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 partially hyperbolic invariant tori. We mainly focus on the tori 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 the contribution of each harmonic is computed after a suitable number of averaging steps, depending on the harmonic. 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.

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1 Introduction and statement of results

1.1 The problem and its motivation

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, known as Arnold's diffusion. This is a classical example which displays a (very slow) drift of the actions for small values of ε, provided μ is small enough. 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 the diffusion mechanism, he used the Poincaré–Melnikov integrals to measure the splitting. The integrals turn 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 if 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 splitting 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. This is a natural starting point. Indeed, consider an integrable system. Adding a perturbation the more important effects will be produced at the resonances. It is reasonable to denote as ε a measure of the size of the perturbation at a simple resonance, and $\varepsilon\mu$ as a measure of the next terms in the perturbation. If these are of the order of ε^2 we have $\mu = \varepsilon$. The parameter μ could also be a power of ε.

In the study of realistic models, we are faced to many physical problems which 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.

Another "practical reason" to consider the case $\mu = \varepsilon$ is that we want to produce numerical estimates of the splitting. Using $\mu = \varepsilon^p$ with some $p > 1$ or μ exponentially small in ε, the range of values of ε that one could explore will be quite narrow, due to numerical difficulties in computing very small quantities. This can be overcome using arbitrary precision arithmetics, but for the moment being we prefer to keep things as simple as possible.

From the mathematical point of view, it is clear that the case $p = 1$ is very interesting because then the perturbation is large. Therefore, from now on, and for scaling purposes, we set $\mu = \varepsilon = \eta^2$. Moreover, we claim that the method proposed here also works with $\mu = \varepsilon^p$ with $p > 1$.

The manifold $\mathbb{T}_\beta$, given by $x = y = 0$, $I_2 = \beta$, $I_3 = 0$, is an invariant two-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. This information will give us a description of the qualitative phenomena and, after future work, a fairly complete description of the dynamics on a vicinity of the former separatrices.

1.2 The present approach to measure the splitting

In order to give an effective measure of the splitting of separatrices several analytical tools have been developed. A very popular tool is known as Melnikov method. The main idea behind this method goes back to Poincaré [10], although it is usually attributed to Melnikov [9]. It reduces to estimate the effect of the first order variational equations with respect some small parameter along the separatrices of the unperturbed problem. Melnikov developed a computable formula (in terms of an integral) for the first order term of the distance between the perturbed invariant manifolds. However, when the splitting turns out to be exponentially small with respect to the perturbation parameter, it cannot be taken for granted, in general, that Melnikov method gives the correct estimates of the splitting, due to its perturbative character, and more sophisticated analytical tools are required. The most common method consists in computing the effective measure of the exponentially small splitting by checking the validity of the Melnikov prediction, that is, by justifying that one can bound the difference between the splitting and the prediction by some amount which is relatively small.

In particular, if the perturbation is a trigonometric polynomial like in (1), this method is also unsuccessful: the standard Melnikov function cannot give all the dominant terms of the splitting, since it only accounts for a finite number of harmonics. A direct application gives exactly the formulas found by Arnold in [1]. Higher order variationals lead to new harmonics (by linear combinations of the initial ones) which can be very close to resonance. From one side these harmonics will have amplitudes which contain higher order powers of η, but from the other side the corresponding frequencies can be very small. Hence the exponentially small term can be close to 1 and give large contributions to the splitting. One has to "optimize" with respect to the harmonic giving larger contributions (see, e.g., a presentation of this idea in [14]). Therefore we need to modify Melnikov's approach in order to get realistic estimates of the splitting.

To be guided on how to modify Melnikov's approach, 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 and give contributions which are larger than the ones obtained before. Furthermore a close to the identity transformation has no essential effect on the geometric objects. Hence, the measure of the splitting in the new variables is essentially the same.

The main ideas of this paper, concerning evaluation of the splitting, are:

- Instead of looking for estimates of the splitting at once, we look for the contributions of the different harmonics to the splitting, individually.
- A given harmonic can be not present in the initial Hamiltonian. It can appear when some steps of averaging are carried out. After every step of averaging the current Hamiltonian contains an integrable part and a remainder. Inside the remainder there are terms containing different powers of η. The *leading terms of the remainder* are the ones which have the smaller power of η as factor. Then a number of steps of averaging are carried out until the desired harmonic appears as one of the leading terms for the first time.

- We proceed then to compute the contribution of this harmonic to the splitting by using Melnikov's approach. The Melnikov integral is computed, hence, after a suitable number of steps of averaging which depends on the harmonic whose contribution we want to obtain. We will denote this procedure as *adapted Melnikov function.*

- The contribution of the different harmonics depends on η. Then, for a given value of η we study which are the dominant contributions to the splitting. The current dominant harmonics depend on η. They are the same on some interval, but when $\eta \to 0$ the order of the dominant harmonics increases and tends to infinity. Correspondingly, the number of averaging steps to have these harmonics as leading terms increases when $\eta \to 0$.

In this way the *most relevant resonances* for every range of values of η are put in evidence. The dominant terms in the splitting are, of course, related to the approximants of β. But for a general diophantine β (or even for constant type numbers, see the end of section 5 for some examples with quadratic irrationals and Conjecture 5.10) some of the best approximants can be not present as dominant harmonics for any value of η.

Using a heuristic approach we can say that one has to give the initial harmonics the opportunity to interact and create new harmonics (or new relevant contributions to an harmonic already present). To detect analytically the contribution of a given harmonic from the initial Hamiltonian we could use a cumbersome higher order Melnikov approach based on higher order variational equations. The desired object is hidden in deep levels of the variationals. Using the suitable number of steps of averaging first, it appears as a leading term in the remainder and the usual first order Melnikov approach is able to catch it.

1.3 Preliminaries

The Hamilton's canonical equations corresponding to (1) are:

$$\begin{aligned}
\dot{y} &= \frac{\partial H}{\partial x} = x, \quad \dot{x} = -\frac{\partial H}{\partial y} = \eta^2 \sin y \left(1 + \eta^2(\cos\theta_2 + \cos\theta_3)\right), \\
\dot{\theta}_2 &= \frac{\partial H}{\partial I_2} = I_2, \quad \dot{I}_2 = -\frac{\partial H}{\partial \theta_2} = \eta^4 \sin\theta_2(\cos y - 1), \\
\dot{\theta}_3 &= \frac{\partial H}{\partial I_3} = 1, \quad \dot{I}_3 = -\frac{\partial H}{\partial \theta_3} = \eta^4 \sin\theta_3(\cos y - 1).
\end{aligned} \tag{2}$$

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 and lower separatrices of the pendulum cross a two-dimensional torus with frequencies $\omega = (\beta, 1)$.

We recall that the lower 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 $z^u = (y = \pi, x = x^u, \theta_2 = \psi_2, I_2 = I_2^u, \theta_3 = \psi_3, I_3 = I_3^u)$. Now consider a point on the stable whisker. Assume that that point has $y \in (\pi, 2\pi)$ and that under the forward flow $y(t) \to 2\pi$ when $t \to \infty$ (where we consider y on the lift, that is, the orbit is not making several revolutions in the y variable before entering the invariant torus). Going back on time, the first intersection with $y = \pi$ takes place at a point $z^s = (y = \pi, x = x^s, \theta_2 = \psi_2, I_2 = I_2^s, \theta_3 = \psi_3, I_3 = I_3^s)$. These points z^u and z^s will be seen as a function of the corresponding angle (ψ_2, ψ_3), to be denoted as $\hat{\psi}$ for shortness. In fact, due to the symmetries of the problem, it is enough to compute only one of the two manifolds.

The splitting vector is defined as

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

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 (see. e.g. [3]), but we shall look for Δ_1 and Δ_2, independently, as an additional check of the computations.

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. We point out that the expansions of the splitting in this paper are formal in the sense of formal power series. We do not claim here that the proposed approach gives the correct estimates. The present objective of the paper is to propose a new method to compute such splitting and provide numerical evidence of its validity. A theoretical study is in progress [17].

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 $\Delta(\hat{\psi}, \eta) = 0$.

1.4 The contents of the sections

In order to numerically compute such splitting vector, approximations of the local invariant stable and unstable manifolds $W^s_{\mathbb{T}_\beta}$ and $W^u_{\mathbb{T}_\beta}$ are obtained in section 2. 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 $W^u_{\mathbb{T}_\beta}$ 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 $W^s_{\mathbb{T}_\beta}$ with $\{y = \pi\}$ is obtained by symmetry because (1) is even in θ_2 and θ_3. Two 2D tori are obtained as those intersections. They can be described by giving the numerical values of x and I_2 as a function of the angles $\hat{\psi}$, as explained before. Let $x_{W^{u,s}_{\mathbb{T}_\beta} \bigcap \{y=\pi\}} = m^{u,s}(\hat{\psi}, \eta)$, $I_{2, W^{u,s}_{\mathbb{T}_\beta} \bigcap \{y=\pi\}} = n^{u,s}(\hat{\psi}, \eta)$. A convenient numerical measure of the splitting is given by

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

where $d_1(\hat{\psi}, \eta)$ and $d_2(\hat{\psi}, \eta)$ are defined as

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

Note that the functions $m^{u,s}$, $n^{u,s}$, d_1, d_2 are nothing else than *numerical* approximations to 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. The Fourier analysis of these functions is carried out and a selected set of results is displayed.

In section 3, using a result in [14] (which in order to make the paper self-contained is given in the Appendix of such section) we give an upper bound of the splitting of separatrices. The role of H_0 and H being entire, and not only analytic, as is happens in the present case, is also stressed. It turns out that an upper bound for the splitting of separatrices is of the form

$$\exp\left(-\hat{c}\left(\frac{|\ln \eta|}{\eta}\right)^{1/2}\right), \tag{5}$$

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

Furthermore, in section 3 we symbolically carry out some steps of an averaging procedure in order to compute the adapted Melnikov vector. It is checked that the predictions made following this approach agree with the numerically computed values of the splitting vector, as least for the lower order harmonics in the splitting, the ones which can be numerically detected.

In section 4 we compute the harmonics of the adapted 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. This section contains cumbersome estimates of the integrals appearing in Melnikov's formula. For clarity, we have included an Appendix that contains the technical proofs of the Lemmas of the section.

In section 5 we carry out a "first order" analysis of the splitting. Melnikov's computation gives a theoretical value for the vector (Δ_1, Δ_2) described before. We do not claim that this approximation is rigorously justified. Assuming that the adapted Melnikov approach gives good estimates to the splitting, we analyze the vector Δ in the case of small values of η. The splitting is given by an infinite sum, each term in $\Delta_j(\hat{\psi}, \eta)$, $j = 1, 2$, 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 dominant 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,

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

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.

Work towards proving 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 is in progress [17].

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 (22), 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 sets of points in $W^{u,s}_{\mathbb{T}_\beta} \bigcap \{y = \pi\}$ giving rise to either $\Delta_1(\hat{\psi}, \eta) = 0$ or $\Delta_2(\hat{\psi}, \eta) = 0$. 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 $W^u_{\mathbb{T}_\beta} \bigcap \{y = \pi\}$, 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, $k \in \mathbb{N}$, $\eta_1 > \eta_2 > \dots$, the set of values at 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.

1.5 Additional comments

Finally, we would like to mention that there are several other works concerning with the effective measure of the splitting of separatrices in the literature. We cite, among others, [2], [4], [5], [8], [11] (see, also the references therein). Most of those works deal with the following topics:

- Upper bounds on the splitting under quite general conditions,
- Correct estimates of the splitting assuming that the perturbation has all the harmonics (or, at least, the ones which play a key role) and the amplitudes of these harmonics are bounded from below by suitable functions. Then a first order Melnikov approach gives the correct estimate of the splitting. The major difficulty of the problem consists in proving last assertion,
- The case of frequencies of different order of magnitude (say, ε, 1 and ε) but with the second difficulty mentioned at the beginning of this introduction present. That is, one has to show, first, that sufficiently many non-maximal dimension tori subsist when the perturbation is added. In that case the "arithmetical" difficulties related to multiple resonances are absent.

The most severe difficulties in the understanding of the diffusion mechanisms are due to multiple resonances. Just the case of double resonances is still open, as far as the authors know. Some numerical experiments show the key role of double resonances. We refer to [16] for several examples and, to a lesser extend, to [15].

2 Symbolic and numerical computations of the splitting

This section is devoted to the numerical computation, as fast as possible, of the splitting of separatrices for several values of the parameter η. We put emphasis on the fact that, as pointed out in the introduction, this splitting is going to be exponentially small. We summarise the strategy: First, we need to find the invariant manifolds of the partially hyperbolic invariant tori till they reach the Poincaré section $\{y = \pi\}$. As it is well known, obtaining the invariant

manifolds involves some computational effort and, thus, we have to use a high order analytical expansion of the local invariant manifolds which will allow us to start the computations at a relatively big distance from the invariant torus of frequency β, $\mathbb{T}_\beta$. Thus, we will write the actions of the torus as graph over the angles. More concretely, we will apply schemes that work with the expansion of the actions as Taylor series in y and Fourier series in the angles (θ_2, θ_3). This part is carried out by means of an ad hoc algebraic manipulator. Second, we globalize the invariant manifolds till they reach the Poincaré section $\{y = \pi\}$, using a Taylor method to numerically integrate the Hamilton equations. Finally, the splitting is computed as the difference of the value of the actions on the Poincaré section.

To obtain approximations of the invariant manifolds of $\mathbb{T}_\beta$, 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 $x = y = 0$, $I_2 = \beta$, 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 (η, y) and Fourier series in (θ_2, θ_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:

$$\begin{aligned}\eta \sin y(1+\eta^2\frac{z_2+z_2^{-1}+z_3+z_3^{-1}}{2}) \;=\; & 2\eta\cos\left(\frac{y}{2}\right)\sin\left(\frac{y}{2}\right)+\sum_{\substack{k,l\geq 1\\ j_2,j_3\in\mathbb{Z}}} a_{k,l,j_2,j_3}\eta^{k+1}y^l\cos\left(\frac{y}{2}\right)z_2^{j_2}z_3^{j_3}\\ &+\sum_{\substack{k,l\geq 1\\ j_2,j_3\in\mathbb{Z}}} 2la_{k,l,j_2,j_3}\eta^{k+1}y^{l-1}\sin\left(\frac{y}{2}\right)z_2^{j_2}z_3^{j_3}\\ &+\sum_{\substack{k,l\geq 1\\ j_2,j_3\in\mathbb{Z}}} i(j_2\beta+j_3)a_{k,l,j_2,j_3}\eta^k y^l z_2^{j_2}z_3^{j_3}\\ &+\sum_{\substack{k+r,l+s\geq 1\\ j_2+q_2,j_3+q_3\in\mathbb{Z}}} la_{k,l,j_2,j_3}a_{r,s,q_2,q_3}\eta^{k+1+r}y^{l+s-1}z_2^{j_2+q_2}z_3^{j_3+q_3}\\ &+\sum_{\substack{k+r,l+s\geq 1\\ j_2+q_2,j_3+q_3\in\mathbb{Z}}} ij_2a_{k,l,j_2,j_3}b_{r,s,q_2,q_3}\eta^{k+1+r}y^{l+s}z_2^{j_2+q_2}z_3^{j_3+q_3}, \end{aligned}\tag{10}$$

$$\begin{aligned}\eta^3(\cos y-1)\frac{z_2-z_2^{-1}}{2i} \;=\; & \sum_{\substack{m,n\geq 1\\ p_2,p_3\in\mathbb{Z}}} i(p_2\beta+p_3)b_{m,n,p_2,p_3}\eta^m y^n z_2^{p_2}z_3^{p_3}\\ &+\sum_{\substack{m,n\geq 1\\ p_2,p_3\in\mathbb{Z}}} nb_{m,n,p_2,p_3}\eta^{m+1}y^{n-1}2\sin\left(\frac{y}{2}\right)z_2^{p_2}z_3^{p_3}\\ &+\sum_{\substack{m+r,n+s\geq 1\\ p_2+q_2,p_3+q_3\in\mathbb{Z}}} nb_{m,n,p_2,p_3}a_{r,s,q_2,q_3}\eta^{m+r+1}y^{n+s-1}z_2^{p_2+q_2}z_3^{p_3+q_3}\\ &+\sum_{\substack{m+r,n+s\geq 1\\ p_2+q_2,p_3+q_3\in\mathbb{Z}}} ip_2b_{m,n,p_2,p_3}b_{r,s,q_2,q_3}\eta^{m+r+1}y^{n+s}z_2^{p_2+q_2}z_3^{p_3+q_3}. \end{aligned}\tag{11}$$

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}. More concretely, as it is easily checked by induction, the exponents j_2, j_3, p_2 and p_3 satisfy:

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

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 $W^u_{\mathbb{T}_\beta}$ 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 $W^u_{\mathbb{T}_\beta} \bigcap \{y = \pi\}$. 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^u_2 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 $w^{(j)}$, $j = 1, \ldots, N$, for $w \in \{y, \theta_2, J_1, J_2\}$. This allows to do accurately integration steps with large step size 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 $W^s_{\mathbb{T}_\beta}$, we obtain x^s and I^s_2 in $W^s_{\mathbb{T}_\beta} \bigcap \{y = \pi\}$ (by backwards integration in time using the correct "branch" of $W^s_{\mathbb{T}_\beta}$). 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 $W^s_{\mathbb{T}_\beta}$ is not needed in the present case.

The splitting between the two manifolds is measured by the functions d_1 and d_2, introduced in (4). As it 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 $\Delta_1(\hat{\psi}) = 0$ and $\Delta_2(\hat{\psi}) = 0$ correspond to homoclinic orbits to the invariant torus. If we denote by $C^1_h(\eta) = \{\hat{\psi} \in \mathbb{T}^2 | \Delta_1(\hat{\psi}, \eta) = 0\}$ and $C^2_h(\eta) = \{\hat{\psi} \in \mathbb{T}^2 | \Delta_2(\hat{\psi}, \eta) = 0\}$, 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

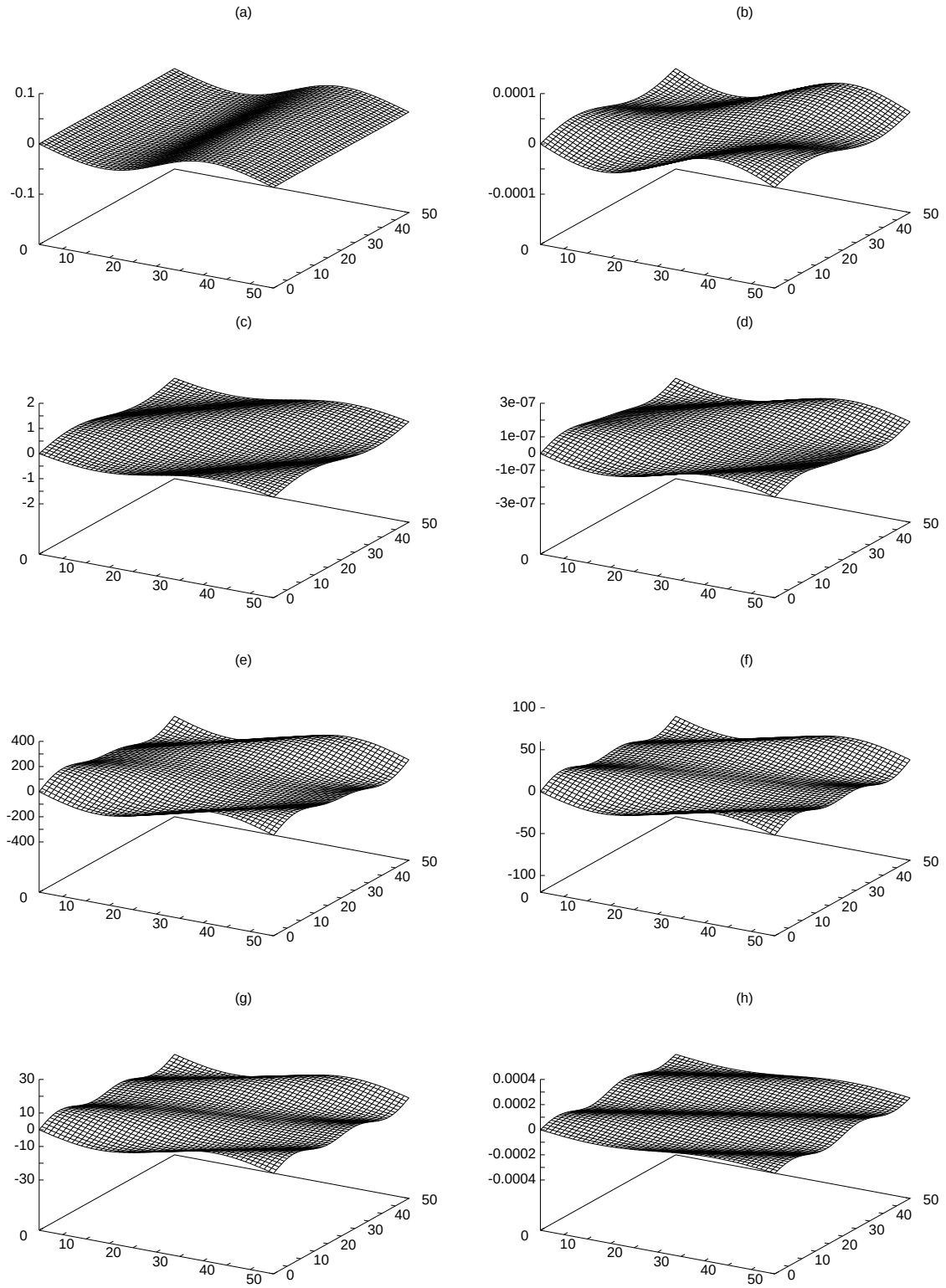

Figure 1: Behaviour of $d_2(\hat{\psi}, \eta)$ for different values of η. a) $\eta = 0.44$; b) $\eta = 0.205$; c) $\eta = 0.065$ (magnified by 10^{10}); d) $\eta = 0.034$ (magn. by 10^{10}); e) $\eta = 0.032$ (magn. by 10^{20}); f) $\eta = 0.030$ (magn. by 10^{20}); g) $\eta = 0.0292$ (magn. by 10^{20});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

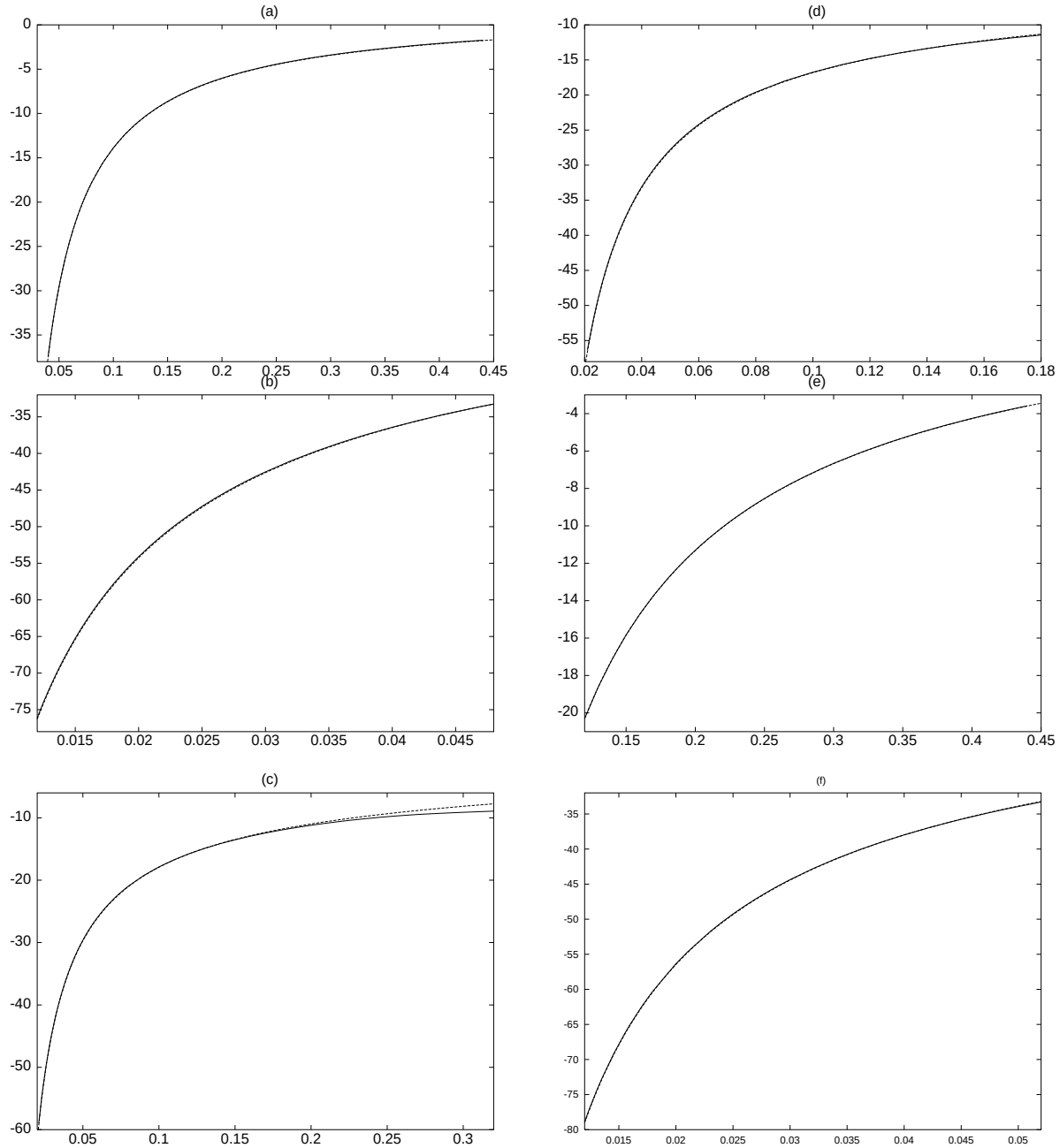

Figure 2: Behaviour of $\ln(d_1)$ and $\ln(d_2)$ for different harmonics, and some functions versus η. It has been even enough to obtain the functions by visual fitting. a) $\ln(d_1(0,1,\eta))$ and $-\pi/(2\eta)+1.8$; b) $\ln(d_1(1,-1,\eta))$ and $-\pi(3-\sqrt{5})/4\eta+2\ln(\eta)-2.5$; c) $\ln(d_1(2,-1,\eta))$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

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 $d_j(\hat{\psi}, \eta)$.

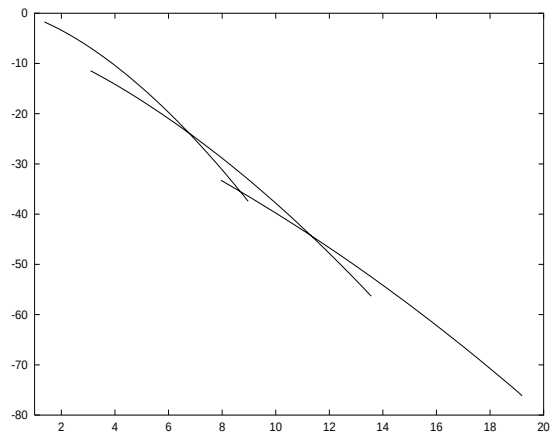

Figure 3: The three harmonics $(0, 1)$, $(1, -1)$, $(2, -1)$, for $\ln(d_1)$ versus $(|\ln(\eta)|/\eta)^{1/2}$.

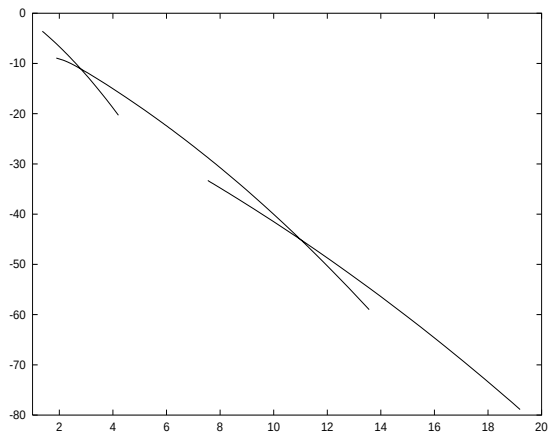

Figure 4: The three harmonics $(1, 0)$, $(1, -1)$, $(2, -1)$, for $\ln(d_2)$ versus $(|\ln(\eta)|/\eta)^{1/2}$.

Figures 3 and 4 show simultaneously the three initial harmonics for d_1 and d_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 $C_h^1(\eta)$ and $C_h^2(\eta)$ for different values of η. Instead of the Δ_j, $j = 1, 2$ functions we have used the computed functions d_j, $j = 1, 2$. 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

This section has two different purposes: The first one deals with the upper bound (5) for the splitting of separatrices and the second one with the study in detail of the averaging procedure used before applying Melnikov formula.

To achieve the first one, let us introduce the change of variables

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

This change extends the one introduced in the previous section and uses (q, p) as variables. Despite it 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

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

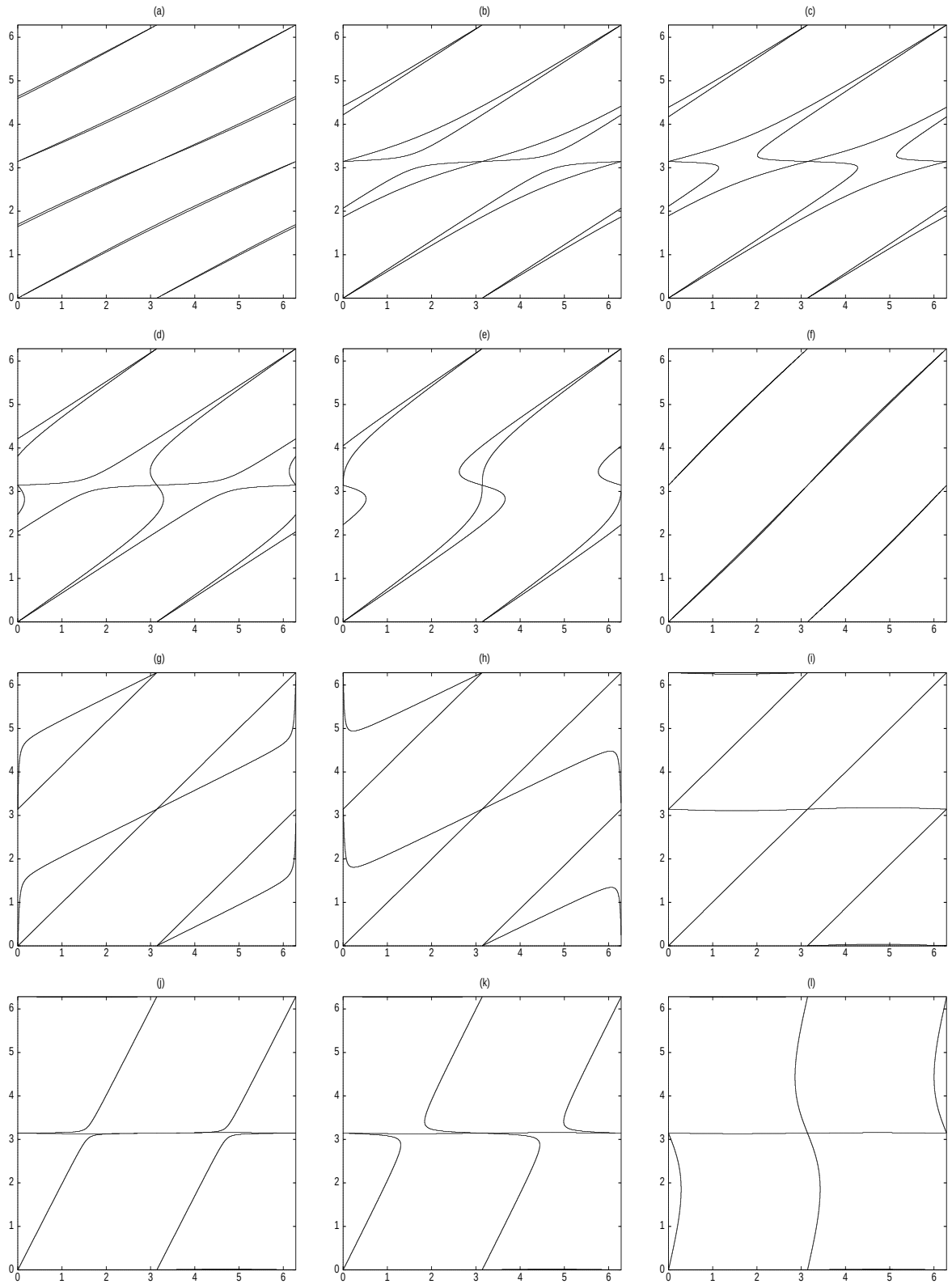

Figure 5: Behaviour of $C_h^j(\eta)$, $j = 1, 2$ for different values of η. a) $\eta = 0.025$; b) $\eta = 0.028$; c) $\eta = 0.0282$; d) $\eta = 0.0293$; e) $\eta = 0.03$; f) $\eta = 0.04$; g) $\eta = 0.062$; h) $\eta = 0.0624$; i) $\eta = 0.12$; j) $\eta = 0.22$; k) $\eta = 0.222$; l) $\eta = 0.3$.

Applying the Averaging Theorem [14] to (13) (see Theorem 3.5 in subsection 3.1 for its formulation and comments, including details on the proof in the Hamiltonian case), 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 variable in the Hamiltonian (13) is q_3 and the dependence on q_3 is quasiperiodic with frequency $\omega = (\beta, 1)$. We average with respect to q_3 and, hence, the averaged Hamiltonian does no longer contain the angles q_3 and βq_3. We claim that cancelling the dependence with respect to βq_3 also cancels the dependence with respect to q_2 up to the desired order.

To prove the claim we should go a little bit into the proof of theorem 3.5 or into the averaging procedure which is described later in this section. Note that both procedures are slightly different. In the proof of theorem 3.5 at every step the transformation it is intended to cancel all the purely quasi–periodic terms in the fast angles θ while the slow variables and the small parameter η (except the η appearing as a factor in the differential equation) are taken as constants to derive the transformation. In the method described below we assume the Hamiltonian expanded in powers of η and, at the n-th step, one intends to cancel the dependence with respect to the fast variable in η^n.

In both cases the angles q_2 and βq_3 appear together and with the same multiples. Using the notation which we shall introduce in (16), if $z_2 = \exp(i(q_2 + \beta q_3)$, we can also define $z_2' = \exp(iq_2)$ and $z_2'' = \exp(i\beta q_3)$. Every time z_2'' appears raised to some power, also z_2' appears with the same power. This is preserved under all the operations: expansions and changes of variables. Hence, as z_2'' disappears in the averaged part (Z^n above), also z_2' should disappear. This proves the claim.

If n is chosen in an optimal way, as a function of η, then the remainder R_{opt} satisfies an exponentially small bound

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

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. [14]), 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, that contains a factor of the form $-c(\eta|\ln(\eta)|)^{-1/2}$ inside the exponential. We recall (cf. [14] 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 $c = \mathrm{O}(|\ln(\eta)|)$. Combining these two facts and the dependence of the invariant manifolds with respect to parameters (see, e.g., [6]) one obtains a priori bounds of the form (5). Note, however, that this exceptional role of $\tau = 1$ could be due to the use of theorem 3.5. In this direction see remark 3.6.

Remark 3.2 *The averaging procedure is close to the identity, because at each step of the averaging procedure we are making a change of coordinates of the form*

$$\left(Id + \mathrm{O}(\eta^{n+2})\right), \quad n\text{=step of averaging.}$$

The composition of the finite number of transformations we are doing is still close to the identity. The differential of the change of variables is also close to the identity. Hence, we are making an small error on the splitting of separatrices, which is a geometrical object, whose influence can be neglected.

To start with the second purpose of this section, let us recall that 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 [7].

Let us explain one of these steps: Step $n-2$; $n \geq 3$. We want to compute a generating function G_n (having η^n as a factor) such that the transformed Hamiltonian

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

has its terms of degree n independent of (q_2, q_3). Every time we refer to degree through this section, must be understood degree in η. If we want to refer to degree on other variables, we will mention explicitly the variables. As we did before for the local expansions of W^u, we introduce the change of variables

$$z_1 = \exp(iq_1), \quad z_2 = \exp(i(q_2 + \beta q_3)), \quad z_3 = \exp(iq_3). \tag{16}$$

Using that $H = H_0 + H_1 + H_3 + \ldots + H_n$, with

$$H_0 = p_3, \;\; H_1 = \eta\frac{p_1^2 + p_2^2 + z_1^1 + z_1^{-1} - 2}{2}$$

and that H_m has degree m for any $3 \leq m \leq n$, one obtains that the terms of degree n of the transformed Hamiltonian H' are

$$H'_n = H_n + \{H_0, G_n\}.$$

We want H'_n to be independent of (q_2, q_3). This equation is easily solved, because of the form of H_0. The expressions of H_n and G_n can be written as

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

where, as we shall do through the paper, $\mathbb{N}$ and $\hat{\mathbb{N}}$ will denote the natural numbers without the zero value and with the zero value, respectively: $\hat{\mathbb{N}} = \mathbb{N} \cup \{0\}$.

Hence, since the frequencies $\omega = (\beta, 1)$ are rationally independent, it is immediate that

$$g_{n,l,k} = \begin{cases} \dfrac{h_{n,l,k}}{i(k_2\beta + k_3)}, & (k_2, k_3) \neq (0,0), \\ 0, & (k_2, k_3) = (0,0). \end{cases}$$

If H_n has zero average, we can manage to obtain $H'_n = 0$, but this is not true in general. In particular, due to the special form of (13) only the terms of degrees $2, 4, 5$ and 6 are absent in (17) if $n \geq 7$.

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

Once G_3 has been obtained, we can apply (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:

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

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 used again 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 the contribution of G_3 has been finished (up to the maximal order N), 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

$$H' = Z^n(p_1, p_2, p_3, q_1, \eta) + R_{n+1}(p_1, p_2, q_1, q_2, q_3, \eta), \tag{17}$$

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 $G_3, \dots G_n$. 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 $k_2 = k_3 = 0$.

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 3.3 *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,

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

$$+ i\overline{k}_2(\tilde{l}_2+1) h_{\overline{m},\overline{l}_1,\overline{l}_2,\overline{k}_1,\hat{\overline{k}}} g_{\tilde{m},\tilde{l}_1,\tilde{l}_2+1,\tilde{k}_1,\hat{\tilde{k}}} - i\tilde{k}_2(\overline{l}_2+1) h_{\overline{m},\overline{l}_1,\overline{l}_2+1,\overline{k}_1,\hat{\overline{k}}} g_{\tilde{m},\tilde{l}_1,\tilde{l}_2,\tilde{k}_1,\hat{\tilde{k}}} \Big\}.$$

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 3.3 is straightforward. □

Lemma 3.3, implies that Z^n and R_{n+1} can be represented as a sum of monomials of the form

$$\sum_{m>n, l\in\hat{\mathbb{N}}^2, k\in\hat{\mathbb{N}}\times\mathbb{Z}^2} C_{m,l,k}\eta^m p^l \left(\delta_1 \cos(k_1 q_1)\cos(\hat{k}\cdot\hat{q}) - \delta_2 \sin(k_1 q_1)\sin(\hat{k}\cdot\hat{q})\right), \tag{18}$$

for R_{n+1} and

$$\sum_{n\geq m\geq 0, l\in\hat{\mathbb{N}}^2, k_1\in\hat{\mathbb{N}}} \delta_1 C_{m,l,k_1,0}\eta^m p^l \cos(k_1 q_1), \tag{19}$$

for Z^n, being $\delta_1 = (1+(-1)^{l_1})/2$, and $\delta_2 = (1-(-1)^{l_1})/2$.

Furthermore, the following Lemma holds:

Lemma 3.4 *For $l_1 = 0$ and every $m, l_2, \hat{k}$ fixed,*

$$\sum_{k_1\in\hat{\mathbb{N}}} C_{m,0,l_2,k_1,\hat{k}} = 0. \tag{20}$$

Moreover, at $p_1 = q_1 = 0$ we have

$$\frac{\partial Z^n}{\partial p_1} = \frac{\partial Z^n}{\partial q_1} = \frac{\partial R_{n+1}}{\partial q_1} = \frac{\partial R_{n+1}}{\partial p_1} = 0. \tag{21}$$

Proof of Lemma 3.4

To prove Lemma 3.4, it suffices to prove that Z^n and R_{n+1} have at least degree 2 in the (p_1, q_1)-variables, because in that case, (21) is readily satisfied and (20) follows imposing that Z^n and R_{n+1} are zero for $p_1 = q_1 = 0$.

The fact that Z^n and R_{n+1} have at least degree two in the (p_1, q_1)-variables, is a direct consequence of the fact that H_3 has degree at least 2 in the (p_1, q_1)-variables, that G_n and H_n have the same degree in the (p_1, q_1)-variables at each step of the averaging process and that the Poisson bracket between two homogeneous polynomials of degrees r and s, is an homogeneous polynomial of degree $r + s - 2$. □

Table 1 summarizes some selected terms which appear inside the remainder in (17) 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 3.3, 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 [17] and the beginning of section 5).

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. This means, for instance, that, after using G_6 as generating function, there are terms in the remainder which contain η^7 as a factor. They are the current leading terms. There are also terms having η^8 which appear for the first time when the effect

of G_6 is computed. When using the G_7 generating function, the terms in η^7 will disappear, of course, but the ones in η^8 are not affected and these ones will be the current leading terms. The same applies to the terms in η^9 and η^{10}. Is in this sense that we state the sentence at the beginning of that paragraph. 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}.

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.

Let us comment a little on Table 1. Consider, for instance, the terms with $m = 7, 8, 9, 10$. All of them contain the harmonic $(-1,1)$ and a coefficient having η^m as factor. The first important contribution to the $(-1,1)$ harmonic in the splitting comes from $m = 7$. But these terms contain also a factor of the form $p_1^{l_1}\cos(k_1 q_1)$. Hence the Melnikov integrals will involve poles of different order. The terms with $m = 8, 9, 10$ give corrections to the contribution of the term with $m = 7$ which are worth to be included.

To detect a given Fibonacci-type harmonic of the form $\pm(F_n, -F_{n-1})$ one should use $m = 4F_{n+1} - 1$, according to (12), and hence the last G to be used, to see that term coming as leading term in the remainder, has index $4F_{n+1} - 2$.

3.1 Appendix: The Averaging Theorem

In this subsection we state the Averaging Theorem [14] and include some comments.

Theorem 3.5 *Let us consider the system of differential equations given by* $\dot{z} = \eta f(z, \theta, \eta)$, $\dot{\theta} = \omega$, $z \in \Omega \subset \mathbb{C}^n$, *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*

$$|r|_{\delta/2} < c_1 \exp\left(-c_2/\eta^{c_3}\right), \tag{22}$$

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* $|\ln \eta|^{-1/p}$.

This theorem deals with a general differential equation. To specialize to the Hamiltonian case and prove that a canonical change of variables can be used, some natural modifications of the proof in [14] must be done. For completeness we sketch here the key idea.

At the j step of the iterative process in the proof of theorem 3.5 we search for a transformation of the form $z = w + \eta v(w, \theta, \eta)$ (cf. (13) in [14]) and the condition

$$\frac{\partial v}{\partial \theta}(w, \theta, \eta)(\omega) = \widetilde{f}_j(w, \theta, \eta) \quad \text{and} \quad \overline{v}(w, \eta) = 0$$

is derived for v (cf. (18) in [14]). Here $\widetilde{f}_j(w, \theta, \eta)$ is the purely quasi–periodic part (with respect to θ) of the current differential equation at the j-th step.

Assume the system is Hamiltonian. Then $z = (q, p)$, the current Hamiltonian at the j-th step can be denoted as $H_j(q, p, \theta, \eta)$ and its purely quasi–periodic part as $\widetilde{H}_j(q, p, \theta, \eta)$. The new variable will be $w = (Q, P)$. Instead of looking for a transformation v we look for a generating function of the transformation of the form

$$q \cdot P + \eta S_j(q, P, \theta, \eta).$$

It is immediately checked that the relation between v and S_j is $v = J\nabla S_j$, J being the standard symplectic matrix. From this follows the condition on S_j

$$\frac{\partial S_j}{\partial \theta} = \widetilde{H}_j \quad \text{and} \quad \overline{S}_j = 0.$$

The proof ends as in [14] with minor modifications on the estimates of the remainder after the change of variables (cf. (30) and (31) in [14]).

Remark 3.6 *During the revision of this paper, the authors were aware of the existence of a preprint of Sauzin [12] from which (see, for example Theorem* 3.2 *formula* 3.5 *in [12]) bound (5) could be deduced without any special treatment nor any exceptional conclusion for the case* $\tau = 1$ *provided the width of the analyticity domain (*h_0 *in [12]) could be taken depending on* η *(in [12], assumption A2, it is taken as a constant).*

4 The adapted Melnikov vector

Before starting this section, let us recall where we are now: We are dealing with perturbations which are trigonometric polynomials and thus the most common method of computing the effective measure of the splitting of separatrices by checking the validity of the Melnikov prediction does not work. Then, we modify Melnikov's approach in order to get realistic estimates of the splitting. The method we propose is to compute the Melnikov function after a suitable number of averaging steps. If $|\hat{k}| = |k_2| + |k_3|$ is the order of the harmonic to be computed, we propose to make steps of averaging until $\hat{k}$ appears as an harmonic in the leading terms of the remainder of the averaged Hamiltonian for the first time. Guided by relation (12) in Section 2, the number of these steps is $4|\hat{k}| - 1$. We recall that from the above section (see (17)), the output of the averaging procedure is an integrable Hamiltonian (that we call averaged Hamiltonian and denote by Z^n) plus a remainder R_{n+1}.

Since the separatrix of the averaged Hamiltonian is not computable, in order to get an effective computation of the *adapted Melnikov function*, such computation has been carried out "only" with the pendulum separatrix cross a rotor, instead of the whole separatrix of Z^n. Of course, one should consider (but we do not do this in this paper) the errors obtained by that simplification and therefore we do not claim that the approximation given here is rigorously justified. However, the results obtained in this way have a good agreement with the numerical ones. An heuristic reason for that is that the singularities of the separatrix could move by a relatively small amount when taking into account the full expression of Z^n.

The variation of the actions due to the perturbation R_{n+1} is

$$\Delta p_2 = \int_{\mathbb{R}} \{H, p_2\} = \int_{\mathbb{R}} \frac{\partial R_{n+1}}{\partial q_2}, \quad \Delta p_3 = \int_{\mathbb{R}} \{H, p_3\} = \int_{\mathbb{R}} \frac{\partial R_{n+1}}{\partial q_3}, \tag{23}$$

where the integration is carried out along the separatrix of the pendulum cross a rotor. Formula (23) gives the contribution of R_{n+1} (if any) to the adapted Melnikov vector. This 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 $q_3^u = q_3^s$:

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

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 (this also follows from the existence of a splitting potential) and it is obvious that Δp_j^u and Δp_j^s, $j = 1, 2, 3$ are, at most, of order η^3. Hence

$$\Delta p_1 = -\frac{\Delta p_3}{2\eta}. \tag{24}$$

Later, we will see that computing the variation of p_1 using (24) has a good agreement with the numerical computation of such variation.

Therefore, we are dealing with the computation of the quantities (23). To this end, we have that the lower 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 $\hat{\mathbb{N}} \times \mathbb{N}^2 \times \mathbb{Z}^2$, 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 from (18) that

$$\begin{aligned} \frac{\partial R_{n+1}}{\partial q_2} &= -2\sum_{(m,l_1,k_1,\hat{k})\in\mathcal{A}} \eta^{m-1} k_2 p_1^{l_1} r_{m,l_1,0,k_1,\hat{k}} \left[\delta_1 \cos(k_1 q_1)\sin(\hat{k}\cdot\hat{q}) + \delta_2 \sin(k_1 q_1)\cos(\hat{k}\cdot\hat{q})\right], \\ \frac{\partial R_{n+1}}{\partial q_3} &= -2\sum_{(m,l_1,k_1,\hat{k})\in\mathcal{A}} \eta^{m-1} (\hat{k}\cdot\omega) p_1^{l_1} r_{m,l_1,0,k_1,\hat{k}} \left[\delta_1 \cos(k_1 q_1)\sin(\hat{k}\cdot\hat{q}) + \delta_2 \sin(k_1 q_1)\cos(\hat{k}\cdot\hat{q})\right], \end{aligned}$$

where $\hat{q} = (q_2, q_3)$, $\sigma_1 = (1 + (-1)^{l_1})/2$, $\sigma_2 = 1 - \sigma_1$ and the factor 2 appears taking into account that, from (16), for $j = 1, 2, 3$, $\cos\theta_j = (z_j + z_j^{-1})/2$. Note that $\hat{q}(0) = \hat{\psi}$, as in (4), when we restrict to the separatrix of the unperturbed system.

Expanding $\cos(k_1 q_1)\sin(\hat{k}\cdot\hat{q})$ and $\sin(k_1 q_1)\cos(\hat{k}\cdot\hat{q})$ over the separatrix of the pendulum times the rotor, denoting $\kappa := \hat{k}\cdot\omega$ and introducing $\mu = \kappa/\eta$, we obtain

$$\cos(k_1 q_1)\sin(\hat{k}\cdot\hat{q}) = (-1)^{k_1}\cos(4k_1\arctan(\tanh(t/2)))\left[\sin(\mu t)\cos(\hat{k}\cdot\hat{\psi}) + \cos(\mu t)\sin(\hat{k}\cdot\hat{\psi})\right],$$

$$\sin(k_1 q_1)\cos(\hat{k}\cdot\hat{q}) = (-1)^{k_1}\sin(4k_1\arctan(\tanh(t/2)))\left[\sin(\mu t)\sin(\hat{k}\cdot\hat{\psi}) - \cos(\mu t)\cos(\hat{k}\cdot\hat{\psi})\right].$$

By the oddness of the functions, we have that the only terms giving a non zero contribution to the integrals in (23) are the ones coming from the terms 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.

For a vector $\hat{k}$ such that $\hat{k}\cdot\omega > 0$, let $\mathcal{B} = \mathcal{B}_{\hat{k}} = \{(m, l_1, k_1) \,|\, (m, l_1, k_1, \hat{k}) \in \mathcal{A}\}$. Note that we consider sets $\mathcal{B}$ 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 $\mathcal{B}$. Taking into account the relation between the coefficients in the normal form given in Lemma 3.3 and using the notation

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

for $j=2,3$, we can distinguish different cases for:

$$\Delta p_j^{\hat{k}} = 2\sum_{(m,l_1,k_1)\in\mathcal{B}} (-1)^{k_1+1} 2^{l_1} \eta^{m-1} |k_2|^{3-j} \kappa^{j-2} r_{m,l_1,0,k_1,\hat{k}} \sum_{\rho\in\{-1,1\}} \left[\delta_1 I(k_1,l_1,\rho,\mu) - \delta_2 \rho I(k_1,l_1,\rho,\mu)\right]. \quad (25)$$

We are faced to the computation of the $I(k_1,l_1,\rho,\mu)$ integrals. This is an elementary but cumbersome task, requiring several Lemmata. We state Lemmata 4.1 and 4.2, whose proof appears in the Appendix of this section. First we proceed with the cases $l_1>0$, the ones with $l_1=0$ being deferred till Lemma 4.2.

Lemma 4.1 *For $k_1\in\hat{\mathbb{N}}$, $l_1\in\mathbb{N}$ and $\rho\in\{-1;1\}$, the values of $I(k_1,l_1,\rho,\mu)$ are:*

1. *If $2k_1\geq l_1$*

$$\frac{4\pi(2\mu\rho)^{\sigma_1}}{2^{l_1}(1-e^{2\mu\rho\pi})} \frac{(-1)^{l_1} e^{\mu\rho\frac{\pi}{2}}}{(l_1+2k_1-1)!} \prod_{m=1}^{\frac{l_1+2k_1-1-\sigma_1}{2}} \left(4\mu^2+z_m\right).$$

2. *If $2k_1\in[0,l_1-1]$*

$$\frac{4\pi(2\mu\rho)^{\sigma_1}}{2^{l_1}(1-e^{2\mu\rho\pi})} \left[\frac{(-1)^{l_1} e^{\mu\rho\frac{\pi}{2}}}{(l_1+2k_1-1)!} \prod_{m=1}^{\frac{l_1+2k_1-1-\sigma_1}{2}} (4\mu^2+z_m) + \frac{e^{\mu\rho\frac{3\pi}{2}}}{(l_1-2k_1-1)!} \prod_{m=1}^{\frac{l_1-2k_1-1-\sigma_1}{2}} (4\mu^2+z_m) \right],$$

where we have introduced several real numbers $z_j\in\mathbb{R}$ satisfying the following properties

$$|z_j|\leq 9\max\{q^2,p^2\}, 1\leq j\leq \frac{q-1-\sigma}{2}, \quad \text{and} \quad \sum_{j=1}^{\frac{q-1-\sigma}{2}} z_j = \binom{q-1}{2}\left(\frac{q}{3}-p\right),$$

with $q=l_1+2k_1$ and $p=-l_1+2k_1$ in case 1., $q=l_1-2k_1$ and $p=-l_1-2k_1$ in case 2.

Taking into account the relation between the coefficients in the normal form given in (20) for $l_1=l_2=0$, and using the notation

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

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

$$-2\sum_{(m,0,k_1)\in\mathcal{B}} \eta^{m-1}|k_2|^{3-j}\kappa^{j-2} r_{m,0,0,k_1,\hat{k}} \sum_{\rho\in\{-1,1\}} \tilde{I}_1(k_1,\rho,\mu). \quad (26)$$

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

Lemma 4.2 *For $l_1=0$, $k_1\in\mathbb{N}$ and $\rho\in\{-1;1\}$, the values of $\tilde{I}_1(k_1,\rho,\mu)$ are*

$$\frac{8\pi\mu\rho(-1)^{k_1}}{(2k_1-1)!}\frac{e^{\mu\rho\frac{\pi}{2}}}{1-e^{2\mu\rho\pi}}\prod_{m=1}^{k_1-1}\left(4\mu^2+z_m\right).$$

Lemma 4.1 and Lemma 4.2 imply that, for any harmonic $\hat{k}$ with $\hat{k}\cdot\omega > 0$, one has

$$\Delta p_j^{\hat{k}} = 8\pi \sum_{(m,l_1,k_1)\in\mathcal{A}_+} (-1)^{k_1+l_1+1}\eta^{m-1}\,|k_2|^{3-j}\,\kappa^{j-2}\frac{r_{m,l_1,0,k_1,\hat{k}}}{1-e^{-2\mu\pi}}e^{-\mu\frac{\pi}{2}}(1+e^{-\mu\pi}) \tag{27}$$
$$\times((-2\mu)^{\sigma_1}+1-\sigma_1)\left\{\frac{1}{(l_1+2k_1-1)!}\mathcal{P}_{\sigma_1}(l_1+2k_1)+\frac{(-1)^{l_1}1_{\{2k_1<l_1\}}e^{-\mu\pi}}{(l_1-2k_1-1)!}\mathcal{P}_{\sigma_1}(l_1-2k_1)\right\}$$

where

$$\mathcal{P}_{\sigma_1}(q) = \prod_{m=1}^{\frac{q-1-\sigma}{2}}\left(4\mu^2+z_m\right), \quad \text{and} \quad 1_{\{2k_1<l_1\}} = \begin{cases} 1 & \text{if } 2k_1<l_1 \\ 0 & \text{otherwise.}\end{cases} \tag{28}$$

We recall that $\sigma = (1+(-1)^{l_1})/2$ and that the zeroes $-z_m$ of $\mathcal{P}_{\sigma_1}$ as a function of μ^2 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 (25) and (26) in the following form:

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

Now, we want to obtain some bounds of $\Delta p_2^{\hat{k}}$ and $\Delta p_3^{\hat{k}}$ that will be used in next section to detect relevant harmonics of the splitting. 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 4.3 *For a fixed $q\geq 4$, let $\dfrac{\max(q^2,p^2)}{\mu^2} := B$, sufficiently small. Then (with 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 4.4.

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:

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

Next we give the low order contributions to the splitting (that is, the contributions of the harmonics of low order), 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:

$$\Delta p_2^{\hat{k}} = (-1)^{|\hat{k}|} 2^{2|\hat{k}|+2} |k_2| \eta^{2|\hat{k}|-1} \pi \frac{e^{-\mu\frac{\pi}{2}}}{1-e^{-2\mu\pi}} \kappa^{2|\hat{k}|-1} \left(1+e^{-\mu\pi}\right) \frac{c^{\hat{k}}}{(2|\hat{k}|-1)!}, \tag{29}$$

$$\Delta p_1^{\hat{k}} = (-1)^{|\hat{k}|+1} 2^{2|\hat{k}|+1} \eta^{2|\hat{k}|-2} \pi \frac{e^{-\mu\frac{\pi}{2}}}{1-e^{-2\mu\pi}} \kappa^{2|\hat{k}|} \left(1+e^{-\mu\pi}\right) \frac{c^{\hat{k}}}{(2|\hat{k}|-1)!}, \tag{30}$$

where

$$\begin{aligned} c^{\hat{k}} &= r_{-1}^0 \prod_{m=1}^{|\hat{k}|-1} (1 + z_m^{2|\hat{k}|,0}/(4\mu^2)) - \frac{r_0^1 \kappa}{|\hat{k}|} \prod_{m=1}^{|\hat{k}|} (1 + z_m^{2|\hat{k}|,1}/(4\mu^2)) \\ &+ \frac{2\kappa^2}{|\hat{k}|(2|\hat{k}|+1)} \left(r_1^2 \prod_{m=1}^{|\hat{k}|} (1 + z_m^{2|\hat{k}|,2}/(4\mu^2)) - r_1^0 \prod_{m=1}^{|\hat{k}|} (1 + z_m^{2|\hat{k}|+2,0}/(4\mu^2)) \right) \\ &- \frac{2\kappa^3}{|\hat{k}|(2|\hat{k}|+1)(|\hat{k}|+1)} \left(r_2^1 \prod_{m=1}^{|\hat{k}|+1} (1 + z_m^{2|\hat{k}|+2,1}/(4\mu^2)) - r_2^3 \prod_{m=1}^{|\hat{k}|+1} (1 + z_m^{2|\hat{k}|,3}/(4\mu^2)) \right), \end{aligned} \tag{31}$$

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 4.4 and the proof of Lemma 4.5.

Therefore, disregarding the exponentially small errors, we have

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

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

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

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

Using (32), taking η small enough and the values of $r_{7,0,0,0,2}$, $r_{8,1,0,0,2}$, $r_{9,0,0,0,2}$, $r_{9,2,0,0,2}$, $r_{10,1,0,0,2}$, $r_{10,3,0,0,2}$, $r_{11,0,0,0,3}$, $r_{12,1,0,0,3}$, $r_{13,0,0,3}$, $r_{13,2,0,0,3}$, $r_{14,1,0,0,3}$, $r_{14,3,0,0,3}$, $r_{19,0,0,0,5}$, $r_{20,1,0,0,5}$, $r_{21,0,0,0,5}$, $r_{21,2,0,0,5}$, $r_{22,1,0,0,5}$, $r_{22,3,0,0,5}$, $r_{31,0,0,0,8}$, $r_{32,1,0,0,8}$, $r_{33,0,0,0,8}$, $r_{33,2,0,0,8}$, $r_{34,1,0,0,8}$, $r_{34,3,0,0,8}$, 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

(33)

$\hat{k}$	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.

4.1 Appendix: Proof of Lemma 4.1 and Lemma 4.2

4.1.1 Proof of Lemma 4.1

Consider the function

$$g(z) = \arctan(\tanh(z/2)). \tag{34}$$

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

$$I(k_1, l_1, \mu) = \int_{\mathbb{R}} \frac{e^{4ik_1 g(\tau)}}{\cosh^{l_1} \tau} e^{i\mu\rho\tau} d\tau.$$

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

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

The number of poles in

$$\Omega_R = \{z \in \mathbb{C} : -\pi \leq \text{Im } z \leq 0, \, |\text{Re } z| \leq R\} \tag{35}$$

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

$$h_{p,q,\mu}(x) = \frac{\cosh^p(x) e^{2i\mu\rho x}}{\sinh^q(x)},$$

where x is obtained by a translation of s to have the pole at $x = 0$. Then,

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

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

   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 $-i\frac{3\pi}{4}$. In this case,

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

   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

$$h_{p,q,\mu}(x) = \frac{e^{\alpha x}\cosh^p(x)}{\sinh^q(x)} = \frac{C(x)}{x^q}. \tag{36}$$

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 (36), the residue is given by

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

Taking logarithms in (36), 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 $n = 3, \ldots, q$,

$$C_{n-1} = \alpha \sum_{k=0}^{\left[\frac{n-2}{2}\right]} \binom{n-1}{2k+1} 2^{2k} \frac{C_{n-2k-2}}{n-1} + \sum_{k=1}^{\left[\frac{n-1}{2}\right]} \binom{n}{2k+1} 2^{2k} \frac{C_{n-2k-1} D(n,k,p,q)}{n(n-1)}, \tag{37}$$

where

$$D(n,k,p,q) = \left(p\left(k+\frac{1}{2}\right) - q\left(k-\frac{1}{2}\right) - (n-2k-1)\right). \tag{38}$$

From (37) we obtain several consequences that are contained in the following Lemma.

Lemma 4.4 *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,

$$C_{q-1}(\alpha) = \alpha^\sigma \prod_{j=1}^{\frac{q-1-\sigma}{2}} (\alpha^2 - z_j). \tag{39}$$

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 (37) 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, (37) can be reduced to $\overline{C}_0 = 1$, $\overline{C}_1 = 1$ and for $n = 3, \ldots, q$

$$\begin{cases} (n-1)\overline{C}_{n-1} &= w \displaystyle\sum_{k=0}^{\left[\frac{n-2}{2}\right]} \frac{\overline{C}_{n-2k-2}}{(2k+1)!} + \sum_{k=1}^{\left[\frac{n-1}{2}\right]} \frac{\overline{C}_{n-2k-1}}{(2k+1)!} D(n,k,p,q), \quad \text{if } n \text{ odd}, \\ (n-1)\overline{C}_{n-1} &= \displaystyle\sum_{k=0}^{\left[\frac{n-2}{2}\right]} \frac{\overline{C}_{n-2k-2}}{(2k+1)!} + \sum_{k=1}^{\left[\frac{n-1}{2}\right]} \frac{\overline{C}_{n-2k-1}}{(2k+1)!} D(n,k,p,q), \quad \text{if } n \text{ even}, \end{cases} \tag{40}$$

where $D(n,k,p,q)$ is given in (38). With (40), (39) is easily obtained.

Proof of 2.

From equation (37), 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 4.1, we need to prove the following Lemma:

Lemma 4.5 *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*

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

The proof of Lemma 4.5 is splitted into 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

$$I_{p,q} := \mathrm{Res}(h_{p,q,\alpha/2i}(x), x = 0) = \frac{1}{2\pi i}\int_\Gamma \frac{e^{\alpha z}\cosh^p(z)}{\sinh^q(z)}dz, \tag{41}$$

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 (41), 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

$$I_{p,q} = \frac{1}{q-1}(\alpha I_{p-1,q-1} + (p-1)I_{p-2,q-2}), \tag{42}$$

   which follows from (41). The relation (42) 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 (42) becomes

$$J_l = \frac{1}{q-p+l-1}(\beta J_{l-1} - (l-1)J_{l-2}), \quad l \geq 1 \quad \text{with} \quad J_0 = 1,\ J_1 = \frac{\beta}{q-p}, \tag{43}$$

   where $\beta = \alpha i$ (β is here a local variable inside the proof). The recurrence (43) 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 $z_j = -\beta_j^2$.

3. If $p = q$, introducing $J_l = i^{l-1}I_{l,l}$ the recurrence (42) 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.

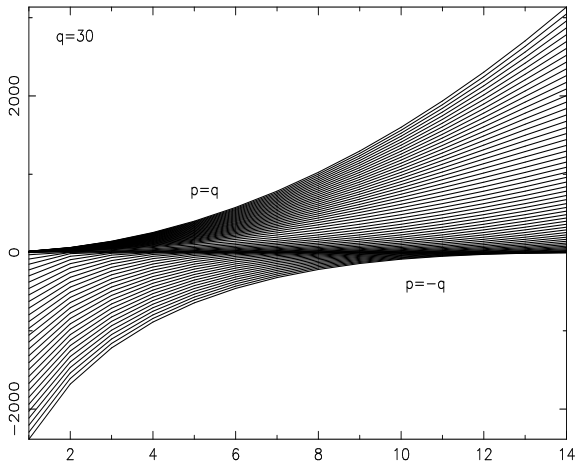

Figure 6: The behaviour of the zeroes for $p \in (-q, q)$, $q = 30$. On the horizontal axis we put the number of the zero, ordered by increasing value.

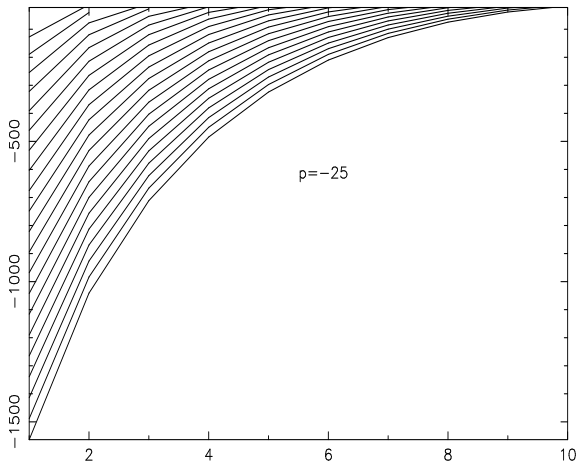

Figure 7: The behaviour of the zeroes for $q \in (4, |p|)$, $p = -25$. The values of q increase from top to bottom. Order of zeroes as in Figure 6.

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 4.5. 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 (40). 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 (40). From Lemma 4.6, we know that $w \in \mathbb{R}$. Let us consider $w = -a^2q^2$, 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 (40) takes the form: $\hat{C}_0 = 1$ and

$$\begin{aligned}(n-1)\hat{C}_{n-1} &= aq \sum_{k=0}^{\left[\frac{n-2}{2}\right]} \frac{\hat{C}_{n-2k-2}}{(2k+1)!}(-1)^k + \sum_{k=1}^{\left[\frac{n-1}{2}\right]} \frac{\hat{C}_{n-2k-1}}{(2k+1)!}(q-n+2k+1)(-1)^k \\ &- \frac{q-p}{2} \sum_{k=1}^{\left[\frac{n-1}{2}\right]} \frac{\hat{C}_{n-2k-1}}{(2k)!}(-1)^k,\end{aligned} \tag{44}$$

both for n odd and even. From (44) 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 (44) 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 $a \geq \frac{7}{5}$,

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

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

$$\begin{aligned}\frac{\hat{C}_{n-1}}{\hat{C}_{n-2}} &= \frac{aq}{n-1}\left[1 - \frac{1}{3!}\frac{\hat{C}_{n-4}}{\hat{C}_{n-2}} + \frac{1}{5!}\frac{\hat{C}_{n-6}}{\hat{C}_{n-2}} - \frac{1}{7!}\frac{\hat{C}_{n-8}}{\hat{C}_{n-2}} + \ldots\right] \\ &+ \frac{1}{n-1}\left[-\frac{q-n+3}{3!}\frac{\hat{C}_{n-3}}{\hat{C}_{n-2}} + \frac{q-n+5}{5!}\frac{\hat{C}_{n-5}}{\hat{C}_{n-2}} + \ldots\right]\end{aligned} \tag{45}$$

All the terms in the first bracket of (45), except the first two, letting aside the factor $1/\tilde{C}_{n-2}$, can be written as a sum of couples:

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

which are positive by the inductive hypothesis.

In the second bracket of (45), 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 $m = 2, \ldots, \left[\frac{n-1}{2}\right]$. 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 (40) takes the form: $C_0^* = 1$ and

$$\begin{aligned}(n-1)C_{n-1}^* &= a\,|p| \sum_{k=0}^{\left[\frac{n-2}{2}\right]} \frac{C_{n-2k-2}^*}{(2k+1)!}(-1)^k + \sum_{k=1}^{\left[\frac{n-1}{2}\right]} \frac{C_{n-2k-1}^*}{(2k+1)!}(q-n+2k+1)(-1)^k \\ &- \left(\frac{|p|+q}{2}\right) \sum_{k=1}^{\left[\frac{n-1}{2}\right]} \frac{C_{n-2k-1}^*}{(2k)!}(-1)^k,\end{aligned} \tag{46}$$

both for n odd and even. From (46) the following lemma holds:

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

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*

$$-z_m \leq \frac{196}{25}\max\{q^2, p^2\}. \tag{47}$$

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 (40) takes the form: $\tilde{C}_0 = 1$ and

$$\tilde{C}_{n-1} = \frac{aq}{n-1}\sum_{k=0}^{\left[\frac{n-2}{2}\right]} \frac{\tilde{C}_{n-2k-2}}{(2k+1)!} + \sum_{k=1}^{\left[\frac{n-1}{2}\right]} \frac{\tilde{C}_{n-2k-1}}{(2k+1)!}\left(\frac{-(2qk+n-2k-1)+(p+q)(k+\frac{1}{2})}{n-1}\right) \tag{48}$$

both for n even and odd.

From (48) the following lemma holds:

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

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

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

$$\begin{aligned} \frac{\tilde{C}_{n-1}}{\tilde{C}_{n-2}} &= \frac{aq}{n-1}\left[1 + \frac{1}{3!}\frac{\tilde{C}_{n-4}}{\tilde{C}_{n-2}} + \frac{1}{5!}\frac{\tilde{C}_{n-6}}{\tilde{C}_{n-2}} + \frac{1}{7!}\frac{\tilde{C}_{n-8}}{\tilde{C}_{n-2}} + \dots\right] \\ &- \frac{1}{n-1}\left[\frac{2q+n-3}{3!}\frac{\tilde{C}_{n-3}}{\tilde{C}_{n-2}} + \frac{4q+n-5}{5!}\frac{\tilde{C}_{n-5}}{\tilde{C}_{n-2}} + \dots\right] \end{aligned} \tag{49}$$

The terms in the brackets of (49) 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,

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

□

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 (40) takes the form: $C_0^{**} = 1$ and

$$\begin{aligned} &(n-1)C_{n-1}^{**} = \\ &= a\,|p| \sum_{k=0}^{\left[\frac{n-2}{2}\right]} \frac{C_{n-2k-2}^{**}}{(2k+1)!} + \sum_{k=1}^{\left[\frac{n-1}{2}\right]} \frac{C_{n-2k-1}^{**}}{(2k+1)!}\left(-(2qk+n-2k-1) - (|p|-q)(k+\frac{1}{2})\right) \end{aligned} \tag{50}$$

both for n even and odd.

From (50) the following lemma holds:

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

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*

$$z_m \leq 9\max\{q^2, p^2\}. \tag{51}$$

Notice that equations (47) and (51) imply that $|z_m| \leq 9\max\{q^2,p^2\}$. Hence, Lemma 4.5 is proved. □

End of proof of Lemma 4.1

Using Lemma 4.4 and Lemma 4.5, integrating along the border of Ω_R and letting $R \to \infty$ Lemma 4.1 follows. □

4.1.2 Proof of Lemma 4.2

Proceeding as in the proof of Lemma 4.1, considering also the function $g(z)$ given in (34), we have to compute

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

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

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

The integrand has only one pole in the domain Ω_R given in (35) 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

$$\int_{\Omega_R} \left((-1)^{k_1} \tan^{2k_1}(is+\pi/4) - 1\right) e^{2i\mu\rho s} ds = \frac{4\pi\mu\rho(-1)^{k_1} e^{\mu\rho\frac{\pi}{2}}}{(2k_1-1)!} \prod_{m=1}^{k_1-1} \left(4\mu^2 + z_m\right). \tag{52}$$

Therefore, (52) can be written as

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

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

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}, that is, the harmonics $\hat{k}$ which, as it will be clear later on, give the largest

contribution into the R_{n+1}. We summarize some data about the exponents appearing then: m must be $4|\hat{k}|-1$, $k_1=|\hat{k}|$, $l_1=0$. From this we can see the contribution to Δp_j, $j=1,2$ in (27). We note also that the $\mathcal{P}_\sigma(q)$ products in (28) must be estimated using $q=p=2|\hat{k}|$. We use Lemma 4.3 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 4.3 is bounded by $\exp(\hat{B}|\hat{k}|)$, with $|\hat{B}|$ bounded. So, its effect is small. This fact, together with the results in the previous section (see (30)-(32)) gives that 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 and we assume that is bounded by $\exp(-M|\hat{k}|)<|\hat{A}_{\hat{k}}|<\exp(M|\hat{k}|)$ for some $M>0$.

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

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

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 (53) have relevant coefficients, specially when η becomes small. Our present goal is to detect the dominant ones, optimizing with respect to $\hat{k}$, depending on η, and bound the effect of the remaining terms.

Let

$$\eta_n^*|\ln\eta_n^*|=\frac{\pi\sqrt{5}\beta^{2n+1}}{8},\quad \hat{\eta}_n^*|\ln\hat{\eta}_n^*|=\frac{\pi\sqrt{5}\beta^{2n+2}}{8},\quad (\eta_n^*,\hat{\eta}_n^*<0.1),\qquad n\geq 1.\tag{54}$$

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

$$\ln\eta_n^*=(2n+1)\ln\beta(1+o(1)),\quad \ln\hat{\eta}_n^*=(2n+2)\ln\beta(1+o(1)),\quad o(1)=\mathrm{O}\left(\frac{\ln n}{n}\right).\tag{55}$$

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

$$c_\beta(\eta)=C_0\cosh\left(\frac{\ln\eta-\ln\eta_n^*}{2\ln\beta}\right),\quad C_0=\sqrt{\frac{8\pi(1+\beta)}{\sqrt{5}}}.\tag{56}$$

We are guided by [14] and [5] to introduce this function. It has a small discontinuity, $o(1)$ as in (55), 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*

$$\mathcal{N}(\hat{\psi},\eta)=\sum_{\hat{k}\in\mathbb{Z}^2\setminus\{0\}}A_{\hat{k}}\exp\left(-2|\hat{k}||\ln\eta|-\frac{\pi|\hat{k}\cdot\omega|}{2\eta}+2|\hat{k}|\ln\frac{|\hat{k}\cdot\omega|}{|\hat{k}|}\right)\sin(\hat{k}\cdot\hat{\psi}). \tag{57}$$

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

$$c_1<\frac{\ln|A_{\hat{k}}|}{|\hat{k}|}<c_2, \tag{58}$$

then, for η small enough,

$$\begin{aligned}\mathcal{N}(\hat{\psi},\eta) &= \sum_{\hat{k}\in\{\hat{k}^*,\hat{k}^{**}\}}A_{\hat{k}}\exp\left(-2|\hat{k}||\ln\eta|-\frac{\pi|\hat{k}\cdot\omega|}{2\eta}+2|\hat{k}|\ln\frac{|\hat{k}\cdot\omega|}{|\hat{k}|}\right)\\ &\quad\times\left(\sin(\hat{k}\cdot\hat{\psi})+\mathrm{O}\left(\exp\left(-g_1\frac{|\ln\eta|^{1/2}}{\eta^{1/2}}\right)\right)\right),\end{aligned} \tag{59}$$

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

$$|\mathcal{N}(\hat{\psi},\eta)| < \exp\left(-[c_\beta(\eta)-g_3]\frac{|\ln\eta|^{1/2}}{\eta^{1/2}}\right), \tag{60}$$

$$|\mathcal{N}(\eta)| > \exp\left(-[c_\beta(\eta)+g_4]\frac{|\ln\eta|^{1/2}}{\eta^{1/2}}\right), \tag{61}$$

where g_3,g_4 are fixed positive constants, as small as desired, and c_β is given in (56) and (54).

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):

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

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 [13].

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 $\beta \notin \mathbb{Q}$ and $n \geq 1$, 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 $\mathbb{T}^2$ given by the Fourier series in (57) where $A_{\hat{k}} = -A_{-\hat{k}}$ will be all non–zero, with the bounds given in (58).

First we need to introduce some auxiliary 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

$$k = \left(\frac{2\gamma}{\eta|\ln\eta|}\right)^{1/2} \times \left(1 + \mathrm{O}\left(\frac{\ln|\ln\eta|}{|\ln\eta|}\right)\right). \tag{62}$$

If we rewrite (57) 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):

$$\sum_{k_2,k_3\in\mathbb{Z},|k_2\beta-k_3|\geq 1/2} + \sum_{|k_2\beta-k_3|<1/2} \left\{ \sum_{k_3,k_2\in\mathbb{Z},k_2>k_{2,\eta}} + \sum_{n\geq 0,k_2^{(n)}\leq k_{2,\eta}} + \sum_{n\geq 0,k_2^{(n-1)}<k_2<\min(k_2^{(n)},k_{2,\eta})} \right\}, \tag{63}$$

the objects added in each sum being

$$\exp\left(\xi_{\hat{k}}|\hat{k}| - 2|\hat{k}||\ln\eta| - \frac{\pi|\hat{k}\cdot\omega|}{2\eta} + 2|\hat{k}|\ln\frac{|\hat{k}\cdot\omega|}{|\hat{k}|}\right)\sin(\hat{k}\cdot\hat{\psi}), \tag{64}$$

where $\xi_{\hat{k}}$ stands for $\ln|A_{\hat{k}}|/|\hat{k}|$ (and, hence, it is bounded by (58)) 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

$$\begin{aligned} \left|\sum\nolimits_1\right| &\leq \exp\left(-\frac{\pi}{4\eta}\right) \sum_{\hat{k}\in\mathbb{Z}^2\setminus\{0\}} \exp\left(c_2|\hat{k}| - 2|\hat{k}||\ln\eta| + 2|\hat{k}|\ln\frac{|\hat{k}\cdot\omega|}{|\hat{k}|}\right) \\ &< \exp\left(-\frac{\pi}{4\eta}\right) \sum_{\hat{k}\in\mathbb{Z}^2\setminus\{0\}} \exp(c_2|\hat{k}| - 2|\hat{k}||\ln\eta|) \leq \exp\left(-\frac{\pi}{4\eta}\right). \end{aligned} \tag{65}$$

Estimate (65) 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

$$F_n = (\beta^{-n} - (-1)^n\beta^n)/\sqrt{5}, \tag{66}$$

then it follows

$$|F_n\beta - F_{n-1}| = \frac{1-(-1)^n\beta^{2n}}{\sqrt{5}F_n} = \frac{1+\mathrm{O}(F_n^{-2})}{\sqrt{5}F_n} \quad \text{and} \quad F_{n+1} = F_n(\beta^{-1} + \mathrm{O}(F_n^{-2})). \tag{67}$$

From now on we shall neglect the $\mathrm{O}(F_n^{-2})$ terms in (67) 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

$$|k_2\beta - k_3| \geq \frac{4}{\sqrt{5}k_2}(1 + \mathrm{O}(k_2^{-2})). \tag{68}$$

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

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

if η is small enough. We have used $\left||\hat{k}| - (1+\beta)k_2\right| < 1/2$, the bounds following from (62), the constant $\hat{c}_2$, which is a minor modification of c_2 to account for some additional terms $\mathrm{O}(k_2)$ 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 (68) we have

$$\left|\sum\nolimits_4\right| \leq \exp\left(\hat{c}_2k_2 - 2(1+\beta)k_2|\ln\eta| - \frac{\pi}{2\eta}\frac{4}{\sqrt{5}k_2} - 4(1+\beta)k_2\ln k_2\right). \tag{69}$$

We shall bound each one of the terms in (69) (there are at most $k_{2,\eta} = \mathrm{O}((\eta|\ln\eta|)^{-1/2})$ 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 (69). Equating the derivative with respect to x to zero, we obtain

$$\eta x^2|\ln\eta|/2 + \eta x^2\ln x + o(1) = \frac{\pi\beta}{2\sqrt{5}}. \tag{70}$$

Let $\gamma = \eta x^2\ln x$. Solving for x as in (62) and replacing in (70) we obtain $\gamma = \dfrac{\pi\beta}{4\sqrt{5}} + o(1)$ and from this the bound

$$\left|\sum\nolimits_4\right| \leq \exp\left(\left(-4\left(\frac{2\pi}{\beta\sqrt{5}}\right)^{1/2} + o(1)\right)\left(\frac{|\ln\eta|}{\eta|}\right)^{1/2}\right). \tag{71}$$

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 (63). 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 (69) but using (67) instead of (68) 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

$$2(1+\beta)x|\ln\eta| + \frac{\pi}{2\eta\sqrt{5}x} + (1+\beta)(x\ln x - x). \tag{72}$$

The first derivative of (72) 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

$$x_{\max} = \left(\frac{2\gamma_F}{\eta|\ln\eta|}\right)^{1/2}\left(1 + \mathrm{O}\left(\frac{\ln|\ln\eta|}{|\ln\eta|}\right)\right) \tag{73}$$

and (72) gives the value

$$\left(\frac{8\pi(1+\beta)}{\sqrt{5}}\right)^{1/2}\left(\frac{|\ln\eta|}{\eta}\right)^{1/2}(1+o(1)), \tag{74}$$

when $\eta \to 0$.

This already shows several things:

- The $\mathrm{O}(x)$ neglected terms behave like (73) and hence they can be included in the $o(1)$ terms in (74) for η small.
- The (absolute value of the numerical) coefficient in (74) is less, by a factor of 2, than the one in (71). 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 (66) and (73) tell us

$$\eta_n|\ln\eta_n| = 10\gamma_F\beta^{2n}\left(1 + \mathrm{O}\left(\frac{\ln n}{n}\right)\right), \quad \eta_n = \frac{10\gamma_F\beta^{2n}}{2n|\ln\beta|}\left(1 + \mathrm{O}\left(\frac{\ln n}{n}\right)\right), \quad \frac{\eta_{n+1}}{\eta_n} \to \beta^2 \tag{75}$$

if $n \to \infty$. We realize that η_n is nothing else than the value η_n^* defined before in (54), 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 (75). We want to express the coefficient in (64) as

$$\exp\left(-\hat{g}(w)\left(\frac{|\ln\eta|}{\eta}\right)^{1/2}\right) \tag{76}$$

for $\eta = \beta^w \eta_n^*$, $|w|$ bounded by a constant. Direct substitution in (64) gives

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

From this it follows that, given η, we select n such that $\hat{\eta}_n^* < \eta \leq \hat{\eta}_{n-1}^*$. We look now for the contribution of the term associated to F_n. It will be of the form (76) with $-1 < w \leq 1$. 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 $\mathrm{O}((|\ln\eta|/\eta)^{1/2})$, 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 (59), (60) and (61). □

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 $A_{\hat{k}}$ cannot 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 Δ_1 and Δ_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 (76) are of the form $\cosh(w/2)$ and $\cosh(w/2 - 1)$ if we assume, for definiteness, $0 < w_0 \leq w \leq 1$, 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 Δ_j is denoted as $\mathcal{E}_{\hat{k}}^{(j)}$ for $j = 1, 2$.

Then we have

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

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 Δ_1, Δ_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 $0 \leq w < w_0$. In this last case, there is a large dominant term but the next two subdominant are of comparable order of magnitude. Hence, they can cancel. The discussion is postponed to the end of next section.

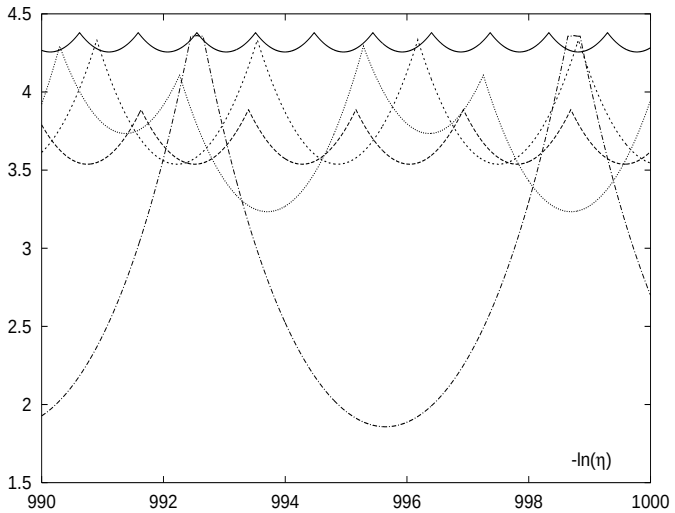

Figure 8: Values of c_β as a function of $|\ln\eta|$ for several quadratic irrationals.

The description of the behaviour of the dominant terms in the splitting, under the assumption (58) on the coefficients, requires the introduction of the function c_β as defined by (56) and (54). 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

$$\exp\left(-(8\pi\underline{c}(1+\beta))^{1/2}\left(\frac{|\ln\eta|}{\eta}\right)^{1/2}\right), \tag{77}$$

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 (58) the 2D invariant tori have a splitting whose upper bound has a sharp estimate of the form (77), 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

In this section we compute the points in $W^u_{\mathbb{T}_\beta} \cap \{y = \pi\}$ or $W^s_{\mathbb{T}_\beta} \cap \{y = \pi\}$ giving rise to either $\Delta_1(\hat{\psi}, \eta) = 0$ or $\Delta_2(\hat{\psi}, \eta) = 0$. These are curves in a two torus whose topology changes when η does. Therefore, the behaviour of the set of bifurcations is described. Furthermore, this section is also devoted to study the homoclinic points and the behaviour of the splitting determinant on these points.

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 $\Delta_1(\hat{\psi}, \eta)$, 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:

$$\Delta_1(\hat{\psi}, \eta) = c_1 \sin(\mathcal{X}) + c_2 \sin(\hat{\mathcal{X}}), \quad c_1 = c_1(\eta), \quad c_2 = c_2(\eta),$$

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 $\Delta_1(\hat{\psi}, \eta) = 0$ 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 Δ_1, $\partial\Delta_1/\partial\psi_2$ and $\partial\Delta_1/\partial\psi_3$ are simultaneously zero, that is

1. $\Delta_1 = c_1 \sin(\mathcal{X}) + c_2 \sin(\hat{\mathcal{X}}) = 0,$
2. $\dfrac{\partial\Delta_1}{\partial\psi_2} = c_1 F_{j+1} \cos(\mathcal{X}) + c_2 F_{j+2} \cos(\hat{\mathcal{X}}) = 0,$
3. $\dfrac{\partial\Delta_1}{\partial\psi_3} = -c_1 F_j \cos(\mathcal{X}) - c_2 F_{j+1} \cos(\hat{\mathcal{X}}) = 0,$

which implies that

$$\begin{pmatrix} F_{j+1}\cos(\mathcal{X}) & F_{j+2}\cos(\hat{\mathcal{X}}) \\ F_j \cos(\mathcal{X}) & F_{j+1}\cos(\hat{\mathcal{X}}) \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{78}$$

If $\cos(\mathcal{X})\cos(\hat{\mathcal{X}}) \neq 0$, it follows from Proposition 5.4 that the determinant of the matrix in (78) is different from zero.

Hence, the unique non-trivial solution of (78) 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

$$\mid c_1 \mid = \mid c_2 \mid .$$

The same occurs for Δ_2. In this case, we have that the general contribution to $\Delta_2(\hat{\psi}, \eta)$ given by the two dominant Fibonacci–type harmonics with coefficients d_1, d_2 is:

$$\Delta_2(\hat{\psi}, \eta) = d_1 \sin(\mathcal{X}) + d_2 \sin(\hat{\mathcal{X}}), \;\; d_1 = d_1(\eta), \;\; d_2 = d_2(\eta).$$

Again the curve C_h^2 given by $\Delta_2(\hat{\psi}, \eta) = 0$, 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 ψ_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 Δ_1, and close to 0.2211 and to 0.0295 in the case of Δ_2 (see Figure 5).

If the analytic approximations given in (33) are used, the critical values of η are, respectively, 0.061345, 0.028, 0.00675 and 0.002614 for Δ_1, and 0.2163, 0.02933, 0.007 and 0.002664 for Δ_2. The moderate lack of agreement is due to the fact that there are exponential terms (see Lemma 4.3) and higher order terms missing in (33). 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 Δ_1 and Δ_2, respectively, then

$$\frac{\eta_1}{\eta_2} = \begin{cases} 2.191 & \text{for } \Delta_1 \\ 7.375 & \text{for } \Delta_2 \end{cases}, \quad \frac{\eta_2}{\eta_3} = \begin{cases} 4.415 & \text{for } \Delta_1 \\ 4.191 & \text{for } \Delta_2 \end{cases} \quad \text{and} \quad \frac{\eta_3}{\eta_4} = \begin{cases} 2.582 & \text{for } \Delta_1 \\ 2.628 & \text{for } \Delta_2 \end{cases}$$

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 (54).

However, one can also give a direct proof of the value of such quotient from the criterion of being η a critical value, when taking into account only the dominant part of the Melnikov function given in (29), (30) and (31). 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 $\eta_1, \eta_2, \dots$, 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:

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

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 (53)) and for the neglected last term inside the function exp in (53). Bearing in mind (67), putting all the terms as a function of F_n, using (66) 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

$$\eta = \frac{A}{F_n^2\,(2\ln F_n - \ln\eta + B)\,.} \tag{79}$$

In order to estimate the behaviour of η_n/η_{n+1} we need to solve (79). We proceed as in (62) with some detail. Let $\gamma = \eta F_n^2 \ln F_n$. Then (79) can be written as

$$\gamma = \frac{A}{4 + (\ln(\ln F_n) + B - \ln\gamma)/\ln F_n}, \tag{80}$$

which has an unique solution, γ_n, in $[\gamma^{(1)}, \gamma^{(2)}] := [A/5, A/3]$. Indeed, writing (80) 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 zeroes of the splitting determinant.

If only the same two dominant harmonics in Δ_1 and Δ_2 are relevant, that is, for example

$$\begin{aligned}\Delta_1 &= A_2 \sin(p_n\psi_2 - q_n\psi_3) + B_2 \sin(p_{n+1}\psi_2 - q_{n+1}\psi_3),\\ \Delta_2 &= A_3 \sin(p_n\psi_2 - q_n\psi_3) + B_3 \sin(p_{n+1}\psi_2 - q_{n+1}\psi_3),\end{aligned}$$

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

$$\begin{pmatrix} A_2 & B_2 \\ A_3 & B_3 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{81}$$

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 Δ_1, Δ_2 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 (81) 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 Δ_1 and Δ_2 appear as the gradient of a function that, after a suitable scaling of the dominant term, is of the form*

$$-c_n - \lambda(\eta)c_{n+1} - \delta(\eta)c_{n-1} + o(\lambda(\eta)^2 + \delta(\eta)^2), \tag{82}$$

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 (56), while the order of the next terms has a similar form with $a = C_0(\cosh(3|\ln\beta|/2) - 1)$. However, from (32), (31) 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

$$\begin{aligned} p_ns_n + \lambda p_{n+1}s_{n+1} + \delta p_{n-1}s_{n-1} &= 0, \\ q_ns_n + \lambda q_{n+1}s_{n+1} + \delta q_{n-1}s_{n-1} &= 0, \end{aligned} \tag{83}$$

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 (83) is equivalent to

$$\begin{aligned} \delta a_{n+1}\sin(\gamma_{n-1}) &= \gamma_n, \\ \lambda\sin(\gamma_{n+1}) + \delta\sin(\gamma_{n-1}) &= 0. \end{aligned} \tag{84}$$

Using $\gamma_{n+1} = \delta a_{n+1}^2\sin(\gamma_{n-1}) + \gamma_{n-1}$ in the second equation in (84), 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 (82). The effect of the terms beyond the subdominant ones can be taken into account using the smallness assumption made in (82) and a routine application of the Implicit Function Theorem, for η small enough. □

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 $\Delta_1 = 0$ and $\Delta_2 = 0$ 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

$$\begin{aligned} \lambda(\eta) &= \exp\left(-C_0\left(\cosh(|\ln\beta|) - \sinh(|\ln\beta|)\tfrac{\Delta\eta}{2\eta'}\right)h(\eta)\right), \\ \delta(\eta) &= \exp\left(-C_0\left(\cosh(|\ln\beta|) + \sinh(|\ln\beta|)\tfrac{\Delta\eta}{2\eta'}\right)h(\eta)\right), \end{aligned} \tag{85}$$

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 (85) we obtain the dominant terms

$$\Delta\eta = \frac{\eta'\exp(-C_0\cosh(|\ln\beta|)h(\eta'))}{h(\eta')2\sinh(|\ln\beta|)}. \tag{86}$$

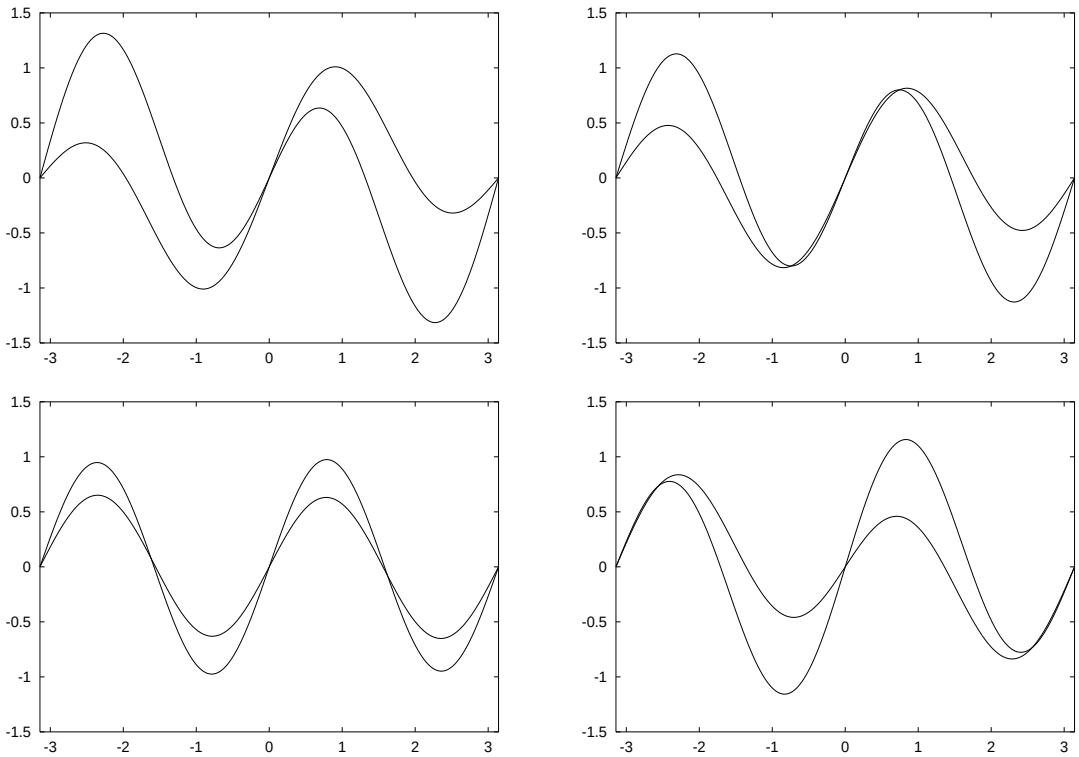

Figure 9: Additional homoclinic points. See the text for explanation.

This clearly shows that the successive intervals of existence of additional homoclinic points decrease very quickly when $\eta \to 0$. The expression (86) 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 must cross each other. At the crossings we are in the situation studied in Proposition 6.2.*

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