

# Effective Hamiltonian for travelling discrete breathers

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## Abstract

Hamiltonian chains of oscillators in general probably do not sustain exact travelling discrete breathers. However solutions which look like moving discrete breathers for some time are not difficult to observe in numerics. In this paper we propose an abstract framework for the description of approximate travelling discrete breathers in Hamiltonian chains of oscillators. The method is based on the construction of an effective Hamiltonian enabling one to describe the dynamics of the translation degree of freedom of moving breathers. Error estimate on the approximate dynamics is also studied. The concept of Peierls-Nabarro barrier can be made clear in this framework. We illustrate the method on two simple examples, namely the Salerno model which interpolates between the Ablowitz-Ladik lattice and the discrete nonlinear Schrödinger system, and the Fermi-Pasta-Ulam chain.

# 1 Introduction

In this paper we present a Hamiltonian framework for the description of travelling discrete breathers in oscillator lattices. The concept of discrete breathers (DB) is well-defined mathematically – a time-periodic solution which is spatially localised [1] – whereas the notion of travelling DB can be formulated in different ways [2, 3]. Here we consider that a travelling DB is a spatially localised solution which has essentially two dynamical degrees of freedom (DOF): a translation DOF which makes the center of the breather move in time, and a vibrational (or rotational) DOF which evolves periodically in time. So a functional form for describing these structures could be written as  $\mathbf{u}_n(t) = \mathbf{F}(t, n - ct, n)$  which is time-periodic with respect to the first variable,  $\mathbf{F}(t + T, \cdot, \cdot) = \mathbf{F}(t, \cdot, \cdot)$ , and spatially localised with respect to its second variable (e.g.  $|\mathbf{F}(\cdot, n, \cdot)|$  is exponentially localised in space variable  $n$ ). Such functional form, however, has not been shown to comply with exact solutions in typical anharmonic lattices. (Notable exception is the family of travelling DB of the Ablowitz-Ladik system (AL) [4].) Moreover, most likely travelling DB are non-generic phenomena [5]. Nevertheless, spatio-temporal structures which resemble travelling DB have been observed in numerous numerical simulations, leading to several theoretical analyses which have attempted to describe these solutions [6]-[11]. For instance in [7] the problem of moving breather is dealt with by perturbation of the AL system; in [9] numerics are compared with high order multiple scale expansions of a Klein-Gordon model, and in [6, 10] the mobility of DB is related to the stability analysis of DB. In the present work, we would like to approach this problem from the general point of view sketched in [11]: if we forget about its internal DOF of vibration, a solution which looks like a travelling discrete breathers should be governed by a 1-DOF effective Hamiltonian that could be constructed, at least perturbatively. In [7] the authors provided an effective dynamics for the motion of DB in the perturbed AL model, and this was obtained with the help of the inverse scattering transform of the AL system. Here we propose a framework which we think is conceptually simpler, and which applies to systems which are not necessarily integrable. Moreover the method is designed in such a way that the error estimate is in principle tractable. All that we require is the existence of a set of loops (i.e. closed curves in phase space) which form a family of approximate discrete breathers indexed by a parameter  $Q$  representing a translation DOF. Then, assuming that one can define another parameter  $P$  from the family, which should be identified with a conjugate variable to  $Q$  (we will see below how to deal with this point), we construct an effective Hamiltonian dynamics for  $P$  and  $Q$  such that the stationary points of  $\mathbf{H}^{\text{eff}}(P, Q)$  correspond to exact discrete breathers, and the

approximate dynamics is accurate for trajectories for which  $|\nabla H^{\text{eff}}|$  remains small. The principle of the method was initiated in [11] and developed from a broader point of view in [12]. The construction of the effective dynamics is variational and consists in considering the family of approximate periodic solutions as exact critical points of the averaged Hamiltonian subjected to constraints of fixed  $P$  and  $Q$ , and fixed area (recall the latter is defined as  $\int p dq$  in canonical coordinates). Then we show that the slow dynamics for  $(P, Q)$  can be deduced from the associated Lagrange multipliers.

The paper is organised as follows. In section 2 and 3 we recall the principle of the method in an abstract way, so that it can be useful for applications in contexts different from those of discrete breathers. Section 3 is devoted to estimating the error made in approximating the actual dynamics by an effective one. In section 4 and 5 the method is applied to specific examples related to travelling discrete breathers. First, in section 4 we consider the Salerno model (a subtle interpolation between the AL model and the discrete nonlinear Schrödinger system), and gives analytical results on moving DB in this model. The latter are illustrated by some numerical simulations. In next section, the method is applied to some travelling localised solutions of the Fermi-Pasta-Ulam model (FPU), both analytically and numerically. Conclusions are drawn in section 6.

## 2 The method of the effective Hamiltonian

The method of the effective Hamiltonian that we consider in this paper was initiated in [11] in the context of dynamics of generalised multibreathers. In the present paper, it is presented in a more general way so that it should be applicable to a broader range of situations. The starting point is the variational formulation of Hamiltonian dynamics. In this framework, one is given  $(\mathcal{E}, \alpha, H)$  where  $\mathcal{E}$  is an exact symplectic manifold (the phase space),  $\alpha$  is a non-degenerate one-form called the area form ( $\sum_j p_j dq_j$  in canonical coordinates) and  $H$  is a Hamiltonian function. Then the dynamics is given by the principle of least action. It says that  $z(t)$  is a solution of the Hamiltonian system if it stationarises the action defined by:

$$W(z) = \int_{t_0}^{t_f} (H(z) - \alpha[\frac{dz}{dt}]) dt$$

in the space of  $C^1$  trajectories with fixed ends  $\delta z(t_0) = \delta z(t_f) = 0$ . This prescription imposes that the dynamics is governed by a vector field  $\frac{dz}{dt}$  which can be computed for each  $z \in \mathcal{E}$  as the (unique) solution of the equation:

$$d\alpha_z[\xi, \frac{dz}{dt}] = dH_z[\xi], \quad \text{for all } \xi \in T_z\mathcal{E} \quad (1)$$

Here  $d\alpha$  is a two-form which is called the symplectic form associated to the Hamiltonian dynamics. Indeed when  $z = (p, q)$  and  $\alpha = \sum_j p_j dq_j$ , the latter equation turns out to be nothing but the canonical Hamiltonian equations

$$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \dot{p} \\ \dot{q} \end{pmatrix} = \begin{pmatrix} \partial_p H \\ \partial_q H \end{pmatrix}, \quad (2)$$

since in this case,  $d\alpha = \sum dp \wedge dq$ , which is the above square matrix when written in components. Below, however, we will see examples with non-canonical coordinates. Moreover, this general formulation of Hamiltonian dynamics can be adapted to defining Hamiltonian dynamics on a set of loops as follows.

Let  $\mathcal{L}_1$  be the space of  $C^1$  period-1 loops in  $\mathcal{E}$ . Then, if  $z \in \mathcal{L}_1$ ,  $\text{T}\mathcal{L}_1$  is the space of  $C^0$  loops  $\xi$  such that  $\xi(s) \in \text{T}_{z(s)}\mathcal{E}$  for all  $s \in [0, 1]$ . The symplectic form  $d\alpha$  given on  $\text{T}\mathcal{E}$  induces a symplectic form  $\Omega$  on  $\text{T}\mathcal{L}_1$  defined by:

$$\Omega[\xi, \zeta] = \oint d\alpha_z[\xi(s), \zeta(s)] ds, \quad (3)$$

Here and in the following the notation  $\oint$  means that we compute the mean value of a periodic function over one period. Then the natural extension of eq. (1) to loop space writes:

$$\Omega[\xi, \frac{dz}{dt}] = \oint dH_{z(s)}[\xi(s)] ds, \quad \text{for all } \xi \in \text{T}_z\mathcal{L}_1. \quad (4)$$

This idea goes back to A. Weinstein [13]. Here  $\frac{dz}{dt}$  represents a vector field on the loop  $z(s)$  whose integration from  $t = 0$  provides a function  $z(t, s)$  describing the deformation of the initial loop in time. So far there is no approximation. The goal of this section is to propose a good estimate of  $z(t, s)$  when we know a family of period-1 loops  $\{z_\mu(s)\}_\mu$  which form an *approximate* invariant manifold  $\mathcal{M}$  of  $\mathcal{L}_1$ . (This means that each loop is nearly a periodic solution of the Hamiltonian system, provided that it is parametrised with the appropriate period, which is not necessarily equal to 1.) We will see later how such a family can in principle be constructed. The loops are indexed by an even number of parameters  $\mu = (a, \phi_0, \mathbf{p}, \mathbf{q})$  where  $a$  is the area of the loop:

$$a = \oint \alpha[\partial_s z_\mu] ds,$$

and  $\phi_0$  is a reference phase along the loop:

$$z_{(a, \phi_0, \mathbf{p}, \mathbf{q})}(s) = z_{(a, 0, \mathbf{p}, \mathbf{q})}(s + \phi_0).$$

The other parameters  $(\mathbf{p}, \mathbf{q}) \in \mathbb{R}^{2m}$  should play the role of conjugate variables and we will see how to check that point below.

Now if we start with an initial loop on  $\mathcal{M}$ , then by assumption it will stay for a long time on this subspace, but with a slow drift in parameters  $\mu$ . The actual trajectory can be approximated by:

$$z(t, s) \approx z_{\mu(t)}(s) \in \mathcal{M}, \quad (5)$$

and we want to find an approximate dynamics for variables  $\mu(t)$ . Thus the latter play the role of “collective coordinates” widely used in the study of solitons [14]. Let us note that in eq. (5) we are not interested in the variable  $s$  and will make it disappear by averaging. Now, we consider eq. (4) as the basic equation to determine the dynamics  $\frac{dz}{dt}$ . A natural simplification of eq. (4) is to “project” it on  $\text{T}\mathcal{M}$  by restricting the vectors  $\frac{dz}{dt}$  and  $\xi$  to be tangent to  $\text{T}\mathcal{M}$ . This is relevant because we assume that space  $\mathcal{M}$  is nearly invariant under the dynamics. So we propose the following equation to compute the evolution of  $\frac{d\mu}{dt}$ :

$$\Omega[\xi, D_\mu z_\mu \frac{d\mu}{dt}] = \oint dH_{z_{\mu(s)}}[\xi(s)] ds, \quad \text{for all } \xi(s) \in \text{T}_{z_\mu} \mathcal{M}. \quad (6)$$

The benefit of this projection is that the number of degrees of freedom has been reduced to the number of components of  $\mu$ , or even better, to the dimension  $m$  of  $(\mathbf{p}, \mathbf{q})$ . To convince oneself that this is true, we consider now the simple case  $\mu = (a, \phi_0, P, Q)$ , and will write the effective Hamiltonian dynamics for  $(P, Q)$ , deduced from (6). The tangent vectors to the loops are decomposed along these coordinates  $\mu$ . In particular, the approximate vector field is written as:

$$\frac{dz_\mu}{dt} = \dot{a} \partial_a z_\mu + \dot{\phi}_0 \partial_{\phi_0} z_\mu + \dot{P} \partial_P z_\mu + \dot{Q} \partial_Q z_\mu,$$

with the dots denoting derivative with respect to time  $t$ . First it is easy to show that  $\dot{a} = 0$  by substituting  $\xi = \partial_s z_\mu (= \partial_{\phi_0} z_\mu)$  in (6), and noticing that

$$\partial_{\mu_k} \oint_{z_\mu} \alpha = \oint d\alpha [\partial_{\mu_k} z_\mu, \partial_s z_\mu],$$

the latter vanishes for any component of  $\mu$ , but the first one, since  $\oint \alpha = a (= \mu_1)$  is constant. Secondly, by using the same fact, and substituting  $\xi = \partial_P z_\mu$  or  $\partial_Q z_\mu$  in (6), one obtains a direct generalisation of the canonical equation (2) as follows:

$$\begin{pmatrix} 0 & \tau_{PQ} \\ -\tau_{PQ} & 0 \end{pmatrix} \begin{pmatrix} \dot{P} \\ \dot{Q} \end{pmatrix} = \begin{pmatrix} \partial_P \text{H}^{\text{eff}} \\ \partial_Q \text{H}^{\text{eff}} \end{pmatrix} \quad (7)$$

where the effective Hamiltonian is defined as the mean energy along the loop indexed by  $(P, Q)$ :

$$\text{H}^{\text{eff}}(a, P, Q) = \oint H(z_{(a, \phi_0, P, Q)}(s)) ds, \quad (8)$$

and is to be used with an effective symplectic form whose components are determined by:

$$\tau_{PQ}(\mu) = \Omega[\partial_P z_\mu, \partial_Q z_\mu]. \quad (9)$$

Equation (7) generalises obviously for multi-component  $(\mathbf{p}, \mathbf{q})$ . Then  $\tau_{p_i q_j}$  becomes a matrix. An important remark is that the effective dynamics is well-defined only if the associated matrix  $\tau$  is invertible for all  $\mu$ . This is what we meant by saying that  $(\mathbf{p}, \mathbf{q})$  should be “conjugate variables”, as we required at the beginning of this section. A second remark is that since  $\dot{a} = 0$  we see directly that the effective dynamics take place in a family of loops with constant area. It is well-known that area is an adiabatic invariant for perturbation of an integrable Hamiltonian system. Notice that here the system is not assumed to be integrable, however.

A third remark is that, in practise, the Hamiltonian system often depends on a small parameter, say  $H_\epsilon$  and  $\alpha_\epsilon$  depending on  $\epsilon$ , but typically the family of loops  $z_\mu$  is only known in the unperturbed case  $\epsilon = 0$ . In this situation, it might be difficult to find explicit continuation of  $z_\mu$  for  $\epsilon \neq 0$ . Nevertheless, equation (7) can generally be written at the first order in  $\epsilon$ , using an approximate effective Hamiltonian  $\mathbf{H}_\epsilon^{\text{eff}} \approx \mathbf{H}_0^{\text{eff}} + \mathbf{V}^{\text{eff}}$  (and an approximate effective symplectic form), where  $\mathbf{V}^{\text{eff}}$  is obtained by averaging the perturbation  $H_\epsilon - H_0$  around the loops  $z_\mu$ . Examples will be provided in sections 4 and 5. Prior to this we will study how to estimate the error  $|\frac{dz_\mu}{dt} - X_H(z_\mu)|$  where  $X_H(z_\mu)$  is the actual Hamiltonian vector field associated with  $H$  and  $\alpha$  and defined by (1).

### 3 Estimating the approximation error

The accuracy of the approximation (6) and (7) will depend on the choice of  $\mathcal{M}$  as a good approximate invariant manifold of the dynamics. In this section we analyse how such an approximate invariant manifold could be constructed and estimate the error  $|\Delta X| = |X_{\mathbf{H}^{\text{eff}}}(z_\mu) - X_H(z_\mu)|$ , where  $X_H(z_\mu)$  and  $X_{\mathbf{H}^{\text{eff}}}(z_\mu)$  are respectively the Hamiltonian vector field and the effective Hamiltonian vector field. The result that we aim to show in this section can be written as follows:

$$\|\Delta X\| \leq K \|\nabla \mathbf{H}^{\text{eff}}\| \cos \gamma \quad (10)$$

where  $K$  is a bounded constant, and  $\gamma$  is an angle between two submanifolds to be defined below. This inequality is useful as it shows in which cases the approximation can be good.

We recall that  $\mathcal{E}$  is a symplectic phase space with the symplectic form  $d\alpha$  defined on the tangent bundle  $T\mathcal{E}$ , and  $\mathcal{L}_1$  is the space of  $C^1$  period-1 loops in  $\mathcal{E}$  which

inherits a symplectic form defined by (3). We suppose that there is also a scalar product  $(\cdot, \cdot)$  on  $T\mathcal{E}$  and endow  $T_z\mathcal{L}_1$  with the scalar product (and the associate norm  $L_2$ ) defined by:

$$\begin{aligned} \langle \xi, \zeta \rangle &= \oint (\xi(s), \zeta(s)) ds \\ &= \|\xi\| \|\zeta\| \cos \varphi, \end{aligned}$$

where  $\varphi$  is called the Euclidean angle between  $\xi$  and  $\zeta$  belonging to  $T_z\mathcal{M}$ . Likewise, we assume that the symplectic form  $\Omega$  can be written as:

$$\Omega[\xi, \zeta] = \|\xi\| \|\zeta\| \cos \theta_s,$$

where  $\theta_s$  is called the symplectic angle between  $\xi$  and  $\zeta$ .

Before using these definitions, we want to specify how one can obtain the family of loops  $\{z_\mu(s) \in \mathcal{L}_1\}_\mu$  considered in the previous section. We suppose that there is a function  $\mathbf{G}$  defined on  $\mathcal{E}$  such that

$$\oint \mathbf{G}(z_\mu) = (\mathbf{p}, \mathbf{q}), \quad (11)$$

and a phase function  $\Phi$  such that

$$\oint \Phi(z_\mu) = \phi_0$$

Then, as already stated in [11], if  $z_\mu(s)$  is an approximate periodic solution of the Hamiltonian system, it can also be viewed as a critical point of the mean energy  $\oint H$  subjected to fixed area,  $a = \oint \alpha(z)$ , fixed phase  $\phi_0 = \oint \Phi$  and fixed parameters  $(\mathbf{p}, \mathbf{q}) = \oint \mathbf{G}$ . Equivalently,  $z_\mu$  is defined as a critical point of the constrained energy:

$$\mathcal{H}(z) = \oint H(z) - f \left( \oint \alpha[\partial_s z] - a \right) - k \left( \oint \Phi(z) - \phi_0 \right) - \boldsymbol{\lambda} \left[ \oint \mathbf{G}(z) - (\mathbf{p}, \mathbf{q}) \right] \quad (12)$$

where  $f, k$  and  $\boldsymbol{\lambda}$  are Lagrange multipliers. Moreover, it is not difficult to prove that [11]:

$$\begin{aligned} f &= \partial_a \mathbf{H}^{\text{eff}} \\ k &= \partial_{\phi_0} \mathbf{H}^{\text{eff}} = 0 \\ \boldsymbol{\lambda} &= \partial_{(\mathbf{p}, \mathbf{q})} \mathbf{H}^{\text{eff}} \end{aligned}$$

with  $\mathbf{H}^{\text{eff}}(\mu) = \oint H(z_\mu)$ . (Here  $\partial_{(\mathbf{p}, \mathbf{q})}$  denotes the vector  $(\partial_{p_1}, \partial_{p_2}, \dots, \partial_{q_1}, \partial_{q_2}, \dots, \partial_{q_m})$ ).

Then  $\mathcal{M}$  can be redefined as the subspace of  $\mathcal{L}_1$  formed by the critical points  $z_\mu$  of  $\mathcal{H}(z)$  and parametrised by  $\mu$ . We also assume that  $\mathcal{L}_1$  can be foliated by the subspaces:

$$\mathcal{F}_\mu = \{z \in \mathcal{L}_1 \mid \oint \alpha[\partial_s z] = a, \oint \Phi(z) = \phi_0, \oint \mathbf{G}(z) = (\mathbf{p}, \mathbf{q})\}$$

in such a way that each tangent loop  $v$  of  $T_{z_\mu}\mathcal{L}_1$  can be written as a sum  $v = \xi + \eta$ , with  $\xi \in T_{z_\mu}\mathcal{M}$  and  $\eta \in T_{z_\mu}\mathcal{F}_\mu$ . Note that the latter is defined as

$$T_{z_\mu}\mathcal{F}_\mu = \{\eta \in T_{z_\mu}\mathcal{L}_1 \mid \oint d\alpha[\eta, \partial_s z_\mu] = 0, \oint d\Phi(\eta) = 0, \oint D\mathbf{G}(\eta) = 0\} \quad (13)$$

Now, to achieve the estimate (10), the main step consists in showing that

$$\Omega[\Delta X, \xi + \eta] = \Omega[X_{\text{H}^{\text{eff}}}, \eta]. \quad (14)$$

Indeed, by using the definition (6) of  $X_{\text{H}^{\text{eff}}}$ , we have that for all  $\xi \in T_{z_\mu}\mathcal{M}$ :

$$\Omega[\xi, X_{\text{H}^{\text{eff}}}] = \oint d\alpha_{z_\mu}[\xi, X_{\text{H}^{\text{eff}}}] = \oint dH[\xi] = \Omega[\xi, X_H] \quad (15)$$

Consequently,  $\Omega[\xi, \Delta X] = 0$ . Secondly, by expressing that  $\delta\mathcal{H} = 0$  (from eq. (12)) in conjunction with eq. (13), one deduces that, for all  $\eta \in T_{z_\mu}\mathcal{F}_\mu$ :

$$\begin{aligned} \Omega[\eta, X_H] &= \oint dH_{z_\mu}[\eta] \\ &= 0. \end{aligned} \quad (16)$$

So, eqs. (15) and (16) imply eq. (14).

On the other hand, as  $\Omega$  is non degenerate, there exists  $v = \xi + \eta$  such that  $\Omega(\Delta X, \xi + \eta) = \|\Delta X\| \|\xi + \eta\| \cos \theta_s$  with non vanishing  $\theta_s$ . Therefore, for this  $v$ :

$$\begin{aligned} \|\Delta X\| &= \frac{\Omega(\Delta X, \xi + \eta)}{\|\xi + \eta\| \cos \theta_s} \\ &= \frac{\Omega(X_{\text{H}^{\text{eff}}}, \eta)}{\|\xi + \eta\| \cos \theta_s} \\ &= \|\nabla \mathbf{H}^{\text{eff}}\| \frac{\|\eta\| \cos \varphi}{\|\xi + \eta\| \cos \theta_s}, \end{aligned}$$

where  $\varphi$  is the Euclidean angle between  $\nabla \mathbf{H}^{\text{eff}}$  and  $\eta$ . By taking the supremum over  $\xi \in T\mathcal{M}$  we get

$$\|\Delta X\| \leq \|\nabla \mathbf{H}^{\text{eff}}\| \frac{\cos \varphi}{\cos \delta \cos \theta_s}$$

with  $\delta$  being the Euclidean angle between  $\xi + \eta$  and  $\eta$ . Finally, one can replace  $\varphi$  by

$$\gamma = \inf_{\xi \in T_z\mathcal{M}, \eta \in T_z\mathcal{F}_\mu} \arccos |\langle \xi, \eta \rangle|, \quad (17)$$

which we define as the angle between  $T_{z_\mu}\mathcal{F}_\mu$  and  $T_{z_\mu}\mathcal{M}$ . In conclusion we obtain the above equation (10). We see that if  $\gamma = \frac{\pi}{2}$  for all  $z_\mu$ , the effective dynamics is exact since we have  $\|\Delta X\| = 0$ . In general it is not the case but nevertheless the error can be quite small in a neighborhood of critical points of  $\mathbf{H}^{\text{eff}}$ , which are true



periodic orbits of the system. Finally notice that estimate (10) depends on the full dynamics, not only on the approximating one. For example modifying the actual system without changing the approximating one amounts to change the foliation  $\mathcal{F}_\mu$ , which in turn will change the angles defined in (17) and in previous equations, and so the constants in estimate (10).

## 4 Salerno's model

In this section we illustrate the theory presented in section 2 on an interesting model proposed by Salerno, whose Hamiltonian can be written as follows [14, 15]:

$$H_\epsilon = - \sum_n \left[ \phi_n^* (\phi_{n+1} + \phi_{n-1}) + \frac{2\epsilon}{\gamma - \epsilon} |\phi_n|^2 - \frac{4\gamma}{(\gamma - \epsilon)^2} \log\left(1 + \frac{\gamma - \epsilon}{2} |\phi_n|^2\right) \right],$$

to be used with the area form:

$$\alpha_\epsilon = i \frac{2}{\gamma - \epsilon} \sum_n \log\left(1 + \frac{\gamma - \epsilon}{2} |\phi_n|^2\right) \frac{d\phi_n}{\phi_n} \quad (18)$$

So the symplectic form  $d\alpha_\epsilon = \Omega_\epsilon$  is computed as:

$$\Omega_\epsilon = i \sum_n \frac{d\phi_n^* \wedge d\phi_n}{1 + \left(\frac{\gamma - \epsilon}{2}\right) |\phi_n|^2}$$

Here the conjugate variables are  $(i\phi_n^*, \phi_n)$ . Note that the symplectic form is canonical only when  $\gamma = \epsilon$ .

The Salerno model has the nice property to provide a Hamiltonian interpolation between two well-studied systems, namely the Ablowitz-Ladik system (AL), for  $\epsilon = 0$ , and the discrete nonlinear Schrödinger system (DNLS), when  $\epsilon = \gamma$  [4, 14]. In the latter limit, the expression of  $H_\gamma$  seems singular, but using the expansion of  $\log(1 + x)$  one easily checks that

$$\lim_{\epsilon \rightarrow \gamma} H_\epsilon = - \sum_n \left[ \phi_n^* (\phi_{n+1} + \phi_{n-1} - 2\phi_n) + \frac{\gamma}{2} |\phi_n|^4 \right] \quad (19)$$

which gives, using  $\Omega_\gamma$ , the DNLS equation:

$$i\dot{\phi}_n + \gamma |\phi_n|^2 \phi_n + (\phi_{n+1} + \phi_{n-1} - 2\phi_n) = 0$$

On the other hand, when  $\epsilon = 0$ , the evolution equation (with the non-canonical form  $\Omega_0$ ) is found to be the AL equation:

$$i\dot{\phi}_n + \frac{\gamma}{2} |\phi_n|^2 (\phi_{n+1} + \phi_{n-1}) + (\phi_{n+1} + \phi_{n-1} - 2\phi_n) = 0$$

which is known to be completely integrable. In particular, the AL system possesses a family of moving discrete breathers that can be explicitly written as:

$$u_n(t) = \sqrt{\frac{2}{\gamma}} \sinh \beta \frac{e^{-i(\omega t - kn)}}{\cosh \beta(n - ct)} \quad (20)$$

with parameters  $\beta, \gamma, k$  and  $\omega = 2(1 - \cos k \cosh \beta)$ . The velocity of the DB is given by

$$c = 2 \sin k \frac{\cosh \beta}{\beta} \quad (21)$$

Our aim is to show that the method of the effective Hamiltonian applies here to analyse moving discrete breathers in the Salerno model. First we will interpret the travelling DB of the AL system (20) as a trivial one degree of freedom dynamics governed by a simple effective Hamiltonian system. Next we will use these exact travelling solutions to describe approximate moving breathers for  $\epsilon \neq 0$ , and in particular for the DNLS system. In the following we set  $\gamma = 2$  for convenience (or equivalently we rescale amplitude of  $\phi_n$  to  $\sqrt{\frac{2}{\gamma}}\phi_n$ ).

We consider the following family of period-1 loops

$$z_n(s) = \sinh \beta \frac{e^{-i(2\pi s - kn)}}{\cosh \beta(n - Q)}, \quad (22)$$

with parameter  $Q, k$  and  $\beta$ . We first compute the area of these loops, using the area form (18), and find that:

$$\oint_z \alpha_0 = 4\pi\beta. \quad (23)$$

Note that this is an exact result, which can be obtained by a Poisson summation. As this technique is frequently used in this section, it is recalled in Appendix A.

So, we note that (22) forms a family of loops with constant area, if  $\beta$  is fixed. Next, it is easy to check that these loops form a family of exact periodic solutions of the AL equation only when  $k = 0$  or  $\pi$ , and if the time  $s$  is scaled properly as in eq. (20). Moreover, the amplitude of these solutions is exponentially localised in space about position  $n_c = Q$ , thus these loops constitute a continuous family of discrete breathers parametrised by a translation coordinate  $Q$  (see Fig. 1(c) and (d)). This is exactly what we want to get moving breathers, except that we need a conjugate variable to  $Q$ . We can try to use variable  $k$  if the symplectic form  $\Omega_0$  restricted to coordinates  $(k, Q)$  is non-degenerate. As explained in section 2, this can be checked by computing eq. (9), viz.,

$$\tau(k, Q) = \oint \Omega_0(\partial_k z, \partial_Q z) = 2\beta,$$

which is non zero for  $\beta \neq 0$ . Now, if  $k$  is near 0 or  $\pi$ , the family of loops (22) is interpreted as forming an approximate invariant manifold in phase space, parametrised by  $(k, Q)$ , on which it could be possible to describe the slow evolution of  $(k, Q)$ . To this end we have just to compute  $H_0^{\text{eff}}$  given by eq. (8). After some computations which involves the same technique as before we find:

$$H_0^{\text{eff}} = -4 \cos k \cosh \beta.$$

Using  $\Omega^{\text{eff}} = 2\beta dk \wedge dQ$ , one gets the following equations of motion:

$$\begin{aligned} \dot{k} &= 0 \\ \dot{Q} &= \frac{2 \sin k \cosh \beta}{\beta} \end{aligned}$$

Therefore the dynamics of discrete breathers is extremely simple in this case, since they move with constant speed  $\dot{Q}$  (which coincides with formula (21)). The corresponding phase portrait is sketched on Fig.1(a).

Let us notice that other “conjugate” variables to  $Q$  could have been chosen. For example it might be natural to think of the following conserved quantity of the AL system, which can be interpreted as the “momentum” of the system:

$$P = -i \sum_n \phi_n^* (\phi_{n+1} - \phi_{n-1}).$$

Computing the momentum of the loops (22) with the same technique as for (23) we get:

$$P(\{z_n\}) = 4 \sin k \sinh \beta. \quad (24)$$

So we have  $P = 0$  for discrete breathers ( $k = 0$  or  $\pi$ ) which is consistent with the fact that these structure are immobile. On the other hand, we can look at (22) with arbitrary  $k$  as periodic solutions of AL system under the constraint that  $\oint P$  has a non-zero value fixed in  $[-\sinh \beta, \sinh \beta]$ . As before, these periodic solutions enable one to construct an effective Hamiltonian in variables  $(P, Q)$ , which has the form  $H_0^{\text{eff}}(P, Q) = 4\beta - \sqrt{16 \sinh^2 \beta - P^2}$ , and the associated dynamics is quite simple:  $\dot{P} = 0$ ;  $\dot{Q} = \frac{P}{2\beta}$ .

The method of effective Hamiltonian generally gives only approximate solutions, but in the special case of AL system, it describes exact moving breathers. (We expect that the symplectic angle defined by (17) is equal to  $\pi/2$  in the present case). Now we want to compute an effective Hamiltonian for the Salerno interpolation, i.e. when  $\epsilon \neq 0$ . In this case we do not know exact periodic solutions of the system with constraints of constant area and fixed  $(k, Q)$  but we can use the family (22) to

produce a perturbative scheme, as explained in section 2. Then at first order in  $\epsilon$ , the effect of perturbation is to change  $H_0^{\text{eff}}$  to  $H_0^{\text{eff}} + V^{\text{eff}}$  with

$$V^{\text{eff}} = -\epsilon 4\pi^2 \frac{\sinh^2 \beta}{\beta^2 \sinh(\frac{\pi^2}{\beta})} \cos(2\pi Q) + O(\epsilon e^{-\frac{2\pi^2}{\beta}} \cos(4\pi Q)) \quad (25)$$

Therefore  $H^{\text{eff}}$  now depends on  $Q$  and the phase portrait of Fig.1(a) is changed to the pendulum-like phase portrait of Fig.1(b). We see that the line of critical points ( $k = 0$  or  $\pi$ ) of the former has turned into a set of isolated equilibria which correspond to (exact) discrete breathers of Salerno's system. More precisely, these discrete breathers are centred at  $Q = \frac{n}{2}$  ( $n \in \mathbb{Z}$ ). The in-phase discrete breathers (i.e.  $k = 0$ ) are stable for  $n$  even and unstable for  $n$  odd, and the converse situation holds for the anti-phase discrete breathers ( $k = \pi$ ). In this picture, if a stable discrete breather is perturbed, its position  $Q$  simply oscillates periodically, since in space ( $k, Q$ ), its trajectory is trapped within the corresponding island. On the other hand, the stable discrete breathers can be set into motion by a kick of momentum which brings the state of the system outside the islands of the stable critical points. This change of momentum amounts to crossing a minimal energy barrier which is called the Peierls-Nabarro barrier by analogy with the theory of moving localized defects in solid. Thus in the context of discrete breathers, as already mentioned in [11], the PN barrier is defined as the difference of potential energy  $\Delta V^{\text{eff}}$  between the stable and the unstable breathers with same area.

In fact, the phase portrait depicted in Fig.1(b) was already presented by Claude et al. [7] in order to analyse the motion of discrete breathers in anharmonic chains with on-site potential. In particular, they pointed out that there is a critical value  $\beta_c$  above which the saddle-nodes of lines  $k = 0$  or those of  $k = \pi$  are no longer connected horizontally, but connect vertically in the plane ( $k, Q$ ). This  $\beta_c$  depends on  $\epsilon$ , and Claude *et al.* obtained  $\beta_c \simeq 3.6862$ , which corresponds to  $\epsilon = 2$  in (25). For  $\beta > \beta_c$ , the trajectories with monotonously increasing (or decreasing)  $Q$  are lost, and so are the moving discrete breathers. This explains, at least qualitatively, why the large amplitude DB (which occurs for large  $\beta$ ), are always trapped in the anharmonic chains of the Salerno family (with  $\epsilon \neq 0$ ). We remark, however, that rigorous conclusions should take into account that the method of the effective Hamiltonian works well only when the size of the islands is small, which is the case for  $\beta \ll \beta_c$ , since only in this case the error estimate is guaranteed to be small (eq. (10)). In fact, numerical simulations reported in [9] demonstrate that the trapping of DB happens with amplitudes corresponding to  $\beta$  much smaller than  $\beta_c$ . This tendency to pinning will also be illustrated below by a numerical simulation.

We also notice that if one is interested in the limit  $\epsilon = 2$ , which indeed cor-

responds to the DNLS limit of the Salerno family, then, in view of eq. (19) (recall  $\gamma = 2$ ), the effective potential should not be determined by setting  $\epsilon = 2$  in (25), but should be estimated by substitution of (22) in  $\sum_n (2\|\phi_n\|^2 - \|\phi_n\|^4)$ . One obtains the new effective potential as:

$$V^{\text{eff}} = 8\pi^2 \frac{\sinh^2 \beta}{\beta^2 \sinh(\frac{\pi^2}{\beta})} \left( 1 - \frac{1}{3} \left[ 1 + \frac{\pi^2}{\beta^2} \right] \sinh^2 \beta \right) \cos(2\pi Q) + O(e^{-\frac{2\pi^2}{\beta}}).$$

For this potential there is also a critical  $\beta$ , but now evaluated as  $\beta_c \simeq 1.695$ . To end this section, we wish to show how the analysis presented above can be matched with direct numerical simulations of the Salerno equations, projected on the effective phase space spanned by coordinates  $(k, Q)$ . To this purpose, we have to find a function  $\mathbf{G} = (G_1, G_2)$  (see eq. (11)), such that

$$\oint \mathbf{G}(\{\phi_n\}) = (k, Q),$$

when  $\phi_n$  is replaced by the loops (22). The function  $G_1$  can be determined from eqs. (24), and the function  $G_2$  can be defined by:

$$G_2(\{\phi_n\}) = \frac{\sum_n n \log(1 + \|\phi_n\|^2)}{\sum_n \log(1 + \|\phi_n\|^2)}.$$

We consider a chain of 99 oscillators with periodic boundary conditions and integrate numerically the Salerno equations with  $\epsilon = 0.1$  and initial conditions given by a member of the loop family (22), with  $\beta = 1$  and small  $k$ . The evolution of variables:

$$(\bar{k}(t), \bar{Q}(t)) = \frac{1}{T} \int_t^{t+T} \mathbf{G}(\{\phi_n(t')\}) dt' \quad (26)$$

is followed in time and plotted in the plane  $(k, Q)$ . The period  $T$  is chosen as the one of the DB ( $k = 0$ ). Figure (2) shows two trajectories which are consistent with the effective separatrices (i.e. the frontiers of the islands). The latter are computed from  $H^{\text{eff}}(k, Q)$ . Let us note that performing the averaging of  $\mathbf{G}$  is crucial to eliminate the effect of global phase of the loops on the dynamics. This point is illustrated on Fig. (3) where trajectories are compared with and without averaging  $\mathbf{G}$ .

Next, increasing slightly  $\epsilon$ , one observes an example of trapping phenomenon which is not predicted by the effective Hamiltonian. Figure (4) shows a trajectory which starts outside the trapping islands, but which ends on pinning due to a decrease of  $k$  in time. For this value of  $\epsilon = 0.2$ , this behaviour is observed for any initial  $k$ . It is presumably related to interaction of the DB with its own radiation, due to finite size of the system, but it could be interesting to investigate this point further. In any case, we numerically observe that the validity of the effective Hamiltonian description in a finite chain is limited to relatively low value of  $\epsilon$ .

## 5 Weakly localised travelling discrete breathers in FPU chains

We consider another situation where the framework of the effective Hamiltonian can be used to describe approximate travelling discrete breathers, namely the Fermi-Pasta-Ulam (FPU) system on a ring. This model has been theoretically studied recently by different authors [16, 17, 18]. It is given by a closed chain of identical masses anharmonically coupled to their first neighbours:

$$H = \sum_{n=-N}^N \left( \frac{p_n^2}{2} + V(x_{n+1} - x_n) \right) \quad (27)$$

The number of particles is assumed to be odd, and equal to  $M = 2N+1$ . We consider the so-called  $\alpha\beta$ -FPU system in which the anharmonicity is at most quartic:

$$V(x) = \frac{x^2}{2} + \alpha \frac{x^3}{3} + \beta \frac{x^4}{4}$$

First we recall some standard results concerning the complete analysis of the harmonic chain  $\alpha = \beta = 0$ . In this case  $H_0$  can be diagonalised by a discrete Fourier transform as follows:

$$z_k = \frac{1}{\sqrt{2M\omega_k}} \sum_{n=-N}^N (\omega_k x_n + i p_n) e^{-i2\pi kn/M} \quad (28)$$

where  $\omega_k = 2|\sin(\frac{k\pi}{M})|$  for  $(k = \pm 1, \pm 2, \dots, \pm N)$ , and the  $k = 0$  component is treated by defining  $\bar{p}_0 = \frac{1}{\sqrt{M}} \sum_n p_n$  and  $\bar{x}_0 = \frac{1}{\sqrt{M}} \sum_n x_n$ . The change of coordinates  $(p_n, x_n) \rightarrow (\bar{p}_0, \bar{x}_0, i z_k^*, z_k)$  is canonical, i.e. the symplectic form writes  $\Omega = \sum_n dp_n \wedge dq_n = d\bar{p}_0 \wedge d\bar{x}_0 + i \sum_k dz_k^* \wedge dz_k$ . The expression of  $H_0$  becomes simply

$$H_0 = \frac{\bar{p}_0^2}{2} + \sum_{k=1}^N \omega_k (|z_k|^2 + |z_{-k}|^2),$$

and we can assume that the center of mass of the chain is at rest, i.e.  $\bar{p}_0 = 0$ . In this setting, it is readily seen that the general (vibrational) solution is a superposition of  $N$  distinct modes (the phonons) which are twofold degenerate.

It is yet simpler to describe the phonons of frequency  $\omega_k$  with the help of action-angle variables defined by:

$$\begin{aligned} z_k &= \sqrt{J_k} e^{-i\psi_k} \\ z_{-k} &= \sqrt{J_{-k}} e^{-i\psi_{-k}} \end{aligned} \quad (29)$$

This second canonical transformation simplifies further the Hamiltonian into

$$H_0 = \sum_{k=1}^N \omega_k (J_k + J_{-k}),$$

such that the evolution of the variables are trivially given by

$$\begin{aligned} \psi_k &= \omega_k t + \psi_k^0 \\ \psi_{-k} &= \omega_k t + \psi_{-k}^0 \end{aligned}$$

and the actions  $J_k$  are constant. Note that we can easily come back to the physical displacement  $x_n$  by inverting the transformations (28) and (29). For instance, the phonons of frequency  $\omega_N$  form a 4-parameter family of periodic solutions which can be written as:

$$x_n(t) = \sqrt{\frac{2}{M\omega_N}} \left[ \sqrt{J_N} \cos(\omega_N t - \sigma_N n + \psi_N^0) + \sqrt{J_{-N}} \cos(\omega_N t + \sigma_N n + \psi_{-N}^0) \right] \quad (30)$$

with  $\sigma_N = \frac{2\pi N}{M}$ .

Strictly speaking there are no discrete breathers in the harmonic chain. Nevertheless we can consider that some periodic solutions of this system are weakly localized in space, namely the phonons with the upper frequency,  $\omega_N$ , and with  $J_N = J_{-N}$ . The latter correspond to the standing wave:

$$x_n(t) = 2\sqrt{\frac{2J_N}{M\omega_N}} \cos\left(\omega_N t + \frac{\psi_k^0 + \psi_{-k}^0}{2}\right) \cos\left(\sigma_N n - \frac{\psi_k^0 - \psi_{-k}^0}{2}\right) \quad (31)$$

By writing  $\sigma_N n = \pi n(1 - \frac{1}{2N+1})$  the spatial shape of this periodic solution can be seen as follows:

$$\cos\left(\sigma_N n - \frac{\psi_k^0 - \psi_{-k}^0}{2}\right) = (-1)^n \cos\left(\frac{\pi}{2N+1} n - \frac{\psi_k^0 - \psi_{-k}^0}{2}\right)$$

so it corresponds to the anti-phase oscillations  $(-1)^n$  modulated by a one-bump envelope which is centred around  $\theta \equiv \frac{\psi_N - \psi_{-N}}{2} = \frac{\psi_N^0 - \psi_{-N}^0}{2}$ . One can check that the energy density (defined as  $h_n = \frac{p_n}{2} + \frac{1}{2}(V(x_{n+1} - x_n) + V(x_n - x_{n-1}))$ ) is also localised in this weak sense. Therefore the relative phase variable  $\theta$  plays the role of a spatial coordinate of a periodic solution which is weakly localised. Let us call it a *weakly localised* discrete breather. This name can be justified a posteriori, because we notice by numerical simulations, that the localisation of this periodic solution is enhanced when the anharmonicity is turned on (see Fig.5).

In order to construct an effective Hamiltonian for  $\theta$  we need to specify its conjugate variable. Here it is natural to consider the relative action  $J_N - J_{-N}$ . This

motivates a further canonical transformation as follows:

$$\begin{aligned} a &= J_N + J_{-N} \\ J &= J_N - J_{-N} \\ \varphi &= \frac{\psi_N + \psi_{-N}}{2} \\ \theta &= \frac{\psi_N - \psi_{-N}}{2} \end{aligned}$$

The first variable  $a$  is proportional to the area of the periodic solutions defined by eq. (30). In fact the exact relation is

$$\text{area} = \sqrt{\frac{2}{M\omega_N}} 2\pi a$$

By extension, let us call  $a$  the area in the sequel. Therefore, for fixed area, eq. (30) define a two-dimensional family (parametrised by  $J$  and  $\theta$ ) of periodic solutions of the chain when  $\beta = 0$ . In the spirit of section 4 this family can be used as a submanifold of loops in order to obtain an effective dynamics of  $J$  and  $\theta$ . Thus we substitute

$$x_n(J, \theta; s) = \sqrt{\frac{2}{M\omega_N}} \left[ \sqrt{\frac{a+J}{2}} \cos(2\pi s - \sigma_N n - \theta) + \sqrt{\frac{a-J}{2}} \cos(2\pi s + \sigma_N n + \theta) \right] \quad (32)$$

in the FPU-Hamiltonian (27) (with  $p_n = \dot{x}_n$ ) and obtain, after averaging over  $s$ , and at the lowest order in  $(\alpha, \beta)$ :

$$\mathbf{H}^{\text{eff}} \simeq \omega a + \frac{3}{16} \beta \frac{\omega^2}{M} (3a^2 - J^2).$$

We remark that this Hamiltonian is a particular case of the (Birkhoff) normal form Hamiltonian obtained by Rink for the periodic  $\beta$ -FPU chains, when only modes  $\omega_N$  are excited [18]. In view of this Hamiltonian, the variable  $\theta$  (or more precisely its averaged value) has now a drift which is given by:

$$\theta(t) = -\frac{3}{8} \beta \frac{\omega^2}{M} J t + \theta_0. \quad (33)$$

The drift (33) is associated with the slow motion of the weakly localised discrete breathers defined by eq. (31). To make this clear, we compute from eq. (32) the averaged square amplitude of  $x_n(J, \theta, s)$ , when  $J$  is small compared to  $a$ :

$$\oint |x_n(J, \theta; s)|^2 ds \approx \frac{a}{M\omega_N} \cos^2(\sigma_N n - \theta(t))$$

Let us note that at this order of approximation  $J$  is constant, since  $\mathbf{H}^{\text{eff}}$  does not depend on  $\theta$ . So the phase portrait is like that of fig.1(a), and at this level of



approximation there is no PN barrier. This may be related to the observations that mobile breathers are easily observed in numerical simulations of the FPU systems. It is likely, however, that a PN barrier would show up at a higher order in  $\alpha$  or in  $\beta$ , and this could be interesting to estimate explicitly.

We have performed some numerical simulations of the FPU model to illustrate the theory. We use a small chain of 25 particles and integrate numerically the dynamics in  $(p_n, x_n)$  variables with a Runge-Kutta method. We monitor the time evolution of the relative phase  $\theta$  which is deduced from the numerics as  $\theta = \frac{1}{2} \arg(z_N z_{-N}^*)$ , where  $z_N$  is computed with the help of eq. (28).

We start with an initial area of  $a = 0.05$ . As mentioned above the effect of anharmonicity reinforces the localisation of the solution, as compared with the shape of the ansatz [Fig.5]. On a time interval of order  $25T$ , where  $T = 2\pi/\omega_N$  is the period of the fast oscillations, we see that the evolution of variable  $\theta$  is almost linear and the slope of the line is in good agreement with eq. (33) [Fig.6(a)]. The fast oscillations of  $\theta$  can be eliminated by averaging, as explained in the previous section. Figure 6(b) shows the evolution of  $\theta$  on a much longer time scale. One sees a discrepancy growing between the actual dynamics  $\theta(t)$  and its linear estimate given by eq. (33). Let us note that in the same time fairly constant values of variables  $a$  and  $J$  were observed. With these parameters, and for any initial value of  $\theta$  we have not observed any trapping of the weakly localised discrete breather. If we consider an initial area which is two times higher but still small,  $a = 0.1$ , we observe that the effective dynamics describes fairly well the actual dynamics for the same time interval as compared with the previous case (of order  $25T$ ). However here the discrepancy grows faster with large amplitude oscillations [Fig. 7(a)], and the numerics show that area  $a$  is no longer constant. Nevertheless, the linear approximation given by (33) describes yet the global drift of the relative phase. In the local phase  $(\theta, J)$ , the trajectory is still drifting in  $\theta$  but not like the simple linear drift predicted for the effective dynamics [Fig. 7(b)]. Again in this case, no pinning state is observed for various initial values of  $\theta$ .

To end this section we point out that recently a proof of existence of DB in FPU chains has been obtained by G. James [20]. These DB can also be described as “weakly localised” for small amplitude since although they are exponentially localised the spatial decay rate goes to zero with the amplitude. So by deducing from his result an analytical form for a family of (approximate) DB solutions it could be interesting to consider the latter as a starting point for constructing the effective Hamiltonian.

## 6 Conclusions

In this paper we have proposed a framework to figure out the approximate travelling DB as trajectories described by an effective 1-DOF Hamiltonian. Our method can also be regarded as a method of collective coordinates for loops in Hamiltonian systems, based on an averaging procedure, and designed so that the error can in principle be estimated. The effective Hamiltonian is constructed as the averaged energy along loops representing approximate DB of the system with fixed area, and indexed by a spatial-like parameter. This Hamiltonian possesses critical points which correspond to exact DB of the chain. Some of them may be stable, others are unstable. Around the stable DB the trajectories of the effective Hamiltonian are closed and form an island of quasi-periodic breathers. The smaller is the size of these islands, the better is the approximation because in this case the error given by eq. (10) is small. In the effective phase portrait, the difference of potential energy between the stable and the (most) unstable DB can be defined as the Peierls-Nabarro barrier for DB. Thus the simple picture which emerges from this framework is that if one starts with an approximate DB with energy slightly above the PN barrier, it travels, drifting along separatrices in the effective phase space.

To illustrate the theory we applied the method to simple tutorial models, both analytically and numerically. In particular the concept of PN barrier for DB is illustrated on the Salerno model. For the FPU model, no PN was found at the lowest order in the anharmonicity parameters. Further applications could be thought of, however, to give insight on travelling DB in more realistic models. For example, a recent paper by Tsironis et al. [21] proposed a modification of the FPU model to take into account the curvature of discrete curvilinear chains that model biopolymers. If this curvature is small enough, it plays the role of a perturbation of the standard FPU model and an effective potential could be computed for the family of loops (30), so that the effect of such curvature could be estimated on loose DB defined in previous section. Another perspective is to consider application of the effective Hamiltonian method to describing travelling DB in Davydov or Holstein-like models [14]. Preliminary work is in progress in this direction.

## A Appendix

In this appendix we briefly recall the technique of Poisson summation and use it to obtain eq. (23). The same method is used to compute various quantities in section 4, as for instance  $P$ ,  $H^{\text{eff}}$ ,  $\Omega^{\text{eff}}$  and  $V^{\text{eff}}$ .

The following result is standard in signal analysis [19] and is known as the Poisson

summation formula:

$$\sum_{n=-\infty}^{\infty} f(n) = \sum_{n=-\infty}^{\infty} \hat{f}(n), \quad (34)$$

where  $\hat{f}$  is the Fourier transform of  $f$  defined by:

$$\hat{f}(\nu) = \int_{-\infty}^{\infty} f(x) e^{-i2\pi\nu x} dx$$

Now we want to compute  $\oint_z \alpha_0$ , i.e. integrate the area form (18) over a loop of the family (22). Integration over time is trivial and gives

$$a(\beta, Q) = 2\pi \sum_n \log\left(1 + \frac{\sinh^2 \beta}{\cosh^2(\beta[n - Q])}\right).$$

First choose  $Q = 0$  and compute:

$$\frac{\partial a}{\partial \beta}(\beta, 0) = 2\pi \frac{2 \sinh \beta}{\beta} \sum_n \frac{\beta \cosh \beta \cosh \beta n - \beta n \sinh \beta \sinh \beta n}{\cosh \beta(n+1) \cosh \beta n \cosh \beta(n-1)}$$

The sum can be written as  $\sum_n g(\beta n)$  with some function  $g(x)$  whose Fourier transform can be computed explicitly using residue calculus:

$$\hat{g}(\nu) = \pi^2 \frac{\sin^2 \pi \nu \beta \cosh \pi^2 \nu}{\sinh \beta \sinh^2 \pi^2 \nu}$$

So application of the Poisson formula (34) yields:

$$\frac{\partial a}{\partial \beta} = 2\pi \frac{2 \sinh \beta}{\beta^2} \sum_n \hat{g}\left(\frac{n}{\beta}\right) = 4\pi$$

On the other hand, the same technique enables one to prove that  $\frac{\partial a}{\partial Q} = 0$ . Therefore equation (23) is obtained.

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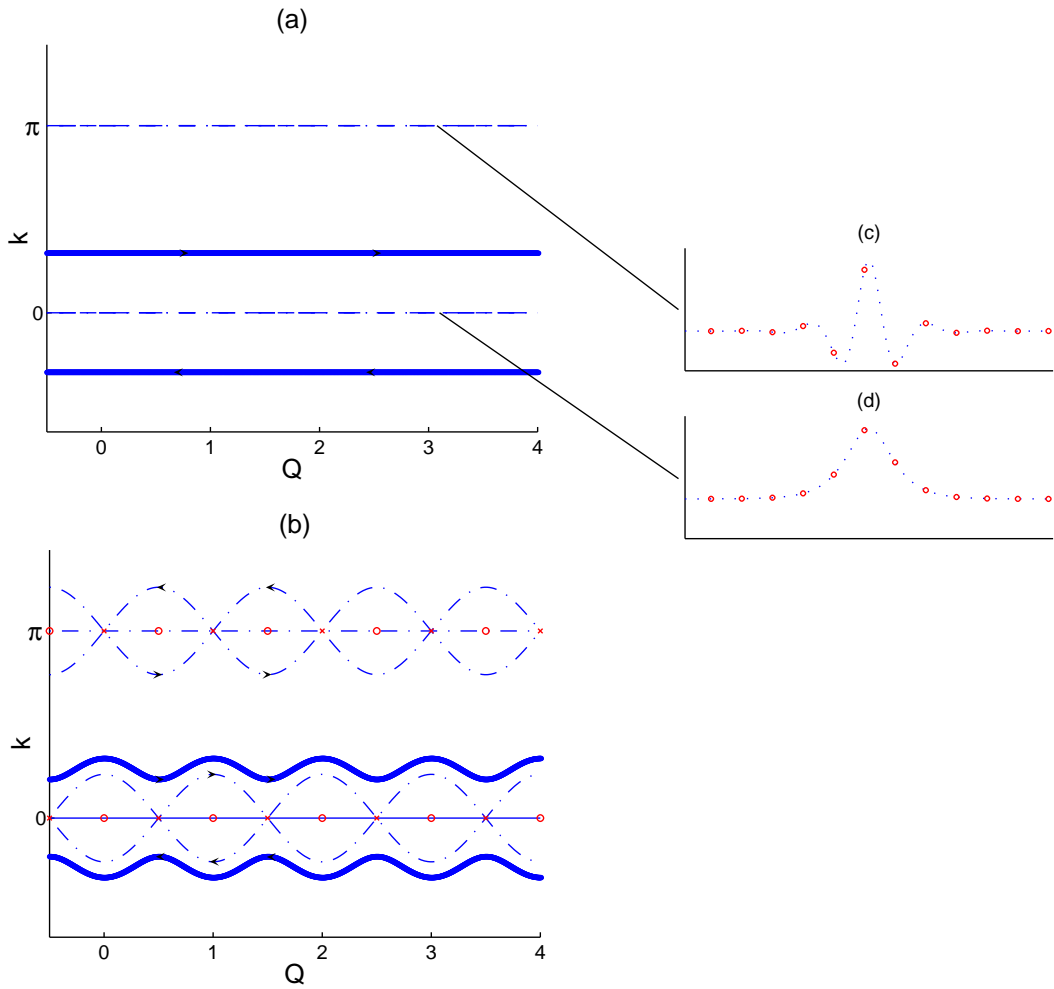


Figure 1: (a) Effective Hamiltonian phase portrait for travelling DB in the AL lattice ( $\epsilon = 0$  in the Salerno model). (b) Perturbation of the ( $\epsilon = 0$ ) phase portrait in the Salerno family.  $\epsilon = 1$ ,  $\beta = 1.5$  (c) “anti-phase” discrete breathers, when  $k = \pi$  in (20), (d) “in-phase” discrete breathers when  $k = 0$ . In both examples, the real part is shown with  $\beta = 1.5$ ,  $Q = 3.15$ .

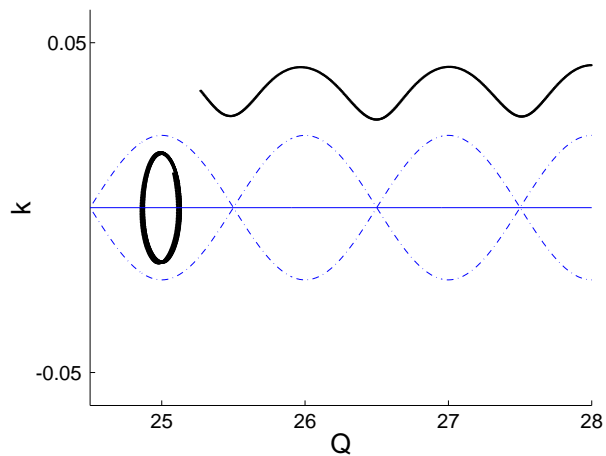


Figure 2: Solid lines: projection of the  $(\bar{k}, \bar{Q})$  variables [eq. (26)] computed from the numerical integration of the Salerno model ( $\epsilon = 0.1$ ) in the effective phase portrait of Fig. 1. Dashed lines correspond to the theoretical separatrices. Parameter  $\beta = 1$ .

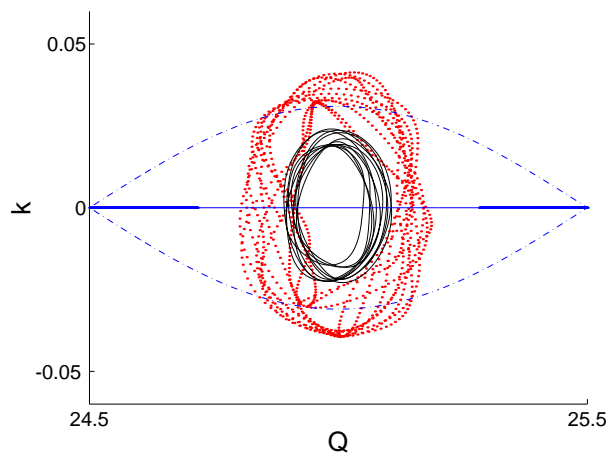


Figure 3: Dotted line shows the evolution of function  $\mathbf{G}$  without averaging (see text). The corresponding averaged trajectory is indicated in solid line. Same parameters as in Fig. 2 but  $\epsilon = 0.2$ .

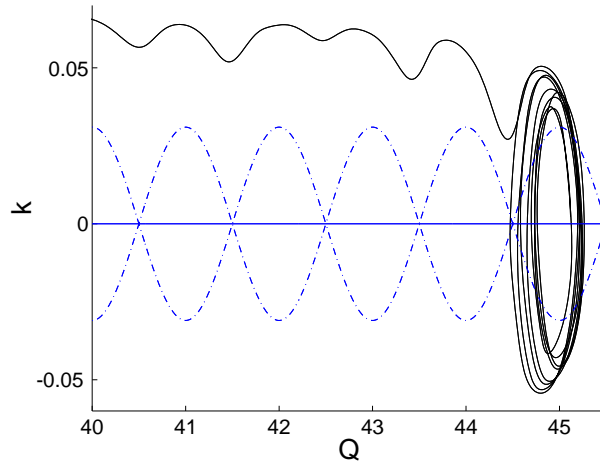


Figure 4: Anomalous trapping of travelling DB (w.r.t. the expected effective Hamiltonian). Parameters are as in Fig. 3.

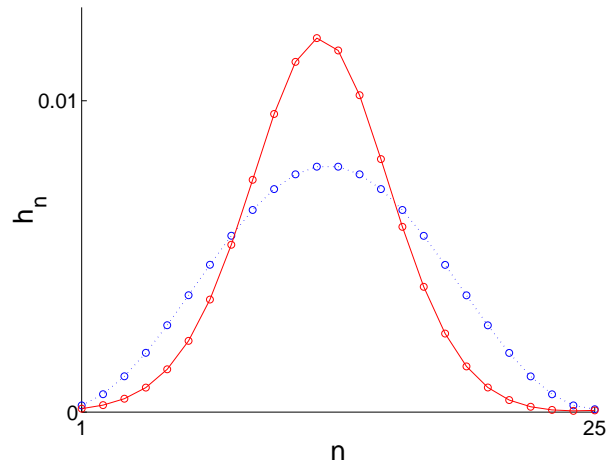


Figure 5: Enhancement of the localisation of energy density  $h_n$  after a lapse of time  $t = 100$  in the numerical simulation of the FPU chain (solid line) , as compared with the initial condition given by the ansatz (32) (dotted line). The parameters are chosen as in Fig. 6.



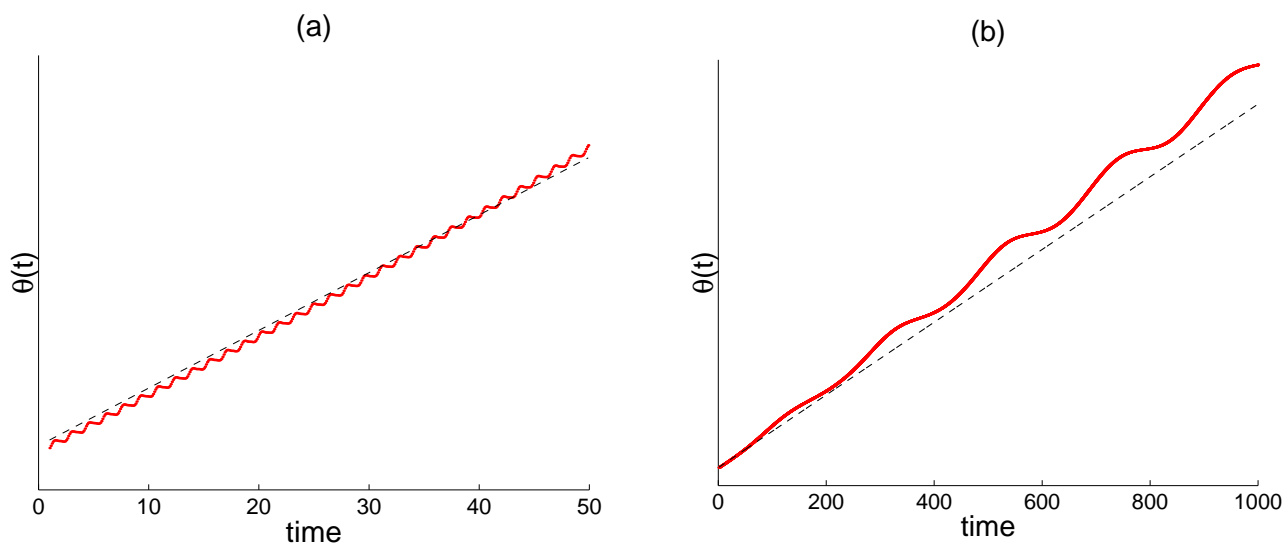


Figure 6: Evolution of the coordinate  $\theta$  in time (see text). The straight lines indicate the prediction of the effective dynamics, given by eq. (33). The parameters of the FPU model as chosen as  $\alpha = 0$ ,  $\beta = 1$ ,  $a = 0.05$ ,  $\theta_0 = -\frac{\pi}{2}$ ,  $J_0 = -0.01$ . Panel (a) is an enlargement of a part of the graphic of panel (b), corresponding to the time lapse  $[0, 50]$ .

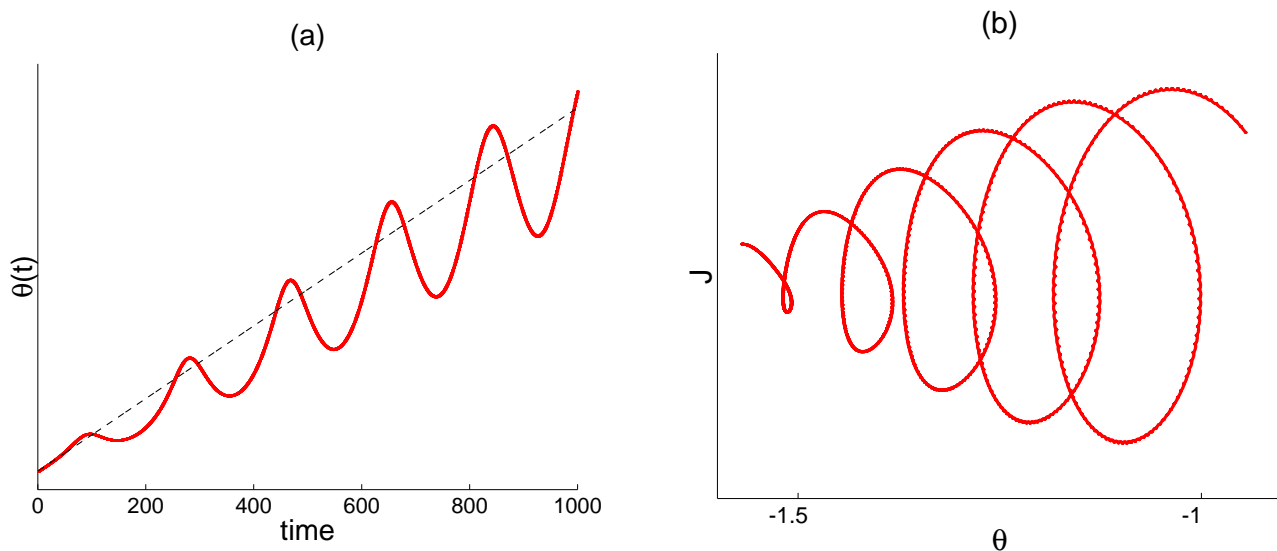


Figure 7: (a) Evolution of  $\theta$  as in Fig. 6 (b), but the area of approximate DB is doubled,  $a = 0.1$ . The straight line shows the simple dynamics given by eq. (33) ; (b) The actual phase trajectory. The effective phase space should be more than 2-dimensional.