



Isochronism and tangent bifurcation of band edge modes in Hamiltonian lattices

J. Dorignac^{a,*}, S. Flach^b

^a College of Engineering, Boston University, 44 Cummington Street, Boston, MA 02215, USA

^b Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, D-01187 Dresden, Germany

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Abstract

In *Physica D* [S. Flach, *Physica D* 91 (1996) 223], results were obtained regarding the tangent bifurcation of the band edge modes ($q = 0, \pi$) of nonlinear Hamiltonian lattices made of N coupled identical oscillators. Introducing the concept of *partial isochronism* which characterises the way the frequency of a mode, ω , depends on its energy, ε , we generalize these results and show how the bifurcation energies of these modes are intimately connected to their degree of isochronism. In particular, we prove that in a lattice of coupled purely isochronous oscillators (oscillators with an energy-independent frequency), the in-phase mode ($q = 0$) never undergoes a tangent bifurcation whereas the out-of-phase mode ($q = \pi$) does, provided the strength of the nonlinearity in the coupling is sufficient. We derive a discrete nonlinear Schrödinger equation governing the slow modulations of small-amplitude band edge modes and show that its nonlinear exponent is proportional to the degree of isochronism of the corresponding orbits. This equation may be seen as a link between the tangent bifurcation of band edge modes and the possible emergence of localized modes such as discrete breathers.

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1. Introduction

Since almost 15 years now, properties of discrete breathers (DB) in nonlinear translationally invariant Hamiltonian lattices are under intense investigation. General features regarding these time periodic, spatially localised excitations are well understood and have been documented in several reviews [1–7]. Mathematical proofs of their existence go

* Corresponding author. Tel.: +1 617 358 1554; fax: +1 617 353 9393.

E-mail addresses: dorignac@bu.edu (J. Dorignac), flach@mpipks-dresden.mpg.de (S. Flach)

back to a paper by MacKay and Aubry [8] which considers lattices of interacting oscillators. It shows the possibility to continue single site oscillations in the decoupled (so-called anti-continuous) limit to nonzero coupling between the oscillators provided the corresponding orbit stays out of resonance with the low amplitude lattice modes. This, in particular, requires the oscillator (onsite) potential to be non isochronous, that is, to possess orbits whose frequency varies with the energy. Other works, either generalising this method [9], or using different approaches [10–12] have added to the variety of rigorous existence proofs of discrete breathers.

One of us has performed an analytical study of the way band edge modes (BEMs) may bifurcate (tangently) to give rise to new periodic orbits breaking the translation invariance of the lattice [13]. It is a common conjecture indeed that discrete breathers are among the orbits bifurcating from these plane waves. The bifurcation analysis investigates the possible existence of almost extended discrete breathers and, in this respect, is complementary to MacKay's and Aubry's theorem which proves the existence of strongly peaked ones in networks of weakly coupled non isochronous oscillators. It provides the critical energy at which tangent bifurcations of BEMs possibly occur according to the mode under consideration (see also [14]). But it is restricted to the generic case where plane wave orbits do not bear any degree of isochronism.

In order to discuss further the specific properties of partially isochronous BEMs, we now define this concept more precisely. Let us first remark that in one-dimensional (1D) convex potentials, the motion is always periodic. To any given energy corresponds a unique orbit whose frequency is determined by the features of the potential (basically, its shape). We will say an orbit to be *isochronous* if its frequency does not depend on its energy. Given the one-to-one correspondence between the potential and its orbits, if the motion is isochronous the potential can be said to be isochronous as well.

In higher dimension however, the concept of isochronous potentials becomes ambiguous due to the possible presence of several families of periodic orbits, each of which having its own energy-frequency dependence. *Isochronism is then a property of a particular family of orbits* rather than a property of the potential itself. Let us notice though, that to give birth to a family of isochronous orbits, the potential must fulfill certain conditions. These constraints simply vary according to the motion under consideration, and may be different for different families of periodic orbits of one and the same potential.

The most famous example of a 1D isochronous potential is the harmonic well $V(x) = \omega^2 x^2/2$ whose frequency ω is well known to be energy-independent. Nevertheless, isochronism is not the privilege of the latter and it can be shown that appropriate shears of the parabolic curve produce other *non symmetric* isochronous potentials $V(x) \neq V(-x)$ [17].

Now, for generic convex potentials, the frequency of a given periodic orbit can be expanded at low energies E (bottom of the potential) as a power series in E . Its behaviour is generally linear with E around the equilibrium position. We will call “partially isochronous” or, more precisely *isochronous up to order n* , orbits whose frequency behaves instead as a nonlinear function of the energy when expanded around $E = 0$. Typically, $\omega^2(E) = \omega_0^2 + \gamma_n E^n + o(E)^n$, $n \geq 2$, $\omega_0 > 0$ and $\gamma_n \neq 0$. For $n = 1$, we recover the case of non isochronous motions or, equivalently in our terminology, of orbits isochronous up to order 1. Completely isochronous orbits verify $\omega^2(E) = \omega_0^2$.

The aim of the present paper is to extend the results [13] to the class of potentials rendering certain periodic motions partially or completely isochronous. As we will see, it turns out that the tangent bifurcation of band edge plane waves is intimately related to the low-energy behaviour of their frequency (hence the above definitions). This remark will enable us to generalise the perturbative analysis performed in [13] and to express the bifurcation energy of BEMs in a very simple way valid for any potential. An immediate conclusion of this generalisation will be that, *families of discrete breathers bifurcating from partially isochronous BEMs possess energy thresholds, even in 1D*. This, to some extent, shall be confirmed by a “multiple-scale” analysis which leads to a discrete nonlinear Schrödinger equation (DNLS) whose nonlinear exponent is related to the degree of isochronism of the BEM. The existence of energy thresholds of DBs for such DNLS models has been confirmed [15] and has been proved by M.I. Weinstein [16].

The paper is organised as follows: in Section 2, we present a low-energy perturbative solution of the in-phase and out-of-phase modes and in Section 3, we use them to derive the constraints imposed to 1D or 2D potentials

to enforce a partial isochronism of these motions. In Section 4, we study the linear stability of these orbits and derive an expression for the energy at which they undergo a tangent bifurcation. Finally, in Section 5, we discuss the implications of these results and present a brief multiple-scale analysis which corroborates our conclusions.

2. Equations of motion

2. 1. Generalities

All along this paper, we will investigate the dynamical properties of a lattice described by the following Hamiltonian

$$H = \sum_{n=1}^N \left[\frac{1}{2} p_n^2 + V(x_n) + W(x_{n+1} - x_n) \right], \tag{1}$$

with periodic boundary conditions $x_{n+N} = x_n$. For the sake of simplicity, we consider an even number of sites N ranging from 2 to infinity. The onsite ($V(x)$) and the interaction ($W(x)$) potentials are both assumed to possess a minimum at $x = 0$ around which they can be expanded as

$$V(x) = \sum_{\mu=2}^{\infty} \frac{1}{\mu} v_{\mu} x^{\mu}; \quad W(x) = \sum_{\mu=2}^{\infty} \frac{1}{\mu} \phi_{\mu} x^{\mu}. \tag{2}$$

The first coefficients of these expansions, v_2 and ϕ_2 , represent harmonic frequencies and are assumed to be strictly positive. The Hamiltonian equations of motion for (1) are given by

$$\begin{aligned} \dot{x}_n &= p_n, \\ \dot{p}_n &= -V'(x_n) - W'(x_n - x_{n-1}) + W'(x_{n+1} - x_n). \end{aligned} \tag{3}$$

Let us introduce the normal coordinates

$$Q_q = \frac{1}{N} \sum_{n=1}^N e^{iqn} x_n, \quad q = \frac{2\pi l}{N}, \quad l \in \left\{ -\frac{N}{2} + 1, \dots, \frac{N}{2} \right\}. \tag{4}$$

Their properties are

$$Q_{q+2\pi} = Q_q \quad \text{and} \quad Q_{-q} = Q_q^* \quad (x_n \in \mathbb{R}), \tag{5}$$

and inverting the transform (4) yields

$$x_n = \sum_q e^{-iqn} Q_q. \tag{6}$$

Rewritten in terms of normal coordinates, Eq. (3) read now

$$\ddot{Q}_q + F_q(Q) = 0, \tag{7}$$

where

$$\begin{aligned} F_q(Q) &= \frac{1}{N} \sum_{n=1}^N e^{iqn} \left[V' \left(\sum_{q'} e^{-iq'n} Q_{q'} \right) + W' \left(\sum_{q'} (1 - e^{iq'}) e^{-iq'n} Q_{q'} \right) \right. \\ &\quad \left. - W' \left(\sum_{q'} (e^{-iq'} - 1) e^{-iq'n} Q_{q'} \right) \right]. \end{aligned} \tag{8}$$

A linearization of $F_q(Q)$ around $Q_q = 0$ leads to the equations of motion of a harmonic lattice, namely

$$\ddot{Q}_q + \omega_{q,0}^2 Q_q = 0, \quad (9)$$

where

$$\omega_{q,0}^2 = v_2 + 4\phi_2 \sin^2\left(\frac{q}{2}\right) \quad (10)$$

represents the squared frequency of each *linear* mode q (hence the additional subscript 0, the frequency of the nonlinear mode being denoted by ω_q).

In what follows, we will be interested in the stability of two particular nonlinear modes corresponding to the natural continuation of the linear $q = 0$ and $q = \pi$ modes defined by (9). These nonlinear modes are periodic solutions of (7) which converge to their respective linear modes as their energy tends to zero. Notice that the linear frequency $\omega_{0,0}$ of the in-phase mode is always nondegenerate and because the number of sites N is even, the linear frequency $\omega_{\pi,0}$ of the out-of-phase mode is nondegenerate as well. All other modes $q \neq 0, \pi$ are twofold degenerate ($\omega_{q,0} = \omega_{-q,0}$). In the next two sections, we define more precisely the two nonlinear in-phase and out-of-phase modes and evaluate them perturbatively by means of a Poincaré–Lindstedt expansion carried out at low energy.

2. 2. In-phase mode (orbit I)

2. 2. 1. Equation of motion

Oscillators are said to be in phase when they perform identical periodic motions. This corresponds to

$$Q_q = Q_0 \delta_{q,0} \quad (11)$$

where $\delta_{q,q'} = 1$ if $q = q' [2\pi]$ and 0 else. The previous expression is a solution of the equations of motion (7) provided

$$\ddot{Q}_0 + V'(Q_0) = 0. \quad (12)$$

The solution $Q_q = Q_0 \delta_{q,0}$ represents the in-phase periodic orbit. We call it orbit I. The total energy of the lattice evolving according to orbit I is

$$E_I = H(\{x_n = Q_0\}) = N \left(\frac{1}{2} \dot{Q}_0^2 + V(Q_0) \right). \quad (13)$$

We will use an energy density (or energy per site) rather than the total energy E_I to describe this orbit. It is given by $\varepsilon_I = E_I/N$ and represents the energy of the oscillator Q_0 evolving according to (12).

2. 2. 2. Solution at low energy

Eq. (12) represents the motion of a single oscillator in the potential $V(x)$. According to our assumptions regarding the latter, the potential is convex in $x = 0$ and at small energy, the motion is bounded and thus periodic. We can solve for it in perturbation by expanding the solution as a Poincaré–Lindstedt series (see e.g. [21]). For this purpose, let us first define a new dimensionless time $\tau = \omega(\varepsilon)t$, where $\omega(\varepsilon)$ is the frequency of Q_0 as a function of its energy ε (for the sake of clarity we have dropped the subscript I). The corresponding period is $T(\varepsilon) = 2\pi/\omega(\varepsilon)$. We show in Appendix A how this period can be expanded as a power series in energy. Let us also define $X = (2\varepsilon/v_2)^{1/2}$, as well as the new dimensionless quantities $\tilde{T}(X) = T(\varepsilon)\sqrt{v_2}/(2\pi)$ and $\tilde{V}(x) = V(x)/v_2$. Eq. (12) now reads

$$\frac{\partial^2 Q_0(X, \tau)}{\partial \tau^2} + \tilde{T}^2(X) \tilde{V}'(Q_0(X, \tau)) = 0, \quad (14)$$

where we have explicitly mentioned the energy dependence of Q_0 on X . To solve this last equation, we expand $Q_0(X, \tau)$ as a series in X around 0:

$$Q_0(X, \tau) = \sum_{n=1}^{\infty} Q_0^{(n)}(\tau) X^n. \quad (15)$$

We choose without loss of generality an initial condition such that $\dot{Q}_0(X, 0) = 0$ which means that $Q_0(X, 0)$ is a turning point of the potential V defined by the relation $V(Q_0(X, 0)) = \varepsilon \Leftrightarrow \tilde{V}(Q_0(X, 0)) = X^2/2$. Inverting the previous relation gives

$$Q_0(X, 0) = X + \sum_{n=2}^{\infty} \sigma_n X^n, \quad (16)$$

where the first odd coefficients σ_n are given in [Appendix A](#). According to the relation above, the initial conditions for the functions $Q_0^{(n)}(\tau)$ are

$$Q_0^{(1)}(0) = 1; \quad Q_0^{(n)}(0) = \sigma_n, \quad \forall n \geq 2 \quad \text{and} \quad \dot{Q}_0^{(n)}(0) = 0, \quad \forall n \geq 1. \quad (17)$$

Moreover, according to [\(A.6\)](#), we know the explicit form of $\tilde{T}(X)$ which reads,

$$\tilde{T}(X) = 1 + \sum_{k=1}^{\infty} \tilde{T}_{2k} X^{2k} \quad \text{where} \quad \tilde{T}_{2k} = \sigma_{2k+1} \frac{(2k+1)!!}{(2k)!!}. \quad (18)$$

Reinstating [\(18\)](#) and [\(15\)](#) in [\(14\)](#) and expanding as a series of X , we derive a set of differential equations for $Q_0^{(n)}(\tau)$. This way is clearly related to the Poincaré–Lindstedt method except that the preliminary calculation [\(18\)](#) of the period $\tilde{T}(X)$ automatically removes all secular terms from Eq. [\(14\)](#).

Using the results of [Appendix A](#), we may derive for example the first differential equations involving $Q_0^{(1)}(\tau)$, $Q_0^{(2)}(\tau)$ and $Q_0^{(3)}(\tau)$.

$$\ddot{Q}_0^{(1)}(\tau) + Q_0^{(1)}(\tau) = 0, \quad (19)$$

$$\ddot{Q}_0^{(2)}(\tau) + Q_0^{(2)}(\tau) + \alpha_2 [Q_0^{(1)}(\tau)]^2 = 0, \quad (20)$$

$$\ddot{Q}_0^{(3)}(\tau) + Q_0^{(3)}(\tau) + \left(\frac{5}{6}\alpha_2^2 - \frac{3}{4}\alpha_3\right) Q_0^{(1)}(\tau) + \alpha_3 [Q_0^{(1)}(\tau)]^3 + 2\alpha_2 Q_0^{(1)}(\tau) Q_0^{(2)}(\tau) = 0, \quad (21)$$

where the double dot stands now for a differentiation with respect to τ and $\alpha_n = v_{n+1}/v_2$. Solving this system together with the initial conditions [\(17\)](#), we obtain

$$Q_0^{(1)}(\tau) = \cos(\tau), \quad (22)$$

$$Q_0^{(2)}(\tau) = \frac{1}{6}\alpha_2(\cos(2\tau) - 3), \quad (23)$$

$$Q_0^{(3)}(\tau) = \frac{1}{96}(2\alpha_2^2 + 3\alpha_3)\cos(3\tau) + \left(\frac{37}{144}\alpha_2^2 - \frac{9}{32}\alpha_3\right)\cos(\tau), \quad (24)$$

where we have used $\sigma_2 = -\alpha_2/3$ and the value for σ_3 given in [Appendix A](#).

The first term of the expansion [\(15\)](#), $Q_0^{(1)}(\tau) = \cos(\tau)$, represents the linear (harmonic) part of the in-phase motion. Higher order corrections in X^n , $n > 1$ (i.e. $\varepsilon^{(n/2)}$) stem from the nonlinearity of the onsite potential. It is important to notice that they appear also for isochronous onsite potentials. In other words, *isochronous motions are generally anharmonic*.

Reinstating the results for the $Q_0^{(n)}(\tau)$ in [\(15\)](#) provides the general perturbative expression for the continuation of the linear in-phase motion, that is, a perturbative expression for the *nonlinear in-phase mode*.

2.3 Out-of-phase mode (orbit II)

2.3.1. Equations of motion

If the potential $V(x)$ is not symmetric ($V(-x) \neq V(x)$), its Taylor expansion around 0 contains at least one nonzero odd coefficient. This has no influence on the previous result concerning the in-phase motion because any oscillator of the chain performs the same motion in the same time. This reduces the set of N Eq. (7) to a single one (12), representing the equation of motion of a single oscillator in the onsite potential V . But as soon as we are interested in an out-of-phase like motion, we have to consider a dimerization of the chain, each dimer being made of two neighbouring units oscillating in opposite phase. The lack of symmetry of V induces two different motions to the right and to the left. This prevents us from finding a pure out-of-phase solution to (7) which would imply $Q_q = Q_\pi \delta_{q,\pi}$ or in real space $x_{2n} = -x_{2n+1}$. Instead, we can look for a solution of the type

$$Q_q = Q_0 \delta_{q,0} + Q_\pi \delta_{q,\pi} \quad (25)$$

involving both in- and out-of-phase variables, the others being zero. Using (6), we obtain $x_n = Q_0 + (-1)^n Q_\pi$ or $x_{2n} = Q_0 + Q_\pi$ and $x_{2n+1} = Q_0 - Q_\pi$. Adding and subtracting the equations of motion for x_{2n} and x_{2n+1} , we finally get

$$\begin{aligned} \ddot{Q}_0 + \frac{1}{2}[V'(Q_0 + Q_\pi) + V'(Q_0 - Q_\pi)] &= 0, \\ \ddot{Q}_\pi + \frac{1}{2}[V'(Q_0 + Q_\pi) - V'(Q_0 - Q_\pi)] + W'(2Q_\pi) - W'(-2Q_\pi) &= 0. \end{aligned} \quad (26)$$

The total energy of the system evolving according to orbit II is

$$\begin{aligned} E_{\text{II}} &= H(\{x_{2n} = Q_0 + Q_\pi, x_{2n+1} = Q_0 - Q_\pi\}) \\ &= \frac{N}{2}(\dot{Q}_0^2 + \dot{Q}_\pi^2 + V(Q_0 + Q_\pi) + V(Q_0 - Q_\pi) + W(2Q_\pi) + W(-2Q_\pi)). \end{aligned} \quad (27)$$

2.3.2. Solution at low energy

System (26) represents a dimer. Applying the method of the first section, we are able to derive its time-periodic solution at low energy by requiring that the corresponding orbit converges towards the linear out-of-phase mode as the energy vanishes. However, at variance with the in-phase mode, we cannot provide an explicit expression for its period in terms of the Taylor coefficients of V and W . Removing the secular terms from (26) yields simultaneously the expressions for the period and for the motions $Q_0(\tau)$ and $Q_\pi(\tau)$.

Contrary to the previous case, we will not use an energy expansion for the diverse quantities to be calculated but merely a *small amplitude* expansion. The small amplitude is denoted by y . We define a dimensionless time $\tau = \omega(y)t$ where $\omega(y)$ stands for the frequency of orbit II as a function of its amplitude y . The corresponding period is denoted by $T(y)$. Moreover, we define the two dimensionless potentials

$$\tilde{V}(x) = \frac{V(x)}{v_2 + 4\phi_2} = \sum_{n=2}^{\infty} \frac{\alpha_{n-1}}{n} x^n; \quad \tilde{W}(x) = \frac{W(x)}{v_2 + 4\phi_2} = \sum_{n=2}^{\infty} \frac{\beta_{n-1}}{n} \left(\frac{x}{2}\right)^n, \quad (28)$$

as well as a dimensionless period $\tilde{T}(y) = \sqrt{v_2 + 4\phi_2} T(y)/2\pi$. Notice the slightly different definition of the coefficients $\alpha_n = v_{n+1}/(v_2 + 4\phi_2)$ of this section as compared to the previous one. We nevertheless keep the same notation for the sake of clarity given that these coefficients are still related to the onsite potential $V(x)$. Functions Q_0 , Q_π and $\tilde{T}(y)$ are expanded as follows,

$$Q_0(y, \tau) = \sum_{n=1}^{\infty} Q_0^{(n)}(\tau) y^n; \quad Q_\pi(y, \tau) = \sum_{n=1}^{\infty} Q_\pi^{(n)}(\tau) y^n; \quad \tilde{T}(y) = \sum_{n=1}^{\infty} \tilde{T}_n y^n. \quad (29)$$

Equations of motion (26) now read

$$\begin{aligned} \ddot{Q}_0 + \frac{\tilde{T}^2(y)}{2} [\tilde{V}'(Q_0 + Q_\pi) + \tilde{V}'(Q_0 - Q_\pi)] &= 0, \\ \ddot{Q}_\pi + \tilde{T}^2(y) \left\{ \frac{1}{2} [\tilde{V}'(Q_0 + Q_\pi) - \tilde{V}'(Q_0 - Q_\pi)] + \tilde{W}'(2Q_\pi) - \tilde{W}'(-2Q_\pi) \right\} &= 0. \end{aligned} \tag{30}$$

The double dot denotes the derivative with respect to τ . Inserting (29) in the previous system and collecting the terms of same order in y gives rise to a set of differential equations involving the functions $Q_0^{(n)}(\tau)$, $Q_\pi^{(n)}(\tau)$ as well as the unknowns \tilde{T}_n (to be determined by requiring the removal of secular terms). Solving them, it is not difficult to obtain the following general features for the motion: by choosing a proper origin of time the solution can be made time-reversal symmetric (the only nonzero Fourier coefficients of $Q_0^{(n)}(\tau)$ and $Q_\pi^{(n)}(\tau)$ are even). Moreover, $Q_0^{(n)}(\tau)$ and $Q_\pi^{(n)}(\tau)$ are respectively even and odd in y . Finally, $\tilde{T}(y)$ is also even in y . Thus, we have

$$Q_0(y, \tau) = \sum_{n=1}^{\infty} Q_0^{(2n)}(\tau) y^{2n}; \quad Q_\pi(y, \tau) = \sum_{n=0}^{\infty} Q_\pi^{(2n+1)}(\tau) y^{2n+1}; \quad \tilde{T}(y) = 1 + \sum_{n=1}^{\infty} \tilde{T}_{2n} y^{2n}. \tag{31}$$

where

$$\begin{aligned} Q_\pi^{(1)}(\tau) &= \cos(\tau), \quad Q_0^{(2)}(\tau) = \frac{1}{2} \alpha_2 \left(\frac{\cos(2\tau)}{4 - \alpha_1} - \frac{1}{\alpha_1} \right), \quad Q_\pi^{(3)}(\tau) = \frac{1}{32} \left[(\alpha_3 + \beta_3) - \frac{2\alpha_2^2}{\alpha_1 - 4} \right] \cos(3\tau), \\ \tilde{T}_2 &= \frac{1}{4} \frac{(3\alpha_1 - 8)\alpha_2^2}{(\alpha_1 - 4)\alpha_1} - \frac{3}{8}(\alpha_3 + \beta_3), \end{aligned} \tag{32}$$

to give a few. Notice that the even coefficients β_{2n} are absent from the equations of motion (30) and consequently from the expressions (32). β_1 has been eliminated thanks to the relation $\beta_1 + \alpha_1 = 1$, which follows from the definition of these coefficients in terms of v_2 and ϕ_2 (see Eqs. (2) and (28)).

Reinstating properly the expressions for $Q_0(y, \tau)$ and $Q_\pi(y, \tau)$ in (27) allows us to derive a perturbative expansion for the energy density $\varepsilon = E_{II}/N$ of the nonlinear out-of-phase mode in terms of its amplitude y . As for the in-phase mode, it is convenient to define a quantity $Y = (2\varepsilon/(v_2 + 4\phi_2))^{1/2}$ playing the same role as X in the previous section. We then obtain

$$\frac{2\varepsilon}{v_2 + 4\phi_2} \equiv Y^2 = y^2 + \left[\frac{9}{16}(\alpha_3 + \beta_3) - \frac{1}{8} \frac{(9\alpha_1^2 - 68\alpha_1 + 96)\alpha_2^2}{\alpha_1(\alpha_1 - 4)^2} \right] y^4 + \mathcal{O}(y^6). \tag{33}$$

The first term of this expansion corresponds to the harmonic limit.

3. Isochronism

In the previous section, we have described the way to obtain a perturbative energy expansion for both the in- and out-of-phase motions, as well as for their respective periods. We are thus in a position to express the conditions required for a (partial) isochronism of these modes. For an isochronism of order n , this is easily achieved by cancelling all coefficients of the energy expansion for the period up to order $n - 1$.

3.1. In-phase mode

Due to its integral representation, the period of the in-phase mode can be explicitly expanded as a power series in energy (see Appendix A). Obtaining an in-phase mode isochronous up to order n then amounts to zeroing the

coefficients σ_{2k+1} , $1 \leq k \leq n-1$. This has been done in [Appendix A](#) up to order $n=4$. The set of equations thus derived induces some constraints on the Taylor (v_k or α_{k-1}) coefficients of the potential V . It leaves nevertheless an entire freedom on the choice of odd coefficients (v_{2k+1} , $k \geq 1$) as already remarked in [\[22\]](#). For a (1D) potential isochronous up to order n , the even coefficients v_{2k} are then determined by the odd ones v_{2k+1} up to $k=2n$. The rest of the expansion is free.

To illustrate this, let us derive the most general expansion of a (\mathcal{C}^∞) 1D potential isochronous up to order 4. Using the results of [Appendix A](#) and $V(x) = \omega^2 \tilde{V}(x)$, we obtain:

$$\begin{aligned} \tilde{V}(x) = & \frac{1}{2}x^2 + \frac{\alpha_2}{3}x^3 + \frac{5}{18}\alpha_2^2x^4 + \frac{\alpha_4}{5}x^5 + \frac{1}{6}\left(-\frac{56}{27}\alpha_2^4 + \frac{14}{5}\alpha_4\alpha_2\right)x^6 + \frac{\alpha_6}{7}x^7 \\ & + \frac{1}{8}\left(\frac{24}{7}\alpha_6\alpha_2 - \frac{592}{45}\alpha_4\alpha_2^3 + \frac{36}{25}\alpha_4^2 + \frac{848}{81}\alpha_2^6\right)x^8 + \sum_{k=9}^{\infty} \frac{\alpha_{k-1}}{k}x^k \end{aligned} \quad (34)$$

This expression is equivalent¹ to Eq. (34) of [\[22\]](#).

3.2. Out-of-phase mode

As for the out-of-phase motion, no explicit (integral) expression is available for the period. However, we have shown in the previous section how to calculate it as a function of the small amplitude y by removing the secular terms at each step of the calculation. The period could of course be converted as a series in energy rather than expressed as a series in amplitude. Such a transformation would be pointless however. Indeed, even if an isochronism of order n has been previously defined through $T = T_0 + T_{2n}\varepsilon^n + o(\varepsilon^n)$ as the energy tends to zero, the dependence of the amplitude on energy [\(33\)](#) shows that this statement is equivalent to $T = T_0 + T_{2n}[(v_2 + 4\phi_2)/2]^n y^{2n} + o(y^{2n})$. It is then equivalent to zero the coefficients of the y or ε expansions up to order $n-1$ as it produces the same constraints on the Taylor coefficients of the potentials V and W , although these two series have different coefficients.

Let us finally provide the reader with an example to illustrate the method described in the previous section. If we require the out-of-phase mode to be isochronous up to order 3, we obtain the following constraints on the coefficients α and β (see Eq. [\(28\)](#) for their definition):

$$\begin{aligned} \beta_3 = & -\alpha_3 + \frac{2(3\alpha_1 - 8)\alpha_2^2}{3(\alpha_1 - 4)\alpha_1} \\ \beta_5 = & -\alpha_5 + \frac{2(96 + 15\alpha_1^2 - 56\alpha_1)}{15\alpha_1^3(\alpha_1 - 4)^2}\alpha_2^4 - \frac{9(32 + 5\alpha_1^2 - 24\alpha_1)}{5\alpha_1^3(\alpha_1 - 4)^2}\alpha_1\alpha_2^2\alpha_3 + \frac{6(5\alpha_1 - 12)}{5\alpha_1^3(\alpha_1 - 4)}\alpha_1^2\alpha_2\alpha_4 \end{aligned} \quad (35)$$

Notice that for the sake of simplicity, we have kept the same notation α_k for the coefficients of \tilde{V} for both modes. However, the definition of these coefficients is mode dependent as they represent v_{k+1}/v_2 for the in-phase mode and $v_{k+1}/(v_2 + 4\phi_2)$ for the out-of-phase mode. As already displayed in the above relations, it can be shown in general that the isochronism of orbit II is easily expressed through a relation of the type $\beta_{2n+1} = f(\{\alpha_k\})$ ($k \in \{1, \dots, 2n+1\}$). This means that once the coefficients $\{\alpha_k\}$ have been chosen for the onsite potential V , the isochronism of the out-of-phase mode fixes the even part of the interaction potential. The odd part of W remains completely free as it does not enter the equations of motion.

¹ Two misprints have to be corrected in this expression. Using the notations of [\[22\]](#), the last coefficient of order 6 reads $-7/2 b_4^4$ and the last coefficient of order 8, $477/16 b_1^6$.

4. Tangent bifurcation of orbits I and II

4.1. Statement of the problem

The system of Eq. (7) is of the form $\ddot{Q} + F(Q) = 0$, where Q and $F(Q)$ denote two vectors of components Q_q and $F_q(Q)$ respectively, $q \in \{0, 2\pi/N, \dots, 2(N-1)\pi/N\}$. A perturbation η of the system around the solution Q gives rise to the following variational system

$$\ddot{\eta} + DF(Q)\eta = 0 \tag{36}$$

where $DF(Q)$ is the Jacobian matrix of F evaluated in Q whose components are $DF_{qk}(Q) = \partial F_q(Q)/\partial Q_k$.

To evaluate the Jacobian matrix, we use (8) and find

$$\begin{aligned} \frac{\partial F_q}{\partial Q_k}(Q) = & \frac{1}{N} \sum_{n=1}^N e^{i(q-k)n} \left[V'' \left(\sum_{q'} e^{-iq'n} Q_{q'} \right) + (1 - e^{ik})W'' \left(\sum_{q'} (1 - e^{iq'})e^{-iq'n} Q_{q'} \right) \right. \\ & \left. - (e^{-ik} - 1)W'' \left(\sum_{q'} (e^{-iq'} - 1)e^{-iq'n} Q_{q'} \right) \right]. \end{aligned} \tag{37}$$

We will now use the method already described in [13] in order to obtain the energy thresholds, if any, at which orbits I and II become unstable and bifurcate tangently to give rise to other types of periodic orbits which break the translational invariance of the lattice. Before to proceed, let us briefly recall how the method works.

Once the periodic solution for Q has been introduced in the Jacobian matrix $DF(Q)$, the variational system (36) presents itself as a vectorial Hill's equation for the perturbation η . This type of systems is known as *parametrically excited* as the Jacobian matrix generally depends on several parameters. In our case, such parameters are the energy (or the amplitude) of the solution Q as well as the frequencies of the modes we are interested in. Once expanded as a Fourier series, the Jacobian matrix may be decomposed into a static (dc-) part (its zero mode) and a driving (ac-) part.

A paradigmatic example of Hill's equation is the Mathieu equation $\ddot{x}(t) + (\delta + 2\epsilon \cos(2t))x(t) = 0$. For a comprehensive treatment of this equation the reader is invited to consult [21], for example. In one dimension (the Jacobian matrix is reduced to a single element in this case), the parameter δ plays the role of the static part and $2\epsilon \cos(2t)$ the role of the driving. It is known from the stability analysis of this equation that the behaviour of its solution varies according to the values of the parameters δ and ϵ . The solution can be either stable, unstable or periodic. In the $\epsilon\delta$ -plane (δ as x -axis and ϵ as y -axis), the regions of instability present themselves as tongues (the so-called Arnold's tongues) starting from the δ -axis at the values $\delta_n = n^2$, $n \in \mathbb{N}$ and widening as ϵ increases. In these regions, the motion is unbounded whereas outside, it is stable (bounded).

Of particular interest are the boundaries of such regions called *transition curves* that separate stable from unstable motions. Along this curves, the solution is periodic of period π (n even) or 2π (n odd). For small ϵ values, a perturbative treatment of the Mathieu equation which consists in expanding both $x(t)$ and the parameter δ as series in ϵ allows for the determination of the transition curves of the form $\delta_n = n^2 + \sum_l A_{nl}^{s/a} \epsilon^l$. The coefficients $A_{nl}^{s/a}$ depend on the tongue (n) as well as on the *branch* (that is, the boundary) we are interested in. It can be shown that one of these branches is related to time reversal symmetric solutions η (denoted by the subscript s) whereas the second one is associated with time reversal antisymmetric solutions (a).

Let us suppose now that we fix the value of δ close to a transition point $\delta_n = n^2$. At $\epsilon = 0$, the point corresponding to the state of the system in the parameter space is located in a region of stability. Let us increase the value of ϵ at fixed δ . If the corresponding vertical line crosses the transition curve nearby, the solution $x(t)$ becomes unstable above the crossing point. And right at the intersecting point, the solution is periodic. Although

the variational Eq. (36) is more complex than the Mathieu equation, we will proceed along the same lines as those described above to derive the energies at which the modes (in- or -out-of-phase) become unstable and bifurcate.

4. 2. In-phase mode

4. 2. 1. Stability analysis

Evaluated along orbit I, the Jacobian matrix (37) is diagonal

$$DF_{qk}(Q_I) = \left[V''(Q_0) + 4\phi_2 \sin^2 \left(\frac{k}{2} \right) \right] \delta_{q,k}. \quad (38)$$

All perturbations decouple from each other and their equations of motion are

$$\ddot{\eta}_q + \left[V''(Q_0) + 4\phi_2 \sin^2 \left(\frac{q}{2} \right) \right] \eta_q = 0. \quad (39)$$

As already stated in [13], the perturbation η_0 describes the continuation of orbit I along itself. It cannot be responsible for a bifurcation of Q_0 as it simply operates a shift in time or modifies the energy (or the frequency) along the one-parameter family. We then look for the perturbation able to give rise to the required tangent bifurcation. The first to occur will be for the closest (linear) frequency to the linear in-phase frequency, that is for $q_c = 2\pi/N$.

Let us now rewrite the system made of the dimensionless equations of motion for $Q_0(\tau)$ and $\eta_{q_c}(\tau)$. We obtain

$$\frac{\partial^2 Q_0(X, \tau)}{\partial \tau^2} + \tilde{T}^2(X) \tilde{V}'(Q_0(X, \tau)) = 0, \quad (40)$$

$$\frac{\partial^2 \eta_{q_c}(X, \tau)}{\partial \tau^2} + \tilde{T}^2(X) [\tilde{V}''(Q_0(X, \tau)) - \Delta] \eta_{q_c}(X, \tau) = 0, \quad (41)$$

where

$$\Delta = -\frac{4\phi_2}{v_2} \sin^2 \left(\frac{\pi}{N} \right) = \frac{\omega_{0,0}^2 - \omega_{q_c,0}^2}{v_2}. \quad (42)$$

The notations used above are the same as in Section 2.2. The energy dependence of all quantities has been emphasized through X .

4. 2. 2. Arnold tongue corresponding to a tangent bifurcation

Recall that due to the time scaling $\tau = \omega(\varepsilon)t$ the period of $Q_0(X, \tau)$ is now 2π . So that looking for a tangent bifurcation of this orbit through $\eta_{q_c}(X, \tau)$ requires $\eta_{q_c}(X, \tau + 2\pi) = \eta_{q_c}(X, \tau)$ as well. However, this condition in itself, although necessary, is not sufficient for our purpose. We have indeed to require the frequency of $\eta_{q_c}(X, \tau)$ to be the same as (and not a multiple of) the driving frequency *in the limit of vanishing energy* (or as $X \rightarrow 0$). In other words, expanding $\eta_{q_c}(X, \tau)$ as a Fourier series, we must have

$$\eta_{q_c}(X, \tau) = \sum_{n \in \mathbb{Z}} A_n(X) e^{in\tau} \quad \text{with} \quad \forall |n| \neq 1, \quad A_n(X) \xrightarrow{X \rightarrow 0} 0. \quad (43)$$

This implies that we have to investigate the *first instability zone* of the Hill's Eq. (41).

At a strictly zero energy ($X = 0$), this imposes $\Delta = 0$ for in this limit, (41) becomes

$$\ddot{\eta}_{q_c} + [1 - \Delta] \eta_{q_c} = 0,$$

(we again use the dot as a derivative with respect to τ). The previous equation has a frequency equal to 1 for $\Delta = 0$ only. Thus, in a diagram (Δ, ε) , the Arnold tongue we are concerned with starts from the point $(\Delta = 0, \varepsilon = 0)$.

To evaluate the boundaries of this instability zone, we need to solve (41) by expanding $\eta_{qc}(X, \tau)$ and Δ as power series in X :

$$\eta_{qc}(X, \tau) = \sum_{m=0}^{\infty} \eta_{qc}^{(m)}(\tau) X^m; \quad \Delta = \sum_{m=0}^{\infty} \Delta^{(m)} X^m. \tag{44}$$

As for the Mathieu equation, removing the secular terms from (41) gives rise to two critical curves $\Delta_s(X)$ and $\Delta_a(X)$ associated respectively with the periodic time reversal symmetric solution $\eta_{qc,s}(X, \tau) = \eta_{qc,s}(X, -\tau)$ and the periodic time reversal antisymmetric solution $\eta_{qc,a}(X, \tau) = -\eta_{qc,a}(X, -\tau)$.

4. 2. 3 First transition curve.

Differentiating (40) with respect to τ and dividing by X shows that

$$\frac{\partial^2}{\partial \tau^2} \left(\frac{\dot{Q}_0}{X} \right) + \tilde{T}^2(X) \tilde{V}''(Q_0(X, \tau)) \left(\frac{\dot{Q}_0}{X} \right) = 0. \tag{45}$$

As $Q_0(X, \tau)$ is time reversal symmetric and equivalent to $\cos(\tau)X + \mathcal{O}(X)$ when X tends to zero (see (15) and (22)), $\dot{Q}_0(X, \tau)/X$ is time reversal antisymmetric and satisfies (43). We then deduce that, for all X , $\dot{Q}_0(X, \tau)/X$ is an eigensolution of (41) for the eigenvalue $\Delta = 0$. In other words, $\eta_{qc,a}(X, \tau) = \dot{Q}_0(X, \tau)/X$ is the eigenfunction corresponding to the eigenvalue $\Delta = 0$ whatever the energy (or X) is. We have then shown that the boundary $\Delta_a(X)$ of the instability zone we are concerned with is the ε -axis of the $\Delta - \varepsilon$ plane.

4. 2. 4 Second transition curve for a partial isochronism of order n

To calculate the second curve, $\Delta_s(X)$ related to the time reversal symmetric solution $\eta_{qc,s}(X, \tau)$ of (41), we differentiate (40) with respect to X :

$$\frac{\partial^2}{\partial \tau^2} \left(\frac{\partial Q_0}{\partial X} \right) + \tilde{T}^2(X) \tilde{V}''(Q_0) \left(\frac{\partial Q_0}{\partial X} \right) + \frac{d\tilde{T}^2(X)}{dX} \tilde{V}'(Q_0) = 0. \tag{46}$$

This equation is not of the Hill type because of its last term which is not linear in $\partial Q_0/\partial X$.

Suppose now that the potential V is isochronous up to order n . By definition, we have $\tilde{T}^2(X) = 1 + 2\tilde{T}_{2n} X^{2n} + o(X^{2n})$. That is $d\tilde{T}^2/dX = 4n\tilde{T}_{2n} X^{2n-1} + o(X^{2n-1})$ and $\tilde{V}'(Q_0) = X Q_0^{(1)}(\tau) + o(X^2)$. The last term of Eq. (46) is then of order X^{2n} .

This means that, up to order X^{2n-1} , Eq. (46) reads

$$\left[\frac{\partial^2}{\partial \tau^2} \left(\frac{\partial Q_0}{\partial X} \right) + \tilde{T}^2(X) \tilde{V}''(Q_0) \left(\frac{\partial Q_0}{\partial X} \right) \right]_k = 0, \quad 0 \leq k \leq 2n - 1. \tag{47}$$

(Here and hereafter, the symbol $[f(X)]_k$ will denote the terms of order X^k of $f(X)$, $[f(X)]_k = \frac{1}{k!} \frac{d^k f}{dX^k}(0)$). Since $\partial Q_0/\partial X = \cos(\tau) + \mathcal{O}(X)$ as $X \rightarrow 0$, it satisfies (43) and is moreover time reversal symmetric. Now, because of (47), up to order X^{2n-1} , $\partial Q_0/\partial X$ represents the time reversal symmetric eigenfunction $\eta_{qc,s}(X, \tau)$ of (41) for an eigenvalue Δ_s which, up to this order, is equal to 0. This means that

$$\Delta_s(X) = \sum_{m=2n}^{\infty} \Delta_s^{(m)} X^m \quad \text{and} \quad \eta_{qc,s}^{(k)}(\tau) \equiv [\eta_{qc,s}(X, \tau)]_k = \left[\frac{\partial Q_0}{\partial X} \right]_k, \quad 0 \leq k \leq 2n - 1. \tag{48}$$

Let us write now

$$\eta_{qc,s}^{(2n)}(\tau) = \left[\frac{\partial Q_0}{\partial X} \right]_{2n} + \zeta(\tau), \quad (49)$$

where $\zeta(\tau)$ is a function to be determined. Taking into account (48) and (47), we are able to calculate the terms of order X^{2n} of (41) and obtain

$$\left[\frac{\partial^2 \eta_{qc}(X, \tau)}{\partial \tau^2} + \tilde{T}^2(X) \{ \tilde{V}''(Q_0(X, \tau)) - \Delta \} \eta_{qc}(X, \tau) \right]_{2n} = 0 \quad (50)$$

$$\implies \ddot{\zeta}(\tau) + \zeta(\tau) - \Delta_s^{(2n)} Q_0^{(1)}(\tau) - 4n \tilde{T}_{2n} Q_0^{(1)}(\tau) = 0.$$

As $Q_0^{(1)}(\tau) = \cos(\tau)$, removing the secular terms from this last equation requires $\Delta_s^{(2n)} = -4n \tilde{T}_{2n}$. Hence, the equation of the second branch of the instability zone

$$\Delta_s(X) = -4n \tilde{T}_{2n} X^{2n} + o(X^{2n}). \quad (51)$$

4. 2. 5. Bifurcation energy

Coming back to the definitions, $\Delta = (\omega_{0,0}^2 - \omega_{qc,0}^2)/v_2$, $X = (2\varepsilon/v_2)^{1/2}$, $\tilde{T}^2(X) = v_2/\omega_0^2$ and $\omega_0^2 = \omega_{0,0}^2 + \gamma_{0,n} \varepsilon^n + o(\varepsilon^n)$ ($\omega_{0,0}^2 = v_2$), we can use (51) to obtain the leading order expression for the energy $\varepsilon_0^{(n)}$ at which a nonlinear in-phase mode isochronous up to order n bifurcates:

$$\varepsilon_0^{(n)} = \left(\frac{\omega_{0,0}^2 - \omega_{qc,0}^2}{2n\gamma_{0,n}} \right)^{1/n} = \left(\frac{-2\phi_2 \sin^2(\pi/N)}{n\gamma_{0,n}} \right)^{1/n} + o(N^{-2/n}), \quad N \rightarrow \infty. \quad (52)$$

Let us first notice that the existence of a critical energy at which the in-phase mode undergoes a bifurcation implies that $\gamma_{0,n}$ is negative which, in turn, requires the corresponding frequency to decrease with increasing energy. This condition, already known for non isochronous potentials (or, in our terminology, isochronous up to order 1) [13], still holds in case of partial isochronism.

As already mentioned in the introduction, expression (52) shows a very deep relation between the low-energy behaviour of the frequency of the in-phase mode and its bifurcation energy. We will see in the next section that the same relation holds in fact for the out-of-phase mode. As n may now take on arbitrary positive integer values, (52) treats the case of all possible analytic potentials with nonzero harmonic frequency ($v_2 > 0$). Its validity is however not restricted to such potentials and we remark that it still holds for the class of non analytic potentials studied recently by Kastner in relation with the possible existence of energy thresholds for discrete breathers [25,26]. From this point of view, this relation seems quite general.

4. 2. 6. Examples

The coefficients $\gamma_{0,n} = -2v_2(2/v_2)^n \tilde{T}_{2n}$ are easily obtained from the expression (A.6) for the period T . Indeed, Eq. (A.6) shows that $\tilde{T}_{2n} = \sigma_{2n+1} (2n+1)!!/(2n)!!$. Then, zeroing the σ_{2k+1} , $k \in \{1, \dots, n-1\}$ as explained in Appendix A and re-introducing the corresponding constraints in σ_{2n+1} , allows us to derive the expression for \tilde{T}_{2n} for a potential isochronous up to order n .

For $n = 1$ (non isochronous potential),

$$\tilde{T}_2 = \frac{3}{2} \sigma_3 = \frac{3}{2} \left(\frac{5}{18} \alpha_2^2 - \frac{1}{4} \alpha_3 \right) \implies \gamma_{0,1} = \frac{3v_4}{2v_2} - \frac{5v_3^2}{3v_2^2}$$

then,

$$\varepsilon_0^{(1)} = \frac{12\phi_2 v_2^2 \sin^2(\pi/N)}{10v_3^2 - 9v_2 v_4} + o(N^{-2}), \quad N \rightarrow \infty, \quad (53)$$

which is exactly the expression (3.13) of [13].

For $n = 2$,

$$\begin{aligned} \tilde{T}_2 = 0 &\implies \alpha_3 = \frac{10}{9}\alpha_2^2 \implies \tilde{T}_4 = \frac{15}{8} \left(-\frac{1}{6}\alpha_5 - \frac{28}{81}\alpha_2^4 + \frac{7}{15}\alpha_4\alpha_2 \right) \\ \implies \gamma_{0,2} &= -\frac{15}{v_2} \left(\frac{7}{15} \frac{v_3 v_5}{v_2^2} - \frac{28}{81} \frac{v_3^4}{v_2^4} - \frac{1}{6} \frac{v_6}{v_2} \right). \end{aligned}$$

Hence,

$$\varepsilon_0^{(2)} = \left(\frac{54v_2^3\phi_2}{378v_3v_5v_2^2 - 280v_3^4 - 135v_6v_2^3} \right)^{1/2} v_2 \sin\left(\frac{\pi}{N}\right) + o(N^{-1}), \quad N \rightarrow \infty. \quad (54)$$

4. 2. 7. Pure isochronism

Let us suppose now that the in-phase mode is purely isochronous. Then, $\tilde{T}(X) = 1$. Differentiating (40) with respect to X as we have done in the previous section gives rise to

$$\frac{\partial^2}{\partial \tau^2} \left(\frac{\partial Q_0}{\partial X} \right) + \tilde{V}''(Q_0) \left(\frac{\partial Q_0}{\partial X} \right) = 0. \quad (55)$$

At variance with Eq. (46), this equation is of the Hill type and $\partial Q_0/\partial X$ represents the time reversal symmetric eigensolution of the instability zone under investigation. Its eigenvalue is $\Delta_s = 0$ for all X , i.e. whatever the energy is. We have thus found that, in case of pure isochronism of the onsite potential, the boundaries $\Delta_a(X)$ and $\Delta_s(X)$ of the instability zone merge and make it disappear. The merging of two transition curves is a phenomenon known in stability theory as a *coexistence*. It occurs for instance in Ince's or Lamé's equations and general conditions for its appearance are given in [27,28]. We notice incidentally that for an "isotonic" potential, $V(x) = \omega^2(x + 1 - 1/(x + 1))^2/8$, which is isochronous (see for example [29]), the variational Eq. (41) reduces to an Ince's equation. This allows for an explicit verification of the general result stated above.

As a consequence of the disappearance of the instability region, *the in-phase mode never undergoes a tangent bifurcation*. Remark that, at variance with the results obtained for a partial isochronism, this result is *non perturbative*. Indeed, Eqs. (45) and (55) are exact and their respective eigensolutions $\eta_{q_c,a}(X, \tau) = \dot{Q}_0/X$ and $\eta_{q_c,s}(X, \tau) = \partial Q_0/\partial X$ as well.

To conclude, let us notice that expression (52) shows how the instability zone shrinks as n tends to infinity (see also Fig. 1). Nevertheless, as it is valid in the limit of vanishing energies only it couldn't have been used to prove the result above.

4. 3 Out-of-phase mode

4. 3 1. Stability analysis

Evaluated along orbit II, the Jacobian matrix (37) now reads

$$\begin{aligned} \text{DF}_{qk}(Q_{\text{II}}) &= \frac{1}{2} \left[V''(Q_0 + Q_\pi) + V''(Q_0 - Q_\pi) + 4 \sin^2 \frac{k}{2} \{ W''(2Q_\pi) + W''(-2Q_\pi) \} \right] \delta_{k,q} \\ &+ \frac{1}{2} \left[V''(Q_0 + Q_\pi) - V''(Q_0 - Q_\pi) - 2i \sin k \{ W''(2Q_\pi) - W''(-2Q_\pi) \} \right] \delta_{k,q+\pi} \end{aligned} \quad (56)$$

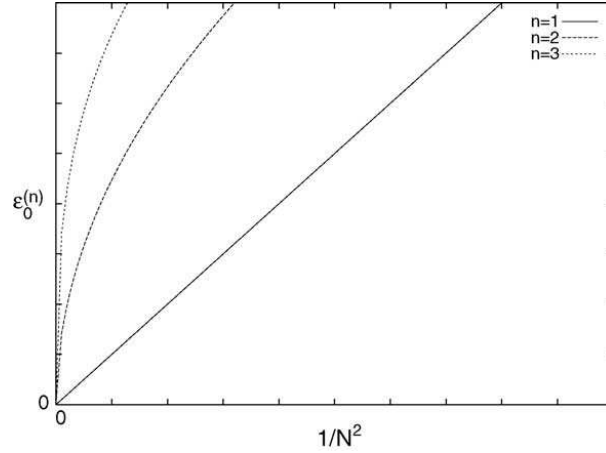


Fig. 1. Schematic representation of the bifurcation energy (41) as a function of the inverse squared number of oscillators N for various degrees of isochronism of the in-phase mode ($n = 1-3$). For a given n , the instability zone lies between the energy-axis (first transition curve, $1/N^2 = 0$) and the curve labelled by n ($=1, 2$ or 3). Below (above) the latter, the in-phase mode is stable (unstable). Right on a transition curve the solution is periodic. We see on this graph how the instability zone shrinks as n increases. In the purely isochronous case, the second transition curve merges with the first one on the energy-axis and the corresponding instability zone disappears.

and the corresponding dynamics,

$$\ddot{\eta}_q + \frac{1}{2} \left[V''(Q_0 + Q_\pi) + V''(Q_0 - Q_\pi) + 4 \sin^2 \frac{q}{2} \{ W''(2Q_\pi) + W''(-2Q_\pi) \} \right] \eta_q + \frac{1}{2} [V''(Q_0 + Q_\pi) - V''(Q_0 - Q_\pi) + 2i \sin q \{ W''(2Q_\pi) - W''(-2Q_\pi) \}] \eta_{q+\pi} = 0. \quad (57)$$

To evaluate the possible bifurcating energies in this case, we will proceed along the same lines as for the in-phase mode. Notice, however, that Eq. (57) do not decouple in the present case and that, due to the very last term, they are complex (real and imaginary parts are not decoupled). To deal with this first difficulty, we will write the system (57) in terms of real and imaginary parts.

Similar to the in-phase mode, the out-of-phase mode will eventually undergo a first tangent bifurcation via the perturbation η_{q_c} whose frequency is the closest to $\omega_{\pi,0}$, that is, for $q_c = \pi - 2\pi/N$. As N tends to infinity, $q = 2\pi/N$ plays the role of the small parameter in the variational equations. But at variance with the in-phase variational equation where $\Delta \propto \sin^2(\pi/N)$ was the unique small parameter, Eq. (57) possess two small parameters through $\sin^2((q_c + \pi)/2) \sim (\pi/N)^2$ and $\sin(q_c) \sim \pi/N$. Notice that these two parameters are not of the same order.

In what follows, for the sake of clarity, we simplify further the notations by using $\eta_{q_c} = r_\pi + i j_\pi$ and $\eta_{q_c+\pi} = r_0 + i j_0$ (with $i = \sqrt{-1}$) rather than the lengthy values for q_c and $q_c + \pi$. We work with dimensionless equations and with the same notations as in Section 2.3. We take $\delta = 4 \sin^2(\pi/N)$ as small parameter. The quantities $r_0, j_0, r_\pi, j_\pi, Q_0, Q_\pi$ and \tilde{T} depend on the amplitude y defined in Section 2.3. As the previous quantities, the small parameter δ has to be expanded as a power series in y . Moreover, we define

$$\begin{aligned} \mathcal{T}_1(\delta, \tau) &= \frac{\tilde{T}^2}{2} [\tilde{V}''(Q_0 + Q_\pi) + \tilde{V}''(Q_0 - Q_\pi) + (4 - \delta) \{ \tilde{W}''(2Q_\pi) + \tilde{W}''(-2Q_\pi) \}], \\ \mathcal{T}_2(\tau) &= \frac{\tilde{T}^2}{2} [\tilde{V}''(Q_0 + Q_\pi) - \tilde{V}''(Q_0 - Q_\pi)], \quad \mathcal{T}_3(\delta, \tau) = \tilde{T}^2 \sqrt{\delta(1 - \delta/4)} [\tilde{W}''(2Q_\pi) - \tilde{W}''(-2Q_\pi)], \\ \mathcal{T}_4(\delta, \tau) &= \frac{\tilde{T}^2}{2} [\tilde{V}''(Q_0 + Q_\pi) + \tilde{V}''(Q_0 - Q_\pi) + 4\delta \{ \tilde{W}''(2Q_\pi) + \tilde{W}''(-2Q_\pi) \}]. \end{aligned} \quad (58)$$

System (57) now reads (from now on, dots denote τ derivative),

$$\begin{cases} \ddot{r}_\pi + \mathcal{T}_1(\delta, \tau)r_\pi + \mathcal{T}_2(\tau)r_0 - \mathcal{T}_3(\delta, \tau)j_0 = 0, \\ \ddot{j}_\pi + \mathcal{T}_1(\delta, \tau)j_\pi + \mathcal{T}_2(\tau)j_0 + \mathcal{T}_3(\delta, \tau)r_0 = 0, \\ \ddot{r}_0 + \mathcal{T}_4(\delta, \tau)r_0 + \mathcal{T}_2(\tau)r_\pi + \mathcal{T}_3(\delta, \tau)j_\pi = 0, \\ \ddot{j}_0 + \mathcal{T}_4(\delta, \tau)j_0 + \mathcal{T}_2(\tau)j_\pi - \mathcal{T}_3(\delta, \tau)r_\pi = 0. \end{cases} \quad (59)$$

As the energy (amplitude y) tends to zero, Q_π and Q_0 tend to zero as well and from (58), (31) and (32), we obtain $\mathcal{T}_1(\delta, \tau) \rightarrow 1 - \delta\beta_1/4$, $\mathcal{T}_4(\delta, \tau) \rightarrow \alpha_1 + \delta\beta_1/4$ and $\mathcal{T}_2(\delta, \tau)$ and $\mathcal{T}_3(\delta, \tau)$ both tend to 0. As δ is a small parameter, the only way to obtain a perturbation whose frequency is exactly 1 (as for the mode itself) is to require $\delta = 0$ for it gives rise to $\mathcal{T}_1 = 1$ which is precisely the desired frequency for the perturbation (r_π, j_π) . Regarding (r_0, j_0) , as $\mathcal{T}_4 = \alpha_1 < 1$ in this limit, we have to require $(r_0 = 0, j_0 = 0)$ in order zero in y . The origin of the instability zone is thus located at $\delta = 0, \varepsilon = 0$ in the parameter space.

4. 3 2. First transition curve

Now, proceeding as in the previous section, let us derive the equations obeyed by $Q_0 = \dot{Q}_0/y$ and $Q_\pi = \dot{Q}_\pi/y$.

$$\begin{cases} \ddot{Q}_\pi + \mathcal{T}_1(0, \tau)Q_\pi + \mathcal{T}_2(\tau)Q_0 = 0, \\ \ddot{Q}_0 + \mathcal{T}_4(0, \tau)Q_0 + \mathcal{T}_2(\tau)Q_\pi = 0. \end{cases} \quad (60)$$

As the out-of-phase mode has been chosen time reversal symmetric, Q_0 and Q_π are time reversal anti-symmetric. Moreover, due to the asymptotic relations given above, they represent a motion of frequency 1 as $y \rightarrow 0$. Having the required properties, they form the antisymmetric eigensolution of the Hill's system (59) for a value of δ equal to zero for all y (or energy). Therefore, $(r_\pi, j_\pi) \propto Q_\pi$ and $(r_0, j_0) \propto Q_0$. We thus deduce that, in a diagram (δ, ε) , one of the boundaries of the Arnold tongue is the ε -axis itself which means that, similar to the result obtained for the in-phase mode, no bifurcation can be expected from this branch.

4. 3 3. Second transition curve for an isochronism of order n

The second branch of the instability zone is the curve associated with the time reversal symmetric eigenfunction. Differentiating (30) with respect to y , we obtain

$$\begin{cases} \frac{\partial^2}{\partial \tau^2} \left(\frac{\partial Q_\pi}{\partial y} \right) + \mathcal{T}_1(0, \tau) \left(\frac{\partial Q_\pi}{\partial y} \right) + \mathcal{T}_2(\tau) \left(\frac{\partial Q_0}{\partial y} \right) - \frac{d \ln \tilde{T}^2}{dy} \frac{\partial^2 Q_\pi}{\partial \tau^2} = 0, \\ \frac{\partial^2}{\partial \tau^2} \left(\frac{\partial Q_0}{\partial y} \right) + \mathcal{T}_4(0, \tau) \left(\frac{\partial Q_0}{\partial y} \right) + \mathcal{T}_2(\tau) \left(\frac{\partial Q_\pi}{\partial y} \right) - \frac{d \ln \tilde{T}^2}{dy} \frac{\partial^2 Q_0}{\partial \tau^2} = 0. \end{cases} \quad (61)$$

Again, the functions $\partial Q_\pi/\partial y$ and $\partial Q_0/\partial y$ have the right time symmetry and Fourier properties. Nevertheless, the system above is not a Hill's system due to the last terms. For an out-of-phase mode isochronous up to order n , $\tilde{T}(y) = 1 + \tilde{T}_{2n}y^{2n} + o(y^{2n})$, and we can evaluate the order of the last terms in (61). Using (31) and (32), we find

$$-\frac{d \ln \tilde{T}^2}{dy} \frac{\partial^2 Q_\pi}{\partial \tau^2} = 4n \tilde{T}_{2n} \cos \tau y^{2n} + o(y^{2n}); \quad -\frac{d \ln \tilde{T}^2}{dy} \frac{\partial^2 Q_0}{\partial \tau^2} = \mathcal{O}(y^{2n+1}). \quad (62)$$

Given this last result, we will first assume, and then verify a posteriori, that the order of δ in y is $2n$, hence

$$\delta = \delta^{(2n)}y^{2n} + o(y^{2n}). \quad (63)$$

We then obtain immediately

$$\begin{aligned} \mathcal{T}_1(\delta, \tau) &= \mathcal{T}_1(0, \tau) - \frac{\beta_1}{4} \delta^{(2n)} y^{2n} + o(y^{2n}), & \mathcal{T}_2(\tau) &= 2\alpha_2 \cos \tau y + o(y), \\ \mathcal{T}_3(\delta, \tau) &= \sqrt{\delta^{(2n)}} \beta_2 \cos \tau y^{n+1} + o(y^{n+1}), & \mathcal{T}_4(\delta, \tau) &= \mathcal{T}_4(0, \tau) + \frac{\beta_1}{4} \delta^{(2n)} y^{2n} + o(y^{2n}). \end{aligned} \quad (64)$$

We deduce from these relations that system (59) verifies

$$\begin{cases} \ddot{r}_\pi + \mathcal{T}_1(0, \tau) r_\pi + \mathcal{T}_2(\tau) r_0 = o(y^n), \\ \ddot{j}_\pi + \mathcal{T}_1(0, \tau) j_\pi + \mathcal{T}_2(\tau) j_0 = o(y^n), \\ \ddot{r}_0 + \mathcal{T}_4(0, \tau) r_0 + \mathcal{T}_2(\tau) r_\pi = o(y^n), \\ \ddot{j}_0 + \mathcal{T}_4(0, \tau) j_0 + \mathcal{T}_2(\tau) j_\pi = o(y^n). \end{cases} \quad (65)$$

We remark now that the solution $(\eta_{q_c}(\tau), \eta_{q_c+\pi}(\tau))$ of (57) is defined up to a global phase only (i.e. if $(\eta_{q_c}(\tau), \eta_{q_c+\pi}(\tau))$ is a solution of (57), $(e^{i\phi} \eta_{q_c}(\tau), e^{i\phi} \eta_{q_c+\pi}(\tau))$, $\phi \in \mathbb{R}$ is also a solution). Using this freedom, we solve (65) by requiring

$$r_\pi^{(k)} = \left[\frac{\partial \mathcal{Q}_\pi}{\partial y} \right]_k; \quad r_0^{(k)} = \left[\frac{\partial \mathcal{Q}_0}{\partial y} \right]_k; \quad j_\pi^{(k)} = 0; \quad j_0^{(k)} = 0, \quad 1 \leq k \leq n, \quad (66)$$

without loss of generality (the brackets have the same meaning as in the previous section). Reinstating in (59) and using (64) we find

$$r_\pi^{(k)} = \left[\frac{\partial \mathcal{Q}_\pi}{\partial y} \right]_k; \quad r_0^{(k)} = \left[\frac{\partial \mathcal{Q}_0}{\partial y} \right]_k, \quad 1 \leq k \leq 2n - 1. \quad (67)$$

As in the last section, we now solve the first and the third equation of (59) at order $2n$ by introducing two functions $\zeta_\pi(\tau)$ and $\zeta_0(\tau)$ according to

$$r_\pi^{(2n)} = \left[\frac{\partial \mathcal{Q}_\pi}{\partial y} \right]_{2n} + \zeta_\pi; \quad r_0^{(2n)} = \left[\frac{\partial \mathcal{Q}_0}{\partial y} \right]_{2n} + \zeta_0 = \zeta_0. \quad (68)$$

From (61) and (62) we have

$$\begin{cases} \left[\frac{\partial^2}{\partial \tau^2} \left(\frac{\partial \mathcal{Q}_\pi}{\partial y} \right) + \mathcal{T}_1(0, \tau) \left(\frac{\partial \mathcal{Q}_\pi}{\partial y} \right) + \mathcal{T}_2(\tau) \left(\frac{\partial \mathcal{Q}_0}{\partial y} \right) \right]_{2n} + 4n \tilde{T}_{2n} \cos \tau = 0, \\ \left[\frac{\partial^2}{\partial \tau^2} \left(\frac{\partial \mathcal{Q}_0}{\partial y} \right) + \mathcal{T}_4(0, \tau) \left(\frac{\partial \mathcal{Q}_0}{\partial y} \right) + \mathcal{T}_2(\tau) \left(\frac{\partial \mathcal{Q}_\pi}{\partial y} \right) \right]_{2n} = 0. \end{cases} \quad (69)$$

and from (59) and (64)

$$\begin{cases} [\ddot{r}_\pi + \mathcal{T}_1(0, \tau) r_\pi + \mathcal{T}_2(\tau) r_0]_{2n} - \frac{\beta_1}{4} \delta^{(2n)} \cos \tau = 0, \\ [\ddot{r}_0 + \mathcal{T}_4(0, \tau) r_0 + \mathcal{T}_2(\tau) r_\pi]_{2n} = 0. \end{cases} \quad (70)$$

Therefore,

$$\begin{cases} \ddot{\zeta}_\pi + \zeta_\pi - \left(\frac{\beta_1}{4} \delta^{(2n)} + 4n \tilde{T}_{2n} \right) \cos \tau = 0, \\ \ddot{\zeta}_0 + \alpha_1 \zeta_0 = 0. \end{cases} \quad (71)$$

Removing the secular term from the first equation leads eventually to the equation of the second transition curve

$$\delta = -\frac{16n\tilde{T}_{2n}}{\beta_1}y^{2n} + o(y^{2n}). \tag{72}$$

Discarding the solution of the homogenous equation [21] gives $\zeta_\pi = 0$. The second equation is satisfied by setting $\zeta_0 = 0$ as well (because its frequency $\alpha_1 \neq 1$). Hence, $r_\pi^{(2n)} = [\partial Q_\pi / \partial y]_{2n}$ and $r_0^{(2n)} = [\partial Q_0 / \partial y]_{2n}$. Remark that these results are correct provided we are able to justify a posteriori the initial assumption (63) regarding the small parameter δ . This amounts to proving that the remaining equations for j_π and j_0 in (59) never develop any secular terms up to order $2n$. This is done in Appendix B by showing that these equations verify the adequate solvability conditions.

4.3.4. Bifurcation energy

Using the leading order relation between the amplitude and the energy density, $y^2 = 2\varepsilon/\omega_{\pi,0}^2 + o(\varepsilon^2)$, $\omega_{\pi,0}^2 = v_2 + 4\phi_2$, together with the relation

$$\omega_\pi^2 = \omega_{\pi,0}^2 + \gamma_{\pi,n}\varepsilon^n + o(\varepsilon^n), \tag{73}$$

and noting that $\delta = 4 \sin^2(\pi/N)$, $\tilde{T}_{2n}y^{2n} = -\gamma_{\pi,n}\varepsilon^n/2\omega_{\pi,0}^2 + o(\varepsilon^n)$, we finally obtain from (72)

$$\varepsilon_\pi^{(n)} = \left(\frac{\omega_{\pi,0}^2 - \omega_{c,0}^2}{2n\gamma_{\pi,n}} \right)^{1/n} = \left(\frac{2\phi_2 \sin^2(\pi/N)}{n\gamma_{\pi,n}} \right)^{1/n} + o(N^{-2/n}), \quad N \rightarrow \infty, \tag{74}$$

which is similar to the expression obtained for the in-phase mode. We notice this time that the existence of a critical energy at which the out-of-phase mode undergoes a bifurcation implies that $\gamma_{0,n}$ is positive. This requires the corresponding frequency to increase with the energy. This condition, already known for non isochronous motions [13], still holds in case of partial isochronism.

As seen in Section 2.3.2, the period of the motion is more conveniently expressed as a series in the square of the amplitude, y^2 , rather than as a series in the energy ε . For this reason, we also provide the bifurcation energy in terms of the coefficients \tilde{T}_{2n} defined in (31),

$$\varepsilon_\pi^{(n)} = \frac{\omega_{\pi,0}^2}{2} \left(\frac{-\phi_2 \sin^2(\pi/N)}{n\omega_{\pi,0}^2 \tilde{T}_{2n}} \right)^{1/n} + o(N^{-2/n}), \quad N \rightarrow \infty. \tag{75}$$

4.3.5. Examples

We are now in a position to give an explicit expression of $\varepsilon_\pi^{(n)}$ for an out-of-phase mode isochronous up to order n in terms of the parameters v_i and ϕ_i defining $V(x)$ and $W(x)$ (see (2) and (28)). This amounts simply to finding the leading order of the low-energy (or low-amplitude) behaviour of the corresponding frequency as explained in Section 2.3.2 (see also Section 3.2).

For a non isochronous out-of-phase mode ($n = 1$), from (32) and (75), we find

$$\varepsilon_\pi^{(1)} = \frac{4(v_2 + 4\phi_2)\phi_2}{3(v_4 + 16\phi_4) + (2v_3^2)/(3v_2 + 16\phi_2) - (4v_3^2)/(v_2)} \sin^2\left(\frac{\pi}{N}\right) + o(N^{-2}), \quad N \rightarrow \infty. \tag{76}$$

Let us notice first that, when $v_3 = 0$ this expression reduces to formula (3.20) of [13] obtained in the special case of a symmetric onsite potential $V(x)$. The correction introduced by the asymmetry of $V(x)$ (i.e. the term proportional to v_3^2 in the denominator of (76)) has the interesting feature to be always negative. Therefore, the following inequality

$$v_3^2 < \frac{3v_2(v_4 + 16\phi_4)(3v_2 + 16\phi_2)}{2(5v_2 + 32\phi_2)} \tag{77}$$

has to be satisfied for the out-of-phase mode to undergo a tangent bifurcation. This corresponds, as we have seen in the section above, to requiring that the frequency increases with the energy.

Another interesting result easily drawn from (76) concerns the case of partially isochronous *onsite* potentials. It is found in this case that a certain amount of nonlinearity (ϕ_4) in the interaction potential is needed in order to ensure a bifurcation of the *out-of-phase mode*. Indeed, the relation between the first coefficients of the Taylor expansion of $V(x)$ is $10v_3^2 = 9v_2v_4$ in this case. The denominator of (76) is then positive provided

$$\phi_4 > \frac{1}{5} \frac{v_4\phi_2}{3v_2 + 16\phi_2} \quad (78)$$

So that, in a chain of harmonically coupled partially isochronous oscillators, no discrete breather (if any) stems from the tangent bifurcation of the out-of-phase mode. At the same time we can conclude, that breathers appear for fully isochronous harmonic oscillators ($v_4 = 0$) when coupled anharmonically ($\phi_4 > 0$). This statement is to some extent confirmed by a recent proof that breathers exist and can be continued from zero anharmonic coupling for harmonic oscillators coupled by a purely quartic interaction [31].

For a first degree of isochronism ($\nu = 2$), we obtain from (75)

$$\varepsilon_\pi^{(2)} = \frac{v_2 + 4\phi_2}{2} \left(\frac{-\phi_2}{2(v_2 + 4\phi_2)\tilde{T}_4} \right)^{1/2} \sin\left(\frac{\pi}{N}\right) + o(N^{-1}), \quad N \rightarrow \infty, \quad (79)$$

where

$$\tilde{T}_4 = \frac{(15\alpha_1^2 + 96 - 56\alpha_1)\alpha_2^4}{24\alpha_1^3(\alpha_1 - 4)^2} - \frac{9(32 + 5\alpha_1^2 - 24\alpha_1)\alpha_3\alpha_2^2}{16\alpha_1^2(\alpha_1 - 4)^2} + \frac{3(5\alpha_1 - 12)\alpha_4\alpha_2}{8\alpha_1(\alpha_1 - 4)} - \frac{5}{16}(\alpha_5 + \beta_5) \quad (80)$$

with $\alpha_n = v_{n+1}/(v_2 + 4\phi_2)$ and $\beta_n = 2^{n+1}\phi_{n+1}/(v_2 + 4\phi_2)$. Notice that, to enforce a partial isochronism of the out-of-phase mode up to order $n = 2$, we have used the first of the relations (35) ($\beta_3 = f(\{\alpha_j\})$) to derive (80). Again, a tangent bifurcation of this mode will take place provided the inequality $\tilde{T}_4 < 0$ is fulfilled.

We remark finally that expression (74) for the bifurcation energy of π -modes still holds in case no onsite potential is present ($V(x) = 0$) *providing the interaction potential is even*. For instance, it can be applied to the generalized (FPU)- β interaction potential, $W(x) = (x^2/2) + x^{2(p+1)}/2(p+1)$, $p \in \mathbb{N}$, investigated in [23]². The case of a zero onsite potential and an interaction potential containing odd terms has to be treated separately (as already proved in [13]) and (74) does not apply in this case. The reader is for example referred to [13] or [24] for the stability analysis of π -modes in such potentials.

4.3.6 Pure isochronism

Similar to the pure isochronism of the in-phase mode, the pure isochronism of the out-of-phase mode leads to a merging of the two transition curves which makes the instability zone disappear. This is clear from the fact that, as $\tilde{T}(y) = 1$, $\partial Q_\pi/\partial y$ and $\partial Q_0/\partial y$ obey

$$\begin{cases} \frac{\partial^2}{\partial \tau^2} \left(\frac{\partial Q_\pi}{\partial y} \right) + \mathcal{T}_1(0, \tau) \left(\frac{\partial Q_\pi}{\partial y} \right) + \mathcal{T}_2(\tau) \left(\frac{\partial Q_0}{\partial y} \right) = 0, \\ \frac{\partial^2}{\partial \tau^2} \left(\frac{\partial Q_0}{\partial y} \right) + \mathcal{T}_4(0, \tau) \left(\frac{\partial Q_0}{\partial y} \right) + \mathcal{T}_2(\tau) \left(\frac{\partial Q_\pi}{\partial y} \right) = 0 \end{cases} \quad (81)$$

² In this case $\ddot{Q}_\pi + 2W'(2Q_\pi) = 0$ (see (30)) with reduced period $\tilde{T}(y) = T(\varepsilon)/\pi = 1 + \tilde{T}_{2p}y^{2p} + o(y^{2p})$ where y is the leading order of the amplitude of Q_π related to its energy by $\varepsilon = 2y^2 + o(y^2)$ and where $\tilde{T}_{2p} = -(2p+1)!/2p!(p+1)!$. This mode is thus partially isochronous up to order p . Using \tilde{T}_{2p} in (75) and $\varepsilon = 2y^2 + o(y^2)$, the bifurcation amplitude y_c reads $y_c = [(p!(p+1)!/(2p+1)!2p) \sin^2(\pi/N)]^{1/2p} + o(N^{-1/p})$, which is the expression (16) derived in [23] when $N \rightarrow \infty$.

and are thus exact solutions of the variational Eq. (59) for $q = 0$ (i.e. $(r_\pi, j_\pi) \propto \partial Q_\pi / \partial y$ and $(r_0, j_0) \propto \partial Q_0 / \partial y$). As a consequence, *if the out-of-phase mode is isochronous it does not undergo a tangent bifurcation.*

5. Summary and discussion

We have examined so far the close link existing between the possible tangent bifurcation of band edge modes and the low-energy behaviour of their frequency. We have introduced the concept of partial isochronism of order n for these modes through the relation $\omega_q^2 = \omega_{q,0}^2 + \gamma_{q,n} \varepsilon^n + o(\varepsilon^n)$ ($q = 0$ or π). By performing a linear stability analysis in the limit of small oscillations, we have derived a simple and general expression for the leading order of their bifurcation energy in terms of $\gamma_{q,n}$. We have shown that the calculation of $\gamma_{0,n}$ (in-phase mode) simply requires to invert a series and thus reduces to a pure algebraic problem. The inversion of this series is easily implemented with the help of any software able to perform formal calculations. The coefficient $\gamma_{\pi,n}$ related to the out-of-phase mode may be derived by means of a Lindstedt–Poincaré expansion for the motion.

In addition, we have proved by means of an *exact* linear stability analysis that, fully isochronous band edge modes (i.e. with an energy-independent frequency) never undergo a tangent bifurcation. At variance with the results quoted above, this one is *non perturbative*.

In order to discuss the implications of these results on discrete breathers, we shall now assume that, at least some of them stem from the tangent bifurcation of the band edge modes investigated so far. To our knowledge, for a Klein–Gordon lattice with smooth (say C^∞) linearizable onsite *and* interaction potentials ($\omega_{0,0}$ and $\omega_{\pi,0}$ both nonzero) no general result exists which proves such an assumption. However, with the additional assumption that, in an infinite lattice, the breather amplitude (measured at the level of its largest oscillation) can be lowered to arbitrary small values [13,15], we come to the conclusion that, in this limit, the breather frequency tends to an edge of the phonon band and merges with the corresponding mode. Indeed, for small amplitudes, the motion enters a quasi-linear regime and then approaches some phonon mode. But in the same time, the breather family (parametrised either by its amplitude, its frequency or its energy) has to lie outside the phonon band to avoid a resonance which would lead to its disappearance. And this is possible by approaching an edge of the phonon band only. Notice however that one can find systems with breather families which do not possess any small amplitude limit (see, e.g. [25]). Such breather families are then not related with the instabilities discussed above.

5.1. Energy thresholds for discrete breathers

We now turn to an important implication of our results on the possible existence of energy thresholds for families of discrete breathers bifurcating tangently from band edge modes. It has already been noticed in many places that such a nonzero activation energy for discrete breathers is of practical relevance [15,25] as it surely affects their experimental detection and presumably their contribution to thermodynamical properties of lattices (see for example [30] for some work in this direction).

Let us consider a Hamiltonian lattice of N coupled oscillators described by (1) with families of periodic orbits parametrised by their amplitude. Let us follow the periodic orbit corresponding to a band edge mode as its amplitude increases from zero. As we have seen in Section 4, under certain conditions, at a finite critical amplitude (or energy density) this mode will become unstable and bifurcate tangently. A family of discrete breathers emerging from this bifurcation is, right at this point, identical to the mode from which it stems and therefore has the same energy. Increasing the amplitude further and following this new orbit, we obtain its energy as a function of its amplitude. It is worth noticing immediately that in finite systems $N < \infty$, discrete breathers arising in this way exist above a certain energy threshold only. Indeed, due to their finite amplitude their energy is surely nonzero. The question is as whether this threshold persists in the thermodynamic limit, $N \rightarrow \infty$.

We then turn to the determination of the (total) bifurcation energy $E_q^{(n)}$ of a BEM partially isochronous up to order n , in the thermodynamic limit. According to (52) and (74), the bifurcation energy density for the two possible modes $q = 0$ or $q = \pi$ can be cast into the general form

$$\varepsilon_q^{(n)} = \left(\frac{\omega_{q,0}^2 - \omega_{q_c,0}^2}{2n\gamma_{q,n}} \right)^{1/n} + o(N^{-2/n}), \quad N \rightarrow \infty, \quad (82)$$

where the coefficient $\gamma_{q,n}$ is defined by the low-energy behaviour of the BEM frequency

$$\omega_q^2 = \omega_{q,0}^2 + \gamma_{q,n}\varepsilon^n + o(\varepsilon^n), \quad (83)$$

and where the wave number q_c is the closest to q ($q_c = 2\pi/N$ if $q = 0$ and $q_c = \pi - 2\pi/N$ if $q = \pi$). In any case, $\omega_{q,0}^2 - \omega_{q_c,0}^2 \sim N^{-2}$. We then find that

$$E_q^{(n)} = N\varepsilon_q^{(n)} \sim N^{1-(2/n)} \quad (N \rightarrow \infty). \quad (84)$$

We note that the same scaling has been recently derived for π -modes in the particular case of generalized (FPU)- β systems ([23] Eq. (18)). As shown in Section 4.3.5, these modes are indeed partially isochronous, hence the result.

Now, if the BEM is not isochronous, ($n = 1$), its total bifurcation energy vanishes as the lattice becomes infinite and so does the breather energy in this limit. No energy threshold exists in this case as already mentioned in [13]. However, as soon as the band edge mode bears some degree of isochronism, ($n > 1$), its total bifurcation energy either converges to a finite value ($n = 2$) or simply diverges ($n > 2$) and energy thresholds are thus expected.

We note incidentally that expression (84), although valid for a one-dimensional chain, bears some striking resemblance with its multi-dimensional counterpart in the *non isochronous* case which reads $E_q^{(d)} \sim N^{1-(2/d)}$ where d is the dimension of the lattice [13,15,23]. Combination of both isochronism (n) and dimensionality (d) leads immediately to the conclusion that the total bifurcation energy of a BEM scales like

$$E^{(n,d)} \sim N^{1-(2/nd)} \quad (N \rightarrow \infty). \quad (85)$$

Energy thresholds for discrete breather families bifurcating tangentially from BEMs are thus expected as soon as one of the positive integers n or d is strictly greater than one.

As already mentioned in Section 4.2.5, the general expression (82) still holds in case the analyticity of the onsite potential is relaxed. Recent results obtained by Kastner in [25,26] prove for example that, for (1D) onsite potentials of the form $V(x) = x^2/2 + |x|^r/r + o(|x|^r)$, where r is any real number greater than 2, (82) and (83) are still valid and that $n = r/2 - 1$. This way, the exponent n governing the low-energy behaviour of the frequency (83) can be tuned continuously over the whole range of positive real numbers and may counterbalance the effect due to the dimensionality d . This *nonintegral* partial isochronism opens up the possibility to satisfy the inequality obtained from (85)

$$nd < 2, \quad n \in \mathbb{R}^+, \quad d \in \mathbb{N}^+, \quad (86)$$

ensuring the absence of energy threshold in dimension d , even in two- or three-dimensional systems.

Finally, we also mention the existence of energy thresholds for breathers in one-dimensional systems with algebraically decaying long range interactions [32]. We can then identify three lattice properties which lead to appearance of breather energy thresholds - dimensionality, interaction range, and (partial) isochronism.

5.2. Energy thresholds for discrete breathers revisited

5.2.1. DNLS equations for the slow modulations of BEMs

To conclude this paper, we propose to revisit certain results of the previous section by deriving a discrete nonlinear Schrödinger equation (DNLS) for the slow modulations of small-amplitude partially isochronous BEMs. We shall

do it with the help of a method based on their nonlinear dispersion relation (see for example [33–35]) which renders its derivation almost straightforward. We would like to mention that this result, obtained by a somehow heuristic method, is also confirmed by a more rigorous multiple-scale analysis at least for the first orders of isochronism.

The method we will use to derive the DNLS equation is not properly speaking a multiple-scale expansion for the motions $x_l(t)$ which would read $x_l(t) = \sum_{j \geq 1} \mu^j F_{j,l}(t_0, t_1, \dots)$ where $\mu \ll 1$ is a small parameter and where the different timescales are given by $t_m = \mu^m t$ (see for example [36–39]). But it represents a similar approximation and has the advantage to be more transparent. It is based on the nonlinear dispersion relation obeyed by a BEM isochronous up to order n .

We first note that in the harmonic limit, plane waves $x_{q;l}(t) \propto e^{i(ql - \omega_{q,0}t)}$, where $\omega_{q,0}$ is given in (10), are solutions of the linearised equations of motion (9). Looking for slow modulations of the $q = 0$ and $q = \pi$ modes, we write them

$$x_{q;l}(t) = A_l e^{i(ql - \omega_{q,0}t)} + \text{c.c.} + o(\mu) \tag{87}$$

where ‘‘c.c.’’ stands for ‘‘complex conjugate’’, $q \in \{0, \pi\}$ and the small amplitude $A_l = \mu \psi_l$. Here μ is some small parameter.

The function ψ_l is slowly varying in space and time. It is found typically from a multiple-scale analysis that, for non isochronous modes, it assumes the form $\psi_l \equiv \psi_l(\mu^2 t, \mu l)$ (see for example [39]). For modes isochronous up to order n , a similar analysis yields $\psi_l \equiv \psi_l(\mu^{2n} t, \mu^n l)$. This is easily understood from the nonlinear dispersion relation $\omega_q^2 \simeq \omega_{q,0}^2 + \gamma_{q,n} \varepsilon^n$. For a slowly modulated plane wave to exist, it is known that nonlinearity has to compensate the dispersion of the wave packet. Now, the nonlinear term in the previous relation is, in leading order, proportional to $\varepsilon^n \sim \mu^{2n}$. Therefore, the nonlinear correction to the frequency introduces the natural long-time scale $\mu^{2n} t$. On another hand, the dispersion of the wave packet arises from a (spatial) Laplacian. If $\mu^p l$ is the space scale, dispersion introduces a correction of order μ^{2p} . This correction is able to compensate the nonlinear effects only if $p = n$, hence the scaling of ψ_l .

Now, in leading order (harmonic regime), the energy density of a BEM reads $\varepsilon_q = 2\omega_{q,0}^2 |A|^2$, $q \in \{0, \pi\}$ (the BEM amplitude A is constant so that it does not depend on l). Re-instating in the nonlinear dispersion and expanding the latter around $q = 0$ or $q = \pi$ yields

$$\begin{aligned} \omega_0 - \omega_{0,0} &\simeq \frac{\phi_2}{\omega_{0,0}} [1 - \cos(q)] + \frac{\gamma_{0,n}}{2\omega_{0,0}} (2\omega_{0,0}^2)^n |A|^{2n} \quad \text{and} \\ \omega_\pi - \omega_{\pi,0} &\simeq -\frac{\phi_2}{\omega_{\pi,0}} [1 - \cos(q - \pi)] + \frac{\gamma_{\pi,n}}{2\omega_{\pi,0}} (2\omega_{\pi,0}^2)^n |A|^{2n}. \end{aligned} \tag{88}$$

As explained in [33–35], we can now use the dispersion relations above to find the equations governing the envelope of the slowly varying amplitude A . This merely amounts to replacing $(\omega_k - \omega_{k,0})$ by $i\partial_t$, $(q - k)$ by $i\partial_l$ (with $k = 0, \pi$), A by the slowly varying amplitude A_l and finally to let it act on the amplitude A_l . We then obtain,

$$i\partial_t A_l = -\frac{\phi_2}{2\omega_{0,0}} (A_{l+1} + A_{l-1} - 2A_l) + \frac{\gamma_{0,n}}{2\omega_{0,0}} (2\omega_{0,0}^2)^n |A_l|^{2n} A_l \quad (\text{in-phase}) \tag{89}$$

$$i\partial_t A_l = \frac{\phi_2}{2\omega_{\pi,0}} (A_{l+1} + A_{l-1} - 2A_l) + \frac{\gamma_{\pi,n}}{2\omega_{\pi,0}} (2\omega_{\pi,0}^2)^n |A_l|^{2n} A_l \quad (\text{out-of-phase}) \tag{90}$$

Several remarks are in order at this stage. First, the above derivation is not rigorous. Nevertheless, it makes the role of isochronism through the nonlinear dispersion relation transparent and allows us to derive the DNLS equations for the modulation of the BEMs very easily. Second, we remark that for non isochronous potentials ($n = 1$), (89) is exactly the Eq. (6) derived by Kivshar in [40] (see also [41], Eq. (5) or [42], Eq. (19)). In this respect, (89) and (90) are generalisations to higher order of isochronism. We would like to mention as well that, for $n = 1$, (89) and (90) have been obtained by a rigorous multiple-scale expansion in [39] (up to the fact that the discrete spatial derivative is replaced by a continuous one).

Eqs. (89) and (90) provide now a physical motivation for studying DNLS with higher order nonlinearities. Indeed, the nonlinear exponent is shown to be directly related to the isochronism of the BEM under consideration. We notice finally that, (89) and (90) describe both the BEMs and their modulations and that, for this reason they make it possible to study the bifurcation process which leads from the plane wave to a breather (within the degree of approximation inherent to their derivation).

5.2.2. Rederivation of discrete breather energy thresholds

Now, the condition for the stability of a plane wave for the cubic DNLS equation on a periodic lattice has been derived by Carr and Eilbeck in [43]. Studying an equation of the type $i\dot{A}_l + \chi(A_{l+1} + A_{l-1} - 2A_l) + \lambda|A_l|^2 A_l$, with $A_{l+N} = A_l$, N being the number of lattice sites and $\mathcal{N} = \sum_l |A_l|^2 = 1$, these authors show that the plane wave $A_l = e^{i\omega t} A$ is stable if and only if $\lambda \leq 2N\chi \sin^2(\pi/N)$. The generalisation of this result to arbitrary nonlinearity ($\lambda|A_l|^{2n} A_l$) and norm \mathcal{N} is straightforward and reads

$$\frac{\mathcal{N}}{N} \leq \left[\frac{2\chi}{n\lambda} \sin^2\left(\frac{\pi}{N}\right) \right]^{1/n}. \quad (91)$$

For a plane wave $\mathcal{N}/N = |A|^2$ and according to the mode q under consideration, the amplitude and the energy density are related via $\varepsilon_q = 2\omega_{q,0}^2 |A_q|^2$. Moreover, in (89) and (90), the ratio of the coupling χ_q and the nonlinear parameter λ_q is $\chi_q/\lambda_q = \pm\phi_2/(2\omega_{q,0}^2)^n \gamma_{q,n}$, “+” for $q = \pi$ and “-” for $q = 0$. Then, eventually, we find the energies at which the in-phase and out-of-phase modes become respectively unstable

$$\varepsilon_0^{(n)} = \left(\frac{-2\phi_2 \sin^2(\pi/N)}{n\gamma_{0,n}} \right)^{1/n}, \quad \text{and} \quad \varepsilon_\pi^{(n)} = \left(\frac{2\phi_2 \sin^2(\pi/N)}{n\gamma_{\pi,n}} \right)^{1/n}, \quad (92)$$

which are precisely the expressions obtained in the previous sections. Notice that, these energies exist provided $\gamma_{0,n} < 0$ and $\gamma_{\pi,n} > 0$ respectively. At the level of (89) and (90), these conditions imply $\chi_q \lambda_q > 0$, ($q = 0, \pi$), which is precisely the condition for these equations to support bright type breathers.

Our concluding remark is that, for nonlinearities higher than the usual cubic one, the DNLS equation is known to possess energy thresholds for discrete breathers (see for example [44,16,15,45]). This allows us to corroborate our previous prediction that discrete breathers stemming from the tangent bifurcation of partially isochronous band edge modes appear above certain energy thresholds only. Eqs. (89) and (90) should provide a way to estimate them.

6. Conclusions

In this paper we have shown that, in network of coupled oscillators described by Hamiltonian (1), the way band edge modes (BEMs) possibly undergo a tangent bifurcation crucially relies on the low-energy behaviour of their frequency. This behaviour is obtained by expanding the frequency as a power series in the energy (see (83)) as explained in Section 2.2.2 and in Appendix A for the in-phase mode or in Section 2.3.2 for the out-of-phase mode.

The energy at which such modes may bifurcate tangently is given in (52) for an in-phase mode and in (74) for an out-of-phase mode. In these expressions, n is the degree of isochronism of the mode under consideration and $\gamma_{q,n}$, the first nonzero nonlinear coefficient of the low-energy expansion of the frequency as defined in (83).

As proved in Sections 4.2.7 and 4.3.6, purely isochronous modes (i.e. with an energy-independent frequency) never undergo a tangent bifurcation. This result is *non perturbative*. Now, in a network of coupled isochronous *onsite* potentials, the in-phase mode is isochronous and never bifurcates tangently according to the previous theorem. But the out-of-phase mode, which is generically non isochronous, may bifurcate as soon as the nonlinearity of the *interaction* potential is strong enough as expressed in (78).

Bifurcation energies obtained in (52) and (74) are used in Section 5.1 to derive a condition for the occurrence of energy thresholds for discrete breathers bifurcating tangently from BEMs. For modes isochronous up to order n and in dimension d , this reads $nd \geq 2$. For analytic potentials (n positive integer) energy thresholds exist whenever $n \geq 2$ (even in 1D) or when $d \geq 2$. For non-analytic potentials, n becomes a positive real number which opens up the possibility of absence of energy threshold even in 2- or 3D.

In Section 5.2.1, we derived two DNLS equations respectively related to the slow modulations of small-amplitude partially isochronous in-phase (Eq. (89)) and out-of-phase (Eq. (90)) modes. These equations are the generalisation to higher degree of isochronism of the usual cubic DNLS equation. Their nonlinearity is proportional to the degree of isochronism of the corresponding mode.³ As shown in Section 5.2.2, they allow for an easy rederivation of the bifurcation energies (52) and (74).

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Appendix A. Energy expansion for the period in a 1D potential

We derive in this appendix a simple method to compute the period of oscillation around the minimum of a potential $V(x)$ as a power series in the energy E . This method is, to our opinion, simpler than other methods which have been developed earlier [18,19]. It yields the coefficients of this power series in terms of the coefficients of the Taylor expansion of $V(x)$ around its minimum. This is used to construct a potential partially isochronous up to order n , which merely amounts to canceling out all the coefficients of the power series in E up to order $n - 1$.

We assume that $V(x)$ has the following properties: $V(0) = 0$, $V'(0) = 0$, $V''(0) = \omega^2 \neq 0$. Moreover, we require that $V'(x)/x > 0$ on an interval I centered around the minimum. In this interval, $V(x)$ can be expanded as a power series in x around 0,

$$V(x) = \frac{1}{2}\omega^2 x^2 + \omega^2 \sum_{n=3}^{\infty} \frac{1}{n} \alpha_{n-1} x^n. \tag{A.1}$$

At a given energy E , the period T is given by

$$T(E) = \sqrt{2} \int_{x_-(E)}^{x_+(E)} \frac{dx}{\sqrt{E - V(x)}} \tag{A.2}$$

where $x_{\pm}(E)$ are the two solutions of $V(x) = E$, ($x_+(E) > 0$ and $x_-(E) < 0$). Let us make a change of variable defined by $V(x) = (1/2)\omega^2 X^2$, with $dX(x)/dx > 0$ for $x \in I$. The last condition ensures that X is a monotonic increasing function of x . Then (A.2) yields,

$$T(E) = \sqrt{2} \int_0^{\sqrt{2E}/\omega} \frac{\Delta'(X)}{\sqrt{E - (1/2)\omega^2 X^2}} dX = \frac{2}{\omega} \int_0^1 \Delta' \left(\frac{\sqrt{2E}}{\omega} u \right) \frac{du}{\sqrt{1 - u^2}} \tag{A.3}$$

³ Note that the in- and out-of-phase degrees are independent of each other. For a given system, Eqs. (89) and (90) will then generally have different nonlinearities.

where $\Delta(X) = x(X) - x(-X)$ with $dx(X)/dX > 0$. Δ' represents the derivative with respect to X . In order to compute the last expression of $T(E)$, we need to invert the change of variable. Taking into account the condition $dx(X)/dX > 0$, we obtain

$$V(x) = \frac{1}{2}\omega^2 X^2 \Rightarrow x(X) = X + \sum_{n=2}^{\infty} \sigma_n X^n \quad (\text{A.4})$$

where the coefficients σ_n are functions of the α_m . Hence

$$\Delta'(X) = 2 \left(1 + \sum_{n=1}^{\infty} (2n+1) \sigma_{2n+1} X^{2n} \right). \quad (\text{A.5})$$

Reinstating this expression into (A.3) and performing a term by term integration over u , we finally get

$$T(E) = \frac{2\pi}{\omega} \left[1 + \sum_{n=1}^{\infty} \sigma_{2n+1} \frac{(2n+1)!!}{(2n)!!} \left(\frac{2E}{\omega^2} \right)^n \right] \quad (\text{A.6})$$

The inversion (A.4) is easily done with the help of any software able to perform formal calculations. Using Maple [20], we have computed the few first odd coefficients σ_{2n+1} :

$$\begin{aligned} \sigma_3 &= \frac{5}{18}\alpha_2^2 - \frac{1}{4}\alpha_3 \\ \sigma_5 &= \frac{77}{216}\alpha_2^4 - \frac{7}{8}\alpha_3\alpha_2^2 + \frac{7}{15}\alpha_4\alpha_2 + \frac{7}{32}\alpha_3^2 - \frac{1}{6}\alpha_5 \\ \sigma_7 &= \frac{3}{7}\alpha_6\alpha_2 - \frac{33}{20}\alpha_4\alpha_3\alpha_2 + \frac{143}{90}\alpha_4\alpha_2^3 + \frac{9}{50}\alpha_4^2 - \frac{715}{288}\alpha_2^4\alpha_3 + \frac{143}{64}\alpha_3^2\alpha_2^2 - \frac{11}{12}\alpha_5\alpha_2^2 + \frac{3}{8}\alpha_3\alpha_5 \\ &\quad + \frac{2431}{3888}\alpha_2^6 - \frac{33}{128}\alpha_3^3 - \frac{1}{8}\alpha_7 \end{aligned}$$

To construct a potential partially isochronous up to order n we need to zero the coefficients σ_{2k+1} up to σ_{2n-1} . This constrains the coefficients α_k to verify certain relations given below⁴:

$$\begin{aligned} \text{Order } n = 2; \quad \alpha_3 &= \frac{10}{9}\alpha_2^2 \\ \text{Order } n = 3; \quad \alpha_5 &= -\frac{56}{27}\alpha_2^4 + \frac{14}{5}\alpha_4\alpha_2 \\ \text{Order } n = 4; \quad \alpha_7 &= \frac{24}{7}\alpha_6\alpha_2 - \frac{592}{45}\alpha_4\alpha_2^3 + \frac{36}{25}\alpha_4^2 + \frac{848}{81}\alpha_2^6 \end{aligned}$$

Appendix B. Solvability condition for system (59)

We prove hereafter that, up to order $2n$ in the amplitude y , system (59) never develops any secular term.

⁴ It is intended that, at order n , all previous relations hold. For example for $n = 4$, α_3 , α_5 and α_7 are given by the relations above.

- Up to order y^{2n} , we have shown in Section 4.3.3 that the real parts r_π and r_0 of the two modes $\eta_{\pi-2\pi/N}$ and $\eta_{2\pi/N}$ obey the system

$$\begin{cases} \ddot{r}_\pi + \mathcal{T}_1(0, \tau)r_\pi + \mathcal{T}_2(\tau)r_0 = 0, \\ \ddot{r}_0 + \mathcal{T}_4(0, \tau)r_0 + \mathcal{T}_2(\tau)r_\pi = 0. \end{cases} \tag{B.1}$$

The functions $\mathcal{T}_i(\tau)$ are 2π -periodic.

- Up to the same order, the two periodic solutions of this system are given by

$$\begin{pmatrix} r_\pi^{(s)} \\ r_0^{(s)} \end{pmatrix} = \begin{pmatrix} \frac{\partial Q_\pi}{\partial y} \\ \frac{\partial Q_0}{\partial y} \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} r_\pi^{(a)} \\ r_0^{(a)} \end{pmatrix} = \begin{pmatrix} \frac{1}{y} \frac{\partial Q_\pi}{\partial \tau} \\ \frac{1}{y} \frac{\partial Q_0}{\partial \tau} \end{pmatrix} \tag{B.2}$$

The first solution is time-symmetric ((s)) whereas the second is time-antisymmetric ((a)).

- From order 0 to n we can take the imaginary parts j_π and j_0 of the modes equal to 0. From $(n + 1)$ to $2n$ they obey,

$$\begin{cases} \ddot{j}_\pi + \mathcal{T}_1(0, \tau)j_\pi + \mathcal{T}_2(\tau)j_0 + \mathcal{T}_3(\delta, \tau)r_0^{(s)} = 0, \\ \ddot{j}_0 + \mathcal{T}_4(0, \tau)j_0 + \mathcal{T}_2(\tau)j_\pi - \mathcal{T}_3(\delta, \tau)r_\pi^{(s)} = 0, \end{cases} \tag{B.3}$$

where \mathcal{T}_3 is time-periodic and time-symmetric (it is a function of Q_π which is time-symmetric itself).

- The problem is to prove that from $y^{(n+1)}$ to y^{2n} , (B.3) never develops secular terms. We will use the solvability condition below (see for example [46]).

Theorem 1 (Fredholm alternative). *Assume the subspace of T -periodic solutions of the homogeneous system*

$$\frac{d}{dt}|x\rangle = A(t)|x\rangle,$$

$A(t + T) = A(t)$, $A \in \text{Mat}(n \times n)$ is of dimension $k \geq 1$. Denote by $|\eta^{(l)}\rangle$, $l \in \{1, \dots, k\}$, k linearly independent T -periodic solutions of the adjoint system

$$\frac{d}{dt}|\eta\rangle = -A^\dagger(t)|\eta\rangle.$$

For $|f(t + T)\rangle = |f(t)\rangle$, the inhomogeneous system

$$\frac{d}{dt}|y\rangle = A(t)|y\rangle + |f(t)\rangle,$$

has T -periodic solutions if and only if

$$\int_0^T \langle \eta^{(l)} | f(t) \rangle dt = 0 \quad (l \in \{1, \dots, k\}). \tag{B.4}$$

- In our case, we rewrite (B.3) as a first order inhomogeneous system with $|y\rangle = \text{col}(r_\pi, r_0, p_\pi, p_0)$ (column vector) and $p_\pi = \dot{r}_\pi, p_0 = \dot{r}_0$. We have

$$A = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -\mathcal{T}_1 & -\mathcal{T}_2 & 0 & 0 \\ -\mathcal{T}_2 & -\mathcal{T}_4 & 0 & 0 \end{pmatrix} \quad \text{and} \quad |f\rangle = \begin{pmatrix} 0 \\ 0 \\ -\mathcal{T}_3 r_0^{(s)} \\ \mathcal{T}_3 r_\pi^{(s)} \end{pmatrix} \quad (\text{B.5})$$

The corresponding homogeneous adjoint system is

$$\frac{d}{dt} |\eta\rangle = -A^\dagger(t) |\eta\rangle \Leftrightarrow \frac{d}{dt} \begin{pmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \\ \eta_4 \end{pmatrix} = \begin{pmatrix} 0 & 0 & \mathcal{T}_1 & \mathcal{T}_2 \\ 0 & 0 & \mathcal{T}_2 & \mathcal{T}_4 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} \begin{pmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \\ \eta_4 \end{pmatrix} \quad (\text{B.6})$$

Its solutions are

$$\begin{pmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \\ \eta_4 \end{pmatrix}^{(s),(a)} = \begin{pmatrix} -p_\pi \\ -p_0 \\ r_\pi \\ r_0 \end{pmatrix}^{(s),(a)} \quad (\text{B.7})$$

- Calculating the two solvability conditions (B.4), we get

$$\int_0^{2\pi} \langle \eta^{(s)} | f \rangle dt = \int_0^{2\pi} \mathcal{T}_3 (-r_\pi^{(s)} r_0^{(s)} + r_0^{(s)} r_\pi^{(s)}) d\tau = 0 \quad (\text{B.8})$$

and

$$\int_0^{2\pi} \langle \eta^{(a)} | f \rangle dt = \int_0^{2\pi} \mathcal{T}_3 (-r_\pi^{(a)} r_0^{(s)} + r_0^{(a)} r_\pi^{(s)}) d\tau = 0 \quad (\text{B.9})$$

Indeed, to compute this last expression, we remember that \mathcal{T}_3 is time-symmetric (series of cosine terms). The term in parenthesis being time-antisymmetric, the integrand is time-antisymmetric. Because it is 2π -periodic, the integral is zero.

- Conclusion: The solvability conditions are fulfilled and consequently (B.3) does not develop any secular terms up to order $2n$. The way we have obtained the critical energy for the tangent bifurcation is thus correct.

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