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LETTER TO THE EDITOR

Exact compact breather-like solutions of two-dimensional Fermi–Pasta–Ulam lattice

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Abstract

We demonstrate that two-dimensional Fermi–Pasta–Ulam lattice support exact discrete compact breather-like solutions. We also find exact compact breather solutions of the same lattice in presence of long-range interaction with r^{-s} dependence on the distance in the continuum limit. The usefulness of these solutions for energy localization and transport in various physical systems are discussed.

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It is now well known that the balance between nonlinearity and dispersion leads to various localized solutions in nonlinear lattices, such as solitons, discrete breathers etc. These solutions are usually exponentially localized in space. On the other hand, recently Rosenau and Hyman showed that the interaction of nonlinear dispersion with nonlinear convection generates exact compact structures free of exponential tails [1]. Such solutions which are termed as *compactons* are basic solutions of Korteweg-de Vries (KdV)-like equations with nonlinear dispersion and in many cases they behave like a power of trigonometric functions inside their domain of nonzero values [1]. Stability analysis has shown that compactons are stable structures [2].

In contrast to continuum systems where the compactons have exact compact support, in nonlinear dispersive lattices the discrete compacton modes become almost compact or compact-like, by acquiring a very small tail which decays faster than exponential (stretched exponential) outside the support. More detailed study of the shape profile of compact-like discrete breathers in nonlinear dispersive lattice systems shows that the tail region decays with a faster than exponential law, such as a superexponential one [3].

The ability of compactons to store energy in a compact region and also transfer energy gives them a particular importance. This property is of the highest importance in biological physics where the mechanism of energy transport in biomolecules, naturally designed for sustaining life, is still not clearly understood. Discrete breathers have been theoretically proposed as the relevant mechanism for energy and charge storage and transfer in biomolecules

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and molecular chains [4]. However, the biological systems or the biological macromolecules, such as proteins, DNA etc have very complex structures and their structure is crucial for their functionality. Also, molecular chains and DNA molecules contain charged groups, and there is long-range dipole–dipole interaction between these charged groups. Therefore, one needs to study models that deviate from simple, typical one-dimensional ones, and incorporate in the models the more complicated effects of structure or geometry of the actual physical systems, long-range interactions, disorder as well as nonlinear dispersion. Some studies along these lines have been reported in the literature recently. Tsironis *et al* [5] addressed the energy localization and transport in discrete curvilinear chains that model bioploymers and showed that above a critical curvature discrete breathers cannot propagate freely in the chains. Dynamics of bent chains of coupled nonlinear oscillators with long-range interaction are also reported [6].

However, most of the two-dimensional studies are limited to the simple case of a particular geometry of the chain with fixed curvature, like the parabolic or wedge shaped chain embedded in a plane or two straight segments joined by a bent section etc [5, 6]. Also, the angles defining the curvature of the chain are considered time independent and only the dynamics of the coupled oscillators on the fixed chain are considered. This puts a limitation on these models to describe actual biological macromolecules such as DNA or other polymers which are usually not static entities due to fluctuations. For example, DNA shows large fluctuational opening, in which the base pairs are temporarily open to allow various biological processes such as processing of proteins, strand separation etc. Moreover, all these studies considered only the discrete breathers as localized excitations in the systems. As has been mentioned above, due to their compact support, the compact breathers are expected to provide better localization of energy at particular points of the chain, for example, in the promoter sites or bases of the DNA sequence etc.

In this letter we consider the more general two-dimensional lattice problem. We include the essential anharmonicity in the system by considering nearest neighbour interaction potential as Fermi–Pasta–Ulam type. In earlier similar studies as mentioned above, the geometries of the chain were restricted to a parabola or to a fixed set of angles between bond vectors at different lattice sites. We remove these constraint conditions on the dynamics of the chain and consider both the radial coordinates as well as the angular coordinates of the position vectors as dynamical variables. This corresponds to a more realistic situation in biological systems. We do not restrict ourselves to any particular shape but consider the arbitrary shape of the chain. We consider both the cases when the arbitrary shape of the chain is time independent as well as time dependent. We obtain various exact discrete compact breather-like solutions for this generalized two-dimensional FPU lattice problem. We also consider the question of the existence of discrete compact breather solutions in nonlinear dispersive lattice with long-range interactions. For this we study the dynamics of the two-dimensional FPU lattice of arbitrary shape with nonlocal dispersive interactions with power dependence r^{-s} on the distance and obtain various exact compacton breather solutions in the continuum limit.

We model the actual biophysical systems by reducing a macromolecule into a simple model of polymer chain consisting of N units, each of mass m, labelled by index n, and denoted by x_n, y_n the longitudinal and transverse positions of the nth mass wrt a 2D-Cartesian coordinate system. The Hamiltonian is

$$H = \sum_n \left[\frac{\dot{x}_n^2}{2} + \frac{\dot{y}_n^2}{2} + V(d_n) \right] \tag{1}$$

where we have considered the unit mass of each particle and d_n is the distance between the adjacent mass points given by $d_n = [(x_n - x_{n-1})^2 + (y_n - y_{n-1})^2]^{\frac{1}{2}}$. We will assume the essential anharmonicity in the system, apart from the geometric one entering through d_n is of the Fermi–Pasta–Ulam (FPU) type viz.,

$$V(d_n) = K_2 \frac{(d_n - a)^2}{2} + K_4 \frac{(d_n - a)^4}{4} \tag{2}$$

where a is the equilibrium distance between particles in the chain, K_2 and K_4 are strength of linear and nonlinear forces. The equations of motion can be written in a compact form as

$$\ddot{z}_n = R_{n+1} + R_{n-1} - 2R_n \tag{3}$$

where time has been normalized to $\sqrt{K_2}t$, $z_n = \xi_n + \mathrm{i}\rho_n$, $\xi_n = \frac{x_n - x_{n-1}}{a}$, $\rho_n = \frac{y_n - y_{n-1}}{a}$, $R_n = \frac{z_n}{|z_n|}[(|z_n| - 1) + \gamma(|z_n| - 1)^3]$ and $\gamma = \frac{K_4 a^2}{K_2}$ is the anharmonicity parameter. Using the polar coordinate $z_n = r_n(t)\mathrm{e}^{\mathrm{i}\theta_n(t)}$ we get two coupled discrete differential equations

$$\ddot{\tau}_n - (\tau_n + 1)\dot{\theta}_n^2 = g_{n+1}\cos(\theta_{n+1} - \theta_n) + g_{n-1}\cos(\theta_{n-1} - \theta_n) - 2g_n \tag{4}$$

$$(\tau_n + 1)\ddot{\theta}_n + 2\dot{\tau}_n\dot{\theta}_n = g_{n+1}\sin(\theta_{n+1} - \theta_n) + g_{n-1}\sin(\theta_{n-1} - \theta_n) \tag{5}$$

where $\tau_n(t) = (r_n(t) - 1)$ and $g_n = \tau_n + \gamma\tau_n^3$. The local variables (τ_n, θ_n) represent the normalized local relative deviation of two adjacent masses of the chain wrt the lattice spacing a and its angles wrt a given axis, respectively. When all local angles are zero, i.e. $\theta_n = 0$ for all values of n, then these equations reduce to a one-dimensional FPU model. Tsironis *et al* [5] considered a constrained dynamics for simplicity and ignored the second equation completely and also considered the angular variables to be time independent, i.e. $\dot{\theta}_n = 0$ for all values of n. Under these approximations, equations (4) and (5) reduce to just one equation, the same as equation (8) in [5]. We remove these constraint conditions used in [5] and consider both equations (4) and (5) for nonlinear compact breather solutions. We further remove the fixed geometry condition assumed in earlier studies [5, 6] and consider arbitrary shape of the chain and consider the cases when all local angles θ_n are time independent as well as time dependent.

Let us first consider the case when $\theta_n(t)$ are independent of time, i.e. $\dot{\theta}_n = 0$ for all n. Substituting equation (5) in equation (4) we get

$$\ddot{\tau}_n = \left[g_{n+1}^2 + g_{n-1}^2 + 2g_{n+1}g_{n-1}\cos(\theta_{n+1} - \theta_{n-1})\right]^{\frac{1}{2}} - 2g_n. \tag{6}$$

We look for static discrete compact breather solutions of the form

$$\tau_n(t) = Af_n\cos(\omega t) \tag{7}$$

where,

$$f_n = \cos(B(n - n_0)), \qquad \text{for} \quad |n - n_0| < \frac{\pi}{2B}$$
$$= 0, \qquad \text{otherwise.} \tag{8}$$

For compacton solutions to exist, the width B should be independent of the amplitude A. Substituting equations (7) and (8) in equation (6) and using rotating wave approximation (RWA), we obtain the exact compact breather solution for the shape of the chain given by

$$\cos(\theta_{n+1} - \theta_{n-1}) = \frac{\mu\cos^2(B(n - n_0)) + p}{\cos^2(B(n - n_0)) - \sin^2(B)} \tag{9}$$

and for a set of parameter values $\{\omega, \mu, p, B\}$. The solutions exist for three set of parameter values given by $\left\{\omega^2 = 4 + 2A^2\gamma_1, \mu = 3, p = -1, B = \frac{\pi}{2}\right\}$; $\left\{\omega^2 = 3 + \frac{9}{4}A^2\gamma_1, \mu = 1, p = -\frac{3}{4}, B = \frac{2\pi}{3}\right\}$; $\left\{\omega^2 = 3 + \frac{9}{4}A^2\gamma_1, \mu = 1, p = -\frac{3}{4}, B = \frac{\pi}{3}\right\}$, where $\gamma_1 = \frac{3}{4}\gamma$. It may be noted that other forms of discrete compact breather solutions may also exist for the system.

It is appropriate to mention here that even the approximate one-dimensional modified FPU model considered by Tsironis *et al* (equation (8) in [5]) also have discrete travelling compacton solutions of the form $\tau_n(t) = A\cos(B(n - vt))$, for $|(n - vt)| < \frac{\pi}{2B}$ and zero otherwise and for the shape of the chain given by

$$\cos(\theta_{n+1} - \theta_n) = \cos(\theta_{n-1} - \theta_n) = \frac{1}{\cos(B)(2\cos(2B) - 1)} \tag{10}$$

and the compacton velocity given by $v^2 = \frac{(\cos(2B)-1)(4+3\gamma A^2)}{B^2(2\cos(2B)-1)}$. The same equation (equation (8) in [5]) also has discrete static compact breather solutions of the form of equations (7) and (8) above for the same shape of the chain given by equation (10). The breather frequency is given by $\omega^2 = \frac{(\cos(2B)-1)(4+3\gamma_1 A^2)}{(2\cos(2B)-1)}$, where $\gamma_1 = \frac{3}{4}\gamma$. Both the static compact breather solutions and the travelling compacton solutions exist for arbitrary amplitude A and width $B = \frac{\pi}{3}, \frac{2\pi}{3}$.

We now look for discrete travelling compact breather solutions of equations (4) and (5) when the curvature of the chain is time dependent, i.e. $\dot{\theta}_n \neq 0$. We use the ansatz

$$\tau_n(t) = A\psi_n(t)\cos(\omega t) \tag{11}$$

where $\psi_n(t) = \cos(B(n - vt))$, for $|n - vt| < \frac{\pi}{2B}$ and zero otherwise.

For large breather amplitude, $A \gg 1$ and for small angular difference between the lattice sites, equations (4) and (5) are approximated respectively as

$$\ddot{\tau}_n - \tau_n\dot{\theta}_n^2 = g_{n+1}\left(1 - \frac{(\theta_{n+1} - \theta_n)^2}{2}\right) + g_{n-1}\left(1 - \frac{(\theta_{n-1} - \theta_n)^2}{2}\right) - 2g_n \tag{12}$$

$$\tau_n\ddot{\theta}_n + 2\dot{\tau}_n\dot{\theta}_n = g_{n+1}(\theta_{n+1} - \theta_n) + g_{n-1}(\theta_{n-1} - \theta_n). \tag{13}$$

Defining the shape of the chain as $\theta_n(t) = \eta\psi_n(t)$ we get exact travelling compact breather solutions for a set of parameter values $\{v, B, \omega, \eta\}$ and arbitrary amplitude A. For FPU lattice with anharmonicity parameter $\gamma < 0$, the solutions exist for $v^2 = \frac{(0.8535+0.546\gamma A^2)}{B^2}$, $\cos(B) = 0.382\,683$, $\eta^2 = \frac{-651.525\gamma A^2}{(263.34+93\gamma A^2)}$, $\omega^2 = \frac{1.252(0.85+\gamma A^2)(2.03+\gamma A^2)}{(2.83+\gamma A^2)}$ and $|\gamma|A^2 < 0.85$. For a lattice with $\gamma > 0$, the solutions exist for two set of parameter values given by $\left\{\cos(B) = 0.923\,88,\ \eta^2 = \frac{1446.95\gamma A^2}{(-159.5+93\gamma A^2)},\ \omega^2 = \frac{0.28(-1.11+\gamma A^2)(0.064+\gamma A^2)}{(-1.715+\gamma A^2)}\right\}$ and $\left\{\cos(B) = -0.923\,88, \eta^2 = \frac{119.17\gamma A^2}{(115.85+93\gamma A^2)}, \omega^2 = \frac{2.1535(1.61+\gamma A^2)(2.66+\gamma A^2)}{(1.25+\gamma A^2)}\right\}$, with $v^2 = \frac{(0.146+0.016\gamma A^2)}{B^2}$ and $\gamma A^2 > 1.715$.

As mentioned earlier, in an actual discrete lattice, the exact discrete compact breather solutions as obtained above may not be exactly zero outside the compact support but the breathers may become compact-like by acquiring a very small tail. Beyond the breathers' support the tail (discrete effects) decay at a super exponential rate [3] and the interplay of nonlinear force and nonlinear dispersion creates a genuine screening effect beyond which there is no measurable motion. In that sense, the discrete compact breather solutions as obtained above may be an approximation in the tails. Hence we term these solutions as exact compact breather-like solutions (also termed as almost compact breather solutions by Rosenau *et al* [3]).

We now consider the question of existence of the discrete compact breather solution in the two-dimensional FPU lattice in presence of long-range nonlinear dispersive interactions. The model is described by the Hamiltonian

$$H = \sum_n \left[\frac{\dot{x}_n^2}{2} + \frac{\dot{y}_n^2}{2} + \sum_p \frac{K_2}{2}\frac{(d_{n,p} - a)^2}{|p|^{s_1}} + \sum_p \frac{K_4}{4}\frac{(d_{n,p} - a)^4}{|p|^{s_2}}\right] \tag{14}$$

where $p = 1, 2, 3, \ldots$ and s_1 and s_2 are the long-range interaction parameters for the harmonic and anharmonic interactions respectively and $d_{n,p} = [(x_n - x_{n-p})^2 + (y_n - y_{n-p})^2]^{\frac{1}{2}}$. The equations of motion are given by

$$\ddot{\tau}_n - (\tau_n + 1)\dot{\theta}_n^2 = \sum_p [g_{n+p,p}\cos(\theta_{n+p} - \theta_n) + g_{n-p,p}\cos(\theta_{n-p} - \theta_n) - 2g_{n,p}] \tag{15}$$

$$(\tau_n + 1)\ddot{\theta}_n + 2\dot{\tau}_n\dot{\theta}_n = \sum_p [g_{n+p,p}\sin(\theta_{n+p} - \theta_n) + g_{n-p,p}\sin(\theta_{n-p} - \theta_n)] \tag{16}$$

where $g_{n,p} = \frac{\tau_n}{|p|^{s_1}} + \gamma\frac{\tau_n^3}{|p|^{s_2}}$. For $p = 1$ these equations reduce to equations (4) and (5), respectively.

It is a very difficult problem to solve these coupled discrete equations analytically. For the case of harmonic interaction between the oscillators, analytic solutions can be obtained by approximate methods like the variational method and lattice Green's function method. Such methods cannot be implemented as easily in the present case with anharmonic nonlocal long-range dispersive interactions. However, we realized that some special solutions in which we are interested here, such as the spatially localized solutions with compact support, can be obtained in the continuum limit. The advantage of obtaining the continuum solutions is that it may be possible to use these solutions as initial conditions to obtain the solutions of the actual discrete lattice numerically. Our earlier studies of the numerical simulations of the dynamics of 1D FPU lattice with long-range interactions showed that the exact continuum compacton breather solutions correctly predict the essential compact span of the corresponding discrete compact breather and also, the continuum solutions survive in the actual discrete lattice for a time over hundreds of periods of the discrete breather [7]. We therefore go to the long wavelength limit and in the weak nonlinear limit we obtain the continuum dynamical equations of motion as

$$\begin{aligned}\tau_{tt} - (\tau + 1)\theta_t^2 &= \zeta(s_1 - 2)\tau_{2x} + \tfrac{1}{12}\zeta(s_1 - 4)\tau_{4x} + \gamma\zeta(s_2 - 2)(\tau^3)_{2x} \\ &\quad - \left[\zeta(s_1 - 2)\tau + \gamma\zeta(s_2 - 2)\tau^3 + \tfrac{1}{2}\zeta(s_1 - 4)\tau_{2x} + \tfrac{1}{2}\gamma\zeta(s_2 - 4)(\tau^3)_{2x}\right]\theta_x^2\end{aligned} \tag{17}$$

$$(\tau + 1)\theta_{tt} + 2\theta_t\tau_t = \left[2\zeta(s_1 - 2)\tau_x + \tfrac{1}{3}\zeta(s_1 - 4)\tau_{3x} + 6\gamma\zeta(s_2 - 2)\tau^2\tau_x\right]\theta_x \tag{18}$$

where subscripts denote partial derivative and $\zeta(s)$ is the Riemann zeta function [7]. For large amplitude we can obtain an exact travelling compacton breather solution of the form $\tau(x, t) = A\phi(x, t)\cos(\omega t)$, where $\phi(x, t) = \cos(B(x - vt))$, for $|x - vt| < \frac{\pi}{2B}$ and zero otherwise and for the shape of the chain given by $\theta(x, t) = \eta\phi(x, t)$. The parameters are given by $B^2 = \frac{2\zeta(s_2-2)}{9\zeta(s_2-4)}$, $v^2 = \zeta(s_1 - 2) - \frac{\zeta(s_2-2)\zeta(s_1-4)}{27\zeta(s_2-4)}$, $\eta^2 = \frac{243\gamma A^2\zeta(s_2-4)}{54\gamma A^2\zeta(s_2-4)-8\zeta(s_1-4)}$, $\omega^2 = \frac{\zeta(s_2-2)}{486(\zeta(s_2-4))^2}[108\zeta(s_1 - 2)\zeta(s_2 - 4) + \zeta(s_2 - 2)(243\gamma A^2\zeta(s_2 - 4) - 2\zeta(s_1 - 4))]$ and the anharmonicity parameter γ and the amplitude A are arbitrary. Thus the set of parameters B, v, η and ω for which the exact travelling compacton breather solutions exist depend on the Riemann zeta functions, which are again functions of the long-range interaction parameters s_1 and s_2. Therefore, the allowed ranges of the parameters s_1 and s_2 are those for which Riemann zeta functions are finite and the set of parameter values are finite and real and are given by $s_1 = 4, s_2 > 5$ and $s_1, s_2 > 5$.

It may also be noted that the continuum limit of equation (8) in [5] with long range interactions as above also has an exact *static* compacton breather solution of the form $\tau(x, t) = A\phi(x)\cos(\omega t)$, $\phi(x) = \cos(Bx)$ for $|x| < \frac{\pi}{2B}$ and zero otherwise and for the time-independent shape of the chain as $\theta_x = \mu\phi(x)$.

In conclusion, we have obtained exact discrete compact breather-like solutions of the two-dimensional FPU lattice. To model various physical processes, such as energy localization and transport in more realistic biophysical systems, we have relaxed the constraint conditions (of fixed geometry) put on the dynamics by earlier similar studies and considered the more general dynamics of nonlinear oscillators on a two-dimensional FPU chain of arbitrary shape. We have considered both the cases when the arbitrary shape of the chain is time independent as well as time dependent. We have also considered the dynamics of the 2D FPU lattice in presence of long-range interactions with r^{-s} dependence on distance and obtained various exact compact breather solutions in the continuum limit. It may be possible to use these continuum solutions as initial conditions in the numerical simulation to look for the existence of discrete compact breather solutions in the actual 2D discrete FPU lattice with long-range interactions. Work along this direction is in progress and will be reported elsewhere.

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