Seminumerical method for tracking multibreathers in Klein-Gordon chains

Vassilis Koukouloyannis*
Department of Physics, University of Thessaloniki, Thessaloniki 54124, Greece
(Received 1 April 2003; published 30 April 2004)

We present a method of numerical calculation of multibreathers in Klein-Gordon chains. This method provides in advance the linear stability of the calculated multibreather solutions. We illustrate the method by calculating initial conditions for multibreathers in a chain of coupled Morse oscillators.

DOI: 10.1103/PhysRevE.69.046613 PACS number(s): 05.45.Yv, 05.45.Xt, 45.05.+x, 63.20.Pw

I. INTRODUCTION

Many researchers (e.g., Refs. [1,2]) are presently interested on spatially localized and time-periodic motions in systems of weakly coupled oscillators, which are called breathers. The first observation of breathers was made by Sievers and Takeno [3]. A generalization of the notion of a breather is the multisite breather or multibreather where in the uncoupled limit more than one oscillators are moving. The first existence proof of breathers in systems of weekly coupled Hamiltonian or time-reversible oscillators has been given in Ref. [4]. This proof led directly to a method of numerical calculation of the breather solutions (e.g., Ref. [5]). Apart from this, there exist also other numerical methods of calculating initial conditions for breathers or multibreathers, such as the method of homoclinic orbits [6].

In Ref. [7], an existence proof of multibreathers is presented, which is based on the ideas of Poincaré ([8],[9] Sec. 42). This proof shows the existence of monoparametric families of multibreathers with the total energy of the system as a parameter. In this work we present a systematic way of using these results in order to acquire initial conditions for multibreathers. The system we study is a chain of one-dimensional oscillators with a nearest-neighbor coupling, through a small nonzero parameter ε. This method provides the orbits, on the phase-space of the system, for $\varepsilon=0$ which are going to be continued, to provide a multibreather, for $\varepsilon\neq 0$. By fixing a point on this orbit we get an initial estimation and, at the same time, we define the Poincaré section on which our root finding method is going to work. The use of the Poincaré section is necessary due to Hamiltonian character of the system. The method also provides, in advance, the linear stability of the calculated multibreather solution, by evaluating, up to order $O(\sqrt{\varepsilon})$ its characteristic exponents. The work is divided in two sections. In Sec. II we construct the method using the required elements from Ref. [7]. Since the formulas provided there make use of the action-angle variables, we provide a way to perform the same calculations when this transformation is not known. In Sec. III, we apply this method to a one-dimensional chain of weakly coupled Morse oscillators.

II. DESCRIPTION OF THE METHOD

We define our oscillator by an autonomous Hamiltonian of one degree of freedom

$$H_{\mathrm{osc}}=\tfrac{1}{2}p^2+V(x),$$

where x is the displacement, p is the conjugate momentum, and $V(x)$ is the potential function. In this case the system is integrable since H_{osc} is always an integral of motion. We assume that $V(x)$ possesses a minimum at $x=0$ with $V''(0)=\omega_p^2$ with $\omega_p\in\mathbb{R}$. The well-known [10] action-angle canonical transformation is defined in the area of the bounded motion of the oscillator, which is after all the motion that interests us. The motion of the oscillator is described, in these variables, by the equations

$$J=J(h),$$

$$w=\omega t+\vartheta, \tag{1}$$

where $\vartheta=w(0)$ is the initial angle of the oscillation and h is the pertinent value of H_{osc} for a specific orbit, which is obviously constant along this orbit. In action-angle variables, the Hamiltonian of the oscillator becomes $H_{\mathrm{osc}}=H_{\mathrm{osc}}(J)$, and the frequency of the oscillation is given by

$$\omega(J)=\frac{\partial H_{\mathrm{osc}}(J)}{\partial J}.$$

The chain, we are going to study, is constructed by considering a countable set of oscillators with a nearest-neighbor coupling through a coupling constant ε. The Hamiltonian of the system becomes

$$H=H_0+\varepsilon H_1 = \sum_{i=-\infty}^{\infty}\left(\frac{1}{2}p_i^2+V_i(x_i)\right)+\frac{\varepsilon}{2}\sum_{i=-\infty}^{\infty}(x_{i+1}-x_i)^2, \tag{2}$$

where x_i is the position, p_i represents the momentum, and V_i denotes the potential of the ith oscillator. Note that H_0 is trivially integrable being separable. The equations of motion for this Hamiltonian are

$$\dot{x}_k=\frac{\partial H}{\partial p_k}=p_k, \tag{3a}$$

*Electronic address: vkouk@skiathos.physics.auth.gr

$$\dot{p}_k = -\frac{\partial H}{\partial x_k} = -V_k'(x_k) + \varepsilon(x_{k+1} - 2x_k + x_{k-1}), \quad k \in \mathbb{Z}, \tag{3b}$$

where

$$V_k'(x_k) = \frac{dV_k(x_k)}{dx_k}.$$

For $\varepsilon = 0$, which is the uncoupled case, we set a number of neighboring oscillators, which we call ''central,'' moving in periodic orbits satisfying the resonance condition

$$\frac{\omega_{-m}}{k_{-m}} = \cdots = \frac{\omega_n}{k_n} = \omega, \quad m, \ldots, n \in \mathbb{N}, \quad k_{-m}, \ldots, k_n \in \mathbb{Z}, \tag{4}$$

while the rest lie on the stable equilibrium point $(x_i, p_i) = (0,0)$. The indices in Eq. (4) denote the oscillator. The total number of central oscillators is $q = m + n + 1$ and we denote by $I = \{-m, \ldots, n\}$ the set of indices for these oscillators and $I^* = \{-m, \ldots, n\} \backslash \{0\}$. Then, a periodic orbit of period $T = 2\pi/\omega$ is defined in the phase space of the complete system, and it corresponds to a time-periodic and trivially spatially localized motion along the chain. We define the *resonant angles* as

$$\phi_i = k_0 \vartheta_i - k_i \vartheta_0, \quad i \in I^*. \tag{5}$$

It is proven [7] that this motion is continued, for $\varepsilon \neq 0$ small enough, forming a discrete multibreather if the following conditions are satisfied

$$T \neq \frac{2\pi}{\omega_p} l = l T_p, \quad \forall \quad l \in \mathbb{Z}, \tag{6}$$

$$\det\left|\frac{\partial^2 H_0}{\partial J_i \partial J_j}\right| \neq 0, \quad i,j \in I, \tag{7}$$

$$\frac{\partial \langle H_1 \rangle}{\partial \phi_i} = 0, \quad i \in I^*, \tag{8}$$

$$\det\left|\frac{\partial^2 \langle H_1 \rangle}{\partial \phi_i \partial \phi_j}\right| \neq 0, \quad i,j \in I^*, \tag{9}$$

where

$$\langle H_1 \rangle = \frac{1}{T}\int_0^T H_1 dt, \tag{10}$$

is the average value of H_1. We note that the integration in Eq. (10) is performed along the periodic orbit of the uncoupled case, defined by Eq. (4). Equation (6) is the nonresonance condition with the phonons of the system and Eq. (7) is the anharmonicity condition for H_0. Since for $\varepsilon = 0$ the system is integrable and we consider q central oscillators, the orbits lie on q-dimensional resonant tori. The solutions of Eq. (8) define the orbits of such a resonant torus which will be continued under a small but non-zero perturbation ($\varepsilon \neq 0$), while Eq. (9) denotes that the zeros of Eq. (8) must be simple. The resonance condition (4) is valid, not only for one torus, but for a monoparametric family of tori with the total energy of the system as a parameter. We can choose a representative of this family by fixing the energy to a value E_0.

We denote by **S** the set of the periodic orbits on the resonant torus that will be continued for $\varepsilon \neq 0$ and $s_i \in \mathbf{S}$. It is known that the solution of a Hamiltonian system, with Hamiltonian analytic with respect to a parameter ε, is analytic with respect to the same parameter [11]. So, for $\varepsilon \neq 0$ the desired periodic orbits, which are essentially the multibreathers we want to construct, will lie in the ε-neighborhood of the respective s_i.

Each distinct set of ϕ_i, which satisfies Eqs. (8) and (9) defines a s_j. In order to attain initial conditions we have to define an initial point on this specific orbit. We fix a specific ϑ_k and we calculate the other ϑ_i through Eq. (5) which defines ϕ_i. We use the action-angle transformation and get this point in coordinates x_i, p_i. We define the Poincaré surface of the section by fixing a specific x_j and taking the conjugate variable to be $p_j > 0$ on it. Let $\bar{x}, \bar{p}$ be the position and momentum vectors, respectively, and let $\Phi(\bar{x}, \bar{p})$ be the Poincaré map. Every point $(\bar{x}, \bar{p})$ on the surface defines an orbit in the phase space, and this map gives the next point that this orbit crosses the surface with $p_j > 0$. Then, if $\bar{\eta} = (\bar{x}, \bar{p})$, for a periodic orbit of this map we have $\Phi(\bar{\eta}) = \bar{\eta}$, or more generally, $\Phi^k(\bar{\eta}) = \underbrace{\Phi \circ \Phi \circ \cdots \circ \Phi(\bar{\eta})}_{k \text{ times}} = \bar{\eta}$.

Then the problem of finding a periodic orbit becomes a problem of finding the zeros of the function

$$\mathbf{F}(\bar{\eta}) \equiv \Phi^k(\bar{\eta}) - \bar{\eta}. \tag{11}$$

To approximate this solution, we have to use a numerical method of root finding in systems of nonlinear equations. We chose to use the Broyden method [12], since its convergence behavior seemed better than Newton's method. This method is shortly described on p. 389 of Ref. [13]. In order to calculate the points of the map we need a method of numerical integration of differential equations and for that we use a fourth to fifth order with adaptive step size Runge-Kutta method, on p. 714 of Ref. [13].

By calculating **S** we do not know yet if the resulting multibreather will be stable or unstable. As it is known [14], the linear stability of the multibreather depends on the eigenvalues of the linearized system (3). As it is described in Ref. [7], for ε small enough, the eigenvalues of the noncentral oscillators lie on the unit circle, while the eigenvalues of the central ones are

$$\lambda_i = e^{\pm \sigma_i T},$$

where σ_i are the *characteristic exponents*. According to Ref. [9] Sec. 79, σ_i are analytic with respect to $\sqrt{\varepsilon}$, so they are expanded as

$$\sigma_i = \sqrt{\varepsilon}\sigma_{i1} + o(\sqrt{\varepsilon}), \quad i \in I, \tag{12}$$

where σ_{i1}^2 are the eigenvalues of the $q \times q$ matrix **E** defined as

$$\mathbf{E} = -\mathbf{A} \cdot \mathbf{B}, \tag{13}$$

where

$$A_{ik}=\frac{\partial^2\langle H_1\rangle}{\partial\vartheta_i\partial\vartheta_k},\quad B_{kj}=\frac{\partial^2 H_0}{\partial J_k\partial J_j},\quad i,k,j\in I. \tag{14}$$

Due to conservation of energy, one pair of eigenvalues λ_i of the central oscillators remains equal to one, i.e., one pair of exponents remains equal to zero in the perturbed system. If all other eigenvalues lie on the unit circle of the complex plane (i.e., the corresponding exponents are purely imaginary), the breather is linearly stable, while if at least one eigenvalue has modulus different from 1 it will be unstable. So, the only case for linear stability is met when all nonzero σ_{i1}^2 are negative and are simple eigenvalues of the above matrix **E**, since if some $\sigma_{i1}^2>0$ the corresponding eigenvalues will leave the unit circle along the real axis, and if all $\sigma_{i1}^2<0$ but are not distinct, complex instability can occur, as explained in Ref. [7]. The multibreather can become unstable if ε becomes large enough, so that the eigenvalues of the central oscillators reach the phonon band. Then, complex instability can also occur.

As is obvious from the above analysis, the action-angle canonical transformation is crucial to the construction of the method. But its explicit form, which is often very hard to be acquired, is not required. To demonstrate this fact we perform the following analysis. Note that using Eq. (5), we get

$$\frac{\partial\langle H_1\rangle}{\partial\phi_i}=-\frac{1}{k_0}\frac{\partial\langle H_1\rangle}{\partial\vartheta_i},\quad \frac{\partial^2\langle H_1\rangle}{\partial\phi_i\partial\phi_j}=\frac{1}{k_0^2}\frac{\partial^2\langle H_1\rangle}{\partial\vartheta_i\partial\vartheta_j},\quad i,j\in I^*. \tag{15}$$

So, conditions (8) and (9) become

$$\frac{\partial\langle H_1\rangle}{\partial\vartheta_i}=0, \tag{16}$$

and

$$\det\left|\frac{\partial^2\langle H_1\rangle}{\partial\vartheta_i\partial\vartheta_j}\right|\neq 0,\quad i,j\in I^*, \tag{17}$$

respectively. By taking under consideration the facts that the action-angle variables w_i, J_i depend only on the corresponding x_i, p_i, that H_1 depends only on the x_i and that

$$\frac{dx_i}{dt}=\omega_i\frac{\partial x_i}{\partial w_i},$$

we get

$$\frac{\partial\langle H_1\rangle}{\partial\vartheta_i}=\frac{1}{T}\int_0^T\frac{\partial H_1}{\partial w_i}dt=\frac{1}{\omega_i T}\int_0^T\frac{\partial H_1}{\partial x_i}p_i dt, \tag{18}$$

and

$$\frac{\partial^2\langle H_1\rangle}{\partial\vartheta_i\vartheta_j}=\frac{1}{T}\int_0^T\frac{\partial^2 H_1}{\partial w_i\partial w_j}dt=\begin{cases}\dfrac{1}{\omega_i^2 T} & \displaystyle\int_0^T\frac{\partial^2 H_1}{\partial x_i^2}p_i^2+\frac{\partial H_1}{\partial x_i}\dot{p}_i dt,\quad i=j\\[2ex] \dfrac{1}{\omega_i\omega_j T} & \displaystyle\int_0^T\frac{\partial^2 H_1}{\partial x_i\partial x_j}p_i p_j dt,\quad i\neq j,\quad i,j\in I.\end{cases} \tag{19}$$

We calculate q orbits in the domain of bounded motion of the oscillator we consider, satisfying the resonance condition (4), calculate the corresponding energies E_i, and consider the q central oscillators moving on them. This can easily be done by numerically defining a function $T(x_0,y_0)$ which calculates the period of an orbit, given its initial conditions. Then finding orbits satisfying the resonance condition (4) becomes a usual shooting problem. Let $\eta_{i_0}=(x_{i_0},p_{i_0})=(x_i(0),p_i(0))$. Condition (16) defines, through Eq. (18), a relationship between the various η_{i_0} condition (8), as defines a relationship between ϑ_i, determining this way the orbits of the resonant q-torus for $\varepsilon=0$, which will be continued for $\varepsilon\neq 0$ to provide the multibreathers. So, in order to acquire initial conditions of these orbits for $\varepsilon=0$, we have to fix some η_{k_0}, usually by also taking care of $p_{k_0}>0$. This way, in order to acquire the rest of the η_{i_0}, we have to solve a system of equations which, because of the form of H_1, decomposes to give $n+m$ independent two branched equations

$$F_i(x_{i_0})=\int_0^T\frac{\partial H_1}{\partial x_i}dt=0, \tag{20}$$

where the value of p_{i_0} is calculated through $p_{i_0}=\pm\sqrt{2(E_i-V(x_{i_0})}$. The fixed value of x_{k_0}, the sign of p_{k_0}, and the value of the total energy for $\varepsilon=0$, $E=\Sigma_{i=-m}^{n}E_i$ defines the Poincaré section on which we are going to work in order to calculate the multibreathers for $\varepsilon\neq 0$ exactly as we did before, where we will use as initial estimates the calculated values of η_{i_0}.

These solutions must satisfy also Eq. (17) for the continuation to be valid. This condition is calculated by substituting the elements of this determinant by Eq. (19).

For the computation of the stability matrix **E** we have to note that

$$B_{ij}=\frac{\partial^2 H_0}{\partial J_i\partial J_j}=\begin{cases}0, & i\neq j\\ \dfrac{d\omega_i}{dJ_i}, & i=j,\end{cases}$$

TABLE I. First estimation for $\phi_{-1}=\phi_1=\pi$.

$\vartheta_{-1}=0.361\,367$	$\vartheta_0=-1.390\,11$	$\vartheta_1=0.361\,367$
$x_{-1}=0.0$	$x_0=3.271\,092$	$x_1=0.0$
$p_{-1}=1.322\,875$	$p_0=-0.294\,0698$	$p_1=1.322\,875$

and

$$\frac{d\omega_i}{dJ_i}=\frac{d\omega_i}{dE_i}\frac{dE_i}{dJ_i}. \tag{21}$$

Function $\omega(E)$ is easily defined by forcing η_0 of the previously defined $T(\eta_0)$ to take values along the positive x axis. Then the specific orbit crosses this axis to $x_{i_{\max}}$ which is related to the corresponding energy by $E_i=V(x_{i_{\max}})$. So $\omega(E)$ is defined as $\omega_i(E_i)=2\pi/T(x_{i_{\max}}(E_i),0)$, while

$$J_i(E_i)=\frac{1}{\pi}\int_{x_{i_{\min}}(E_i)}^{x_{i_{\max}}(E_i)} p_i dx_i\,.$$

On the other hand, **A** in Eq. (13) is calculated using relations (19).

Relations (19)–(21) are not very hard to be computed since functions x_i, y_i are sufficiently well behaving, being solutions of differential equations which describe the motion of an oscillator and are easily implemented using a software package which performs both analytical and numerical calculations as, e.g., MATHEMATICA. Note also that the accuracy much higher than $O(\varepsilon)$ is not very useful if we are going to use the results as initial estimates for multibreathers since the actual orbit lies in an ε-neighborhood of this estimation.

III. AN EXAMPLE: CHAIN CONSISTING OF COUPLED MORSE OSCILLATORS

The Morse oscillator is defined by the potential $V_M(x)=(e^{-x}-1)^2$ and its Hamiltonian is

$$H_M=\tfrac{1}{2}p^2+(e^{-x}-1)^2. \tag{22}$$

The action-angle canonical transformation for this system, in the domain of bounded motions, is given by

$$w=\arccos\left(\frac{1-(1-E)e^x}{\sqrt{E}}\right),$$

$$J=\sqrt{2}(1-\sqrt{1-E}), \tag{23}$$

TABLE II. Second estimation for $\phi_{-1}=\phi_1=3\pi$.

$\vartheta_{-1}=0.361\,367$	$\vartheta_0=-4.531\,71$	$\vartheta_1=0.361\,367$
$x_{-1}=0.0$	$x_0=3.628\,595$	$x_1=0.0$
$p_{-1}=1.322\,875$	$p_0=0.205\,678$	$p_1=1.322\,875$

TABLE III. Initial conditions for a 2:1:2 multibreather with $\varepsilon=0.0001$.

Site	x	p
0	3.627 812 858 975	0.207 299 776 628
1	0.0	1.322 289 057 449
2	$1.361\,989\,220\,8\times10^{-5}$	$-7.953\,790\,414\,34\times10^{-5}$
3	$-1.834\,285\,35\times10^{-8}$	$4.618\,550\,6\times10^{-8}$
4	-7.203×10^{-13}	$-1.261\,58\times10^{-11}$
5	$-3.250\,21\times10^{-11}$	$1.961\,46\times10^{-11}$
6	$4.137\,00\times10^{-11}$	$1.290\,02\times10^{-11}$
7	$-2.387\,64\times10^{-11}$	$-1.647\,55\times10^{-11}$
8	3.5055×10^{-12}	1.6442×10^{-12}
9	-7.3×10^{-15}	5.82×10^{-14}
10	0.0	0.0

where E is the energy of the oscillator, i.e., the value of H_M for a specific bounded orbit. The Hamiltonian in action-angle variables becomes

$$H_M=\tfrac{1}{2}(2\sqrt{2}J-J^2).$$

The frequency of the oscillation is

$$\omega=\sqrt{2(1-E)}. \tag{24}$$

Note that, for periodic motion, it holds that $0<E<1$. The value $E=0$ corresponds to the stable equilibrium at $x=0$, while $E=1$ corresponds to the unstable equilibrium at infinity and its separatrix. Consequently, the Hamiltonian of the complete chain is

$$H=H_0+\varepsilon H_1=\sum_{i=-\infty}^{\infty}\left(\frac{1}{2}p_i^2+(e^{-x_i}-1)^2\right)+\frac{\varepsilon}{2}\sum_{i=-\infty}^{\infty}(x_{i+1}-x_i)^2.$$

At this point we need to decide the number q of central oscillators. We choose $q=3$, on sites -1, 0, and 1 (i.e., $m=n=1$). So, for $\varepsilon=0$, we assume that all the oscillators lie on the stable equilibrium $(x_k,p_k)=(0,0)$, except the three central ones, which move in periodic orbits, satisfying the resonance condition $k_{-1}T_{-1}=k_0T_0=k_1T_1=T$. In order to evaluate the conditions which must be fulfilled for this motion to be continued for $\varepsilon\neq0$ to provide the multibreather, we have, first of all, to calculate $\langle H_1\rangle$. The perturbative term of the Hamiltonian for this specific case is

$$H_1=\tfrac{1}{2}[x_{-1}^2+(x_{-1}-x_0)^2+(x_0-x_1)^2+x_1^2], \tag{25}$$

and its average value will be

$$\langle H_1\rangle=-\int_0^T x_{-1}x_0dt-\int_0^T x_0x_1dt+c, \tag{26}$$

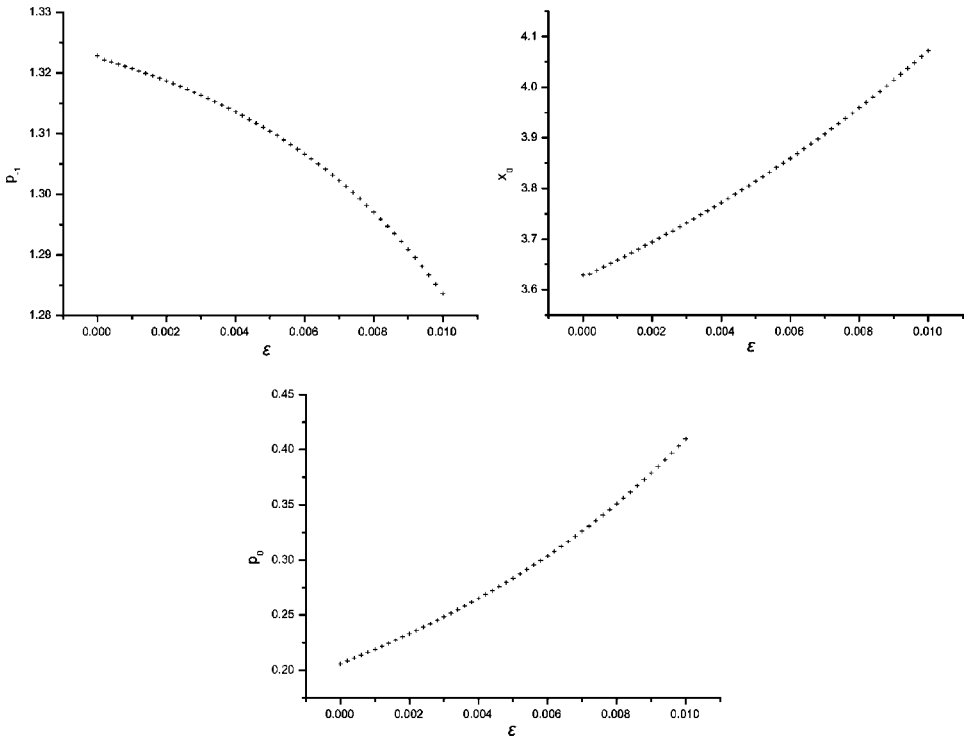

FIG. 1. The variation of the initial conditions for the "central" oscillators with respect to ε.

since the quadratic terms of Eq. (25) will provide terms independent of ϑ_i, because their average value is independent of the initial conditions on the torus. This has been evaluated in Ref. [7], and it is

$$\langle H_1\rangle = \sum_i \frac{2}{k_0 k_i}\int \arctan\left(\frac{\sin\phi_i}{z_i-\cos\phi_i}\right)d\phi_i + c, \quad i=\pm 1, \tag{27}$$

where $z_i = e^{k_i a_0 + k_0 a_i}$ and $\cosh a_i = E_i^{-1/2}$. The orbits that will be continued are these which satisfy

$$\frac{\partial\langle H_1\rangle}{\partial\phi_i} = 0 \Rightarrow \phi_i = 0,\pi. \tag{28}$$

TABLE IV. Initial conditions for a 2:1:2 multibreather with $\varepsilon = 0.0064$.

Site	x	p
0	3.878 723 990 992	0.312 409 333 321
1	0.0	1.304 931 271 741
2	$9.235\,355\,787\,833\times10^{-4}$	$7.048\,630\,765\,4203\times10^{-3}$
3	$2.193\,440\,215\,51\times10^{-5}$	$2.291\,014\,387\,809\times10^{-4}$
4	$1.739\,764\,5567\times10^{-6}$	$5.794\,311\,3468\times10^{-6}$
5	$4.779\,390\,88\times10^{-8}$	$1.744\,568\,404\times10^{-7}$
6	$1.548\,9699\times10^{-9}$	$5.046\,149\times10^{-9}$
7	$-3.846\,35\times10^{-11}$	$9.792\,29\times10^{-11}$
8	$-3.872\,50\times10^{-11}$	6.8740×10^{-12}
9	$2.918\,50\times10^{-11}$	-3.7176×10^{-12}
10	$4.504\,83\times10^{-11}$	4.47934×10^{-11}

These solutions satisfy also $\det\left|(\partial^2\langle H_1\rangle/\partial\phi_i\partial\phi_j)\right| \neq 0$ and the continuation is valid.

To define the stability of the breather solution, we need to calculate the matrix **E** defined in Eq. (13). Since in this case

$$\frac{\partial^2 H_0}{\partial J_l \partial J_j} = -\delta_{lj},$$

it holds that

$$E_{ij} = \frac{\partial^2\langle H_1\rangle}{\partial\vartheta_i\partial\vartheta_j} \quad \forall \;\; i,j\in\{-1,0,1\},$$

and finally we get

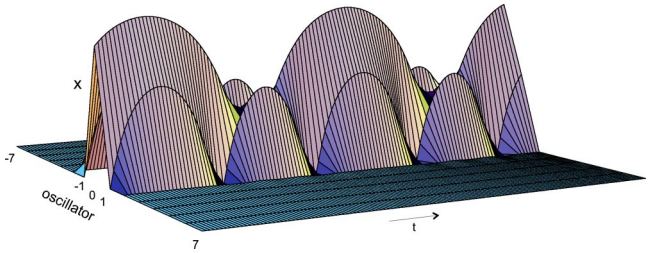

FIG. 2. Time evolution of a 2:1:2 multibreather, for $\varepsilon = 0.0064$.

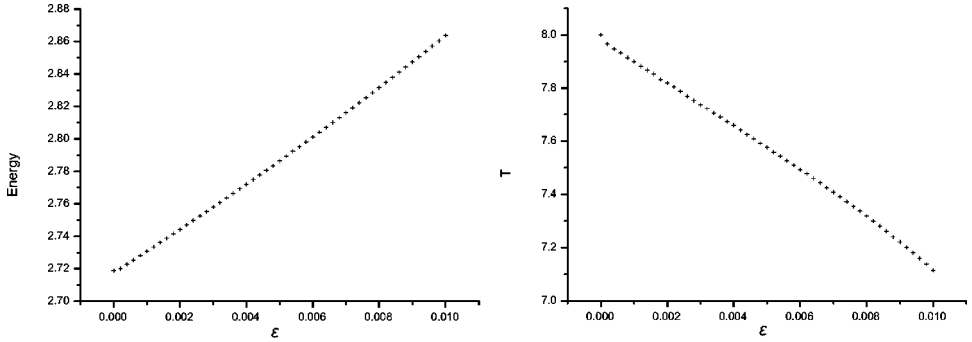

FIG. 3. The variation of the energy and the period of the calculated multibreathers with respect to ε.

$$E_{ij}=\frac{\partial^2\langle H_1\rangle}{\partial\vartheta_i\partial\vartheta_j}=\begin{cases}0, & i=-j=\pm 1\\ k_0^2\dfrac{\partial^2\langle H_1\rangle}{\partial\phi_i^2}, & i=j=\pm 1\\ -k_0k_i\dfrac{\partial^2\langle H_1\rangle}{\partial\phi_i^2}, & i=\pm 1, j=0\\ \displaystyle\sum_{l=\pm 1}k_l^2\frac{\partial^2\langle H_1\rangle}{\partial\phi_l^2}, & i,j=0.\end{cases} \tag{29}$$

Using Eq. (27) the elements of the matrix **E** become

$$E_{11}=\frac{2k_0}{k_1}\frac{z_1\cos\phi_1-1}{z_1^2-2z_1\cos\phi_1+1},$$

$$E_{10}=-2\frac{z_1\cos\phi_1-1}{z_1^2-2z_1\cos\phi_1+1},$$

$$E_{-1-1}=\frac{2k_0}{k_{-1}}\frac{z_{-1}\cos\phi_{-1}-1}{z_{-1}^2-2z_{-1}\cos\phi_{-1}+1},$$

$$E_{-10}=-2\frac{z_{-1}\cos\phi_{-1}-1}{z_{-1}^2-2z_{-1}\cos\phi_{-1}+1},$$

$$E_{00}=\frac{2k_1}{k_0}\frac{z_1\cos\phi_1-1}{z_1^2-2z_1\cos\phi_1+1}+\frac{2k_{-1}}{k_0}\frac{z_{-1}\cos\phi_{-1}-1}{z_{-1}^2-2z_{-1}\cos\phi_{-1}+1},$$

$$E_{-11}=0.$$

We now have to choose a family with a specific resonance. We choose $k_{-1}=k_1=2$ and $k_0=1$ that define the 2:1:2 resonance. We calculate the eigenvalues of **E** which coincide to σ_{i1}^2 in Eq. (12). We always have a zero eigenvalue. Apart from this, for every $\phi=0$ we get, for this resonance, a positive eigenvalue and for $\phi=\pi$ we get a negative eigenvalue. In the box below we see the linear stability of the continued multibreather for the different s_i.

s_i	ϕ_{-1}	ϕ_1	Stability
s_1	π	π	Stable
s_2	π	0	Unstable
s_3	0	π	Unstable
s_4	0	0	Unstable

We choose for example s_1. We define our section with $x_{-1}=0$, $p_{-1}>0$, and for $\omega=1/4$ in Eq. (4) which gives for the total energy $E=E_{-1}+E_0+E_1=\frac{81}{32}$. We calculate ϑ_{-1} by the action-angle transformation (23), and ϑ_1 from Eq. (5). Note that, since the resonance between the -1 oscillator, through which we defined the surface of section, and the 0 oscillator is 2:1 the same orbit will cross the surface of section in two distinct points. To calculate the second point we put $\phi_1=\phi_{-1}=3\pi$. We can use these two points as initial estimations to calculate the initial conditions for the stable

TABLE V. Initial conditions for a 3:1:2 multibreather with $\varepsilon=0.003$

Site	x	p
10	-1.6082×10^{-12}	6.883×10^{-13}
9	-2.57×10^{-14}	-3.759×10^{-13}
8	3.403×10^{-13}	7.249×10^{-13}
7	-1.76×10^{-14}	-8.905×10^{-13}
6	-5.5455×10^{-12}	1.92253×10^{-11}
5	$8.257\,078\times10^{-10}$	$-2.472\,7360\times10^{-9}$
4	$-4.386\,186\,97\times10^{-8}$	$1.935\,814\,499\times10^{-7}$
3	$1.448\,213\,911\,77\times10^{-5}$	$-2.595\,187\,926\,20\times10^{-5}$
2	$3.374\,092\,576\,531\times10^{-3}$	$2.019\,169\,816\,698\times10^{-3}$
1	2.761 549 204 437	$-8.907\,506\,361\,151\times10^{-2}$
0	4.459 826 334 650	$-3.156\,430\,138\,958\times10^{-2}$
-1	0.0	1.183 358 227 340
-2	$5.321\,016\,762\,607\times10^{-4}$	$-2.874\,821\,181\,95\times10^{-3}$
-3	$-1.362\,784\,997\,12\times10^{-5}$	$3.964\,585\,013\,87\times10^{-5}$
-4	$9.175\,537\,64\times10^{-8}$	$-3.260\,196\,926\times10^{-7}$
-5	$-1.068\,3378\times10^{-9}$	$3.389\,6598\times10^{-9}$
-6	$1.378\,34\times10^{-11}$	$-3.557\,11\times10^{-11}$
-7	4.840×10^{-13}	4.5190×10^{-12}
-8	-1.9042×10^{-12}	-2.929×10^{-12}
-9	4.139×10^{-13}	-6.02×10^{-14}
-10	5.364×10^{-13}	1.7401×10^{-12}

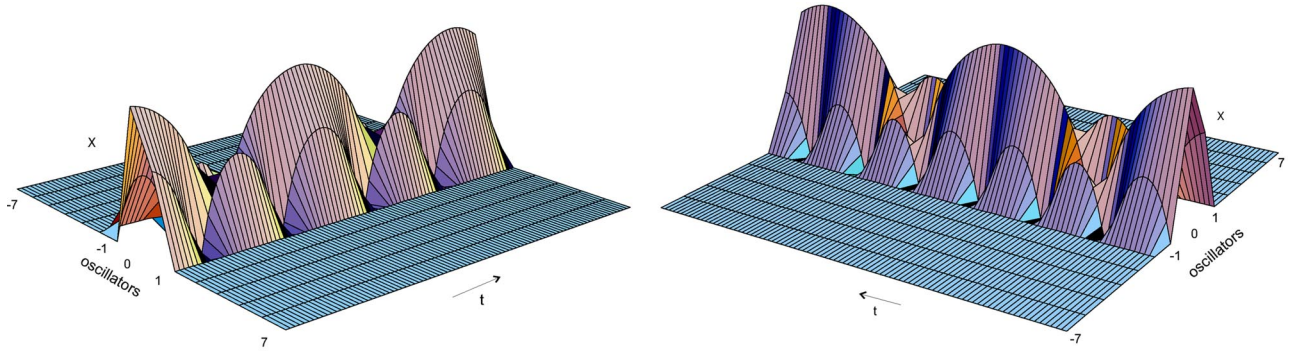

FIG. 4. Time evolution of a 3:1:2 multibreather, for $\varepsilon=0.003$. Both sides of the multibreather are shown. The one showing the 2:1 resonance and the other showing the 3:1 resonance.

2:1:2 multibreather on the surface of section (Tables I and II). We recall that the initial estimation for all the non-central oscillators it is $(x_i,p_i)=(0,0)$. Note that, since $\phi_1=\phi_{-1}$, we have also $x_{-1}=x_1$ and $p_{-1}=p_1$. We chose to work with the second one.

Now, the numerics come in to play and we have to use a finite chain. We use a chain of 21 oscillators with periodic conditions at the edges. We set $\varepsilon\neq 0$ and calculate the solution using the Broyden method, for $\varepsilon=0.0001$ (Table III). All the presented solutions are, at least, 10^{-10} near the periodic orbit.

Note that since the initial estimation is symmetric so is the multibreather, i.e., $x_{-i}=x_i$ and $p_{-i}=p_i$. The maximum deviation of the initial conditions from the initial estimations is $O(10^{-3})$. Using the values of the initial conditions of the calculated multibreather as input we can calculate the next member of the family for $\varepsilon=0.0002$, and so on. In Fig. 1 we see the variation of the initial conditions for the central oscillators with respect to the coupling constant ε with a step in ε of 2×10^{-4}. We recall that it is always $x_{-1}=0$. For example the solution for $\varepsilon=0.0064$ is presented in Table IV and its time evolution is shown in Fig. 2. By this method, the energy and the period T of the calculated multibreathers also vary. This variation (Fig. 3) appears because we use as initial estimation for the initial conditions for the multibreather, the initial conditions of the previously computed multibreather which correspond to a smaller value of the coupling constant ε. But the same values for x_i,y_i with larger ε correspond to a larger value of the energy of the system. Since the period is a function of the energy, it varies too.

In the same way we calculated initial conditions for a 3:1:2 multibreather for $\varepsilon=0.003$ (Table V). Note that, since in this case the multibreather is not symmetric $(\vartheta_{-i}\neq\vartheta_i)$, we have $x_i\neq x_{-i}$ and $p_i\neq p_{-i}$, so both (x_{-i},p_{-i}) and (x_i,p_i) are shown. The time evolution for this multibreather is shown in Fig. 4.

If the action-angle transformation was not known, we could have used the method described in the end of the preceding section in order to calculate the above results. Equation (18) transforms, for the particular example, to the following relation

$$\frac{\partial\langle H_1\rangle}{\partial\vartheta_i}=-\frac{1}{\omega_i T}\int_0^T x_0 p_i dt,\quad i=\pm 1,$$

while (17) becomes

$$\frac{\partial^2\langle H_1\rangle}{\partial\vartheta_i\vartheta_j}=\begin{cases}\dfrac{1}{\omega_i^2 T}\displaystyle\int_0^T\{p_i^2+2(2x_i-x_0)(e^{-x_i}-1)e^{-x_i}\}dt, & i=j\\ 0, \quad i\neq j \quad i,j\in\{-1,0,1\}.\end{cases}\tag{30}$$

So, Eq. (20) becomes

$$F(x_{i_0})=\int_0^T x_0 p_i dt=0.$$

The solutions of the above equation must also satisfy Eq. (17) which, taking under consideration (30), becomes

$$\int_0^T\{p_i^2+2(2x_i-x_0)(e^{-x_i}-1)e^{-x_i}\}dt\neq 0.$$

As for the linear stability of these solutions, the elements of the stability matrix **E** can be computed following the procedure described at the end of Sec. II, where we also make use of Eq. (30). The results of these numerical calculations are obviously the same as the ones calculated using the action-angle variables. Once programmed, this implementation of the method, can provide all the information we can get in less than 1 min. So, one could wonder about the utility of the time-consuming calculations using the action-angle variables. The answer is that the results provided using the action-angle variables have a much nicer geometrical interpretation as it can be shown from Eqs. (28) and (5).

IV. CONCLUSIONS

We presented a method of numerical calculation of the multibreathers which are predicted in Ref. [7]. This method has the advantage of calculating analytically an $O(\varepsilon)$ estimation of the initial conditions for a multibreather solution and its stability, provided the action-angle canonical transformation for the specific on-site potential of the oscillators of the chain is known. But even when the explicit form of the

action-angle transformation is not known we provide formulas with respect to the x_i, p_i variables only, which can be easily solved and provide us the same results. Finally these results are used to calculate a spatially symmetric and a spatially nonsymmetric multibreather in a chain consisting of coupled Morse oscillators. We have to note also, that one could use other methods of root finding, with probably better results on the accuracy and the convergence rate. The latter is reduced when Newton or approximate Newton methods are used, due to the near unity eigenvalues of the Newton matrix. For future work, we plan to perform a comparison between the different methods that can be used.

ACKNOWLEDGMENTS

The author would like to thank Assistant Professor S. Ichtiaroglou for his constructive criticism and Professor M. Vrahatis for suggesting the root finding numerical method. This work has been partially supported by the Greek Scholarship Foundation (IKY).

[1] S. Aubry, Physica D **103**, 201 (1997).
[2] S. Flach and C.R. Willis, Phys. Rep. **295**, 181 (1998).
[3] S. Takeno, K. Kisoda, and A.J. Sievers, Prog. Theor. Phys. Suppl. **94**, 242 (1988).
[4] R.S. MacKay and S. Aubry, Nonlinearity **7**, 1623 (1994).
[5] J.L. Marín and S. Aubry, Nonlinearity **9**, 1501 (1996).
[6] T. Bountis, H.W. Capel, M. Kollmann, J.C. Ross, J.M. Bergamin, and J.P. van der Weele Phys. Lett. A **268**, 50 (2000).
[7] V. Koukouloyannis and S. Ichtiaroglou, Phys. Rev. E **66**, 066602 (2002).
[8] H. Poincaré, Acta Math. **13**, 1 (1890).
[9] H. Poincaré, Les Méthodes Nouvelles de la Méchanique Céleste (Gauthier-Villars, Paris, 1892), Vol I. [English translation: *New Methods in Celestial Mechanics*, edited by D.L. Goroff (American Institute of Physics, New York, 1993).]
[10] H. Goldstein, *Classical Mechanics*, 2nd ed. (Addison-Wesley, Reading, 1980).
[11] G.D. Birkhoff, *Dynamical Systems*, Colloquium Publications Vol. 9 (American Mathematical Society, Providence, RI, 1927).
[12] C.G. Broyden, Math. Comput. **19**, 577 (1965).
[13] W.H. Press, S.A. Teukolsky, W.T. Vettering, and B.P. Flannery, *Numerical Recipes in C: The Art of Scientific Computing*, 2nd ed. (Cambridge University Press, Cambridge, 1992).
[14] V.A. Yakubovich and V.M. Starzhinskii, *Linear Differential Equations with Periodic Coefficients* (Wiley, New York, 1975).