Exact traveling breather solutions in a discrete Klein-Gordon ring

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Following an earlier work relating to traveling kinks and pulses in a discrete reaction-diffusion system, we construct exact traveling breather solutions on a closed Klein-Gordon type lattice with a double-well potential at each site. The dynamics consists of a succession of linear regimes and the problem reduces to an appropriate matching for successive regimes. The analysis shows that the so-called marginal modes are not essential for the existence of traveling breathers. Results are shown for a ring with $N=3$ sites for the sake of illustration of the principles involved, while a number of basic results are also presented for the open lattice ($N\rightarrow\infty$, see below).

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I. INTRODUCTION

Moving breathers in nonlinear discrete lattices are by now well-studied objects, from both analytical and numerical points of view, and appear to be as ubiquitous as their stationary counterparts. They were observed numerically even in early days of exploration of localized nonlinear excitations,[1,2] and were later extensively studied, especially for FPU chains and anti-ferromagnetic lattices (see, e.g., Refs. 3 and 4). While the existence of traveling breathers is theoretically well-understood for integrable lattices like the Toda lattice and Ablowitz-Ladik lattice, and also for spatially continuous systems,[5] their existence for nonintegrable discrete systems is a more subtle phenomenon. In some situations (e.g., FPU systems and Klein-Gordon chains; see Refs. 3 and 4) one can describe moving breathers in terms of a Peierls-Nabarro potential,[6–9] but this does not seem to be the generic picture for spatially discrete systems.[8] Special models have been constructed where the Peierls-Nabarro potential does not exist and one can establish the existence of traveling NLE's (to be more precise, traveling kink solutions) with reference to a topological lower bound to the energy of the NLE.[10] Some of these traveling NLE's radiate energy into the phonon modes as they wobble along the lattice, while some others continue to remain truly localized during their motion. Approximate traveling breather solutions with possible small-amplitude oscillations in the tails have been studied in the context of energy transport in alpha-helices and in DNA.[11–15]

An important work by Aubry and Cretegny[7] elucidates the mechanism underlying the occurrence of a class of traveling breather solutions, namely the emergence of *marginal modes*. The latter pertains to the onset of instability of the so-called pinning mode—a localized internal mode of a stationary breather, which may be even or odd depending on the symmetry of the breather itself. As the pinning mode gets destabilized, there occurs a regime of linear growth, leading to breather mobility. In a related approach, Flach and Willis[8] explain the emergence of traveling breathers in terms of the crossing of a separatrix barrier pertaining to a set of collective internal degrees of freedom associated with a stationary breather. An algorithm for finding moving breather and kink solutions in nonlinear lattices was proposed in Ref. 5 on the basis of tail analysis of the breathers where a linear approximation can be employed. As observed there, the transition from moving to trapped breathers cannot be obtained from the tail analysis since such transitions essentially depend on the dynamics at the breather center, involving the pinning modes.

In a recent work James and Sire[16] have (in this context, see also Ref. 17) proven the existence of small amplitude traveling breathers with exponentially small tails in a discrete Klein-Gordon chain and have followed it up[18] with numerical computations, continued into the large amplitude regime. They employ a technique of center manifold reduction, once again related to marginal stability.

In the present paper we consider a closed nonlinear discrete Klein-Gordon (NDKG) type chain with piecewise parabolic double-well on-site potentials (i.e., piecewise linear restitution forces) for which the analysis reduces to an appropriate matching between successive regimes described by linear evolution equations, and construct exact traveling breather solutions, following the approach adopted in an earlier work relating to a Nagumo type discrete reaction-diffusion system.

II. EXACT TRAVELING KINK SOLUTIONS IN A DISCRETE REACTION-DIFFUSION SYSTEM

In this Nagumo-type model,[19] where the dynamics is piecewise linear, one can construct a stable stationary kink solution all of whose eigenmodes can be calculated exactly. There exists a linear regime where the general solution for the model can be set up by superposing all these eigenmodes, and one can demand that this be of the form of a traveling kink, choosing the superposition coefficients appropriately. The linear regime is eventually terminated, giving way to a new linear regime as there occurs the crossing of a threshold at one of the sites, and one has to perform a matching of the superposition coefficients for the successive regimes. The resulting traveling kink solution can be obtained as an exact integral expression or as a series involving Bessel functions.

It is important to note that the stationary and the traveling kink solutions exist in the model simultaneously, and the traveling kink emerges as simply a *response* of the stationary kink to appropriate perturbations, all of which are temporally stable. As a result of these perturbations, the stationary kink gets "dressed" as it becomes mobile, and the profiles of the stationary and the moving kinks look different. This is to be contrasted with the situation where one of the eigenmodes of a localized stationary excitation becomes unstable as one or more parameters characterizing the system are varied, and the excitation becomes mobile at the marginal stability border, with its shape modified only marginally. Co-existence of stationary and traveling solutions in nonlinear lattices is known, for instance, in d.c.-driven sine-Gordon models with damping.[20]

III. NDKG RING WITH A DOUBLE QUADRATIC ON-SITE POTENTIAL

The model consists of a ring of, say, N oscillators, with the oscillator at site n $(n=1,2,\ldots,N)$ described by conjugate variables u_n, $\dot{u}_n$. The oscillators are coupled linearly to nearest neighbors, and each moves in a piecewise parabolic double-well potential so that the system is described by the coupled equations

$$\ddot{u}_n = u_{n+1} - 2u_n + u_{n-1} + F(u_n), \tag{1a}$$

where $F(x)(=-V'(x))$ stands for the restitution force in the double well potential

$$V(X) = \tfrac{1}{2}\alpha x^2 \ (x < a), \tag{1b}$$

$$= \tfrac{1}{2}\beta(1-x)^2 \ (x > a). \tag{1c}$$

Here α and $a(<1)$ are constants characterizing the potential, the latter being a *threshold* parameter determining the boundary between the two wells, and

$$\beta = \alpha\frac{a^2}{(1-a)^2}, \tag{1d}$$

ensuring that the two wells are of the same height. More general situations involving wells of different heights can also be considered. The choice $a=1/2$ corresponds to a symmetric double well. In (1a) the sites are numbered in accordance with the periodic boundary condition appropriate to the ring:

$$u_{n+N} = u_n, \tag{2a}$$

$$\dot{u}_{n+N} = \dot{u}_n, \tag{2b}$$

so that, for instance,

$$u_0 \equiv u_N, \quad u_{-1} \equiv u_{N-1}.$$

Discrete Klein-Gordon type lattices with symmetric double-quadratic on-site potentials given above have been considered in Ref. 21 where a large class of stationary breather solutions have been constructed. The more general situation involving asymmetric double-quadratic potentials was considered in Ref. 22 where an exact zero frequency stationary breather together with a class of monochromatic perturbed breather solutions was presented.

IV. ZERO FREQUENCY STATIONARY BREATHER SOLUTION

We now proceed to outline the construction of exact traveling breather solutions in the NDKG ring under consideration using the approach indicated above. For this, we first construct, along lines followed in Ref. 22, an exact stationary zero-frequency breather ($\dot{u}_n=0$ for all n) on the ring. Calling the nth site *high* (resp. *low*) if $u_n>a$ (resp. $u_n<a$), and assuming that the only high site is at $n=0$ so that, for all other sites one has the system of linear equations

$$u_{n+1} - (2+\alpha)u_n + u_{n-1} = 0, \tag{3}$$

and finally, assuming the breather to be *symmetric* about the site $n=0$, it is easy to see that the required solution is given by

$$\bar{u}_n = \frac{\beta(\lambda^n + \lambda^{N-n})}{(2+\beta)(1+\lambda^N) - 2(\lambda + \lambda^{N-1})}(n=0,1\ldots,N-1), \tag{4}$$

where λ satisfies

$$\lambda + \frac{1}{\lambda} = 2 + \alpha, \quad |\lambda| < 1, \tag{5}$$

and where the parameters of the model are to satisfy the consistency requirement

$$\frac{\alpha a^2}{(1-a)^2\left(\dfrac{\lambda+\lambda^{N-1}}{a} - a(1+\lambda^N)\right)} < 2(1-\lambda)(1-\lambda^{N-1}) < \frac{a\alpha}{1-a}, \tag{6a}$$

corresponding to our assumption

$$\bar{u}_0 > a, \quad \bar{u}_1 < a. \tag{6b}$$

V. EIGENMODES AND EIGENFREQUENCIES

For the traveling breather obtained by the dressing of the above stationary solution, u_0 continues to be *high* and all other sites continue to be *low* for the time-interval taken by the breather to move through one lattice site during which the system evolves linearly, and the general solution pertaining to this time interval is obtained by superposing with the above stationary solution all its eigenmodes, a typical eigenmode being of the form

$$\tilde{u}_n = \phi_n(A\cos\omega t + B\sin\omega t), \tag{7a}$$

where the ϕ_n's satisfy

$$\phi_{n+1} + \phi_{n-1} - (2 + h_n - \omega^2) = 0, \tag{7b}$$

and where

$$h_n = \beta(n=0), \quad h_n = \alpha(n \neq 0), \tag{7c}$$

A, B being constants. Since the stationary breather we start from is symmetric about $n=0$, all the eigenmodes can be chosen to be either symmetric or antisymmetric.

Each eigenmode is characterized by a spatial variation rate (say, μ, $|\mu| \leqslant 1$, see below) analogous to the spatial variation rate (λ) of the stationary breather itself, and the eigen-frequencies are related to μ as

$$\omega^2 = 2 + \alpha - \left(\mu + \frac{1}{\mu}\right), \tag{8a}$$

with μ solving

$$\mu^{N+2} + \gamma\mu^{N+1} - \mu^N - \mu^2 + \gamma\mu + 1 = 0(\gamma \equiv \beta - \lambda), \tag{8b}$$

for the *symmetric* mode, and

$$\mu^N = 1, \tag{8c}$$

for the *antisymmetric* mode.

Comparing with the open lattice[22] a root satisfying $|\mu| < 1$, if it exists, can be said to correspond to a "localized" mode while the roots with μ lying on the unit circle can be said to correspond to "extended" modes (this becomes evident as one goes to $N \to \infty$). For instance, all the antisymmetric modes are extended in this sense, while a symmetric mode may be localized, depending on the parameters of the model (see below for an example; in the limit $N \to \infty$, i.e., for the open lattice, there occurs exactly one localized symmetric mode). One also observes that there are certain unacceptable roots in Eqs. (8b) and (8c), namely $\mu=-1$ for a symmetric mode, which occurs when N is odd, and $\mu = \pm 1$ (even N), $\mu=1$ (odd N) for an antisymmetric mode. Discounting these, it turns out that, for N even, there are $(N/2+1)$ pair of symmetric and $(N/2-1)$ pair of antisymmetric modes, while for N odd, there are $((N-1)/2+1)$ pair of symmetric and $((N-1)/2)$ pair of antisymmetric modes making up, in each case, N pair of roots $(\mu, 1/\mu)$ in all, as expected.

Given a root μ (and a corresponding eigenfrequency ω) it is straightforward to obtain the eigenmode (up to a normalization), namely,

$$\textit{symmetric}: \phi_n = \frac{\mu^n + \mu^{N-n}}{1 + \mu^N} + c.c., \tag{9a}$$

$$\textit{antisymmetric}: \phi_n = (\mu^n - \mu^{N-n}) + c.c., \tag{9b}$$

where "c.c." stands for complex conjugate (notice that, for the antisymmetric mode, (9b) implies $\phi_0=0$).

VI. DRESSING OF THE STATIONARY BREATHER: THE TRAVELING BREATHER SOLUTION

We choose initial conditions such that u_0 crosses the threshold a from below, at $t=0$, while all other lattice sites are *low*. Denoting the speed of the traveling breather by χ we note that the system will evolve linearly during $0 < t < 1/\chi$, and hence during this interval the solution for the u_n's will be given by a superposition involving the stationary breather and the eigenmodes, as indicated above. Launching such a superposition at $t=0$ and demanding that it be of the form of a traveling breather, we introduce the propagation variable $\zeta \equiv \chi t + n$ (solutions with positive and negative values of χ occur in pairs; we choose positive values of χ in our examples), and note that during the next interval of length $1/\chi$ the site $n=-1$ will be *high* like the site $n=0$ during the previous interval, while all other sites will be *low*, so that the evolution will be similar with t replaced by the *local time* $\tau = (\zeta - [\zeta])/\chi$, where $[\zeta]$ stands for the integer part of the propagation variable ζ. The local time gives the time at site n that corresponds to the time t $(0 < t < 1/\chi)$ at site 0. In other words, the traveling breather solution we seek will be of the form

$$u_n(t) \equiv g(\zeta) = \bar{u}_m + \sum_{k=1}^{N} [\phi^{(k)}{}_m \{a_k \cos \omega_k \tau + b_k \sin \omega_k \tau\}]. \tag{10}$$

Here we have written m for $[\zeta]$, and have used the index k to label the different eigenmodes and eigenfrequencies. The superposition constants a_k, b_k are to be chosen appropriately so as to satisfy appropriate matching conditions, stated below, between successive time intervals of length $1/\chi$. Finally, $\bar{u}_m$, with $m \equiv [\zeta]$, is given by Eq. (4).

The breather profile function g, together with its derivative has to be continuous at each instant of threshold crossing and, moreover, according to the initial condition chosen, $g(0)$ has to be the threshold a. In other words, the constants a_k, b_k are to be determined from the conditions

$$g(m^+) = g(m^-), \tag{11a}$$

$$g'(m^+) = g'(m^-), \tag{11b}$$

$$g(0) = a, \tag{11c}$$

where the superscripts $+$, $-$ refer to instants just after and just before the crossing of the threshold, respectively.

Thus, finally, we have obtained the exact form (10) of the traveling breather solution determined by the matching conditions (11a)–(11c), where the symbols have all been explained above. This solution has to satisfy the consistency condition

$$u_0 > a, \quad u_n < a(n = 1, \ldots, N-1), \tag{12a}$$

for

$$0 < t < \frac{1}{\chi}. \tag{12b}$$

We illustrate below a few results for the simple case $N=3$. More elaborate results will be presented elsewhere.

VII. NDKG RING WITH THREE SITES (N=3)

We consider the simplest case $N=3$ for the sake of concreteness. The eigenfrequencies ω_k $(k=1,2,3)$ depend on μ through $\nu \equiv \mu + 1/\mu$. For the symmetric eigenmodes, ignoring the root $\mu=-1$ (this root gives $u_n=0$ for all n), one has

$$\nu^2 + (\gamma - 1)\nu - (\gamma + 2) = 0(\gamma \equiv \beta - \alpha), \quad (13a)$$

giving

$$\nu_{1,2} = \tfrac{1}{2}[-(\gamma - 1) \pm \sqrt{\{\gamma^2 + 2\gamma + 9\}}], \quad (13b)$$

$$\omega_{1,2}^2 = 2 + \alpha - \nu. \quad (13c)$$

The corresponding eigenmodes are (we choose a convenient normalization)

$$\phi^{(1)} = \begin{pmatrix} \nu_1 - 1 \\ 1 \\ 1 \end{pmatrix}, \quad \phi^{(2)} = \begin{pmatrix} \nu_2 - 1 \\ 1 \\ 1 \end{pmatrix}. \quad (14)$$

Note that, for $0 < \gamma < 4/3$, one of the two symmetric modes is localized (as explained above, this term is used by analogy with the eigenmodes for the open lattice), while outside this range both the modes are extended.

The single antisymmetric eigenmode is similarly obtained as

$$\phi^{(3)} = \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix}, \quad (15a)$$

with

$$\nu_3 = -1, \quad \omega_3 = \sqrt{(3 + \alpha)}. \quad (15b)$$

With these eigenmodes and eigenfrequencies, the traveling breather is given by (10), there being three terms in the summation on the right hand side, involving the six constants a_k, b_k $(k=1,2,3)$, while a seventh unknown to be determined is the speed χ. These seven parameters are obtained by solving Eqs. (11a)–(11c) which, for $N=3$, make up a total of precisely seven equations, thereby giving a complete determination of the traveling breather, subject to the consistency requirements (12a) and (12b).

For instance, with $a=0.7, \alpha=6$, the stationary breather is

$$\begin{pmatrix} \bar{u}_0 \\ \bar{u}_1 \\ \bar{u}_{-1} \equiv \bar{u}_2 \end{pmatrix} = \begin{pmatrix} 0.9501 \\ 0.1357 \\ 0.1357 \end{pmatrix},$$

and one has, for the traveling breather, $\chi = 1.040\,723\,77\ldots$, while the consistency conditions (12a) and (12b) are met with, as seen in Fig. 1, where we plot the time variation of $u_0(t)$, $u_1(t)$, $u_2(t) \equiv u_{-1}(t)$, confirming that (10) does indeed represent a traveling breather solution on the NDKG ring considered. As one varies one or more of the parameters, the speed gets changed; e.g., with $a=0.695, \alpha=6.0$, one has $\chi = 1.131\,304\,98\ldots$. Precisely the same time variation is obtained on integrating (1a)–(1c) with an initial condition given by (10) with $\tau=0$, thereby corroborating the correctness of our analysis.

VIII. THE OPEN NDKG LATTICE ($N \to \infty$)

For the open lattice, we assign site numbers so that the *high* site during $0 < t < 1/\chi$ is located at $n=0$, while the other sites on either side correspond to $n = \pm 1, \pm 2, \ldots$, and one arrives at results for the open lattice from those for the ring with N sites by identifying site number $N-k$ $(0 < k \leq N/2)$ with $-k$. Using this procedure, one notes from (4) that the zero-frequency stationary breather solution is now given by

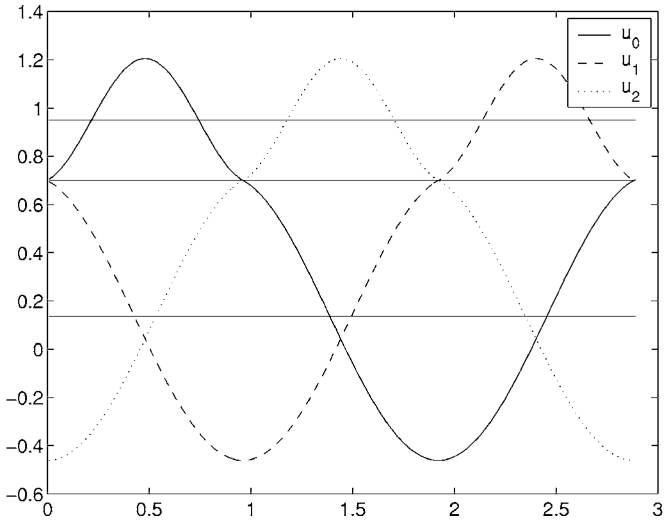

FIG. 1. Variation of u_0, u_1, $u_2 = u_{-1}$ with time for the traveling breather on a ring with three sites ($a=0.7$, $\alpha=6$); the horizontal lines depict: (Top) value of $\bar{u}_0$ for the stationary breather, (middle) value of threshold a, (bottom) value of $\bar{u}_1 = \bar{u}_2$ for the stationary breather; the time interval between successive threshold crossings is $1/\chi = 0.960\,869\,76$; as u_0 becomes *low*, u_{-1} becomes *high* (see text), indicating that the breather has moved through one lattice site.

$$\bar{u}_n = \frac{\beta}{2 + \beta - 2\lambda}\lambda^{|n|}, \quad (16)$$

precisely the result arrived as in Ref. 22. The perturbations around this solution are characterized by a continuous band of eigenfrequencies given by

$$\omega(\theta) = \alpha + 4\sin^2\frac{\theta}{2}(0 \leq \theta \leq \pi), \quad (17a)$$

together with a single isolated frequency satisfying

$$\omega^2 = \alpha + 2 \pm \sqrt{(\gamma^2 + 4)}, \quad (17b)$$

where the upper (resp. lower) sign corresponds to $\alpha < \beta$ (resp. $\alpha > \beta$). Each eigenfrequency in the continuum is doubly degenerate with an even and an odd eigenmode associated with it, respectively, given by

$$\phi_n^{(e)}(\theta) = 2\sin\theta\cos(n\theta) + \gamma\sin(|n|\theta), \quad (18a)$$

and

$$\phi_n^{(o)} = \sin(n\theta), \quad (18b)$$

where the normalization has been chosen arbitrarily. The general form of an eigenfunction belonging to the band is thus

$$\phi_n(\theta) = 2\sin\theta\cos(n\theta) + (f(\theta) \pm \gamma)\sin(n\theta), \qquad (18c)$$

where the upper (resp. lower) sign corresponds to $n>0$ (resp. $n<0$), and where $f(\theta)$ is an arbitrary function indicating a superposition of the even and odd eigenmodes. The isolated frequency, on the other hand, is nondegenerate, and is associated with an even eigenmode given by

$$\phi_n^{(0)} = \rho^{|n|}, \qquad (19a)$$

where

$$\rho = \tfrac{1}{2}(\gamma \pm \sqrt{(\gamma^2 + 4)}), \qquad (19b)$$

the upper and lower signs being once again applicable as in (17b).

Following principles outlined above one can then obtain the traveling breather solution in the open lattice as an exact integral expression:

$$u_n(t) \equiv (\zeta) = \bar{u}_m + A\phi_m^{(0)} + \int_0^\pi d\theta[\phi_m(\theta)\{a(\theta)\sin(\omega(\theta)\tau) + b(\theta)\cos(\omega(\theta)u)\}]. \qquad (20)$$

Here, as before, ζ stands for the propagation variable ($\zeta=\chi t+n$, χ=speed of the traveling breather), the index m equals $[\zeta]$, the integer part of ζ, τ stands for the local time $(\zeta-[\zeta])/\chi$, $\phi_m^{(0)}$ and $\phi_m(\theta)$ represent eigenmodes as in (19a) and (18c), respectively, and the functions $a(\theta)$, $b(\theta)$ (together with the superposition coefficient $f(\theta)$ and the speed χ) are to be determined from the matching conditions. The latter are once again given by (11a)–(11c), with m now running through the values $0, \pm 1, \pm 2, \ldots$.

One can replace the integral in (20) by a sum over a discrete index by looking at the open lattice as the limit of a ring with N sites as indicated above, and going over to the limit $N\to\infty$ at the end. Details relating to (17a)–(20), as also to numerical construction of the traveling breather and a number of exact results will be published elsewhere.

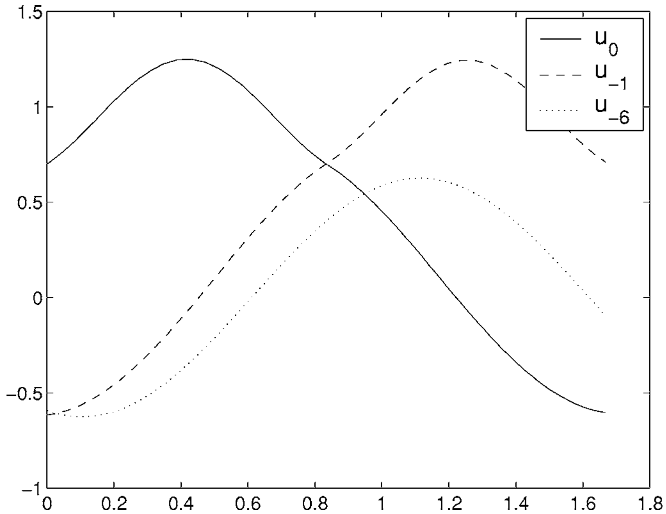

FIG. 2. Variation of u_0, $u_{-1}\equiv u_{N-1}$, $u_{-6}\equiv u_{N-6}$ with time for the traveling breather on a ring with N=20 sites (a=0.7, α=6); the time interval between successive threshold crossings is $1/\chi$ =0.833 575 282 3…; as u_0 becomes *low*, u_{-1} becomes *high* (see text), indicating that the breather has moved through one lattice site in the time-interval $0<t<1/\chi$.

Figure 2 shows the time variation of u_n for three chosen values of n (resp. 0, $N-1$, $N-6$, corresponding to sites 0, −1, −6, respectively, in the open lattice) for a lattice with N=20, a=0.7, α=6. One has here χ=1.199 651 69…, and observes that the breather has shifted through exactly one lattice site in time $1/\chi$ with the site at n=0 remaining *high* during $0<t<1/\chi$ while sites with $n\neq 0$ (only two are shown in the figure) all remain *low*. This once again confirms that Eq. (20) does indeed represent a traveling breather solution in the open NDKG lattice considered here.

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