Two-dimensional map for a curved Fermi-Pasta-Ulam chain

Ranja Sarkar
Department Of Physics, University Of Pune, Pune-411007, India
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A two-dimensional map is derived from the model of a curved Fermi-Pasta-Ulam (FPU) chain which supports exact discrete breather (DB) solutions with frequencies lying outside the linear spectrum or phonon band. The stability of the equilibrium points of the two-dimensional map is examined and the nature of the trajectories is numerically studied. The map displays regular orbits and commensurate states in the phase space for different choices of curvature strength of the FPU chain. The homoclinic map orbits are attributed to the stationary DB solutions of the lattice system.

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The importance of discrete breathers (DBs) or intrinsic localized modes in nonlinear lattices has been emphasized in the modeling of biopolymers and conducting polymers during recent years. It is suggested that these nonlinear localized excitations may provide a possible physical mechanism for energy storage and transport as well as for structural properties of biopolymers [1], charge transport in conducting polymers [2]. They may play relevant roles in energy trapping and other dynamical properties [3] such as folding in polypeptide chains and targeted breaking of chemical bonds in molecular chains [4]. Conformational changes may occur in response to the excitation of DBs and therefore may prove to be crucial in the kinetics of conformational phase transitions of semiflexible biopolymers [3]. It thus becomes necessary to find out whether such modes are sturdy against changes in the geometrical curvatures or structures of the polymer chains.

Exact analytic solutions in the form of static DBs have been presented recently for a model of a curved Fermi-Pasta-Ulam (FPU) chain confined to a two-dimensional (2D) plane [5]. Since the model involves a quadratic (apart from quartic) nearest-neighbor interaction, it is not free from linear dispersion. Due to phonon resonances, the strong localization of the nonlinear excitations may be destroyed [6]. Therefore it becomes important to show that localization resulting from nonlinear dispersion can be a robust property even in the presence of linear dispersion in the curved chain.

The FPU chain considered in [5] is an infinite chain consisting of unit masses lying in the x-y plane and coupled to their nearest neighbors by a potential which is minimized whenever the nearest neighbors lie the lattice constant ''a'' apart. A relative distance is defined between the nearest neighbors as

$$z_n = \frac{1}{a}[(x_n - x_{n-1}) + i(y_n - y_{n-1})].$$

The potential (P) and kinetic (T) energies of the planar chain are respectively given by

$$P = \frac{1}{2}(r_n - 1)^2 + \frac{\gamma}{4}(r_n - 1)^4, \quad T = \frac{1}{2}(\dot{x}_n^2 + \dot{y}_n^2),$$

where $r_n = |z_n| = \frac{1}{a}[(x_n - x_{n-1})^2 + (y_n - y_{n-1})^2]^{1/2}$ and γ denotes the quartic anharmonicity parameter. A transformation to the polar coordinate representation simplifies the calculations and accordingly $z_n = r_n e^{i\theta_n}$ is used. This leads to

$$x_n - x_{n-1} = a r_n \cos(\theta_n), \quad y_n - y_{n-1} = a r_n \sin(\theta_n).$$

It is easily seen that only the kinetic energy depends on the angles θ_n between adjacent links in the chain and not the potential energy. The total energy $E = P + T$ is therefore dependent on the angles. While the links of the curved chain resist compression and stretching, it is rigid in nature.

Having briefly described the system under consideration, the focus is now on the linear stability analysis of DBs existing in the system. The present paper is aimed at investigating the stability of possible orbits of the system. For this, the equation of motion in plane polar coordinates (r_n, θ_n) governing the displacement field dynamics of the curved chain is taken from [5] and is given by

$$\ddot{\tau}_n = g_{n+1}\cos(\theta_{n+1} - \theta_n) + g_{n-1}\cos(\theta_{n-1} - \theta_n) - 2g_n, \quad (1)$$

where $\tau_n = (r_n - 1)$ and $g_n = \tau_n + \gamma\tau_n^3$. This is Eq. (12) in [5], and Eq. (13) therein simply expresses the generalized forces in terms of the appropriate acting torques on the chain which is treated as a constraint condition here, since calculating these forces is not the concern of the present study. Equation (1) contains all the dynamics of the anisotropic (θ_n-dependent) chain, the geometry of which is time independent and defined as

$$\cos(\theta_{n+1} - \theta_n) = \frac{\mu}{(1 + \gamma_1 \phi_{n+1}^2)},$$

$$\cos(\theta_{n-1} - \theta_n) = \frac{\mu}{(1 + \gamma_1 \phi_{n-1}^2)}, \quad (2)$$

like in [5], where $\gamma_1 = \frac{3}{4}\gamma$. The curvature of the chain depends only parametrically on μ. In other words, the chain geometry is only inhomogeneous (n-dependent) in the sense that it is determined by the lattice displacement pattern. Here ϕ_n is the spatial profile of the stationary DB mode. When all local angles are equal to the same constant nonzero value $\theta_n = \theta^0$, the modified FPU model represented by Eq. (1) reduces to the one-dimensional FPU chain rotated through an angle θ^0 wrt a horizontal axis. Motion in a third dimension (perpendicular to the chain) is ignored here in the model to reduce its complexity, which in no way blurs the essential results.

Such a nonlinear chain embedded in a plane can describe polymers in general. The dynamics of the chain taken into consideration is fixed in time and it evolves only by changing the lengths of its links, i.e., moves with the orientations of the links altering with the sites n to accommodate the expansion and contraction of the links. This can be viewed as a conformational flexibility of the chain arising in response to the excitation of nonlinear localized modes.

The existing DB solutions given by the ansatz $\tau_n = \phi_n \cos(\omega t)$ are allowed for the particular chain geometry (2) within the framework of the rotating wave approximation (RWA). RWA means considering a monochromatic anharmonic oscillation and neglecting all the higher harmonics. The equation in the amplitudes ϕ_n thus obtained after substituting the DB ansatz and Eq. (2) in Eq. (1) is

$$-\omega^2 \phi_n = \mu \phi_{n+1} + \mu \phi_{n-1} - 2(\phi_n + \gamma_1 \phi_n^3), \tag{3}$$

which supports odd and even-parity DB modes whose frequencies lie well above the linear spectrum band [5]. The dynamics of the system evolves in space, not in time. Equation (3) is of prime interest and can be cast into a 2D map for a mapping stability analysis.

We define a map on phase space and search for fixed points of this map. An explicit construction of a 2D map is possible by introducing the relation $\psi_{n+1}=(\phi_{n+1}-\phi_n)$ that can be solved uniquely for ϕ_{n+1} and ψ_{n+1} in terms of ϕ_n and ψ_n. The map determines the displacement of the nth mass "ϕ_n" at all subsequent sites along the curved FPU chain for a choice of the model parameter "μ". For a chosen arbitrary value (ϕ_0, ψ_0) near the fixed point of the map and a fixed strength of the coupling constant, the map illustrates the phase portrait of the lattice system.

It is convenient to analyze the stability aspects of the static DBs associated with the given system from the viewpoint of mapping orbit stability [7]. The real-valued equation (3) is thus investigated as a map where the lattice index n plays the role of discrete time. The corresponding map $\mathbf{M}$ is given as

$$\psi_{n+1} = \psi_n - a\phi_n + b\phi_n^3,$$

$$\phi_{n+1} = \phi_n + \psi_{n+1}, \tag{4}$$

where $a=\frac{1}{\mu}[\omega^2+2(\mu-1)]$ and $b=\frac{3\gamma}{2\mu}$. To examine the structural stability of the stationary DBs with frequencies lying above the linear band, studying the stability of the fixed points and associated homoclinic orbits of $\mathbf{M}$ is sufficient.

As is apparent from the map $\mathbf{M}$, the origin $(0,0)$ represents a fixed point of the map. The other fixed points are located at $(\pm\sqrt{\frac{a}{b}},0)$ which exist if $a>0$, $b>0$ $(\gamma>0)$ and $a<0$, $b<0$ $(\gamma<0)$ for the curvature parameter $\mu>0$. In the following discussion, the first case is taken into consideration, i.e., the focus is on localized states whose frequencies lie above the plane wave spectrum $\omega>\omega_m$ for a "hard" nonlinearity $\gamma>0$ where "ω_m" is the maximum plane wave frequency [5]. The stability of the fixed points is governed by their values for the corresponding residues:

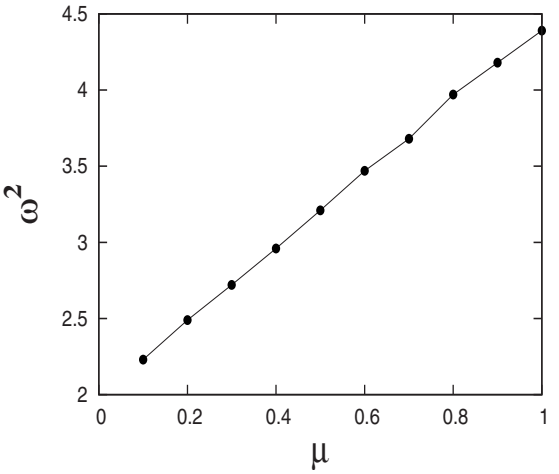

FIG. 1. DB frequency as a function of the curvature parameter.

$$\rho = \frac{1}{4}[2 - Tr(D\mathbf{M})], \tag{5}$$

where the tangent map $D\mathbf{M}$ is determined by

$$D\mathbf{M} = \begin{bmatrix} 1 & w_n \\ 1 & 1+w_n \end{bmatrix}, \tag{6}$$

with $w_n=(-a+3b\phi_n^2)$. It is clear from Eq. (6) that $\mathbf{M}$ is an area-preserving map. The value of residue at fixed point $\phi_n=0$ is $\rho=\frac{a}{4}$ and that at fixed points $\phi_n=\pm\sqrt{\frac{a}{b}}$ is $\rho=-\frac{a}{2}$. For DB frequency fulfilling the nonresonance condition $\omega>\omega_m$ [8], the map parameter $a>0$. Hence for the fixed points $(\pm\sqrt{\frac{a}{b}},0)$ the residue is $\rho<0$ which therefore lose stability. However, for the fixed point $(0,0)$ the value is $\rho>0$ and hence the system (4) is studied by plotting the map orbits initialized near the origin, simulated over 1000 lattice sites. It is further noted that the highest frequency which the DB can attain above the harmonic spectrum for a particular curvature of the chain increases with increasing μ, in a manner shown in Fig. 1. For $\mu=0$, $\omega^2=\omega_m^2=2$ represents the upper edge or cutoff of the linear band and is readily seen in the plot. For the present study, the two values of ω^2 corresponding to $\mu=0.1$ and $\mu=0.3$ are chosen from the figure without losing generality.

The iterates of $\mathbf{M}$ are obtained with some chosen sets of initial conditions and $\gamma=1$ is fixed for convenience. The stability of a fixed point is determined by the eigenvalues of the tangent map $D\mathbf{M}$. For the map origin $(0,0)$, $|\mathrm{Tr}(D\mathbf{M})|>2$ makes the eigenvalues real and reciprocals representing growing and decaying solutions [9]. Thus the equilibrium point $(0,0)$ is an unstable hyperbolic having one-dimensional stable and unstable manifolds in the 2D phase space, and is connected to itself by a homoclinic orbit created by the (invariant) unstable and stable manifolds. The value of residue at the zero equilibrium point is $\rho>1$ for the set of chosen parameters $0<\mu\leq 1$ and $\omega>\omega_m$, and it is converted into an unstable hyperbolic point with reflection. The map orbits are located on the line $\phi_n=-\psi_n$. Therefore the homoclinic map orbit of the curved FPU chain supports

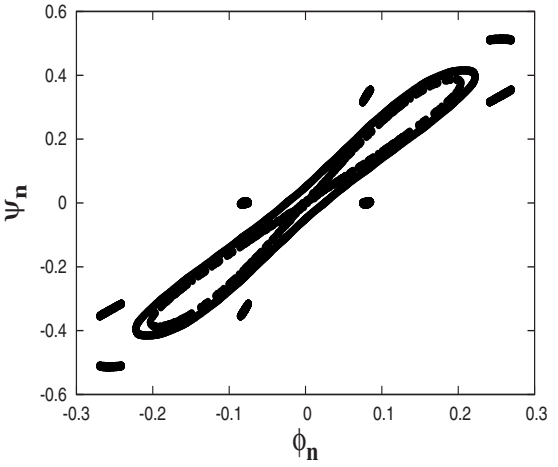

FIG. 2. ψ_n vs ϕ_n plot for $\mu=0.1$.

DBs which have frequencies existing above the linear spectrum, and have alternating signs for adjacent amplitudes, i.e., $\mathrm{sgn}(\phi_{n+1})=-\mathrm{sgn}(\phi_n)$ as a characteristic feature. Such DBs are said to have a staggered form that is, neighboring particles in the chain oscillate out of phase. This striking feature has been revealed in the previous study [5] of the same model for both odd and even-parity DB modes.

The ψ_n versus ϕ_n plot for $\mu=0.1$ ($\omega^2=2.23$) shown in Fig. 2 displays regular orbits and a chain of islands (high-order commensurate states) for different chosen initial conditions. When μ value is increased to 0.3 ($\omega^2=2.72$), the lattice displacement patterns show similar behavior as can be seen from Fig. 3. For even higher values of μ (the range considered in Fig. 1), the map orbits still remain periodic. One can find a host of similar trajectories corresponding to such localized states for different positive nonlinearity strengths.

It is evident that localized stationary states correspond to map orbits lying on the stable and unstable manifolds of hyperbolic equilibrium. In particular, if the map origin represents an unstable hyperbolic equilibrium point, exponential DBs in the curved FPU chain are excitable. Each homoclinic orbit "ϕ_n" is attributed to a localized state pinned by the lattice chain. Figure 4 shows the spatial profiles of stationary DBs of the FPU chain with its two curvature values (μ

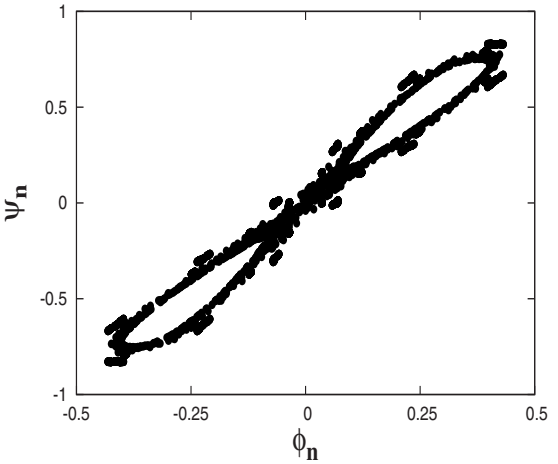

FIG. 3. ψ_n vs ϕ_n plot for $\mu=0.3$.

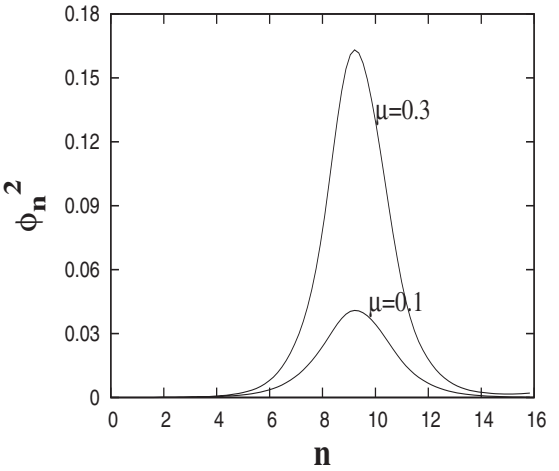

FIG. 4. Amplitude profiles of the stationary DB states of Eq. (3).

$=0.1, 0.3$), the real-valued amplitudes being obtained from the homoclinic map orbits. It is observed that the curved FPU chain with smaller μ values bears stationary DB states of absolute amplitudes smaller than the ones with larger μ values. In the latter case, the decay of the DB tails is less rapid which is clearly seen from Fig. 4. The extent of localization thus changes with changing μ values, i.e., for smaller μ values the DBs are intensely localized. This result agrees with that obtained in [5] for the same μ values. Thus the stationary DBs are robust under changes in curvature strengths of the chain. They adapt to the curvature change to sustain themselves in the chain by changing their amplitudes and hence, total energies.

In this paper, the map approach for the construction of sturdy DB states in a curved FPU chain with nearest-neighbor interaction is presented. A similar brief discussion can be found for next-nearest-neighbor interaction in the Discrete Nonlinear Schrodinger (DNLS) lattice in [10]. Beyond this, for a longer range of interaction, the map approach can be invoked by considering a higher dimensional map.

Generally stable stationary localized states are related to homoclinic and heteroclinic orbits of the corresponding map interpreting the system, even though there exist neighboring map orbits that are strongly chaotic, the reason being the dependence of localized states on the structural stability of orbits which are homoclinic or heteroclinic to unstable hyperbolic fixed points. Based on this, the stability properties of the DB modes in the curved FPU chain are considered from the perspective of the corresponding map orbit stability. In summary, the results obtained here show that in the case of an unstable hyperbolic equilibrium point of the 2D map, the construction of exact DB solutions can be achieved. The DB amplitudes grow and the DB widths diminish with changing curvature strengths of the FPU chain. Such spontaneous adaptation to the degree of localization is the inherent mechanism of the lattice system to maintain its localized structures and to protect them against dispersion. The numerical iterates of the 2D map display periodic orbits and a great number of commensurate states (islands). Hence one can conclude that there is no breakdown of the DB states which may have been caused via the mechanism of reso-

nances with linear coupling terms, and this accounts for longer lifetimes of DBs admitted by the curved FPU chain. In view of the localization properties of polymer chains, the curved FPU chain can serve as a minimal model to achieve states with excitation patterns of different amplitude heights and localization strengths.

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