

Localized vibrations and standing waves in anharmonic lattices

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A sequence of nonlinear, time-dependent second order differential equations describing the motion of an infinite one-dimensional periodic lattice of arbitrary anharmonicity is considered. It is converted to an equivalent time-independent integrodifferential system, solved for all localized vibrational modes and standing waves. As illustrated by several examples this approach provides an accurate and efficient computational tool. An existence criterion to be satisfied by the potential is worked out for the considered vibrational modes. [S1063-651X(98)05001-6]

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I. INTRODUCTION

Unlike a harmonic, spatially periodic lattice, an anharmonic one can sustain breathers, that is, time-periodic, spatially localized vibrational modes even without broken periodicity. Breathers and standing waves experience currently a budding interest because they are believed to be instrumental in energy localization or equipartition and heat transfer [1–4]. The problem has been mostly tackled from a classical point of view but a quantum mechanical treatment has also been published [5].

As the KAM theorem is ill suited here because it produces many, rather than single, time period solutions, early attempts have resorted to approximate expansions [6,7]. Significant progress was achieved when the existence of breathers could be proved [8] in the uncoupled oscillator limit and the method was turned into a practical tool [9]. However, the problem of the existence of breathers remains unsolved in the general case, i.e., for plenty of models where no uncoupled oscillator limit is available.

The method presented here affords the determination of all breathers and standing waves for the most general anharmonic potential. The key point is to work out the restoring force at each site as a function of the displacement at this site only, which means that integrable modes of the anharmonic model are achieved in this way. Not only does this provide the frequency and the vibrational amplitude at every site for all integrable breathers and standing waves but it also enables us to work out an existence condition to be obeyed by the potential for these vibrational modes to arise.

II. THE METHOD

Let us consider an infinite chain of oscillators coupled by a pair potential $V = \sum_i W(u_i, u_{i+1})$ where u_i designates the displacement of site i and i takes all positive and negative integer values. $W(u_i, u_{i+1})$ is assumed to be symmetric with respect to u_i and u_{i+1} but is otherwise an arbitrary anharmonic function. The equations of motion read

$$\frac{d^2 u_i}{dt^2} = - \frac{\partial V}{\partial u_i} = f(u_{i-1}, u_i, u_{i+1}), \quad (1)$$

where t stands for time. Breathers and standing waves are characterized respectively by $u_i \rightarrow 0, \forall t$ for $i \rightarrow \infty$ and $u_{i+p}(t) = u_i(t), \forall i, t$ where the integer p denotes the wave-length. $W(u_i, u_{i+1})$ is chosen so that $f(x, y, z)$ has one equilibrium position at $x = y = z = 0$, which entails that $f(0, 0, 0) = 0$. The vibrational amplitude of oscillator i is assigned to $a_i^+ > 0, a_i^- < 0$, i.e., the velocity du_i/dt vanishes when u_i reaches the values a_i^\pm . This work is concerned with all vibrational modes, such that $u_i = 0, u_i = a_i^+$, and $u_i = a_i^-$ at $t = 0, t = T^+ > 0$ and $t = T^- < 0$ for every i , respectively. Equation (1) is time reversible, i.e., neither t nor du_i/dt appear explicitly therein. Consequently $u_i(2T^\pm - t) = u_i(t), \forall i, t$. It suffices thence to confine oneself to the range $T^- < t < T^+$. As the lattice is periodic, $f(x, y, z)$ does not exhibit any explicit i dependence. If $f(x, y, z)$ were linear in x, y, z , thanks to the Bloch-Floquet theorem the relation $u_{i+1}(t) = r u_i(t)$ would hold for any t where r is generally a complex number. Thus u_{i+1} can be expressed as a function of u_i by dropping any t dependence. The present work extends this result to the nonlinear case by looking for the unknown function g_i defined so that $u_{i+1} = g_i(u_i)$. The main difference with the linear case is that g_i depends explicitly on i , unlike the Bloch phase shift r , even though the lattice is periodic but the following analysis is valid for a nonperiodic lattice too. Having g_i at hand enables one to apply the kinetic energy theorem as in the single oscillator case and thus to express each velocity du_i/dt as a function of u_i only. Further integration yields time t as a function of u_i .

The function $u_i(t)$ is assumed to be monotonous versus t for every i inside the range $T^- < t < T^+$ so that each $u_i(t)$ can be inverted to give t versus u_i . This ensures that there is a one-to-one mapping $t \rightarrow u_i \rightarrow u_{i+1}$, which in turn warrants the existence of the functions g_i and g_i^{-1} defined as $u_{i+1}(t) = g_i(u_i(t))$ and $u_i(t) = g_i^{-1}(u_{i+1}(t))$. In addition, it is assumed that $u_i(t=0) = 0$ for every i , which entails by virtue of the definition of g_i that $g_i(0) = g_i^{-1}(0) = 0$. The system of Eqs. (1) is then recast into

$$\frac{d^2 u_i}{dt^2} = h_i(u_i), \quad h_i(x) = f(g_{i-1}^{-1}(x), x, g_i(x)). \quad (2)$$

TABLE I. Vibrational amplitudes a_i and initial velocities v_i for a breather sustained by potential W_1 .

i	0	1	2	3	4
a_i	8.6665	4.6692	0.39029	$2.2326E-4$	$4.1794E-14$
v_i	100	-53.876	4.5034	$-2.5762E-3$	$4.8225E-13$

The kinetic energy theorem is applied to Eq. (2) to yield the velocity du_i/dt :

$$\frac{du_i}{dt} = \pm \sqrt{e_i(u_i(t))}, \quad e_i(x) = (v_i)^2 + 2 \int_0^x h_i(y) dy, \quad (3)$$

where $v_i = (du_i/dt)(0)$ is the initial velocity of oscillator i . The differential equation in Eq. (3) is then integrated to give

$$t = \pm \int_0^{u_i} \frac{dx}{\sqrt{e_i(x)}}, \quad (4)$$

where $+$ or $-$ signs refer to $t > 0$ and $t < 0$, respectively. Since the system of Eqs. (1) is assumed to have a restoring force, there is a_i^\pm such that $e_i(a_i^\pm) = 0$. Moreover the following value is ascribed to T^\pm :

$$T^\pm = \int_0^{a_i^\pm} \frac{dx}{\sqrt{e_i(x)}}, \quad T = 2(T^+ - T^-), \quad (5)$$

where T stands for the time period. That the relations $e_i(a_i^\pm) = 0$ and $a_{i+1}^\pm = g_i(a_i^\pm)$ hold for every i ensures that the values of T^+, T^-, T can be calculated as well by selecting any i value in Eq. (5).

Applying Eq. (4) to i and $i+1$ gives

$$\int_0^{u_i} \frac{dx}{\sqrt{e_i(x)}} = \int_0^{u_{i+1}=g_i(u_i)} \frac{dx}{\sqrt{e_{i+1}(x)}}. \quad (6)$$

Differentiating Eq. (6) with respect to u_i results in

$$\frac{du_{i+1}}{du_i} = \frac{dg_i}{du_i} = \sqrt{\frac{e_{i+1}(u_{i+1})}{e_i(u_i)}}, \quad (7)$$

where $u_{i+1} = g_i(u_i)$. The system of Eqs. (7) is complemented by a matching equation taken at site $i=0$:

$$\frac{du_1}{du_0} = \frac{dg_0}{du_0} = \sqrt{\frac{e_1(u_1)}{e_0(u_0)}}, \quad h_0(x) = f(g_0(x), x, g_0(x)), \quad (8)$$

which ensures that $u_i(t) = u_{-i}(t)$ for every i and t . An additional matching equation is required in case of a standing wave:

$$\frac{du_n}{du_{n-1}} = \frac{dg_{n-1}}{du_{n-1}} = \sqrt{\frac{e_n(u_n)}{e_{n-1}(u_{n-1})}}, \quad h_n(x) = f(g_{n-1}^{-1}(x), x, g_n(x)), \quad (9)$$

where $u_{n-i}(t) = u_{n+i}(t)$, $g_n(x) = g_{n-1}^{-1}(x)$ or $u_{n-i}(t) = u_{n+i+1}(t)$, $g_n(x) = x$ for the wave-lengths $p=2n$ or $p=2n+1$, respectively. The system to be solved reads finally:

TABLE II. Vibrational amplitudes a_i and initial velocities v_i for a breather sustained by potential W_2 .

i	0	1	2	3	4
a_i	0.89182	0.60287	0.10361	$5.5163E-4$	$8.2879E-11$
v_i	0.94809	0.62966	0.10607	$5.5769E-4$	$8.3565E-11$

$$\frac{dg_i}{du_i} = \sqrt{\frac{e_{i+1} \circ g_i(u_i)}{e_i(u_i)}}, \quad i=0,1,\dots,n, \quad (10)$$

where for breathers n is assigned to so big a value that $a_n^+, |a_n^-|$ are both smaller than the required accuracy. The system of first order differential equations (10) is known to have a single solution $\{g_0, g_1, \dots, g_n\}$ if it is integrated with the initial condition $g_i(0) = 0$, $\forall i$. The solution depends implicitly on the set of initial velocities $\{v_{i=0,1,\dots,n}\}$ via the definition of $e_i(u_i)$ in Eqs. (3). Each v_i must be matched such that $du_i/dt(T^\pm) = 0$. Because of $du_i/dt(T^\pm) = \sqrt{e_i(a_i^\pm)}$ due to Eqs. (3),(5), the system of Eqs. (10) must be solved under the constraints $e_i(a_i^\pm) = 0$ and $a_{i+1}^\pm = g_i(a_i^\pm)$ for every i .

III. EXISTENCE CRITERION

The second derivative $[d^2 g_i/d(u_i)^2](0)$ is found to vanish for every i . Actually the lowest integer $j > 1$ such that $[d^j g_i/d(u_i)^j](0) \neq 0$ is equal to $k+2$ where k is the smallest integer such that $[\partial^k f/\partial(u)^k](0,0,0) \neq 0$ where $u=x,y$, or z and $f(x,y,z)$ is defined in Eq. (1). Consequently the exact identity $g_i(u_i) = dg_i/du_i(0)u_i$ in the case of a harmonic potential remains an excellent approximation for an anharmonic one too, even for $|u_i|$ as big as $|a_i^\pm|$. Likewise the relation $u_{i+1}(t) = g_i(u_i(t))$ implies that $r_i = (dg_i/du_i)(0) = [du_{i+1}/dt](0)/[du_i/dt](0)$. Thus the bigger the integer k , that is, the more anharmonic the potential is, regardless of its magnitude, the less the $g_i(x)$'s deviate from a linear law $g_i(x) = r_i x$, which ensures in particular $a_{i+1}^\pm \approx r_i a_i^\pm$. This feature enables us to recast the integrodifferential system of equations (10) into an equivalent system of ordinary equations:

$$\tilde{e}_i(v_i, a_i^\pm) = 0, \quad i=0,1,\dots,n, \quad (11)$$

where $\tilde{e}_i(v_i, a_i^\pm)$ is calculated by inserting $g_{i-1}^{-1}(x) = x/r_{i-1}$, $g_i(x) = r_i x$ into $e_i(x)$ in Eq. (3) and assuming $v_i = r_{i-1} v_{i-1}$, $a_i^\pm = r_{i-1} a_{i-1}^\pm$; the unknowns are a_0^\pm , $r_{i=0,1,\dots,n-1}$, and v_0 is the only disposable parameter.

Because we are interested in a localized mode, that is, $|a_i^\pm| < |a_{i-1}^\pm|$, Eqs. (11) are solved for a decreasing sequence $\{v_{i=0,1,\dots,n}\}$ such that $|v_i| < |v_{i-1}|$. We use a Newton's

TABLE III. Vibrational amplitudes a_i and initial velocities v_i for a breather sustained by potential W_3 .

i	0	1	2	3	4
a_i	1.8079	0.36855	$7.3857E-2$	$1.4796E-2$	$2.8544E-3$
v_i	3.0512	-0.68933	0.1398	$-2.8039E-2$	$5.4096E-3$

TABLE IV. Vibrational amplitudes a_i and initial velocities v_i for a $p=8$ standing wave sustained by potential W_3 .

i	0	1	2	3	4
a_i	1.808	0.36857	$7.3978E-2$	$1.5416E-2$	$5.9476E-3$
v_i	3.0513	-0.68937	0.14003	$-2.9213E-2$	$1.1272E-2$

method based iterative procedure starting with $n=2$ and increasing n repeatedly by 1 until n reaches the value requested by Eq. (10). The values resulting from step n are used as estimates to launch iteration $n+1$.

The property that $v_i \rightarrow 0$ for $i \rightarrow \infty$ implies that at large enough i one has $|r_i| \ll 1$ and the pair potential $W(u_{i-1}, u_i)$ can be approximated near $u_i=0$ by keeping only the leading power in its Taylor expansion. Writing then the equation of motion (1) results in

$$\begin{aligned} W(u_{i-1}, u_i) &= u_i^{m-l+1} u_{i-1}^l + u_i^l u_{i-1}^{m-l+1} \Rightarrow \frac{d^2 u_i}{dt^2} \\ &= h(u_i) = -(m+1) \frac{u_i^m}{r_{i-1}^l}, \end{aligned} \quad (12)$$

where we take $m-2l+1 \leq 0$, u_{i+1} has been neglected versus u_i because of $|r_i| \ll 1$, u_{i-1} has been replaced by u_i/r_{i-1} , and m is odd for Eq. (12) to secure a restoring force. Inserting this expression of $h(u_i)$ into that of \tilde{e}_i in Eq. (11) leads to

$$(a_i^+)^{m+1} = \frac{v_i^2 |r_{i-1}|^l}{2}, \quad |v_i| = \left| \frac{v_{i-1}^l}{c^2} \right|^{1/(l+1-m)}, \quad (13)$$

where $c = (\sqrt{8}/T) \int_0^1 dx / \sqrt{1-x^{m+1}}$. Within the limit $|r_i| \ll 1$ where Eqs. (13) are valid, the restoring force $h_i(x)$ in Eq. (12) is odd with respect to x , which implies that $a_i^+ = -a_i^-$. This latter result entails that $T^+ = -T^-$ in Eq. (5) and thence $T = 4T^+$ for every potential V , even though $W(u_{i-1}, u_i)$ is not even with respect to u_{i-1}, u_i . It is also inferred from Eqs. (12) and (13) that $T \rightarrow 0$ when $|v_0| \rightarrow \infty$, whereas T is known to be independent of v_0 for a harmonic potential.

Seeking a decreasing sequence $\{v_{i=0, \dots, n}\}$ requires that $m-l+1 > 0$ and $l > 0$. In addition, $l+1-m > 0$ is inferred from Eqs. (13). The above inequalities imply that $l=m$ and $l > 0$. Hence m being odd causes l to be odd too. The sought condition for the existence of integrable breathers and standing waves then states that *the Taylor expansion of the pair potential $W(u_{i-1}, u_i)$ must include the term $u_i u_{i-1}^l$ where the integer $l > 0$ is odd*. Furthermore v_i is seen in Eq. (13) to behave like v_{i-1}^l . Consequently a_i^\pm behaves also like $(a_{i-1}^\pm)^l$ and a_i^\pm decays exponentially towards zero versus $i \rightarrow \infty$ for $l=1$ and faster than exponentially for $l > 1$. Given v_0 , the above quoted necessary condition may prove not sufficient in two cases: (i) Equation (11) does not have any solution $\{v_{i=0, \dots, n}\}$, such that $|v_{i+1}| < |v_i|$; (ii) $2|\int_0^x h_i(y) dy|$ has an upper bound v_M^2 . Then there is no a_0^\pm solution of $e_0(a_0^\pm) = 0$ for $|v_0| > |v_M|$.

TABLE V. Vibrational amplitudes a_i and initial velocities v_i for a $p=9$ standing wave sustained by potential W_3 .

i	0	1	2	3	4
a_i	1.8079	0.36855	$7.3839E-2$	$1.4701E-2$	$2.3774E-3$
v_i	3.0512	-0.68932	0.13977	$-2.7858E-2$	$4.5055E-3$

These conclusions will be now illustrated by several examples. As shown in the discussion of Eq. (13), it is of little significance whether $W(u_{i-1}, u_i)$ is even or not. Therefore it has been assumed for simplicity to be even in all examples below, which implies that $a_i = a_i^+ = -a_i^-$. Given v_0 in each studied case, we have solved Eqs. (11) for the unknown amplitudes a_i and initial velocities $v_{i>0}$. In all but one case, the resulting $a_{i=0, \dots, n}, v_{i=1, \dots, n}$'s have been then inserted as estimates into a shooting procedure aimed at solving Eq. (1) and converging very fast because the solution of Eq. (11) was close to that of Eq. (10).

IV. THE $l > 1$ CASE

Results are given first for the $l=3$ potential $W_1(u_i, u_{i+1}) = -(u_i u_{i+1}^3 + u_i^3 u_{i+1})$. The linear approximation $g_i(x) \approx r_i x$ works so well that the final a_i, v_i values are available with an accuracy better than 10^{-11} right after solving Eqs. (11). Due to the steep decay of the vibrational amplitude observed for $l=3$ in agreement with Eq. (13), the results obtained for the breather and the standing waves turn out to differ only at the matching site $n=4$. Therefore the breather data, reported in Table I, are to be complemented by giving furthermore $a_4 = 8.3588E-14$, $4.1794E-14$ and $v_4 = 9.6449E-13$, $4.8225E-13$ for standing waves of wavelengths $p=8$ and $p=9$, respectively. The period T has been found equal to 0.45448.

In regard to the breather solution for the $l=3$ potential $W_2(u_i, u_{i+1}) = \sin(u_i) \sin^3(u_{i+1}) + \sin^3(u_i) \sin(u_{i+1})$, the results are gathered in Table II. The period has been found equal to 5.2045. As for W_1 , these results must be complemented by $a_4 = 1.6576E-10$, $8.2879E-11$ and $v_4 = 1.6713E-10$, $8.3565E-11$ for $p=8$ and $p=9$, respectively. But as $|\int_0^x h_i(y) dy|$ has an upper bound, there is no solution for $v_0 \geq 2$ consistent with the above reservation (ii). Previous methods [8,9] break down because no uncoupled oscillator limit can be defined for the potentials W_1, W_2 . As there is no harmonic ($l=1$) term in both potentials W_1, W_2 , this method proves well suited to studying soft phonon-induced dispersive transitions [10].

V. THE $l = 1$ CASE

This quasiharmonic case is the major concern of previous works [1,2,5,9] in that they rely heavily on the presence of

TABLE VI. Vibrational amplitudes a_i and initial velocities v_i for a breather sustained by potential FPU.

i	0	1	2	3	4
a_i	1.3133	0.56734	$7.4399E-2$	$1.2402E-2$	$2.0224E-3$
v_i	-1.9288	0.78584	0.14832	$2.5147E-2$	$4.1085E-3$

TABLE VII. Vibrational amplitudes a_i and initial velocities v_i for a $p=8$ standing wave sustained by potential FPU.

i	0	1	2	3	4
a_i	1.3133	0.56737	$7.4458E-2$	$1.276E-2$	$4.1614E-3$
v_i	-1.929	0.78596	0.14845	$2.5876E-2$	$8.4543E-3$

traveling phonons. A typical pair potential reads $W_3(u_i, u_{i+1}) = [\lambda(u_i - u_{i+1})^2 + u_i^4 + u_{i+1}^4]/4$. The calculation has been done with $\lambda = 1$. The period has been found to be equal to 3.3153. Consistent with Eq. (13), the vibrational amplitude decays more smoothly than in the $l=3$ case, the matching equation in Eq. (9) causes the results, given in Tables III, IV, and V for the breather and the $p=8$ and $p=9$ standing waves, respectively, to differ slightly from one another.

The presence of a traveling phonon band, typical of the harmonic limit, entails that the existence of a solution of Eqs. (11) is still more severely restricted than for the $l>1$ case. Calculating $e_0(x)$ and T for W_3 yields

$$v_0^2 = \lambda(1 + r_0)a_0^2 + a_0^4,$$

$$T = 4 \int_0^{a_0} \frac{dx}{\sqrt{(v_0^2 - \lambda(1 + r_0)x^2 - x^4)/2}}, \quad (14)$$

where $u_1 = -r_0 u_0$ and $0 < r_0 < 1$. Because $a_i \rightarrow 0$ for $i \rightarrow \infty$, the anharmonic term u_i^4 becomes negligible and the harmonic case is retrieved, i.e., $u_{i+1} = -r_\infty u_i$ where $0 < r_\infty < 1$ is independent of i . In addition r_∞ and T are related by

$$\left(\frac{2\pi}{T}\right)^2 = \frac{\lambda}{2} \left(r_\infty + \frac{1}{r_\infty} + 2 \right). \quad (15)$$

At large enough $|v_0|$, the a_0^4 term in Eq. (14) overwhelms the a_0^2 one, so that T increases if $|v_0|$ is taken to decrease at fixed λ . But Eq. (15) sets an upper bound $T \leq T_M = \pi\sqrt{2/\lambda}$ where $1/T_M$ is the highest traveling phonon frequency. Moreover, decreasing $|v_0|$ causes a_0 to decrease too and a_0^4 becomes eventually negligible versus a_0^2 , so that we are brought back to the harmonic case, which cannot sustain any solution of Eqs. (10). Finally for decreasing $|v_0|$, any localized mode, either breather or standing wave, is bound to vanish when T reaches its maximum value T_M , that is, no solution of Eqs. (10) can be degenerate with a traveling phonon. This explains why in a previous work [9] the search for a breather failed eventually while increasing T or equivalently decreasing $|v_0|$. Similarly if λ increases at fixed v_0 , the localized mode disappears too because the harmonic regime is restored at large enough λ .

TABLE VIII. Vibrational amplitudes a_i and initial velocities v_i for a $p=9$ standing wave sustained by potential FPU.

i	0	1	2	3	4
a_i	1.3133	0.56735	$7.441E-2$	$1.247E-2$	$2.4299E-3$
v_i	-1.9289	0.78587	0.14835	$2.5286E-2$	$4.9365E-3$

We focus finally on the Fermi-Pasta-Ulam (FPU) potential, which belongs in the $l=1$ type and has attracted recent interest [3,9]. In both works the traveling phonons available in the harmonic limit are used as a prerequisite to find breathers and standing waves and to analyze their stability. Therefore we turn to a peculiar version of the FPU potential $W_4(u_i, u_{i+1}) = -(u_i - u_{i+1})^2/2 + (u_i - u_{i+1})^4/4$, which cannot sustain any traveling phonon because there is no restoring force in the harmonic limit. Hence this case is well outside the purview of previous work [3,9]. Nevertheless because it satisfies the existence criterion quoted above, breathers and standing waves may still arise as induced by anharmonicity provided $|v_0|$ or equivalently a_0 is high enough so that W_4 gives rise to a finite restoring force and the period is smaller than some upper bound T_M . The period has been computed to be equal to 3.0919, 3.0917, 3.0918 and other results are reported in in Tables VI, VII, and VIII for the breather and the $p=8$ and $p=9$ standing waves, respectively. As in the W_1, W_2 cases, anharmonicity is seen to restore dynamical stability in an unstable lattice in the harmonic limit. This emphasizes the drawbacks of the stability analysis in the harmonic approximation [3,9,11].

VI. CONCLUSION

Regardless of whether the uncoupled oscillator limit is available or the crystal is stable in the harmonic limit, every anharmonic potential may sustain infinitely many breathers and standing waves provided it fulfills the above stated criterion with respect to l being odd. Each vibrational mode is completely determined by a single parameter, e.g., the initial velocity v_0 at an arbitrary site. In the $l=1$ case a vibrational mode may arise only for high enough $|v_0|$, which gives rise to a forbidden gap for $T > T_M$. These conclusions have been achieved by looking for the functions $g_i(x)$ such that $u_{i+1} = g_i(u_i)$ and $g_i(x)$ deviates very little from $g_i(x) = r_i x$ even though the potential is strongly anharmonic. This prominent property has enabled us to derive an existence criterion. In addition, it offers a practical tool to assess the integrable vibrational modes. As it sheds new light on the significance of lattice stability, it also paves the way for investigating anharmonicity driven instabilities [10].

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