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An algebraic approach to discrete breather construction

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Abstract

We obtain useful analytic discrete breather solutions in the form of elliptic functions for a large class of physically relevant nonlinear lattices through the application of an algebraic approach. The method we introduce is quite accurate and applies equally well to optic and acoustic chains. We present explicit results for ϕ^4 and Fermi–Pasta–Ulam lattices and discuss their implications to breather properties such as generation and mobility. The method is useful also in cases where no explicit analytic solutions can be obtained. In the context of the present approach, discrete breathers are shown to be localized cnoidal modes of nonlinear lattices.

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Ever since their introduction by Sievers and Takeno [1], intrinsic localized modes (ILMs) or discrete breathers (DBs) have been the object of intense scrutiny both from theoretical and experimental viewpoints [1–22]. Discrete breathers are time-periodic and space-localized modes of extended, typically translationally invariant systems, that are discrete and weakly coupled. In the frequency domain, DBs appear as impurity or gap states in nonallowed spectral regions of the standard linear modes. Many theoretical issues regarding DBs, such as rigorous mathematical existence [7, 8, 10], generation [1–13], mobility [5, 12], statistical dynamics [14, 15], etc have been addressed. Recent DB experimental observation in man-made systems [18–20], quasi-one-dimensional solids [21] and possibly in biological systems [22] has increased the interest for understanding their role in a large class of systems. Even though there has been tremendous progress in DB research during the last few years through the use of mathematical and numerical techniques, the lack of analytic DB solutions for physically relevant models has inhibited somehow large scale DB applications. The most widely used approaches for DB study are either approximate, relying on the rotating wave approximation (RWA) [1–3], or numerically exact, utilizing the DB construction from the anticontinuous limit [7, 8, 10, 11]. While the former approach is straightforward, it is nonetheless approximate and cumbersome in complicated models. The construction from the anticontinuous limit, on the other hand, while very general and numerically exact, relies on long, complex computations

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and, furthermore, does not furnish analytical functional forms for DBs. The algebraic method we present has the advantage of providing straightforwardly simple analytical DB solutions within the elliptic function subset of periodic functions, is both simpler to apply and superior in accuracy to the RWA, and works well for relevant models.

Let us introduce our method utilizing a one-dimensional lattice of oscillators each of mass m that are coupled linearly with coupling strength C, while at the same time experiencing the local on-site potential:

$$V(x_n) = \frac{\beta}{2}{x_n}^2 + \frac{\gamma}{4}{x_n}^4 \tag{1}$$

where x_n is the displacement of the nth oscillator from its equilibrium position and β, γ are constant parameters. The Hamiltonian of the chain for $m = 1$ is

$$H = \sum_n \left(\frac{\dot{x}_n^2}{2} + \frac{C}{2}(x_{n+1} - x_n)^2 + V(x_n) \right) \tag{2}$$

where the index n runs over the entire one-dimensional infinite lattice; we obtain the following equations of motion:

$$\ddot{x}_n = C(x_{n+1} + x_{n-1} - 2x_n) - \beta x_n - \gamma x_n^3. \tag{3}$$

If we were to use the anticontinuous limit approach for constructing a single breather [11], we would have to first construct in a given lattice site a trivial breather of frequency ω_b for zero coupling, i.e. for $C = 0$, and subsequently continue analytically the trivial solution to finite couplings C, keeping the oscillation frequency constant. As a result, we would obtain a spatially localized solution where each site has a slightly different functional form in its time evolution but all sites would oscillate with exactly the same frequency ω_b. In order to find analytically a good approximation to this exact breather and since there is no dramatic difference in the evolution of distinct breather sites, we assume that the whole lattice oscillates collectively in a fashion similar to the oscillations at the zone boundary of the Brillouin zone [6], i.e.

$$x_n(t) = \alpha_n x(t) \tag{4}$$

where $x(t)$ represents the coherent lattice oscillation and the sequence of constants $\{\alpha_n\}$ determines the local oscillation amplitudes at each lattice site. Upon substituting the decoupling ansatz of equation (4) into equation (3) and some rearrangements we obtain the equation for $x(t)$:

$$\ddot{x} = -A_n x - B_n x^3 \tag{5}$$

with

$$A_n = \beta - C\frac{\alpha_{n+1} + \alpha_{n-1} - 2\alpha_n}{\alpha_n} \tag{6}$$

$$B_n = \gamma {\alpha_n}^2. \tag{7}$$

Equation (5) for $x(t)$ is a simple nonlinear equation of second order; its solutions are

$$x(t) = cn[\epsilon_n t | k_n] \tag{8}$$

$${\epsilon_n}^2 = A_n + B_n \tag{9}$$

$${k_n}^2 = \frac{B_n}{2(A_n + B_n)} \tag{10}$$

where we assume presently for simplicity the initial conditions $x(0) = 1$ and $\dot{x}(0) = 0$. The function cn is the Jacobian elliptic cosine of modulus k_n; for the solution to be real and

periodic, ϵ_n must be real and for the elliptic modulus k_n, $0 \leqslant k_n < 1$. The Jacobian elliptic cosine is a doubly periodic function with real period equal to $4K_n$, where $K_n \equiv K(k_n)$ is the complete elliptic integral of the first kind [23]. As a result, the frequency of the periodic solution determined through equations (8)–(10) with (6) and (7) is

$$\omega_n \equiv \omega(\epsilon_n, k_n) = \frac{\epsilon_n}{\frac{2}{\pi}K_n}. \tag{11}$$

The analytical DB solution at frequency ω_b is then obtained through the localized sequences of amplitudes $\{\alpha_n\}$ that are solutions of the transcendental equation

$$\omega_n = \omega_b. \tag{12}$$

In other words, for a given ω_b, sequences of the amplitudes $\{\alpha_n\}$ that are finite in a region of the lattice, decay asymptotically in n and are roots of the transcendental equation (12), give the amplitude part of the DB solution for finite C, while the time dependence is provided by the elliptic function solution. We note that after the solution of equation (12) each pair of (ϵ_n, k_n) results in different cn evolution but with the same frequency ω_b. Since, due to the localized nature of the DB solution, there is a lattice breaking of symmetry manifested in the local amplitudes $\{\alpha_n\}$, the pair (ϵ_n, k_n) is directly associated with site n. We can thus parametrize the DB at frequency ω_b in terms of k_n:

$$x_n(t) = \alpha_n cn\left[\frac{2}{\pi}K_n\omega_b\, t|k_n\right] \tag{13}$$

while the amplitudes α_n in this case can be expressed as $\alpha_n = (8/\pi^2\gamma)^{1/2}k_nK_n\omega_b$. We note that while elliptic function modulus k_n and non-time-dependent parts of the argument ϵ_n are local, i.e. depend directly on lattice site indices through equations (6), (7), (9) and (10), the DB analytical solution, and in particular the DB oscillation frequency, determined through the transcendental eigenvalue equations (11) and (12), are global and independent of the lattice location. The DB of frequency ω_b is then brought into existence when the appropriate local elliptic modulus–amplitude relation is achieved that makes ω_b global for all sites; this local DB interpretation can be quite useful in non-homogeneous and disordered lattices. When α_n amplitudes become zero, we truncate equations (6) and (7) appropriately. The maximal coupling C for localized solution existence [8] is connected here to conditions for equation (5) to have periodic solutions; a necessary condition is clearly $k_n < 1$.

We will study some approximate forms of the transcendental equation (12) below; presently we resort to numerics for obtaining its roots. In order to avoid the tedious evaluation of Jacobian matrix derivatives required in the Newton method, we use the straightforward Broyden root finding method [24]. In figure 1 we present the amplitudes of DBs generated through the root finding numerical solution of the nonlinear eigenvalue problem of equations (11) and (12) for the hard ($\gamma > 0$) as well as soft ($\gamma < 0$) unimodal ϕ^4 potentials. Substitution of these states as initial conditions into equation (3) results in the breather modes determined analytically through equations (8) or (13). The analytical algebraic method in the present case, besides being numerically fast and conceptually simple, provides analytical time dependence of the localized states. Furthermore, it can readily tackle breather amplitude stability issues; a Fourier expansion of the periodic solution of equation (13) gives [23]

$$x_n(t) = \frac{2\pi\alpha_n}{k_nK_n}\sum_{m=0}^{\infty}\frac{q^{m+1/2}}{1+q^{2m+1}}\cos\left[(2m+1)\omega_b t\right] \tag{14}$$

where $q \equiv q_n = \exp(-\pi K_n'/K_n)$ and K' is the elliptic integral of the first kind evaluated at the complementary modulus k', with $k'^2 = 1 - k^2$. From equation (14) we observe that ω_b

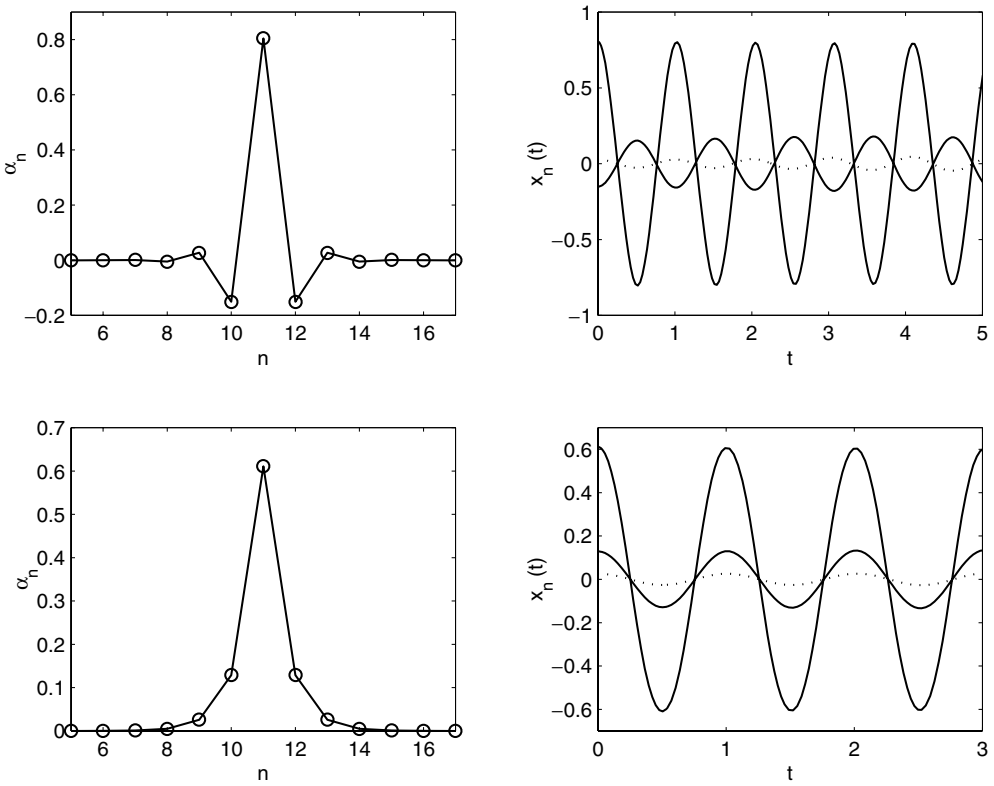

Figure 1. Analytic breathers: in the upper plots initial DB amplitudes (left) generated through equation (12) and cnoidal evolution after substitution in equation (3) for the central and next two breather sites (right) for a hard ϕ^4 potential ($\beta = \gamma = 1$, $\omega = 1.403\,94$, $C = 0.025$). In the lower plots the same plots are given for a soft ϕ^4 potential with solution $x_n(t) = \alpha_n cd\left[\frac{2}{\pi}K_n\omega_b t|k_n\right]$, nonlinear eigenvalue equation $\omega^2 = (A_n + B_n/2)/\left[\frac{2}{\pi}K_n\right]^{-2}$, ${k_n}^2 = |B_n|/(2A_n + B_n)$ for $\gamma < 0$, where cd is a Jacobian elliptic function ($\beta = -\gamma = 1$, $\omega = 0.872\,20$, $C = 0.06$). In both cases, time is in units of DB period and the numerical evolution agrees with the corresponding analytical solutions.

as well as its harmonics cannot coincide with the linear frequency spectrum, since otherwise the breather decays due to resonance with phonons, in agreement with the standard breather theory [8, 11, 13]. We note that the expansion of the elliptic function breather expression in trigonometric functions determines through the nome q the order at which the breather decays, should a resonance of its harmonics with linear modes occur. Finally, we comment that linear stability analysis of equation (5) results in Lamé's differential equation that can give conditions for DB linear stability, although numerics might be preferable.

Let us now come to acoustic chain models and in particular to the celebrated Fermi–Pasta–Ulam (FPU) model with Hamiltonian [1, 11]

$$H = \sum_n \left(\frac{\dot{x}_n^2}{2} + \frac{C}{2}(x_{n+1} - x_n)^2 + \frac{\gamma}{4}(x_{n+1} - x_n)^4 \right) \tag{15}$$

where C, γ denote now the strengths of the couplings for the linear and nonlinear nearest neighbour interactions, respectively. The equations of motion are

$$\ddot{x}_n = C(x_{n+1} + x_{n-1} - 2x_n) + \gamma\left((x_{n+1} - x_n)^3 + (x_{n-1} - x_n)^3\right). \tag{16}$$

Use of the decoupling ansatz of equation (4) results in identical equations for the internal DB variable $x(t)$ as before, i.e. equation (5), but with new coefficients A_n and B_n given by

$$A_n = -C\frac{\alpha_{n+1} + \alpha_{n-1} - 2\alpha_n}{\alpha_n} \tag{17}$$

$$B_n = \gamma\frac{(\alpha_n - \alpha_{n+1})^3 + (\alpha_n - \alpha_{n-1})^3}{\alpha_n}. \tag{18}$$

The expressions for the analytic solution equations (8)–(10) and the mode frequency equation (11) are also valid but with the new coefficients.

Let us investigate some limiting cases of the new transcendental system. In the purely linear case with $\gamma = 0$, equations (9)–(11), (17) and (18) result in the linear eigenvalue problem

$$\alpha_n {\omega_0}^2 = C(2\alpha_n - \alpha_{n+1} - \alpha_{n-1}) \tag{19}$$

where $\omega \equiv \omega_0$ provides the linear phonon spectrum of the problem. In the purely nonlinear case, on the other hand, for $C = 0$ we have $A_n = 0$, the elliptic modulus becomes a constant, namely $k = 1/\sqrt{2}$ and the transcendental equation reduces to an algebraic equation

$$\alpha_n {\omega_b}^2 = \gamma\left[(\alpha_n - \alpha_{n+1})^3 + (\alpha_n - \alpha_{n-1})^3\right]. \tag{20}$$

Consequently, our expressions reduce to known exact analytical results [2, 3, 6, 9, 11]. Finally, in the general case, we can expand the elliptic integral K in powers of the (assumed small) modulus k, make the drastic approximation of retaining only the first term, namely $2K(k)/\pi \approx 1$, and obtain

$$\alpha_n {\omega_b}^2 = C(2\alpha_n - \alpha_{n+1} - \alpha_{n-1}) + \gamma\left[(\alpha_n - \alpha_{n+1})^3 + (\alpha_n - \alpha_{n-1})^3\right]. \tag{21}$$

The nonlinear eigenvalue equation (21) is identical to that obtained by Sievers and Takeno for the FPU lattice through the use of the RWA[1] [1]. Clearly, successively improved algebraic approximations can be derived if needed. The construction of the FPU breather amplitudes can be done straightforwardly as in the previous cases with on-site potentials.

The use of the algebraic method in the previous cases depended directly on the separability of the nonlinear potential $V(x_n)$ and the possibility of finding exact solutions to the resulting nonlinear differential equation. It is possible however that either one or both these conditions are not met. In this case, while the method does not furnish analytical expressions it nevertheless provides readily accurate numerical DBs. Using equations (1) and (2) with the ansatz (4) we obtain

$$\ddot{x} = -\frac{\partial}{\partial x}W(\{\alpha_n\}, x) \tag{22}$$

$$\alpha_n W(\{\alpha_n\}, x) = \frac{C}{2}\left[(\alpha_{n+1} - \alpha_n)^2 + (\alpha_{n-1} - \alpha_n)^2\right]x^2 + V(\alpha_n x). \tag{23}$$

Equation (23) represents the motion of an effective particle in the general potential $W(\{\alpha_n\}, x)$ that contains both the reduced variable x as well as the local amplitudes $\{\alpha_n\}$ that need to be determined selfconsistently. The expression for the period of the nth oscillator is obtained easily and given by

$$T_n = 4\int_0^1 \frac{\mathrm{d}x}{\sqrt{2(W(\{\alpha_n\}, 0) - W(\{\alpha_n\}, x))}}. \tag{24}$$

The breather solution is now obtained through the numerical solution of the following algebraic system:

$$T_n = T_b \tag{25}$$

[1] Except for a factor of 3/4 in the nonlinear term that stems from the RWA.

where T_b is the desired breather period. Different breather and multibreather states can be found as different roots of this system that have to be accessed by judicial selection of the initial codes for the local amplitudes $\{\alpha_n\}$.

The algebraic method we presented is quite general and can be applied to a large class of problems, including higher dimensional lattices, long range interactions and disordered lattices. The essence of the method is that instead of making the RWA in equation (5), i.e. $x^3 \simeq Dx$, where D is an appropriate constant [1–3], we solve the latter equation exactly. Numerical work has shown that the method is more accurate than the RWA and agrees generally with the results obtained from the numerically exact anticontinuous limit method, typically to 10^{-3} or sometimes better. Application of the algebraic method in the present study resulted in Jacobian elliptic function DB time-dependence, with spatial distribution determined through the roots of a transcendental equation associated with a dispersion relation-like nonlinear eigenvalue problem. Root sequences relevant to DBs are decaying ones, while other classes of roots give rise to linear and nonlinear extended modes. Explicit analytical breather expressions can be obtained for both even and odd power potentials as well as some other functional cases. We note that the algebraic method can easily be adapted to generate multibreathers and also be applied to disordered lattices where DB amplitudes adjust to local imperfections. The nature of the analytical solution clearly suggests that DBs can be thought of to a good approximation as discrete, localized, particle-like entities with cnoidal wave internal structure, that adapt to local environments and move by coupling translational motion to their internal dynamics. We also comment in passing here, that the availability of analytic expressions can also be used to describe approximately the depinned DB uniform dynamics. In the spirit of the study by Hori and Takeno [4] we make the ansatz $x_n(t) = \alpha_n(t)cn[\mu n - \epsilon_n t|k_n]$ where μ is a parameter. Upon substituting it into equation (3) we obtain approximate closed equations for the time-dependent amplitudes $\alpha_n(t)$ (using however a nonlinear extension of the rotating wave approximation, i.e. $dn[\mu n - \epsilon_n t|k_n] \approx 1$, where dn is an elliptic function). Approximate solution of the latter, results finally in $x_n(t) = a_n \,\mathrm{sech}[\zeta(n - \upsilon t)]cn[\mu n - \epsilon_n t|k_n]$, representing a DB travelling with velocity υ and a_n, ζ, μ are determined parameters that depend on the specific model. The parameters ζ, μ are homogeneous functions of the breather velocity, whereas to low order, a_n and ϵ_n can be obtained by using the algebraic method as in the static breather case. Localized mode evolution of this type was considered earlier utilizing the RWA [4], as well as being observed numerically [5, 12]. The explicit use of the algebraic method in determining breather mobility demands extensive numerics and will be presented elsewhere. We conclude that the approach presented here produces quite accurate static and approximate moving breathers, provides useful breather functional forms and by using minimal numerics proves to be quite fast.

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