Numerical approximation of breathers in lattices with nearest-neighbor interactions

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A numerical method is presented for accurately approximating time-periodic and spatially localized solutions known as (discrete) breathers, of the equations of motion describing lattices with one degree-of-freedom per lattice site and nearest-neighbor interactions. Our method is an extension of an approximation suggested by Tsironis [J. Phys. A **35**, 951 (2002)], gives more accurate results than the rotating wave approximation and is more universally applicable for these lattices. As an illustration, the method is applied here to several one- and two-dimensional lattices.

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I. GENERAL IDEA

We consider the system described by the Hamiltonian

$$H=\sum_{\vec{n}\in\mathbb{Z}^d}\frac{1}{2}p_{\vec{n}}^2+V(u_{\vec{n}})+\sum_{\vec{m}\in B_{\vec{n}}}W(u_{\vec{m}}-u_{\vec{n}}), \tag{1}$$

giving the equations of motion

$$\ddot{u}_{\vec{n}}+V'(u_{\vec{n}})=\sum_{\vec{m}\in B_{\vec{n}}}W'(u_{\vec{m}}-u_{\vec{n}}),\quad \forall\ \vec{n}\in\mathbb{Z}^d \tag{2}$$

(dots denote differentiation with respect to time and primes denote differentiation with respect to the argument) where $u_{\vec{n}}(t)\in\mathbb{R}$ is a dimensionless coordinate describing the position of a particle at the lattice site indicated by $\vec{n}$ as a function of time. With $\mathbb{Z}^d$ we refer to the set of all d-dimensional vectors whose elements are integers and define the norm on this set as $\|\vec{n}\|=\Sigma_{i=1}^d|n_i|$. With the set $B_{\vec{n}}$ we denote the set of all possible vectors $\vec{m}\in\mathbb{Z}^d$ for which $\|\vec{m}-\vec{n}\|=1$ (i.e., the set of nearest neighbors of the site denoted by $\vec{n}$). The potentials V: $\mathbb{R}\to\mathbb{R}$ and W: $\mathbb{R}\to\mathbb{R}$ are referred to as the on-site and interaction potential, respectively. For one-dimensional lattices we take $W(u_m-u_n)=W_+(u_m-u_n)$ if $m>n$ and $W(u_m-u_n)=W_-(u_m-u_n)$ if $m<n$, with the property $W_+(x)=W_-(-x)$.

These equations describe the motion of a system of coupled particles on a d-dimensional lattice with nearest-neighbor interactions. Since the late 1980s, it is known that these structures can sustain intrinsic localized modes, also known as discrete breathers [1].

In 1994, a proof of their existence was given for a certain class of one-dimensional lattices, which gave rise to a method for finding them using continuation from a suitable limit in which the equations of motion become uncoupled [2,3]. Outside the region of applicability of this proof one has to rely on numerical methods to find breathers. This paper describes such a numerical method.

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It is important to note that in recent years discrete breathers have been observed experimentally in a number of problems ranging from Josephson junction arrays to nonlinear optical waveguide systems [4].

A breather is defined as a time-periodic and spatially localized solution of Eq. (2), i.e., $u_{\vec{n}}(t)=u_{\vec{n}}(t+\tau)$ and $u_{\vec{n}}\to 0$ as $\|\vec{n}\|\to\infty$. For this definition to hold we require that $u_{\vec{n}}=0$ is a fixed point of Eq. (2) and $V'(0)=W'(0)=0$. Following other authors [5], we introduce new variables $a_{\vec{n}}$ and $T_{\vec{n}}(t)$ by

$$u_{\vec{n}}(t)=a_{\vec{n}}T_{\vec{n}}(t) \tag{3}$$

and set $T_{\vec{n}}(0)=1$ without loss of generality. In these variables a breather is equivalent to a solution with the properties (1) $T_{\vec{n}}(t)=T_{\vec{n}}(t+\tau)$ (time periodic) and (2) $a_{\vec{n}}\to 0$ as $\|\vec{n}\|\to\infty$ (spatially localized).

In a one-dimensional setting, the second property [6] is the definition of a homoclinic orbit in the spatial coordinate n. Thus, the method proposed in this paper has been inspired by a family of numerical methods using homoclinic orbits in two- or higher-dimensional maps to find breathers [7,8]. As will be shown, for one-dimensional lattices an approximation proposed by Tsironis [9] gives far better approximations than the standard rotating wave method [i.e., using the ansatz $T_{\vec{n}}=\cos(\omega t)$ in Eq. (3)], while keeping the dimension of the recurrence relation low (equal to $2d$) unlike the Fourier-series expansion method which, in general, requires higher dimensions to reach the same accuracy.

The approximation proposed by Tsironis can be written as [9]

$$u_{\vec{m}}-u_{\vec{n}}\approx(a_{\vec{m}}-a_{\vec{n}})T_{\vec{n}}, \tag{4}$$

with $\vec{n}\in Z^d$ and $\vec{m}\in B_{\vec{n}}$. We can estimate a relative error E by dividing the difference between the left- and right-hand sides by the approximate value:

$$E=\left|\frac{(a_{\vec{m}}-a_{\vec{n}})T_{\vec{n}}-a_{\vec{m}}T_{\vec{m}}+a_{\vec{n}}T_{\vec{n}}}{(a_{\vec{m}}-a_{\vec{n}})T_{\vec{m}}}\right|=\left|\frac{a_{\vec{m}}}{a_{\vec{m}}-a_{\vec{n}}}\right|\left|\frac{T_{\vec{n}}}{T_{\vec{m}}}-1\right|. \tag{5}$$

This error is small if either $|a_{\vec{m}}| \ll |a_{\vec{n}}|$ and/or $T_{\vec{m}} \approx T_{\vec{n}}$. Thus, when using this approximation, we expect the largest error to be made in the case that $|a_{\vec{n}}| \ll |a_{\vec{m}}|$ and $T_{\vec{n}}$ is significantly different from $T_{\vec{m}}$. However, in this case the amplitude at site $\vec{n}$ will not influence the calculation of the time function at site $\vec{m}$ since $|a_{\vec{n}}| \ll |a_{\vec{m}}|$ and hence this error is regarded as unimportant for the overall accuracy. In the case $|a_{\vec{m}}| \approx |a_{\vec{n}}|$ we need $T_{\vec{m}} \approx T_{\vec{n}}$ to make the error small. We can split this in two parts, for $a_{\vec{m}} \approx a_{\vec{n}}$ and for $a_{\vec{m}} \approx -a_{\vec{n}}$. As will be shown below, this can lead to forbidden combinations of neighboring amplitudes, depending on the behavior of $T_{\vec{n}}$ and $T_{\vec{m}}$.

The approximation (4) transforms the equations of motion (2) to

$$a_{\vec{n}} \ddot{T}_{\vec{n}} + V'(a_{\vec{n}} T_{\vec{n}}) = \sum_{\vec{m} \in B_{\vec{n}}} W'((a_{\vec{m}} - a_{\vec{n}}) T_{\vec{n}}), \tag{6}$$

which is a second-order ordinary differential equation (ODE) for $T_{\vec{n}}$. We restrict our solutions to time-reversible ones so that we have sufficient initial conditions [an initial value $T_{\vec{n}}(0) = 1$ and an initial derivative $\dot{T}_{\vec{n}}(0) = 0$] to be able to solve this ODE.

For certain potentials (e.g., some potentials which are low-order polynomials in their arguments) an analytical solution is possible [9]. In this paper, we will not try to solve the ODE analytically. Instead, we shall exploit the fact that the ODE (6) is overdetermined by fixing the period of the solution τ.

We then use this extra information about the solution for $T_{\vec{n}}(t)$ of Eq. (6) to numerically determine a relation between the amplitude at site $\vec{n}$ with the amplitudes of its nearest neighbors. Any set of values for the $a_{\vec{n}}$ satisfying this recurrence relation at each site $\vec{n}$ and simultaneously the asymptotic condition $a_{\vec{n}} \to 0$ as $\|\vec{n}\| \to \infty$ gives an approximate breather solution to the original equations of motion (2), since knowledge of the $\vec{a}_n$ completely determines $T_{\vec{n}}(t)$ through Eq. (6).

When such an approximate solution has been found we improve the approximation using a Newton-Raphson method, finding a zero of the system of equations $u_{\vec{n}}(\tau) - u_{\vec{n}}(0) = 0$ for all $\vec{n}$. If this method converges to a zero within a tolerance limit [10], we call the solution a numerically exact breather.

This paper is organized as follows: In Sec. II, we show how the method works for one-dimensional lattices, in particular Klein-Gordon lattices (i.e., anharmonic on-site and harmonic interaction potentials) and Fermi-Pasta-Ulam lattices (i.e., no on-site potential and anharmonic interaction potentials). A comparison is made with the rotating wave approximation in the case of a hard ϕ^4 potential in a Klein-Gordon lattice. In Sec. III, we apply the method to a two-dimensional Klein-Gordon lattice. In Sec. IV, we give some concluding remarks. The Appendix explains the numerical method used to find solutions to the recurrence relations.

II. APPLICATION TO ONE-DIMENSIONAL LATTICES

In one dimension, the equations of motion are

$$\ddot{u}_n + V'(u_n) = W'(u_{n+1} - u_n) - W'(u_n - u_{n-1}) \tag{7}$$

(where we replaced W_+ by W to simplify notation) which after applying approximation (4) becomes

$$a_n \ddot{T}_n + V'(a_n T_n) = W'((a_{n+1} - a_n) T_n) - W'((a_n - a_{n-1}) T_n). \tag{8}$$

This can be written in terms of an effective potential as

$$\ddot{T}_n = -\frac{\partial V_{\mathrm{eff}}(a_n, a_{n-1}, a_{n+1}, T_n)}{\partial T_n}, \tag{9}$$

where

$$V_{\mathrm{eff}}(a_n, a_{n-1}, a_{n+1}, T_n) = \frac{1}{a_n^2} V(a_n T_n) - \frac{1}{a_n (a_{n+1} - a_n)} W((a_{n+1} - a_n) T_n) + \frac{1}{a_n (a_n - a_{n-1})} W((a_n - a_{n-1}) T_n). \tag{10}$$

If $V(x)$ and $W(x)$ are even functions, the effective potential has the symmetry

$$V_{\mathrm{eff}}(a_n, a_{n-1}, a_{n+1}, T_n) = V_{\mathrm{eff}}(-a_n, -a_{n-1}, -a_{n+1}, T_n). \tag{11}$$

Later on, this symmetry can be used to determine further symmetries between the amplitudes and time functions.

Returning to the discussion about the relative error in Sec. I, we are now in a position to state that if the effective potential V_{eff} is even with respect to T_n [i.e., $V_{\mathrm{eff}}(a_n, a_{n-1}, a_{n+1}, T_n) = V_{\mathrm{eff}}(a_n, a_{n-1}, a_{n+1}, -T_n)$], the functions T_n determined for a_n and $a_m = -a_n$ are the same since $V_{\mathrm{eff}}(a_n, a_{n-1}, a_{n+1}, -T_n) = V_{\mathrm{eff}}(-a_n, a_{n-1}, a_{n+1}, T_n)$ and thus the approximation will hold for the stronger case $|a_m| \approx |a_n|$. If the effective potential is not even, only the weaker case $a_m \approx a_n$ will yield accurate approximations.

We can therefore categorize the amplitudes of breathers in one-dimensional lattices found with this method in three classes: A_+ whose amplitudes are large and positive, A_- whose amplitudes are large and negative, and A_0 whose amplitudes are small compared to those of classes A_+ and A_-. In an even effective potential there is no restriction on the classes to which neighboring amplitudes belong. If the effective potential is not even, we can only expect good results if an amplitude from class A_+ or A_- is followed by an amplitude of the same class or of the class A_0. A similar distinction of a breather's amplitudes in such classes has proven useful to a classification of breathers based on ideas of symbolic dynamics [11].

A. Klein-Gordon lattices

For Klein-Gordon lattices, the interaction potential is harmonic. Thus, we write $W(x)=(C/2)x^2$. The constant C is referred to as the coupling strength. The ODE for T_n becomes

$$a_n\ddot{T}_n+V'(a_nT_n)=C(a_{n+1}+a_{n-1}-2a_n)T_n, \qquad (12)$$

from which it is clear that a time-periodic solution T_n with period τ depends on the two parameters $f=a_{n+1}+a_{n-1}$ and a_n, for a certain coupling strength C. The period τ is a function of these two parameters, i.e., $\tau=\tau(f,a_n)$. If this function can be inverted we have $f=f(a_n;\tau)$ which can be determined numerically (if not analytically), such that we have a two-dimensional invertible map

$$M:\begin{cases} a_{n+1}=f(a_n;\tau)-b_n \\ b_{n+1}=a_n. \end{cases} \qquad (13)$$

Inversion of the relationship between τ and f is possible if $\partial\tau/\partial f\neq 0$ on an appropriate interval $X\subset\mathbb{R}$, for any $a_n\in X$, through the inverse function theorem. We now make this more explicit by deriving an expression for τ. First, we rewrite Eq. (12) as

$$\ddot{T}_n=-\frac{\partial V_{\mathrm{eff}}(a_n,f,T_n)}{\partial T_n}, \qquad (14)$$

where

$$V_{\mathrm{eff}}(a_n,f,T_n)=\frac{1}{a_n^2}V(a_nT_n)-\frac{1}{2a_n}C(f-2a_n)T_n^2, \qquad (15)$$

from which we infer that $f=0$ if $a_n=0$ to make Eq. (15) compatible with Eq. (12) at $a_n=0$. Notice also that if V_{eff} is even with respect to T_n one finds $f(a_n;\tau)=-f(-a_n;\tau)$, since $V_{\mathrm{eff}}(a_n,f(a_n;\tau),T_n)=V_{\mathrm{eff}}(a_n,f(a_n;\tau),-T_n)$ implies $V_{\mathrm{eff}}(a_n,f(a_n;\tau),T_n)=V_{\mathrm{eff}}(-a_n,f(-a_n;\tau),T_n)$, in accordance with Eq. (11) if the potentials $V(x)$ and $W(x)$ are even.

We can thus write an effective Hamiltonian for this system in the form

$$H_{\mathrm{eff}}=\frac{1}{2}S_n^2+V_{\mathrm{eff}}(a_n,f,T_n), \qquad (16)$$

with S_n the generalized momentum corresponding to T_n. Introducing an action I and an angle θ in the standard way, such that $H_{\mathrm{eff}}=H_{\mathrm{eff}}(I)$, we see that the frequency of motion is $\omega=dH/dI$ such that the period is $\tau=2\pi\omega^{-1}$. The requirement $d\tau/df\neq 0$ is commonly referred to as the anharmonicity condition and needs to hold for all $a_n\in X$ [2]. In all our calculations this condition holds for the range of amplitudes considered.

Since the map is invertible, we can use the techniques presented in Ref. [12] to find homoclinic orbits of this map. In the appendix an easily applied and very fast algorithm is given, based on the ideas presented in Ref. [12], to find large numbers of homoclinic orbits. In order for Eq. (13) to have any homoclinic orbits at all, we need the origin to be of the saddle type. The eigenvalues of the map at the origin are

$$\lambda_{\pm}=\frac{1}{2}\left(\frac{\partial f}{\partial a_n}(0)\pm\sqrt{\left(\frac{\partial f}{\partial a_n}(0)\right)^2-4}\right),$$

hence a necessary condition for a saddle is $|(\partial f/\partial a_n)(0)|>2$. If this condition is not fulfilled, the origin will be of the center type. Consequently, one cannot approach the equilibrium as $n\to\pm\infty$ and localized solutions are not possible.

By linearizing the equations of motion around $a_n=0$ we see that $T_n=\Sigma_{k=1}^{\infty}\alpha_k\cos(k\omega t)$ is the general solution. Inserting this in the linearized equations we have $(\partial f/\partial a_n)(0)=2+C^{-1}[V''(0)-k^2\omega^2]$ with $k=1,2,\ldots$. Therefore, we require either $k^2\omega^2<V''(0)$ or $k^2\omega^2>4C+V''(0)$ which is known as the nonresonance condition, since we can identify $V''(0)$ with the ground frequency of the harmonic part of the potential and the interval $V''(0)\leqslant k^2\omega^2\leqslant V''(0)+4C$ with the phonon band [2].

1. A Klein-Gordon lattice with hard ϕ^4 potential

As a first example, we present results for finding breathers in a Klein-Gordon lattice with coupling strength $C=0.25$ and on-site potential

$$V(x)=\frac{3}{20}x^2+x^4, \qquad (17)$$

which is often referred to as a hard ϕ^4 potential.

Figure 1 shows how the method compares with the rotating wave approximation, using $T_n=\cos(\omega t)$ on the same lattice. To estimate the accuracy, we calculated breathers using a Newton-Raphson method to solve the equations of motion for periodic solutions with homoclinic orbits as an initial guess for the breather shape at time $t=0$. Since the effective potential is even with respect to T_n we can use any homoclinic orbit as an initial guess. Then, we suppose that the breather shape locally follows a map of the form $\hat{f}(u_n(0))=u_{n+1}(0)+u_{n-1}(0)$ and compare the shape of the function $\hat{f}$ with f. For the case considered here, the method is more accurate than the rotating wave approximation by a factor of 2.

2. A Klein-Gordon lattice with soft Morse potential

As a second example, we take a potential for which the ODE is difficult to solve analytically, namely, the Morse potential

$$V(x)=[1-\exp(-x)]^2, \qquad (18)$$

using $C=0.01$ for this Klein-Gordon (KG) lattice.

A rotating wave approximation with $T_n=\cos(\omega t)$ is not possible due to the asymmetry of the potential. Using a Fourier-series method requires higher than two-dimensional

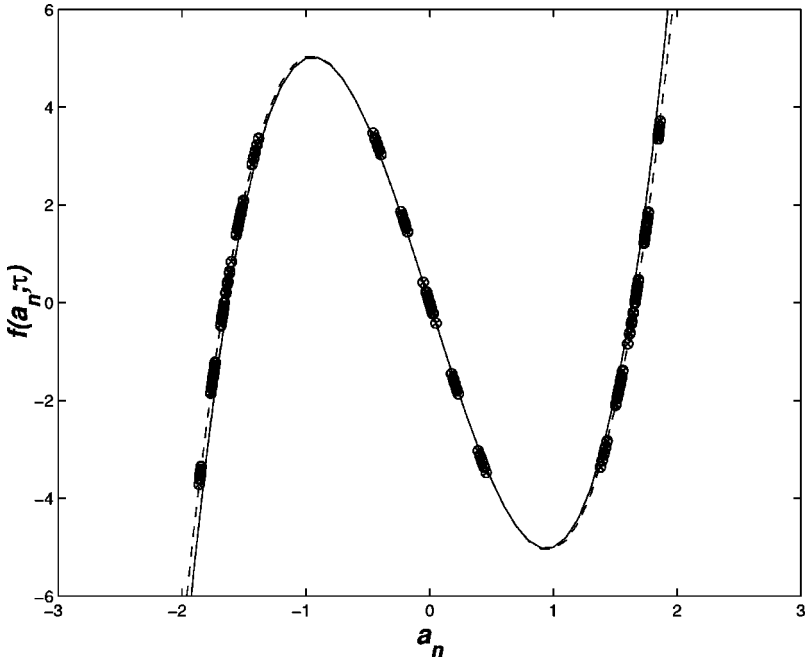

FIG. 1. Accuracy results for a Klein-Gordon lattice with hard ϕ^4 potential (17), $C=0.25$ and the period $\tau=2(2.8)^{-1/2}\pi$. The figure shows the function $f(a_n)=a_{n+1}+a_{n-1}$ as determined numerically using approximation (4) (dashed line), by the rotating wave approximation (solid line) and the data $\hat{f}(u_n(0))=u_{n+1}(0)+u_{n-1}(0)$ determined from breather solutions (dots). The maximum distance between the dots and the line using approximation (4) is within 1% of the maximum amplitude, whereas the rotating wave approximation reaches only 2%.

mappings. Therefore, Tsironis' approximation combined with our homoclinic orbit approach is very well suited for this potential since we work with a two-dimensional map. However, since the effective potential is not even with respect to T_n, not all homoclinic orbits are suitable candidates for finding breathers. We can only use those orbits whose neighboring amplitudes have the same sign or when one of them is very small compared to the other.

In Fig. 2, we show the accuracy of this approach in the same way as for the ϕ^4 potential in Fig. 1. We have also compared the homoclinic orbits with their corresponding breathers by calculating the distance using the max norm $\|\vec{u}(0)-\vec{a}\|=\max|u_n(0)-a_n|$, where $\vec{u}(0)=(\ldots,u_{-1}(0),u_0(0),u_1(0),\ldots)$ and $\vec{a}$ likewise. Although the maximum absolute distance was observed to be 7×10^{-2} the average absolute distance was only 7×10^{-3}. In Fig. 3, some of the shapes of the calculated breathers are given.

B. General lattices and Fermi-Pasta-Ulam (FPU) lattices

For general lattices we have the effective potential:

$$V_{\text{eff}}(a_n,a_{n-1},a_{n+1},T_n)$$
$$=\frac{1}{a_n^2}V(a_nT_n)-\frac{1}{a_n(a_{n+1}-a_n)}W((a_{n+1}-a_n)T_n)$$
$$+\frac{1}{a_n(a_n-a_{n-1})}W((a_n-a_{n-1})T_n). \qquad (19)$$

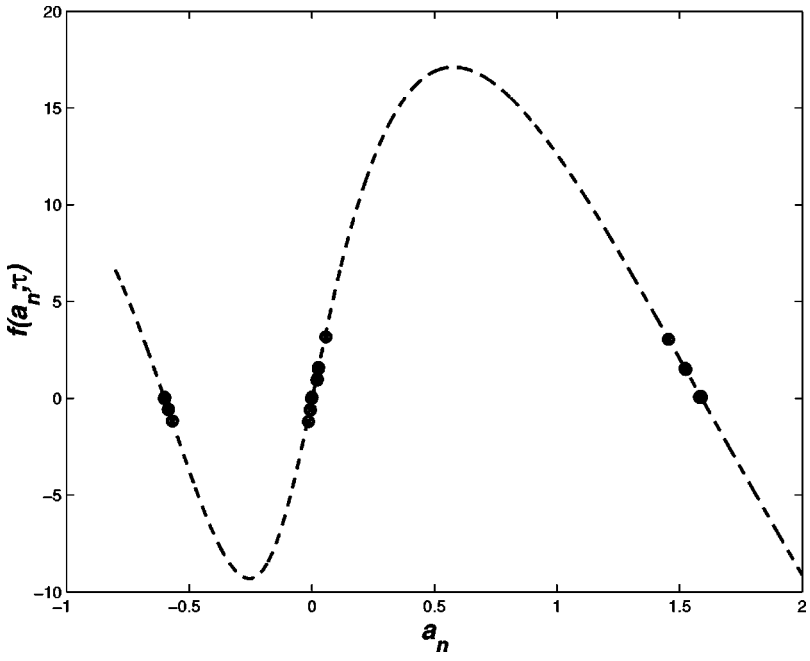

FIG. 2. Accuracy results for a Klein-Gordon lattice with Morse potential (18). Here, we use $C=0.01$ and the period $\tau=2(0.41)^{-1/2}\pi$. The figure shows the function $f(a_n)=a_{n+1}+a_{n-1}$ as determined numerically (dashed line) and the data $\hat{f}(u_n(0))=u_{n+1}(0)+u_{n-1}(0)$ determined from the exact breather solutions (dots). The maximum distance between the dots and the line is within 5% of the maximum amplitude.

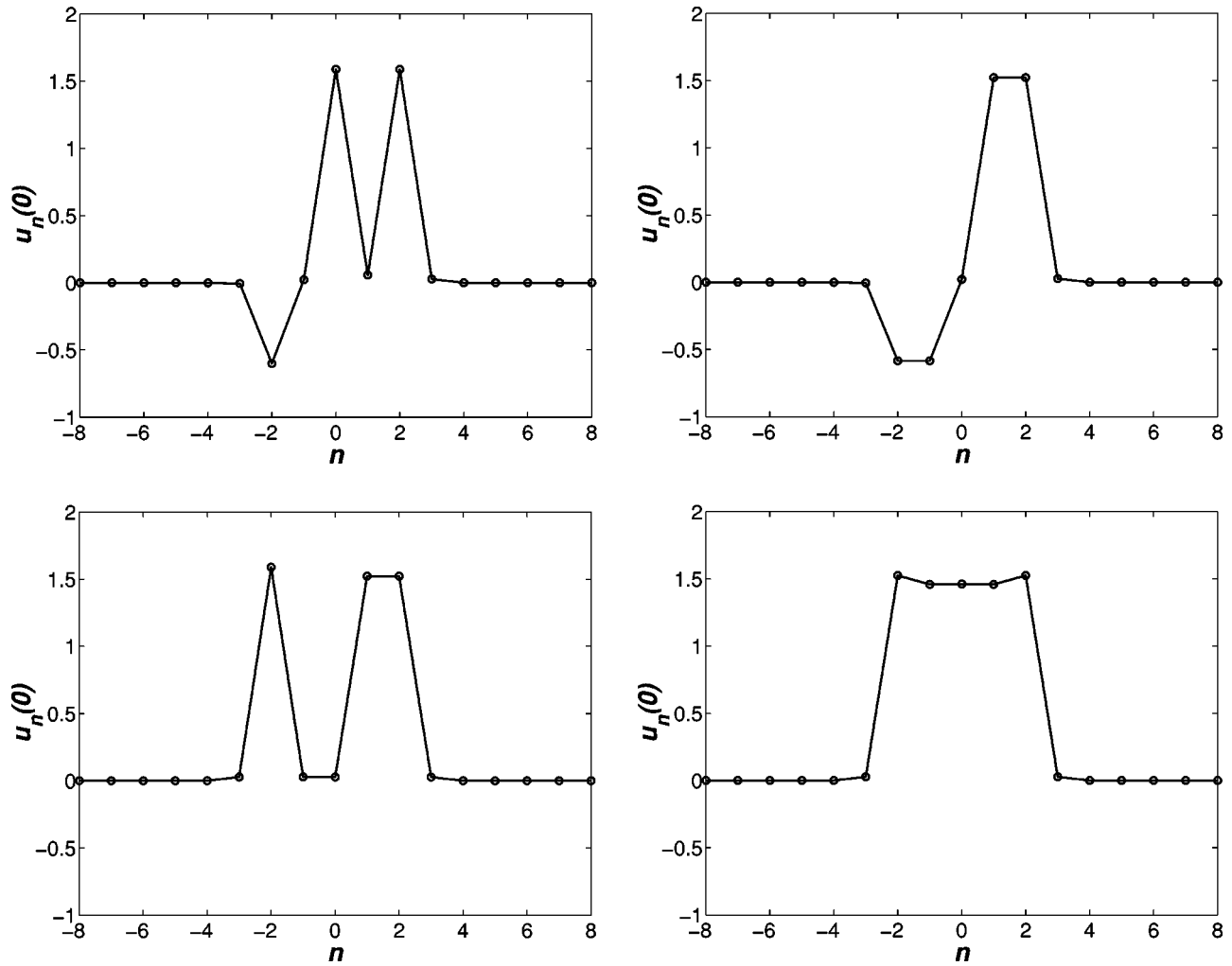

FIG. 3. Several simple breather shapes determined with the method presented here for the Morse potential (18) in a Klein-Gordon lattice. The coupling strength is $C=0.01$ and the period $\tau=2(0.41)^{-1/2}\pi$. The maximum observed absolute distance on a site between a homoclinic orbit and the corresponding breather (i.e., $\max|u_n(0)-a_n|$) is 7×10^{-2} which is 4.5% of the breather amplitude at that site. On average, the observed maximum distance is 7×10^{-3}.

In order to apply the methods from Ref. [12] to find homoclinic orbits we need to define a map and its inverse. Therefore, we first use the extra knowledge of the period τ to determine $a_{n+1}=f(a_n,a_{n-1};\tau)$ and $a_{n-1}=g(a_n,a_{n+1};\tau)$. Thus, we can define a map for the amplitudes a_n as

$$M:\begin{cases} a_{n+1}=f(a_n,b_n;\tau) \\ b_{n+1}=a_n \end{cases} \tag{20}$$

and its inverse

$$M^{-1}:\begin{cases} a_{n-1}=g(a_n,b_n;\tau) \\ b_{n-1}=a_n\,. \end{cases} \tag{21}$$

Existence conditions for the functions f and g are equivalent to the ones derived for KG lattices. The anharmonicity condition becomes $\partial\tau/\partial a_{n+1}\neq0$ and $\partial\tau/\partial a_{n-1}\neq0$. In our investigations this condition is always fulfilled for the range of amplitudes considered. The nonresonance condition is derived with the coupling strength C now replaced by $W''(0)$ in comparison with KG lattices, as can be seen by linearizing the effective potential V_{eff} around $a_n=0$ for small perturbations a_{n+1} and a_{n-1}. Thus, we need either $k^2\omega^2<V''(0)$ or $k^2\omega^2>4W''(0)+V''(0)$.

An FPU lattice with hard ϕ^4 potential

In Fig. 4, several breather shapes for a Fermi-Pasta-Ulam lattice [i.e., the on-site potential $V(x)=0$] with a hard ϕ^4 interaction potential

$$W(x)=\frac{3}{20}x^2+x^4 \tag{22}$$

are given. The effective potential is even with respect to T_n, such that all homoclinic orbits calculated should give accurate approximations of breathers.

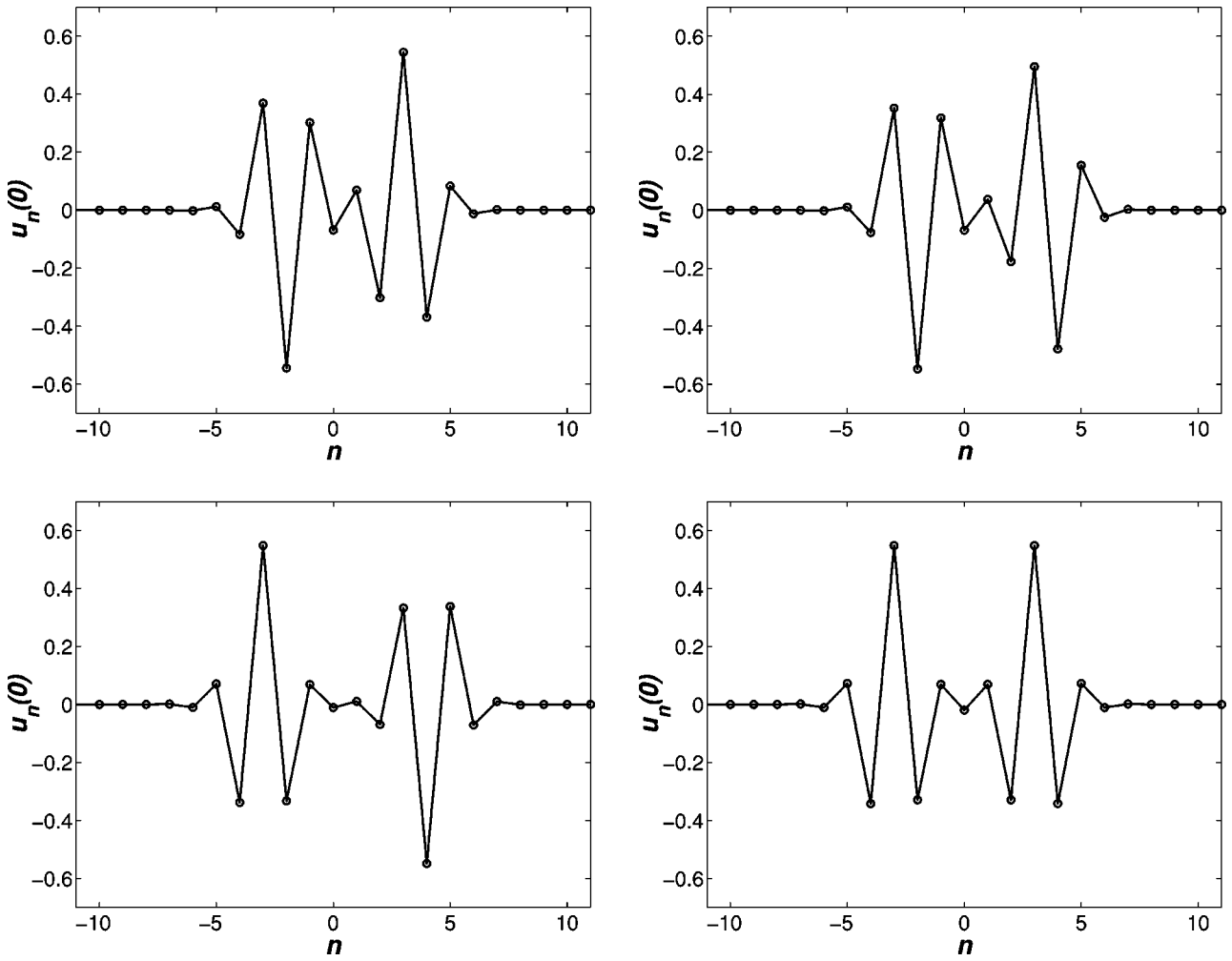

FIG. 4. Several breather shapes determined with the method presented here for the hard ϕ^4 potential (22) in a Fermi-Pasta-Ulam lattice. The period is $\tau=2(2.8)^{-1/2}\pi$. The maximum observed absolute distance on a site between a homoclinic orbit and the corresponding breather is $\max|u_n(0)-a_n|=5\times10^{-3}$ which is about 1% of the maximum amplitude $\max|u_n(0)|$.

The function f is a function of two variables and is shown in Fig. 5. Notice that since the interaction potential W is symmetric with the property $W(x)=W(-x)$, the function g is identical to f with the role of a_{n+1} and a_{n-1} interchanged. Furthermore, due to Eq. (11), we have the symmetry $f(x,y)=-f(-x,-y)$ for all $(x,y)\in\mathbb{R}\times\mathbb{R}$. Comparison of homoclinic orbits and breathers using the max norm shows an accuracy of about 1% distance relative to the largest amplitude.

III. APPLICATION TO TWO-DIMENSIONAL LATTICES

We consider now a two-dimensional lattice with one degree of freedom per lattice site [13]. The equations of motion are

$$\begin{aligned}\ddot{u}_{n,m}+V'(u_{n,m})=&W'(u_{n+1,m}-u_{n,m})+W'(u_{n-1,m}-u_{n,m})\\&+W'(u_{n,m+1}-u_{n,m})\\&+W'(u_{n,m-1}-u_{n,m}),\end{aligned}\tag{23}$$

with $(n,m)\in\mathbb{Z}\times\mathbb{Z}$. After inserting $u_{n,m}(t)=a_{n,m}T_{n,m}(t)$ and applying approximation (4), the ODE for $T_{n,m}$ becomes

$$\begin{aligned}&a_{n,m}\ddot{T}_{n,m}+V'(a_{n,m}T_{n,m})\\&\quad=[W'(a_{n+1,m}-a_{n,m})+W'(a_{n-1,m}-a_{n,m})\\&\quad+W'(a_{n,m+1}-a_{n,m})+W'(a_{n,m-1}-a_{n,m})]T_{n,m}.\end{aligned}\tag{24}$$

For general interaction potentials $W(x)$ one derives four separate recurrence relations using knowledge of the period τ to determine functions for $a_{n+1,m}$, $a_{n-1,m}$, $a_{n,m+1}$, and $a_{n,m-1}$, respectively. It is again possible to write the problem in an effective potential setting. The statements about which solutions to the recurrence relations are accurate approximations to breather solutions hold exactly as for one-dimensional Klein-Gordon lattices (see Sec. II).

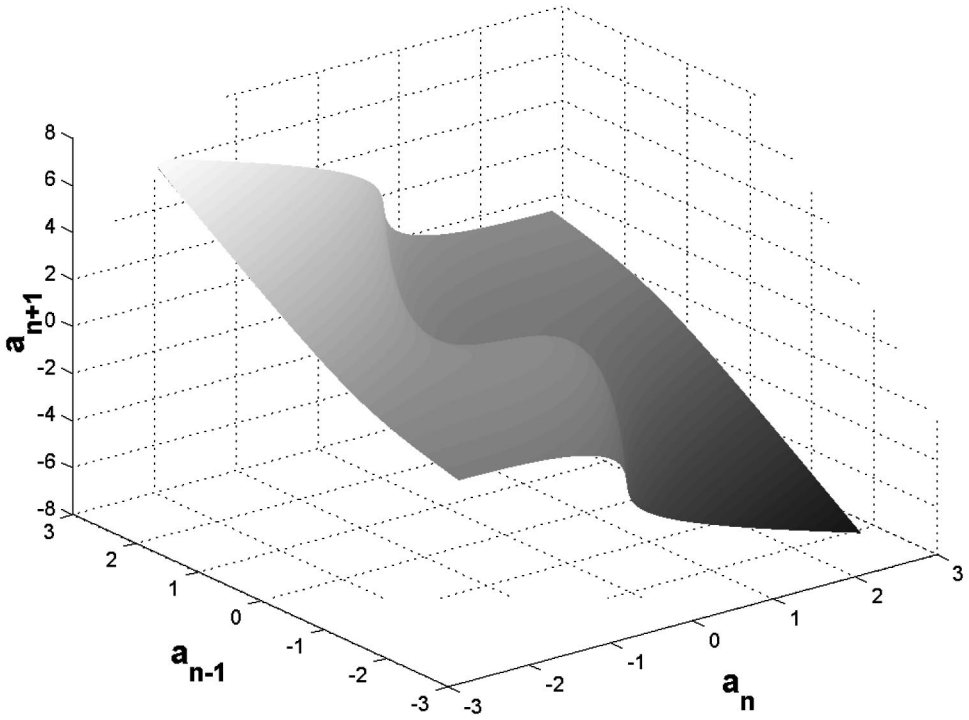

FIG. 5. The function $a_{n+1}=f(a_n,a_{n-1};\tau)$ for a Fermi-Pasta-Ulam lattice with a hard ϕ^4 potential (22). The function $a_{n-1}=g(a_n,a_{n-1};\tau)$ is identical to f with the role of a_{n-1} and a_{n+1} interchanged, due to the potential being even.

A. A two-dimensional Klein-Gordon lattice with hard ϕ^4 potential

In case of a harmonic interaction potential (i.e., a Klein-Gordon lattice), the ODE is reduced to

$$a_{n,m}\ddot{T}_{n,m}+V'(a_{n,m}T_{n,m})=C(a_{n+1,m}+a_{n-1,m}+a_{n,m+1}+a_{n,m-1}-4a_{n,m})T_{n,m}, \quad (25)$$

such that we need to determine only a single function $(a_{n+1,m}+a_{n-1,m}+a_{n,m+1}+a_{n,m-1})=f(a_{n,m};\tau)$. Anharmonicity and nonresonance conditions can be derived as easily as for one-dimensional lattices and are also checked to hold in all cases studied.

Setting the coupling $C=0.25$ and the on-site potential to be the familiar hard ϕ^4 potential (17), we first determine this function f. Using the techniques described in the Appendix, several solutions to the recursion relations

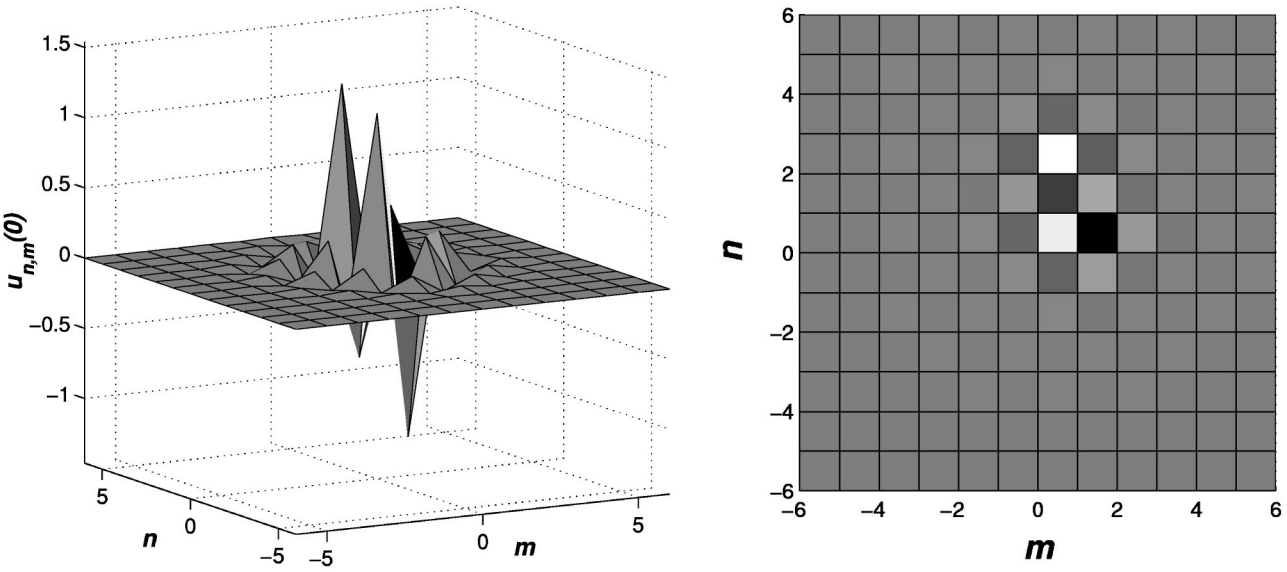

FIG. 6. The shape of a breather in a two-dimensional lattice with ϕ^4 potential. The coupling is $C=0.25$ and the period $\tau=2(2.8)^{-1/2}\pi$. Left: A three-dimensional image of the breather amplitudes $u_{n,m}$ at time $t=0$. Right: A projection on a two-dimensional plane, with colors indicating the relative values of $u_{n,m}(0)$, with lighter shades indicating higher values. The difference between the solution of the recurrence relations (the "homoclinic plane") and the breather, measured by $\max|u_{n,m}(0)-a_{n,m}|$, is 6.7×10^{-3}, which is about 0.5% of the maximum amplitude $\max|u_{n,m}(0)|$.

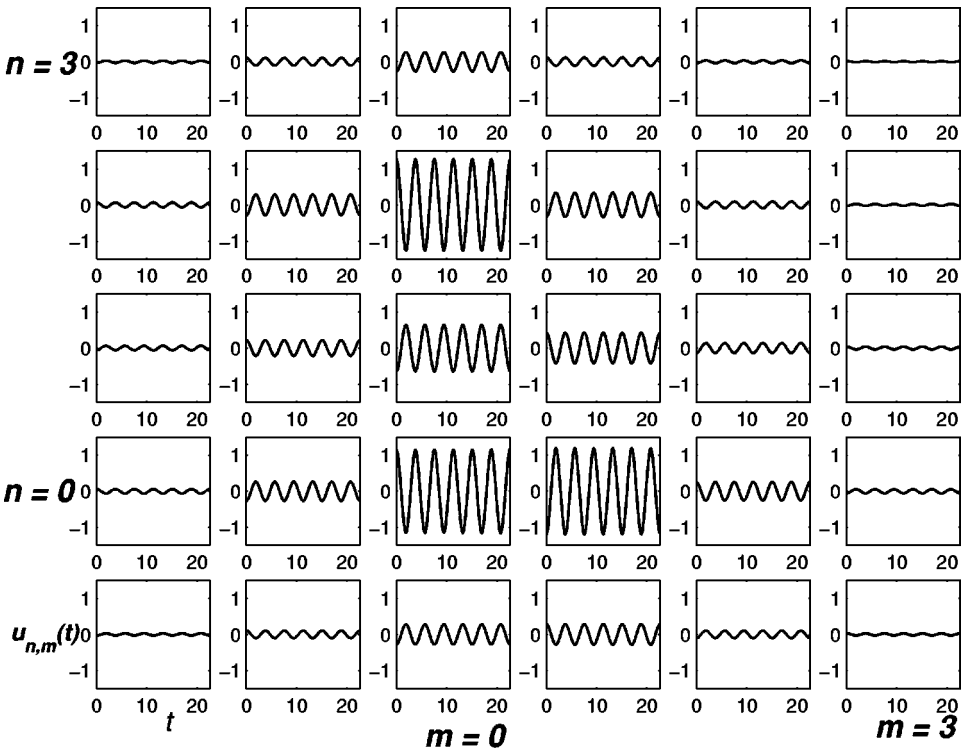

FIG. 7. Time evolution of the breather in a two-dimensional lattice with ϕ^4 potential, whose shape is depicted in Fig. 6. Shown here are the first six periods of the breather evolution. Each image shows $u_{n,m}(t)$, where n goes from -1 to 3 (bottom to top) and m from -2 to 3 (left to right).

$$a_{n+1,m}+a_{n-1,m}+a_{n,m+1}+a_{n,m-1}=f(a_{n,m};\tau) \quad (26)$$

under the asymptotic conditions

$$\lim_{n\to\pm\infty} a_{n,m}=0, \quad \forall \quad m$$
$$\lim_{m\to\pm\infty} a_{n,m}=0, \quad \forall \quad n, \quad (27)$$

have been constructed. Such a solution might be called a ''homoclinic plane'' in analogy with the name ''homoclinic orbit'' in one dimension. Since the effective potential for this problem is even, all homoclinic planes should give accurate approximations to breather solutions and $f(a_{n,m};\tau) = -f(-a_{n,m};\tau)$. Using these approximations, breathers can be found using a Newton-Raphson method. In Figs. 6 and 7, the shape and behavior of one such solution is presented. The difference between the homoclinic plane and the breather is about 6.7×10^{-3}, measured with the max norm $\max|u_{n,m}(0) - a_{n,m}|$.

IV. CONCLUDING REMARKS

In this paper, we have shown that using recurrence relations with appropriate asymptotic conditions is a useful tool for approximating breather solutions in one- and two-dimensional lattices. The conjecture is made that this can be done for higher dimensions as well, as long as there is only a single scalar variable per lattice site. Our work also shows that Tsironis' approximation [9] gives more accurate approximations than the rotating wave approximation with a single cosine as basis function. It can also be applied to lattices for which cosines are clearly the wrong basis function, for instance when dealing with asymmetric potentials. Furthermore, the method presented here uses the lowest possible dimension of the recurrence relations [i.e., the same dimension as the equation of motion, when seen as a recurrence relation in function space for the $u_{\vec{n}}(t)$].

In many cases, the way to find solutions to the recurrence relations can be applied as presented in the Appendix. When this is not possible, one can resort to more reliable methods such as the ones presented in Ref. [12]. The computation of these solutions requires relatively little effort, considering the complexity and accuracy of the solutions found in comparison to the breathers being approximated. Based on the discussion of the relative error made when using approximation (4), we were able to predict which solutions would give accurate approximations. All results confirmed these predictions.

Determining the recurrence relations themselves is a very rewarding task on its own. Once they are determined for a certain set of on-site potentials and interaction potentials as well as a specific period, one can generate an infinite number of solutions by the techniques mentioned above. Therefore, large numbers of numerically accurate breathers in lattices with a single scalar variable per lattice site and nearest-neighbor interactions can be generated using this method, in a relatively short time.

Finally, identifying the stability of these localized solutions is a problem of great interest, especially with a view towards applications and experiments. In a future publication, we intend to return to this question not only using linear stability analysis but also applying more global methods to explore the extent of the stability region of breathers in phase space.

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APPENDIX: SOLVING THE RECURRENCE RELATIONS

In the following, we present a fast method for computing solutions of a system of recurrence relations

$$f(a_{\vec{n}}) + \sum_{\vec{m} \in B_{\vec{n}}} g(a_{\vec{m}} - a_{\vec{n}}) = 0, \quad \forall\ \vec{n} \in \mathbb{Z}^d, \tag{A1}$$

with $a_{\vec{n}} \in \mathbb{R}$, f: $\mathbb{R} \to \mathbb{R}$, and g: $\mathbb{R} \to \mathbb{R}$ with $f(0) = g(0) = 0$, under the asymptotic condition $a_{\vec{n}} \to 0$ as $\|\vec{n}\| \to \infty$ with the norm on $\mathbb{Z}^d$ defined as $\|\vec{n}\| = \Sigma_{i=1}^{d} |n_i|$.

For this numerical calculation, we limit ourselves to a finite subspace $\vec{n} \in S \subset \mathbb{Z}^d$. If this subspace is taken large enough, we can set the boundary condition such that $a_{\vec{n}} = 0$ if $\vec{n} \in \partial S$, since the boundaries will have no influence on the behavior of the solution in the numerical method proposed below. Numerical solutions of Eq. (A1) can be found starting from an initial guess using a Newton-Raphson method. As shown by Beyn and Kleinkauf, this method converges if a solution is present, in the case of finite-dimensional mappings [14]. We conjecture that this holds also in the case of Eq. (A1). The idea of the method is to provide accurate initial conditions for a Newton-Raphson search.

Observe first that $a_{\vec{n}} = 0$ for all $\vec{n} \in S$ is an exact solution of Eq. (A1). We call this the initial seed O_0. The first generation of solutions O_1 is found as follows. First, we set $O_1 = M(O_0)$, with M an operator which can be chosen in different ways, e.g., to preserve some symmetry. For now, we choose M to be the identity map. Then, we allow a single site of O_1 to regain its freedom (i.e., we set the amplitude at this site to be equal to some unknown variable x). Without loss of generality, we can choose this site to be the origin $\vec{n} = 0$. We solve (numerically) Eq. (A1) with $\vec{n} = 0$ for $a_{\vec{n}}$. This is a single equation with a single unknown, but, in general, with several solutions for $a_{\vec{n}=0}$. Each of these solutions now defines a member of O_1 and is a suitable initial condition for applying a Newton-Raphson search. The numerically exact solutions found by this procedure obey the recurrence relations and the boundary conditions. Each of these can be the seed for a new generation of solutions, obtained in the same way as above, but with the allowed freedom at a different site, if the map M is the identity map.

This method for solving Eq. (A1) was also mentioned in the context of homoclinic orbits in the concluding remarks of Ref. [12]. In the spirit of that paper, the operator M can be chosen in such a way as to generate a well-defined family of solutions preserving a symmetry. For the one-dimensional lattices of Sec. II, this operator M can be a shift matrix, preserving, e.g., the symmetry $a_n = a_{-n}$, if M is such that $\hat{a}_{n-1} = a_n$ for $n < 0$ and $\hat{a}_{n+1} = a_n$ for $n > 0$, with the hat denoting a solution in the new generation. By allowing the site at the origin to regain its freedom we generate (starting from O_0) all symmetric homoclinic orbits of the two-dimensional map, with the symmetry $a_n = a_{-n}$.

Using the ideas of Ref. [12] we can as easily determine *asymmetric* homoclinic orbits as long as the map is invertible. For higher-dimensional lattices, similar methods can be derived. Application of this method is limited by the existence of solutions for the amplitude of the free lattice site. If there are no solutions, one has to resort to the full method for finding homoclinic orbits in the case of one-dimensional lattices or to make a guess about approximate solutions for higher-dimensional lattices and depend on the convergence of the Newton-Raphson scheme.

[1] See the works by S. Takeno and A.J. Sievers, e.g., A.J. Sievers and S. Takeno, Phys. Rev. Lett. **61**, 970 (1988); S. Takeno, K. Kisoda, and A.J. Sievers, Prog. Theor. Phys. Suppl. **94**, 242 (1988).

[2] R.S. MacKay and S. Aubry, Nonlinearity **7**, 1623 (1994).

[3] J.L. Marin and S. Aubry, Nonlinearity **9**, 1501 (1996); S. Aubry, Physica D **103**, 201 (1997).

[4] See, e.g., H.S. Eisenberg *et al.*, Phys. Rev. Lett. **81**, 3383 (1998); B.I. Swanson, *et al.*, *ibid.* **82**, 3288 (1999); E. Trias, J.J. Mazo, and T.P. Orlando, *ibid.* **84**, 741 (2000); P. Binder, *et al.*, *ibid.* **84**, 745 (2000).

[5] See for instance, Ref. [9]; S.A. Kiselev, Phys. Lett. A **148**, 95 (1990); F. Fischer, Ann. Phys. (Leipzig) **2**, 296 (1993); Y.S. Kivshar, Phys. Rev. E **48**, R43 (1993).

[6] See, e.g., Ref. [1]; J.B. Page, Phys. Rev. B **41**, 7835 (1990); S.R. Bickham and A.J. Sievers, *ibid.* **43**, 2339 (1991); S.R. Bickham, A.J. Sievers, and S. Takeno, *ibid.* **45**, 10 344 (1992); K.W. Sandusky, J.B. Page, and K.E. Schmidt, *ibid.* **46**, 6161 (1992); V.M. Burlakov, S.A. Kiselev, and V.I. Rupasov, Phys. Lett. A **147**, 130 (1990); S. Takeno, J. Phys. Soc. Jpn. **59**, 1571 (1990); S. Takeno, *ibid.* **59**, 3861 (1990); S. Takeno and K. Hori, *ibid.* **59**, 3037 (1990); K. Hori and S. Takeno, *ibid.* **61**, 4263 (1992).

[7] T. Bountis *et al.*, Phys. Lett. A **268**, 50 (2000).

[8] For example, S. Takeno and K. Hori, J. Phys. Soc. Jpn. **60**, 847 (1991); S. Takeno, *ibid.* **61**, 2821 (1992); Y.S. Kivshar, Phys. Lett. A **173**, 172 (1993); S. Flach, Phys. Rev. E **50**, 3134 (1994); S. Flach, *ibid.* **51**, 1503 (1995); S. Flach, *ibid.* **51**, 3579 (1995); O. Bang and M. Peyrard, *ibid.* **53**, 4143 (1996); J.L. Marin, S. Aubry, and L.M. Floria, Physica D **113**, 283 (1998); J.F.R. Archilla, R.S. MacKay, and J.L. Marin, *ibid.* **134**, 406 (1999).

[9] G.P. Tsironis, J. Phys. A **35**, 951 (2002).

[10] We accept a solution as numerically exact when $\max|u_{\vec{n}}(\tau)$

$-u_{\vec{n}}(0)|<\epsilon$ with ϵ small; in our calculations we use $\epsilon=10^{-6}$.
[11] J.M. Bergamin, T. Bountis, and C. Jung, J. Phys. A **33**, 8059 (2000).
[12] J.M. Bergamin, T. Bountis, and M.N. Vrahatis, Nonlinearity **15**, 1603 (2002).
[13] For some other numerical approximations to breathers in two-dimensional lattices see, e.g., V.M. Burlakov, S.A. Kiselev, and V.N. Pyrkov, Phys. Rev. B **42**, 4921 (1990); S. Flach, K. Kladko, and C.R. Willis, Phys. Rev. E **50**, 2293 (1994).
[14] W.-J. Beyn and J.-M. Kleinkauf, SIAM (Soc. Ind. Appl. Math.) J. Numer. Anal. **34**, 1207 (1997); W.-J. Beyn and J.-M. Kleinkauf, Numer. Algorithms **14**, 25 (1997).