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Integrable discrete static Hamiltonian with a parametric double-well potential

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ABSTRACT

A one-dimensional discrete conservative Hamiltonian with a generalized form of the Schmidt potential, is constructed with the help of a non-integrable discrete Hamiltonian whose parametrized double-well potential can be reduced to the ϕ^4 potential. The new conservative Hamiltonian is completely integrable in the discrete static regime, and the associate exact nonlinear solution is shown to coincide with the continuum nonlinear periodic solution of the non-integrable Hamiltonian. Numerical simulations and nonlinear stability analysis suggest that the discrete mapping derived from the completely integrable Hamiltonian undergoes a bifurcation which does not leads to the chaotic phase with randomly pinned states, but instead to a phase where real solutions become rare forming a cluster of periodic points around an elliptic fixed point.

1. Introduction

One-dimensional (1D) discrete nonlinear conservative systems show a wealth of fascinating features that make their interest [1–3]. In particular, the variety of phase patterns due to the interplay of lattice discreteness and on-site potential provides rich insight on near-critical phenomena in structural phase transition processes. Two most attracting among these phase patterns are modulated structures [2,4] and the so-called spatial chaos [5–8], they are manifest in several contexts of structural instabilities such as commensurate–incommensurate, ferroelectric and metal–insulator transitions [2] where randomly pinned states with chaotic features populate pretransitional phases.

However, while the account of all phase patterns is relevant to a global understanding of discrete conservative systems from a theoretical standpoint, real contexts exist where only few of them interplay. For systems undergoing structural transitions without chaotic precursors, modulated structures are most relevant so that obtaining periodic solutions of the associate discrete nonlinear Hamiltonians can be far more useful in the characterization of their ordered phases.

In recent years, two main approaches emerged in attempts to construct integrable discrete models. In one [9–14] of them, one seeks for the potential admitting the continuum kink of a given generic potential as exact discrete solutions, and in the other a judicious discretization of the continuum equation of motion is done [14–17]. The first approach has demonstrated high efficiency in the study of critical processes in discrete conserved energy systems, in addition the resulting discrete map has a standard topology characteristic of discrete conservative Hamiltonians [2] unlike artificially discretized equations [14–17] which give rise to nonstandard mappings. Concerning the discrete ϕ^4 model, Jensen et al. [9] established that the associate continuum periodic kink was unpinned in a discrete system based on the Schmidt potential [18]. They pointed that the discrete 2D mapping of the Schmidt Hamiltonian displayed a period-doubling bifurcations but without the infinite cascade to a spatially chaotic regime.

In this Letter, following closely Ref. [9], we construct a spatial chaos-free discrete Hamiltonian from a non-integrable discrete double-well Hamiltonian [19,20]. The generic double-well model is member of a family of parametrized double-well potential (PDWP) models [21–24] admitting exact continuum kink solutions. In view of the fact that it reduces exactly to the ϕ^4 in a specific limit, constructing the equivalent completely integrable discrete Hamiltonian is of fundamental importance for bistable systems that the ϕ^4 model may not adequately describe from both quantitative and qualitative points of view.

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2. The integrable discrete static Hamiltonian

The total Hamiltonian of a 1D chain of N harmonically coupled identical atoms with a one-body potential is given by:

$$H=\sum_{n=1}^{N}\left[\frac{K}{2}(u_{n+1}-u_n)^2+V_\mu(u_n)\right], \tag{1}$$

where u_n is the relative displacement of the nth atom from its commensurate position. The equilibrium configurations of the lattice that result from the interplay of the interatomic interaction and the on-site potential $V_\mu(u_n)$, are determined by minimizing the Hamiltonian (1) with respect to u_n leading to the following set of discrete difference equations:

$$u_{n+1}-2u_n+u_{n-1}-\frac{1}{K}V'_\mu(u_n)=0, \quad V'_\mu(u_n)\equiv\frac{\partial V_\mu(u_n)}{\partial u_n}. \tag{2}$$

We choose an on-site potential with the following double-well shape [19,20]:

$$V_\mu(u)=\frac{a_\mu}{2}\left[\frac{1}{\mu^2}\sinh^2(\alpha_\mu u)-1\right]^2, \quad \mu\neq 0, \tag{3}$$

where:

$$\alpha_\mu=\operatorname{arsinh}(\mu), \qquad a_\mu=\frac{a\mu^2}{(1+\mu^2)\operatorname{arsinh}^2(\mu)}, \tag{4}$$

with μ the deformability parameter. Note that in a strict sense the quantity $a/2$ in (4) represents the bare magnitude of the ϕ^4 potential barrier. However, to keep a one-to-one correspondence with the ϕ^4 model studied in Ref. [9] we shall also set $K\equiv 1$.

In a previous study [20], we discussed the Peierls–Nabarro problem for the discrete equation (2) with the PDWP (3), (4). Then, we established that its exact continuum kink solution was pinned to the lattice structure, and derived the Peierls–Nabarro potential whose height was dependent on μ. The variation of the Peierls–Nabarro barrier with the deformability that we obtained, showed that the pinning effect was always sizeable to empede translational invariance of the parametric continuum kink in the discrete medium.

In the present work, we wish to construct a discrete Hamiltonian for which the continuum periodic kink structure of equation (2) with the PDWP (3), (4) is an exact solution free from the Peierls–Nabarro effect. In this purpose, it is useful to first obtain the analytical expression of this continuum periodic kink solution. Thus, applying the continuum limit approximation on (2) in the weak dispersion regime, then integrating the resulting continuum equation with periodic boundary conditions we find:

$$u(n)=\frac{1}{\alpha_\mu}\tanh^{-1}\left[u_\mu \operatorname{sn} q_\mu(x-x_o)\right], \quad x\equiv n\ell, \tag{5}$$

where ℓ is the lattice spacing, sn is the Jacobi elliptic function and κ will be used to designate the associate modulus. The quantity u_μ, and the size $d_\mu=1/q_\mu$ of individual kinks in the periodic kink lattice (5), are defined as:

$$u_\mu=\beta\sqrt{\frac{1+8\beta^2\zeta}{1+8\beta^4\zeta}}u_0(\kappa), \qquad q_\mu=\sqrt{1+8\beta^2\zeta}\,q_0(\kappa), \tag{6}$$

with $\beta=\mu/\sqrt{1+\mu^2}$,

$$u_0(\kappa)=\kappa\sqrt{\frac{2}{1+\kappa^2}}, \qquad \ell q_0(\kappa)=\sqrt{\frac{2a}{1+\kappa^2}}. \tag{7}$$

The constant of first integral, i.e. the parameter ζ in (6), is expressed in terms of the modulus κ of the Jacobi elliptic function as:

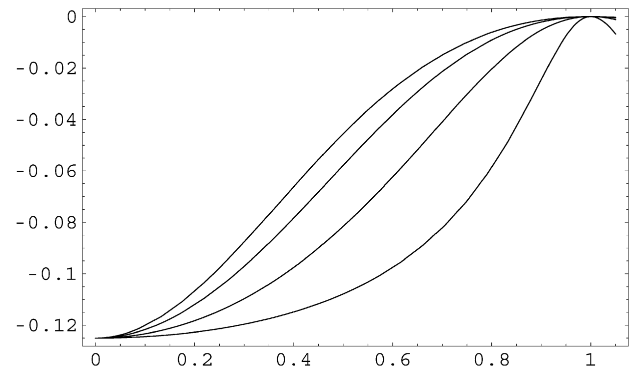

Fig. 1. Variation in κ of the constant of first-integral ζ. From the lowest to the upper curve in the range $0\leqslant\kappa\leqslant 1$: $\mu=2$, 1, 0.5, 0.1.

$$\zeta=\frac{8\kappa^2\beta^2-(1+\kappa^2)^2(1+\beta^4)-(1+\kappa^2)(1-\beta^2)F_\mu(\kappa)}{16\beta^4(1-\kappa^2)^2}, \tag{8}$$

$$F_\mu(\kappa)=\sqrt{(1+\kappa^4)(1+\beta^2)^2+2\kappa^2(1-6\beta^2+\beta^4)}. \tag{9}$$

According to Fig. 1, irrespective of the value of μ the parameter ζ increases with increasing κ in the negative branch. It reaches its maximum value of zero at $\kappa=1$, a limit where the periodic kink lattice sharpens into a single kink with shape extending from $x\to-\infty$ to $x\to\infty$. It is also instructive to stress that when $\mu\to 0$, i.e. when the parametrized potential becomes the ϕ^4 potential, the periodic kink solution (5) reduces to the well-known [9,25] periodic kink solution of the continuum ϕ^4 model.

We now seek for a discrete Hamiltonian with an appropriate on-site potential $W_\mu(u)$ admitting the continuum periodic kink (5) as exact static solution in the discrete regime. To simplify we rewrite (5) as:

$$u_n=\frac{1}{\alpha_\mu}\tanh^{-1}\phi_n, \quad \phi_n=u_\mu\operatorname{sn}(q_\mu n\ell). \tag{10}$$

In terms of this notations Eq. (2) becomes:

$$\tanh^{-1}\phi_{n+1}-2\tanh^{-1}\phi_n+\tanh^{-1}\phi_{n-1}=\alpha_\mu W'_\mu. \tag{11}$$

At this step, it is useful to recall the following identities:

$$\tanh^{-1}x\pm\tanh^{-1}y=\tanh^{-1}\left(\frac{x\pm y}{1\pm xy}\right), \tag{12}$$

and [26]

$$\phi_{n\pm1}=\frac{\nu_1\phi_n\pm\nu_2\operatorname{cn}(q_\mu n\ell)\operatorname{dn}(q_\mu n\ell)}{1-\nu_3^2\phi_n^2}, \tag{13}$$

$$\nu_1=\operatorname{cn}(q_\mu\ell)\operatorname{dn}(q_\mu\ell), \qquad \nu_2=u_\mu\operatorname{sn}(q_\mu\ell),$$
$$\nu_3=(\kappa/u_\mu^2)\nu_2. \tag{14}$$

With the help of these identities we get:

$$\phi_{n+1}+\phi_{n-1}=\frac{2\nu_1\phi_n}{1-\nu_3^2\phi_n^2}, \tag{15}$$

$$1+\phi_{n+1}\phi_{n-1}=\frac{(1-\nu_2^2)+(1-\nu_3^2)\phi_n^2}{1-\nu_3^2\phi_n^2}, \tag{16}$$

$$\frac{\phi_{n+1}+\phi_{n-1}}{1+\phi_{n+1}\phi_{n-1}}=\frac{2\eta_1\phi_n}{1-\eta_2\phi_n^2}. \tag{17}$$

Ultimately, replacing

$$\operatorname{cn}(q_\mu\ell)\operatorname{dn}(q_\mu\ell)=\sqrt{1-\operatorname{sn}^2(q_\mu\ell)}\sqrt{1-\kappa^2\operatorname{sn}^2(q_\mu\ell)} \tag{18}$$

everywhere we find:

$$W'_\mu(u)=\frac{1}{\alpha_\mu}\tanh^{-1}\left[\frac{2\eta_1\tanh(\alpha_\mu u)}{1-\eta_2\tanh^2(\alpha_\mu u)}\right]-2u, \tag{19}$$