPU $\lambda = 0$ case yields the vibrational patterns $u_i(t)$ and amplitudes $a_i(= u_i(\frac{T}{4}))$ reported in Figures 5, 6. The breather and phonon frequencies are checked not to be degenerate as the breather displacement field vanishes allover the phonon frequency range.

A breather-like solution of equations (7) requires $\lambda \gtrsim 0.05$. It is noteworthy that the same minimum λ-value is needed for a soliton [21] to arise. This low value indicates how efficiently the quartic term contributes to building up a restoring force in both cases.

3.2 Nonlinear periodic waves

A nonlinear periodic wave of vibrational period T and phase velocity τ^{-1} (the lattice parameter is set equal to 1) is characterised in an infinite crystal by

$$u_{i\in\mathbb{Z}}(t + T) = u_i(t) \ , \ u_{i+1}(t) = u_i(t + \tau) \ , \ \forall \ t. \tag{8}$$

The wave-length l, wave-vector k and frequency ω fulfil $l\tau = T$ and $kl = \omega T = 2\pi$, which results in $k = \omega\tau$. Equation (8) implies $\tau \leq T$, which assigns the size of the one-dimensional Brillouin zone $k \in [0, 2\pi]$. A nonlinear periodic wave propagating in the infinite FK lattice is obtained as a solution of

$$\begin{aligned}\ddot{u}(t) = u(t-\tau) + u(t+\tau) - 2u(t) - \sin(u(t)) \\ +\lambda\left((u(t-\tau) - u(t))^3 - (u(t) - u(t+\tau))^3\right).\end{aligned} \tag{9}$$

A solution $u(t)$ such that $u(t) = -u(-t)$ is consistent with equation (9). Owing to $W_2(u_i, u_{i+1}) = W_2(-u_i, -u_{i+1})$ equation (9) will be solved under the boundary conditions

$$\begin{aligned} &t \in \left[0, \tfrac{T}{4}\right], && u(0) = 0, \\ &u(t < 0) = -u(-t), && u\left(t > \tfrac{T}{4}\right) = u\left(\tfrac{T}{2} - t\right). \end{aligned} \tag{10}$$

To solve equation (9) we proceed by combining the finite difference and Newton methods, as done elsewhere [11,12]. Accordingly the $u(t)$'s, reported in Figure 7, display the sine-wave shape, typical of $k \gtrsim \frac{\pi}{2}$ and the profile turns gradually into a square wave for $k \lesssim \frac{\pi}{2}$.

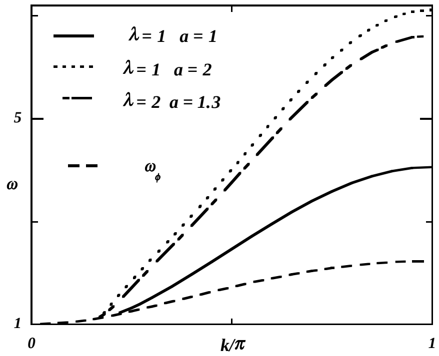

Fig. 8. Plots of (a, λ) dependent dispersion curves $\omega(k)$ for nonlinear periodic waves sustained by W_2.

λ dependent dispersion data $\omega(k)$ have been reported in Figure 8 throughout the Brillouin zone. As expected for anharmonic excitations, they depend also upon the amplitude $a = u(\frac{T}{4})$. There is no solution for $k \leq k_m \simeq 0.17$. This feature stands out prominently where dispersion data have been depicted and k_m corresponds to the crossing point of the dispersion curve of anharmonic phonons $\omega(k)$ with that of harmonic ones $\omega_\phi(k)$. k_m is found to depend weakly on λ. Thus the condition $\omega(k) > \omega_\phi(k)$ is fulfiled as for W_1 [12]. Besides as for breathers and solitons [21], there is no solution for $\lambda \lesssim 0.05$ and thence in the usual $\lambda = 0$ case either.

We have checked by simulation that the anharmonic phonon patterns $u(t)$, computed for W_2, prove to be exact and stable solutions of equation (9). To that end we integrate iteratively over $[0, \frac{T}{4}]$

$$\ddot{v}_j(t) = \frac{\mathrm{d}W}{\mathrm{d}x}(v_{j-1}(t-\tau) - v_j(t)) \\ - \frac{\mathrm{d}W}{\mathrm{d}x}(v_j(t) - v_{j-1}(t+\tau))$$

for the sequence of unknown functions $\{v_j(t)\}$ taking as initial conditions $v_j(0) = v_{j-1}(0), \dot{v}_j(0) = \dot{v}_{j-1}(0)$. The iteration is started for $v_1(t)$, taking $v_0(t) = u(t)$. Note that the hereabove equation is an ordinary differential equation with respect to the unknown $v_j(t)$ since the previously determined $v_{j-1}(t)$ plays the role of a known parameter field. As the iteration number j grows towards its final value $j_f \gg 1$, thus mimicking a propagation over a large crystal comprising j_f of unit-cells, the sequence $v_j(t)$ is found to converge towards $u(t)$ as far as the error $\max_{t\in[0,t_W]}(|v_j(t) - u(t)|)$ remains $< 10^{-6}$ for every $j = 1, ...j_f$. By contrast the Brillouin zone boundary anharmonic phonon calculated by RWA has been reported [28] to be unstable in simulations.

4 Unstable systems

It has been shown [30] how nonlinearity can restore dynamical stability into a macroscopic, mechanically unstable system. But a similar conclusion was also noticed to prevail in the microscopic realm, namely the solid phase of rare gases [31] since the second derivative of the interatomic potential is negative at the thermal equilibrium position. The numerical tools developed here permit to study this issue on the harmonically unstable FPU potential W_3

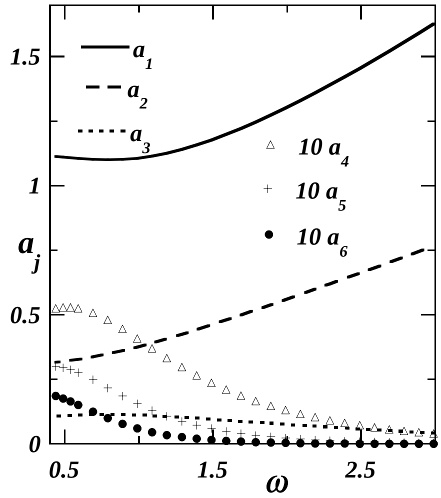

Fig. 9. Plots of $\{a_{i=1,..6} = |u_i(\frac{T}{4})|\}$ *versus* ω for breathers sustained by W_3.

$$W_3(x) = -\frac{x^2}{2} + \frac{x^4}{4},$$

where $x_i = u_i - u_{i+1}$. As the phonon branch of W_3 is of imaginary frequency ($\omega_\phi^2 = 2(\cos(k) - 1) < 0 \Rightarrow \omega_\phi \in \mathbb{C}$), it is said to be soft [4]. Because the associated static configuration is not stable, the solid should undergo a structural change. However it was noticed that the unstable equilibrium configuration regains some dynamical stability in spite of its soft phonon as far as breathers [20] and solitons [27] can still arise with infinite lifetimes. To get further insight we have worked out the breathers and anharmonic phonons of W_3.

The vibrational amplitudes calculated for breathers have been represented in Figure 9. The comparison with the results achieved for the stable FPU potential is illuminating. Whereas the amplitude field vanishes for $\omega < \omega_M$ in the stable case, it remains $\neq 0$ while ω can decrease practically down to nought for the unstable potential W_3. Actually $|\dot{u}_i(0)|$ decreases with ω and eventually $\dot{u}_i(t)$ changes sign several times over $[0, \frac{T}{4}]$ for $\omega \lesssim 0.5$ while the amplitudes a_i tend toward a limiting value $\neq 0$. These results are consistent with those obtained for anharmonic phonons which have been pictured in Figure 10. As a matter of fact the amplitude a decreases for every $k \gtrsim 0.3\pi$ with decreasing frequency ω down to a minimum value $a_m \simeq 0.7$, depending but weakly on k. Likewise for $\omega \to 0.3^+$ the initial velocity $|\dot{u}_i(0)|$ decreases so strongly that $u(t)$ is no longer monotonous over $[0, \frac{T}{4}]$. Furthermore no monotonous solution could be found for $k < 0.3\pi$. This can be understood by noticing that for $|u(t)| \ll 1$ the restoring force is determined by the harmonic limit of the potential. But as no restoring force is available in

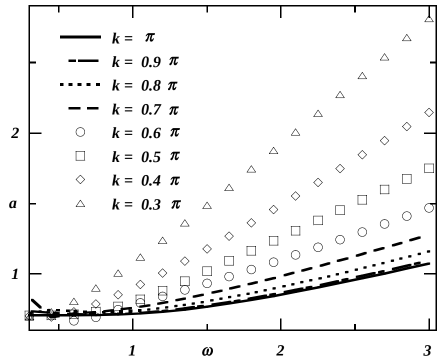

Fig. 10. Plots of $a(\omega)$ for nonlinear periodic waves sustained by W_3.

case of the unstable potential W_3 for small $|u(t)|$, a large enough amplitude a_m must be reached as a prerequisite for the anharmonic part of the potential to prevail over the harmonic one, thus giving rise to a finite restoring force. As this latter grows like $|u_i(t) - u_{i+1}(t)|$ which rises through a maximum at $k = \pi$ because of $u_i(t) = -u_{i+1}(t)$, the amplitude a tends to decrease with increasing k at fixed $\omega > 0.4$. By contrast with the stable case characterized by a phonon mediated minimum frequency so that $\omega(k) \geq \omega_\phi(k)$, there appears instead a soft phonon induced minimum amplitude a_m.

5 Conclusion

The effect of the cubic term on the existence of breathers has been investigated for the FPU potential. Too large a cubic term thwarts the arising of any breather because it cancels the restoring force. Inversely the quartic one contributes very efficiently to arousing such modes in the FK model. A minimum value of the quartic term is even required for every localized and nonlinear periodic wave, including solitons [21] to arise. Both breathers and anharmonic phonons of this work show up as exact solutions of the equations of motion in an infinite crystal. Finally it has been shown how a lattice driven to instability by a soft phonon may still sustain breathers and nonlinear periodic waves owing to anharmonicity. This statement conveys a particular significance for solid rare gases and could also cast some new light on the role of soft phonons in displacive transitions [4].

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