A FORMAL APPROXIMATION OF THE SPLITTING OF SEPARATRICES IN THE CLASSICAL ARNOLD'S EXAMPLE OF DIFFUSION WITH TWO EQUAL PARAMETERS

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Abstract

We consider the classical Arnold's example of diffusion with two equal parameters. Such system has two dimensional normally hyperbolic invariant tori. We focus on the torus whose ratio of frequencies is the golden mean. We present formal approximations of the three dimensional invariant manifolds associated to this torus and numerical globalization of these manifolds. This allows to obtain the splitting (of separatrices) vector and to compute its Fourier components. It is apparent that the Melnikov vector provides the dominant order of the splitting provided it is computed after a suitable number of averaging steps. We carry out the first order analysis of the splitting based on that approach, mainly looking for bifurcations of the zero level curves of the components of the splitting vector and of the homoclinic points.

Contents

1 Introduction and statement of results

In this paper we study the following Hamiltonian:

$$H(x,I_2,I_3,y,\theta_2,\theta_3)=\frac{1}{2}\left(x^2+I_2^2\right)+I_3+\varepsilon(\cos y-1)\left(1+\mu(\cos\theta_2+\cos\theta_3)\right) \tag{1}$$

In an equivalent form, this system was introduced by Arnold [1] to illustrate the transition chain mechanism, called Arnold's diffusion. This is a classical example which displays a (very slow) drift of the actions for any value of ε, provided μ is small enough. Nowadays Arnold's diffusion is one of the outstanding topics in Hamiltonian dynamics.

Present model (1) has two difficulties to be considered as a typical example of diffusion.

On one hand, how small must be the dependence of μ with respect to ε. In particular, when Arnold tried to illustrate Arnold's diffusion, he used the Poincaré–Melnikov integrals to measure the splitting. The integrals turned out to be exponentially small with respect to ε. If μ and ε are regarded as independent, it gives a valid measure of the splitting, provided μ is small enough for a fixed value of ε. However, if μ is regarded as a function of ε, Melnikov integrals are only a valid measure of the distance provided μ is exponentially small with respect to ε. This is a consequence of a naive use of Melnikov formula to measure the splitting of separatrices.

On the other hand, it has a strong degeneracy because all the "normally" hyperbolic tori which appear for $\mu=0$, subsist when introducing the perturbation. This paper deals with the first difficulty. To this end the two parameters are taken as equal, but μ could also be a power of ε. This is done in order to study more realistic models, since many physical problems are described with only one perturbative parameter or, in case they contain several parameters, there is no reason why one of them should be exponentially small with respect to another one. From now on, and for scaling purposes, we set $\mu=\varepsilon=\eta^2$.

The manifold $\mathbb{T}_\beta$, given by $x=y=0$, $I_2=\beta$, $I_3=0$, is an invariant three-dimensional whiskered torus for any value of β. Our purpose is to show that, under a suitable diophantine condition on β, the separatrices of these tori have a transversal intersection and to have quantitative information on the splitting.

We note that the Melnikov function is not invariant with respect to canonical changes of variables. After a change of variables, for instance after a step of a classical averaging procedure, a lot of non-zero harmonics, which were not present in the original system, can appear. So, the key idea of this paper is to do, for a given value of η, some steps of a normal form procedure *before applying Melnikov method.* The goal, then, is to capture a given harmonic of the splitting. For the ones having larger amplitude the number of steps is constant for η on some interval, but when η goes to zero it increases and tends to infinity. In this way the *most relevant resonances* for this range of values of η are put in evidence. The dominant terms in the splitting are, of course, related to the approximants of β. This result is not trivial since the Melnikov function is exponentially small with respect to η. So, we introduce what can be named as *adapted Melnikov method.*

The Hamilton's canonical equations are:

$$\begin{aligned}
\dot y &= \frac{\partial H}{\partial x}=x, & \dot x &= -\frac{\partial H}{\partial y}=\eta^2\sin y\left(1+\eta^2(\cos\theta_2+\cos\theta_3)\right),\\
\dot\theta_2 &= \frac{\partial H}{\partial I_2}=I_2, & \dot I_2 &= -\frac{\partial H}{\partial \theta_2}=\eta^4\sin\theta_2(\cos y-1),\\
\dot\theta_3 &= \frac{\partial H}{\partial I_3}=1, & \dot I_3 &= -\frac{\partial H}{\partial \theta_3}=\eta^4\sin\theta_3(\cos y-1).
\end{aligned} \tag{2}$$

The action I_3 has only been used to put the Hamiltonian in autonomous form but it is not relevant from a dynamical point of view.

The Hamiltonian (1) can be considered as a perturbation of a pendulum cross a rotor

$$H_0 = \frac{x^2}{2} + \eta^2 (\cos y - 1) + \frac{I_2^2}{2} + I_3.$$

Note that the unperturbed problem is obtained from (2) by retaining the η^2 terms and dropping the η^4 ones.

The unperturbed system has an invariant two dimensional whiskered torus located at $x = y = I_3 = 0$, $I_2 = \beta$, the whiskers being three-dimensional. For most of the paper β will be taken as the golden mean number ($\beta = (\sqrt{5}-1)/2$). These invariant manifolds are the upper separatrix of the pendulum cross a two dimensional torus with frequencies $\omega = (\beta, 1)$. We recall that the upper separatrix of the pendulum, corresponding to the Hamiltonian function $x_0^2/2 + \cos y_0 - 1$, with $y(0) = \pi$, is given by

$$y_0(t) = 4\arctan(e^t) = \pi - 4\arctan(\tanh(t/2)), \quad x_0(t) = \dot{y}_0(t).$$

We will consider intersections of the whiskers with the Poincaré section $y = \pi$.

As we have pointed out before, the complete system (1) with $\mu = \varepsilon$ has a whiskered torus $\mathbb{T}_\beta$. The whiskers are three dimensional, being close to the ones of the unperturbed pendulum cross a rotor.

Since for the unperturbed problem I_2 and I_3 are integrals of motion, their values on this intersection coincide if $\mu = 0$. This is no longer true in the perturbed case and the differences of the values of these functions, on the mentioned section, can be used to measure how these manifolds break up under the perturbation.

Consider an orbit on the unstable whisker of $\mathbb{T}_\beta$ for the perturbed problem. For $t \to -\infty$ one has $y(t) \to 0$. Assume that the initial conditions (for $t = 0$) are taken with $y \in (0, \pi)$. The first intersection (i.e., the first with $t > 0$) of the orbit through $y = \pi$ takes place at some point $(y = \pi, x = x^u, \theta_2 = \psi_2, I_2 = I_2^u, \theta_3 = \psi_3, I_3 = I_3^u)$. A similar point is obtained for the stable whiskers, starting at some $y \in (\pi, 2\pi)$ and going back on time obtaining x^s, I_2^s, I_3^s. Those final points in both the unstable and stable case will be seen as a function of the corresponding angle (ψ_2, ψ_3), to be denoted as $\hat{\psi}$ for shortness.

The splitting vector is defined as

$$\begin{array}{rcll}
\Delta(\beta, \hat{\psi}, \eta) & = & (\Delta_1, \Delta_2, \Delta_3)(\beta, \hat{\psi}, \eta), & \text{with} \\
\Delta_1(\beta, \hat{\psi}, \eta) & = & x^u(\beta, \hat{\psi}, \eta) - x^s i(\beta, \hat{\psi}, \eta), & \text{and} \\
\Delta_j(\beta, \hat{\psi}, \eta) & = & I_j^u(\beta, \hat{\psi}, \eta) - I_j^s(\beta, \hat{\psi}, \eta), & \text{for } j = 2, 3\,.
\end{array}$$

It is enough to measure the splitting using two of those components because of the energy conservation. And, in fact, it is enough to compute a single function, due to the existence of a splitting potential, but we shall compute Δ_1 and Δ_2, independently, as additional check.

From now on, we restrict ourselves to Δ_1 and Δ_2. Together they are denoted again as Δ. As all the computations in this paper are done for a fixed value of β, the dependence of Δ on β will be skipped.

One of the first goals of this work is to numerically compute the value of the splitting vector as a function of $\hat{\psi}$ and η, and to show that the *adapted Melnikov method* gives a good first approximation. This will provide insight on the splitting relevant terms, their evolution and bifurcations.

To measure the transversality, or the angle between both invariant manifolds, it is also usual to compute the quantity

$$\Upsilon = \left|\det \partial_{\hat{\psi}} \Delta\right|,$$

evaluated at the homoclinic points, i.e., points for which $\Delta(\hat{\psi}, \eta) = 0$.

In order to numerically compute such splitting vector, approximations of the invariant stable and unstable manifolds $W^s_{\mathbb{T}^2}$ and $W^U_{\mathbb{T}^2}$ are obtained in section 2. Here $\mathbb{T}^2 = \mathbb{T}_\beta$. The algorithm to obtain such approximations is given in detail and effective computations have been implemented and carried out. In section 2, we show how to globalize $W^u_{\mathbb{T}^2}$ starting at points given by the previous approximation and integrating (2) numerically by means of a power series method. This is done until the points reach $\{y = \pi\}$ for the first time. The intersection of $W^s_{\mathbb{T}^2}$ with $\{y = \pi\}$ is obtained by symmetry because (1) is even in θ_2 and θ_3. Two tori are obtained as "that intersections". They can be described by giving the values of x as a function of the angles, $\hat{\psi}$, and I_2 as a function of the same angles as explained before. Let $x_{W^{u,s}_{\mathbb{T}^2} \bigcap \{y=\pi\}} = m^{u,s}(\hat{\psi}, \eta)$, $I_{2, W^{u,s}_{\mathbb{T}^2} \bigcap \{y=\pi\}} = n^{u,s}(\hat{\psi}, \eta)$. A convenient measure of the splitting is given by

$$\Delta(\hat{\psi}, \eta) = (d_1(\hat{\psi}, \eta), d_2(\hat{\psi}, \eta)), \tag{3}$$

where each $d_1(\hat{\psi}, \eta)$ and $d_2(\hat{\psi}, \eta)$ are given by

$$\begin{aligned} d_1(\hat{\psi}, \eta) &= m^u(\hat{\psi}, \eta) - m^s(\hat{\psi}, \eta), \\ d_2(\hat{\psi}, \eta) &= n^u(\hat{\psi}, \eta) - n^s(\hat{\psi}, \eta). \end{aligned} \tag{4}$$

Note that the functions $m^{u,s}$, $n^{u,s}$, d_1, d_2 are nothing else than the *numerical* approximations of the previously defined functions $x^{u,s}$, $I_2^{u,s}$, Δ_1 and Δ_2.

The functions (4) have been numerically computed for several values of η and a selected set of results has been displayed.

In section 3 we symbolically carry out some steps of an averaging procedure in order to compute the Melnikov vector, just to check if it agrees with the computed values of the splitting vector.

A result in [6] shows that if one considers the system of differential equations given by $\dot{z} = f(z, \theta, \eta)$, $z \in \Omega \subset \mathbb{C}^n$, being $\Omega = D + \delta$ a δ-neighbourhood of D in $\mathbb{C}^n$, D a compact set in $\mathbb{R}^n$ and $\theta \in \mathbb{T}^p + \delta$, $p \geq 2$, and one assumes that $|\hat{k} \cdot \omega| \geq b|\hat{k}|^{-\tau}$, where $b > 0$, $\tau > p - 1$ and $|\hat{k}| = \sum_{k=1}^p |k_i|$, then, if η_0 is small enough, for a fixed η with $|\eta| \leq \eta_0$, there exists a change of variables $z = h(w, \theta, \eta)$, analytic in (w, θ) for $w \in D + \delta/2$, $\theta \in \mathbb{T}^p + \delta/2$, such that the new equation is $\dot{w} = \eta\,(g(w, \eta) + r(w, \theta, \eta))$ and the remainder satisfies an exponentially small bound

$$|r|_{\delta/2} < c_1 \exp\left(-c_2/\eta^{c_3}\right), \tag{5}$$

where c_1, $c_2 > 0$ and $c_3 = \frac{1}{\tau+1}$. The constants depend on $|f|_\delta$, on the dimensions and on the constants appearing in the diophantine condition. If $\tau = p - 1$, then one has to change the bound by replacing c_2 by a multiple of $|\ln \eta|^{-1/p}$. Using this result, we will give, in section 3, an upper bound of the splitting of separatrices. The role of the fact that H_0 and H are entire, and not only analytic, as is happens in the present case, will be also stressed.

In section 4 we formally compute the Melnikov vector, after a suitable number of steps of averaging. The final result of the computation is given explicitly only for a few harmonics, in order to show the mechanism.

In section 5 we carry out a "first order" analysis of the splitting. Melnikov's computation gives a theoretical value for the vector (d_1, d_2) described before. We do not claim that this approximation is rigorously justified, but the results are in good agreement with the numerical ones.

Assuming that the Melnikov approach gives a good approximation to the splitting, we analyze the vector (3) in the case of small values of η. The splitting is given by an infinite sum, each term in $d_1(\hat{\psi}, \eta)$ and $d_2(\hat{\psi}, \eta)$, being essentially of the form:

$$A_{\hat{k}} \exp\left(-2|\hat{k}||\ln\eta| - \frac{\pi|\hat{k}\cdot\omega|}{2\eta} + 2|\hat{k}|\ln\frac{|\hat{k}\cdot\omega|}{|\hat{k}|}\right)\sin(\hat{k}\cdot\hat{\psi}), \quad \hat{k}\in\mathbb{Z}^2, \tag{6}$$

where $\omega = (\beta, 1)$. The coefficients $A_{\hat{k}}$ depend on $\hat{k}$, and they take into account the combinatorics of the interactions of the initial harmonics. However, if for some positive constant M, the coefficients $|A_{\hat{k}}|$ never grow (respectively, decrease) faster than $\exp\left(M|\hat{k}|\right)$ (respectively, $\exp\left(-M|\hat{k}|\right)$), as $|\hat{k}|\to\infty$, then we can state the main theorem, which assures that there are at most two terms in the Fourier series for the splitting distance given by (6), which will account for its leading–order behaviour.

Theorem 1.1 *Let*

$$\mathcal{N}(\hat{\psi}, \eta) = \sum_{\hat{k}\in\mathbb{Z}^2\setminus\{0\}} A_{\hat{k}} \exp\left(-2|\hat{k}||\ln\eta| - \frac{\pi|\hat{k}\cdot\omega|}{2\eta} + 2|\hat{k}|\ln\frac{|\hat{k}\cdot\omega|}{|\hat{k}|}\right)\sin(\hat{k}\cdot\hat{\psi})$$

and

$$|\mathcal{N}(\eta)| = \max_{\hat{\psi}\in\mathbb{T}^2}|\mathcal{N}(\hat{\psi},\eta)|.$$

If β is the golden mean number and for some positive constant M, the coefficients $|A_{\hat{k}}|$ are such that they never grow (respectively, decrease) faster than $\exp\left(M|\hat{k}|\right)$ (respectively, $\exp\left(-M|\hat{k}|\right)$), as $|\hat{k}|\to\infty$, then, for η small enough,

$$\begin{aligned}
\mathcal{N}(\hat{\psi},\eta) &= \sum_{\hat{k}\in\{\hat{k}^*,\hat{k}^{**}\}} A_{\hat{k}} \exp\left(-2|\hat{k}||\ln\eta| - \frac{\pi|\hat{k}\cdot\omega|}{2\eta} + 2|\hat{k}|\ln\frac{|\hat{k}\cdot\omega|}{|\hat{k}|}\right) \\
&\qquad \times\left(\sin(\hat{k}\cdot\hat{\psi}) + \mathrm{O}\left(\exp\left(-g_1\frac{|\ln\eta|^{1/2}}{\eta^{1/2}}\right)\right)\right), \\
|\mathcal{N}(\hat{\psi},\eta)| &\le \exp\left(-g_2(\eta)\frac{|\ln\eta|^{1/2}}{\eta^{1/2}}\right), \\
|\mathcal{N}(\eta)| &\ge \exp\left(-\underline{g}_2(\eta)\frac{|\ln\eta|^{1/2}}{\eta^{1/2}}\right),
\end{aligned}$$

where $\hat{k}^* = (F_n, -F_{n-1})$, and $\hat{k}^{**} = (F_{n+1}, -F_n)$, being F_{n-1}, F_n and F_{n+1} consecutive Fibonacci numbers. The index n increases as η goes to 0, g_1 is a positive constant and $g_2, \underline{g}_2$ are functions of η, bounded from above and below by positive numbers.

The proof that, under the assumptions made on $|A_{\hat{k}}|$, the function $\mathcal{N}(\hat{\psi},\eta)$ with the above properties, gives the right estimate of the splitting can be found in [7].

The dependence of n, g_2 and $\underline{g}_2$ in η, will be described in section 5. We want to note that the above bound is in perfect agreement with the modification of (5), when $\tau = 1$. Also at this point we remark why it is natural to make the assumption on the behaviour of $A_{\hat{k}}$ and that the fact that the Hamiltonian is entire and the choice we made $\varepsilon = \mu = \eta^2$, produce a splitting which is much less than the one we would find for a generic analytical Hamiltonian. Some comments on the behaviour of $\mathcal{N}(\hat{\psi}, \eta)$ when β is taken as a quadratic irrational, as well as a natural conjecture about the behaviour for β of constant type, follow after the proof of the Theorem.

Concerning the splitting determinant, Υ, the given expression of $\mathcal{N}(\hat{\psi}, \eta)$ will be enough to decide that it is different from zero (under the assumptions of the Theorem), provided the two dominant terms are not too different. The discussion is also given in section 5.

Section 6 is devoted to the set of points in $W^u_{\mathbb{T}^2} \bigcap \{y = \pi\}$ or $W^s_{\mathbb{T}^2} \bigcap \{y = \pi\}$ giving rise to either $d_1(\hat{\psi}, \eta) = 0$ or $d_2(\hat{\psi}, \eta) = 0$. These are curves in a two-torus. The topology of the curves changes when η does. This is a very natural phenomenon. Indeed, when η goes to zero, the "pendulum part" of the motion is almost "frozen", and if a point belongs to $W^u_{\mathbb{T}^2} \bigcap \{y = \pi\}$, say, its orbit under the flow must be very close to such curve. But the (θ_2, θ_3) components of the orbit are close to the line with slope β^{-1}, so the curves must tend to this line. This forces the topological changes. The behaviour of the set of bifurcations is described. Let η_k, $k \in \mathbb{N}$, $\eta_1 > \eta_2 > \ldots$, the set of values for which a bifurcation is produced. Then $\lim_{k\to\infty} \eta_k/\eta_{k+1} = \beta^{-2}$. The curves close after n_1 revolutions in the ψ_2 direction, and n_2 in the ψ_3 direction. The successive values of the pairs (n_1, n_2) are given by two successive Fibonacci numbers (F_j, F_{j+1}), where we use the convention $F_0 = 0$, $F_1 = 1$, and $F_j = F_{j-1} + F_{j-2}$ for $j \geq 2$.

When there are two subdominant Fourier harmonics of comparable size (and then they are small compared to the dominant one), besides the homoclinic points $(0,0)$, $(0,\pi)$, $(\pi,0)$, (π,π), which are always present by symmetry, additional homoclinic points can appear. Also the splitting determinant is zero at some of these points for a sequence of values of η tending to zero. The related analysis closes section 6.

Several technicalities, mainly concerning the relation between indices of terms in the normal form, can be found in [7]. This paper contains also the complete proof that the terms dominating the splitting are indeed the ones found in the present paper, under the same assumption on the behaviour of the coefficients $A_{\hat{k}}$. Concerning the geometrical and dynamical consequences, we refer to [4] where, based on the results of the splitting, a kind of "return map" (a *generalized separatrix map*) is obtained. It allows to prove the existence of different kinds of orbits and, in particular, the existence of some diffusion to a local level: the variations of the action variables are of the order of a power (with exponent less than 1) of the perturbing parameter, that is, until a second resonance of low enough order is found.

2 Symbolic and numerical computations of the splitting

To obtain approximations of the invariant manifolds of the invariant torus $\mathbb{T}_\beta$, we will proceed, formally, in a direct way. We do not claim that the method proposed here is convergent. But it is, at least, enough to produce local approximations with error exponentially small in η.

We start directly with the two and a half degrees of freedom Hamiltonian given by (1). We introduce a non-symplectic change of variables

$$J_1 = \frac{x}{\eta}, \quad J_2 = \frac{I_2 - \beta}{\eta},$$

such that, in the new variables the equations of motion are still Hamiltonian and have the form

$$\dot{y}=\eta J_1, \quad \dot{\theta}_2=\beta+\eta J_2, \quad \dot{J}_1=\eta\sin y(1+\eta^2(\cos\theta_2+\cos\theta_3)), \quad \dot{J}_2=\eta^3(\cos y-1)\sin\theta_2. \tag{7}$$

As we have seen, when ε is not zero and μ is equal to zero, the manifold $\mathbb{T}_\beta$, defined by the equations $x=y=0$, $I_2=\beta$, is a two-dimensional whiskered torus of the unperturbed system, the whiskers being three-dimensional and having the representation

$$J_2=0, \quad J_1=2\sin\left(\frac{y}{2}\right).$$

In the perturbed system with $\mu=\varepsilon=\eta^2$, we search for the invariant manifolds (unstable and stable) writing J_1, J_2 as a power series in $(\eta,\, y)$ and Fourier series in $(\theta_2,\, \theta_3)$. Note that other representations are possible. Let us introduce $z_2=\exp(i\theta_2)$ and $z_3=\exp(i\theta_3)$. Then

$$\begin{aligned} J_1 &= 2\sin\left(\frac{y}{2}\right)+\sum_{k\geq 1} a_k(y,z_2,z_3)\eta^k = 2\sin\left(\frac{y}{2}\right)+\sum_{k,l\geq 1} a_{k,l}(z_2,z_3)\eta^k y^l \\ &= 2\sin\left(\frac{y}{2}\right)+\sum_{\substack{k,l\geq 1\\ j_2,j_3\in\mathbb{Z}}} a_{k,l,j_2,j_3}\eta^k y^l z_2^{j_2} z_3^{j_3}, \end{aligned} \tag{8}$$

$$\begin{aligned} J_2 &= \sum_{m\geq 1} b_m(y,z_2,z_3)\eta^m = \sum_{m,n\geq 1} b_{m,n}(z_2,z_3)\eta^m y^n \\ &= \sum_{\substack{m,n\geq 1\\ p_2,p_3\in\mathbb{Z}}} b_{m,n,p_2,p_3}\eta^m y^n z_2^{p_2} z_3^{p_3}, \end{aligned} \tag{9}$$

where a_{k,l,j_2,j_3} and b_{m,n,p_2,p_3} are complex coefficients.

The invariance of (8) and (9) under the flow of (7) gives (10) and (11), respectively:

$$\begin{aligned} \eta\sin y(1+\eta^2\frac{z_2+z_2^{-1}+z_3+z_3^{-1}}{2}) &= 2\eta\cos\left(\frac{y}{2}\right)\sin\left(\frac{y}{2}\right)+\sum_{\substack{k,l\geq 1\\ j_2,j_3\in\mathbb{Z}}} a_{k,l,j_2,j_3}\eta^{k+1}y^l\cos\left(\frac{y}{2}\right)z_2^{j_2}z_3^{j_3} \\ &+ \sum_{\substack{k,l\geq 1\\ j_2,j_3\in\mathbb{Z}}} 2l a_{k,l,j_2,j_3}\eta^{k+1}y^{l-1}\sin\left(\frac{y}{2}\right)z_2^{j_2}z_3^{j_3} \\ &+ \sum_{\substack{k,l\geq 1\\ j_2,j_3\in\mathbb{Z}}} i(j_2\beta+j_3)a_{k,l,j_2,j_3}\eta^k y^l z_2^{j_2}z_3^{j_3} \\ &+ \sum_{\substack{k+r,l+s\geq 1\\ j_2+q_2,j_3+q_3\in\mathbb{Z}}} l a_{k,l,j_2,j_3}a_{r,s,q_2,q_3}\eta^{k+1+r}y^{l+s-1}z_2^{j_2+q_2}z_3^{j_3+q_3} \\ &+ \sum_{\substack{k+r,l+s\geq 1\\ j_2+q_2,j_3+q_3\in\mathbb{Z}}} i j_2 a_{k,l,j_2,j_3}b_{r,s,q_2,q_3}\eta^{k+1+r}y^{l+s}z_2^{j_2+q_2}z_3^{j_3+q_3}, \end{aligned} \tag{10}$$

$$\begin{aligned} \eta^3(\cos y-1)\frac{z_2-z_2^{-1}}{2i} &= \sum_{\substack{m,n\geq 1\\ p_2,p_3\in\mathbb{Z}}} i(p_2\beta+p_3)b_{m,n,p_2,p_3}\eta^m y^n z_2^{p_2}z_3^{p_3} \\ &+ \sum_{\substack{m,n\geq 1\\ p_2,p_3\in\mathbb{Z}}} n b_{m,n,p_2,p_3}\eta^{m+1}y^{n-1}2\sin\left(\frac{y}{2}\right)z_2^{p_2}z_3^{p_3} \end{aligned}$$

$$
\begin{aligned}
&+ \sum_{\substack{m+r,n+s\geq 1\\ p_2+q_2,p_3+q_3\in\mathbb{Z}}} n b_{m,n,p_2,p_3} a_{r,s,q_2,q_3} \eta^{m+r+1} y^{n+s-1} z_2^{p_2+q_2} z_3^{p_3+q_3}\\
&+ \sum_{\substack{m+r,n+s\geq 1\\ p_2+q_2,p_3+q_3\in\mathbb{Z}}} i p_2 b_{m,n,p_2,p_3} b_{r,s,q_2,q_3} \eta^{m+r+1} y^{n+s} z_2^{p_2+q_2} z_3^{p_3+q_3}. \qquad (11)
\end{aligned}
$$

The symbolic computation of the invariant manifolds has been done by keeping η, y, z_2 and z_3 as symbols and using complex numerical coefficients, a_{k,l,j_2,j_3} and b_{m,n,p_2,p_3}, in FORTRAN quadruple precision.

By looking at the terms of degrees $0, 1$ and 2 in η we have that the coefficients a_{k,l,j_2,j_3} and b_{m,n,p_2,p_3} appearing in (8) and (9) are identically zero for $k \leq 2$ (or $m \leq 2$). Equating the terms in η^r for $r \geq 3$ and, among them, the terms in y^l for $l \geq 1$ in (10) and (11) we recurrently obtain the functions $a_{k,l}(z_2, z_3)$ and $b_{m,n}(z_2, z_3)$.

Furthermore, the functions $a_{k,l}(z_2, z_3)$ and $b_{m,n}(z_2, z_3)$ are polynomials in z_2, z_3, z_2^{-1} and z_3^{-1}. That is, the exponents j_2, j_3, p_2 and p_3 satisfy:

$$
|j_2| + |j_3| \leq \frac{k+1}{4}, \quad \forall l, \qquad |p_2| + |p_3| \leq \frac{m+1}{4}, \quad \forall n, \qquad (12)
$$

which is very useful to save computer memory.

Another important fact that saves computer memory is the following: J_1 and J_2 have to be real for η, y, θ_2 and θ_3 real. This implies that $a_{k,l,-j_2,-j_3}$ (respectively, $b_{m,n,-p_2,-p_3}$) is the complex conjugate of a_{k,l,j_2,j_3} (respectively, b_{m,n,p_2,p_3}). It is, therefore, enough to store terms with $j_2, p_2 \geq 0$ and if $j_2 = 0$ with $j_3 \geq 0$, or if $p_2 = 0$ with $p_3 \geq 0$.

The previous algorithm has been implemented to obtain the coefficients a_{k,l,j_2,j_3} and b_{m,n,p_2,p_3} with $1 \leq k \leq 50$, $1 \leq l \leq 50$, $1 \leq n \leq 50$, $1 \leq m \leq 50$ and $|j_2|, |j_3|, |p_2|, |p_3| \leq 12$, the latter satisfying the rule given in (12). This limitation can set up some upper bound on the values of η which can be used. But we are interested in small values of η.

After having passed some tests of invariance, we have globalized the manifold $W^u_{\mathbb{T}^2}$ starting with a moderate value of $y : y = y_{in}$ till y reaches the value π. We have fixed a lattice on $\mathbb{T}^2$ (50×50 equispaced points, for instance) as target values $\hat{\psi}$ of the variables (θ_2, θ_3) on $W^u_{\mathbb{T}^2} \bigcap \{y = \pi\}$. An initial point, beyond $y = y_{in}$, requires values, (ϕ_2, ϕ_3), of the variables (θ_2, θ_3). Then the values of x and I_2 are recovered from (8) and (9). With y_{in} fixed, only (ϕ_2, ϕ_3) are needed to obtain the final point. As the passage from $y = y_{in}$ to $y = \pi$ requires different travelling times, depending on (ϕ_2, ϕ_3), these initial values have been found by an iterative process. This is possible because the map $(\phi_2, \phi_3) \to (\psi_2, \psi_3)$ is a diffeomorphism close to a shift. In this way x^u and I_2^u are obtained as a function of $\hat{\psi}$.

As we are interested in efficient high accuracy computations, the integration of (7) has been done using Taylor method up to order 50. Let us sketch the main ideas. Let w denote a generic variable and let

$$
w^{(j)} = \frac{1}{j!} \frac{d^j w}{dt^j}.
$$

From (7) it follows that, $y^{(j)} = \frac{1}{j} \eta J_1^{(j-1)}$, for $j > 1$. In a similar way $\theta_2^{(j)} = \frac{1}{j} \eta J_2^{(j-1)}$, for $j > 1$. For an expression like $w = w_1 w_2$, Leibniz rule gives $w^{(j)} = \sum_{l=0}^{j} w_1^{(l)} w_2^{(j-l)}$. For an expression like $w = \sin y$ we introduce also $v = \cos y$. Then $\dot{w} = v \cdot \dot{y}$, $\dot{v} = -w \cdot \dot{y}$. Again Leibniz rule gives

$$
w^{(j)} = \frac{1}{j} \sum_{l=0}^{j-1} (j-l) v^{(l)} y^{(j-l)}, \quad v^{(j)} = -\frac{1}{j} \sum_{l=0}^{j-1} (j-l) w^{(l)} y^{(j-l)}.
$$

Combining these ideas it is immediate to compute $w^{(j)}$, $j=1,\dots,N$, for $w\in\{y,\theta_2,J_1,J_2\}$. This allows to do accurately integration steps with large stepsize which are only affected, essentially, by rounding errors. Note that, for efficiency, we work with numeric (and not with symbolic) values of $w^{(j)}$.

Doing the same process for $W^s_{\mathbb{T}^2}$, we obtain x^s and I^s_2 in $W^s_{\mathbb{T}^2}\bigcap\{y=\pi\}$ (by backwards integration in time using the correct "branch" of $W^s_{\mathbb{T}^2}$). We get $x^s=m^s(\hat\psi,\eta)$ and $I^s_2=n^s(\hat\psi,\eta)$. By symmetry one has $m^s(\psi_2,\psi_3,\eta)=m^u(2\pi-\psi_2,2\pi-\psi_3,\eta)$, $n^s(\psi_2,\psi_3,\eta)=n^u(2\pi-\psi_2,2\pi-\psi_3,\eta)$. Hence, the computation of $W^s_{\mathbb{T}^2}$ is not needed in the present case.

The splitting between the two manifolds is measured by the functions

$$d_1(\eta)=m^{u,s}(\hat\psi,\eta)=m^u(\hat\psi,\eta)-m^s(\hat\psi,\eta),\qquad d_2(\eta)=n^{u,s}(\hat\psi,\eta)=n^u(\hat\psi,\eta)-n^s(\hat\psi,\eta).$$

As the splitting is exponentially small with respect to η, even using quadruple precision in the computations we can only be confident on the results for η in the range $[0.012,0.5]$.

We note that the values of $\hat\psi$ such that $\Delta x(\hat\psi)=0$ and $\Delta I_2(\hat\psi)=0$ correspond to homoclinic orbits to the invariant torus. If we denote by $C^1_h(\eta)=\{\hat\psi\in\mathbb{T}^2|\Delta x(\hat\psi,\eta)=0\}$ and $C^2_h(\eta)=\{\hat\psi\in\mathbb{T}^2|\Delta I_2(\hat\psi,\eta)=0\}$, we remark that the topology of $C^1_h(\eta)$ and $C^2_h(\eta)$ changes with η. We will return to this point in section 6. Of course, the homoclinic points are given by $C^1_h(\eta)\bigcap C^2_h(\eta)$.

The results of the computations described so far are given in the figures as follows. Figure 1 shows views of $d_2(\hat\psi,\eta)$ for different values of η. From top to bottom an increase of the order of the leading harmonics is produced. Then the numerical computations of the splitting, as functions on $\mathbb{T}^2$, are Fourier analyzed, and a sample of the dependence of the different coefficients on η is displayed in Figure 2. Despite the fitting of the data by a function of the suitable form has been done just "visually", the agreement is remarkable. Note that on this figure $d_j(k_2,k_3,\eta)$ means the modulus of the (k_2,k_3)–harmonic in $d_j(\hat\psi,\eta)$.

Figures 3 and 4 show simultaneously the three initial harmonics for Δx and Δp_2. As independent variable we are using here $z:=(|\ln(\eta)|/\eta)^{1/2}$. One can check that, roughly, the "envelope" of the current dominant harmonics behaves like $\alpha_1 z+\alpha_0$, $\alpha_1<0$ and α_0 being suitable constants. This agrees with the form of the a priori bounds (see next section).

Finally, Figure 5 illustrates the shape of the curves $C^1_h(\eta)$ and $C^2_h(\eta)$ for different values of η. On the right lower corner the situation for large values of η is depicted. The two curves tend to be independent (just as in the case studied by Arnold). Moving to the left upper corner the value of η decreases and both lines tend to a line with the golden mean slope. In the mean time several bifurcations take place. The discussion of these bifurcations is presented in section 6.

3 A priori results on averaging. Carrying out the first steps

Let us introduce the change of variables

$$y=q_1,\quad \theta_2=q_2+\beta q_3,\quad \theta_3=q_3,\quad x=\eta p_1,\quad I_2=\beta+\eta p_2,\quad I_3=\eta(p_3-\beta p_2).$$

Despite the change is not symplectic, the equations are still canonic. The new Hamiltonian is

$$H(p_1,p_2,p_3,q_1,q_2,q_3)=\eta\left(\frac{p_1^2+p_2^2}{2}+(\cos q_1-1)(1+\eta^2(\cos(q_2+\beta q_3)+\cos q_3))\right)+p_3. \quad (13)$$

Let $\omega=(\beta,1)$ be the frequency vector on a given torus. Let us introduce the set $\Omega_{\tau,b}$ as the set of frequency vectors satisfying the diophantine condition

$$\Omega_{\tau,b}=\{\omega\in\mathbb{R}^2\quad|\quad|k\cdot\omega|\geq b|k|^{-\tau},\forall k\in\mathbb{Z}^2\setminus\{(0,0)\}\}. \quad (14)$$

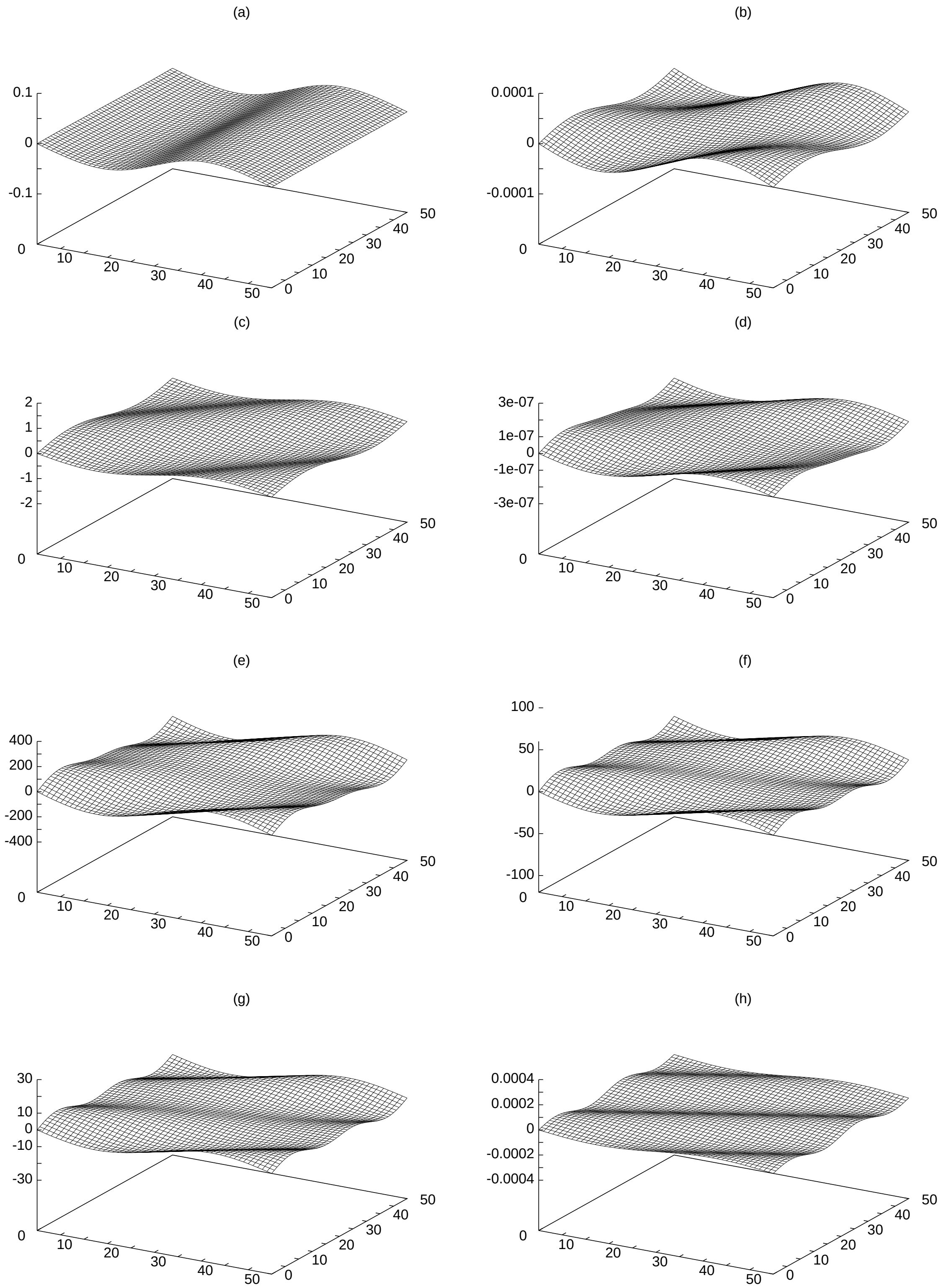

Figure 1: Behaviour of $d_2(\hat{\psi}, \eta)$ for different values of η. a) $\eta = 0.44$; b) $\eta = 0.205$; c) $\eta = 0.065$ (magnified by 10^{10}); d) $\eta = 0.034$ (magn. by 10^{10}); e) $\eta = 0.032$ (magn. by 10^{20}); f) $\eta = 0.030$ (magn. by 10^{20}); g) $\eta = 0.0292$ (magn. by 10^{20}); h) $\eta = 0.020$ (magn. by 10^{20}).

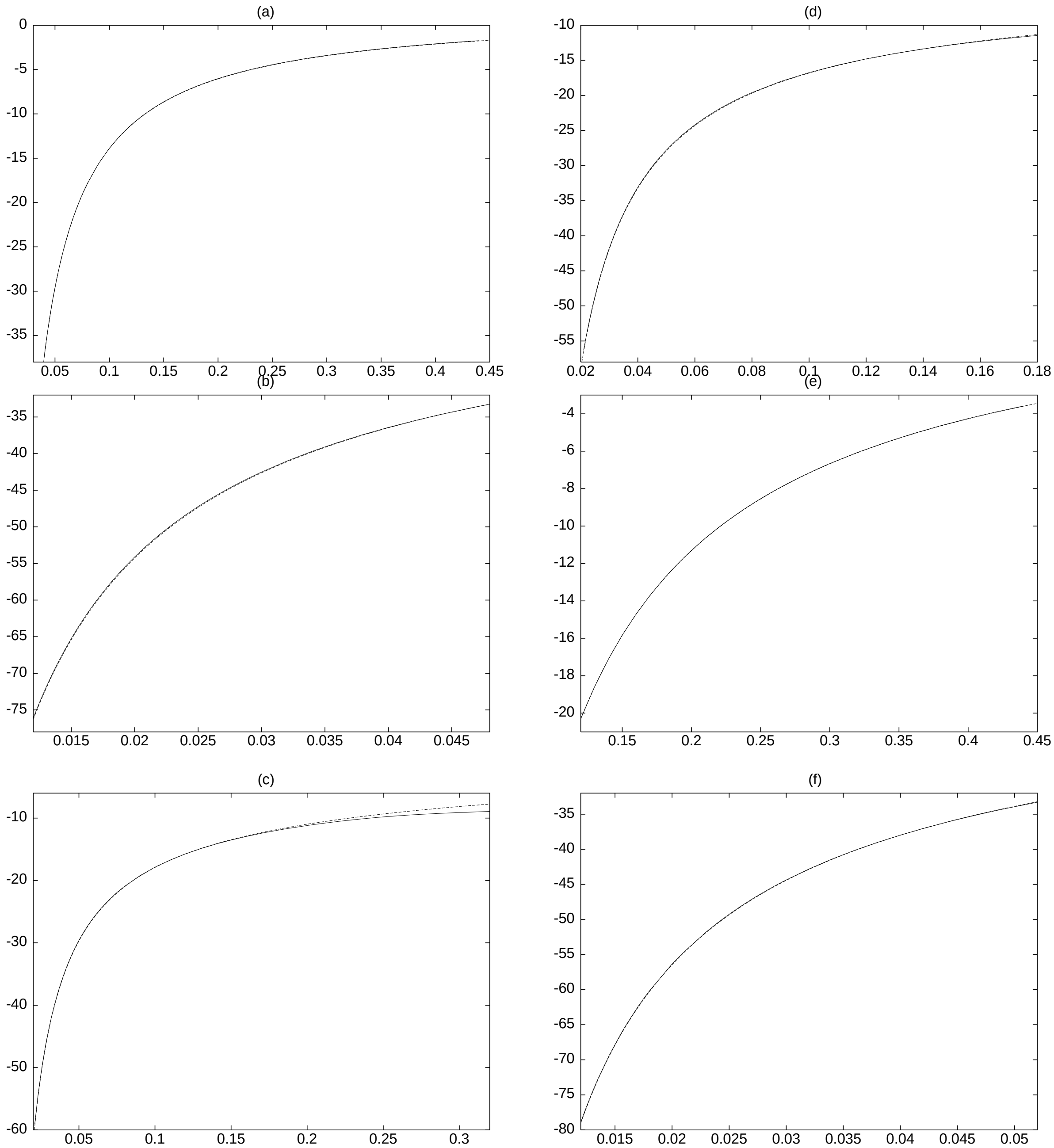

Figure 2: Behaviour of $\ln(d_1)$ and $\ln(d_2)$ for different harmonics, and some functions versus η. It has been even enough to obtain the functions by visual fitting. a) $\ln(d_1(0,1,\eta))$ and $-\pi/(2\eta)+1.8$; b) $\ln(d_1(1,-1,\eta))$ and $-\pi(3-\sqrt{5})/4\eta+2\ln(\eta)-2.5$; c) $\ln(d_1(2,-1,\eta))$ and $-\pi(\sqrt{5}-2)/2\eta+4\ln(\eta)-8.6$; d) $\ln(d_2(1,0,\eta))$ and $-\pi(\sqrt{5}-1)/4\eta+\ln(\eta)+3$; e) $\ln(d_2(1,-1,\eta))$ and $-\pi(3-\sqrt{5})/4\eta+3\ln(\eta)-1.3$; f) $\ln(d_2(2,-1,\eta))$ and $-\pi(\sqrt{5}-2)/2\eta+5\ln(\eta)-6.9$.

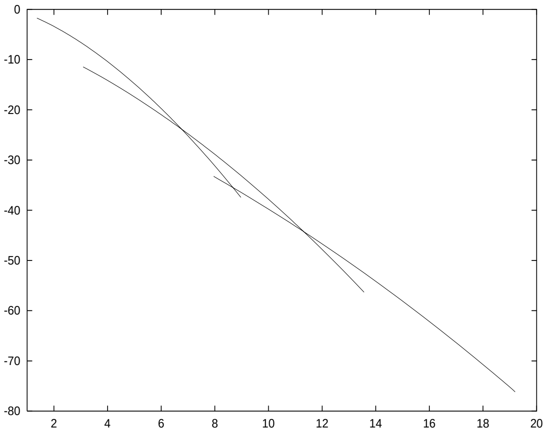

Figure 3: The three harmonics $(0,1)$, $(1,-1)$, $(2,-1)$, for $\ln(\Delta x)$ versus $(|\ln(\eta)|/\eta)^{1/2}$.

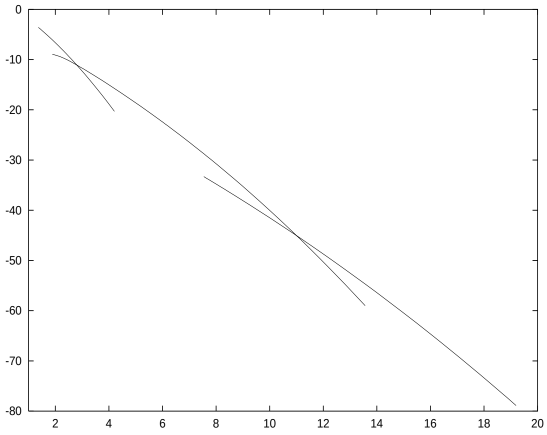

Figure 4: The three harmonics $(1,0)$, $(1,-1)$, $(2,-1)$, for $\ln(\Delta p_2)$ versus $(|\ln(\eta)|/\eta)^{1/2}$.

Applying the Averaging Theorem [6] to (13), if η_0 is small enough, for a fixed value of η with $|\eta| \leq \eta_0$, there exists a canonical change of variables such that the Hamiltonian becomes

$$H(p,q,\eta) = Z^n(p,q_1,\eta) + R_{n+1}(p,q,\eta),$$

with n related to the number of steps in the averaging and $R_{n+1} = \mathrm{O}(\eta^{n+1})$ as $\eta \to 0$. It is necessary to take n depending on η to minimize the norm of R_{n+1}. Note that the "fast" variables which are averaged are q_3 and βq_3, but cancelling the dependence with respect to βq_3 also cancels the dependence with respect to q_2 up to the desired order. If n is chosen in an optimal way, as a function of η, then the remainder R_{opt} satisfies an exponentially small bound

$$|R_{\text{opt}}|_{D_{\rho/2,\nu/2}} < c_1 \exp(-c_2/\eta^{c_3}),$$

where c_1, c_2 are positive constants depending only on the dimension, the diophantine condition and $|H|_{D_{\rho,\nu}}$. Moreover $c_3 = 1/(\tau+1)$ if $\tau > 1$ (see later for the case $\tau = 1$). Here D denotes a real compact set large enough to contain all the interesting dynamics and $D_{\rho,\nu}$ denotes a complex extension.

The following theorem gives an upper bound for the splitting of separatrices, since the system of Hamiltonian $Z^n(p,q_1,\eta)$ is integrable.

Theorem 3.1 *Assume $\omega \in \Omega_{\tau,b}$ as defined in (14), with exponent $\tau > 1$ and some $b > 0$. Then the splitting is bounded from above by $\exp(-c\eta^{-\frac{1}{\tau+1}})$, for some $c > 0$. If β is a quadratic irrational (as it has been taken in the numerical examples, where $\beta = \frac{\sqrt{5}-1}{2}$ and, hence, $\tau = 1$), one has to change the result by replacing c by a term of the form $c|\ln(\eta)|^{-1/2}$.*

At this point we would like to add some comments on two facts concerning a priori bounds: the role of $\tau = 1$ and the role of the entire character of H. As $\tau = 1$ with $p = 2$ in the problem we shall study, bounds based on averaging have a slightly different form than for larger values of τ. It turns out that, along the iterative method to average (cf. [6]), the effect of the "non–small divisors" is more relevant than the one of the small divisors (there are, comparatively, "too many" non–small divisors). This produces a bound for the remainder, after averaging,

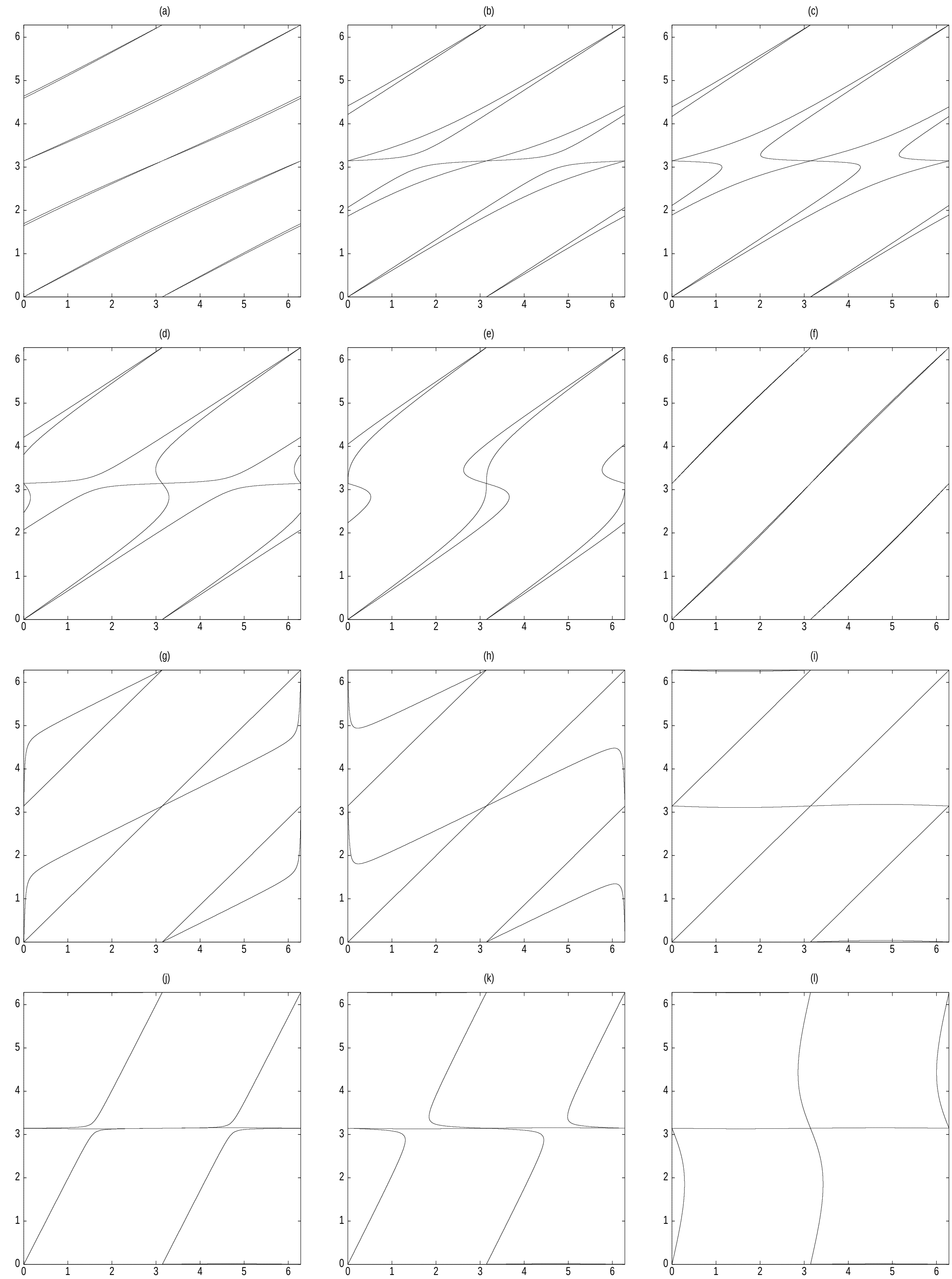

Figure 5: Behaviour of $C_h^j(\eta)$, $j = 1, 2$ for different values of η. a) $\eta = 0.025$; b) $\eta = 0.028$; c) $\eta = 0.0282$; d) $\eta = 0.0293$; e) $\eta = 0.03$; f) $\eta = 0.04$; g) $\eta = 0.062$; h) $\eta = 0.0624$; i) $\eta = 0.12$; j) $\eta = 0.22$; k) $\eta = 0.222$; l) $\eta = 0.3$.

that contains a factor of the form $-c(\eta|\ln(\eta)|)^{-1/2}$ inside the exponential. We recall (cf. [6] again) that c is proportional to the width of the analyticity domain. If H is entire c can be chosen as large as we want, but one is interested in having the norm of H in (13) bounded by some constant not depending on η. This means that we can allow for values of c of the order of $|\ln(\eta)|$. Combining these two facts and the dependence of the invariant manifolds with respect to parameters (see, e.g., [2]) one obtains a priori bounds of the form

$$\exp\left(-\hat{c}\left(\frac{|\ln(\eta)|}{\eta}\right)^{1/2}\right),$$

where $\hat{c}$ is a constant independent of η.

As it has been pointed out in the introduction, the main idea of this paper is the following: To obtain information on the dominant harmonics of the splitting for a given value of η, one can use directly the "first order" Melnikov method but the terms obtained in this way are not enough. One has to include all the effects up to a suitable order (physically, one can say that one has to give the harmonics the opportunity to interact). What we propose is to do some steps of a normal form procedure (averaging) *before applying a first order Melnikov method.* Instead of looking for the "full" splitting we want to detect the different harmonics on it. It turns out that for the harmonics having larger amplitude, the number of steps is constant for η on some interval, but when η goes to zero it increases and tends to ∞. In this way *the most relevant resonances for this range of values of η are put in evidence.* Therefore, it is crucial to keep a good control on the averaging method used before applying Melnikov method.

In order to obtain the normal form, we use Lie series, since they are suitable to perform explicit computations. This is done in several steps, one for each degree in η, following the method of [3].

Let us explain the first of these steps. We want to compute a generating function G_3 (a polynomial of degree 3 in η) such that the transformed Hamiltonian

$$H' = H + \{H, G_3\} + \frac{1}{2!}\{\{H, G_3\}, G_3\} + \frac{1}{3!}\{\{\{H, G_3\}, G_3\}, G_3\} + \ldots \tag{15}$$

has no terms with zero average of degree 3. Every time we refer to degree through this section, must be understood degree in η. As we did before for the local expansions of W^u, we introduce the change of variables

$$z_1 = \exp(iq_1), \quad z_2 = \exp(i(q_2 + \beta q_3)), \quad z_3 = \exp(iq_3).$$

Using that $H = H_0 + H_1 + H_3$, where

$$H_0 = p_3, \;\; H_1 = \eta\frac{p_1^2 + p_2^2 + z_1^1 + z_1^{-1} - 2}{2}, \;\; H_3 = \eta^3\frac{(z_1 + z_1^{-1} - 2)(z_2 + z_2^{-1} + z_3 + z_3^{-1})}{4},$$

one obtains that the terms of degree 3 of the transformed Hamiltonian H' are

$$H_3' = H_3 + \{H_0, G_3\}.$$

Hence, we can ask for $H_3' = 0$. This equation is easily solved, because of the form of H_0. The expressions of H_3 and G_3 can be written as

$$H_3 = \sum_{\substack{l=(l_1,l_2)\in\hat{\mathbb{N}}^2, \\ k=(k_1,k_2,k_3)\in\mathbb{Z}^3}} \eta^3 h_{3,l,k} p_1^{l_1} p_2^{l_2} z_1^{k_1} z_2^{k_2} z_3^{k_3}, \quad G_3 = \sum_{\substack{l=(l_1,l_2)\in\hat{\mathbb{N}}^2, \\ k=(k_1,k_2,k_3)\in\mathbb{Z}^3}} \eta^3 g_{3,l,k} p_1^{l_1} p_2^{l_2} z_1^{k_1} z_2^{k_2} z_3^{k_3},$$

where $\hat{\mathbb{N}} = \mathbb{N} \cup \{0\}$. Hence, since the frequencies $\omega = (\beta, 1)$ are rationally independent, it is immediate that

$$g_{3,l,k} = \frac{h_{3,l,k}}{i(k_2\beta + k_3)}.$$

It turns out that $\quad G_3 = (\cos q_1 - 1)(\sin q_2 + \sin q_3)$.

Notice that if one wants to perform the normal form up to degree N (included) it is enough to ask for $k \cdot \omega \neq 0$ when $0 < |k| \leq N$.

Once G_3 has been obtained, we can use (15) to compute the transformed Hamiltonian. Let us see the implementation we have used to this end. Let $H = \sum_k H_k$, where H_k collects all the terms containing η^k. Of course, initially only H_0, H_1 and H_3 are different from 0. If we want to transform it up to degree N using G_3 as generating function, we can proceed as follows:

To save memory the result will be stored in the same space used for H. We write explicitly the first steps of this method:

Step 1.1	H_N	$\leftarrow$	H_N	$+$	$\{H_{N-3}, G_3\}$
Step 2.1	H_{N-1}	$\leftarrow$	H_{N-1}	$+$	$\{H_{N-4}, G_3\}$
Step 2.2	H_N	$\leftarrow$	H_N	$+$	$\frac{1}{2!}\{\{H_{N-6}, G_3\}, G_3\}$
Step 3.1	H_{N-2}	$\leftarrow$	H_{N-2}	$+$	$\{H_{N-5}, G_3\}$
Step 3.2	H_{N-1}	$\leftarrow$	H_{N-1}	$+$	$\frac{1}{2!}\{\{H_{N-7}, G_3\}, G_3\}$
Step 3.3	H_N	$\leftarrow$	H_N	$+$	$\frac{1}{3!}\{\{\{H_{N-9}, G_3\}, G_3\}, G_3\}$
Step 4.1	H_{N-3}	$\leftarrow$	H_{N-3}	$+$	$\{H_{N-6}, G_3\}$
Step 4.2	H_{N-2}	$\leftarrow$	H_{N-2}	$+$	$\frac{1}{2!}\{\{H_{N-8}, G_3\}, G_3\}$
Step 4.3	H_{N-1}	$\leftarrow$	H_{N-1}	$+$	$\frac{1}{3!}\{\{\{H_{N-10}, G_3\}, G_3\}, G_3\}$
Step 4.4	H_N	$\leftarrow$	H_N	$+$	$\frac{1}{4!}\{\{\{\{H_{N-12}, G_3\}, G_3\}, G_3\}, G_3\}$
$\vdots$					

Note that the Poisson bracket computed in step 2.2 can be re-used in step 4.1, the one in 3.2 will be used in 5.1, the one in 3.3 will be re-used in 6.1 and so on. In this way, we are minimizing the number of arithmetic operations (each Poisson bracket is done only once), we can work with the area taken by the initial Hamiltonian (the parts of it that are overwritten are not needed in further steps) and the need of working space is not very big: at most for three polynomials of degree N, one of them being the current generating function.

After G_3 has been finished, we compute G_4, we transform up to order N using G_4, then we proceed with G_5 and so on up to G_N.

Therefore, making n steps of averaging, the transformed Hamiltonian has the form

$$H' = Z^n(p_1, p_2, p_3, q_1, \eta) + R_{n+1}(p_1, p_2, q_1, q_2, q_3, \eta), \tag{16}$$

where Z^n is the averaged Hamiltonian and $R_{n+1} = \mathrm{O}(\eta^{n+1})$ is the remainder, which is analytic in η. Note that we denote again by H' the transformed Hamiltonian, after using $G_3, \ldots G_n$. The terms in R_{n+1} are of the form $r_{m,l,k}\eta^m p^l z^k$, for $m \geq n+1$, $l = (l_1, l_2) \in \hat{\mathbb{N}}^2$, $k = (k_1, \hat{k}) = (k_1, k_2, k_3) \in \mathbb{Z}^3$. Here, as usual, $p^l = p_1^{l_1} p_2^{l_2}$ and $z^k = z_1^{k_1} z_2^{k_2} z_3^{k_3}$. Reality conditions imply that $r_{m,l,-k} = \overline{r}_{m,l,k}$. In Z^n the terms are similar but with $k_2 = k_3 = 0$. Due to the special form of (13) the terms of degree $2, 4, 5$ and 6 do not appear in (16) if $n \geq 7$.

Now we are interested in some symmetry properties of the remainder R_{n+1}, which will be useful in the computation of the Melnikov function. To this end we introduce five function spaces $\mathcal{B}$, $\mathcal{B}_1$, $\mathcal{B}_2$, $\mathcal{B}_3$ and $\mathcal{B}_4$, whose elements will be represented as (formal) sums of monomials,

$$C_{m,l,k}\eta^m p^l z^k$$

for $m \geq 1$, $l \in \hat{\mathbb{N}}^2$ and $k \in \mathbb{Z}^3$. $\mathcal{B}$ is defined as containing the monomials satisfying

$$C_{m,l,k_1,\hat{k}} = (-1)^{l_1} C_{m,l,k_1,-\hat{k}},$$

$\mathcal{B}_1$ as containing the monomials $C_{m,l,k} = 0$ if m and $|l|$ have the same parity, $\mathcal{B}_3$ as containing the monomials $C_{m,l,k} = 0$ if m and $|l|$ have different parity, $\mathcal{B}_2$ as containing the monomials with real coefficient, $C_{m,l,k}$, and $\mathcal{B}_4$ as containing the monomials with pure imaginary coefficient, $C_{m,l,k}$.

Lemma 3.2 *It holds that* $R_{n+1}, Z^n \in \mathcal{B} \cap \mathcal{B}_1 \cap \mathcal{B}_2$.

Proof

The proof is based on the following properties of $\mathcal{B}$, $\mathcal{B}_1$, $\mathcal{B}_2$, $\mathcal{B}_3$ and $\mathcal{B}_4$:

1. H_1, H_3 belong to $\mathcal{B} \cap \mathcal{B}_1 \cap \mathcal{B}_2$.

2. If $h_{m,l,k} \in \mathcal{B} \cap \mathcal{B}_1 \cap \mathcal{B}_2$ then

$$g_{m,l,k_1,\hat{k}} := \frac{-h_{m,l,k_1,\hat{k}}}{i\,(k_2\beta + k_3)} = (-1)^{l_1+1} g_{m,l,k_1,-\hat{k}}, \quad \text{if } \hat{k} \neq 0, \qquad g_{m,l,k_1,\hat{k}} := 0, \quad \text{if } \hat{k} = 0.$$

   Moreover, $g \in \mathcal{B}_1 \cap \mathcal{B}_4$.

3. $\mathcal{B}$ is closed under addition and multiplication and $\mathcal{B}_1$, $\mathcal{B}_2$ are closed under addition. Moreover, $H_1 \cdot H_2 \in \mathcal{B}_2$ if and only if $H_1, H_2 \in \mathcal{B}_2$, or $H_1, H_2 \in \mathcal{B}_4$. On the other hand $H_1 \cdot H_2 \in \mathcal{B}_4$ if and only if $H_1 \in \mathcal{B}_2$ and $H_2 \in \mathcal{B}_4$ or $H_1 \in \mathcal{B}_4$ and $H_2 \in \mathcal{B}_2$. Furthermore, $H_1 \cdot H_2 \in \mathcal{B}_1$ if and only if $H_1 \in \mathcal{B}_1$ and $H_2 \in \mathcal{B}_3$ or $H_1 \in \mathcal{B}_3$ and $H_2 \in \mathcal{B}_1$.

4. If $H \in \mathcal{B} \cap \mathcal{B}_1 \cap \mathcal{B}_2$ then $\{H, G\} \in \mathcal{B} \cap \mathcal{B}_1 \cap \mathcal{B}_2$. Indeed,

$$\begin{aligned}\{h,g\}_{m,l,k_1,\hat{k}} = \sum_{\substack{\overline{m}+\tilde{m}=m,\\ \bar{l}_1+\tilde{l}_1=l_1,\ \bar{l}_2+\tilde{l}_2=l_2,\\ \bar{k}_1+\tilde{k}_1=k_1,\ \bar{k}_2+\tilde{k}_2=k_2,\\ \bar{k}_3+\tilde{k}_3=k_3}} \Big\{ & i\bar{k}_1(\tilde{l}_1+1) h_{\overline{m},\bar{l}_1,\bar{l}_2,\bar{k}_1,\bar{\hat{k}}}\, g_{\tilde{m},\tilde{l}_1+1,\tilde{l}_2,\tilde{k}_1,\tilde{\hat{k}}} - i\tilde{k}_1(\bar{l}_1+1) h_{\overline{m},\bar{l}_1+1,\bar{l}_2,\bar{k}_1,\bar{\hat{k}}}\, g_{\tilde{m},\tilde{l}_1,\tilde{l}_2,\tilde{k}_1,\tilde{\hat{k}}} \\ & + i\bar{k}_2(\tilde{l}_2+1) h_{\overline{m},\bar{l}_1,\bar{l}_2,\bar{k}_1,\bar{\hat{k}}}\, g_{\tilde{m},\tilde{l}_1,\tilde{l}_2+1,\tilde{k}_1,\tilde{\hat{k}}} - i\tilde{k}_2(\bar{l}_2+1) h_{\overline{m},\bar{l}_1,\bar{l}_2+1,\bar{k}_1,\bar{\hat{k}}}\, g_{\tilde{m},\tilde{l}_1,\tilde{l}_2,\tilde{k}_1,\tilde{\hat{k}}} \Big\}.\end{aligned}$$

   Bearing in mind that $H \in \mathcal{B} \cap \mathcal{B}_1 \cap \mathcal{B}_2$, the second and third properties stated above, that if $H_1 \in \mathcal{B}_4$ then $iH_1 \in \mathcal{B}_2$, it is straightforward that $\{H, G\} \in \mathcal{B} \cap \mathcal{B}_1 \cap \mathcal{B}_2$.

Using the above properties and the way R_{n+1} and Z^n are constructed, the claim of Lemma 3.2 is straightforward. □

Lemma 3.2, implies that Z^n and R_{n+1} can be represented as a sum of monomials of the form

$$\sum_{m>n,\, l\in\hat{\mathbb{N}}^2,\, k\in\hat{\mathbb{N}}\times\mathbb{Z}^2} C_{m,l,k}\eta^m p^l \left(\delta_1 \cos(k_1 q_1)\cos(\hat{k}\cdot\hat{q}) - \delta_2 \sin(k_1 q_1)\sin(\hat{k}\cdot\hat{q})\right), \tag{17}$$

for R_{n+1} and

$$\sum_{n\geq m\geq 0,\, l\in\hat{\mathbb{N}}^2,\, k_1\in\hat{\mathbb{N}}} \delta_1 C_{m,l,k_1,0}\eta^m p^l \cos(k_1 q_1), \tag{18}$$

for Z^n, being $\delta_1 = (1+(-1)^{l_1})/2$, and $\delta_2 = (1-(-1)^{l_1})/2$. Since the original Hamiltonian H has a continuum of whiskered 2D tori located at $p_1 = q_1 = 0$, it follows that Z^n and R_{n+1} are zero for $p_1 = q_1 = 0$. The C coefficients in (17) and (18) should satisfy that if $l_1 = 0$, then

$$\sum_{k_1 \in \hat{\mathbb{N}}} C_{m,0,l_2,k_1,\hat{k}} = 0 \tag{19}$$

for every $m, l_2, \hat{k}$ fixed. Note that $\partial/\partial p_1 = \partial/\partial q_1 = 0$ at $p_1 = q_1 = 0$ because of the forms of (17) and (18).

Table 1 summarizes some selected terms which appear inside the remainder in (16) when the computation is stopped at different values of n. These terms will play a key role in the splitting estimates. Stopping averaging at some order n yields terms in the remainder of order $m > n$. For reasons which will be clear later, the interesting values of k_2 and $-k_3$ are consecutive Fibonacci numbers (perhaps changing sign of some or both) (if $\beta =$ golden mean). Note that, due to Lemma 3.2, it is enough to display the terms giving $\hat{k}\cdot\omega > 0$. Working around $p_2 = 0$ the exponent l_2 has to be zero. The exponents l_1 and k_1 are not independent (see [7] and the beginning of section 5).

m :=degree of η	(l_1, l_2, k_1)	k_2	k_3	coef : $r_{m,l_1,k}$
3	$(0,0,1)$	1	0	2.500000000000000E-01
	$(0,0,1)$	0	1	2.500000000000000E-01
7	$(0,0,2)$	-1	1	-4.253510734375189E-02
8	$(1,0,2)$	-1	1	-3.739012590402631E-02
9	$(0,0,3)$	-1	1	5.855378067600916E-02
	$(2,0,2)$	-1	1	-7.193171719185818E-02
10	$(1,0,3)$	-1	1	1.129428339443463E-01
	$(3,0,2)$	-1	1	-3.459965199302226E-02
11	$(0,0,3)$	2	-1	2.385665478959481E-02
12	$(1,0,3)$	2	-1	6.474194839591554E-02
13	$(0,0,4)$	2	-1	-1.609101147998339E-01
	$(2,0,3)$	2	-1	3.947278831794541E-01
14	$(1,0,4)$	2	-1	-9.294779845771670E-01
	$(3,0,3)$	2	-1	8.081996376414760E-01
19	$(0,0,5)$	-3	2	2.229687893990839E-02
20	$(1,0,5)$	-3	2	1.833950253104235E-01
21	$(0,0,6)$	-3	2	-6.516518975748299E-01
	$(2,0,5)$	-3	2	2.868787806886720E+00
22	$(1,0,6)$	-3	2	-4.311933282037920E+00
	$(3,0,5)$	-3	2	8.932723103041311E+00
31	$(0,0,8)$	5	-3	-7.033638786008045E-02
32	$(1,0,8)$	5	-3	-1.541762726656330E+00
33	$(0,0,9)$	5	-3	8.516150078812856E+00
	$(2,0,8)$	5	-3	-6.670323265174216E+01
34	$(1,0,9)$	5	-3	2.171358825583065E+02
	$(3,0,8)$	5	-3	-6.963543393735017E+02

Table 1: The relevant coefficients of selected remainders of the normal form when the harmonics $(1,0)$, $(0,1)$, $(-1,1)$, $(2,-1)$, $(-3,2)$ and $(5,-3)$ appear for the first time.

Notice that the terms with $m = 7, 8, 9, 10$ come from R_7, which requires to compute the generating functions up to G_6. Similarly, terms with $m = 11, 12, 13, 14$ come from R_{11} requiring to compute the generating function up to G_{10}, terms with $m = 19, 20, 21, 22$ come from R_{19} requiring to compute the generating function up to G_{18} and, finally, terms with $m = 31, 32, 33, 34$ come from R_{31} requiring to compute the generating function up to G_{30}.

4 The Melnikov Vector

In this section we formally compute the harmonics contributing to the splitting by using the *adapted Melnikov method*, i.e., using (16). The number of steps before applying Melnikov formula is given by $4|\hat{k}|-1$ (this comes from the relation similar to (12), where $|\hat{k}| = |k_2|+|k_3|$ is the order of the harmonic to be computed). We do not claim here that this approximation is rigorously justified. However, results obtained in this way have a good agreement with the numerical ones.

From the form of Z^n given in the above section, the separatrix of Z^n has the same symmetry properties as the separatrix of the pendulum part.

The variation of the actions due to the perturbation R_n is

$$\Delta p_2 = \int_{\mathbb{R}} \frac{\partial R_{n+1}}{\partial q_2}, \quad \Delta p_3 = \int_{\mathbb{R}} \frac{\partial R_{n+1}}{\partial q_3}, \tag{20}$$

where the integration is carried out along the separatrix of Z^n. The definition of the Melnikov vector as (20) comes from the fact that for the non-perturbed Hamiltonian p_2 and p_3 are integrals of motion, so that Δp_2 and Δp_3 give the first formal approximation to the splitting vector.

In fact, we want to compute the quantity Δp_1, and this is possible recalling that Δp_1 and Δp_3 are dependent via energy conservation. We can decompose the variations of the Hamiltonian H (see (13)) on the Poincaré section $q_1 = \pi$, recalling that we are comparing points that, before the perturbation, had $q_2^u = q_2^s$ and $q_3^u = q_3^s$:

$$\begin{aligned} \Delta H^u &= \eta \left(\frac{(p_1^u)^2}{2} + \frac{(p_2^u)^2}{2} - 2 \right) - 2\eta^3 \left(\cos(q_2^u + \beta q_3^u) + \cos q_3^u \right) + p_3^u = 0, \\ \Delta H^s &= \eta \left(\frac{(p_1^s)^2}{2} + \frac{(p_2^s)^2}{2} - 2 \right) - 2\eta^3 \left(\cos(q_2^s + \beta q_3^s) + \cos q_3^s \right) + p_3^s = 0. \end{aligned}$$

Using

$$p_1^u = 2 + \Delta p_1^u, \quad p_1^s = 2 + \Delta p_1^s$$

and

$$0 = \eta \left(2(\Delta p_1^u - \Delta p_1^s) + \frac{(\Delta p_1^u)^2 - (\Delta p_1^s)^2}{2} \right) + \frac{1}{2} \left((\Delta p_2^u)^2 - (\Delta p_2^s)^2 \right) + \Delta p_3,$$

we conclude that

$$\frac{\eta \Delta p_1}{2} (4 + \Delta p_1^u + \Delta p_1^s) = -\Delta p_3 - \frac{1}{2} \Delta p_2 (\Delta p_2^u + \Delta p_2^s).$$

It will be shown later that Δp_2 and Δp_3 differ only in numerical coefficients and it is obvious that Δp_j^u and Δp_j^s, $j = 1, 2, 3$ are, at most, of order η^3. Hence, assuming that the numerical coefficient of Δp_3 is different from zero, one has

$$\Delta p_1 = -\frac{\Delta p_3}{2\eta} \left(1 + \mathrm{O}(\eta^3) \right).$$

We will compute Δp_2 and Δp_1, with the integral carried out along the separatrix of "the pendulum" part of Z^n times the rotor. That is, we shall neglect, in this paper, the difference between both separatrices.

The upper separatrix motion of the pendulum $\frac{p^2}{2}+\cos q-1$ starting at $q=\pi$ is of the form:

$$\begin{aligned} q_1(t) &= 4\arctan(e^{-t}) = \pi - 4\arctan(\tanh(t/2)), \quad p_1(t)=\frac{2}{\cosh t}, \\ \cos q_1(t) &= 1-\frac{2}{\cosh^2 t}, \quad \sin q_1(t)=\frac{-2\sinh t}{\cosh^2 t}. \end{aligned}$$

Due to the fact that H has η as a factor, we can scale t by the change $t=\tau/\eta$ and, then, we denote again τ as t, as usual. This will decrease by one unit the exponents of η.

Moreover, denoting by $\mathcal{A}$ the subset of $\mathbb{N}^3\times\mathbb{Z}^2$, containing the values of $(m,l_1,k_1,\hat{k})$ present in the remainder, R_{n+1}, with $l_1\neq 0$ and $k_1\neq 0$, it follows that

$$\begin{aligned} \frac{\partial R_{n+1}}{\partial q_2} &= -\sum_{(m,l_1,k_1,\hat{k})\in\mathcal{A}} \eta^{m-1}k_2 p_1^{l_1} r_{m,l_1,k_1,\hat{k}}\left(\sin(k_1q_1+\hat{k}\cdot\hat{q})\right), \\ \frac{\partial R_{n+1}}{\partial q_3} &= -\sum_{(m,l_1,k_1,\hat{k})\in\mathcal{A}} \eta^{m-1}(\hat{k}\cdot\omega) p_1^{l_1} r_{m,l_1,k_1,\hat{k}}\left(\sin(k_1q_1+\hat{k}\cdot\hat{q})\right), \end{aligned}$$

where $\hat{q}=(q_2,q_3)$. Note that $\hat{q}(0)=\hat{\psi}$, as in (4), when we restrict to the separatrix of the unperturbed system.

Expanding $\sin(k_1q_1+\hat{k}\cdot\hat{q})$ over the separatrix of the pendulum times the rotor, denoting $\kappa:=\hat{k}\cdot\omega$ and introducing $\mu=\kappa/\eta$, we obtain

$$\sin(k_1q_1+\hat{k}\cdot\hat{q}) = (-1)^{k_1}[\sin(\gamma(t))\cos(\hat{k}\cdot\psi)+\cos(\gamma(t))\sin(\hat{k}\cdot\psi)],$$

where $\gamma(t)=-4k_1\arctan(\tanh(t/2))+\mu t$. By the oddness of the functions, we have

$$\int_{\mathbb{R}}\cosh^{-l_1} t\sin(\gamma(t))dt = 0.$$

Therefore the only terms giving a non zero contribution to the integrals in (20) (using the pendulum separatrix) are the ones coming from the terms even in t and odd in $\hat{\psi}$. Hence

$$\Delta p_2=\sum_{\hat{k}\in\mathbb{Z}^2}\Delta p_2^{\hat{k}}\sin(\hat{k}\cdot\hat{\psi}), \quad \Delta p_3=\sum_{\hat{k}\in\mathbb{Z}^2}\Delta p_3^{\hat{k}}\sin(\hat{k}\cdot\hat{\psi}),$$

where $\Delta p_2^{\hat{k}}$ and $\Delta p_3^{\hat{k}}$ denote the coefficients of the respective harmonics.

Let $\mathcal{A}_+=\{(m,l_1,k_1,\hat{k})\mid \hat{k}\cdot\omega>0\}$. Note that we consider sets $\mathcal{A}_+$ for fixed indices $\hat{k}$. Hence, all the sums below range over m,l_1,k_1, and we shall skip $\hat{k}$ from the indices in $\mathcal{A}_+$. Taking into account the relation between the coefficients in the normal form given in Lemma 3.2 and using the notation

$$I(k_1,l_1,\mu)=\int_{\mathbb{R}}\frac{\exp\left(i\left(-\mu s+4k_1\arctan(\tanh(s/2))\right)\right)}{\cosh^{l_1}s}ds,$$

we can distinguish different cases for:

$$\Delta p_j^{\hat{k}} = 2\sum_{(m,l_1,k_1)\in\mathcal{A}_+}(-1)^{k_1+1}2^{l_1}\eta^{m-1}\left|k_2\right|^{3-j}\kappa^{j-2}r_{m,l_1,k_1,\hat{k}}I(k_1,l_1,\mu), \quad j=2,3. \tag{21}$$

First we proceed with the cases $l_1>0$, the ones with $l_1=0$ being deferred till Lemma 4.4.

Lemma 4.1 *For $k_1 \in \hat{\mathbb{N}}$, $l_1 \in \mathbb{N}$, the values of $I(k_1, l_1, \mu)$ are:*

1. *If $2k_1 \geq l_1$*
$$\frac{4\pi(-2\mu)^\sigma}{2^{l_1}(1-e^{-2\mu\pi})}\frac{(-1)^{l_1}e^{-\mu\frac{\pi}{2}}}{(l_1+2k_1-1)!}\prod_{m=1}^{\frac{l_1+2k_1-1-\sigma}{2}}\left(4\mu^2+z_m\right).$$

2. *If $2k_1 \in [0, l_1-1]$*
$$\frac{4\pi(-2\mu)^\sigma}{2^{l_1}(1-e^{-2\mu\pi})}\left[\frac{(-1)^{l_1}e^{-\mu\frac{\pi}{2}}}{(l_1+2k_1-1)!}\prod_{m=1}^{\frac{l_1+2k_1-1-\sigma}{2}}(4\mu^2+z_m)+\frac{e^{-\mu\frac{3\pi}{2}}}{(l_1-2k_1-1)!}\prod_{m=1}^{\frac{l_1-2k_1-1-\sigma}{2}}(4\mu^2+z_m)\right],$$

where $\sigma = (1+(-1)^{l_1})/2$. Moreover,
$$z_j \in \mathbb{R}, \quad |z_j| \leq 9\max\{q^2, p^2\}, 1 \leq j \leq \frac{q-1-\sigma}{2}, \quad \textit{and} \quad \sum_{j=1}^{\frac{q-1-\sigma}{2}} z_j = \binom{q-1}{2}\left(\frac{q}{3}-p\right),$$
where $q = l_1+2k_1$ and $p = -l_1+2k_1$ in case 1., $q = l_1-2k_1$ and $p = -l_1-2k_1$ in case 2.

Proof

Consider the function
$$g(z) = \arctan(\tanh(z/2)). \tag{22}$$
First, notice that
$$g(z) = \ln(\tan(iz/2+\pi/4))/(2i),$$
where we are considering the principal branch of the logarithm in $\mathbb{C}\backslash\{\text{Im } z = 0, \text{Re } z \leq 0\}$. Indeed, the two expressions coincide at $z=0$ and their derivatives are both equal to $(2\cosh z)-1$.

Therefore, we have to compute
$$I(k_1, l_1, \mu) = \int_{\mathbb{R}} \frac{e^{4ik_1 g(\tau)}}{\cosh^{l_1}\tau} e^{-i\mu\tau} d\tau.$$
Since $k_1 \in \hat{\mathbb{N}}$, the function $e^{4ik_1 g(s)}$ is meromorphic in $\mathbb{C}$.

The integral to obtain now is
$$\begin{aligned} I(k_1, l_1, \mu) &= \int_{\mathbb{R}} \frac{\tan^{2k_1}(i\tau/2+\pi/4)}{\cosh^{l_1}\tau} e^{-i\mu\tau} d\tau = 2\int_{\mathbb{R}} \frac{\tan^{2k_1}(is+\pi/4)}{\cosh^{l_1}2s} e^{-2i\mu s} ds \\ &:= 2\int_{\mathbb{R}} B(s)ds = 2\hat{I}(k_1, l_1, \mu). \end{aligned}$$

The number of poles in
$$\Omega_R = \{z \in \mathbb{C} : -\pi \leq \text{Im } z \leq 0, |\text{Re } z| \leq R\} \tag{23}$$
of the function to integrate depends on k_1 : If $2k_1 \geq l_1$ there is a unique pole at $-i\pi/4$ (of multiplicity l_1+2k_1). If $2k_1 \in [0, l_1-1]$, there are two poles: one at $-i\pi/4$ (of multiplicity l_1+2k_1) and the other at $-i3\pi/4$ (of multiplicity l_1-2k_1). To compute the value of the residue at the poles of the function $\hat{I}(k_1, l_1, \mu)$, we will distinguish between both poles.

Let
$$h_{p,q,\mu}(x) = \frac{\cosh^p(x)e^{-2i\mu x}}{\sinh^q(x)},$$
where x is obtained by a translation of s to have the pole at $x=0$. Then,

1. Pole at $-i\dfrac{\pi}{4}$. We obtain

$$\mathrm{Res}\left(B(z), z=-i\frac{\pi}{4}\right) = \frac{(-1)^{k_1+l_1}e^{-\mu\frac{\pi}{2}}}{2^{l_1}i^{l_1}}\mathrm{Res}(h_{p,q,\mu}(x), x=0),$$

where $p=-l_1+2k_1$ and $q=l_1+2k_1$. Note that $q>0$. On the other hand, $p>0$ if $2k_1\geq l_1$, and $p<0$ otherwise. Anyway, $|p|\leq q$.

2. Pole at $-i\dfrac{3\pi}{4}$. In this case,

$$\mathrm{Res}\left(B(z), z=-i\frac{3\pi}{4}\right) = \frac{(-1)^{k_1}e^{-\mu\frac{3\pi}{2}}}{2^{l_1}i^{l_1}}\mathrm{Res}(h_{p,q,\mu}(x), x=0),$$

where $p=-l_1-2k_1$ and $q=l_1-2k_1$. Since $2k_1<l_1$, we note that $q>0$ and $p<0$.

In order to study more properties of the residue of $h_{p,q,\mu}(x)$ in $x=0$, we will introduce $\alpha=-2i\mu$ and the function

$$C(x)=\sum_{j\geq 0}\frac{C_j}{j!}x^j,$$

such that

$$h_{p,q,\mu}(x)=\frac{e^{\alpha x}\cosh^p(x)}{\sinh^q(x)}=\frac{C(x)}{x^q}. \tag{24}$$

Notice that $\forall j\geq 0$, C_j is a function of α, q and p. If we are interested on the explicit dependence of C_j in any of the above mentioned α, q or p we will write it explicitly as

$$C_j(\xi),\quad \text{where } \xi=q,p,\alpha.$$

Moreover, from (24), the residue is given by

$$\frac{C_{q-1}}{(q-1)!}.$$

Taking logarithms in (24), differentiating and computing the n-th order terms in x, we have the recursive formula for C_n, $n=0,\ldots,q-1:$ $C_0=1$, $C_1=\alpha$ and, for $n=3,\ldots,q$,

$$C_{n-1}=\alpha\sum_{k=0}^{\left[\frac{n-2}{2}\right]}\binom{n-1}{2k+1}2^{2k}\frac{C_{n-2k-2}}{n-1}+\sum_{k=1}^{\left[\frac{n-1}{2}\right]}\binom{n}{2k+1}2^{2k}\frac{C_{n-2k-1}D(n,k,p,q)}{n(n-1)}, \tag{25}$$

where

$$D(n,k,p,q)=\left(p\left(k+\frac{1}{2}\right)-q\left(k-\frac{1}{2}\right)-(n-2k-1)\right). \tag{26}$$

From (25) we obtain several consequences that are contained in the following Lemma.

Lemma 4.2 *The following properties hold:*

1. *The function $C_{q-1}(\alpha)$ satisfies*

$$C_{q-1}(\alpha)=\alpha^{q-1}+a_{q-3}(q,p)\alpha^{q-3}+\ldots+a_\sigma(q,p)\alpha^\sigma,$$

where $\sigma=(1+(-1)^q)/2$. Moreover,

$$C_{q-1}(\alpha)=\alpha^\sigma\prod_{j=1}^{\frac{q-1-\sigma}{2}}(\alpha^2-z_j). \tag{27}$$

2. For every q and p fixed, the sum of all the zeroes, z_j, of $\dfrac{C_{q-1}(q,p,\alpha^2)}{\alpha^\sigma}$ satisfies

$$\sum_{j=1}^{\frac{q-1-\sigma}{2}} z_j = \binom{q-1}{2}\left(\frac{q}{3}-p\right),$$

with σ as before.

Proof

Proof of 1.

The first part of 1. is straightforward by induction using (25) and bearing in mind that $C_0 = 1$ and $C_1 = \alpha$. In order to prove the second part, it is convenient to introduce the variable $w = \alpha^2/4 = -\mu^2$ and the scalings

$$\overline{C}_j = \frac{C_j}{j!2^j} \ \text{ if } j \text{ is even}, \quad \overline{C}_j = \frac{C_j}{j!2^{j-1}\alpha} \ \text{ if } j \text{ is odd}.$$

In these new variables, (25) can be reduced to $\overline{C}_0 = 1$, $\overline{C}_1 = 1$ and for $n = 3, \ldots, q$

$$\left\{\begin{array}{rcl} (n-1)\overline{C}_{n-1} & = & w\displaystyle\sum_{k=0}^{\left[\frac{n-2}{2}\right]} \frac{\overline{C}_{n-2k-2}}{(2k+1)!} + \sum_{k=1}^{\left[\frac{n-1}{2}\right]} \frac{\overline{C}_{n-2k-1}}{(2k+1)!} D(n,k,p,q), \quad \text{if } n \text{ odd}, \\ (n-1)\overline{C}_{n-1} & = & \displaystyle\sum_{k=0}^{\left[\frac{n-2}{2}\right]} \frac{\overline{C}_{n-2k-2}}{(2k+1)!} + \sum_{k=1}^{\left[\frac{n-1}{2}\right]} \frac{\overline{C}_{n-2k-1}}{(2k+1)!} D(n,k,p,q), \quad \text{if } n \text{ even}, \end{array}\right. \tag{28}$$

where $D(n,k,p,q)$ is given in (26). With (28), (27) is easily obtained.

Proof of 2.

From equation (25), we have that minus the coefficient of degree $q-3$ in C_{q-1}, $\gamma_{q-3}^{(q-1)}$, gives the sum of the squares of the zeroes of C_{q-1}. Therefore we only need to compute such coefficient, which is given by

$$\begin{aligned} \gamma_{q-3}^{(q-1)} &= \frac{1}{q(q-1)}\left(q(q-1)\gamma_{q-4}^{(q-2)} + \frac{4q(q-1)(q-2)(q-3)}{6}\right. \\ &+ \left.\frac{4q(q-1)(q-2)}{6}\left(\frac{3p-q}{2} - q + 3\right)\right) = (q-2)\frac{3p-q}{3} + \gamma_{q-4}^{(q-2)} \end{aligned}$$

Proceeding by induction we deduce

$$\gamma_{q-3}^{(q-1)} = \frac{3p-q}{3}\sum_{l=1}^{q-2} l = \binom{q-1}{2}\left(p - \frac{q}{3}\right).$$

□

To conclude the proof of Lemma 4.3, we need to prove the following Lemma:

Lemma 4.3 *For $k \geq 1$, $l_1 \in \hat{\mathbb{N}}$, $j = 1, \ldots, \left[\frac{q-1}{2}\right]$, the zeroes z_j are real and satisfy*

$$|z_j| \leq \left\{\begin{array}{ll} 9q^2 & \text{for } p \in [-q, q] \\ 9p^2 & \text{for } p \in (-\infty, -q). \end{array}\right.$$

The proof of Lemma 4.3 will require, in turn, some additional Lemmata. We postpone the proof till the end of this section. Before we finish the proof of Lemma 4.1, give the corresponding Lemma in the case $l_1 = 0$ and we shall obtain some relevant bounds from them.

End of proof of Lemma 4.1

Using Lemma 4.2 and Lemma 4.3, integrating along the border of Ω_R and letting $R \to \infty$ Lemma 4.1 follows. $\square$

Taking into account the relation between the coefficients in the normal form given in (19) for $l_1 = l_2 = 0$, and using the notation

$$\tilde{I}_1(k_1, \mu) = \int_{\mathbb{R}} \exp(-i\mu s) \left((-1)^{k_1} \exp\left(i4k_1 \arctan(\tanh(s/2))\right) - 1 \right) ds,$$

we have that the contribution to $\Delta p_j^{\hat{k}}$ coming from $l_1 = 0$ is given by

$$-2 \sum_{(m,0,k_1) \in \mathcal{A}_+} \eta^{m-1} \left|k_2\right|^{3-j} \kappa^{j-2} r_{m,0,k_1,\hat{k}} \tilde{I}_1(k_1, \mu). \tag{29}$$

As $\tilde{I}_1(0, \mu) = 0$, we deduce the following result:

Lemma 4.4 *For $l_1 = 0$ and $k_1 \in \mathbb{N}$, the values of $\tilde{I}_1(k_1, \mu)$ are*

$$\frac{4\pi(-1)^{k_1}(-2\mu)}{(2k_1 - 1)!} \frac{e^{-\mu\frac{\pi}{2}}}{1 - e^{-2\mu\pi}} \prod_{m=1}^{k_1 - 1} \left(4\mu^2 + z_m\right).$$

Proof

Proceeding as in the proof of Lemma 4.1, considering also the function $g(z)$ given in (22), we have to compute

$$\tilde{I}(k_1, \mu) = \int_{\mathbb{R}} \left((-1)^{k_1} e^{4ik_1 g(\tau)} - 1 \right) e^{-i\mu\tau} d\tau.$$

Since $k_1 \in \mathbb{N}$, the function is meromorphic in $\mathbb{C}$. The integral to compute is

$$\tilde{I}(k_1, \mu) = 2 \int_{\mathbb{R}} e^{-2i\mu s} \left((-1)^{k_1} \tan^{2k_1}(is + \pi/4) - 1 \right) ds.$$

The integrand has only one pole in the domain Ω_R given in (23) at $-i\pi/4$. Then, since the residue to obtain $\tilde{I}(k_1, \mu)$ is the same as given in Lemma 4.1, we have

$$\int_{\Omega_R} \left((-1)^{k_1} \tan^{2k_1}(is + \pi/4) - 1 \right) e^{-2i\mu s} ds = \frac{4\pi(-1)^{k_1+1} \mu e^{-\mu\frac{\pi}{2}}}{(2k_1 - 1)!} \prod_{m=1}^{k_1 - 1} \left(4\mu^2 + z_m\right). \tag{30}$$

Therefore, (30) can be written as

$$(1 - e^{2\mu\pi}) \int_{-R}^{R} \left((-1)^{k_1} \tan^{2k_1}(is + \pi/4) - 1 \right) e^{-2i\mu s} ds + \int_{R}^{R+\pi} + \int_{-R+\pi}^{R} =$$
$$\frac{2\pi(-1)^{k_1}(-2\mu) e^{-\mu\frac{\pi}{2}}}{(2k_1 - 1)!} \prod_{m=1}^{k_1 - 1} \left(4\mu^2 + z_m\right).$$

Letting $R \to \infty$, last two integrals before the $=$ sign are $O(e^{-2|R|})$. This concludes the proof of the Lemma. $\square$

Lemma 4.1 and Lemma 4.4 imply that, for any harmonic $\hat{k}$ with $\hat{k}\cdot\omega > 0$, one has

$$\Delta p_j^{\hat{k}} = 8\pi \sum_{(m,l_1,k_1)\in\mathcal{A}_+} (-1)^{k_1+1}\eta^{m-1}\,|k_2|^{3-j}\,\kappa^{j-2}(-2\mu)^{\sigma}\frac{r_{m,l_1,k_1,\hat{k}}}{1-e^{-2\mu\pi}}(-1)^{l_1}e^{-\mu\frac{\pi}{2}i}$$
$$\times\left\{\frac{1}{(l_1+2k_1-1)!}\mathcal{P}(l_1+2k_1)+\frac{(-1)^{l_1}1_{\{2k_1<l_1\}}e^{-\mu\pi}}{(l_1-2k_1-1)!}\mathcal{P}(l_1-2k_1)\right\} \tag{31}$$

where

$$\mathcal{P}(q) = \prod_{m=1}^{\frac{q-1-\sigma}{2}}\left(4\mu^2+z_m\right), \quad \text{and} \quad 1_{\{2k_1<l_1\}} = \begin{cases} 1 & \text{if } 2k_1<l_1 \\ 0 & \text{otherwise.}\end{cases} \tag{32}$$

We recall that $\sigma = (1+(-1)^{l_1})/2$ and that the zeroes z_m depend on q (equal to $l_1 \pm 2k_1$) and also on p (equal to $-l_1 \pm 2k_1$).

We remind that the adapted Melnikov function we have constructed follows from (21) and (29) in the following form:

$$\Delta p_j(\hat{\psi}) = \sum_{\hat{k}\in\mathbb{Z}^2}\Delta p_j^{\hat{k}}\sin(\hat{k}\cdot\hat{\psi}), \quad j=2,3.$$

To bound $\Delta p_2^{\hat{k}}$ and $\Delta p_3^{\hat{k}}$ we need bounds of the products appearing in the expressions above.

Lemma 4.5 *For a fixed $q \geq 4$, let $\dfrac{\max(q^2,p^2)}{\mu^2} := B$, sufficiently small. Then (σ as before),*

$$\prod_{m=1}^{\frac{q-1-\sigma}{2}}\left(4\mu^2+z_m\right) = (4\mu^2)^{\frac{q-1-\sigma}{2}}\exp\left(\frac{1}{4\mu^2}\binom{q-1}{2}\left(\frac{q}{3}-p\right)(1+B)\right).$$

The proof follows by dividing both sides by the power of μ^2, taking logarithms, expanding, using the bounds of z_m and 2. of Lemma 4.2.

On the other hand, if $\max(q^2,p^2)/\mu^2$ does not satisfy the condition of B sufficiently small, then, one can assume that there exists a constant $N>0$ such that $\mu^2 \leq N\max(q^2,p^2)$, and for $\sigma = 0$ or 1 one has:

$$\left|\prod_{m=1}^{\frac{q-1-\sigma}{2}}\left(4\mu^2+z_m\right)\right| \leq \left[(4N^2+9)\max(q^2,p^2)\right]^{\frac{q-1-\sigma}{2}}.$$

These bounds will be used in next section to detect the relevant harmonics of the splitting.

Next we give the low order contributions to the splitting, to be checked against the previous numerical results. Assuming that only the terms of the remainder given in Table 1 give significant contribution to the harmonics $(1,0),(0,1),(-1,1),(2,-1),(-3,2)$ and $(5,-3)$ of the splitting vector, one has

$$\begin{aligned}
\Delta p_2^{1,0} &= \eta^2\int_{-\infty}^{\infty} r_{3,0,0,1,0}\frac{2\cos\frac{\beta}{\eta}t}{\cosh^2 t}dt = -2\pi\eta e^{-\frac{\pi\beta}{2\eta}}\beta H(\beta),\\
\Delta p_1^{0,1} &= \frac{-\Delta p_3^{0,1}}{2\eta} = -\frac{\eta}{2}\int_{-\infty}^{\infty} r_{3,0,0,0,1}\frac{2\cos\frac{t}{\eta}}{\cosh^2 t}dt = \pi e^{-\frac{\pi}{2\eta}}H(1),
\end{aligned}$$

where $\delta H(\delta)$ is a function which converges to $2\eta/\pi$ as $\delta \to 0$.

For the rest of the harmonics (remember that we choose $\hat{k}$ such that $\kappa = \hat{k}\cdot\omega > 0$) one has:

$$\Delta p_2^{\hat{k}} = (-1)^{|\hat{k}|} 2^{2|\hat{k}|+2} |k_2| \eta^{2|\hat{k}|-1} \pi \frac{e^{-\mu\frac{\pi}{2}}}{1-e^{-2\mu\pi}} \kappa^{2|\hat{k}|-1} \left(1+e^{-\mu\pi}\right) \frac{c^{\hat{k}}}{(2|\hat{k}|-1)!}, \tag{33}$$

$$\Delta p_1^{\hat{k}} = (-1)^{|\hat{k}|+1} 2^{2|\hat{k}|+1} \eta^{2|\hat{k}|-2} \pi \frac{e^{-\mu\frac{\pi}{2}}}{1-e^{-2\mu\pi}} \kappa^{2|\hat{k}|} \left(1+e^{-\mu\pi}\right) \frac{c^{\hat{k}}}{(2|\hat{k}|-1)!}, \tag{34}$$

where

$$\begin{aligned} c^{\hat{k}} &= r_{-1}^0 \prod_{m=1}^{|\hat{k}|} (1 + z_m^{2|\hat{k}|,0}/(4\mu^2)) - \frac{r_0^1 \kappa}{|\hat{k}|} \prod_{m=1}^{|\hat{k}|} (1 + z_m^{2|\hat{k}|,1}/(4\mu^2)) \\ &+ \frac{2\kappa^2}{|\hat{k}|(2|\hat{k}|+1)} \left(r_1^2 \prod_{m=1}^{|\hat{k}|+1} (1 + z_m^{2|\hat{k}|,2}/(4\mu^2)) - r_1^0 \prod_{m=1}^{|\hat{k}|+1} (1 + z_m^{2|\hat{k}|+2,0}/(4\mu^2)) \right) \\ &- \frac{2\kappa^3}{|\hat{k}|(2|\hat{k}|+1)(|\hat{k}|+1)} \left(r_2^1 \prod_{m=1}^{|\hat{k}|+1} (1 + z_m^{2|\hat{k}|+2,1}/(4\mu^2)) - r_2^3 \prod_{m=1}^{|\hat{k}|+1} (1 + z_m^{2|\hat{k}|,3}/(4\mu^2)) \right), \end{aligned} \tag{35}$$

being

$$\begin{aligned} r_{-1}^0 &= r_{4|\hat{k}|-1,0,0,\hat{k}}, \quad r_0^1 = r_{4|\hat{k}|,1,0,\hat{k}}, \quad r_1^2 = r_{4|\hat{k}|+1,2,0,\hat{k}}, \\ r_1^0 &= r_{4|\hat{k}|+1,0,0,\hat{k}}, \quad r_2^3 = r_{4|\hat{k}|+2,3,0,\hat{k}}, \quad r_2^1 = r_{4|\hat{k}|+2,1,0,\hat{k}}, \end{aligned}$$

and $z_m^{r_1,r_2}$ means the zero associated to the residue with $p = r_1 - r_2$ and $q = r_1 + r_2$. The values of such zeroes are given in Table 2, where we have omitted all the zeroes which can be easily obtained bearing in mind 2. of Lemma 4.2 and the proof of Lemma 4.3.

Therefore, disregarding the exponentially small errors, we have

$$\begin{aligned} \Delta p_2^{-1,1} &= \eta^4 \frac{32\kappa^3 \pi e^{-\frac{\pi\kappa}{2\eta}}}{3} c^{-1,1}, \quad \Delta p_1^{-1,1} = -\eta^3 \frac{16\kappa^4 \pi e^{-\frac{\pi\kappa}{2\eta}}}{3} c^{-1,1}, \\ \Delta p_2^{2,-1} &= -\eta^5 \frac{32\kappa^5 \pi e^{-\frac{\pi\kappa}{2\eta}}}{15} c^{2,-1}, \quad \Delta p_1^{2,-1} = \eta^4 \frac{16\kappa^6 \pi e^{-\frac{\pi\kappa}{2\eta}}}{15} c^{2,-1}, \\ \Delta p_2^{-3,2} &= -\eta^9 \frac{64\kappa^9 \pi e^{-\frac{\pi\kappa}{2\eta}}}{2835} c^{-3,2}, \quad \Delta p_1^{-3,2} = \eta^8 \frac{16\kappa^{10} \pi e^{-\frac{\pi\kappa}{2\eta}}}{2835} c^{2,-3}, \\ \Delta p_2^{5,-3} &= \eta^{15} \frac{128\kappa^{15} \pi e^{-\frac{\pi\kappa}{2\eta}}}{212837625} c^{5,-3}, \quad \Delta p_1^{5,-3} = -\eta^{14} \frac{64\kappa^{14} \pi e^{-\frac{\pi\kappa}{2\eta}}}{638512875} c^{5,-3}, \end{aligned} \tag{36}$$

where in $\Delta p_1^{k_2,k_3}$ and $\Delta p_2^{k_2,k_3}$ we have $\kappa = k_2\beta + k_3 > 0$.

Taking logarithms in the expression of $\left|\Delta p_j^{\hat{k}}\right|$ as

$$\Delta p_j^{\hat{k}} = c_2 \eta^{c_1} \exp\left(-\frac{\pi\kappa}{2\eta}\right),$$

we have

$$\ln|\Delta p_j^{\hat{k}}| = c_1 \ln\eta - \frac{\pi\kappa}{2\eta} + \ln c_2.$$

$\hat{k}$	r_1	r_2	$z_m^{r_1,r_2}$
$(-1,1)$	6	0	3.469693845669E+01
			5.303061543300E+00
$(2,-1)$	6	0	3.469693845669E+01
			5.303061543300E+00
	6	2	2.956465996625E+01
			2.435340033749E+00
	8	0	8.379949748426E+01
			2.400000000000E+01
			4.200502515735E+00
$(-3,2)$	10	0	1.572418695220E+03
			5.998113148991E+02
			1.919434643548E+02
			3.582652552545E+00
	10	2	1.512790260257E+03
			5.542062840986E+02
			1.577615527647E+02
			1.524190287856E+00
	12	0	2.562191202563E+03
			1.156781714946E+03
			4.853527054016E+02
			1.638706115368E+02
			3.180376555107E+00
	10	3	1.394784084281E+03
			4.665139699194E+02
			9.870194579882E+00

$\hat{k}$	r_1	r_2	$z_m^{r_1,r_2}$
$(5,-3)$	16	0	5.338544723145E+03
			2.923721794014E+03
			1.594101120838E+03
			8.160699537285E+01
			3.690382487994E+01
			1.317424269938E+01
			2.678173247920E+00
	16	2	5.273571454571E+03
			2.869239317844E+03
			1.547786191728E+03
			7.767638979731E+02
			3.361949385675E+02
			1.056506747430E+02
			1.079352457168E+00
	18	0	7.135876665263E+03
			4.154992860903E+03
			2.440728330460E+03
			1.381592489983E+03
			7.255793623335E+02
			3.346907864863E+02
			1.215212527420E+02
			2.508250369346E+00
	16	3	5.143931806252E+03
			2.760963959326E+03
			1.456423878475E+03
			7.004615831793E+02
			2.750118780768E+02
			6.320689468962E+00

Table 2: Zeroes z_m

Using (36), taking η small enough and the values of $r_{7,0,0,2}$, $r_{8,1,0,2}$, $r_{9,0,0,2}$, $r_{9,2,0,2}$, $r_{10,1,0,2}$, $r_{10,3,0,2}$, $r_{11,0,0,3}$, $r_{12,1,0,3}$, $r_{13,0,0,3}$, $r_{13,2,0,3}$, $r_{14,1,0,3}$, $r_{14,3,0,3}$, $r_{19,0,0,5}$, $r_{20,1,0,5}$, $r_{21,0,0,5}$, $r_{21,2,0,5}$, $r_{22,1,0,5}$, $r_{22,3,0,5}$, $r_{31,0,0,8}$, $r_{32,1,0,8}$, $r_{33,0,0,8}$, $r_{33,2,0,8}$, $r_{34,1,0,8}$, $r_{34,3,0,8}$, given in Table 1, we obtain the following table for c_1 and $\ln c_2$:

Δp_j	k_2	k_3	c_1	$\ln c_2$
Δp_1	0	1	0	1.837877066E+00
Δp_1	-1	1	2	-2.359941519E+00
Δp_1	2	-1	4	-8.427147970E+00
Δp_1	-3	2	8	-2.239514714E+01
Δp_1	5	-3	14	-4.088183294E+01
Δp_2	1	0	1	3.012236072E+00
Δp_2	-1	1	3	-1.185582513E+00
Δp_2	2	-1	5	-6.771577139E+00
Δp_2	-3	2	9	-1.956521731E+01
Δp_2	5	-3	15	-3.716522617E+01

(37)

which agree quite well with the values given in figure 2 (obtained numerically).

Now we return to the proof of the pending Lemma and auxiliar results. The proof of Lemma 4.3 is splitted in several parts.

Lemma 4.6 *For any $p \in (-\infty, q)$, $q \geq 1$, the zeroes z_j, for $j = 1, \ldots, \frac{q-1-\sigma}{2}$, are real.*

Proof

To prove Lemma 4.6, let us introduce

$$I_{p,q} := \mathrm{Res}(h_{p,q,\alpha/2i}(x), x = 0) = \frac{1}{2\pi i} \int_\Gamma \frac{e^{\alpha z} \cosh^p(z)}{\sinh^q(z)} dz, \tag{38}$$

where Γ is a closed curve of index 1 around zero. We have to distinguish several cases:

1. If $p = 0$ we want to study $I_{0,q}$. Integrating by parts (38), it is easily obtained by recurrence that

$$I_1 = 1, \quad I_2 =, \quad I_q = I_{q-2[\frac{q-1}{2}]} \frac{1}{(q-1)!} \prod_{l=1}^{[\frac{q-1}{2}]} (\alpha^2 - (q-2l)^2).$$

   Hence, for $j = 1, \ldots, [\frac{q-1}{2}]$, z_j, the zeroes are real. Of course, whenever we refer to zeroes, it should be clear from the context if we mean with respect to the variable α^2. The trivial zero at $\alpha = 0$, if it appears, will be usually disregarded.

2. Case $p \in (0, q)$. As well as in other cases to follow we shall need the recurrence

$$I_{p,q} = \frac{1}{q-1}(\alpha I_{p-1,q-1} + (p-1) I_{p-2,q-2}), \tag{39}$$

   which follows from (38). The relation (39) will be applied until we reach either $p = 0$ or $q = 0$. In the present case let

$$J_l = i^l I_{l,q-p+l} / I_{0,q-p}.$$

   We know from case 1. that the zeroes of $I_{0,q-p}$ are real. The recurrence (39) becomes

$$J_l = \frac{1}{q-p+l-1}(\beta J_{l-1} - (l-1) J_{l-2}), \quad l \geq 1 \quad \text{with} \quad J_0 = 1,\ J_1 = \frac{\beta}{q-p}, \tag{40}$$

   where $\beta = \alpha i$ (β is here a local variable inside the proof). The recurrence (40) is of the same type as the ones which appear for symmetric (in β) orthogonal polynomials. Hence all the zeroes of J_l are real, they occur in couples, $\pm\beta_j$, and furthermore $\beta = 0$ appears if l is odd. From the recurrence we have

$$I_{p,q} = I_{0,p-q} \frac{(q-p-1)!}{(q-1)!} \alpha^{p-2[p/2]} \prod_{j=1}^{[p/2]} (\alpha^2 + \beta_j^2),$$

   proving the assertion for this case, if we take $z_j = -\beta_j^2$.

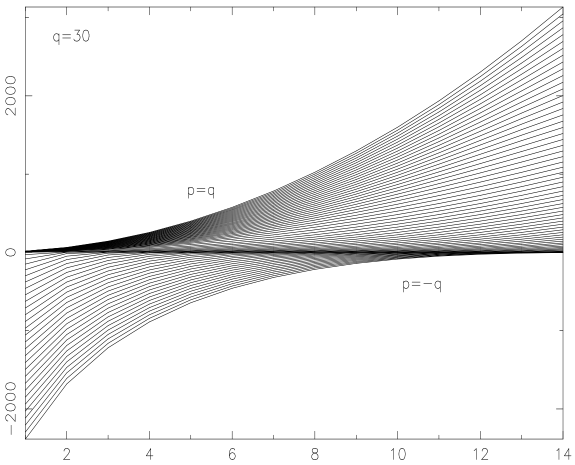

Figure 6: The behaviour of the zeroes for $p \in (-q, q)$, $q = 30$. On the horizontal axis we put the number of the zero, ordered by increasing value.

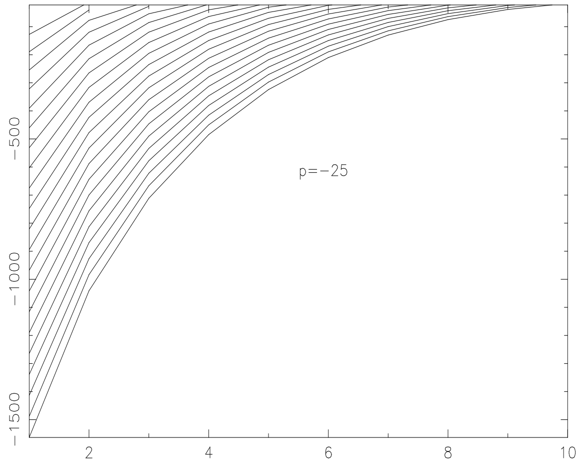

Figure 7: The behaviour of the zeroes for $q \in (4, |p|)$, $p = -25$. The values of q increase from top to bottom. Order of zeroes as in Figure 6.

3. If $p = q$, introducing $J_l = i^{l-1} I_{l,l}$ the recurrence (39) gives

$$J_l = \frac{\beta}{l-1} J_{l-1} - J_{l-2}, \quad l \geq 2, \quad \text{with} \quad J_0 = 0,\ J_1 = 1,$$

   where $\beta = \alpha i$. The same argument of case 2. applies until we reach J_q, which finishes the proof in that case.

4. If $p < 0$ we introduce $J_l = I_{p-q+l,l}$ and the recurrence reduces to

$$J_l = \frac{1}{l-1}(\alpha J_{l-1} + (p - q + l - 1) J_{l-2}), \quad l \geq 2, \quad \text{with} \quad J_0 = 0,\ J_1 = 1.$$

   We want J_q and, hence, we have to use the recurrence with $l = 2, \ldots, q$. As $p - q + l - 1 \leq p - 1 < 0$, a reasoning as before applies also now.

Hence, Lemma 4.6 is proved. □

Remark 4.7 *In Figures 6 and 7, we have plotted numerical evidence that the zeroes z_j for $j = 1, \ldots, [(q-1)/2]$, are real. The horizontal (vertical) axis contains the value of j (z_j). Looking at plots of this kind suggested most of the properties derived here.*

Having proved that all z_m are real, we are in situation to bound them, and hence, to prove the last claim of Lemma 4.3. This has been done by means of four Lemmas: Lemma 4.8, Lemma 4.10, Lemma 4.12 and Lemma 4.14, all of them working with the residue as given by a proper recursive formula derived from (28). Lemmas 4.8 and 4.10 (see later) give bounds for the zeroes z_m, when considering $\sqrt{z_m} \in \mathbb{R}$, for the cases $|p| \leq q$ and $p < -q$, respectively. On the other hand, Lemmas 4.12 and 4.14 give bounds for the zeroes z_m when considering $\sqrt{z_m} \in i\mathbb{R}$, for the cases $|p| \leq q$ and $p < -q$, respectively.

Given p, q, $q \geq 3$, $|p| < q$ and $w = -\mu^2$, we know that the residue is given by the recursive formula (28). From Lemma 4.6, we know that $w \in \mathbb{R}$. Let us consider $w = -a^2 q^2$, with $a > 0$

to be determined later on. Let us define

$$\hat{C}_j = (aq)^{-1}(-1)^{\frac{j}{2}}\overline{C}_j, \quad \text{if } j \text{ is even} \quad \text{and} \quad \hat{C}_j = (-1)^{\frac{j-1}{2}}\overline{C}_j, \quad \text{if } j \text{ is odd.}$$

With this definition, the recursive formula (28) takes the form: $\hat{C}_0 = 1$ and

$$\begin{aligned}(n-1)\hat{C}_{n-1} &= aq\sum_{k=0}^{[\frac{n-2}{2}]}\frac{\hat{C}_{n-2k-2}}{(2k+1)!}(-1)^k + \sum_{k=1}^{[\frac{n-1}{2}]}\frac{\hat{C}_{n-2k-1}}{(2k+1)!}(q-n+2k+1)(-1)^k \\ &- \frac{q-p}{2}\sum_{k=1}^{[\frac{n-1}{2}]}\frac{\hat{C}_{n-2k-1}}{(2k)!}(-1)^k,\end{aligned} \tag{41}$$

both for n odd and even. From (41) the following lemma holds:

Lemma 4.8 *If $a \geq \frac{7}{5}$ and $|p| \leq q$, then* $\dfrac{\hat{C}_j}{\hat{C}_{j-1}} > \dfrac{q}{j}, \quad j = 1, \ldots, q-1.$

Remark 4.9 *The optimal value of a is given by* $a = \dfrac{1}{\sin 1} - \dfrac{1}{q\sin^2 1} + \mathrm{O}\left(\dfrac{1}{q^2}\right).$

Proof

Notice that the last line of (41) is non–negative since all the $\hat{C}_k$ are increasing by the induction hypothesis. Therefore, if we prove that Lemma 4.8 holds for $p = q$, it holds for all $|p| \leq q$. First of all, let us point out that Lemma 4.8 holds for $n = 1$, $n = 2$ and $n = 3$ because for $a \geq \frac{7}{5}$,

$$\frac{\hat{C}_1}{\hat{C}_0} = aq > q, \quad \frac{\hat{C}_2}{\hat{C}_1} = \frac{aq}{2} - \frac{1}{12a} > \frac{q}{2} \quad \text{and} \quad \frac{\hat{C}_3}{\hat{C}_2} = \frac{aq}{3}\left(1 - \frac{1}{3a^2q - \frac{1}{2}}\right) > \frac{q}{3}.$$

For $n = 4, \ldots, q-1$, and setting $p = q$, we have:

$$\begin{aligned}\frac{\hat{C}_{n-1}}{\hat{C}_{n-2}} &= \frac{aq}{n-1}\left[1 - \frac{1}{3!}\frac{\hat{C}_{n-4}}{\hat{C}_{n-2}} + \frac{1}{5!}\frac{\hat{C}_{n-6}}{\hat{C}_{n-2}} - \frac{1}{7!}\frac{\hat{C}_{n-8}}{\hat{C}_{n-2}} + \ldots\right] \\ &+ \frac{1}{n-1}\left[-\frac{q-n+3}{3!}\frac{\hat{C}_{n-3}}{\hat{C}_{n-2}} + \frac{q-n+5}{5!}\frac{\hat{C}_{n-5}}{\hat{C}_{n-2}} + \ldots\right]\end{aligned} \tag{42}$$

All the terms in the first bracket of (42), except the first two, letting aside the factor $1/\tilde{C}_{n-2}$, can be written as a sum of couples:

$$\frac{1}{(2m-1)!}\hat{C}_{n-2m} - \frac{1}{(2m+1)!}\hat{C}_{n-2m-2}, \quad \text{for } m = 3, \ldots, [\tfrac{n}{2}],$$

which are positive by the inductive hypothesis.

In the second bracket of (42), all the terms except the first one, letting aside the factor $1/\hat{C}_{n-2}$, can be written as a sum of couples:

$$\begin{aligned}&\hat{C}_{n-2m-1}\frac{q-n+2m+1}{(2m+1)!} - \hat{C}_{n-2m-3}\frac{q-n+2m+3}{(2m+3)!} \\ &> \left(\frac{q}{n-2m-1}\frac{q}{n-2m-2}\frac{q-n+2m+1}{(2m+1)!} - \frac{q-n+2m+3}{(2m+3)!}\right)\hat{C}_{n-2m-3} \\ &> \frac{1}{(2m+3)!}\left((2m+3)(2m+2)(q-n+2m+1) - (q-n+2m+3)\right) > 0,\end{aligned}$$

for $m=2,\dots,\left[\frac{n-1}{2}\right]$. Therefore,

$$\frac{\hat{C}_{n-1}}{\hat{C}_{n-2}} > \frac{aq}{n-1}\left(1-\frac{1}{3!}\frac{(n-2)(n-3)}{q^2}\right)-\frac{(n-2)(q-n+3)}{3!q(n-1)} > \frac{q}{n-1}\left(\frac{5}{6}a-\frac{1}{6}\right)\geq\frac{q}{n-1}.$$

□

On the other hand, if $p<0$ with $|p|>q$ then we take $w=-(a\,|p|)^2$, with $a>0$ to be determined later on. Moreover, we define

$$C_j^* = (a|p|)^{-1}(-1)^{\frac{j}{2}}\overline{C}_j, \quad \text{if } j \text{ is even} \quad \text{and} \quad C_j^* = (-1)^{\frac{j-1}{2}}\overline{C}_j, \quad \text{if } j \text{ is odd.}$$

With this definition, the recursive formula (28) takes the form: $C_0^*=1$ and

$$\begin{aligned}(n-1)C_{n-1}^* &= a\,|p|\sum_{k=0}^{\left[\frac{n-2}{2}\right]}\frac{C_{n-2k-2}^*}{(2k+1)!}(-1)^k+\sum_{k=1}^{\left[\frac{n-1}{2}\right]}\frac{C_{n-2k-1}^*}{(2k+1)!}(q-n+2k+1)(-1)^k\\ &- \left(\frac{|p|+q}{2}\right)\sum_{k=1}^{\left[\frac{n-1}{2}\right]}\frac{C_{n-2k-1}^*}{(2k)!}(-1)^k,\end{aligned} \tag{43}$$

both for n odd and even. From (43) the following lemma holds:

Lemma 4.10 *If $a\geq\frac{7}{5}$ and $p<0$ with $|p|>q$, then* $\quad \dfrac{C_j^*}{C_{j-1}^*}>\dfrac{|p|}{j}, \quad j=1,\dots,q-1.$

The proof of lemma 4.10 is completely analogous to the respective one of lemma 4.8, taking into account that $p<0$ and $|p|\geq q$.

Remark 4.11 *Lemmas 4.8 and 4.10 imply that all the zeroes z_m related to $C_{q-1}(q,p,\alpha)$ satisfy*

$$-z_m\leq\frac{196}{25}\max\{q^2,p^2\}. \tag{44}$$

Let $w=a^2q^2$ and

$$\tilde{C}_j=\overline{C}_j, \quad \text{if } j \text{ is even} \quad \text{and} \quad \tilde{C}_j=\overline{C}_j(aq)^{-1} \quad \text{if } j \text{ is odd.}$$

With this definition, the recursive formula (28) takes the form: $\tilde{C}_0=1$ and

$$\tilde{C}_{n-1}=\frac{aq}{n-1}\sum_{k=0}^{\left[\frac{n-2}{2}\right]}\frac{\tilde{C}_{n-2k-2}}{(2k+1)!}+\sum_{k=1}^{\left[\frac{n-1}{2}\right]}\frac{\tilde{C}_{n-2k-1}}{(2k+1)!}\left(\frac{-(2qk+n-2k-1)+(p+q)(k+\frac{1}{2})}{n-1}\right) \tag{45}$$

both for n even and odd.

From (45) the following lemma holds:

Lemma 4.12 *If $a\geq\frac{3}{2}$, with $|p|\leq q$, then* $\quad \dfrac{\tilde{C}_j}{\tilde{C}_{j-1}}>\dfrac{q}{j}, \quad j=1,\dots,q-1.$

Remark 4.13 *The optimal value of a is given by the value of* $\quad a=\dfrac{\cosh 1}{\sinh 1}\left(1-\dfrac{1}{q}\right)+\mathrm{O}\left(\dfrac{1}{q^2}\right).$

Proof

First of all, let us note that since $p \geq -q$, then $(p+q)(k+\frac{1}{2}) \geq 0$, and therefore, if we prove Lemma 4.12 without this last term (that is considering case $p = -q$), then the proof for the case $p \geq -q+1$ is obvious.

Lemma 4.12 holds for $j=1$, $j=2$ and $j=3$ since for $a \geq \frac{3}{2}$,

$$\frac{\tilde{C}_1}{\tilde{C}_0} = aq > q, \quad \frac{\tilde{C}_2}{\tilde{C}_1} = \frac{aq}{2} - \frac{1}{6a} > \frac{q}{2} \quad \text{and} \quad \frac{\tilde{C}_3}{\tilde{C}_2} = \frac{aq}{3}\left(1 - \frac{q}{3\tilde{C}_2}\right) > \frac{q}{3}.$$

For $j = 4, \ldots q-1$, and setting $p = -q$, we have:

$$\begin{aligned} \frac{\tilde{C}_{n-1}}{\tilde{C}_{n-2}} &= \frac{aq}{n-1}\left[1 + \frac{1}{3!}\frac{\tilde{C}_{n-4}}{\tilde{C}_{n-2}} + \frac{1}{5!}\frac{\tilde{C}_{n-6}}{\tilde{C}_{n-2}} + \frac{1}{7!}\frac{\tilde{C}_{n-8}}{\tilde{C}_{n-2}} + \ldots\right] \\ &- \frac{1}{n-1}\left[\frac{2q+n-3}{3!}\frac{\tilde{C}_{n-3}}{\tilde{C}_{n-2}} + \frac{4q+n-5}{5!}\frac{\tilde{C}_{n-5}}{\tilde{C}_{n-2}} + \ldots\right] \end{aligned} \tag{46}$$

The terms in the brackets of (46) except the first ones in each bracket can be put together in couples as

$$\begin{aligned} &\frac{aq}{n-1}\frac{1}{(2m+1)!}\frac{\tilde{C}_{n-2(m+1)}}{\tilde{C}_{n-2}} - \frac{1}{n-1}\frac{\tilde{C}_{n-2m-3}}{\tilde{C}_{n-2}}\frac{1}{(2m+3)!}(2q(m+1)+n-2m-3) \\ &> \frac{q}{(n-1)\tilde{C}_{n-2}}\left(\frac{a}{(2m+1)!} - \frac{1}{(2m+2)!}\right)\tilde{C}_{n-2m-3} > 0, \quad m \geq 1, \end{aligned}$$

where we have used the inductive hypothesis and that $2q(m+1)+n-2m-3 < q(2m+3)$.

Therefore,

$$\frac{\tilde{C}_{n-1}}{\tilde{C}_{n-2}} > \frac{aq}{n-1} - \frac{\tilde{C}_{n-3}(2q+n-3)}{6(n-1)\tilde{C}_{n-2}} > \frac{aq}{n-1} - \frac{q}{2(n-1)} = \frac{q}{n-1}\left(a - \frac{1}{2}\right) \geq \frac{q}{n-1}. \qquad \square$$

On the other hand, if $p < 0$ with $|p| < q$, then we take $w = (a|p|)^2$. Moreover, we define

$$C_j^{**} = \overline{C}_j, \quad \text{if } j \text{ is even} \quad \text{and} \quad C_j^{**} = \overline{C}_j(a\,|p|)^{-1} \quad \text{if } j \text{ is odd.}$$

With this definition, the recursive formula (28) takes the form: $C_0^{**} = 1$ and

$$\begin{aligned} &(n-1)C_{n-1}^{**} = \\ &= a\,|p| \sum_{k=0}^{[\frac{n-2}{2}]} \frac{C_{n-2k-2}^{**}}{(2k+1)!} + \sum_{k=1}^{[\frac{n-1}{2}]} \frac{C_{n-2k-1}^{**}}{(2k+1)!}\left(-(2qk+n-2k-1) - (|p|-q)(k+\frac{1}{2})\right) \end{aligned} \tag{47}$$

both for n even and odd.

From (47) the following lemma holds:

Lemma 4.14 *If $a \geq \frac{3}{2}$ and $p < 0$ with $|p| > q$, then* $\dfrac{C_j^{**}}{C_{j-1}^{**}} > \dfrac{|p|}{j}, \quad j = 1, \ldots, q-1.$

Remark 4.15 *Lemmas 4.12 and 4.14 imply that all the zeroes z_m related to $C_{q-1}(q,p,\alpha)$ satisfy*

$$z_m \leq 9\max\{q^2, p^2\}. \tag{48}$$

Notice that equations (44) and (48) imply that $|z_m| \leq 9\max\{q^2,p^2\}$. Hence, Lemma 4.3 is proved. $\square$

5 Dominant terms for the formal splitting and a posteriori upper bounds. The splitting determinant in the simplest case

In this section, guided by results of the previous one, we make explicit assumptions on the form of some coefficients which contain the combinatorial part of the averaging process. Then we will derive the behaviour of the splitting vector as a function of η.

We look for the first occurrence of a given harmonic, $\hat{k}\cdot\psi$, as belonging to the leading–order terms of R_{n+1}. We summarize some data about the exponents appearing then: m must be $4|\hat{k}|-1$, $k_1=|\hat{k}|$, $l_1=0$ (see [7] for an inductive proof of these facts). From this we can see the contribution to Δp_j, $j=1,2$ in (31). We note also that the $\mathcal{P}(q)$ products in (32) must be estimated using $q=p=2|\hat{k}|$. We use Lemma 4.5 to bound his effect. Let us take for granted that $B^{1/2}=|\hat{k}|/\mu$ is small enough in the dominant terms (this fact will be checked later). Then, as $\binom{q-1}{2}\left(\frac{q}{3}-p\right)=-\frac{16}{3}|\hat{k}|^3(1+\mathrm{O}(|\hat{k}|^{-1}))$, the exponential correction in Lemma 4.5 is bounded by $\exp(\hat{B}|\hat{k}|)$, with $|\hat{B}|$ bounded. So, its effect is small and, in any case, it can be added to the effect produced by the $\hat{A}_{\hat{k}}$ coefficients. Finally, the contribution of the harmonic to the splitting, computed in that way, has a coefficient of the form

$$\hat{A}_{\hat{k}}\eta^{\sigma_j}\cdot\eta^{2|\hat{k}|}\exp\left(-\frac{\pi|\hat{k}\cdot\omega|}{2\eta}\right)\frac{(2|\hat{k}\cdot\omega|)^{2|\hat{k}|}}{(2|\hat{k}|)!},$$

where $\sigma_j=-2$ if $j=1$, $\sigma_j=-1$ if $j=2$. The coefficient $\hat{A}_{\hat{k}}$ depends on $\hat{k}$ and ω (and, in particular, on β), but not on η.

Collecting the contributions coming from different $\hat{k}$, we obtain for $d_1(\hat{\psi},\eta)$ and $d_2(\hat{\psi},\eta)$ expressions of the following type

$$\eta^{\sigma_j}\sum_{\hat{k}\in\mathbb{Z}^2\setminus\{0\}}A_{\hat{k}}\exp\left(-2|\hat{k}||\ln\eta|-\frac{\pi|\hat{k}\cdot\omega|}{2\eta}+2|\hat{k}|\ln\frac{|\hat{k}\cdot\omega|}{|\hat{k}|}\right)\sin(\hat{k}\cdot\hat{\psi}),\tag{49}$$

where the $A_{\hat{k}}$ coefficients are a minor modification of the previous $\hat{A}_{\hat{k}}$, but they are still bounded by $\exp(-M|\hat{k}|)<|A_{\hat{k}}|<\exp(M|\hat{k}|)$ for some $M>0$.

Only very few of the harmonics present in (49) have relevant coefficients, specially when η becomes small.

Let

$$\eta_n^*|\ln\eta_n^*|=\frac{\pi\sqrt{5}\beta^{2n+1}}{8},\quad \hat{\eta}_n^*|\ln\hat{\eta}_n^*|=\frac{\pi\sqrt{5}\beta^{2n+2}}{8},\quad (\eta_n^*,\hat{\eta}_n^*<0.1),\qquad n\geq 1.\tag{50}$$

It is clear that $\ldots>\eta_n^*>\hat{\eta}_n^*>\eta_{n+1}^*>\ldots$. It follows also

$$\ln\eta_n^*=(2n+1)\ln\beta(1+o(1)),\quad \ln\hat{\eta}_n^*=(2n+2)\ln\beta(1+o(1)),\quad o(1)=\mathrm{O}\left(\frac{\ln n}{n}\right).\tag{51}$$

Consider the function $c_\beta(\eta)$ defined on each one of the intervals $(\hat{\eta}_{n-1}^*,\hat{\eta}_n^*]$ by

$$c_\beta(\eta)=C_0\cosh\left(\frac{\ln\eta-\ln\eta_n^*}{2\ln\beta}\right),\quad C_0=\sqrt{\frac{8\pi(1+\beta)}{\sqrt{5}}}.\tag{52}$$

The function has a small discontinuity, $o(1)$ as in (51), at the points $\hat{\eta}_n^*$, but this is irrelevant. Furthermore, it tends to be $2|\ln\beta|-$periodic when $\eta \to 0$. We note that the maxima of c_β are attained at $\eta = \hat{\eta}_n^*$, having the limit value

$$\sqrt{\frac{8\pi(1+\beta)}{\sqrt{5}}}\cosh\left(\frac{1}{2}\ln\left(\frac{1+\sqrt{5}}{2}\right)\right) \approx 3.450078\sqrt{1+\beta} \approx 4.388567.$$

In the next statement $\mathcal{N}$ will denote one of the functions d_j, $j = 1, 2$ ignoring the η^{σ_j} factor.

Theorem 5.1 *Let*

$$\mathcal{N}(\hat{\psi}, \eta) = \sum_{\hat{k}\in\mathbb{Z}^2\setminus\{0\}} A_{\hat{k}} \exp\left(-2|\hat{k}||\ln\eta| - \frac{\pi|\hat{k}\cdot\omega|}{2\eta} + 2|\hat{k}|\ln\frac{|\hat{k}\cdot\omega|}{|\hat{k}|}\right)\sin(\hat{k}\cdot\hat{\psi}). \tag{53}$$

If β is the golden mean and there exist two constants, $c_1 < 0 < c_2$, such that

$$c_1 < \frac{\ln|A_{\hat{k}}|}{|\hat{k}|} < c_2, \tag{54}$$

then, for η small enough,

$$\begin{aligned}\mathcal{N}(\hat{\psi}, \eta) &= \sum_{\hat{k}\in\{\hat{k}^*, \hat{k}^{**}\}} A_{\hat{k}} \exp\left(-2|\hat{k}||\ln\eta| - \frac{\pi|\hat{k}\cdot\omega|}{2\eta} + 2|\hat{k}|\ln\frac{|\hat{k}\cdot\omega|}{|\hat{k}|}\right) \\ &\quad \times \left(\sin(\hat{k}\cdot\hat{\psi}) + \mathrm{O}\left(\exp\left(-g_1\frac{|\ln\eta|^{1/2}}{\eta^{1/2}}\right)\right)\right),\end{aligned} \tag{55}$$

where $\hat{k}^* = (F_n, -F_{n-1})$, and $\hat{k}^{**} = (F_{n+1}, -F_n)$, being F_{n-1}, F_n and F_{n+1} consecutive Fibonacci numbers with n increasing as η goes to zero and g_1 a positive constant. Moreover

$$|\mathcal{N}(\hat{\psi}, \eta)| < \exp\left(-[c_\beta(\eta) - g_3]\frac{|\ln\eta|^{1/2}}{\eta^{1/2}}\right), \tag{56}$$

$$|\mathcal{N}(\eta)| > \exp\left(-[c_\beta(\eta) + g_4]\frac{|\ln\eta|^{1/2}}{\eta^{1/2}}\right), \tag{57}$$

where g_3, g_4 are fixed positive constants, as small as desired, and c_β is given in (52) and (50).

Remark 5.2 *The number of leading terms depends on η. In small neighbourhoods of the values $\hat{\eta}_n^*$ (these vicinities are called critical intervals), there are two terms which dominate the Fourier series $\mathcal{N}(\hat{\psi}, \eta)$. In the complement, i.e., the intervals around the η_n^*, just one term dominates the splitting, but there are two subdominant terms of comparable size.*

We need to recall some definitions and facts from continued fraction (CF) theory. For each real number $\beta > 0$ there exists a continued fraction expansion (CFE):

$$\beta = [a_0, a_1, \ldots] = a_0 + \frac{1}{[a_1, a_2, \ldots]} = a_0 + \frac{1}{a_1 + \frac{1}{[a_2, a_3, \ldots]}} = [a_0, \ldots, a_{n-1}, [a_n, a_{n+1}, \ldots]],$$

where $a_i \in \mathbb{N}$ for all $i > 0$, $a_0 \in \hat{\mathbb{N}}$.

We remind that the indexes $\hat{k} = (k_2, k_3)$ for which $A_{\hat{k}}$ is not null, are of the form $k_3 \geq 1$, $k_2 \in \mathbb{Z}^*$. We pay special attention to the values of $\hat{k}$ for which $k_2 > 0$, $k_3 < 0$ or vice versa (these are the ones which can make $|\hat{k}\cdot\omega|$ small because $0 < \beta < 1$.)

Definition 5.3 *A fraction k_3/k_2, where $k_3, k_2 \in \mathbb{N}$, is called a best approximation, or convergent to β, if for any integer k_2' with $0 < k_2' < k_2$ and any integer k_3' one has:*

$$\min_{k_3' \in \mathbb{N}} |k_2'\beta - k_3'| > |k_2\beta - k_3|.$$

It is well–known that, for every β, there is an increasing sequence $\{k_2^{(n)}\}_{n\in\mathbb{N}}$ of positive integers with $k_2^{(0)} = 1$ and a sequence $\{k_3^{(n)}\}_{n\in\mathbb{N}}$ (positive if $\beta > 0$) such that $k_3^{(n)}/k_2^{(n)}$ are the best approximations to β, these sequences being finite for $\beta \in \mathbb{Q}$ and infinite if $\beta \notin \mathbb{Q}$. With some abuse of terminology we will apply the term "convergents" only to the members of the sequence $\{k_2^{(n)}\}_{n\in\mathbb{N}}$ whereas the members of the sequence $\{k_3^{(n)}/k_2^{(n)}\}_{n\in\mathbb{N}}$ will be referred as "best approximations".

The convergents to β are obtained from the CFE by the relations:

$$k_3^{(-2)} = 0, \quad k_2^{(-2)} = 1, \quad k_3^{(-1)} = 1, \quad k_2^{(-1)} = 0,$$

and for $n \geq 0$

$$k_3^{(n)} = a_n k_3^{(n-1)} + k_3^{(n-2)}, \quad k_2^{(n)} = a_n k_2^{(n-1)} + k_2^{(n-2)}.$$

Let $\|k_2\beta\| = \min_{k_3\in\mathbb{N}} |k_2\beta - k_3|$. Then, by Dirichlet's theorem, every best approximation $k_3^{(n)}/k_2^{(n)}$ to β satisfies

$$\left\|k_2^{(n)}\beta\right\| \leq \frac{1}{k_2^{(n+1)}}.$$

The following Propositions are well–known facts concerning best approximations. The proofs can be found in [5].

Proposition 5.4 *For $n \geq -2$, we have $k_2^{(n+1)}k_3^{(n)} - k_3^{(n+1)}k_2^{(n)} = (-1)^{(n+1)}$.*

Proposition 5.5 *If $\beta \in \mathbb{Q}$, β has precisely two simple CFE: One is of the form $[a_0, a_1, \ldots a_{n-1}, a_n]$ with $a_n \geq 2$ and the other is $[a_0, a_1, \ldots, a_{n-1}, a_n - 1, 1]$. If $\beta \notin \mathbb{Q}$ the CFE is unique.*

Proposition 5.6 *If $n \geq 1$, then for any k_2 with $k_2^{(n-1)} < k_2 < k_2^{(n)}$ there exist $(r_1, r_2) \in \mathbb{Z}$, with $|r_2| \geq 2$ if $r_1 = 0$ and otherwise $|r_1|, |r_2| \geq 1$, such that*

$$\|k_2\beta\| = |r_2| \left\|k_2^{(n-1)}\beta\right\| + |r_1| \left\|k_2^{(n)}\beta\right\|.$$

If β is the golden mean, this can be refined as follows

$$\|k_2\beta\| \geq 2\left(\left\|k_2^{(n-1)}\beta\right\| + \left\|k_2^{(n)}\beta\right\|\right),$$

the equal sign being achieved if and only if $k_2 = F_n + F_{n-3}$.

Moreover, if we define

$$x_n := \frac{1}{[a_n, a_{n-1}, \ldots a_1]} = \frac{k_2^{(n-1)}}{k_2^{(n)}} = \frac{1}{a_n + x_{n-1}}, \quad \text{and} \quad z_n := [a_{n+1}, a_{n+2}, \ldots] = a_{n+1} + \frac{1}{z_{n+1}},$$

then it follows that

Proposition 5.7

$$\left\|k_2^{(n)}\beta\right\| = \frac{1}{k_2^{(n)}(z_n+x_n)}, \quad \textit{and} \quad \left\|k_2^{(n-1)}\beta\right\| = \frac{z_n}{k_2^{(n)}(z_n+x_n)} = z_n\left\|k_2^{(n)}\beta\right\|.$$

Proof of Theorem 5.1

Let $\mathcal{N}(\hat\psi,\eta)$ (or $\mathcal{N}(\hat\psi)$ for shortness) be the function on the $2D$–torus, given by the Fourier series in (53) where $\hat\psi\in\mathbb{T}^2$, and the coefficients $A_{\hat k}=-A_{-\hat k}$ will be all non–zero, with the bounds given in (54).

First we need to introduce some auxiliar notation. Given a real number $\gamma>0$, consider the equation $\eta k^2\ln k=\gamma$ for η small enough. It is checked that it can be solved for k as

$$k=\left(\frac{2\gamma}{\eta|\ln\eta|}\right)^{1/2}\times\left(1+\mathrm{O}\left(\frac{\ln|\ln\eta|}{|\ln\eta|}\right)\right). \tag{58}$$

If we rewrite (53) as four separate sums, we can express $\mathcal{N}(\hat\psi)$ as follows (note that we assume $k_2^{(n)}>0$ or, if $k_2^{(n)}=0$ then $k_3^{(n)}>0$, the other terms being obtained by symmetry):

$$\sum_{k_2,k_3\in\mathbb{Z},|k_2\beta-k_3|\geq 1/2}+\sum_{|k_2\beta-k_3|<1/2}\left\{\sum_{k_3,k_2\in\mathbb{Z},k_2>k_{2,\eta}}+\sum_{n\geq 0,k_2^{(n)}\leq k_{2,\eta}}+\sum_{n\geq 0,k_2^{(n-1)}<k_2<\min(k_2^{(n)},k_{2,\eta})}\right\}, \tag{59}$$

the objects added in each sum being

$$\exp\left(\xi_{\hat k}|\hat k|-2|\hat k||\ln\eta|-\frac{\pi|\hat k\cdot\omega|}{2\eta}+2|\hat k|\ln\frac{|\hat k\cdot\omega|}{|\hat k|}\right)\sin(\hat k\cdot\hat\psi), \tag{60}$$

where $\xi_{\hat k}$ stands for $\ln|A_{\hat k}|/|\hat k|$ (and, hence, it is bounded by (54)) and where we introduce $k_{2,\eta}$ as the solution of $\eta k^2\ln k=\gamma_1$ with γ_1 to be determined later. Moreover, the last three sums, really have only one index, because for each integer $k_2>0$ there is only one k_3 such that $|k_2\beta-k_3|<1/2$. The third sum (the second inside $\{\}$) only includes the convergents $k_2^{(n)}$ to β and the fourth one (the third inside $\{\}$) all the k_2 that sit in between. To estimate the first sum we use that $|\hat k\cdot\omega|<|\hat k|$ and η is small enough, to conclude that

$$\begin{aligned}\left|\sum\nolimits_1\right| &\leq \exp\left(-\frac{\pi}{4\eta}\right)\sum_{\hat k\in\mathbb{Z}^2\setminus\{0\}}\exp\left(c_2|\hat k|-2|\hat k||\ln\eta|+2|\hat k|\ln\frac{|\hat k\cdot\omega|}{|\hat k|}\right)\\ &< \exp\left(-\frac{\pi}{4\eta}\right)\sum_{\hat k\in\mathbb{Z}^2\setminus\{0\}}\exp(c_2|\hat k|-2|\hat k||\ln\eta|)\leq\exp\left(-\frac{\pi}{4\eta}\right).\end{aligned} \tag{61}$$

Estimate (61) will turn out to be exponentially small in relation with the asymptotics of the third sum.

For the resonant sums we need bounds for $|\hat k|$ and for the small divisors $|k_2\beta-k_3|$. If $k_2=k_2^{(n)}=F_n$, a Fibonacci number, then $k_3=F_{n-1}$ and $|\hat k^{(n)}|=F_{n+1}$. As

$$F_n=(\beta^{-n}-(-1)^n\beta^n)/\sqrt5, \tag{62}$$

then it follows

$$|F_n\beta-F_{n-1}|=\frac{1-(-1)^n\beta^{2n}}{\sqrt5 F_n}=\frac{1+\mathrm{O}(F_n^{-2})}{\sqrt5 F_n}\quad\text{and}\quad F_{n+1}=F_n(\beta^{-1}+\mathrm{O}(F_n^{-2})). \tag{63}$$

From now on we shall neglect the $O(F_n^{-2})$ terms in (63) because, as we shall see later, its effect can be incorporated inside $\xi_{\hat{k}}$. On the other hand, for the resonant terms which are not of Fibonacci type, from Proposition 5.6 it follows the bound

$$|k_2\beta - k_3| \geq \frac{4}{\sqrt{5}k_2}(1 + O(k_2^{-2})). \tag{64}$$

The second sum (first inside {}), or sum of the resonant terms with $k_2 \geq k_{2,\eta}$, can be estimated as:

$$\begin{aligned}
\left|\sum\nolimits_2\right| &\leq \sum_{k_2 \geq k_{2,\eta}} \exp\left(c_2|\hat{k}| - 2|\hat{k}||\ln\eta| + 2|\hat{k}|\ln\frac{|\hat{k}\cdot\omega|}{|\hat{k}|}\right) \\
&< \sum_{k_2 \geq k_{2,\eta}} \exp\left(k_2(\hat{c}_2 - 2(1+\beta)|\ln\eta| - 2(1+\beta)\ln k_2)\right) \\
&< \sum_{k_2 \geq k_{2,\eta}} \exp\left(k_2(-3(1+\beta)|\ln\eta| + O(\ln|\ln\eta|))\right) \\
&< \exp\left((-3(1+\beta)(2\gamma_1)^{1/2} + o(1))\left(\frac{|\ln\eta|}{\eta}\right)^{1/2}\right),
\end{aligned}$$

if η is small enough. We have used $\left||\hat{k}| - (1+\beta)k_2\right| < 1/2$, the bounds following from (58), the constant $\hat{c}_2$, which is a minor modification of c_2 to account for some additional terms $O(k_2)$ inside the exponent, and the $o(1)$ terms which tend to 0 if $\eta \to 0$.

Now we estimate the resonant terms with $1 \leq k_2 < k_{2,\eta}$, which enter in the third and fourth sums. The number of such terms is large, but finite.

First let us bound the sum containing all the terms which are not Fibonacci numbers, that is, the last sum. Using the same ideas as for $\sum_2$ and the bound (64) we have

$$\left|\sum\nolimits_4\right| \leq \exp\left(\hat{c}_2 k_2 - 2(1+\beta)k_2|\ln\eta| - \frac{\pi}{2\eta}\frac{4}{\sqrt{5}k_2} - 4(1+\beta)k_2\ln k_2\right). \tag{65}$$

We shall bound each one of the terms in (65) (there are at most $k_{2,\eta} = O((\eta|\ln\eta|)^{-1/2})$ of them) by the worst one. To this end let us consider a real variable, x, instead of k_2 inside the exponential function in (65). Equating the derivative with respect to x to zero, we obtain

$$\eta x^2|\ln\eta|/2 + \eta x^2\ln x + o(1) = \frac{\pi\beta}{2\sqrt{5}}. \tag{66}$$

Let $\gamma = \eta x^2 \ln x$. Solving for x as in (58) and replacing in (66) we obtain $\gamma = \dfrac{\pi\beta}{4\sqrt{5}} + o(1)$ and from this the bound

$$\left|\sum\nolimits_4\right| \leq \exp\left(\left(-4\left(\frac{2\pi}{\beta\sqrt{5}}\right)^{1/2} + o(1)\right)\left(\frac{|\ln\eta|}{\eta|}\right)^{1/2}\right). \tag{67}$$

Already at this point, we see that the choice $\gamma_1 \geq \dfrac{16\pi\beta}{4\sqrt{5}}$ produces bounds of $|\sum_2|$ like the ones of $|\sum_4|$ and both of them are much larger than the bounds of $|\sum_1|$ if η is small.

So, we are basically left with $\sum_3$ to evaluate, that is, the second sum inside {} in (59). We must find the dominant terms and compare also them to the bound of $|\sum_4|$.

For the moment being we consider an expression as (65) but using (63) instead of (64) and neglecting the linear term $\hat{c}_2 k_2$, bounded uniformly in η. We also consider k_2 as a positive real number, x, despite we are interested in the values it takes at the F_n with $F_n < k_{2,\eta}$. First we look for the maxima and, hence, we have to minimize

$$2(1+\beta)x|\ln\eta| + \frac{\pi}{2\eta\sqrt{5x}} + (1+\beta)(x\ln x - x). \tag{68}$$

The first derivative of (68) with respect to x is a monotonically increasing function and its range covers $\mathbb{R}$. Hence the minimum is unique. Proceeding as before we obtain $\gamma = \gamma_F := \dfrac{\pi\beta}{16\sqrt{5}} + o(1)$ and therefore

$$x_{\max} = \left(\frac{2\gamma_F}{\eta|\ln\eta|}\right)^{1/2}\left(1+\mathrm{O}\left(\frac{\ln|\ln\eta|}{|\ln\eta|}\right)\right) \tag{69}$$

and (68) gives the value

$$\left(\frac{8\pi(1+\beta)}{\sqrt{5}}\right)^{1/2}\left(\frac{|\ln\eta|}{\eta}\right)^{1/2}(1+o(1)), \tag{70}$$

when $\eta \to 0$.

This already shows several things:

- The $\mathrm{O}(x)$ neglected terms behave like (69) and hence they can be included in the $o(1)$ terms in (70) for η small.
- The (absolute value of the numerical) coefficient in (70) is less, by a factor of 2, than the one in (67). Hence, all the contributions coming from $\sum_1, \sum_2$ and $\sum_4$ can be neglected in front of the ones in $\sum_3$. Furthermore one checks $\gamma_F < \gamma_1$.
- The value of $B^{1/2} = |\hat{k}| : \mu = \eta|\hat{k}|/|(\hat{k}\cdot\omega)| = \mathrm{O}(\eta k_2^2)$ is $\mathrm{O}(|\ln\eta|^{-1})$ for the dominant terms. This was one of the pending things to check.
- The neglected terms in the estimates of the small divisors contribute as $\mathrm{O}(1/(\eta k_2^4))$, again negligible. This was the other pending item.

As a conclusion, it is enough, to prove the theorem, to restrict the study to a few F_n numbers close to the optimal value x_{max}, to see that the difference between the behaviour for x_{max} and those F_n is not relevant. And that the F_n numbers which are not so close to x_{max} can also be neglected. For this, the "security factor" $\gamma_2/\gamma_F = 4$ will be useful (and much larger than what it is really needed).

We shall proceed in an inverse way. Let η_n such that $x_{\max} = F_n$. The expressions (62) and (69) tell us

$$\eta_n|\ln\eta_n| = 10\gamma_F\beta^{2n}\left(1+\mathrm{O}\left(\frac{\ln n}{n}\right)\right), \quad \eta_n = \frac{10\gamma_F\beta^{2n}}{2n|\ln\beta|}\left(1+\mathrm{O}\left(\frac{\ln n}{n}\right)\right), \quad \frac{\eta_{n+1}}{\eta_n} \to \beta^2 \tag{71}$$

if $n \to \infty$. We realize that η_n is nothing else than the value η_n^* defined before in (50), entering in the definition of c_β.

Now we consider the value of the term associated to F_n when η ranges around the values η_n^* given in (71). We want to express the coefficient in (60) as

$$\exp\left(-\hat{g}(w)\left(\frac{|\ln\eta|}{\eta}\right)^{1/2}\right) \tag{72}$$

for $\eta = \beta^w \eta_n^*$, $|w|$ bounded by a constant. Direct substitution in (60) gives

$$\hat{g}(w) = \cosh\left(\frac{w}{2}\right) + o(1).$$

From this it follows that, given η, we select n such that $\hat{\eta}_n^* < \eta \le \hat{\eta}_{n-1}^*$. We look now for the contribution of the term associated to F_n. It will be of the form (72) with $-1 < w \le 1$. If we are not too close to one of the extrema (i.e., we are not in one of the critical intervals) $|w|$ will be bounded away from 1. On the other side, the contributions of F_{n+j}, $|j| > 0$, will have $\hat{g}(2j - w)$ instead of $\hat{g}(w)$. Hence these terms can be neglected in front of the one coming from F_n. The difference in the exponents is $O((|\ln \eta|/\eta)^{1/2})$, enough to allow for a coefficient $A_{\hat{k}^{(n)}}$ of the form $c_1|\hat{k}^{(n)}|$ and for a coefficient $A_{\hat{k}^{(n+j)}}$ of the form $c_2|\hat{k}^{(n+j)}|$.

On the other hand, assume we are in one of the critical intervals. For definiteness, assume w close to 1. Then the contributions of the terms associated to F_n and F_{n+1} are comparable, and we have to keep both of them as dominant terms in $\mathcal{N}(\hat{\psi}, \eta)$. This proves all the parts of the Theorem, summarized in (55), (56) and (57). $\square$

Remark 5.8 *The entire character of H has produced the extra $|ln\,\eta|$ terms inside the exponent of the exponentially small bounds. This implies that one has to be more careful in the bounds that what is needed in the general analytic case. It follows also from the proof that one can be more generous in the bounds of the $A_{\hat{k}}$ coefficients. Indeed, anything which contributes to the exponents in quantities small compared to $|ln\,\eta|/\eta$, like $(|\hat{k}|^\alpha)!$ with $\alpha < 1$ could be allowed.*

Remark 5.9 *We want to point out that there exists numerical evidence that moving the value of the frequency β, some coefficients $A_{\hat{k}^{(n)}}$ which were expected to be the dominant, can be zero. This is due to the fact that the coefficients $A_{\hat{k}}$ are rational functions of β and implies that the assumption on the lower behaviour of the coefficients $A_{\hat{k}}$ can not be removed.*

Let us denote as $\mathcal{E}_{\hat{k}}$ the coefficient of $\sin(\hat{k}\cdot\psi)$ in $\mathcal{N}(\psi, \eta)$. If we turn to the splitting determinant, it is clear that if only one such term is used, and it is the same for both ΔI_1 and ΔI_2, its contribution to Υ is zero. Hence, at least two terms should be considered to show $\Upsilon \neq 0$ at the homoclinic points, say at $(0, 0)$. If η is not too close to some of the η_n^*, then the respective coefficients of the contributions of the two most relevant harmonics inside the exponent in (72) are of the form $\cosh(w/2)$ and $\cosh(w/2 - 1)$ if we assume, for definiteness, $0 < w_0 \le w \le 1$, w_0 being a small positive fixed number. The third contribution, in order of importance, comes from $\cosh(w/2+1)$ (or, eventually, from $\cosh(w/2-1)$ if $w = 1$). As $\cosh(w_0/2+1) < \cosh(w_0/2-1)$, this third contribution can be neglected.

Let $\hat{k}^*$ and $\hat{k}^{**}$ be the two dominant harmonics and we assume that the third (and subsequent ones, of course) are much less. The coefficient of $\sin(\hat{k}\cdot\psi)$ in ΔI_j is denoted as $\mathcal{E}_{\hat{k}}^{(j)}$ for $j = 1, 2$. Then we have

$$\Upsilon = 4\left[\mathcal{E}_{\hat{k}^*}^{(1)}\mathcal{E}_{\hat{k}^{**}}^{(2)} - \mathcal{E}_{\hat{k}^{**}}^{(1)}\mathcal{E}_{\hat{k}^*}^{(2)}\right] \times \{k_2^* k_3^{**} - k_2^{**} k_3^*\} \times \left(1 + \mathrm{O}\left(\exp\left(-g_5\left(\frac{|\ln \eta|}{\eta}\right)^{1/2}\right)\right)\right),$$

where the constant 4 appears from the parity and $g_5 > 0$, independent of η. The term inside $\{\ \}$ has absolute value 1, by the expression of the indices as Fibonacci numbers. If the expression inside $[\ ]$ is also not zero, then $\Upsilon \neq 0$. This turns out to be true because $\Delta I_1, \Delta I_2$ are the gradient of a *splitting potential*.

As a conclusion, the splitting determinant is non zero if η is not too close to some η_n^*, that is, if we exclude the case $0 \le w < w_0$. In this last case, there is a large dominant term but the next two subdominants are of comparable order of magnitude. Hence, they can cancel. The discussion is postponed to the end of next section.

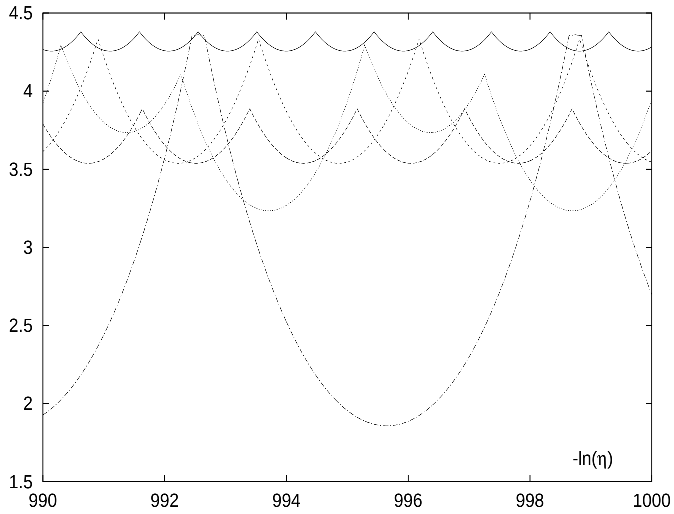

Figure 8: Values of c_β as a function of $|\ln\eta|$ for several quadratic irrationals.

The description of the behaviour of the dominant terms in the splitting, under the assumption (54) on the coefficients, requires the introduction of the function c_β as defined by (52) and (50). If other irrationals are used c_β should be defined correspondingly. As an example, if quadratic irrationals are considered, the function c_β is also periodic. Figure 8 shows plots of c_β as a function of $|\ln\eta|$ for $\beta_1 = (\sqrt{5}-1)/2$, $\beta_2 = \sqrt{2}-1$, $\beta_3 = \sqrt{3}-1$, $\beta_4 = (\sqrt{37}-4)/6$ and $\beta_5 = (\sqrt{122}-10)/2$. The corresponding quotients in the CFE are periodic, with periods [1], [2], [1, 2], [1, 2, 3] and [1, 1, 10], respectively. On the Figure we have selected the interval $|\ln\eta| \in [990, 1000]$ and on the left hand side the values of c_β are ordered as follows: $c_{\beta_1} > c_{\beta_4} > c_{\beta_2} > c_{\beta_3} > c_{\beta_5}$. Not all the best approximants give rise to dominant terms for some range of η. Some of them are "skipped", as occurs in the cases of β_3 and β_4 (but note that all the best approximants can be "seen" in the case of β_5). The corresponding periods in $\ln\eta$ tend to be $2|\ln\beta_1|$, $2|\ln\beta_2|$ in the first two cases and then $2\ln(2+\sqrt{3})$, $2\ln(6+\sqrt{37})$, $2\ln(11+\sqrt{122})$ in the remaining ones. It is easily checked that in all these cases the upper bound of the splitting is of the form

$$\exp\left(-(8\pi\underline{c}(1+\beta))^{1/2}\left(\frac{|\ln\eta|}{\eta}\right)^{1/2}\right), \tag{73}$$

where $\underline{c}$ is the best diophantine constant, that is, $\liminf\{|q\beta - p|q \text{ for } (p,q) \in \mathbb{Z}^2\}$. It seems natural to state the following.

Conjecture 5.10 *Let β be a constant type number, that is, the quotients a_n of the CFE are bounded. Then, for the Hamiltonian (1) and under the assumption (54) the 2D invariant tori have a splitting whose upper bound has a sharp estimate of the form (73), where $\underline{c}$ is the best diophantine constant. In general, the function c_β will be not periodic.*

A lower bound seems to depend strongly on the sequences of quotients to be found in the CFE of β. Furthermore there is the effect of $(1+\beta)^{1/2}$ (β could be chosen large).

6 Bifurcation of the levels of the splitting vector. Additional homoclinic points and the behaviour of the splitting determinant

From the discussion in the previous section, we have seen that for some values of η (the ones called critical values) two different consecutive Fibonacci-type harmonics give contributions of the same order. On this section, for $n \geq 0$, we will denote them as F_n instead of $k_2^{(n)}$, but some final discussion will be done for arbitrary irrational β. Let us consider the contribution to $\Delta x(\hat{\psi}, \eta)$, coming from the two dominant harmonics, of the form $(F_{j+1}, -F_j)$ and $(F_{j+2}, -F_{j+1})$, with coefficients c_1 and c_2:

$$\Delta x(\hat{\psi}, \eta) = c_1 \sin(\mathcal{X}) + c_2 \sin(\hat{\mathcal{X}}), \quad c_1 = c_1(\eta), \quad c_2 = c_2(\eta),$$

where

$$\mathcal{X} = F_{j+1}\psi_2 - F_j\psi_3, \quad \text{and} \quad \hat{\mathcal{X}} = F_{j+2}\psi_2 - F_{j+1}\psi_3.$$

The relation $\Delta x(\hat{\psi}, \eta) = 0$ defines a curve in $\mathbb{T}^2$. If, say, $|c_2/c_1|$ is small, then the $C_h^1(\eta)$ curve (see the end of section 2) is close to the line in $\mathbb{T}^2$ with slope F_{j+1}/F_j. Changes in the topology of $C_h^1(\eta)$ are produced when Δx, $\partial \Delta x/\partial \psi_2$ and $\partial \Delta x/\partial \psi_3$ are simultaneously zero, that is

1. $\Delta x = c_1 \sin(\mathcal{X}) + c_2 \sin(\hat{\mathcal{X}}) = 0,$
2. $\dfrac{\partial \Delta x}{\partial \psi_2} = c_1 F_{j+1} \cos(\mathcal{X}) + c_2 F_{j+2} \cos(\hat{\mathcal{X}}) = 0,$
3. $\dfrac{\partial \Delta x}{\partial \psi_3} = -c_1 F_j \cos(\mathcal{X}) - c_2 F_{j+1} \cos(\hat{\mathcal{X}}) = 0,$

which implies that

$$\begin{pmatrix} F_{j+1}\cos(\mathcal{X}) & F_{j+2}\cos(\hat{\mathcal{X}}) \\ F_j \cos(\mathcal{X}) & F_{j+1}\cos(\hat{\mathcal{X}}) \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{74}$$

If $\cos(\mathcal{X})\cos(\hat{\mathcal{X}}) \neq 0$, it follows from Proposition 5.4 that the determinant of the matrix in (74) is different from zero.

Hence, the unique non-trivial solution of (74) appears for $\cos(\mathcal{X}) = 0$ and $\cos(\hat{\mathcal{X}}) = 0$, that is for $m_1, m_2 \in \mathbb{Z}$ verifying

$$\mathcal{X} = \pm\frac{\pi}{2} + 2m_1\pi \quad \text{and} \quad \hat{\mathcal{X}} = \pm\frac{\pi}{2} + 2m_2\pi.$$

This leads to the solution

$$\psi_2 = \pm\frac{\pi F_{j-1}}{2}, \quad \psi_3 = \pm\frac{\pi F_j}{2} \quad \text{and} \quad |\sin(\mathcal{X})| = |\sin(\hat{\mathcal{X}})| = 1,$$

which implies that the condition to have a bifurcation of $C_h^1(\eta)$ is

$$| c_1 | = | c_2 | \ .$$

The same occurs for ΔI_2. In this case, we have that the general contribution to $\Delta I_2(\hat{\psi}, \eta)$ given by the two dominant Fibonacci–type harmonics with coefficients d_1, d_2 is:

$$\Delta I_2(\hat{\psi}, \eta) = d_1 \sin(\mathcal{X}) + d_2 \sin(\hat{\mathcal{X}}), \quad d_1 = d_1(\eta), \quad d_2 = d_2(\eta).$$

Again the curve C_h^2 given by $\Delta I_2(\hat{\psi}, \eta) = 0$, is a curve in $\mathbb{T}^2$. With the same argument as above, changes in the topology of C_h^2 are produced if and only if $|d_1| = |d_2|$. Then the values of the arguments, $\mathcal{X}$, $\hat{\mathcal{X}}$, must belong to $\{\frac{\pi}{2}, -\frac{\pi}{2}\}$ and the corresponding values of psi_2, ψ_3 are multiples of $\frac{\pi}{2}$.

Going back to the numerical results, it is seen that a bifurcation is produced for values of η close to 0.0621 and to 0.0281, in the case of Δx, and close to 0.2211 and to 0.0295 in the case of ΔI_2 (see Figure 5).

If the analytic approximations given in (37) are used, the critical values of η are, respectively, 0.061345, 0.028, 0.00675 and 0.002614 for Δx, and 0.2163, 0.02933, 0.007 and 0.002664 for ΔI_2. The moderate lack of agreement is due to the fact that there are exponential terms (see Lemma 4.5) and higher order terms missing in (37). If we denote by η_1, η_2, η_3 and η_4 the above theoretical values of η for which a bifurcation takes place for Δx and ΔI_2, respectively, then

$$\frac{\eta_1}{\eta_2} = \begin{cases} 2.191 & \text{for } \Delta x \\ 7.375 & \text{for } \Delta I_2 \end{cases}, \quad \frac{\eta_2}{\eta_3} = \begin{cases} 4.415 & \text{for } \Delta x \\ 4.191 & \text{for } \Delta I_2 \end{cases} \quad \text{and} \quad \frac{\eta_3}{\eta_4} = \begin{cases} 2.582 & \text{for } \Delta x \\ 2.628 & \text{for } \Delta I_2 \end{cases}$$

Notice that the quotient η_n/η_{n+1} for $n = 1, 2$ is far away from β^{-2}, while for $n = 3$ it is close to β^{-2}. As far as n increases the possible irregularities introduced by the values of $A_{\hat{k}}$ become negligible.

It is important to notice that from Theorem 5.1, if the successive bifurcations are produced for values of η equal to $\eta_1, \eta_2, \ldots$ one has that

$$\lim_{n\to\infty} \frac{\eta_n}{\eta_{n+1}} = \beta^{-2}.$$

Indeed, they occur for the values of $\eta_n = \hat{\eta}_n^*(1 + o(1))$, $n \in \mathbb{N}$, introduced in (50).

However, one can also give a direct proof of the value of such quotient from the criterium of being η a critical value, when taking into account only the dominant part of the Melnikov function given in (33), (34) and (35). This is what the following Lemma claims:

Lemma 6.1 *In the same hypothesis as in Theorem 5.1, if the successive bifurcations are produced for values of η equal to $\eta_1, \eta_2, \ldots$, one has*

$$\lim_{n\to\infty} \frac{\eta_n}{\eta_{n+1}} = \beta^{-2}.$$

Proof

Notice that η is a value of bifurcation if the following condition holds:

$$\begin{aligned} 2F_{n+1}\ln\eta - \frac{\pi|F_n\beta - F_{n-1}|}{2\eta} + 2F_{n+1}(\ln|F_n\beta - F_{n-1}| - \ln F_{n+1}) + \xi_n F_{n+1} = \\ 2F_{n+2}\ln\eta - \frac{\pi|F_{n+1}\beta - F_n|}{2\eta} + 2F_{n+2}(\ln|F_{n+1}\beta - F_n| - \ln F_{n+2}) + \xi_{n+1}F_{n+2}, \end{aligned}$$

where ξ_n and ξ_{n+1} are bounded real numbers which account for the contribution of $A_{\hat{k}}$ (essentially bounding $|\xi_n|, |\xi_{n+1}|$ by some M, see Theorem 5.1), for the missing e factor (see (49)) and for the neglected last term inside the function exp in (49). Bearing in mind (63), putting all the terms as a function of F_n, using (62) and neglecting F_n^{-1} in front of F_n, we obtain

$$-\frac{\pi}{2\eta}\frac{\beta^2}{\sqrt{5}F_n} = 2F_n\ln\eta + F_n\left(\frac{6-2\beta}{\beta^2}\ln\beta - \ln 5 - 4\ln F_n + \frac{\xi_{n+1}}{\beta} - \xi_n\right).$$

Letting $A = \dfrac{\pi\beta^2}{4\sqrt{5}}$ and being B a bounded quantity, it follows that we can obtain the value $\eta = \eta_n$, for which the bifurcation takes place, by solving

$$\eta = \frac{A}{F_n^2\,(2\ln F_n - \ln\eta + B)\ .} \tag{75}$$

In order to estimate the behaviour of η_n/η_{n+1} we need to solve (75). We proceed as in (58) with some detail. Let $\gamma = \eta F_n^2 \ln F_n$. Then (75) can be written as

$$\gamma = \frac{A}{4 + (\ln(\ln F_n) + B - \ln\gamma)/\ln F_n}, \tag{76}$$

which has an unique solution, γ_n, in $[\gamma^{(1)}, \gamma^{(2)}] := [A/5, A/3]$. Indeed, writing (76) as $\gamma = g(\gamma)$, we check $g(\gamma^{(1)}) > \gamma^{(1)}$, $g(\gamma^{(2)}) < \gamma^{(2)}$ if n is large enough, for any fixed B. It is clear that g is a contraction and that $\gamma_n \to A/4$ if $n \to \infty$. This implies Lemma 6.1, because

$$\lim_{n\to\infty} \frac{\eta_n}{\eta_{n+1}} = \lim_{n\to\infty} \frac{\gamma_n}{\gamma_{n+1}} \cdot \frac{F_{n+1}^2 \ln F_{n+1}}{F_n^2 \ln F_n} = \beta^{-2}.$$

□

At the bifurcation some of the orbits associated to $C_h^j(\eta)$, $j = 1, 2$, are no longer transversal. It is precisely at those orbits where the change of topology of $C_h^j(\eta)$ is produced. Figure 5 displays the $C_h^j(\eta)$, $j = 1, 2$ curves for some selected values of η. Note that case (l) in figure 5 is similar to what is obtained by direct application of Melnikov method to the initial Hamiltonian, that is, the classical Arnold situations. The other cases are uncovered by a naive direct use of Melnikov formulas.

Now we are interested in the possible appearance of homoclinic points besides the ones at $\psi_2, \psi_3 = 0 \pmod{\pi}$ which are always present due to the symmetry. In the forthcoming discussion we will assume that β is an irrational number (in general different from the golden mean) and that the dominant harmonics in the splitting vector correspond to the best approximants to β. We shall also discuss on the possible zeros of the splitting determinant.

If only the same two dominant harmonics in ΔI_2 and ΔI_3 are relevant, that is, for example

$$\begin{aligned} \Delta I_2 &= A_2 \sin(p_n\psi_2 - q_n\psi_3) + B_2 \sin(p_{n+1}\psi_2 - q_{n+1}\psi_3), \\ \Delta I_3 &= A_3 \sin(p_n\psi_2 - q_n\psi_3) + B_3 \sin(p_{n+1}\psi_2 - q_{n+1}\psi_3), \end{aligned}$$

letting $x = \sin(p_n\psi_2 - q_n\psi_3)$ and $y = \sin(p_{n+1}\psi_2 - q_{n+1}\psi_3)$, we have the following linear system

$$\begin{pmatrix} A_2 & B_2 \\ A_3 & B_3 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{77}$$

If $A_2B_3 \neq B_2A_3$, the only possible solution is $x = y = 0$ which implies

$$\hat{\psi} = (l_1\pi, l_2\pi), \quad l_1, l_2 \in \mathbb{N}.$$

That is, the only homoclinic points are the ones coming from parity. Taking into account that ΔI_2, ΔI_3 appear as the gradient of a *splitting potential*, the coefficients A_2, A_3 are proportional to p_n, q_n, while B_2, B_3 are proportional to p_{n+1}, q_{n+1}. This implies that the determinant in (77) is non–zero. The same argument shows that the splitting determinant is also non–zero. The case with three harmonics, one dominant, two subdominant of similar size, and the other much less important, is quite different.

Proposition 6.2 *Assume that the ΔI_2 and ΔI_3 appear as the gradient of a function that, after a suitable scaling of the dominant term, is of the form*

$$-c_n - \lambda(\eta)c_{n+1} - \delta(\eta)c_{n-1} + o(\lambda(\eta)^2 + \delta(\eta)^2), \tag{78}$$

where $q_{n-1}/p_{n-1}, q_n/p_n$ and q_{n+1}/p_{n+1} are consecutive best approximations to some β, the scaled coefficients $\lambda(\eta)$ and $\delta(\eta)$ are $\ll 1$ and c_m denotes $\cos(p_m\psi_2 - q_m\psi_3)$. Then, if there exists η' such that $\kappa(\eta) := \lambda(\eta) \pm \delta(\eta)$ satisfies $\kappa(\eta') = 0$ and $\kappa(\eta)$ changes from $-m\delta(\eta)^2$ to $m\delta(\eta)^2$ in a neighbourhood of η' (m larger than a constant to be found below) the following holds

1. *For some η close to η', say η'', the splitting determinant at the homoclinic points $(0,0)$ and (π,π) is zero if the $+$ sign is used in κ. If the $-$ sign is used then the splitting determinant is zero at $(\pi,0)$ and $(0,\pi)$.*

2. *On a neighbourhood of $\eta = \eta'$ there are additional homoclinic points. The splitting determinant on them is non–zero for $\eta = \eta''$.*

Remark 6.3 *In the golden mean case, the assumption on the smallness of the terms beyond the subdominant ones is satisfied. The values of $|\lambda(\eta)|$ and $|\delta(\eta)|$ are of the order of* $\exp\left(-a\frac{|\ln\eta)|^{1/2}}{\eta^{1/2}}\right)$, *where $a = C_0(\cosh(|\ln\beta|/2) - 1)$ with C_0 as in (52), while the order of the next terms has a similar form with $a = C_0(\cosh(3|\ln\beta|/2) - 1)$. However, from (36), (35) and table 1 we have that, for the first harmonics, the signs turn out to be equal. So $\lambda(\eta) + \delta(\eta) \neq 0$, but then $\lambda(\eta) - \delta(\eta)$ should be zero (the one or the other are zero if $|\lambda(\eta)| = |\delta(\eta)|$. For other irrationals it can happen that the three more relevant harmonics do not correspond to consecutive best approximations (see the end of the previous section).*

Proof

We restrict the study to the $(0,0)$ case, the others being similar. So the sign $+$ is assumed in κ. A computation of the splitting determinant, using that q_m/p_m are best approximations, gives the value $\lambda(\eta)c_nc_{n+1} + \delta(\eta)c_nc_{n-1} + \mathrm{O}(\lambda(\eta)\delta(\eta))$. If $\hat{\psi} = (0,0)$ and $\eta = \eta'$ the dominant contribution is zero. The condition on the variation of $\kappa(\eta)$ ensures the existence of a nearby η'' where the claim holds.

To look for other homoclinics we skip for the moment the terms beyond the subdominant ones and we write the conditions

$$\begin{aligned} p_ns_n + \lambda p_{n+1}s_{n+1} + \delta p_{n-1}s_{n-1} &= 0, \\ q_ns_n + \lambda q_{n+1}s_{n+1} + \delta q_{n-1}s_{n-1} &= 0, \end{aligned} \tag{79}$$

where s_m denotes $\sin(\gamma_m)$, $\gamma_m = p_m\psi_2 - q_m\psi_3$ and in λ and δ we skipped the dependence in η, for shortness. It is clear that one should have s_n small. Assume γ_n close to zero (if close to π everything is similar). Let a_{n+1} the $(n+1)$–th quotient of the CFE of β, so that $p_{n+1} = a_{n+1}p_n + p_{n-1}$ and similar for q_{n+1}. The system (79) is equivalent to

$$\begin{aligned} \delta a_{n+1}\sin(\gamma_{n-1}) &= \gamma_n, \\ \lambda\sin(\gamma_{n+1}) + \delta\sin(\gamma_{n-1}) &= 0. \end{aligned} \tag{80}$$

Using $\gamma_{n+1} = \delta a_{n+1}^2 \sin(\gamma_{n-1}) + \gamma_{n-1}$ in the second equation in (80), introducing c by means of $\lambda + \delta = c\delta^2$ and collecting the dominant terms in δ^2, we find that, beyond the homoclinic at

$(0,0)$, two new homoclinics appear with $\cos(\gamma_{n-1}) = c/a_{n+1}^2$. If $\eta = \eta''$ (essentially $c = 0$) the splitting determinant at them is $a_{n+1}^2\delta^2 + \mathrm{O}(\delta^3)$. Note that this is not the true value, because initially everything has been scaled by the value of the dominant term in (78). The effect of the terms beyond the subdominant ones can be taken into account using the smallness assumption made in (78) and a routine application of the Implicit Function Theorem, for η small enough. □

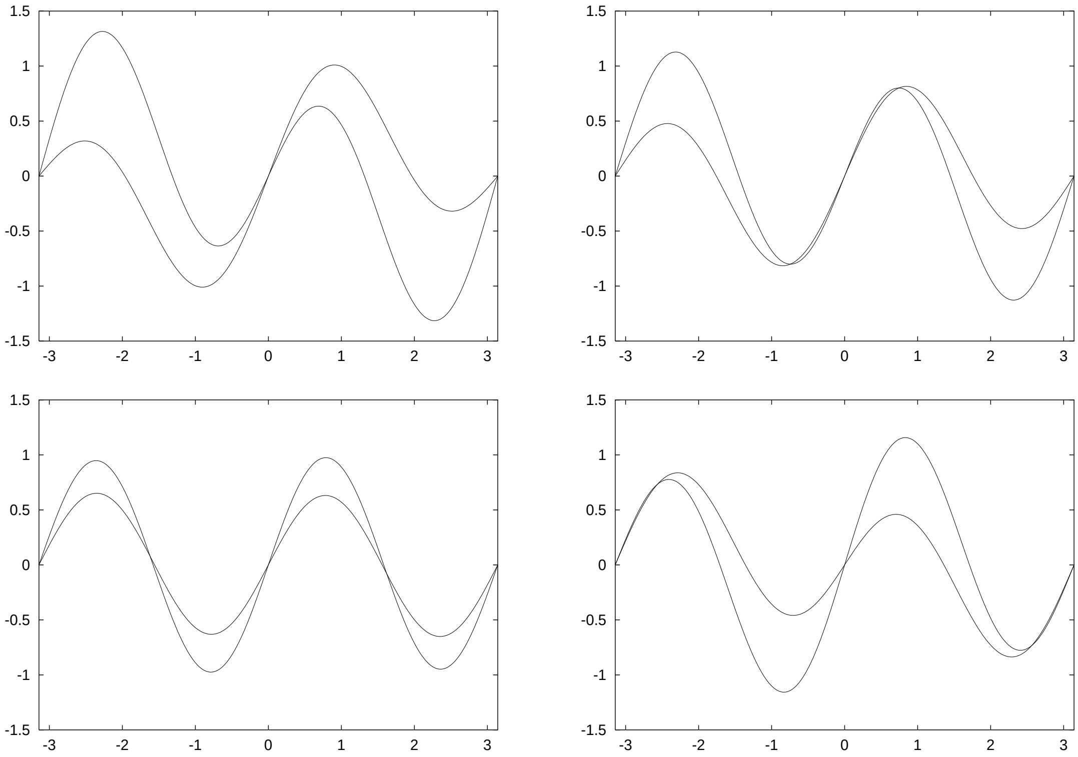

Figure 9: Additional homoclinic points. See the text for explanation.

An illustration of the apparition of additional homoclinic points is presented in Figure 9. The value of η decreases from left to right and from top to bottom. The lines where $\Delta I_2 = 0$ and $\Delta I_3 = 0$ are plotted. We display ψ_2 as horizontal coordinate and $\psi_3 - \psi_2 - \pi$, subtracting a suitable multiple of $\sin(\psi_2)$ and multiplying by a (big) scaling factor to make evident the separation between both curves, as vertical one. On the upper left part only the homoclinics at $\hat{\psi} = (\pi, 0)$ and $(0, \pi)$ exist. On the upper right two new homoclinics are born, bifurcating from the center. They move towards $\psi_2 = \pm\pi$ in the lower figures. At the bifurcation the splitting determinant is zero. Compare with Figure 1, cases (a) and (f).

We can also ask for the range of existence of these additional points. For this discussion we assume that we are in the golden mean case. Around η' the dominant behaviour of λ and δ is

$$\begin{aligned} \lambda(\eta) &= \exp\left(-C_0\left(\cosh(|\ln\beta|) - \sinh(|\ln\beta|)\tfrac{\Delta\eta}{2\eta'}\right)h(\eta)\right), \\ \delta(\eta) &= \exp\left(-C_0\left(\cosh(|\ln\beta|) + \sinh(|\ln\beta|)\tfrac{\Delta\eta}{2\eta'}\right)h(\eta)\right), \end{aligned} \tag{81}$$

where $\Delta\eta = \eta - \eta'$ and $h(\eta) = (|\ln\eta|/\eta)^{1/2}$. From the condition $\lambda(\eta) \pm \delta(\eta) = \pm\delta(\eta)^2$ (now $a_{n+1} = 1$) and (81) we obtain the dominant terms

$$\Delta\eta = \frac{\eta' \exp(-C_0 \cosh(|\ln\beta|) h(\eta'))}{h(\eta') 2 \sinh(|\ln\beta|)}. \tag{82}$$

This clearly shows that the successive intervals of existence of additional homoclinic points decrease very quickly when $\eta \to 0$. The expression (82) gives that each interval is of the order of the power β^{-1} of the previous one.

Remark 6.4 *The existence of points where the splitting determinant is zero can also be proved, at least in the golden mean case, by the changes in the topology of the curves* $\Delta_1 = 0$ *and* $\Delta_2 = 0$. *Between two consecutive bifurcations of the type described at the beginning of this section, either at* $(0,0)$ *and* (π,π) *or at* $(\pi,0)$ *and* $(0,\pi)$, *these curves most cross each other. At the crossings we are in the situation studied in Proposition 6.2.*

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