On the connection between the Nekhoroshev theorem and Arnold Diffusion

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Abstract. The analytical techniques of the Nekhoroshev theorem are used to provide estimates on the coefficient of Arnold diffusion along a particular resonance in the Hamiltonian model of Froeschlé et al. (2000). A resonant normal form is constructed by a computer program and the size of its remainder \( \| R_{\text{opt}} \| \) at the optimal order of normalization is calculated as a function of the small parameter \( \epsilon \). We find that the diffusion coefficient scales as \( D \propto \| R_{\text{opt}} \|^3 \), while the size of the optimal remainder scales as \( \| R_{\text{opt}} \| \propto \exp(1/\epsilon^{0.21}) \) in the range \( 10^{-4} \leq \epsilon \leq 10^{-2} \). A comparison is made with the numerical results of Lega et al. (2003) in the same model.

Keywords: Normal forms, Nekhoroshev theorem, Arnold diffusion

1. Introduction

In a series of instructive papers, Froeschlé et al. (2000, 2005), Lega et al. (2003), and Guzzo et al. (2005) presented the results of a detailed numerical investigation of the phenomenon of Arnold diffusion (Arnold 1964) in a Hamiltonian system of three degrees of freedom that satisfies sufficient conditions for the holding of the Nekhoroshev theorem (Nekhoroshev 1977, Benettin et al. 1985, Lochak 1992, Pöschel 1993). The aim of these studies was to establish quantitative estimates as regards a) the critical value of the small parameter \( \epsilon_c \) below which the system enters into the so-called ‘Nekhoroshev regime’, and b) the dependence of the local diffusion coefficient \( D \), along a particular resonance, on \( \epsilon \). In Guzzo et al. (2005) the authors reported to have also numerically observed global diffusion over an extended domain of the Arnold web. Other numerical studies over the years related to the same problem are: Kaneko and Konishi (1989), Wood et al. (1990), Dumas and Laskar (1993), Laskar (1993), Skokos et al. (1997), Giordano and Cincotta (2004). Some early results of the literature are briefly commented in the discussion.

In what follows we focus on an analysis of point (b) above. According to Lega et al. (2003), a tedious numerical calculation yields that the local diffusion coefficient \( D \) along a resonance depends monotonically on \( \epsilon \). While the limited range of the numerical data did not allow for
a precise fitting, the authors presented evidence that the numerical function $D(\epsilon)$ was decreasing faster than a power-law $D(\epsilon) \propto \epsilon^b$, while it was consistent with an exponential law $D(\epsilon) \propto \exp(-1/\epsilon^a)$ for some unspecified constant $a$. A subsequent study in a mapping model analogous to the above Hamiltonian model yielded the concrete estimate $a \simeq 0.28$ (Froeschlé et al. 2005).

In the present paper our aim is to provide a deeper understanding of these numerical results by having recourse, precisely, to the analytical apparatus of the Nekhoroshev theory, that is, the construction of a resonant Birkhoff normal form and of estimates on the size of the remainder $R$ of the normal form at the optimal order of normalization. The optimal remainder function $R_{\text{opt}}$ is a crucial quantity for the dynamics because it represents the true size of the perturbation of the system that corresponds to its deviation from an integrable system. Indeed, in Nekhoroshev theory all bounds on the variations of the actions follow from estimates on the size of $R_{\text{opt}}$. In order, therefore, to establish the link between the Nekhoroshev theory, on the one hand, and the problem of the speed of diffusion, on the other hand, in the present paper we seek to determine:

a) the dependence of the local diffusion coefficient $D$ on the size of the remainder $||R_{\text{opt}}||$ at the optimal order of normalization, and

b) the precise dependence of $||R_{\text{opt}}||$ on $\epsilon$. In particular, we seek to calculate $||R_{\text{opt}}||$ when $\epsilon$ becomes small enough so that the exponentially small scaling of $||R_{\text{opt}}||$ with $\epsilon$ clearly shows up. This required to consider values of $\epsilon$ one order of magnitude smaller than the values considered in the numerical experiments of Lega et al. (2003).

We can immediately state a brief summary of our main results. We find that:

a) $D$ scales with $||R_{\text{opt}}||$ as a power law $D \propto ||R_{\text{opt}}||^c$, with $c \simeq 3$. To determine this relation, use was made of the data of Lega et al. (2003) for the numerical values of $D$, and a program was written by the author in order to compute the Birkhoff normal form and thereby the remainder $R_{\text{opt}}$.

b) In the range $10^{-4} \leq \epsilon \leq 10^{-2}$, $||R_{\text{opt}}||$ scales as $||R_{\text{opt}}|| = \exp(-b/\epsilon^a)$ with $a \simeq 0.21$ and $b \simeq 3.22$. This also yields the exponential scaling $D \propto \exp(-3b/\epsilon^a)$. Note that the exponentially small scaling shows up clearly only for $\epsilon \leq 0.001$, while in the range $0.001 < \epsilon \leq 0.02$ a power-law fitting $||R_{\text{opt}}|| \propto \epsilon^{2.45}$ yields marginally better results than the exponential fitting. In fact, we find that although the onset of the ‘Nekhoroshev regime’ can be placed at a threshold value $\epsilon \approx 0.01$, the deviation of the remainder from a power law becomes clear only for $\epsilon$ one order of magnitude smaller than this value.
The computational algorithm used to obtain the above results is described in section 2. It follows essentially the normalization scheme described in the lecture notes on exponential stability of Giorgilli (2002, pp.86-87). This scheme is different from the traditional scheme based on normalization by successive orders of $\epsilon$. We further modify it to avoid using $K$-truncated resonant modules (see section 2). People working on mathematical aspects of the Nekhoroshev theory are definitely familiar with all related notions. However, a somewhat extended description is given in section 2, to help rendering the subject more accessible also to people oriented towards the applications.

Section 3 then focuses on the implementation of the algorithm in the particular model of Froeschlé et al. (2000). By constructing the normal form and identifying the optimal order of normalization, the size of $R_{opt}$ is evaluated for various values of $\epsilon$. This yields the exponential scaling of $|R_{opt}|$ on $\epsilon$. Using also the data of Lega et al. (2003) yields the power-law relation of $D$ with $|R_{opt}|$. Section 4 contains a brief discussion of the results.

2. The normal form algorithm

2.1. The classical construction

The analytical part of the Nekhoroshev theorem is based on the construction of a normal form for a $n$ degrees of freedom Hamiltonian system of the form

$$H(J, \phi) = H_0(J) + \epsilon H_1(J, \phi)$$

(1)

where $(J, \phi) \equiv (J_1, J_2, ..., J_n, \phi_1, \phi_2, ..., \phi_n)$ are action-angle variables, $H_0$ satisfies appropriate non-degeneracy and convexity conditions, and $H$ is analytic in a complexified domain of the actions and the angles. We shall be concerned with a local construction of a normal form for the Hamiltonian (1), valid within some (small) preselected open domain $W_a$ of the action space (the index $a$ means action space). The analyticity condition implies that if $H_1$ is Fourier expanded

$$H_1(J, \phi) = \sum_{k \in \mathbb{Z}^n} H_{1,k}(J) \exp(ik \cdot \phi)$$

(2)

there are positive constants $A, \sigma$ such that for all values of $J \in W_a$ the coefficients $H_{1,k}$ are bounded by

$$|H_{1,k}(J)| \leq A \exp(-|k|\sigma) .$$

(3)
The function $H_1$ is analytic in the domain $\mathcal{W}_a \times \mathbb{T}_\sigma^n$, where $\mathbb{T}_\sigma^n \equiv \{ \phi : \text{Re} \phi \in \mathbb{T}^n, |\text{Im} \phi_i| < \sigma, i = 1, \ldots, n \}$. Furthermore, bounds on the function $H_1$ can be found in domains $\mathcal{W}_a \times \mathbb{T}_{\sigma'}^n$, for any positive $\sigma' < \sigma$.

Now, the purpose of the normal form construction is to perform a series of canonical transformations $(J, \phi) \rightarrow (J^{(1)}, \phi^{(1)}), \rightarrow (J^{(2)}, \phi^{(2)}), \ldots$, such that, after $r$ normalization steps, the Hamiltonian is expressed as

$$H^{(r)}(J^{(r)}, \phi^{(r)}) \equiv H(J(J^{(r)}, \phi^{(r)}), \phi(J^{(r)}, \phi^{(r)})) = Z^{(r)}(J^{(r)}, \phi^{(r)}) + R^{(r)}(J^{(r)}, \phi^{(r)}) \quad (4)$$

In the last expression, the first term $Z^{(r)}(J^{(r)}, \phi^{(r)})$, called the normal form, is constructed in such a way as to yield a simple dynamics in the variables $(J^{(r)}, \phi^{(r)})$ (e.g. in the non-resonant or simply resonant case the Hamiltonian $Z^{(r)}(J^{(r)}, \phi^{(r)})$ is integrable). On the other hand, the second term $R^{(r)}(J^{(r)}, \phi^{(r)})$, called the remainder, represents a perturbation to the dynamics induced by the normal form. The goal of the theory is to proceed with the normalization as far as necessary in order to minimize the size of the remainder. In exceptional cases of integrable Hamiltonian systems one may proceed by infinitely many steps, within some domain of convergence, and show that the remainder tends to zero in the limit $r \rightarrow \infty$. In the generic case of non-integrable systems, however, one can only reduce $R^{(r)}(J^{(r)}, \phi^{(r)})$ to a finite minimum size. This is found at a specific order of normalization which is hereafter called the optimal order of normalization $r_{\text{opt}}$. The size of the remainder $R^{(r_{\text{opt}})}(J^{(r_{\text{opt}})}, \phi^{(r_{\text{opt}})})$ for any other order $r \neq r_{\text{opt}}$ is bigger than the size of $R^{(r_{\text{opt}})}(J^{(r_{\text{opt}})}, \phi^{(r_{\text{opt}})})$. Standard theory yields estimates $r_{\text{opt}} \sim 1/e^b$ and $||R^{(r_{\text{opt}})}|| \sim \exp(-1/e^a)$ for some positive integers $a, b$ depending on the number of degrees of freedom.

The classical construction leading to expressions of the form (4) is nowadays analyzed in many books (see e.g. Boccaletti and Pucacco (1996), Contopoulos (2002), Morbidelli (2002), or Ferraz-Mello (2007) for instructive introductions). The main steps can be summarized as follows:

a) One makes a choice as regards which Fourier terms $H_{1,k}(J) \exp(ik \cdot \phi)$ in $H_1$ will be retained and which terms will be eliminated in the normalized Hamiltonian. The terms to be retained are specified by their integer vector $k$ belonging to a particular subset of $\mathbb{Z}^n$ called resonant module (denoted hereafter by $\mathcal{M}$). The choice of resonant module is dictated by the location of the domain $\mathcal{W}_a$ in the action space, i.e., by whether this domain is close to or far from particular resonances (see subsection 2.3).

b) The Fourier terms not belonging to $\mathcal{M}$ are the ones to be eliminated by a canonical transformation. Let us consider the first nor-
malization step. We shall consider canonical transformations of old variables \((J, \phi)\) to new variables \((J^{(1)}, \phi^{(1)})\) obtained via a Lie generating function \(\chi_1(J^{(1)}, \phi^{(1)})\). The function \(\chi_1(J^{(1)}, \phi^{(1)})\) will be selected so as to be of the ‘first order of smallness’ (the precise meaning of this sentence is analyzed below). The canonical transformation is defined by

\[
J = \exp(L_{\chi_1})J^{(1)}, \quad \phi = \exp(L_{\chi_1})\phi^{(1)}
\]

where \(L_{\chi_1} \equiv \{\cdot, \chi_1\}\) is the Poisson bracket operator, and \(\exp(L_{\chi_1})\) is the formal exponential development of \(L_{\chi_1}\). A well known property of Lie transformations is that for any function of the canonical variables \(f(q, p)\) one has

\[
\exp(L_{\chi_1})f(q, p) = f(\exp(L_{\chi_1})q, \exp(L_{\chi_1})p)
\]

As a result, the transformed Hamiltonian, after the action of the generating function \(\chi_1\) is given by

\[
H^{(1)} = \exp(L_{\chi_1})H = H + L_{\chi_1}H + \frac{1}{2}L^2_{\chi_1}H + \ldots
\]

In order to specify the function \(\chi_1(J^{(1)}, \phi^{(1)})\), we select from \(H_1\) all the terms satisfying the following two conditions: a) being of the ‘first order of smallness’, and b) not belonging to \(\mathcal{M}\). Denoting by \(h_1\) the sum of these terms, the terms are eliminated by selecting \(\chi_1\) so as to satisfy:

\[
L_{\chi_1}H_0 + h_1 = 0.
\]

Equation (8) is called homological. It is reduced to a diagonal system of linear algebraic equations. Namely, writing \(h_1\) as

\[
h_1 = \sum_k h_{1,k}(J)\exp(ik \cdot \phi)
\]

and setting

\[
\chi_1 = \sum_k \chi_{1,k}(J)\exp(ik \cdot \phi)
\]

we find, through (8), the solution for the coefficients \(\chi_{1,k}(J)\) given by:

\[
\chi_{1,k}(J) = \frac{h_{1,k}(J)}{ik \cdot \omega(J)}
\]

where

\[
\omega(J) = \nabla_J H_0(J)
\]

is the frequency vector of the unperturbed Hamiltonian at the point \(J\) of the action space.
c) In the same way we eliminate the terms of the second order of smallness in $H^{(1)}$ or, in general, the terms of the $r$-th order of smallness in $H^{(r-1)}$. The recursive formulae for the $r$-th canonical transformation $J^{(r-1)} = \exp(L_{\chi_r})J^{(r)}$, $\phi^{(r-1)} = \exp(L_{\chi_r})\phi^{(r)}$ are:

\[ \{H_0, \chi_r\} + h^{(r-1)}_r = 0 \]
\[ H^{(r)} = \exp(L_{\chi_r})H^{(r-1)} . \]  

(11)

Following iteratively the above procedure, the function $H^{(r)}$ takes the form (4). The remainder consists of all the terms of $H^{(r)}$ of ‘order of smallness’ larger than $r$. It can be written as

\[ R^{(r)} = h^{(r)}_{r+1} + h^{(r)}_{r+2} + \ldots \]  

(12)

This series is an analytic function in a restriction of the domain of analyticity of the original hamiltonian provided that the Lie transformation in (11) is convergent at every step (which is ensured for ‘small enough’ generating functions $\chi_r$).

2.2. Book-keeping

A clarification of the meaning of ‘order of smallness’ is now in order. When one implements the recursive scheme of Eqs.(5) and (11), one needs to decide how should $H^{(r)}$ at every step be split into terms of different orders. Such a splitting should be based on the size of each term relative to the size of the other terms. In a computer program, it is customary to introduce a so-called ‘book-keeping’ parameter $\lambda$. This is a parameter the powers of which appear as coefficients in front of the various terms in the expansion. A term with coefficient $\lambda^p$ is said to be ‘of order of smallness’ $p$. This helps separating the terms in the program by, say, recalling the Coefficient($h^{(r-1)}, \lambda, r$) in an algebraic program like Mathematica in order to get the term $h^{(r-1)}_r$ in Eq.(11). As the program carries on the normalization, the book-keeping coefficients change according to the rule that the coefficient of the Poisson bracket of two terms with coefficients $\lambda^p$ and $\lambda^q$ is $\lambda^{p+q}$. In the end we set $\lambda = 1$ to recover the correct values of all the coefficients.

This way of organizing the series is practical, but it also reflects a fundamental decision on what quantity we consider to represent ‘smallness’ in the perturbation series. If the overall size of $H_1$ is an $O(1)$ quantity, then it is customary to identify $\epsilon$ itself as the small parameter. In that case the normalization scheme proceeds by ascending powers of $\epsilon$, and the generating functions $\chi_r$ are of order $O(\lambda^r) \equiv O(\epsilon^r)$. We shall see in subsection 2.4 how to modify the ‘book-keeping’ so as to separate terms of different smallness which co-exist within $H_1$, and then within
$H^{(r)}$, provided that the function $H_1$ satisfies analyticity conditions of the form (3).

2.3. Resonant K-module

The choice of resonant module depends on the location of the domain $W_a$ in the action space and on the properties of the unperturbed Hamiltonian $H_0$. Let us consider the homological equation of the first order under the choice of book-keeping $\lambda \equiv \epsilon$. This reads:

$$\{H_0, \chi_1\} = -\epsilon \tilde{H}_1$$

where $\tilde{H}_1$ is the part of $H_1$ containing terms to be eliminated. The solution of (13) is

$$\chi_1 = \epsilon \sum_{k \in \mathbb{Z}/M} \frac{H_{1, k}(J) \exp(ik \cdot \phi)}{ik \cdot \omega(J)}.$$  

Provided that the resonant manifolds $k \cdot \omega(J) = 0$ are dense in the action space, for any small open domain $W_a$ there are infinitely many resonant manifolds crossing $W_a$. This implies that there is a dense set of values of the actions $J$ within $W_a$ for which a divisor in (14) becomes exactly equal to zero. In practice, this means that a generating function like $\chi_1$ in (14) cannot in fact be determined in any open domain $W_a$. In Nekhoroshev theory, an often stated remedy to this problem consists of splitting the set of Fourier harmonics $\exp(ik \cdot \phi)$ into low order and high order harmonics according to whether $|k| \equiv |k_1| + \ldots + |k_n|$ is smaller or larger than some positive integer $K$ (see, for example, Morbidelli and Guzzo 1997). The choice of value of $K$ is arbitrary, but the choice $K \sim 1/\epsilon^a$, for some constant $a$, is suggested by the request that there be no overlapping of the resonant domains (of width $O(\epsilon^{1/2})$) formed around each of the resonant manifolds $k \cdot \omega(J) = 0$, with $|k| \leq K$, other than the overlapping near the loci at which the manifolds intersect each other (see Morbidelli 2002, p.119). Fixing $K$ and requesting that only the harmonics with $|k| \leq K$ be normalized ensures that divisors $k \cdot \omega(J)$ with $|k| > K$ will not appear in the series. Furthermore, the domain $W_a$ is crossed by only a finite number of resonant manifolds with $|k| \leq K$. More precisely, denoting by $\mathcal{R}_a$ the subset of integer vectors $k$ for which the resonant manifolds $k \cdot \omega(J) = 0$ intersect the domain $W_a$, and by $b_{\mathcal{R}_a}$ a subset of $\mathcal{R}_a$ such that any vector of $\mathcal{R}_a$ can be produced by a linear combination of the vectors of $b_{\mathcal{R}_a}$ with integer coefficients, the relevant property is that $b_{\mathcal{R}_a}$ contains only a finite number of vectors $k$ with $|k| \leq K$ and an infinite number of vectors with $|k| > K$. Denoting by $b_{\mathcal{R}_a}^{<K}$ the subset of vectors $k \in b_{\mathcal{R}_a}$.
with $|k| \leq K$, the resonant module $\mathcal{M}_{\alpha, \leq K}$ is determined by:

$$
\mathcal{M}_{\alpha, \leq K} = \text{span}\{b^{\leq K}_{R_{\alpha}}\} .
$$

(15)

Let $\mathcal{M}_{\alpha, > K}$ be the complement of $\mathcal{M}_{\alpha, \leq K}$ with respect to $R_{\alpha}$. Under the ’book-keeping’ choice $\lambda \equiv \epsilon$, one then has the following iterative algorithm of determination of the normal form locally, i.e., within the domain $W_{\alpha}$:

a) Assuming that $(r - 1)$ normalization steps were completed, split $H_{\chi}^{(r-1)}$ as $\tilde{H}_{\chi}^{(r-1)} + h_{\chi}^{(r-1)}$, where $\tilde{H}_{\chi}^{(r-1)}$ contains all the terms with $|k| \leq K$ not belonging to $\mathcal{M}_{\alpha, \leq K}$.

b) Determine the generating function $\chi_{\chi}$ by solving

$$
\{H_{0}, \chi_{\chi}\} = -\tilde{H}_{\chi}^{(r-1)}
$$

(16)

c) Find the new Hamiltonian

$$
H^{(r)} = \exp(\epsilon^{r} L_{\chi_{\chi}}) H^{(r-1)} = Z_{0} + \epsilon Z_{1} + \ldots + \epsilon^{r} Z_{r} + H^{(r)}_{\text{res}} + H^{(r)}_{\text{nonres}}
$$

(17)

in which $Z_{j}$, $j = 0, \ldots, r$ are normal form terms belonging to the resonant module $\mathcal{M}_{\alpha, \leq K}$, $H^{(r)}_{\text{res}}$ contains all the Fourier terms belonging to $\mathcal{M}_{\alpha, > K}$, and $H^{(r)}_{\text{nonres}}$ contains the remaining Fourier terms that are not in any of the previously determined sets. This completes one step of the iteration algorithm. As shown in Morbidelli and Giorgilli (1997), while all the terms of order higher than $r$ in these two functions are bounded by a quantity $O(\exp(-K\sigma))$, i.e., they are both exponentially small in $K$, the terms of $H^{(r)}_{\text{res}}$ are the ones making the leading contribution to the remainder.

2.4. A modified algorithm

Two problems arise in the implementation of the above algorithm:

a) Eqs.(9) or (14) imply that the denominators of all the series coefficients are functions of the actions, in the form of products of divisors $k \cdot \omega(J)$. This implies that even if $H_{0}(J)$ is polynomial in the actions, the Fourier coefficients of the terms $\exp(ik \cdot \phi)$ in $H^{(r)}$ or $\chi^{(r)}$ are in general rational in the actions. The extra computational load of dealing with rational expressions (and their derivatives entering into Poisson brackets) makes the whole algorithm hardly tractable in this form. We defer the solution of this problem after the analysis of point (b) below, to which it is linked.

b) One needs to store many more intermediate coefficients than those eventually needed in order to have a complete knowledge of the transformed Hamiltonian or of the generating function within any specified
domain of interest. This is a rather technical problem, the solution of which is, nevertheless, crucial in constructing an efficient algorithm for the computation of the normal form. A detailed quantitative discussion of this problem is deferred to the appendix. Here we state the main result: Under the book-keeping scheme $\lambda \equiv \epsilon$, assume we are interested in specifying the transformed Hamiltonian in a ‘domain of interest’ defined by the maximum orders $(r_{\text{max}}, K_{\text{max}})$, where $r_{\text{max}}$ denotes the maximum order in the book-keeping variable $\epsilon$ and $K_{\text{max}}$ denotes the maximum order in Fourier space. Then, in order to be able to specify all the terms belonging to the ‘domain of interest’, we must store, at intermediate normalization orders $r \leq r_{\text{max}}$, all the Hamiltonian terms of Fourier order $|k| \leq K(r_{\text{max}} - r) + K_{\text{max}}$. As shown in the appendix, these intermediate terms outnumber by far the terms finally stored within the ‘domain of interest’.

Issue (b) can be resolved by introducing a different book-keeping of the terms, on the basis of their Fourier order rather than $\epsilon$-order. This organization of the series is analyzed in detail in Giorgilli (2002, pp.86-87) and we present the main points of this analysis in the appendix. Essentially, it reflects the fact that for any order $r \leq r_{\text{max}}$, many Fourier terms with a coefficient $\epsilon^r$ in front, which would thus be formally stored as of order $\lambda^r$ under the book-keeping $\epsilon \equiv \lambda$, are actually of much smaller size than $\epsilon^r$, because the size of any $\exp(ik \cdot \phi)$ term scales as $(e^{-\sigma})^{|k|}$ by virtue of the analyticity condition. This scaling is already present in the original Hamiltonian and it propagates at all subsequent normalization steps. Precisely, this fact is recognized by ‘book-keeping’ the terms on the basis of their Fourier rather than $\epsilon$-order. The exact algorithm, which replaces the algorithm of subsection (2.3), reads as follows:

1) Define $K' = \max\{[1/\sigma], 1\}$.
2) Place a book-keeping coefficient $\lambda^p$ in front of each Fourier term of the form $\exp(ik \cdot \phi)$ in $H_1$, where $p = [|k|/K'] + 1$.
3) Carry on the normalization (Eqs.(11)) by successive powers of $\lambda$.

As shown in the appendix, with such an algorithm there are no extra terms, outside the domain of interest, that need to be computed.

Furthermore, it is possible to incorporate a solution to issue (a) in the same algorithm. First, we notice that, as defined in step (1) above, the constant $K'$ does not pose an upper bound (like $K$) in the order of the Fourier harmonics being normalized at successive steps, since the algorithm requests that terms of increasing order $rK'$ be normalized at the $r$-th normalization step. In principle, this would cause a problem when $r$ becomes larger than $K/K'$. But in practice, one wishes to avoid the problem of the appearance of the actions in the denominators of the Fourier coefficients for both $|k| \leq K$ or $|k| > K$, that is for both
$r \leq K/K'$ and $r > K/K'$. It can be shown (section 3) that if the domain $W_a$ is 'resonant', that is $M_{\alpha \leq K} \neq \{0,0,\ldots,0\}$, the width of $W_a$ scales with $\varepsilon$ as $O(\varepsilon^{1/2})$. Non-resonant domains can also be covered by subdomains of size $O(\varepsilon^{1/2})$. Choosing a point $J_*$ in the interior of the domain $W_a$, we then develop the Hamiltonian locally, within $W_a$, by expanding the actions as

$$J = J_* + \varepsilon^{1/2} I.$$  

(18)

The transformation $J \rightarrow I$ is not canonical under the usual Poisson structure, but the dynamics remains unaltered if a new Hamiltonian

$$H' = \varepsilon^{-1/2} H$$  

(19)

substitutes $H$ as generator of the equations of motion. For example, in a Thirring-type model

$$H = \frac{J_1^2 + J_2^2}{2} + \varepsilon \sum_{k_1,k_2} c_{k_1,k_2} \exp(i(k_1\phi_1 + k_2\phi_2))$$  

(20)

we get, introducing also the 'book-keeping' parameter $\lambda$:

$$H' = \text{const} + J_1 I_1 + J_2 I_2 + \varepsilon^{1/2} \left( \lambda I_1^2 + I_2^2 \right)$$

$$+ \sum_{k_1,k_2} \lambda^{||k||/K'} + 1 c_{k_1,k_2} \exp(i(k_1\phi_1 + k_2\phi_2)) \right).$$  

(21)

Consequently, the perturbation has been rescaled to $\varepsilon^{1/2}$, i.e., it follows the size $O(\varepsilon^{1/2})$ of the domain $W_a$. Nevertheless, the unperturbed frequencies are now $\omega(J_*) \equiv \omega_*$, thus they do not depend on the actions, since the terms quadratic in the actions are now formally of order $\lambda$. This implies that the divisors are of the form $k \cdot \omega_*$, i.e., independent of the actions. Consequently, the algorithm proceeds with polynomial rather than rational (in the actions) Fourier coefficients at every step. This also means that there is no longer need for introducing a $K$-truncated resonant module. Thus, in all calculations the resonant module is specified only by the resonances between the frequencies $\omega_*$. If $\omega_*$ are incommensurable, one may specify a module corresponding either to no resonance or to an approximate resonance between the frequencies $\omega_*$. As discussed by Morbidelli (2002, p.48-49), such a construction is still consistent with the appearance of an exponentially small remainder at the optimal order of normalization. This is because, as demonstrated in the appendix, the order of normalization has a linear relation with the maximum Fourier order of the terms contained
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in the normal form. Furthermore, we find that $r_{opt} \sim \epsilon^{-1/2}$ which also
implies $|k|_{opt} \sim \epsilon^{-1/2}$. Hence the dominant terms in the remainder are
of Fourier order $|k| > |k|_{opt}$, i.e., they have a size $O(\exp(-\sigma \epsilon^{-1/2}))$.
This means that $|k|_{opt}$ plays now a role similar to $K$ in subsection 2.3.
It is interesting to note, however, that such a result is obtained here
a posteriori, i.e., after the construction of the series. That is, with the
present algorithm one may proceed by calculating the series up to any
desired value of $r$, and then by checking whether the optimal order
$|k|_{opt}$ was reached. This will also specify automatically the optimal order
$|k|_{opt}$. On the contrary, following the algorithm of subsection (2.3), one
would have to fix a value of $K$ in advance and then check whether such
a value yields the optimal estimate for the remainder. Otherwise, the
calculation should be repeated from the start, by making a different
choice of $K$.

3. Results

3.1. Hamiltonian model and resonant dynamics

The Hamiltonian model of Froeschl´e et al. (2000) reads:

$$H = H_0 + \epsilon H_1 = \frac{I_1^2 + I_2^2}{2} + I_3 + \frac{\epsilon}{4 + \cos \phi_1 + \cos \phi_2 + \cos \phi_3}$$ (22)

where $(I_i, \phi_i)$, $i = 1, 2, 3$ are action-angle variables and $\epsilon$ is a perturbation parameter (note the change of notation for the actions, $J \rightarrow I$, with respect to the previous section, for consistency with the notation of Froeschl´e et al. (2000)).

The integrable part $H_0$ produces a simple dynamics: $\dot{I}_1 = 0$ and
$\dot{\phi}_1 = \omega_{0,1} = I_1$, $\dot{\phi}_2 = \omega_{0,2} = I_2$, $\dot{\phi}_3 = \omega_{0,3} = 1$. Thus all three actions are integrals of motion and all three angles circulate with constant frequencies. The surface of constant energy $H = E$ is a paraboloid in the action space given by $I_1^2 + I_2^2 + 2I_3 = 2E$ (Fig. 1a). On the other hand, the resonances $k_1 \omega_{0,1} + k_2 \omega_{0,2} + k_3 \omega_{0,3} = k_1 I_1 + k_2 I_2 + k_3 = 0$, with $k \equiv (k_1, k_2, k_3) \in \mathbb{Z}^3$, $|k| \equiv |k_1| + |k_2| + |k_3| \neq 0$, define planes in the action space which are always normal to the plane $(I_1, I_2)$. The intersections of the resonant planes with the surface of constant energy define the web of resonances on this surface which is a set of parabolic curves (Fig. 1a). When viewed from the top of Fig.1a, the projection of these curves on the plane $(I_1, I_2)$ defines a set of straight lines (Fig. 1b).

When $\epsilon = 0$ all the points on the surface of constant energy of Fig.1a are neutral equilibria, which correspond to invariant 3-tori in the six-dimensional phase space. If, however, $\epsilon \neq 0$, an $O(\epsilon)$ volume of invariant
Figure 1. (a) The white grid-lined surface is a part of the paraboloid of constant energy $I_1^2 + I_2^2 + 2I_3 = 2E$ in the action space for the value of the energy $E = 1$. The three gray-shaded planes correspond to the resonances $I_1 - 2I_2 = 0$ (parallel to the double arrow), $3I_1 + I_2 - 1 = 0$, (to the left of the double arrow), and $2I_1 + 2I_2 - 1 = 0$ (to the right of the double arrow). The intersection of all the resonant planes with the paraboloid of constant energy produces a set of parabolic curves which is the ‘web of resonances’. (b) The projection of the web of resonances $k_1I_1 + k_2I_2 + k_3 = 0$ for $|k| \leq 5$ on the $(I_1, I_2)$ plane. Whenever the coefficient of the term (for one particular resonant vector $k$) of the Fourier development of $H_1$ is positive, we only plot a single line corresponding to the projection of the associated parabolic curve on the plane $(I_1, I_2)$. If this coefficient is negative, we plot the central line and two other parallel lines marking the borders of the resonance as obtained by an analytic estimate of the associated separatrix width when $\epsilon = 0.003$. These rules correspond to a Poincaré surface of section $\phi_R = 0$, where $\phi_R$ is the resonant angle associated with each resonance (see text for details), and due to this reason Fig.1b is directly comparable to Fig.1 of Lega et al. (2003). The analysis in that paper and below refers to orbits exhibiting chaotic diffusion along the direction indicated by the double arrows at the borders of the resonance $I_1 - 2I_2 = 0$. 
tori of the phase space are destroyed, according to the KAM theorem, and replaced by a chaotic subset of orbits. The constant energy condition foliates the phase space into 5-dimensional hypersurfaces. For any fixed value of the angles, the projection of one hypersurface on the space of actions defines a manifold resembling to a paraboloid, like in Fig. 1a, which, however, has some deformation of order $O(\epsilon)$. The chaotic orbits can drift on this manifold. We shall focus on orbits sliding on the manifold of constant energy along the chaotic borders of resonances in the direction indicated by the arrows of Figs.1a,b. As shown below, the planes of resonances $k \cdot (I_1, I_2, 1) = 0$ of the unperturbed system are transformed to resonant manifolds of the perturbed system that also resemble to planes, but with some thickness of order $O(|h_k\epsilon|^{1/2})$, where $h_k$ is the coefficient of the term $\exp(ik \cdot \phi)$ in the Fourier development of the perturbation $H_1$. Thus the intersections of the resonant manifolds with the manifold of constant energy form resonant zones of thickness $O(|h_k\epsilon|^{1/2})$. When projected on the plane $(I_1, I_2)$ the web of resonances looks like in Fig.1b (the reason why in some cases we show one single line for one resonance while in other cases we show a triple line is discussed below). The chaotic orbits studied by Lega et al. (2003) are calculated at a value of $\epsilon$ at which the system is in the so-called ‘Nekhoroshev regime’, i.e. the width of the resonant zones is small and there is no significant resonance overlap. The orbits drift slowly along the border of the resonance $(k_1, k_2, k_3) = (1, -2, 0)$, starting with initial conditions close to, but outside the intersection of this resonance with a different resonance, namely $(k_1, k_2, k_3) = (3, 1, -1)$. The chaotic drift along the zone of the resonance $(1, -2, 0)$ produces a slow secular change of the value of the action $I_F = 2I_1 + I_2$ (see Eqs.(26 – 28) below), which is the action associated with the oscillation in the so-called “direction of fast drift”, i.e., normal to the resonant plane. The change of the value of $I_F$ with time was used by Lega et al. (2003) in order to measure numerically the coefficient of the chaotic diffusion. The latter causes also a slow change of the value of the action $I_3$, due to the confinement of the orbits on the manifold of constant energy.

An estimate of the width of resonances can be made as follows. If we complexify the angles in a domain of $\mathbb{C}$ containing the real 3-torus, i.e., if we make the replacement $\phi_j \rightarrow \phi_j + iu_j$ in $H_1$, with $\phi_j, u_j$ real, then in any direction of the space $(u_1, u_2, u_3)$ the quantities $u_j$ can vary from zero up to a value at which $H_1$ becomes singular. However, there is a lower bound on the distance of all the singularities of $H_1$ from the real 3-torus, i.e., from the value $(u_1, u_2, u_3) = (0, 0, 0)$. Thus, the values of $u_j$ at the point of the closest singularity cannot be all infinitesimally small. In fact, if we develop the denominator of $H_1$ up to terms of second degree in $u_j$, we find an estimate of the position
of the singularities of \( H_1 \) close to the real 3-torus given by the values 
\[ u_j = u_{j,s} \text{ satisfying} \]
\[ u_{1,s}^2 \cos \phi_1 + u_{2,s}^2 \cos \phi_2 + u_{3,s}^2 \cos \phi_3 + 8 + 2(\cos \phi_1 + \cos \phi_2 + \cos \phi_3) = 0 \]
and
\[ u_{1,s} \sin \phi_1 + u_{2,s} \sin \phi_2 + u_{3,s} \sin \phi_3 = 0 \, . \]
The first of the above equalities implies
\[ u_{1,s}^2 + u_{2,s}^2 + u_{3,s}^2 \geq |u_{1,s}^2 \cos \phi_1 + u_{2,s}^2 \cos \phi_2 + u_{3,s}^2 \cos \phi_3| \geq 2 \, . \]
The interior of any parallelepiped in the u-space defined by the three inequalities \( |u_j| < \sigma_j \), for some positive constant numbers \( \sigma_j, j = 1, 2, 3 \), constitutes a domain of analyticity of \( H_1 \) if it is contained within the sphere \( u_1^2 + u_2^2 + u_3^2 = \sqrt{2} \). The optimal estimate for the domain of analyticity corresponds to the parallelepiped with maximum volume \( 8\sigma_1\sigma_2\sigma_3 \), that is to the choice \( \sigma_1 = \sigma_2 = \sigma_3 = \sqrt{\frac{2}{3}} = 0.82\ldots \leq \sigma \).

On the other hand, a more precise value of \( \sigma \) can be found by expressing \( H_1 \) as a triple Fourier series

\[ \frac{1}{4 + \cos \phi_1 + \cos \phi_2 + \cos \phi_3} = \sum_{k_1=\infty}^{\infty} \sum_{k_2=\infty}^{\infty} \sum_{k_3=\infty}^{\infty} h_k \exp(ik \cdot \phi) \, (23) \]

where \( k \equiv (k_1, k_2, k_3) \), \( \phi \equiv (\phi_1, \phi_2, \phi_3) \). According to the Fourier theorem on analytic functions, the coefficients \( |h_k| \) are bounded from above.
by
\[ |h_k| \leq A \exp(-|k|\sigma) \] (24)
with \( |k| = |k_1| + |k_2| + |k_3| \) and \( A, \sigma \) positive constants. Thus Eq. (24) predicts that the coefficients \( h_k \) decay exponentially. This is shown in Fig. 2, where we plot the values \( |h_k| \), calculated by a series development of \( H_1 \) using Mathematica up to the 40th order, against \( |k| \). A numerical fitting to the upper bound of this diagram (solid line) yields \( A = 0.046 \), and \( \sigma = 0.87 \). The latter value is close to the estimate \( \sigma = \sqrt{2/3} = 0.82 \) found above heuristically.

Having determined the size of the Fourier coefficients \( h_k \), the normal form construction described in subsection (2.4) eliminates all harmonics in the Hamiltonian perturbation \( H_1 \) (written in the form (23)), except for the harmonic \( h_k \exp(ik \cdot \phi) \) corresponding to the particular resonance under consideration. To the lowest order, the resonant normal form reads:
\[ H_{res} = I_1^2 + I_2^2 + I_3 + 2\epsilon h_k \cos(k \cdot \phi) + \ldots , \] (25)
where we have used the property \( h_k = h_{-k} \) following from the reality and even parity with respect to the angles \( \phi_i \) of the Hamiltonian perturbation \( H_1 \). Introducing resonant action-angle variables \((I_R, \phi_R), (I_F, \phi_F)\) via the generating function:
\[ S = (k \cdot \phi)(I_R - \frac{k_3}{k_1^2 + k_2^2}) + (m_1\phi_1 + m_2\phi_2)I_F + \phi_3I'_3 \] (26)
where the integers \( m_1, m_2 \) are any pair satisfying \( m_1k_1 + m_2k_2 = 0 \), the resulting canonical transformation is
\[ I_1 = k_1(I_R - \frac{k_3}{k_1^2 + k_2^2}) + m_1I_F, \quad I_2 = k_2(I_R - \frac{k_3}{k_1^2 + k_2^2}) + m_2I_F, \quad \phi_R = k_1\phi_1 + k_2\phi_2 + k_3\phi_3, \quad \phi_F = m_1\phi_1 + m_2\phi_2, \quad I_3 = I'_3, \quad \phi'_3 = \phi_3 . \] (27)
By virtue of (27), the resonant Hamiltonian (25) takes the form (apart from a constant):
\[ H_{res} = \frac{1}{2}(m_1^2 + m_2^2)I_F^2 + I_3 + \frac{1}{2}(k_1^2 + k_2^2)I_R^2 + 2\epsilon h_k \cos \phi_R \] (28)
i.e., it is split in two parts depending only on the actions \( I_F, I_3 \), and a third part which is the pendulum Hamiltonian:
\[ H_{pend} = \frac{1}{2}(k_1^2 + k_2^2)I_R^2 + 2\epsilon h_k \cos \phi_R . \] (29)
The actions $I_3$ and $I_F = (m_1 I_1 + m_2 I_2)/(m_1^2 + m_2^2)$ are integrals of the Hamiltonian $H_{res}$ (in the case of the resonance $(k_1, k_2, k_3) = (1, -2, 0)$ we have $m_1 = 2$, $m_2 = 1$ and the precise definition of the fast action is $I_F = (2I_1 + I_2)/5$ which differs by a factor 1/5 from the definition given at the beginning of this section for that particular resonance). On the other hand, the width of the resonance is determined by the separatrix half-width of the pendulum Hamiltonian $H_{pend}$

$$\Delta I_{R, sep} = \sqrt{\frac{8|\hbar_k\epsilon|}{k_1^2 + k_2^2}}.$$ (30)

The phase portrait of $H_{pend}$ is shown schematically in Fig. 3. In reality, the ideal separatrix given by (29) should be replaced by a thin chaotic layer produced by the weakly chaotic motion near the separatrix due to to higher order coupling terms of the Hamiltonian. When $\epsilon$ is small, however, the width of the chaotic zones is very small. In that case, Eq. (30) can be used to approximate the maximum normal distance to the resonance between the upper and lower branches of the separatrix-like chaotic zones.

The resonant action $I_R$ changes in time according to

$$\dot{I}_R = -\frac{\partial H_{pend}}{\partial \phi_R} = \hbar_k \sin \phi_R .$$

Any variation $\Delta I_R$ of the resonant action results in variations $\Delta I_1$, $\Delta I_2$, such as to respect the integral $I_F$, i.e., $\Delta I_F = 0$. Eq.(27) then gives

$$\Delta I_1 = k_1 \Delta I_R, \quad \Delta I_2 = k_2 \Delta I_R \quad (31)$$

When the resonance web is projected on the $(I_1, I_2)$ plane, as in Fig. 1b, the variations $\Delta I_1$ and $\Delta I_2$ of Eq.(31) correspond to motions across the resonance, i.e., along a line normal to the resonance line $k_1 I_1 + k_2 I_2 + k_3 = 0$ (this is called the “direction of the fast drift” by Froeschlé et al. 2000) On the other hand, when the web of resonances is visualized numerically in the action space, as, for example, by the method of the Fast Lyapunov indicator (Froeschlé et al. 2000), one has to make an appropriate choice of Poincaré surface of section in order to eliminate the angles from the calculation. The choice $\phi_3 = 0$, $|\phi_1| + |\phi_2| \leq 0.05$ made by these authors corresponds essentially to setting the resonant angle $\phi_R = k_1 \phi_1 + k_2 \phi_2 + k_3 \phi_3$ to a value very close to zero, i.e., $\phi_R \approx 0$. We then see that this means to plot (a) two sets of points in the plane $(I_1, I_2)$, corresponding to passing close to the maxima or minima of the theoretical separatrices, when $h_k < 0$, or (b) one set of points on the plane $(I_1, I_2)$, corresponding to passing close to the X-point of each separatrix, when $h_k > 0$. Consequently,
the thin chaotic borders of the resonances will appear as follows on the surface of section: In case (a) \((h_k < 0)\) we see two lines parallel to the resonant line \(k_1 I_1 + k_2 I_2 + k_3 = 0\). These lines define a zone of width determined by Eq.(31). In case (b) \((h_k > 0)\) we see only one line coinciding with the resonance line itself. These rules are followed in the plot of Fig.1b, for all the resonances with \(|k| \leq 5\). This figure is to be compared with Fig.1 of Lega et al. (2003). The two figures compare well not only qualitatively, but also quantitatively, i.e., the theoretical resonance widths found above are very close to the widths determined numerically by the FLI method.

### 3.2. Normal form and Nekhoroshev estimates

The resonance dealt with by Lega et al. (2003) is \(I_1 - 2I_2 = 0\). The diffusion takes place on the thin chaotic border along this resonance (Fig.2 of Lega et al. (2003)) when the initial conditions are taken in a small region of the thin chaotic border. In order to perform a transformation of the type given by Eqs.(18) and (19), we have to specify the central values \((I_{1s}, I_{2s}) \equiv (\omega_{1s}, \omega_{2s})\) with respect to which the Hamiltonian is expanded. By visual inspection of Fig.2 of Lega et al.(2003) a convenient choice compromising the central values of \(I_{is}\) in all the panels is \(I_{1s} = 0.31, I_{2s} = 0.155\). Renaming the variables of Eq.(22) by the same symbols according to \(\epsilon^{-1/2} H \rightarrow H, \quad \epsilon^{-1/2}(I_i - I_{is}) \rightarrow I_i, \quad i = 1, 2, 3,\) and Fourier-expanding up to order 40, the Hamiltonian reads (apart from a constant):

\[
H = H_{0s}(I) + \epsilon^{1/2} H_{1s}(I, \phi) = \omega_{1s} I_1 + \omega_{2s} I_2 + I_3 +
\]
\[ \epsilon^{1/2}\left(\frac{I_1^2 + I_2^2}{2} + \sum_{|k| \leq 40} c_k \exp(i k \cdot \phi)\right). \quad (32) \]

According to the definition of \( K' \) given in subsection 2.4, the term \( \epsilon^{1/2}(I_1^2 + I_2^2)/2 \) should be considered of order of smallness \( p = 1 \). Then, it is convenient to slightly modify the definition of \( K' \) so as to render \( e^{-K'\sigma} \) comparable to the factor \( \epsilon^{1/2} \). We thus set:

\[ K' = \left[ -\frac{\log(\epsilon^{1/2})}{\sigma} \right] + 1. \quad (33) \]

The range of values of \( \epsilon \) for which Lega et al. (2003) provide numerical data on the diffusion coefficient is \( 30 \leq \epsilon^{-1} \leq 1000 \). For most values within this range \( K' \) is equal to a constant value \( K' = 3 \). We thus simply set \( K' = 3 \) in all the calculations. This means that the Fourier modes of \( H_{1*} \) with \( 0 \leq |k| \leq 2 \) are book-kept as of order 1, modes with \( 3 \leq |k| \leq 5 \) as of order 2, etc. The terms of \( H_{0*} \) are of order zero, i.e., they are the ones to be used in the kernel operator \( \{\cdot, H_{0*}\} \) of the homological equation.

Although the computer program allows the user to carry along the powers of \( \epsilon^{1/2} \) in the expansion, the extra requirement of memory in order to store the associated exponents of \( \epsilon^{1/2} \) is prohibitive. We thus had to make separate runs of the computation of the normal form for various numerical values of \( \epsilon \). That is, one numerical value of \( \epsilon \) was supplied to the file storing the coefficients of (32) for each run. Even so, a memory limit of 2GB was reached by computing about \( 5 \times 10^7 \) complex coefficients of the Hamiltonian and of the Lie generating function per run. Such a number of terms corresponds to a truncation \( r \leq 15 \) in the normalization order, or \( K = 3 \cdot 15 - 1 = 44 \) in Fourier space. Despite these limits, it was in the end possible to observe the asymptotic properties of the Birkhoff series within the whole range of values of \( \epsilon \) down to a value \( \epsilon = 0.0001 \), which is one order of magnitude smaller than the value reached in the numerical experiments of Lega et al. (2003).

After \( r \) normalization steps, the Hamiltonian reads:

\[ H^{(r)} = Z^{(r)}(I, \phi) + R^{(r)}_{r+1} + R^{(r)}_{r+2} + \ldots \quad (34) \]

The normal form \( Z^{(r)}(I, \phi) \) contains all the Fourier terms up to \( |k| \leq 3r - 1 \) belonging to the resonant module \( \mathcal{M} = \{k : k_1 - 2k_2 = 0 \text{ and } k_3 = 0\} \). The normal form \( Z^{(r)}(I, \phi) \) is an integrable hamiltonian, the integrals, besides the energy, being \( I_3 \) and \( I_F = 2I_1 + I_2 \). The level lines \( I_F = c \) are normal to the resonance line \( I_1 - 2I_2 = 0 \). Since we are interested in measuring the drift along the chaotic border of the
Nekhoroshev theorem and Arnold diffusion

Figure 4. (a) The size of the truncated remainder $||R^{(r)}||_{\leq r_t}$ as a function of the truncation order $r_t > r$ after one and after two normalization steps (upper and lower points respectively) when $\epsilon = 0.001$. (b) The size of the remainder as a function of the order of the normalization for three different values of $\epsilon$. $||R_{\text{opt}}||$ as a function of $\epsilon$ is given by the size of the remainder at the minimum of each curve.

According to standard theory, the remainder series $R^{(r)}(I, \phi)$ should be convergent. This is shown in Fig.4a, in which the truncated sum

$$||R^{(r)}||_{\leq r_t} \equiv \sum_{j=r+1}^{r_t} ||R^{(r)}_j||$$

(35)

is plotted against the truncation order $r_t$ for the remainders of the first two normalization steps $r = 1$ and $r = 2$ for $\epsilon = 0.001$ (the norm $|| \cdot ||$ is taken as the sum of moduli of all the trigonometric coefficients of the involved function). Clearly, the remainder shows the tendency to converge to its final size after summing just its first two or three successive terms. Furthermore, the size of the remainder, estimated as
$|R^{(r)}|_{<15}$ exhibits the well known behavior expected for an asymptotic series (Fig.4b). Namely, the size of the remainder initially decreases, as $r$ increases, up to an optimal order $r_{opt}(\epsilon)$ corresponding to the minima of the curves of Fig.4b for different values of $\epsilon$. Beyond the optimal order, however, the remainder becomes an increasing function of $r$ and one has $\lim_{r \to \infty} |R^{(r)}| = \infty$, marking the eventual divergence of the normalization procedure. From Fig.5b we see clearly that the optimal order $r_{opt}$ increases as $\epsilon$ decreases.

Figures 5 and 6 show now the main result. The abscissa in Fig.5 shows the value of $|R_{opt}| \equiv |R^{(r_{opt}(\epsilon))}|_{<15}$ for ten different values of $\epsilon$ in the range $0.001 \leq \epsilon \leq 0.02$. The ordinate shows the value of the diffusion coefficient $D(\epsilon)$ for the same values of $\epsilon$ as given by Lega et al. (2003). The straight line represents a power-law fitting of the relation between the optimal remainder and the diffusion coefficient. The best fit law is $D = 1.02 |R_{opt}|^{2.97}$. Thus, the scaling is essentially:

$$D \propto |R_{opt}|^{3}. \quad (36)$$

On the other hand, Fig.6 shows the scaling of $|R_{opt}|$ with $1/\epsilon$ when $\epsilon$ reaches values as small as $\epsilon = 0.0001$, i.e., one order of magnitude smaller than the last point of Fig.7 of Lega et al. (2003) (the right vertical dashed line shows the last point where the numerical calculation of Lega et al. (2003) was stopped). The two solid lines passing through the data correspond to a power-law (lower curve) and an exponential law (upper curve) fitting the data. For small values of $1/\epsilon$ (i.e. for large values of $\epsilon$), the power-law fitting is better than the exponential fitting. The limit beyond which the exponential fitting is acceptable is around $\epsilon = 0.01$ (indicated by the left vertical dashed line of Fig.6 at $1/\epsilon = 100$). We may identify this limit as roughly corresponding to the threshold of the Nekhoroshev regime. On the other hand, in the interval $100 \leq 1/\epsilon \leq 1000$, both the power law and the exponential law yield acceptable fittings. Nevertheless, beyond the value $1/\epsilon > 1000$, the power-law clearly fails while the exponential fitting follows now narrowly the data. The numerical best fit exponential law yields

$$|R_{opt}| \propto \exp(-\epsilon_{*}/\epsilon^{0.21}).$$

We note that Froeschlé et al. (2005), making numerical experiments of the diffusion of orbits in a mapping model resembling to the Hamiltonian (22), found an exponential scaling of the diffusion coefficient with $\epsilon$ in which the best-fit exponent is $a = 0.28$. However, in that paper too the exponential scaling was unraveled by considering values of $\epsilon$ smaller by more than one orders of magnitude from a critical threshold value below which resonances do not significantly overlap. We conclude
Figure 5. The diffusion coefficient $D$ reported in Lega et al. (2003) as a function of the size of the optimal remainder $||R_{opt}||$ of the Birkhoff normal form calculated for different values of $\epsilon$.

Figure 6. The size of the optimal remainder $||R_{opt}||$ as a function of $1/\epsilon$. The data clearly deviate from a power law beyond $1/\epsilon = 1000$, and they are well fitted by an exponential law, as predicted by the Nekhoroshev theorem. The left vertical dashed line gives a lower threshold of $1/\epsilon$ below which the exponential law is no longer valid. The data are well fitted also by a power law in the range $10 \leq 1/\epsilon \leq 1000$. The right vertical dashed line shows the last point of the numerical calculation of the diffusion coefficient by Lega et al. (2003).
that the exponential law predicted by the Nekhoroshev theorem can be unambiguously seen in the real data by various methods when \( \epsilon \) becomes at least one order of magnitude smaller than the critical value characterizing the onset of the ‘Nekhoroshev regime’.

4. Conclusions and Discussion

The present paper demonstrates the applicability of the analytical apparatus of the Nekhoroshev theory in recovering the exponential scaling of the coefficient of Arnold diffusion \( D = O(\exp(-1/\epsilon)) \) along a particular resonance in the model Hamiltonian system of three degrees of freedom of Froeschlé et al. (2000). In particular:

1) The normalization algorithm for the Hamiltonian, based on an organization of the perturbation series in terms of the Fourier order of the terms (rather than on powers of \( \epsilon \)), is presented, and its benefits are analyzed in detail.

2) The implementation of this algorithm on the computer allowed us to reach the optimal order of normalization, at which the size of the remainder \( ||R_{opt}|| \) of the normal form becomes minimal.

3) The coefficient of Arnold diffusion \( D \), as determined numerically by Lega et al. (2003), is found to scale with the size of the optimal remainder like \( D \propto R_{opt}^3 \).

4) The size of the optimal remainder is found to scale exponentially with the inverse of the perturbation parameter, namely \( ||R_{opt}|| \propto \exp(-1/\epsilon^a) \), with \( a \simeq 0.21 \). The exponential scaling clearly shows when one considers values of \( \epsilon \) as small as \( \epsilon = 10^{-4} \), i.e., one order of magnitude smaller than in the numerical experiments of Lega et al. (2003).

Estimates on the speed of Arnold diffusion based on numerical experiments have been given in the literature by a number of authors. We note in particular the early work of Kaneko and Konishi (1989), in which an exponential scaling law is found with \( a \) between 0.1 and 0.3, i.e., consistent with the present results.

On the other hand, Wood et al. (1990) provided estimates of the diffusion coefficient in standard-like multidimensional symplectic maps on the basis of the Arnold-Melnikov method, i.e., the exponentially small splitting of separatrices due to the presence of higher order coupling terms in the resonant Hamiltonian. An exponential scaling of \( D \) with \( 1/\epsilon \) was also found in that case, favoring though a value of \( a \) rather close to \( a = 1/2 \). Thus, a detailed comparison of the results by the Nekhoroshev and Arnold-Melnikov theories is in order. To our knowledge, the only hint in that direction is a paper by Morbidelli and
Giorgilli (1997). Nevertheless, more work is necessary in order to clarify this connection by specific quantitative studies, as well as to compare the predictions of the two theories for Arnold diffusion in various types of multidimensional systems.

Finally, the fact that the scaling of $|R_{opt}|$ with $\epsilon$ appears also as a power law in a transient interval of values of $\epsilon$, before the onset of the exponential regime, is consistent with some past theoretical work (Chirikov et al. 1985) calling such a transient regime ‘modulational diffusion’. According to this theory, there is an intermediate interval of values of $\epsilon$ within which many high order resonances, located in the chaotic border of the low-order resonance along which the diffusion takes place, still overlap. We conjecture that these are resonances of some order $|k|$ which must be above, but close to a truncation order $K$ estimated as $K \sim 1/\epsilon^a$ (according to the analysis of subsection 2.3).

At any rate, the results of the present paper provide a clear relation between the local value of the diffusion coefficient $D$ along a resonance, on the one hand, and the size of the optimal remainder $|R_{opt}|$ of the normal form for the same resonance, on the other hand. Furthermore, for $\epsilon$ sufficiently small $|R_{opt}|$ is found to scale with $\epsilon$ precisely as predicted by the Nekhoroshev theory. Thus, the final conclusion of our study that the analytical techniques of the Nekhoroshev theory can be used with much profit, in order to construct precise quantitative estimates of the speed of Arnold diffusion in Hamiltonian systems.

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The following is a more technical analysis of point (b) of subsection 2.4 referring to the organization of the perturbation series in powers of the small parameter $\epsilon$.

Let $r_{\text{max}}$ be the maximum order in the book-keeping variable $\lambda \equiv \epsilon$, $K_{\text{max}}$ be the maximum order in Fourier space specifying a domain in which we are interested in computing the Hamiltonian, and $K$ the order of truncation in Fourier space beyond which terms are not normalized (in general we have to set $K_{\text{max}} > K$ so that some remainder terms of the Hamiltonian be also stored). Figure 7a shows this domain as a gray-shaded parallelogram in the space $(r, |k|)$. Now, it can be readily seen that many terms of the Hamiltonian which lie outside the domain of interest at some particular order $r$ interact with the generating function in such a way as to produce, at some subsequent order, terms which lie inside the domain of interest, despite the fact that the Hamiltonian term from which it originated lies outside the domain of interest.

A careful examination of all the Lie operations taking place up to the order $r_{\text{max}}$ shows that in order to obtain complete knowledge...
of the transformed Hamiltonian in a domain \((r_{\text{max}}, K_{\text{max}})\), one must store, for every order \(r \leq r_{\text{max}}\), all the Hamiltonian terms of Fourier order \(|k| \leq K(r_{\text{max}} - r) + K_{\text{max}}\). This extended domain, shown by the triangular domain of figure 1a, contains many more terms than those of the domain of interest (the ratio of the number of terms in the two domains is proportional to the ratio of the areas of the domains raised to a power \(\simeq 2n\), where \(n\) is the number of degrees of freedom).

At this point we may argue that, for sufficiently large \(K_{\text{max}}\), the terms with \(|k| > K_{\text{max}}\) have very small size because of the analyticity condition (Eq. (3)), so that they can probably be ignored without great modification of the results. However, precisely this type of argument brings about the real source of the above problem, which is the choice of ‘book-keeping’ \(\lambda \equiv \epsilon\). The fact that the triangular domain of figure 1a contains many more terms than the gray parallelogram in the same figure simply depicts failure to recognize that for any order \(r \leq r_{\text{max}}\), many Fourier terms formally stored as of order \(\lambda^r\) are actually of much smaller size than \(\epsilon^r\). For example, while \(H_1\) is an overall \(O(1)\) quantity, not all the Fourier terms in \(H_1\) have a similar size, because the size of an \(\exp(ik \cdot \phi)\) term in \(H_1\) scales as \((e^{-\sigma})|k|\). This initial scaling propagates also at subsequent orders of normalization. This fact suggests that the

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{hamiltonian_domains}
\caption{(a) The gray parallelogram shows the ‘domain of interest’ defined as the domain in Fourier space (orders of \(|k|\)) of the terms that we wish to store in the transformed Hamiltonian up to an order \(r = r_{\text{max}}\) in the book-keeping parameter \(\lambda \equiv \epsilon\). The inclined line, given by \(|k| = K_{\text{max}}(r_{\text{max}} - r + 1)\), represents the upper limit of a larger domain in Fourier space within which intermediate terms must be stored at an order \(r\), yielding contributions in the gray-shaded domain at orders larger than \(r\). (b) Under an appropriate book-keeping (see subsection (2.4)) the domain of interest can be made to coincide with the domain in which terms must be stored.}
\end{figure}
terms should be ‘book-kept’ differently, i.e., on the basis of their Fourier order rather than their $\epsilon$-order.

Following the algorithm exposed in subsection 2.4 (steps (1) to (3)), the domain of interest (figure 1b) is made to coincide with the domain in which terms should be stored, i.e., terms within the gray-shaded area can only be produced by Poisson bracket operations between terms which are also within the gray shaded area. In particular, the meaning of step (2) is that in a Hamiltonian like (1) the parameter $\epsilon$ is not so relevant in characterizing the smallness of the various terms in $H_1$ ($\epsilon$ can in fact be incorporated in the book-keeping scheme, as was done in section 3). A formal analogy can be made with a polynomial Hamiltonian around an elliptic equilibrium:

$$H \equiv \sum_{i=1}^{n} \omega_i \frac{p_i^2 + q_i^2}{2} + \epsilon \sum_{m_i \geq 3} \alpha_{m_1, m_2, \ldots, m_n} q_1^{m_1} q_2^{m_2} \ldots q_n^{m_n}. \quad (37)$$

In the case of the Hamiltonian (37) it is customary to proceed by normalizing iteratively by the degrees of the monomial terms in the canonical variables rather than by powers of $\epsilon$. Such a choice underlines that the real smallness in the polynomial case is the distance $\rho = \sqrt{\sum (q_i^2 + p_i^2)}$ from the equilibrium point. In fact, it is often convenient to rescale the whole Hamiltonian (37) so that $\epsilon$ disappears from the lowest order terms of the polynomial expansion in the r.h.s. of (37). The analogy with the generic case becomes clear by introducing action-angle variables $q_i = \sqrt{2J_i} \sin \phi_i$, $p_i = \sqrt{2J_i} \cos \phi_i$, $i = 1, \ldots, n$. We then readily find that a Fourier term of order $\rho^r \sim J^{r/2}$ is always of Fourier order $|k| \leq r$ (and $|k|$ has the same parity as $r$). The relevant domain of interest is thus limited by the equation $|k| = r$ which yields a domain very similar to Fig.7b (the only difference is in the slope of the limiting upper line, which is $1/\sigma$ in Fig.7b and 1 in the polynomial case).