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Preservation and destruction of periodic orbits by symplectic integrators

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Abstract We investigate what happens to periodic orbits and lower-dimensional tori of Hamiltonian systems under discretisation by a symplectic one-step method where the system may have more than one degree of freedom. We use an embedding of a symplectic map in a quasi-periodic non-autonomous flow and a KAM result of Jorba and Villaneuva (J Nonlinear Sci 7:427–473, 1997) to show that periodic orbits persist in the new flow, but with slightly perturbed period and an additional degree of freedom when the map is non-resonant with the periodic orbit. The same result holds for lower-dimensional tori with more degrees of freedom. Numerical experiments with the two degree of freedom Hénon–Heiles system are used to show that in the case where the method is resonant with the periodic orbit, the orbit is destroyed and replaced by two invariant sets of periodic points—analogous to what is understood for one degree of freedom systems.

Keywords Periodic orbit · Lower dimensional invariant tori · KAM theory · Symplectic integrators · Hénon-Heiles · Geometric numerical integration

1 Introduction

In the numerical solution of ordinary differential equations (ODEs) it is desirable that the numerical solution should possess as many as possible of the structures inherent to the exact solution of the ODE. Sometimes it is necessary

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to know about these structures in advance and to take specific steps in order to preserve them but the preferable situation is when one is able to use a numerical integrator of a particular class which can guarantee the preservation of certain structures whenever those structures are present. Such integrators are known as geometric numerical integrators (GNIs) or structure-preserving integrators.

Here we investigate a class of GNIs known as symplectic integrators. These integrators preserve the symplectic form associated with a Hamiltonian vector field and are one of the most popular GNIs. Symplectic integrators also preserve other properties of dynamical systems; amongst these are phase space volume, KAM tori and stable/centre/unstable-manifolds near fixed points [7].

When a symplectic integrator using step size h is applied to a d-degree of freedom Hamiltonian vector-field f it gives a symplectic map $\Psi_{h,f} : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$. We are interested in what happens to periodic orbits of a dynamical system when the system is discretized by a symplectic integrator. Does the numerical solution given by $\Psi_{h,f}$ preserve the periodic orbits of the original vector field $f = X_H$? The question can be split into two cases: the resonant case where some multiple of the integrator step size exactly divides the period T of the orbit ($nT/h \in \mathbb{Z}$, $n \in \mathbb{N}$), and the non-resonant case, when it does not ($nT/h \in \mathbb{R} \setminus \mathbb{Z}$). We find that in the resonant case the periodic orbit is destroyed and splits into $2T/h$ points which lie close to the original periodic orbit and which are alternately elliptic and hyperbolic. In the nonresonant case the orbits generally persist but are slightly perturbed—similar to what happens to full dimensional invariant tori in KAM theory. A point of difference between the result for full dimensional invariant tori and periodic orbits or lower dimensional tori is that the frequency of the periodic orbit/lower dimensional torus is shifted from the original frequency while for full dimensional invariant tori, the frequencies of the torus are unchanged by the perturbation.

Knowing that particular geometric structures persist in numerical solutions is important if we are correctly understand the dynamical systems which the solutions represent. In Hamiltonian systems full dimensional tori can partition the phase space of the system and thus form bounds to chaotic regions of the systems; dividing the phase space into regions of regular and chaotic motion. This has implications for the study of ergodicity since sets of invariant tori with positive measure are incompatible with true ergodicity.

At the other end of the dimensional spectrum, one can view fixed points as invariant tori with dimension zero. Clearly, preserving the fixed points and the nature (stable/centre/unstable sets, hyperbolic/parabolic/elliptic) of the eigenvalues of their linearisation is essential to correctly representing a dynamical system with a numerical solution. Fortunately, fixed points are easy to preserve in numerical solutions and the nature of their eigenvalues can also be easily preserved by using symplectic integrators.

Periodic orbits and other lower-dimensional tori with dimension between zero and full dimension also help us better understand the dynamical properties of Hamiltonian systems—celestial mechanics being one obvious example where preservation of periodic orbits can be important. For non-Hamiltonian systems, periodic orbits are preserved by numerical algorithms if the periodic orbit is isolated and hyperbolic. Isolated hyperbolic periodic orbits are not possible for Hamiltonian systems and so we need more subtle methods such as KAM theory to determine the preservation, or otherwise, of the periodic orbits.

In its original form, KAM theory [1, 13, 19] says that if a real-analytic Hamiltonian $H(\theta, I)$ posses quasi-periodic/non-resonant invariant tori then those tori survive small real-analytic, Hamiltonian perturbations. One begins with a real-analytic Hamiltonian defined for $I \in \mathbb{R}^d$ in a neighbourhood of zero and $\theta \in \mathbb{T}^d$, for which the linearisation of $H(\theta, I)$ about $I = 0$ takes the θ-independent form

$$H(\theta, I) = c + \omega^\top I + \frac{1}{2} I^\top M(\theta, I) I,$$

where the frequencies $\omega \in \mathbb{R}^d$ satisfy a diophantine condition $|\omega^\top k| \geq \gamma |k|^{-\nu}$ for $k \in \mathbb{Z}^d \setminus \{0\}$ and where the angular average $\bar{M}_0 := \frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} M(\theta, 0) \mathrm{d}\theta$ of $M(\cdot, 0)$ is an invertible $d \times d$ matrix satisfying $\|\bar{M}_0 v\| \geq \mu \|v\|$, $v \in \mathbb{R}^d$, $\gamma, \nu, \mu > 0$.

For

$$H_\varepsilon(\theta, I) = H(\theta, I) + \varepsilon G(\theta, I),$$

a real-analytic perturbation of H, there exists $\varepsilon_0 > 0$ such that for all $|\varepsilon| < \varepsilon_0$ there is an analytic, symplectic coordinate transformation $\chi : (\theta', I') \mapsto (\theta, I)$ which is order ε close to the identity, has analytic dependence on ε and which puts $H_\varepsilon(\theta, I)$ back into the form

$$H_\varepsilon(\theta, I) = c_\varepsilon + \omega^\top I' + \frac{1}{2} I'^\top M_\varepsilon(\theta', I') I',$$

for $(\theta, I) = \chi(\theta', I')$. The perturbed system therefore also has an invariant torus $\{\theta' \in \mathbb{T}^d, I' = 0\}$ whose quasi-periodic flow has the same frequencies ω as the unperturbed system.

Initially, KAM theory was particularly interested in the case of $H(\theta, I) = H_0(I)$; i.e. perturbations of fully integrable systems. Since then, KAM theory has been extended in many directions, to the point where it is now difficult to succinctly state all the results covered by the theory. Roughly speaking, modern KAM theory says that for open sets of d degree of freedom dynamical systems posessing some geometric property (e.g. Hamiltonian, volume-preserving, reversible, etc.) there exist sets of positive measure covered by invariant tori. The tori need not have dimension d (e.g. lower dimensional tori) and d need not be finite (e.g. infinite dimensional KAM theory, KAM for PDEs). See [14] and the references therein for comprehensive surveys and expositions of KAM theory.

For one degree of freedom systems a periodic orbit is also a full dimensional invariant torus and both the resonant and non-resonant cases are well understood. The non-resonant case was dealt with by Z.-J. Shang [25–27] who proved that the original KAM theory for full dimensional invariant tori of area-preserving/symplectic flows also holds for symplectic maps. That is, a symplectic integrator applied to a Hamiltonian system which is integrable in some domain preserves invariant tori with unchanged frequencies for a Cantor set's worth of strongly non-resonant step sizes. The tori are only slightly deformed by the integrator and the density of the set of step sizes tends to one as $h \to 0$. We state Shang's result more precisely in Theorem 1 of Section 2.

In the resonant case with one degree of freedom, results go back as far as Poincaré who realised that an area preserving twist map of an annulus to itself, with a rational rotation number, must have an even number of periodic points. These periodic points are alternately hyperbolic and elliptic and lie close to the original periodic orbit. Homoclinic tangles originate at the hyperbolic periodic points, trapping the points of the original periodic orbit in a chaotic band within which Poincaré famously described the behaviour "These interactions form a type of trellis, tissue or grid with infinitely fine mesh ... The complexity of this figure is striking, and I shall not even try to draw it." [22].

This article is split into two main parts; we deal with preservation of non-resonant periodic orbits using a KAM type result in Section 2. In Section 3 we consider the case where a periodic orbit is discretised by a symplectic integrator whose step size is resonant with the period of the orbit. We report on numerical investigations which suggest that the periodic orbit is destroyed and is replaced by two invariant sets, one elliptic, the other hyperbolic, analogous to the case for resonant periodic orbits of one degree of freedom systems.

2 Non-resonant step sizes

When a symplectic integrator is applied to a Hamiltonian system containing an invariant torus or periodic orbit, and when the step size of the integrator is not resonant with any of the frequencies of the invariant torus, it is reasonable to hope that the torus persists in the numerical solution. The proof that such tori/periodic orbits persist is possible through a KAM theory for symplectic maps. We begin this section by stating a numerical KAM theorem due to Z.-J. Shang [25–27] which shows that for full dimensional tori of a non-degenerate Hamiltonian system there is a Cantor set, with positive measure, of step sizes for which finitely many different tori with strongly non-resonant frequencies are simultaneously preserved.

Theorem 1 (Shang [26]) *Given an analytic, non-degenerate, and integrable Hamiltonian system of d-degrees of freedom, and given N diophantine*[1] *frequency vectors ω^j, $j = 1, 2, \ldots, N$ in the domain of frequencies of the system, there exists a Cantor set $\mathcal{I} \subset \mathbb{R}$, depending on the N frequency vectors, such that for any symplectic algorithm applied to the system, there exists a positive number δ_0 such that if the step size h of the algorithm falls in the set $(-\delta_0, \delta_0) \cap \mathcal{I}$, then*

[1] I.e. each $\omega^j \in \mathbb{R}^d$ satisfies $|k^\top \omega| \geq \frac{\gamma}{|k|^\nu}$, $0 \neq k = (k_1, \ldots, k_d) \in \mathbb{Z}^d$ for some $\gamma > 0$ and $\nu > 0$.

the algorithm has N invariant tori with frequency vectors $h\omega^j$, $j = 1, 2, \ldots, N$ when applied to the integrable system. These invariant tori approximate the corresponding ones of the system, in the sense of Hausdorff, with the order equal to the order of accuracy of the algorithm. The Cantor set $\mathcal{I}$ has density one at the origin.

Our goal in this section is to develop a similar result for preservation of periodic orbits (and other lower dimensional tori). To do so, two possible approaches are available. The first is to follow the example of Shang who re-proved the original KAM theorem in the setting of analytic symplectic maps. This is not a trivial undertaking. The second approach is to use interpolation to embed the map produced by a symplectic integrator into an analytic symplectic flow. One can then use a suitable result for preservation of periodic orbits of perturbed symplectic flows to prove that such orbits are also preserved by the symplectic map. This has the advantage that it is often easier to think of a problem in terms of maps while it is simpler to give a proof in terms of flows. Many KAM style results for lower dimensional invariant tori already exist. Using interpolation one can avoid redoing lengthy proofs for maps and so it is this approach we take in this paper.

We will assume that the Hamiltonian system $\mathcal{H}$ we are working with has the following properties.

1. The Hamiltonian has d degrees of freedom and is autonomous and analytic with respect to all its variables. It contains an invariant torus with irrational/quasi-periodic flow with frequencies $\hat{\omega}^{(0)} \in \mathbb{R}^r$, $0 \le r \le d$ ($r = 1$ corresponds to a periodic orbit).
2. The invariant torus is reducible; that is the time-dependent linear equations which describe the flow on the torus (e.g. $\dot{x} = A(\phi + \omega t)x$) can be transformed into linear constant coefficient equations. It is known, from Floquet's theorem, that reducibility holds automatically for periodic orbits. For invariant tori with more degrees of freedom there are various positive results concerning when a system is reducible (see, for example, [4, 5, 8–10, 12, 20, 24]), however, the question of reducibility remains open in general.
3. The initial periodic orbit or invariant torus is isotropic; that is the symplectic form evaluates to zero everywhere on it. Any one-dimensional subspace of a symplectic vector space is isotropic so the property holds automatically for periodic orbits.

There is a canonical change of coordinates such that the initial Hamiltonian can be written as a function of the coordinates $\hat{\theta}$, $\hat{I}$, x, y with $\hat{\theta}, \hat{I} \in \mathbb{C}^r$, $x, y \in \mathbb{C}^m$, $d = r + m$, and $z^\top = (x^\top, y^\top)$. Here $\hat{\theta}$ and x are the position variables, with $\hat{\theta}$ being the angle coordinates on the periodic orbit or torus. $\hat{I}$ and y are their respective conjugate momenta. (We use hats to denote variables pertaining to the initial torus. The x and y coordinates are the "normal" directions to the torus.) Since the original Hamiltonian was assumed to be analytic, it has a Taylor expansion (about $z = 0$, $\hat{I} = 0$). For periodic orbits, Floquet theory ensures that the expansion has constant coefficients for the $\hat{I}$ and $z^\top z$ terms and that the only linear term is $\hat{\omega}^{(0)}\hat{I}$ where $\hat{\omega}^{(0)} \in \mathbb{R}$ is the frequency of the periodic orbit. (For invariant tori of dimension two, or greater, the frequency is replaced by a frequency vector $\hat{\omega}^{(0)} \in \mathbb{R}^r$ and the linear term is $\hat{\omega}^{(0)\top}\hat{I}$.) More generally, the assumption of linear, reducible flow on the invariant torus ensures that the initial Hamiltonian can be put into the semi-normal form

$$\mathcal{H}(\hat{\theta}, x, \hat{I}, y) = \hat{\omega}^{(0)\top}\hat{I} + \frac{1}{2}z^\top \mathcal{B} z + \mathcal{H}_*(\hat{\theta}, x, \hat{I}, y). \tag{1}$$

This is sometimes referred to as Floquet form. The terms in the Taylor expansion of $\mathcal{H}_*$ begin at second order in $\hat{I}$ and z. The assumption that the flow on the torus can be reduced to the case of constant coefficients means that $\mathcal{H}_*$ has no quadratic terms in the z variables — all such terms are included in $\frac{1}{2}z^\top\mathcal{B}z$. In these variables $\mathcal{B}$ is a symmetric $2m \times 2m$ complex matrix. $\mathcal{H}_*$ is analytic with respect to all its arguments and is periodic in $\hat{\theta}$.

We also assume that:

4. The analyticity of $\mathcal{H}_*$ holds in a neighbourhood of $z = 0$, $\hat{I} = 0$ (the periodic orbit/torus is assumed to be centered about this point — if it is not, then a change of variables can be used to reduce to this case) and in a complex strip about the variable $\hat{\theta}$, that is for $|\mathrm{Im}(\hat{\theta}_j)| \leq \rho$, $\quad j = 1, 2, \ldots, r$, $\quad \rho \in \mathbb{R}$. Also, the matrix $J_m\mathcal{B}$ is diagonal with distinct eigenvalues[2]

$$\lambda^\top = (\lambda_1, \ldots, \lambda_m, -\lambda_1, \ldots, -\lambda_m).$$

We will also require that the periodic orbit/torus satisfies a strong non-resonance condition and that the normal 'frequencies' λ satisfy a non-degeneracy condition. We delay giving the details of these conditions until later where they arise naturally.

Our method is as follows: we first put the Hamiltonian into the form of (1). Before considering any perturbation it is helpful to put the initial Hamiltonian into a (semi-) normal form. One does this by expanding $\mathcal{H}_*$, the higher order part of (1), as a power series in $\hat{I}$ and z about $\hat{I} = 0$, $z = 0$. Individual monomials in the expansion of $\mathcal{H}_*$ can be eliminated with a convergent change of variables using a generating function. The procedure is similar to that used at each step of the usual KAM method [7] with a point of difference being that the small divisors which appear in the construction of the generating function take the form $ik^\top\hat{\omega}^{(0)} + l^\top\lambda$, with $k \in \mathbb{Z}^r \setminus 0$, $l \in \mathbb{N}^{2m}$. To ensure convergence, the diophantine condition

$$\left|ik^\top\hat{\omega}^{(0)} + l^\top\lambda\right| \geq \frac{\mu_0}{|k|_1^\gamma}, \quad |l|_1 \leq 2 \tag{2}$$

[2] J_m is the matrix of the canonical symplectic form on $\mathbb{C}^{2m}$, $\begin{bmatrix} 0 & I_m \\ -I_m & 0 \end{bmatrix}$.

is assumed to hold. This differs from the usual non-resonance condition of KAM theory in that it includes the effect of the normal frequencies λ. Details of the procedure are in [11], Section 2.2. The resulting Hamiltonian has the form

$$\mathcal{H} = \hat{\omega}^{(0)\top}\hat{I} + \frac{1}{2}z^\top\mathcal{B}z + \frac{1}{2}\hat{I}^\top\mathcal{C}\hat{I} + H_*(\hat{\theta}, x, \hat{I}, y) \tag{3}$$

where $\mathcal{C}$ is a constant matrix with $\det(\mathcal{C}) \neq 0$ and where $H_*(\hat{\theta}, x, \hat{I}, y)$ satisfies the conditions **P1** and **P2**—given in the Appendix—which require that particular monomials of order three, four and five in H_* vanish.

Associated with $\mathcal{H}$ is the real analytic vector field $X_\mathcal{H} = f(u)$, $u^\top = (\hat{\theta}^\top, x^\top, \hat{I}^\top, y^\top)$. When a symplectic integrator with step size h is applied to the vector field f it induces a symplectic map $\Psi_{h,f}$. In order to study whether periodic orbits of $f(u)$ persist in the numerical solution given by the integrator we want to embed $\Psi_{h,f}$ in the flow of a modified vector field close to $f(u)$ and ask whether the modified vector field still contains a periodic orbit. We assume that the symplectic integrator is given by a one-step method, $\Psi_{h,f}$, analytic in both h and u. Iterating the numerical method gives a numerical trajectory $\{u_n\}$ by generating the sequence of vectors u_n:

$$u_{n+1} = \Psi_{h,f}(u_n), \quad n = 0, 1, \ldots \quad u_0 = u(0).$$

The problem of embedding the map $\Psi_{h,f}$ in a flow means finding an analytic modified vector field $\bar{f}$ which exactly interpolates u_n.

It is well known that it is possible to find an autonomous vector field whose flow is close to the numerical trajectory. The following theorem, presented in [18], states that there is always a local modified vector field which comes exponentially close to interpolating the numerical solution.

Theorem 2 (Moan [18]) *Let f be an analytic vector field with $\|f\|_{\delta_1+\delta_2}$ bounded. ($\|f(x)\|_\delta = \sup_{z\in\mathcal{D}_\delta} \|f(z)\|_\infty$, $\mathcal{D}_\delta := \{z \in \mathbb{C}^d : |z_i - x_i| \leq \delta, i = 1, \ldots, d\}$ with $\delta > 0$ and $x \in \mathbb{R}^d$.) Let $u_1 = \Psi_{h,f}(u_0) = u_0 + hf(u_0) + \mathcal{O}(h^2)$ be the approximation produced by a one-step method, and let $\phi_{h,f}$ be the time-h flow of f. Then, for sufficiently small h there exists an autonomous modified vector field $\bar{f}$, bounded on the smaller domain $\mathcal{D}_{\delta_1} \subset \mathcal{D}_{\delta_1+\delta_2}$ such that*

$$\|u_1 - \phi_{h,\bar{f}}(u_0)\|_{\delta_1} = \mathcal{O}(\exp(-c\delta_2/h\|f\|_{\delta_1+\delta_2})).$$

Proofs of Theorem 2 are given by Hairer and Lubich [6] for any B-series methods (e.g. Runge-Kutta methods) and by Benettin and Giorgilli [3] for any symplectic map.

Iterating the bound in Theorem 2 for each step of a numerical integrator, one sees that the numerical trajectory stays exponentially close to $\phi_{nh,\bar{f}}$, the flow of the modified vector field, for some finite time. Unfortunately this result is too weak for our intended use since a trajectory which is close to an invariant curve may diverge from it and may do so after only a short time in the case of exponentially divergent systems. For an arbitrary numerical trajectory, an autonomous flow interpolating the trajectory need not exist, and, in general, rarely does [21]. The following proposition from [18] is an example of the failure of maps, or diffeomorphisms, to embed into flows. Further discussion and examples of this point can be found in the book by Banyaga [2, 1.3.6].

Proposition 1 *There exist vector fields f and one-step methods $\Psi_{h,f}$ for which no time-independent vector field $\bar{f}$ exists with time-h flow $\phi_{h,\bar{f}}$ equal to $\Psi_{h,f}$.*

Pronin and Treschev [23] use a time-averaging procedure to construct an analytic, non-autonomous, periodic flow which exactly interpolates analytic maps isotopic to the identity.[3] If the original map is symplectic then the modified flow is Hamiltonian, (similarly for volume preserving or reversible maps). Other versions of the theorem also hold for maps without such geometric properties.

Theorem 3 (Pronin and Treschev [23]) *Let $(\mathcal{M}, \omega)$ be a compact real-analytic symplectic manifold, where ω is a symplectic structure, and let the analytic map $\Psi : \mathcal{M} \to \mathcal{M}$ be symplectic and isotopic to the identity. Then there exists a function $H(z, t)$, $z \in \mathcal{M}$, $t \in \mathbb{R}$, analytic in t and z and 2π-periodic in t, such that the shift $z(0) \to z(2\pi)$ along trajectories of the Hamiltonian system $\dot{z} = X_H(z, t)$ coincides with Ψ.*

In [16–18] Moan presents the following theorem which gives estimates on the size of the non-autonomous component of the modified vector field $\bar{f} = X_{\bar{H}}$.

Theorem 4 (Moan [17]) *Let $\Psi_{h,f}$ be a one-step method and assume that $f(u)$ is analytic for $u \in \mathcal{D}_{\delta_1+\delta_2} \subset \mathbb{C}^d$. Then there exists a modified vector field*

$$\bar{f}(u, t, h) = f(u) + \varepsilon r_1(u) + \varepsilon r_2(u, t; h) \tag{4}$$

analytic in $\mathcal{D}_{\delta_1}$, analytic and h-periodic in t and with a flow that exactly interpolates the numerical trajectory u_n for all time. Additionally, if the step size is sufficiently small then the time-dependent term is exponentially small in h. More precisely, for $h\|f\|_{\delta_1+\delta_2} < \frac{2\pi\delta_2}{e}$ the size of the non-autonomous term is bounded by $\|\varepsilon r_2\|_{\delta_1} \le C \cdot \exp\left(\frac{-2\pi\delta_2}{eh\|f\|_{\delta_1+\delta_2}}\right)$.

One can now see the $\mathcal{O}(\exp(-c\delta_2/h\|f\|_{\delta_1+\delta_2}))$ term in Theorem 2 as being a consequence of the non-autonomous term εr_2 in Theorem 4.

By Theorem 4 of Moan, and Theorem 3 of Pronin and Treschev, we know that there exists an analytic vector field $\bar{f}(u, t; h) = f(u) + \varepsilon r_1(u) + \varepsilon r_2(u, t; h)$

[3] Two smooth maps $\Psi_i : M \to M'$, $i = 0, 1$ of manifolds M, M' are called *isotopic* if there exists a family of maps $\hat{\Psi}_s : M \to M'$ of the same smoothness class and continuous in the parameter $s \in [0, 1]$, such that $\hat{\Psi}_0 = \Psi_0$ and $\hat{\Psi}_1 = \Psi_1$.

which is also analytic and h-periodic in t. This modified vector field exactly interpolates the numerical trajectory $\{u_n\}$ and is symplectic. Now we associate a perturbed Hamiltonian with the modified vector field, $\bar{f} = X_H,\ H = \mathcal{H} + \varepsilon\mathcal{H}_{\text{pert}}$. Since the perturbation to the vector field is periodic in time we extend the phase space of the original system; $\theta^\top = (\hat{\theta}^\top, \tilde{\theta}),\ I^\top = (\hat{I}^\top, \tilde{I})$ where $\tilde{\theta}$ is the new time/angle variable, with frequency $\tilde{\omega}^{(0)},\ \omega^{(0)\top} = (\hat{\omega}^{(0)\top}, \tilde{\omega}^{(0)})$, and $\tilde{I}$ is its conjugate variable. The perturbed Hamiltonian associated with the modified vector field is written as

$$H(\theta, x, I, y, \varepsilon) = \underbrace{\hat{\omega}^{(0)\top}\hat{I} + \tilde{\omega}^{(0)}\tilde{I}}_{=\omega^{(0)\top} I} + \frac{1}{2}z^\top \mathcal{B} z + \frac{1}{2}\hat{I}^\top \mathcal{C}\hat{I} + H_*(\hat{\theta}, x, \hat{I}, y)$$
$$+ \varepsilon\tilde{\mathcal{H}}(\theta, x, I, y, \varepsilon), \tag{5}$$

that is, $\mathcal{H}_{\text{pert}} = \tilde{w}^{(0)}\tilde{I} + \varepsilon\tilde{\mathcal{H}},\ X_{\mathcal{H}_{\text{pert}}} = \varepsilon R := \varepsilon(r_1 + r_2) = \bar{f} - f$. The dependence of H and $\tilde{\mathcal{H}}$ on ε is due to the dependence of the perturbation size of the modified vector field $\|R\|$ on the step size h. However, we don't make any use of ε as a parameter.

Having found a perturbed Hamiltonian whose flow interpolates the numerical trajectory we are in a position to apply a KAM type method to H in order to prove that it still contains the periodic orbit/lower dimensional torus of the initial $\mathcal{H}$ and thus, state our main result.

Theorem 5 *Consider a Hamiltonian of the form (3) which contains a periodic orbit (r-dimensional invariant torus) about $z = 0,\ \hat{I} = 0$ and satisfying the following assumptions*

(i) *H_* is analytic with respect to $(\hat{\theta}, x, \hat{I}, y)$ about $z = 0,\ \hat{I} = 0$ and satisfies the conditions* **P1** *and* **P2** *specified in the Appendix.*
(ii) *$\mathcal{B}$ is a constant symmetric matrix such that $J_m\mathcal{B}$ is diagonal with distinct eigenvalues $\lambda^\top = (\lambda_1, \ldots, \lambda_m, -\lambda_1, \ldots, -\lambda_m)$.*
(iii) *$\mathcal{C}$ is a constant symmetric matrix with non-zero determinant.*
(iv) *For $\mu_0 > 0$ and $\gamma > 1$ ($\gamma > r$ for the r-dimensional torus case) the following diophantine condition holds.*

$$\left|ik^\top\omega^{(0)} + l^\top\lambda\right| \geq \frac{\mu_0}{|k|_1^\gamma}, \quad k \in \mathbb{Z}^{r+s}\setminus\{0\}, \quad l \in \mathbb{N}^{2m}, \quad |l|_1 \leq 2. \tag{6}$$

Then under the ε independent version of the non-degeneracy condition **NDC** *specified in the Appendix, the following assertion holds.*

Given a fixed ε satisfying $0 \leq \varepsilon \leq R_0^{\frac{\gamma}{\gamma+1}}$ for $R_0 \in \mathbb{R}$ small enough, there exists a Cantor set $\mathcal{W}_*(\varepsilon, R_0) \subset \{\hat{\omega} \in \mathbb{R} : |\hat{\omega} - \hat{\omega}^{(0)}| \leq R_0\} =: \mathcal{V}(R_0)$ ($\hat{\omega} \in \mathbb{R}^r$ for the r-dim. torus) such that for every $\hat{\omega} \in \mathcal{W}_*(\varepsilon, R_0)$ the Hamiltonian H corresponding to this fixed value of ε has a reducible 2-dimensional ($(r+1)$-dim.) invariant torus with a vector of frequencies $\omega^\top = (\hat{\omega}^\top, \tilde{\omega}^{(0)})$ on the torus. Moreover, if R_0 is small enough (depending on σ) then for $0 < \sigma < 1$, *mes* $(\mathcal{V}(R_0)\setminus\mathcal{W}_*(\varepsilon,R_0))\le\exp\left(-R_0^{\frac{-\sigma}{\gamma+1}}\right)$ *where mes*(A) *denotes the Lebesgue measure of the set* A.

Since the additional period of the motion is h, the numerical method sees only a periodic orbit (or r-dim. torus), rather than a 2-torus (or $r+1$-dim. torus). That is, the numerical method is the time-h flow of the modified vector field and this flow has a component with period h.

The theorem above is an application of a more general result due to À. Jorba and J. Villaneuva [11] which we now state.

Theorem 6 (Jorba and Villaneuva [11]) *Consider a* d*-degree of freedom Hamiltonian of the form* (5)*, containing an* r*-dimensional invariant torus and where the perturbation* $\tilde{\mathcal{H}}$ *is quasi-periodic in* $s\ge 1$ *time-like coordinates* $\tilde\theta\in\mathbb{C}^s$. *Assume that* $\tilde{\mathcal{H}}$ *is analytic with respect to* $(\theta,x,\hat I,y)$, $\theta^\top=(\hat\theta^\top,\tilde\theta^\top)$ *about* $z=0$, $\hat I=0$ *with* 2π *periodic dependence on* θ *for any* $\varepsilon\in\mathcal{I}_0:=[0,\varepsilon_0]$, *in a domain that is independent of* ε. *The dependence of* $\tilde{\mathcal{H}}$ *on* ε *is assumed to be* C^2 *and the derivatives of* $\tilde{\mathcal{H}}$ *with respect to* ε *are also analytic in* $(\theta,x,\hat I,y)$ *on the same domain. Then, if assumptions* (i) *to* (iv) *of Theorem* 5 *are satisfied, along with the full* ε*-dependent version of* **NDC** *as given in the Appendix, then the following two assertions hold.*

(a) *There exists a Cantor set* $\mathcal{I}_*\subset\mathcal{I}_0$, *such that for every* $\varepsilon\in\mathcal{I}_*$ *the Hamiltonian* H *has a reducible* $(r+s)$*-dimensional invariant torus with a vector of basic frequencies* $\omega^{(0)}$.
Moreover, for every $0<\sigma<1$, *and for* $\bar\varepsilon$ *small enough (depending on* σ*), mes*$([0,\bar\varepsilon]\setminus\bar{\mathcal{I}}_*)\le\exp(-(1/\bar\varepsilon)^{\frac{\sigma}{\gamma}})$, *where mes*$(A)$ *denotes the Lebesgue measure of the set* A *and where, for every* $\bar\varepsilon$, $\bar{\mathcal{I}}_*:=\bar{\mathcal{I}}_*(\bar\varepsilon)=[0,\bar\varepsilon]\cap\mathcal{I}_*$.

(b) *Given* R_0 *small enough and a fixed* $0\le\varepsilon\le R_0^{\frac{\gamma}{\gamma+1}}$, *there exists a Cantor set* $\mathcal{W}_*(\varepsilon,R_0)\subset\{\hat\omega\in\mathbb{R}^r:|\hat\omega-\hat\omega^{(0)}|\le R_0\}=:\mathcal{V}(R_0)$, *such that for every* $\hat\omega\in\mathcal{W}_*(\varepsilon,R_0)$ *the Hamiltonian* H *corresponding to this fixed value of* ε *has a reducible* $r+s$*-dimensional invariant torus with vector of basic frequencies* ω, $\omega^\top=(\hat\omega^\top,\tilde\omega^{(0)\top})$.
Moreover, if R_0 *is small enough (depending on* σ*), then for every* $0<\sigma<1$, *mes*$(\mathcal{V}(R_0)\setminus\mathcal{W}_*(\varepsilon,R_0))\le\exp\left(-R_0^{\frac{-\sigma}{\gamma+1}}\right)$.

In contrast to Shang's result which gives preservation of a (full dimensional) torus with fixed frequencies for a Cantor set's worth of fixed step sizes, our theorem gives preservation of a Cantor set's worth of frequencies (close to the initial frequencies) for a Cantor set's worth of fixed step sizes, namely, those step sizes that are strongly non-resonant in the sense of (6). The continuous one-parameter family of periodic orbits of the original Hamiltonian system is perturbed to a nearby, discontinuous one-parameter family for a Cantor set of parameter values. The gaps in the set of parameter values correspond to intervals where the strong non-resonance condition fails, that is, where the period of the orbit is resonant, or close to resonant, with the step size of the numerical integrator. We illustrate this idea in Fig. 1.

Proof of Theorem 5 therefore requires that for a Hamiltonian (3) there exists a modified Hamiltonian (5) with a corresponding modified vector field as described by Theorem 4 such that the Hamiltonian (5), and in particular the perturbation $\varepsilon\tilde{\mathcal{H}}$, satisfies all the necessary assumptions of Theorem 6.

Proof of Theorem 5 By Theorems 3 and 4 we have that the modified vector field $\bar{f}(u, t; h) = f(u) + \varepsilon r_1(u) + \varepsilon r_2(u, t; h)$, and hence $\tilde{\mathcal{H}}$, is analytic with respect to all its arguments and is periodic in the new time-like variable. The C^2 dependence of $\tilde{\mathcal{H}}$ on ε required in Theorem 6 is not essential to us since we only require that the second result *(b)* of Theorem 6 holds—this involves fixing the perturbation size ε, not varying it as a parameter to control the normal frequencies.

Properties *(ii)* and *(iii)* of Theorem 6 apply to the initial Hamiltonian $\mathcal{H}$ (i.e (1) and (3)) hence are unaffected by the perturbation $\varepsilon(r_1 + r_2)$ to the vector field. Similarly, once the initial frequencies $\hat{\omega}^{(0)}$ are given the diophantine condition *(iv)* is further affected only by the choice of a (strongly non-resonant) step size h, not on the particular form of the perturbation $R = r_1 + r_2$ (though the choice of h clearly affects the size of R). We can therefore impose condition *(iv)* as an initial assumption on the frequencies of the initial torus, its normal frequencies and on the step size of the numerical method. These frequencies are preserved in the initial component f of the modified vector field $\bar{f}$ given by (4) and so, the perturbed Hamiltonian $H = \mathcal{H} + \varepsilon\tilde{\mathcal{H}}$ satisfies those assumptions of Theorem 6 necessary for the result *(b)* of that theorem. Hence, Theorem 5 holds. □

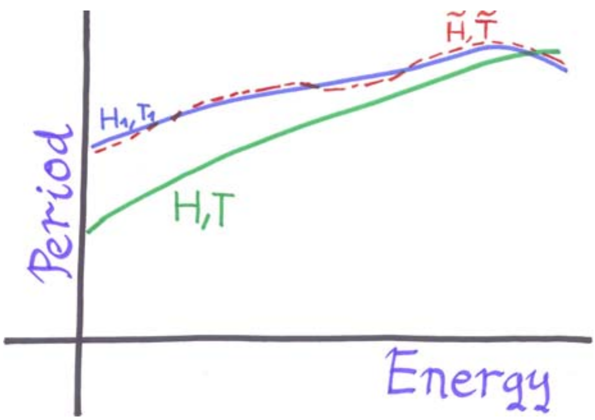

Fig. 1 Possible one-parameter families of periodic orbits for a Hamiltonian H and an autonomous modified Hamiltonian H_1 which is an $\mathcal{O}(\varepsilon = h^p)$ perturbation of H. The (non-autonomous) Hamiltonian $\tilde{H}$ is generated by including the trajectory of a symplectic integrator in the flow of the original Hamiltonian vector field $X_{\tilde{H}}$ and my be thought of as an $\mathcal{O}(e^{-1/\varepsilon})$ perturbation of H_1. The set of periodic orbits of $\tilde{H}$ exist for a Cantor set of periods $\tilde{T}$

Part *(a)* of Theorem 6 seems to suggest that it should be possible to use the perturbation size ε of the modified vector field as a parameter and to achieve a result similar to that of KAM theory for full dimensional tori; namely that periodic orbits or invariant tori are preserved *with their frequencies unchanged*. However, our proof does not allow for this. The parameter ε arises directly from the step size of the symplectic integrator, it also directly affects the frequency of the periodic non-autonomous perturbation. Hence, if one uses the perturbation size, (and thus, the step size), as a parameter, one can no longer ensure that the frequency of the non-autonomous perturbation is not resonant with the existing frequency of the periodic orbit (or the vector of existing frequencies of the lower dimensional torus).

In order to use the perturbation size as a parameter, one would need to show that for a particular step size, the resulting perturbation size was in the Cantor set of values of ε for which the periodic orbit/invariant torus persists *and* that the frequency corresponding to that step size continued to satisfy the strong non-resonance conditions. That is, there must be a non-empty intersection of the Cantor set of step sizes allowed by the perturbation size, and the Cantor set of step sizes allowed by the non-resonance requirement. It does not seem likely that such an intersection would have positive measure.

3 Resonant step sizes

In this section we investigate the case of a symplectic integrator applied to a Hamiltonian system containing a periodic orbit when the step size of the integrator is exactly resonant with the period of the orbit (i.e. $T/h \in \mathbb{Z}$). From the results of the previous section we do not expect the orbit to persist in general.

The resonant, one degree of freedom case is well understood; in fact, it is none other than the Poincaré–Birkhoff fixed point theorem. Consider an annulus $A = \{(\theta, I) : 0 \leq \theta \leq 2\pi, a \leq I \leq b\}$ and an area-preserving twist map $T : A \to A, T : (\theta, I) \mapsto (\theta + \alpha(I), I)$. Let T_ε be an area-preserving perturbation of T; i.e.

$$T_\varepsilon : (\theta, I) \mapsto (\theta + \alpha(I) + f(\theta, I, \varepsilon), I + g(\theta, I, \varepsilon))$$

such that for all ε

$$\int_\Gamma I \mathrm{d}\theta = \int_{T_\varepsilon \Gamma} I \mathrm{d}\theta$$

for Γ any closed curve in A. Then, given any rational number m/n, satisfying $\alpha(a)/2\pi \leq n/m \leq \alpha(b)/2\pi$ there exist $2n$ fixed points of T_ε^n satisfying $T_\varepsilon^n : (\theta, I) \mapsto (0 + 2\pi m, I)$ for ε sufficiently small. The fixed points of T_ε^n (i.e. the n-periodic points of T_ε) are alternately hyperbolic and elliptic. The eigenvalues of T_ε^n must satisfy $\lambda\lambda' = 1$ since the map is area preserving. The return map of the original periodic orbit described by T has a pair of degenerate eigenvalues $(1, 1)$. Under the perturbation, these split to give eigenvalues for the elliptic and hyperbolic fixed points which satisfy $\lambda = \bar{\lambda}'$, $|\lambda| = 1$ and $0 < \lambda < 1 < \lambda' = 1/\lambda$ respectively.

We expect the periodic orbits of Hamiltonian systems with more degrees of freedom to behave in an analogous way when treated with a symplectic map which is resonant with the period of the orbit. More specifically, the return map of a periodic orbit within a d-degree of freedom Hamiltonian system has eigenvalues with a single degenerate pair $\lambda_0 = \lambda_0' = 1$ and $d-1$ non-degenerate pairs satisfying $\lambda_i\lambda_i' = 1$, for $i = 1, \ldots, d-1$. Applying a symplectic integrator whose step size exactly divides the period of a closed orbit, we expect the periodic orbit to be destroyed leaving $n(= T/h)$ elliptic and n hyperbolic periodic points with eigenvalues corresponding to the degenerate pair of the original orbit splitting as either $\lambda_0 = \bar{\lambda}_0'$ or $\lambda_0 = 1/\lambda_0'$ respectively. The remaining $2(d-1)$ eigenvalues are expected to remain of the same type (elliptic or hyperbolic) as for the original periodic orbit but with a small perturbation due to the integrator.

We take, for our symplectic integrator, the leapfrog or Störmer–Verlet method:

$$q_{n+1/2} = q_n + \frac{h}{2}p_n, \quad p_{n+1} = p_n - h\nabla V(q_{n+1/2}), \quad q_{n+1} = q_{n+1/2} + \frac{h}{2}p_{n+1}.$$

As a test system we use the two degree of freedom Hénon–Heiles system given by the Hamiltonian,

$$H(q, p) = T(p) + V(q), \quad q, p \in \mathbb{R}^2, \quad q^\top = (q_1, q_2), \quad p^\top = (p_1, p_2),$$

with

$$T(p) = \frac{1}{2}\|p\|^2 \quad \text{and} \quad V(q) = \frac{1}{2}\|q\|^2 + q_1q_2^2 - \frac{1}{3}q_1^3.$$

The system is non-integrable and when $H < \frac{1}{6}$ the orbits of the system are bounded. For higher energies there are unbounded orbits which escape.

By fixing the energy of the system (we use initial conditions satisfying $H = 0.1$ throughout this section) we can reduce the system from four to three dimensions. Then, taking a transverse section[4] of the flow we can reduce the system by a further dimension leaving a two dimensional map from the plane to itself. Fixed points of the reduced system correspond to periodic orbits of the full four dimensional system. The phase portrait for the reduced system is shown in Fig. 2 where the elliptic and hyperbolic periodic orbits can be seen near $(q_1, p_1) = (0.27, 0)$ and $(-0.15, 0)$ respectively. The periods of the orbits are roughly 5.76 for the elliptic orbit and 6.47 for the hyperbolic.

The two dimensional system in Fig. 2 also shows invariant curves—these correspond to full dimensional invariant tori of the four dimensional system. The tori bound the chaotic regions of the system, leading to bands of chaos trapped between areas of regular motion.

[4]We choose $q_1 = 0$, $p_2 > 0$

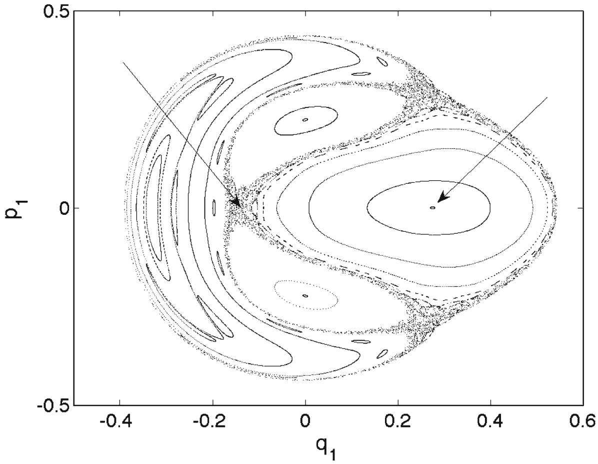

Fig. 2 The Poincaré section of the Hénon–Heiles system calculated with the leapfrog method for $H = 0.1$, with step size $h = 0.1$. The section shows two fixed points (indicated by arrows)—the approximate locations of two periodic orbits of the full system—a hyperbolic point near $(q_1, p_1) = (-0.15, 0)$ and an elliptic point near $(q_1, p_1) = (0.27, 0)$

Table 1 Periodic points corresponding to one elliptic and one hyperbolic perioic orbit of the Hénon–Heiles system after discretisation with $n = 6$ and with $n = 12$ steps of size h per period

	n	h	q_1	q_2	p_1	p_2	Eigenvalues
Ellip.	6	5.67/6	0.24947	0	0	0.40239	$-0.26057 \pm 0.96545i$
							$0.99278 \pm 0.11993i$
Ellip.	6	5.76/6	0.21945	−0.15126	0.09332	0.31512	$-0.18830 \pm 0.98211i$
							1.12557
							0.88844
Hyp.	6	6.47/6	−0.16707	0.24590	0.18003	0.45607	7.47324
							0.13381
							1.34600
							0.74294
Hyp.	6	6.47/6	−0.14100	0.24422	−0.13168	0.22807	$0.59441 \pm 0.80416i$
							1.38670
							0.72114
Ellip.	12	6.03/12	0.26409	−0.00000	0.00000	0.37047	$1.00000 \pm 0.00004i$
							$0.04451 \pm 0.99901i$
Ellip.	12	6.03/12	0.25775	0.088842	−0.04954	0.35192	1.00003
							0.99997
							$0.04451 \pm 0.99901i$
Hyp.	12	6.77/12	−0.17440	−0.00000	−0.00000	0.45137	3.63872
							0.27482
							1.00050
							0.99950
Hyp.	12	6.77/12	−0.16637	0.12413	0.06132	0.44055	3.63872
							0.27482
							$1.00000 \pm 0.00050i$

Eigenvalues are given for the corresponding return map, Ψ_h^n, $n = 6, 12$. Figures are rounded to 5 d.p. but in all cases the pairs of eigenvalues satisfied the property $\lambda\lambda' = 1$ before rounding. A value of 0 indicates zero to machine precision

After using the reduced system to estimate good starting points, we return to the full four-dimensional system and use a combination of nonlinear least squares minimisation and Newton iterations to minimise $\Psi_h^n(x) - x$ for $n = 6, 12$, where Ψ_h^n means taking n steps of size h using the leapfrog method. That is, we find period six and twelve points near the original periodic orbits. The points, along with the eigenvalues of their return maps Ψ_h^n, $n = 6, 12$ are summarised in Table 1.

The results in Table 1 show that in each case the periodic orbits of the original system give rise to pairs of sets of n-periodic points. As expected from the one degree of freedom case, the $(1, 1)$ pair of degenerate eigenvalues corresponding to the original periodic orbit splits into an elliptic and a hyperbolic pair; one pair associated with each of the sets of n-periodic points. Results in the table are rounded to five decimal places. In all cases, the un-rounded eigenvalues satisfy the property $\lambda\lambda' = 1$ to machine precision—as required for the exact preservation of the symplectic property of the system.

Numerical searches in the vicinity of the periodic points and along the line segments joining them found only one elliptic and one hyperbolic set of periodic points per orbit, suggesting that the sets are unique and that the periodic orbit is indeed destroyed by the resonant discretisation.

It is worth noting also, the rapid convergence of the eigenvalues of the six and twelve step return maps towards the eigenvalues of the original periodic orbit. With only 12 steps per period, the eigenvalues corresponding to the degenerate pair differed from one only in the fifth decimal place or, more frequently, smaller. This made it necessary to consider also six steps per period in order to be confident that the results seen were not due to loss of accuracy during numerical calculations.

A full description of the numerical flow in the neighbourhood of a periodic orbit under resonant symplectic discretization, and a proof of the behaviour conjectured here on the basis of our numerical study, remains to be undertaken. Apart from the direct application (to time integration) considered here, there are others that we plan to develop in the future. For example, a steady state or travelling wave of a Hamiltonian PDE with periodic boundary conditions can correspond to a periodic orbit of a Hamiltonian ODE with fixed period. Under spatial semi-discretization the step size is necessarily resonant and the situation we have developed in this section applies.

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Appendix: The P1, P2 and NDC conditions

In order to describe the conditions **P1, P2** and **NDC** in Theorems 5 and 6 it is necessary to give a brief description of the method by which Theorem 6 is arrived at. (For a more detailed description see [11].)

The first step is to rearrange (1), the initial Hamiltonian $\mathcal{H}(\hat{\theta}, x, \hat{I}, y) = \hat{\omega}^{(0)\top}\hat{I} + \frac{1}{2}z^\top\mathcal{B}z + \mathcal{H}_*(\hat{\theta}, x, \hat{I}, y)$, into a suitable form. This involves expanding the $\mathcal{H}_*$ term in a power series about the origin with respect to z and $\hat{I}$. We get

$$\mathcal{H}_* = \sum_{p\geq 2}\mathcal{H}_p^{(0)},$$

where the degree p of a monomial $z^l\hat{I}^j$ is defined as $p = |l|_1 + 2|j|_1$ and where $\mathcal{H}_p^{(0)}$ are homogeneous polynomials of degree p;

$$\mathcal{H}_p^{(0)} = \sum_{\substack{l\in\mathbb{N}^{2m},\ j\in\mathbb{N}^r,\\ |l|_1+2|j|_1=p}} h_{l,j}^{(0)}(\hat{\theta})z^l\hat{I}^j.$$

The periodic coefficients are defined by their Fourier series,

$$h_{l,j}^{(0)}(\hat{\theta}) = \sum_{k\in\mathbb{Z}^r} h_{l,j,k}^{(0)}\exp(ik^\top\hat{\theta}). \tag{7}$$

It is then possible to use three steps of an iterative KAM-like procedure to rewrite the initial Hamiltonian (1) in the form

$$\mathcal{H} = \hat{\omega}^{(0)\top}\hat{I} + \frac{1}{2}z^\top\mathcal{B}z + \frac{1}{2}\hat{I}^\top\mathcal{C}\hat{I} + H_*(\hat{\theta}, x, \hat{I}, y). \tag{8}$$

Each step involves a generating function of the form

$$S^{(n)}(\hat{\theta}, x, \hat{I}, y) = \sum_{\substack{l\in\mathbb{N}^{2m},\ j\in\mathbb{N}^r,\\ |l|_1+2|j|_1=n}} s_{l,j}^{(n)}(\hat{\theta})z^l\hat{I}^j, \quad n = 3, 4, 5, \tag{9}$$

where the periodic coefficients $s_{l,j}^{(n)}(\hat{\theta})$ are defined by their Fourier coefficients allowing us to give an expansion for $S^{(n)}$ based on $\mathcal{H}_n^{(n-3)}$;

$$s_{l,j,k}^{(n)} = \frac{h_{l,j,k}^{(n-3)}}{ik^\top\hat{\omega}^{(0)} + l^\top\lambda}. \tag{10}$$

At each step $S^{(n)}$ is constructed so that the term H_* satisfies the two following conditions hold for monomials of degree= 3, 4, 5:

P1 The coefficients of the monomials $(z, \hat{I})$ (degree 3) and $(z, \hat{I}, \hat{I})$ (degree 5) are zero.

P2 The coefficients of the monomials $(z, z, \hat{I})$ and $(\hat{I}, \hat{I})$ (both of degree 4) do not depend on $\hat{\theta}$ and the coefficients of $(z, z, \hat{I})$ vanish, except for the trivial resonant terms.

The Diophantine condition (6) of *(iv)* Theorem 5 must hold in order that the procedure converges and that the above two conditions can be satisfied.

The condition **NDC** requires yet more details of the procedure used in [11] before it can be stated. We begin by recalling the perturbed Hamiltonian (5):

$$H(\theta, x, I, y, \varepsilon) = \omega^{(0)\top}I + \frac{1}{2}z^\top\mathcal{B}z + \frac{1}{2}\hat{I}^\top\mathcal{C}\hat{I} + H_*(\hat{\theta}, x, \hat{I}, y) + \varepsilon\tilde{\mathcal{H}}(\theta, x, I, y, \varepsilon)$$

and expanding the perturbation in a power series about $\hat{I}=0$, $z=0$. Doing so allows us to group together the terms of the initial Hamiltonian and the perturbation giving the following expression for the Hamiltonian (without explicitly writing the ε dependence)

$$H(\theta, x, I, y) = \tilde{\omega}^{(0)\top}\tilde{I} + H^*(\theta, x, \hat{I}, y), \tag{11}$$

where

$$\begin{aligned} H^* &= a(\theta) + b(\theta)^\top z + c(\theta)^\top \hat{I} \\ &\quad + \frac{1}{2} z^\top B(\theta) z + \hat{I}^\top E(\theta) z + \frac{1}{2}\hat{I}^\top C(\theta)\hat{I} + \Omega(\theta, x, \hat{I}, y), \end{aligned} \tag{12}$$

and where Ω includes all the higher order term in the expansion. The terms $a - \bar{a}$,[5] b, $c - \hat{\omega}^{(0)}$, $B - \mathcal{B}$, $C - \mathcal{C}$ and E are all of order ε.

The idea is to then use a generating function to give a canonical change of coordinates and to kill one power of ε with a procedure similar to that of Kolmogorov [13]. (Although the terms in (12) don't initially depend on θ they do during the iteration.) The smallness of ε and the diophantine condition (6) satisfied by the initial torus means the first step of the procedure can be taken with no small divisor problems. The resulting Hamiltonian is

$$H^{(1)} = H \circ X_S = \tilde{\omega}^{(0)\top}\tilde{I} + H^{(1)*}(\theta, x, \hat{I}, y), \tag{13}$$

with

$$\begin{aligned} H^{(1)*}(\theta, x, \hat{I}, y) &= a^{(1)}(\theta) + b^{(1)}(\theta)^\top z + c^{(1)}(\theta)^\top \hat{I} \\ &\quad + \frac{1}{2} z^\top B^{(1)}(\theta) z + \hat{I}^\top E^{(1)}(\theta) + \frac{1}{2}\hat{I}^\top C^{(1)}(\theta)\hat{I} + \Omega^{(1)}(\theta, x, \hat{I}, y). \end{aligned} \tag{14}$$

If we rewrite the Hamiltonian (13) in the original form (5) we have

$$\begin{aligned} H^{(1)} &= \omega^{(0)\top} I + \frac{1}{2} z^\top \mathcal{B}^{(0)}(\varepsilon) z + \frac{1}{2}\hat{I}^\top \mathcal{C}^{(0)}(\theta, \varepsilon)\hat{I} \\ &\quad + H_*^{(0)}(\hat{\theta}, x, \hat{I}, y) + \varepsilon^2 \tilde{\mathcal{H}}(\theta, x, I, y, \varepsilon), \end{aligned} \tag{15}$$

where $\mathcal{B} - \mathcal{B}^{(0)}$, $\mathcal{C} - \mathcal{C}^{(0)}$ and $H^* - H^{*(0)}$ are all of order ε and where the properties **P1** and **P2** no longer hold for $H^{*(0)}$. The dependence of $\mathcal{B}^{(0)}$ and $\mathcal{C}^{(0)}$ on ε is due to the perturbation size affecting the choice of the generating function and, hence, the coefficient matrices of the new system. However, ε has been fixed throughout this procedure, that is, the C^2 dependence of the Hamiltonian perturbation on ε has not played a role so far. (If the dependence was initially C^2, however, this property is preserved by the step above.)

We would now like to repeat the step above in order to further reduce the size of the perturbation, however, since the normal frequencies change

[5] $\bar{f}(\theta)$ denotes the angular average of the periodic function f.

during each step, we can no longer be sure that the diophantine property which allows convergence by preventing the small divisor problem will hold for the eigenvalues of $J_m\mathcal{B}^{(0)}$. In order to control these eigenvalues at each step we introduce a new parameter. One possible parameter is the perturbation size ε. ε is one possibility for this (and one we want to avoid since it is dependent on the step size h). We introduce the frequencies of the invariant torus as a parameter $\hat{\omega}$, or, more precisely, the difference between the perturbed frequencies and the initial frequencies $\hat{\omega} - \hat{\omega}^{(0)}$. We also introduce the change of variables $\hat{I} \mapsto \hat{I} + \mathcal{C}^{-1}(\hat{\omega} - \hat{\omega}^{(0)})$ and the parameter vector $\varphi^\top = (\hat{\omega}^\top, \varepsilon)$, $\varphi^{\top(0)} = (\hat{\omega}^{(0)\top}, 0)$. With the change of variables (15) becomes

$$\begin{aligned} H^{(1)}(\theta, x, I, y, \varphi) = \tilde{\omega}^{(0)\top}\tilde{I} + \hat{\omega}^{(0)\top}(\hat{I} + \mathcal{C}^{-1}(\hat{\omega} - \hat{\omega}^{(0)})) + \frac{1}{2}z^\top\mathcal{B}^{(0)}z \\ + \frac{1}{2}(\hat{I} + \mathcal{C}^{-1}(\hat{\omega} - \hat{\omega}^{(0)}))^\top\mathcal{C}^{(0)}(\hat{I} + \mathcal{C}^{-1}(\hat{\omega} - \hat{\omega}^{(0)})) \\ + H_*^{(0)}(\theta, x, \hat{I} + \mathcal{C}^{-1}(\hat{\omega} - \hat{\omega}^{(0)}), y, \varepsilon) \\ + \varepsilon^2\mathcal{H}^{(0)}(\theta, x, \hat{I} + \mathcal{C}^{-1}(\hat{\omega} - \hat{\omega}^{(0)}), y, \varepsilon). \end{aligned}$$

Now, if we expand and use the fact that $H_*^{(0)}$ is ε-close to H_* which is in semi-normal form we get

$$\begin{aligned} H^{(1)} = \phi^{(1)}(\varphi) + \omega^\top I + \frac{1}{2}z^\top\mathcal{B}^{(1)}(\varphi)z + \frac{1}{2}\hat{I}^\top\mathcal{C}^{(1)}(\theta, \varphi)\hat{I} \\ + H_*^{(1)}(\theta, x, \hat{I}, y, \varphi) + \tilde{H}^{(1)} \end{aligned} \tag{16}$$

where $\tilde{H}^{(1)}$ contains all the terms that are of order $(\varphi - \varphi^{(0)})^2$ and higher.

By construction, the matrix $J_m\mathcal{B}^{(1)}$ is diagonal. Using the C^2 differentiability with respect to φ its eigenvalues can be written as

$$\lambda_j^{(1)}(\varphi) = \lambda_j + iu_j\varepsilon + iv_j^\top(\hat{\omega} - hw^{(0)}) + \tilde{\lambda}_j^{(1)}(\varphi), \tag{17}$$

for $j = 1, \ldots, 2m$ with $u_j \in \mathbb{C}$ and $v_j \in \mathbb{C}^r$ and where the Lipschitz constant of $\tilde{\lambda}_j^{(1)}$ on the set $\mathcal{E}^{(1)} := \{\varphi \in \mathbb{R}^{r+1} : |\varphi - \varphi^{(0)}| \leq \nu,\ 0 \leq \nu \leq 1\}$ is of $\mathcal{O}(\nu)$. (If we don't have C^2 differentiability with respect to the ε component of φ then the ε term can be fixed to give an ε independent result.[6])

The remaining condition from Theorem 5 can now be given explicitly.

NDC For any j such that $\mathbf{Re}(\lambda_j) = 0$ we have $u_j \neq 0$ and $\mathbf{Re}(v_j) \notin \mathbb{Z}^r$. Moreover, these same conditions hold for $u_{j,l} := u_j - u_l$ and $V_{j,l} := v_j - v_l$ for any $j \neq l$ such that $\mathbf{Re}(\lambda_j - \lambda_l) = 0$.

[6]In [11] it is claimed that even with C^1 dependence on φ the results still hold though the details are more tedious.

References

1. Arnold, V.I.: Proof of a theorem of A.N. Kolmogorov on the preservation of conditionally periodic motions under a small perturbation of the Hamiltonian. Ups. Mat. Nauk **18**(5), 91–192 (1963)
2. Banyaga, A.: The structure of classical diffeomorphism groups. In: Mathematics and Its Applications, vol. 400. Kluwer Academic, Boston (1997)
3. Benettin, G., Giorgilli, A.: On the Hamiltonian interpolation of near-to-the-identity symplectic mappings with application to symplectic integration algorithms. J. Stat. Phys. **74**(5/6), 1117–1143 (1994)
4. Chierchia, L.: Absolutely continuous spectra of quasi-periodic Schrödinger operators. J. Math. Phys. **28**, 2891–2898 (1987)
5. Eliasson, L.H.: Floquet solutions for the 1-dimensional quasi-periodic Schrödinger equation. Commun. Math. Phys. **146**(3), 447–482 (1992)
6. Hairer, E., Lubich, C.: The life-span of backward error analysis for numerical integrators. Numer. Math. **76**, 441–462 (1997)
7. Hairer, E., Lubich, C., Wanner, G.: Geometric Numerical Integration: Structure-preserving Algorithms for Ordinary Differential Equations, 2nd edn., pp. 179–236. Springer, Berlin (2006)
8. Johnson, R.A., Sell, G.R.: Smoothness of spectral subbundles and reducibility of quasi-periodic linear differential equations. J. Differ. Equ. **41**, 262–288 (1981)
9. Jorba, À., Simó, C.: On the reducibility of linear differential equations with quasi-periodic coefficients. J. Differ. Equ. **98**(1), 111–124 (1992)
10. Jorba, À., Simó, C.: On quasi-periodic perturbations of elliptic equilibrium points. SIAM J. Math. Anal. **27**(6), 1704–1737 (1996)
11. Jorba, À., Villanueva, J.: On the persistence of lower dimensional invariant tori under quasi-periodic perturbations. J. Nonlinear Sci. **7**, 427–473 (1997)
12. Jorba, À.: A methodology for the numerical computation of normal forms, centre manifolds, and first integrals of Hamiltonian systems. Exp. Math. **8**(2), 155–195 (1999)
13. Kolmogorov, A.N.: On conservation of conditionally periodic motions under small perturbations of the Hamiltonian. Dokl. Akad. Nauk SSSR **98**, 527–530 (1954)
14. de la Llave, R.: A tutorial on KAM theory. In: Proceedings of the AMS Summer Research Institute on Smooth Ergodic Theory and its Applications, Seattle, 1999, Proc. Sympos. Pure Math., vol. 69, Amer. Math. Soc., vol. 175292 (2001). Expanded version available at ftp.ma.utexas.edu/pub/papers/llave/tutorial.pdf
15. MacKay, R.S., Meiss, J.D.: Hamiltonian Dynamical Systems: A Reprint Selection. Adam Hilger, Bristol (1987)
16. Moan, P.C.: On the KAM and Nekhoroschev theorems for symplectic integrators and implications for error growth. Nonlinearity **17**, 67–83 (2004)
17. Moan, P.-C.: On rigorous modified equations for discretizations of ODEs. (2005). Available at http://www.focm.net/gi/gips/2005/3.html
18. Moan, P.-C.: On modified equations for discretizations of ODEs. J. Phys. A Math. Gen. **39**, 5545–5561 (2006)
19. Moser, J.: On invariant curves of area-preserving mappings of an annulus. Nachr. Akad. Wiss. Gott. Math.-Phys. Kl. **2**, 1–20 (1962)
20. Moser, J., Pöschel, J.: An extension of a result by Dinaburg and Sinai on quasiperiodic potentials. Comment. Math. Helv. **59**(1), 39–85 (1984)
21. Palis, J.: Vector fields generate few diffeomorphisms. Bull. Am. Math. Soc. **80**(3), 503–505 (1974)
22. Poincaré, H.: Les Méthodes Nouvelles de la Mécanique Céleste, pp. 366–401. NASA English translation of the Dover publication (1957)
23. Pronin, A.V., Treschev, D.V.: On the inclusion of analytic symplectic maps into analytic flows. Regul. Chaotic Dyn. **2**(2), 14–24 (1997)
24. Rychlik, M.: Renormalization of cocycles and linear ODE with almost periodic coefficients. Invent. Math. **110**(1), 173–206 (1992)

25. Shang, Z.-J.: KAM theorm of symplectic algorithms for Hamiltonian systems. Numer. Math. **83**, 477–496 (1999)
26. Shang, Z.-J.: Resonant and diophantine step sizes in computing invariant tori of Hamiltonian systems. Nonlinearity **13**, 299–308 (2000)
27. Shang, Z.-J.: A note on the KAM theorem for symplectic mappings. J. Dyn. Differ. Equ. **12**(2), 357–383 (2000)