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KAM theorem of symplectic algorithms for Hamiltonian systems

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Summary. In this paper we prove that an analog of the celebrated KAM theorem holds for symplectic algorithms, which Channel and Scovel (1990), Feng Kang (1991) and Sanz-Serna and Calvo (1994) suggested a few years ago. The main results consist of the existence of invariant tori, with a smooth foliation structure, of a symplectic numerical algorithm when it applies to a generic integrable Hamiltonian system if the system is analytic and the time-step size of the algorithm is sufficiently small. This existence result also implies that the algorithm, when it is applied to a generic integrable system, possesses n independent smooth invariant functions which are in involution and well-defined on the set filled by the invariant tori in the sense of Whitney. The invariant tori are just the level sets of these functions. Some quantitative results about the numerical invariant tori of the algorithm approximating the exact ones of the system are also given.

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1. Introduction and results

Since the pioneering work of Channel (1983), Feng Kang (1985, 1986) and Ruth (1983), the problem of numerically solving Hamiltonian systems in the symplectic way has become a widely interested subject. Feng and Wang (1994) and Sanz-Serna (1995) surveyed most of the interesting results and Hairer, Norsett and Wanner (1993) and Sanz-Serna and Calvo (1994) collected a large number of references related to this problem. The symplectic way consists in the requirement that the step-transition maps of numerical algorithms be symplectic when the algorithms apply to Hamiltonian systems, and in this sense, the corresponding algorithms are called symplectic ones. It turns out that apart from some very rare exceptions (Lasagni (1988), Sanz-Serna (1988) and Suris (1989) discovered independently symplectic algorithms in the classical Runge-Kutta class), all the conventional algorithms are non-symplectic. Great success has been achieved in the construction of symplectic schemes and a considerable enriched arsenal of available symplectic algorithms has been well built up (see [13], [15] and [22]). Extensive computer experimentation, by some typical models of Hamiltonian systems, has shown the overwhelming superiority of symplectic algorithms over the conventional non-symplectic ones, especially in simulating the global and structural dynamic behavior of the systems [10, 11, 12]. The present paper is just to show that the above experimental results lay in fact on the solid basis of a general mathematical theory. On the other hand, in the class of Hamiltonian systems, the most well-understood systems are perhaps only completely integrable ones. Completely integrable systems exhibit regular dynamic behavior which corresponds to periodic and quasi-periodic motions in the phase spaces. A basic question arises accordingly: whether can symplectic algorithms simulate qualitatively and approximate quantitatively the periodic and quasi-periodic phase curves of integrable Hamiltonian systems?

This question fits into the content of the well-known KAM theory, which was already suggested by Channel and Scovel (1990), Feng Kang (1991) and Sanz-Serna and Calvo (1994). KAM theory says that for a generic integrable Hamiltonian system or exact symplectic mapping, most of invariant tori supporting quasi-periodic motions survive small Hamiltonian or symplectic perturbations [2]. A symplectic algorithm may be characterized as a perturbation of the phase flow of the integrable system to which the algorithm is applied. Here the smallness of the perturbation is described by the time-step size of the algorithm which also enters into the frequency map of the integrable system. Therefore the small twist version of KAM theorem for mappings is relevant to this question. For the small twist problem, however, only the special case of two dimension has been tackled by Moser (1962) and no references for the general case can be referred to. The estimates obtained recently by Shang (1996) automatically lead to a generalization of Moser's result to high dimensions which may be applied to give a proper answer to the above question.

There has already appeared recently some nice work about the numerical analysis of symplectic algorithms for Hamiltonian systems, for example, by Benettin and Giorgilli (1994) and Hairer and Lubich (1997). Moreover, Hairer and Lubich (1997) proved, as a corollary of their main theorem, that a numerical solution of a symplectic algorithm, when it is applied to an analytic Hamiltonian system with a nondegenerate critical invariant torus with diophantine frequencies, follows “almost exactly” the solution of some perturbed Hamiltonian system, which is determined by the algorithm, with initial values on the invariant torus of the perturbed system (by KAM theorem the perturbed system has also an invariant torus with the same diophantine frequencies as long as the time-step size of the algorithm is sufficiently small). Here “almost exactly follows” means that the numerical solution by the algorithm differs from the exact solution of the perturbed Hamiltonian system only exponentially small in $1/t$ within the interval of the time evolution exponentially large in $1/t$ if the starting points of the two solutions are the same, where t is the time-step of the algorithm. This result shows that the perturbed system is an efficient approximant to the algorithm in the orbit sense and therefore, may be viewed as an “almost KAM theorem” of symplectic algorithms. In contrast, the results obtained in this paper are exact in the spirit of KAM.

We formulate the main results of the paper as follows. In Sect. 3 we will give more quantitative details.

Theorem 1. *If a Hamiltonian system is integrable in a connected bounded open domain D of $\mathbb{R}^{2n}$, and if it is real analytic and nondegenerate in the sense of Kolmogorov after being expressed as action-angle variables (see [2]), then for any analytic symplectic difference scheme*[1] *compatible with the system, as long as the time-step t of the scheme is small enough, most nonresonant invariant tori of the integrable system do not vanish, but are only slightly deformed, so that in the phase space D, the symplectic difference scheme also has invariant tori densely filled with phase orbits winding around them quasi-periodically, with a number of independent frequencies equal to the number of degrees of freedom. These invariant tori are all analytic manifolds and form a Cantor set, say D_t, in the phase space D, which depends on the time-step t and whose Lebesgue measure mD_t tends to mD as t tends to zero. Moreover, if the difference scheme is restricted to D_t, then it is conjugate to a one parameter family of rotations of the form $(p,q) \to (p, q + t\omega_t(p))$ defined on $B_t \times \boldsymbol{T}^n$, by a C^∞-symplectic conjugation $\Psi_t : B_t \times \boldsymbol{T}^n \to D_t$, with (p,q) as action-angle coordinates and ω_t the frequency map defined on a Cantor set $B_t \subset \mathbb{R}^n$. Furthermore, we have that $\Psi_t \to \Psi$ and $\omega_t \to \omega$ as $t \to 0$ in the sense explained in the last part of Sect. 3.1, where Ψ is the symplectic conjugation of one parameter group $(p,q) \to (p, q + t\omega(p))$ to the phase flow of the system and ω is the frequency map of the integrable system which is defined on the domain, say $B \subset \mathbb{R}^n$, of the action variables with $B_t \to B$ as $t \to 0$ in the Lebesgue*

[1] The referees suggested the notion of *an analytic algorithm* which is an algorithm generating an analytic step-transition map whenever the Hamiltonian is analytic. Note that all the existing available symplectic algorithms are analytic in this sense.

measure sense. Note that functions and mappings of class C^∞ on Cantor sets are defined in the sense of Whitney (see [18] for the exact definition)[2].

A more quantitative result holds. For any given and sufficiently small $\gamma > 0$, if the time step t is sufficiently small, then there exist closed subsets $B_{\gamma,t}$ of B_t and $D_{\gamma,t}$ of D_t such that $D_{\gamma,t} = \Psi_t(B_{\gamma,t} \times \boldsymbol{T}^n)$ and the following hold:

1) $mD_{\gamma,t} \geq (1 - c_1'\gamma)mD$, where c_1' is a positive constant not depending on t and γ;

2) $\|\Psi_t - \Psi\|_{\beta,\beta\lambda;B_{\gamma,t}\times\boldsymbol{T}^n}$, $\|\omega_t - \omega\|_{\beta+1;B_{\gamma,t}} \leq c_2'\gamma^{-(2+\beta)} \cdot t^s$ for any $\beta \geq 0$, where s is the accuracy order of the difference scheme approximating the system, $\lambda > n+2$, c_2' is a positive constant not depending on γ and t. The norms here are understood in the sense of Whitney and will be explained in the next section;

3) every invariant torus in $D_{\gamma,t}$ of the difference scheme is an approximant of order t^s in the sense of Hausdorff[3] *to the invariant torus with the same frequencies of the original integrable system.*

A natural corollary of the above theorem is

Corollary 1. *Under the assumptions of the above theorem, there exist n functions $F_1^{\mathrm{t}}, \cdots, F_n^{\mathrm{t}}$ which are defined on the Cantor set D_t and are of class C^∞ in the sense of Whitney such that*

1) $F_1^{\mathrm{t}}, \cdots, F_n^{\mathrm{t}}$ are functionally independent and in involution (i.e., the Poisson bracket of any two functions vanishes on D_t);

2) every F_j^{t}, $j = 1, \cdots, n$, is invariant under the difference scheme and the invariant tori are just the intersection of the level sets of these functions.

3) F_j^{t}, $j = 1, \cdots, n$ approximate n independent integrals in involution of the integrable system, with a suitable order of accuracy with respect to the time-step t which will be explained in the proof.

2. Small twist version of the KAM theorem

In this section we state a theorem of KAM type for small twist mappings. Such a theorem first appeared in Moser's celebrated paper [17] for two dimensional area-preserving mappings. Its generalization to higher dimen-

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2 One may simply consider a function or a mapping of class C^r ($0 < r \leq \infty$) defined on $I \times \boldsymbol{T}^n$ for a closed set $I \subset \mathbb{R}^n$ in the sense of Whitney as a restriction of some C^r-counterpart, well-defined on $\mathbb{R}^n \times \boldsymbol{T}^n$ in the usual sense, to the set $I \times \boldsymbol{T}^n$.

3 The Hausdorff distance of two sets A and B is defined as [5]

$$d(A, B) = \max(\sup_{x\in A} \mathrm{dist}(x, B), \sup_{y\in B} \mathrm{dist}(y, A)),$$

where $\mathrm{dist}(x, B) = \inf_{y\in B} |x - y|$.

sions is not difficult essentially but, to my knowledge, no reference for it is available.

Consider a one parameter family of exact symplectic mappings S_t : $(p,q) \to (\hat{p},\hat{q})$ with $S_0 =$ identity, to be defined implicitly in phase space $B \times \boldsymbol{T}^n$ by

$$\begin{cases} \hat{p} = p - t\frac{\partial H}{\partial q}(\hat{p},q) = p - t\frac{\partial h}{\partial q}(\hat{p},q) \\ \hat{q} = q + t\frac{\partial H}{\partial \hat{p}}(\hat{p},q) = q + t\omega(\hat{p}) + t\frac{\partial h}{\partial \hat{p}}(\hat{p},q) \end{cases} \tag{2.1}$$

with generating function $H(\hat{p},q) = H_0(\hat{p}) + h(\hat{p},q)$ well-defined for $(\hat{p},q) \in B \times \boldsymbol{T}^n$. In (2.1), $\omega(\hat{p}) = \frac{\partial H_0}{\partial \hat{p}}(\hat{p})$. Here B is an open and usually bounded set of $\mathbb{R}^n$ and $\boldsymbol{T}^n = \mathbb{R}^n/(2\pi\mathbb{Z})^n$ is the usual torus. Note that functions on $B \times \boldsymbol{T}^n$ can be identified with functions on $B \times \mathbb{R}^n$ with 2π-periods in the last n variables. For $t = 1$, the ordinary KAM theorem applies to S_1, which says that for sufficiently smooth generating function $H(\hat{p},q) = H_0(\hat{p}) + h(\hat{p},q)$, if the frequency map $\omega = \frac{\partial H_0}{\partial \hat{p}} : B \to \mathbb{R}^n$ of the integrable system is nondegenerate and if the perturbation h is sufficiently small, then the mapping S_1 has n-dimensional invariant tori, supporting quasi-periodic motions, which fill up a large portion of the phase space $B \times \boldsymbol{T}^n$ in the sense that the relative Lebesgue measure of the union of the invariant tori tends to one as the perturbation h tends to zero [1, 3]. The small twist problem concerns the question as to whether the same results hold for S_t, $0 < t < 1$, under the above conditions of S_1 without further assumptions. For $n = 1$, Moser affirmed that this is true [17]. The theorem below gives a positive answer to the question for general dimension $n \geq 1$.

To formulate the theorem more precisely, we introduce some notations and assumptions. As in [18], for given (ν_1,ν_2), a pair of non-negative numbers, and given I, an open or closed set of $\mathbb{R}^n$, denote by $C^{\nu_1,\nu_2}(I \times \boldsymbol{T}^n)$ the class of functions defined on $I \times \boldsymbol{T}^n$ with anisotropic Whitney derivatives up to order (ν_1,ν_2), and by $\|\cdot\|_{\nu_1,\nu_2;I\times\boldsymbol{T}^n}$ the associated Whitney norm. By $C^a(I \times \boldsymbol{T}^n)$ and $C^a(I)$ we denote the classes of functions on $I \times \boldsymbol{T}^n$ and I, respectively, with isotropic Whitney derivatives up to order a and by $\|\cdot\|_{a;I\times\boldsymbol{T}^n}$ and $\|\cdot\|_{a;I}$ the respective associated norms. These classes with the corresponding norms are all Banach spaces. We also use another norm $\|\cdot\|_{\nu_1,\nu_2;I\times\boldsymbol{T}^n,\rho}$ for $\rho > 0$ defined by

$$\|u\|_{\nu_1,\nu_2;I\times\boldsymbol{T}^n,\rho} = \|u \circ \sigma_\rho\|_{\nu_1,\nu_2;\sigma_\rho^{-1}(I\times\boldsymbol{T}^n)} \tag{2.2}$$

for $u \in C^{\nu_1,\nu_2}(I \times \boldsymbol{T}^n)$, where σ_ρ denotes the partial stretching $(x,y) \to (\rho x, y)$ for $(x,y) \in I \times \boldsymbol{T}^n$. Note that the following relation between these two norms is valid for $0 < \rho \leq 1$:

$$\|u\|_{\nu_1,\nu_2;\rho} \leq \|u\|_{\nu_1,\nu_2} \leq \rho^{-\nu_1}\|u\|_{\nu_1,\nu_2;\rho}\,, \tag{2.3}$$

where we dropped the domains to simplify the notations.

Write $\Omega = \omega(B)$. For $\gamma > 0$ and $0 < t \le 1$ denote by $\Omega_{\gamma,t}$ the set of those frequencies $\omega = (\omega_1, \cdots, \omega_n) \in \Omega$ which satisfy the diophantine condition

$$\left| \mathrm{e}^{\mathrm{i}\langle k, t\omega\rangle} - 1 \right| \ge \frac{t\gamma}{|k|^\tau}, \quad \text{for } 0 \ne k = (k_1, \cdots, k_n) \in \mathbb{Z}^n \tag{2.4}$$

with a fixed constant $\tau > 0$, where $\langle k, \omega\rangle = \sum_{j=1}^n k_j\omega_j$ and $|k| = \sum_{j=1}^n |k_j|$ for integers $k \in \mathbb{Z}^n$, and whose distance to the boundary of Ω is at least equal to 2γ. The difference $\Omega \setminus \bigcup_{\gamma>0} \Omega_{\gamma,t}$ is a zero set for any $0 < t \le 1$ if $\tau > n+1$ (the proof easily follows from the case when $t = 1$ which is referred to [3]). Therefore $\Omega_{\gamma,t}$ is large, uniformly in $0 < t \le 1$, for small γ.

Let $B + r$ be the complex domain of radius r of the real set B. Assume the function $H_0(p)$ is analytic in $p \in B + r$ and that the frequency map $\omega = \frac{\partial H_0}{\partial p} : B \to \mathbb{R}^n$ satisfies the following nondegenerate condition

$$\theta|dp| \le |d\omega(p)| \le \Theta|dp|, \quad \text{for } p \in B + r \tag{2.5}$$

with constants $0 < \theta \le \Theta$, where $|\cdot|$ denotes the maximal norm of vectors in $\mathbb{C}^n$.

The main result of the section is as follows

Theorem 2. *With given positive integer n and given $\tau > n+1$, consider a one parameter family of mappings S_t of the form (2.1) defined in phase space $B \times \boldsymbol{T}^n$ by some function $H(\hat{p}, q) = H_0(\hat{p}) + h(\hat{p}, q)$, where $H_0(\hat{p})$ is analytic in $\hat{p} \in B + r$ with $r > 0$ and $h(\hat{p}, q)$ belongs to the class $C^{\alpha\lambda+\lambda+\tau}(B \times \boldsymbol{T}^n)$ with fixed $\lambda > \tau + 1$ and $\alpha > 1$ not in the discrete set*

$$\Lambda = \{i/\lambda + j : i, j \ge 0 \, \text{integer}\}.$$

Suppose that the frequency map $\omega = \frac{\partial H_0}{\partial \hat{p}} : B \to \Omega$ satisfies the nondegeneracy condition (2.5) with the constants θ and Θ satisfying $0 < \theta \le \Theta$. Then there exists a positive constant δ_0, depending only on n, τ, λ and α, such that for any $0 < \gamma \le \min(1, \frac{1}{2}r\Theta)$, if

$$\|h\|_{\alpha\lambda+\lambda+\tau, I\times \boldsymbol{T}^n; \gamma\Theta^{-1}} \le \delta_0 \gamma^2 \theta^2 \Theta^{-3}, \tag{2.6}$$

then there exist a Cantor set $B_{\gamma,t} \subset B$, a surjective map $\omega_{\gamma,t} : B_{\gamma,t} \to \Omega_{\gamma,t}$ of class $C^{\alpha+1}$ and a symplectic mapping $\Phi_t : B_{\gamma,t} \times \boldsymbol{T}^n \to \mathbb{R}^n \times \boldsymbol{T}^n$ of class $C^{\alpha,\alpha\lambda}$, in the sense of Whitney, such that

(1) Φ_t is a conjugation between S_t and R_t. That is, the following equation holds:

$$S_t \circ \Phi_t = \Phi_t \circ R_t, \tag{2.7}$$

where R_t is the integrable rotation on $B_{\gamma,t} \times \boldsymbol{T}^n$ with the frequency map $t\omega_{\gamma,t}$, i.e., $R_t(P,Q) = (P, Q + t\omega_{\gamma,t}(P))$. Moreover, this equation may be differentiated as often as Φ_t allows.

(2) If Ω is a bounded open set of type D in the sense of Arnold[4] [1]*, then we have the following measure estimate*

$$m\mathcal{E}_{\gamma,t} \geq \Big(1 - c_4\Big(\theta\Theta^{-1}\Big)^{-n}\gamma\Big)m\mathcal{E}, \tag{2.8}$$

where m denotes the Lebesgue measure[5] *of the phase space $\mathcal{E} = B \times \boldsymbol{T}^n$ and $\mathcal{E}_{\gamma,t} = \Phi_t(B_{\gamma,t} \times \boldsymbol{T}^n)$; c_4 is a positive constant depending on n, τ, λ and α and the geometry of the domain Ω.*

(3) If h is of class $C^{\beta\lambda+\lambda+\tau}$ with $\alpha \leq \beta$ not in Λ, then we have further that $\omega_{\gamma,t} \in C^{\beta+1}(B_{\gamma,t})$ and $\Phi_t \in C^{\beta,\beta\lambda}(B_{\gamma,t} \times \boldsymbol{T}^n)$. Moreover,

$$\begin{aligned} &\left\|\sigma^{-1}_{\gamma\Theta^{-1}} \circ (\Phi_t - I)\right\|_{\beta,\beta\lambda;\gamma\Theta^{-1}}, \\ &\gamma^{-1}\left\|\omega_{\gamma,t} - \omega\right\|_{\beta+1;\gamma\Theta^{-1}} \leq c_5\gamma^{-2}\Theta\left\|h\right\|_{\beta\lambda+\lambda+\tau;\gamma\Theta^{-1}} \end{aligned} \tag{(2.9)}$$

with constant c_5 depending on n, τ, λ and β, here we have dropped the domains to simplify the notations of norms.

(4) For each $\omega^* \in \Omega_{\gamma,t}$, there exist $p^* \in B$ and $P^* \in B_{\gamma,t}$ such that $\omega(p^*) = \omega_{\gamma,t}(P^*) = \omega^*$ and

$$|P^* - p^*| \leq c_6\Big(\gamma\theta\Theta^{-1}\Big)^{-1}\|h\|_{a,I\times\boldsymbol{T}^n;\gamma\Theta^{-1}}, \tag{2.10}$$

where c_6 is a positive constant depending on n, τ, λ and α.

Remark 1. If $h \in C^\infty(B \times \boldsymbol{T}^n)$, then $\omega_{\gamma,t} \in C^\infty(B_{\gamma,t})$ and $\Phi_t \in C^\infty(B_{\gamma,t} \times \boldsymbol{T}^n)$ with the estimates (2.9) for any $\beta \geq \alpha$.

Remark 2. If h is analytic with the domain of analyticity containing

$$\begin{aligned} S(r',\rho') = \Big\{&(p,q) \in \mathbb{C}^{2n} : |p - p'| < r', |\operatorname{Im} q| < \rho' \\ &\text{with } p' \in B \text{ and } \operatorname{Re} q \in \boldsymbol{T}^n\Big\} \end{aligned}$$

for some $r' > 0$ and $\rho' > 0$ where $\operatorname{Re} q$ and $\operatorname{Im} q$ denote the real and imaginary parts of q respectively and if, instead of (2.6) in Theorem 2, h satisfies

$$\|h\|_{r',\rho'} = \sup_{(p,q)\in S(r',\rho')} |h(p,q)| \leq \delta_0\gamma^2\theta^2\Theta^{-3}, \tag{2.11}$$

for some sufficiently small $\delta_0 > 0$, depending on n, τ, r' and ρ', then all the conclusions of Theorem 2 are still true with $\omega_{\gamma,t} \in C^\infty(B_{\gamma,t})$, $\Phi_t \in C^{\infty,\omega}(B_{\gamma,t} \times \boldsymbol{T}^n)$ and the estimate (2.9) for any $\beta \geq 0$.

[4] A domain with piece-wise smooth boundary is of type D in the sense of Arnold.
[5] Lebesgue measure of the phase space is compatible with the invariant Liouville measure.

Remark 3. It is clear that if h depends on the parameter t continuously, then Theorem 2 also holds with constants independent of t.

Proof of Theorem 2. Theorem 2 has been proved in [23] for the case $t = 1$. We denote this well-proved case as $(\mathrm{Th})_1$. The validity of the theorem for the case $0 < t < 1$, apart from the measure estimate (2.8), follows directly from $(\mathrm{Th})_1$ with the observation of the facts that $(\mathrm{Th})_1$ may apply to S_t with the replacement of relevant functions and parameters, say H, H_0, h, γ, θ and Θ by tH, tH_0, th, $t\gamma$, $t\theta$ and $t\Theta$ respectively and that the smallness condition (2.5) implies the corresponding smallness condition for S_t as required by $(\mathrm{Th})_1$. As to the estimate (2.8), the direct application of $(\mathrm{Th})_1$ leads to the following

$$m\mathcal{E}_{\gamma,t} \geq \Big(1 - c_4^{\mathrm{t}}\Big(\theta\Theta^{-1}\Big)^{-n} \cdot t\gamma\Big)m\mathcal{E}$$

with the constant $c_4^{\mathrm{t}} > 0$ depending also on t. Note that, for a bounded open set Ω of type D in the sense of Arnold, we have (see [1])

$$m(\Omega \setminus \Omega_{\gamma,1}) \leq D\gamma m\Omega,$$

with a positive constant D not depending on γ, which implies that

$$m(t\Omega \setminus t\Omega_{\gamma,t}) \leq D'\gamma m(t\Omega)$$

with another constant D', possibly larger than D but not depending on γ and t. So, from the standard argument for measure estimate in KAM theorem [1], we find $c_4^{\mathrm{t}} = c_4 t^{-1}$ with $c_4 = c_4^1$ which verifies the estimate (2.8). This completes the proof of Theorem 2. □

The proof of the remarks 1 and 2 follows from the similar arguments and the corresponding remarks of [18].

3. Invariant tori of symplectic algorithms: proofs of the main results

In this section we prove the main results of the paper stated in Sect. 1.

We consider a Hamiltonian system with n degrees of freedom in canonical form

$$\dot{x} = -\frac{\partial K}{\partial y}(x,y), \quad \dot{y} = \frac{\partial K}{\partial x}(x,y), \quad (x,y) \in D, \tag{3.1}$$

where D is a connected bounded open subset of $\mathbb{R}^{2n}$; x and y are both n-dimensional Euclidean coordinates with $\dot{x}$ and $\dot{y}$ the derivatives of x and y with respect to the time "t" respectively; $K : D \to \mathbb{R}^1$ is the Hamiltonian.

A symplectic algorithm that is compatible with the system (3.1) is a discretization scheme such that, when applied to the system (3.1), it uniquely determines a one parameter family of symplectic step-transition maps G_K^t that approximates the phase flow g_K^t in the sense that

$$\lim_{t\to 0}\frac{1}{t^s}\Big(G_K^t(z)-g_K^{\mathrm{t}}(z)\Big)=0,\qquad \text{for any } z=(x,y)\in D \tag{3.2}$$

for some $s\geq 1$, here $t>0$ is the time-step size of the algorithm and s, the largest integer such that (3.2) holds, is the order of accuracy of the algorithm approximating the continuous systems. Note that the domain in which G_K^{t} is well-defined, say $\widetilde{D}_t$, depends on t generally and converges to D as $t\to 0$ — this means that any $z\in D$ is contained in $\widetilde{D}_t$ when t is sufficiently close to zero.

From (3.2), we may assume

$$G_K^{\mathrm{t}}(z)=g_K^{\mathrm{t}}(z)+t^sR_K^{\mathrm{t}}(z), \tag{3.3}$$

where

$$R_K^{\mathrm{t}}(z)=\frac{1}{t^s}\Big(G_K^{\mathrm{t}}(z)-g_K^{\mathrm{t}}(z)\Big)$$

is well-defined for $z\in\widetilde{D}_t\subset D$ and has the limit zero as $t\to 0$ for $z\in D$. Below we prove the results of Sect. 1 by simply regarding the approximant G_K^{t} to the phase flow g_K^{t} of the above form as a symplectic discretization scheme of order s.

3.1. Proof of Theorem 1

We assume the system (3.1) is integrable. That is, there exists a system of action-angle coordinates (p,q) in which the domain D can be expressed as the form $B\times\boldsymbol{T}^n$ and the Hamiltonian depends only on the action variables, where B is a connected bounded open subset of $\mathbb{R}^n$ and $\boldsymbol{T}^n$ the standard n-dimensional torus. Let us denote by $\Psi: B\times\boldsymbol{T}^n\to D$ the coordinate transformation from (p,q) to (x,y), then Ψ is a symplectic diffeomorphism from $B\times\boldsymbol{T}^n$ onto D and the new Hamiltonian

$$K\circ\Psi(p,q)=H(p),\quad (p,q)\in B\times\boldsymbol{T}^n \tag{3.4}$$

only depends on p. Therefore, in the action-angle coordinates (p,q), (3.1) takes the simple form

$$\dot p=0,\quad \dot q=\omega(p)=\frac{\partial H}{\partial p}(p) \tag{3.5}$$

and the phase flow g_H^t is just the one parameter group of rotations $(p,q)\to(p,q+t\omega(p))$ which leaves every torus $\{p\}\times\boldsymbol{T}^n$ invariant.

Assume K is analytic and, without loss of generality, assume the domain of analyticity of K contains the following open subset of $\mathbb{C}^{2n}$

$$\mathcal{D}_{\alpha_0} = \left\{ z = (x, y) \in \mathbb{C}^{2n} : d(z, D) < \alpha_0 \right\}, \tag{3.6}$$

with some $\alpha_0 > 0$, where

$$d(z, D) = \inf_{z' \in D} |z - z'|$$

denotes the distance from the point $z \in \mathbb{C}^{2n}$ to the set $D \subset \mathbb{C}^{2n}$ in which $|z| = \max_{1 \le j \le 2n} |z_j|$ for $z = (z_1, \cdots, z_{2n})$. Also, we assume that Ψ extends analytically to the following complex domain

$$S(r_0, \rho_0) = \left\{ (p, q) \in \mathbb{C}^{2n} : d(p, B) < r_0, \operatorname{Re} q \in \boldsymbol{T}^n, |\operatorname{Im} q| < \rho_0 \right\} \tag{3.7}$$

with $r_0 > 0$, $\rho_0 > 0$ and has period 2π in each component of q. In (3.7), B is considered as a subset of $\mathbb{C}^{2n}$. Without loss of generality, we suppose $\widetilde{\mathcal{D}}(r_0, \rho_0) = \Psi\Big(S(r_0, \rho_0)\Big) \subset \mathcal{D}_{\alpha_0}$ and further that Ψ is a diffeomorphism from $S(r_0, \rho_0)$ onto $\widetilde{\mathcal{D}}(r_0, \rho_0)$. So the equation (3.4) is valid for $(p, q) \in S(r_0, \rho_0)$ and

$$\Psi^{-1} \circ g_K^{\mathrm{t}} \circ \Psi = g_H^{\mathrm{t}} \tag{3.8}$$

on this complex domain of coordinates (p, q).

Checking existing available symplectic algorithms, we find that G_K^{t} is always analytic if the Hamiltonian K is analytic. Since the domain in which G_K^{t} is well-defined converges to the domain of the definition of g_K^{t} as t approaches zero, we may assume, without loss of generality, that G_K^{t} is well-defined and analytic in the complex domain $\mathcal{D}_{\alpha_0}$ for t sufficiently close to zero. Moreover, in the analytic case, we have

$$\Big| G_K^{\mathrm{t}}(z) - g_K^{\mathrm{t}}(z) \Big| \le t^{s+1} M(z, t)$$

with an everywhere positive continuous function $M : \mathcal{D}_{\alpha_0} \times [0, \delta_1] \to \mathbb{R}$ for some sufficiently small $\delta_1 > 0$.

Lemma 3.1 *There exists $\delta_2 > 0$ such that for $t \in [0, \delta_2]$, $\widetilde{G}_K^{\mathrm{t}} = \Psi^{-1} \circ G_K^{\mathrm{t}} \circ \Psi$ is well-defined and real analytic on the closed complex domain $\overline{S(\frac{r_0}{2}, \frac{\rho_0}{2})}$ and*

$$\Big| \widetilde{G}_K^{\mathrm{t}}(p, q) - g_H^{\mathrm{t}}(p, q) \Big| \le M t^{s+1}, \quad (p, q) \in \overline{S\left(\frac{r_0}{2}, \frac{\rho_0}{2}\right)}, \quad t \in [0, \delta_2], \tag{3.9}$$

where M is a positive constant depending on r_0, ρ_0, α_0, δ_1, Ψ and K, not on t.

Proof. Let $\mathcal{U}_1 = \overline{S(\frac{r_0}{2}, \frac{\rho_0}{2})}$ and $\mathcal{V}_1 = \Psi\Big(\overline{S(\frac{r_0}{2}, \frac{\rho_0}{2})}\Big)$. Since $\mathcal{U}_1$ is a closed subset of $S(r_0, \rho_0)$ and Ψ is a diffeomorphism from $S(r_0, \rho_0)$ onto $\mathcal{D}_{\alpha_0}$, $\mathcal{V}_1$ is closed in $\mathcal{D}_{\alpha_0}$. Let ξ be the distance from $\mathcal{V}_1$ to the boundary of $\mathcal{D}_{\alpha_0}$, then $\xi > 0$. The compactness of $\mathcal{V}_1$ implies that there exists $0 < \delta_1^{'} < \delta_1$ such that g_K^{t} maps $\mathcal{V}_1$ into $\mathcal{V}_1 + \frac{\xi}{2}$ for $t \in [0, \delta_1^{'}]$, where $\mathcal{V}_1 + \frac{\xi}{2}$ denotes the union of all complex open balls centered in $\mathcal{V}_1$ with radius $\frac{\xi}{2}$. Since $M(z,t)$ is continuous and positive for $(z,t) \in \mathcal{V}_1 \times [0, \delta_1^{'}]$, there exists a constant $M_0 > 0$ which is an upper bound of $M(z,t)$ on $\mathcal{V}_1 \times [0, \delta_1^{'}]$. Let $\delta_2 = \min\{1, \delta_1^{'}, \sqrt{\frac{\xi}{4M_0}}\}$, then for $t \in [0, \delta_2]$, G_K^{t} maps $\mathcal{V}_1$ into $\mathcal{D}_{\alpha_0}$ and hence $\widetilde{G}_K^{\mathrm{t}} = \Psi^{-1} \circ G_K^{\mathrm{t}} \circ \Psi$ is well-defined on $\mathcal{U}_1$. The real analyticity of the map follows from the real analyticity of Ψ and K. To verify equation (3.9), we first note that the analyticity of Ψ^{-1} on $\overline{\mathcal{V}_1 + \frac{3\xi}{4}} \subset \mathcal{D}_{\alpha_0}$ implies that there exists a constant $M_1 > 0$ such that for all $z \in \overline{\mathcal{V}_1 + \frac{3\xi}{4}}$,

$$\Big|\frac{\partial \Psi^{-1}}{\partial z}(z)\Big| \leq M_1,$$

and then use the Taylor formula, we get that for $(p,q) \in \mathcal{U}_1$ and $t \in [0, \delta_2]$, $\Psi(p,q) \in \mathcal{V}_1$ and $\Big|R_K^{\mathrm{t}}\Big(\Psi(p,q)\Big)\Big| = \Big|G_K^{\mathrm{t}}\Big(\Psi(p,q)\Big) - g_K^{\mathrm{t}}\Big(\Psi(p,q)\Big)\Big| \leq M_0 t^{s+1} \leq \frac{\xi}{4}$, and therefore,

$$\begin{aligned}\Big|\widetilde{G}_K^{\mathrm{t}}(p,q) - g_H^{\mathrm{t}}(p,q)\Big| &= \Big|\Psi^{-1}\Big(g_K^{\mathrm{t}}\Big(\Psi(p,q)\Big) + R_K^{\mathrm{t}}\Big(\Psi(p,q)\Big)\Big) \\ &\quad - \Psi^{-1}\Big(g_K^{\mathrm{t}}\Big(\Psi(p,q)\Big)\Big)\Big| \\ &\leq 2nM_1M_0t^{s+1}.\end{aligned}$$

Let $M = 2nM_1M_0$, then (3.9) is verified. □

The above lemma shows that $\widetilde{G}_K^{\mathrm{t}}$ is an approximant to the one parameter group of integrable rotations g_H^{t} up to order t^{s+1} as t approaches zero. To apply Theorem 2, we need to verify the exact symplecticity of $\widetilde{G}_K^{\mathrm{t}}$ so that it can be expressed by globally defined generating function. Because Ψ is not necessarily exact symplectic, the exact symplecticity of $\widetilde{G}_K^{\mathrm{t}} = \Psi^{-1} \circ G_K^{\mathrm{t}} \circ \Psi$ is not trivially observed.

Lemma 3.2 *Let G be an exact symplectic mapping of class C^1 from D into $\mathbb{R}^{2n}$ where D is an open subset of $\mathbb{R}^{2n}$ and let Ψ be a symplectic diffeomorphism from $B \times \boldsymbol{T}^n$ onto D. Then $\Psi^{-1} \circ G \circ \Psi$ is an exact symplectic mapping in the domain in which it is well-defined.*

Proof. Let $(\hat{p}, \hat{q}) = \Psi^{-1} \circ G \circ \Psi(p,q)$ and let γ be any given closed curve in the domain of definition of $\widetilde{G} =: \Psi^{-1} \circ G \circ \Psi$ which is an open subset of

$B \times \boldsymbol{T}^n$. The exact symplecticity of $\widetilde{G}$ will be implied by (see [2])

$$I(\gamma) = \int_\gamma \hat{p} d\hat{q} - \int_\gamma p dq = 0 \tag{3.10}$$

which we verify below. Let $(x, y) = \Psi(p, q)$ and $(\hat{x}, \hat{y}) = \Psi(\hat{p}, \hat{q})$. Then $(\hat{x}, \hat{y}) = G(x, y)$. Since G is exact symplectic, we have $\int_\gamma \hat{x} d\hat{y} - \int_\gamma x dy = 0$, where x, y, $\hat{x}$, $\hat{y}$ are considered as functions of (p, q), which vary over γ. Therefore, with these conventions and with $\gamma' = \Psi^{-1} \circ G \circ \Psi(\gamma)$,

$$\begin{aligned} I(\gamma) &= \int_\gamma \hat{p} d\hat{q} - \int_\gamma \hat{x} d\hat{y} + \int_\gamma x dy - \int_\gamma p dq \\ &= \int_{\gamma'} p dq - \int_{\Psi(\gamma')} x dy + \int_{\Psi(\gamma)} x dy - \int_\gamma p dq \\ &= \int_{\gamma' - \gamma} p dq - \int_{\Psi(\gamma') - \Psi(\gamma)} x dy. \end{aligned} \tag{3.11}$$

Note that G is exact and hence it is homotopic to the identity. This implies that $\Psi^{-1} \circ G \circ \Psi$ is homotopic to the identity too. So γ' and γ belong to the same homological class in the fundamental group of the manifold $B \times \boldsymbol{T}^n$. Therefore one may find a 2-dimensional surface, say σ, in the phase space $B \times \boldsymbol{T}^n$, which is bounded by γ' and γ. $\Psi(\sigma)$ is then a 2-dimensional surface in D bounded by $\Psi(\gamma')$ and $\Psi(\gamma)$. By stokes formular and from (3.11), we get

$$I(\gamma) = \int_\sigma dp \wedge dq - \int_{\Psi(\sigma)} dx \wedge dy$$

which is equal to zero because Ψ preserves the two form $dp \wedge dq$. Lemma 3.2 is proved. $\square$

Checking existing available symplectic algorithms, we observe that they are generally constructed by discretizing Hamiltonian systems, therefore, they generate exact symplectic step transition maps. In our case, this means that G_K^{t} is a one parameter family of exact symplectic mappings. By Lemma 3.2, so is $\widetilde{G}_K^{\mathrm{t}}$. As a result, $\widetilde{G}_K^{\mathrm{t}}$ can be re-expressed by some generating function. On the other hand, by Lemma 3.1, we see that $\widetilde{G}_K^{\mathrm{t}}$ is near the identity and approximates g_H^{t} up to order t^{s+1} on $S\left(\frac{r_0}{2}, \frac{\rho_0}{2}\right)$ for $t \in [0, \delta_2]$. A simple argument of the implicit function theorem, with the notice of the exact symplecticity of $\widetilde{G}_K^{\mathrm{t}}$, will show the following

Lemma 3.3 *There exists a function h^{t} which depends on the time step t such that it is well-defined and real analytic on the domain $S\left(\frac{r_0}{4}, \frac{\rho_0}{4}\right)$ for*

$t \in [0, \delta_3]$ *with* δ_3 *being a sufficiently small positive number so that* $\widetilde{G}_K^{\mathrm{t}} : (p, q) \to (\hat{p}, \hat{q})$ *can be expressed by* h^{t} *as follows:*

$$\hat{p} = p - t^{s+1}\frac{\partial h^{\mathrm{t}}}{\partial q}(\hat{p}, q), \quad \hat{q} = q + t\omega(\hat{p}) + t^{s+1}\frac{\partial h^{\mathrm{t}}}{\partial \hat{p}}(\hat{p}, q). \tag{3.12}$$

It follows immediately from Lemmas 3.1 and 3.3 that

$$\left\|\frac{\partial h^{\mathrm{t}}}{\partial \hat{p}}\right\|_{\frac{r_0}{4},\frac{\rho_0}{4}} \leq M, \quad \left\|\frac{\partial h^{\mathrm{t}}}{\partial q}\right\|_{\frac{r_0}{4},\frac{\rho_0}{4}} \leq M.$$

Fix $(\hat{p}_0, q_0) \in D$ and let $h^{\mathrm{t}}(\hat{p}_0, q_0) = 0$. For any $(\hat{p}, q) \in S\left(\frac{r_0}{4}, \frac{\rho_0}{4}\right)$, integrating the exact differential one form $\frac{\partial h^{\mathrm{t}}}{\partial \hat{p}} d\hat{p} + \frac{\partial h^{\mathrm{t}}}{\partial q} dq$ along one of the shortest curves from $(\hat{p}_0, q_0)$ to $(\hat{p}, q)$ in $S\left(\frac{r_0}{4}, \frac{\rho_0}{4}\right)$ and then taking the maximal norm of the integration for $(\hat{p}, q)$ over $S\left(\frac{r_0}{4}, \frac{\rho_0}{4}\right)$, we obtain the estimate

$$\|h^{\mathrm{t}}\|_{\frac{r_0}{4},\frac{\rho_0}{4}} \leq 2nML, \quad \text{for } t \in [0, \delta_3], \tag{3.13}$$

where M is the constant in Lemma 3.1 and L is an upper bound of the length of the shortest curves from $(\hat{p}_0, q_0)$ to points of $S\left(\frac{r_0}{4}, \frac{\rho_0}{4}\right)$, which is clearly a finite positive number. Note that B is a connected bounded open subset of $\mathbb{R}^n$ and therefore $S\left(\frac{r_0}{4}, \frac{\rho_0}{4}\right)$ is bounded too.

Now the analytic version of Theorem 2 can be applied to $S_t = \widetilde{G}_K^{\mathrm{t}}$ since the conditions required by Theorem 2 are satisfied clearly according to the assumptions of Theorem 1, say, the nondegeneracy of the integrable system in the sense of Kolmogorov means that the frequency map $\omega : B \to \mathbb{R}^n$ is nondegenerate and therefore, there exist positive constants $\theta \leq \Theta$ such that ω satisfies (2.5) with some positive number $r \leq r_0$. In Theorem 2, the function h is replaced by $t^s h^{\mathrm{t}}$ which satisfies the estimate (2.11) with $r' = r_0/4$ and $\rho' = \rho_0/4$ if we choose

$$\gamma = \gamma_t =: \Gamma t^d, \quad \text{with } 0 < d \leq s/2 \text{ and } \Gamma = \sqrt{\frac{2nML}{\delta_0}}\theta^{-1}\Theta^{3/2} \tag{3.14}$$

and if t is sufficiently small, where δ_0 is the bound given in (2.6) by Theorem 2. It is clear that the so chosen γ satisfies the condition $\gamma \leq \min(1, \frac{1}{2}r\Theta)$ required by Theorem 2 for t sufficiently close to zero. By Theorem 2, we then have the Cantor sets $B_t = B_{\gamma,t} \subset B$ and $\Omega_t = \Omega_{\gamma,t} \subset \omega(B)$, a surjective map $\omega_t = \omega_{\gamma,t} : B_t \to \Omega_t$ of class C^∞ and a symplectic mapping $\Phi_t : B_t \times \boldsymbol{T}^n \to \mathbb{R}^n \times \boldsymbol{T}^n$ of class $C^{\infty,\omega}$, in the sense of Whitney, such that the conclusions (1)-(4) of Theorem 2 hold with $\gamma = \Gamma t^d$. From (2.8), invariant tori of $\widetilde{G}_K^{\mathrm{t}}$ fill out a set $\mathcal{E}_t = \mathcal{E}_{\gamma,t} = \Phi_t(B_t \times \boldsymbol{T}^n)$ in phase space $\mathcal{E} = B \times \boldsymbol{T}^n$ with measure estimate

$$m\mathcal{E}_t \geq \Big(1 - c_4 \Gamma \Big(\theta \Theta^{-1}\Big)^{-n} t^d\Big) m\mathcal{E}. \tag{3.15}$$

From (2.9), with the notice of (2.3) and the fact that

$$\|h^{\mathrm{t}}\|_{\beta\lambda+\lambda+\tau} \leq c_7 \|h^{\mathrm{t}}\|_{\frac{r_0}{4},\frac{\rho_0}{4}}$$

by Cauchy's estimate for derivatives of an analytic function, we have

$$\begin{aligned} \|\Phi_t - I\|_{\beta,\beta\lambda;B_t\times \boldsymbol{T}^n} &\leq \Big(\gamma\Theta^{-1}\Big)^{-\beta} \|\sigma_{\gamma\Theta^{-1}}^{-1} \circ (\Phi_t - I)\|_{\beta,\beta\lambda;\gamma\Theta^{-1}} \\ &\leq c_5 c_7 \gamma^{-(2+\beta)} \Theta^{1+\beta} \|t^s h^{\mathrm{t}}\|_{\frac{r_0}{4},\frac{\rho_0}{4}} \\ &\leq c_8 \theta^{2+\beta} \Theta^{-(2+\beta/2)} \cdot t^{s-(2+\beta)d} \end{aligned} \tag{(3.16)}$$

for t sufficiently close to zero, where

$$c_8 = c_5 c_7 (2nML)^{-\beta/2} \delta_0^{1+\beta/2}.$$

In the last inequality of (3.16) we have used the estimate (3.13) for h^{t}. From (2.9) we also get

$$\begin{aligned} \|\omega_t - \omega\|_{\beta+1;B_t} &\leq \big(\gamma\Theta^{-1}\big)^{-(\beta+1)} \|\omega_t - \omega\|_{\beta+1;\gamma\Theta^{-1}} \\ &\leq c_8 \theta^{2+\beta} \Theta^{-(1+\beta/2)} \cdot t^{s-(2+\beta)d}. \end{aligned} \tag{3.17}$$

Let $\Psi_t = \Psi \circ \Phi_t$ and $D_t = \Psi(\mathcal{E}_t)$, then $G_K^{\mathrm{t}} \circ \Psi_t = \Psi_t \circ R_t$, which means that Ψ_t realizes the conjugation from G_K^{t} to $R_t : (p,q) \to (p, q + t\omega_t(p))$ and for any fixed $P \in B_t$, $\Psi_t(P, \boldsymbol{T}^n)$ is an invariant torus of G_K^{t}, which is an analytic Lagrangian manifold since Ψ_t is a symplectic diffeomorphism and analytic with respect to the angle variables. On the torus the iterations of G_K^{t} starting from any fixed point are quasi-periodic with frequencies $t\omega_t(p)$ which are rationally independent and satisfy the diophantine condition (2.4) with $\omega = \omega_t(p)$ and $\gamma = \Gamma t^d$. These invariant tori distribute C^∞-smoothly in the phase space due to the C^∞-smoothness of the conjugation Ψ_t. Moreover, we have the same estimates for the measure of D_t and for the closeness of Ψ_t to Ψ as (3.15) and (3.16), with larger constants c_4 and c_8, in which $\mathcal{E}_t$, $\mathcal{E}$, Φ_t and I are replaced by D_t, D, Ψ_t and Ψ respectively. For $\beta \geq 0$, if we choose d satisfying

$$0 < d < s/(2+\beta), \tag{3.18}$$

then, from the above estimates, we see that Ψ_t, with the domain of definition $B_t \times \boldsymbol{T}^n$, converges to the Ψ with respect to the $C^{\beta,\beta\lambda}$-norm and ω_t, with the domain of definition B_t, converges to ω with respect to the $C^{\beta+1}$-norm as t tends to zero; the measure of D_t, the union of invariant tori of G_K^{t}, tends to the measure of the phase space D. These arguments just complete the proof of the first part of Theorem 1.

Now we prove the remainder of Theorem 1. From the estimates (3.15)-(3.17) and the uniform boundedness of the diffeomorphism Ψ and its inverse as well as their derivatives, we see that if we choose γ being fixed in advance and not depending on the time-step size t of the difference scheme, then we have

$$mD_{\gamma,t} \geq \Big(1 - \widetilde{c}_4\Big(\theta\Theta^{-1}\Big)^{-n}\gamma\Big)mD \tag{3.19}$$

with constant $\widetilde{c}_4 > 0$ not depending on γ and t, where $D_{\gamma,t} = \Psi(\mathcal{E}_{\gamma,t})$ with $\mathcal{E}_{\gamma,t} = \Phi_t(B_{\gamma,t} \times \boldsymbol{T}^n)$ and with $B_{\gamma,t}$ being the subset of B as indicated above. Note that $B_{\gamma,t}$ is a closed subset of B_t and $D_{\gamma,t}$ a closed subset of D_t if t is sufficiently small. Moreover, the estimate

$$\|\Psi_t - \Psi\|_{\beta,\beta\lambda;B_{\gamma,t}\times\boldsymbol{T}^n} \leq \widetilde{c}_8\gamma^{-(2+\beta)}\Theta^{1+\beta} \cdot t^s \tag{3.20}$$

and

$$\|\omega_t - \omega\|_{\beta+1;B_{\gamma,t}} \leq \widetilde{c}_8\gamma^{-(2+\beta)}\Theta^{2+\beta} \cdot t^s \tag{3.21}$$

hold for any $\beta \geq 0$ with $\widetilde{c}_8 > 0$ not depending on γ and t. The conclusions 1) and 2) of the last part of Theorem 1 are proved if we set $c_1' = \widetilde{c}_4\Big(\theta\Theta^{-1}\Big)^{-n}$ and $c_2' = \widetilde{c}_8 \cdot \max(\Theta^{1+\beta}, \Theta^{2+\beta})$. From (3.19) it follows that for sufficiently small $\gamma > 0$, $D_{\gamma,t}$ has a positive Lebesque measure. From (2.10) it follows that for any $\omega^* \in \Omega_{\gamma,t}$, there exist $p^* \in B$ and $P^* \in B_{\gamma,t}$ such that $\omega(p^*) = \omega_t(P^*) = \omega^*$ and

$$|P^* - p^*| \leq 2nMLc_6c_7\Big(\gamma\theta\Theta^{-1}\Big)^{-1} \cdot t^s,$$

which implies that

$$|\Psi(P^*, q) - \Psi(p^*, q)| \leq 4n^2ML\widetilde{M}_1c_6c_7\Big(\gamma\theta\Theta^{-1}\Big)^{-1} \cdot t^s,$$

uniformly for $q \in \boldsymbol{T}^n$, where $\widetilde{M}_1$ is an upper bound of the norm of $\dfrac{\partial\Psi}{\partial z}(p,q)$ for $(p,q) \in \overline{S\Big(\dfrac{r_0}{2}, \dfrac{\rho_0}{2}\Big)}$. This estimate, together with (3.20), proves the third conclusion of the second part of Theorem 1. Theorem 1 is completely proved.

3.2. Proof of Corollary 1

By Theorem 1, we have

$$G_K^{\mathrm{t}} \circ \Psi_t(p,q) = \Psi_t \circ R_t(p,q), \quad \text{for } (p,q) \in B_t \times \boldsymbol{T}^n, \tag{3.22}$$

where R_t is the integrable rotation $(p,q) \to (p, q + t\omega_t(p))$ which admits n invariant functions, say, $p_1, \cdots, p_n$, analytically defined on $B_t \times \boldsymbol{T}^n$. Let

$$F_i^{\mathrm{t}} = p_i \circ \Psi_t^{-1}, \quad i = 1, \cdots, n,$$

then they are well-defined on the Cantor set D_t and of class C^∞ in the sense of Whitney due to the C^∞-smoothness of Ψ_t^{-1} on D_t. Moreover, we easily verify, by (3.22), that

$$F_i^{\mathrm{t}} \circ G_K^{\mathrm{t}} = F_i^{\mathrm{t}}, \quad i = 1, \cdots, n,$$

which means that F_i^{t}, $i = 1, \cdots, n$ are n invariant functions of G_K^{t}. These n invariant functions are functionally independent because p_i, $i = 1, \cdots, n$ are functionally independent and Ψ_t is a diffeomorphism. The claim that F_i^{t} and F_j^{t} are in involution for $1 \le i,\ j \le n$ simply follows from the fact that p_i and p_j are in involution and Ψ_t is symplectic. Note that the Poisson bracket is invariant under symplectic coordinate transformations. Finally, it is observed from the arguments of Sect. 3.1 that for each of $j = 1, \cdots, n$, F_j^{t} approximates

$$F_j = p_j \circ \Psi^{-1}$$

as $t \to 0$, with the order of accuracy equal to $t^{s-(2+\beta)d}$ ($0 < d < s/(2+\beta)$ is given) on the set D_t (note that this set depends also on d by definition) and equal to t^s on $D_{\gamma,t}$, a subset of D_t, in the norm of the class C^β for any given $\beta \ge 0$. It is clear that the functions F_j, $j = 1, \cdots, n$ are integrals of the integrable system and that any two of them are in involution by the symplecticity of Ψ^{-1}. Corollary 1 is then proved.

4. A remark on the application to nearly integrable systems

We can prove a result similar to Theorem 1 but of less interest, by using the same argument as before, if we apply symplectic algorithms to nearly integrable Hamiltonian systems. In this case the considered Hamiltonian K may be written in the form

$$K = K_\varepsilon(x,y) = K_0(x,y) + \varepsilon K_1(x,y,\varepsilon), \quad (x,y) \in D \tag{4.1}$$

with K_0 representing the Hamiltonian of the integrable system and ε a real parameter which is required to be sufficiently close to zero so that the system with Hamiltonian K_ε has invariant tori by KAM theory. We assume, for the convenient use of Theorem 2, that K_0 and K_1 are analytic with respect to all variables with the domain of analyticity containing, say, $\mathcal{D}_{\alpha_0}$, as in the integrable case, for $|\varepsilon| < \Delta_0$ with some $\Delta_0 > 0$. Let $\Psi : B \times \boldsymbol{T}^n \to D$ be the symplectic coordinate transformation from action-angle variables (p, q) to the Euclidean variables (x, y) such that (3.4) holds for $K = K_0$ and $H = H_0$. Assume

$$H_1(p, q, \varepsilon) = K_1(\Psi(p, q), \varepsilon) \quad \text{and} \quad H_\varepsilon(p, q) = H_0(p) + \varepsilon H_1(p, q, \varepsilon),$$

then

$$H_\varepsilon(p, q) = K_\varepsilon(\Psi(p, q), \varepsilon)$$

and (3.8) holds for $K = K_\varepsilon$ and $H = H_\varepsilon$. We also assume Ψ is a diffeomorphism from $S(r_0, \rho_0)$, a complex extension of the real domain $B \times \boldsymbol{T}^n$, onto $\widetilde{\mathcal{D}}(r_0, \rho_0) = \Psi(S(r_0, \rho_0))$, a subset of $\mathcal{D}_{\alpha_0}$, and that the above relations hold on this complex domain. By a similar argument to that of Sect. 3.1, we can show that Lemma 3.1 is also true for $K = K_\varepsilon$ and $H = H_\varepsilon$ for $|\varepsilon| \leq \Delta_1$ with some $\Delta_1 > 0$, there δ_2 and M also depend on Δ_1. On the other hand, by a standard argument of the theory of ordinary differential equations, we see that, for $|\varepsilon| \leq \Delta_1$,

(4.2)
$$\left|g^{\mathrm{t}}_{H_\varepsilon}(p, q) - g^{\mathrm{t}}_{H_0}(p, q)\right| \leq M_2|\varepsilon t|, \quad (p, q) \in \overline{S\left(\frac{r_0}{2}, \frac{\rho_0}{2}\right)}, \quad t \in [0, \delta_4]$$

with $M_2 > 0$ and $\delta_4 > 0$, depending on r_0, ρ_0, H_0, H_1 and Δ_1, not on t and ε. Therefore, we have, with $\widetilde{G}^{\mathrm{t}}_{K_\varepsilon} = \Psi^{-1} \circ G^{\mathrm{t}}_{K_\varepsilon} \circ \Psi$, that for $|\varepsilon| \leq \Delta_1$,

$$\left|\widetilde{G}^{\mathrm{t}}_{K_\varepsilon}(p, q) - g^{\mathrm{t}}_{H_0}(p, q)\right| \leq M_3(t^{s+1} + |t\varepsilon|),$$

((4.3))
$$(p, q) \in \overline{S\left(\frac{r_0}{2}, \frac{\rho_0}{2}\right)}, \quad t \in [0, \delta_5],$$

where $M_3 = \max(M, M_2)$ and $\delta_5 = \min(\delta_2, \delta_4)$. Since, by Lemma 3.2, $\widetilde{G}^{\mathrm{t}}_{K_\varepsilon}$ is exact symplectic, there is a globally defined (ε, t)-dependent generating function for it, say $H_0(\hat{p}) + h^{\varepsilon,t}(\hat{p}, q)$, which is well-defined and real analytic on the domain $S\left(\frac{r_0}{4}, \frac{\rho_0}{4}\right)$ for $|\varepsilon| \leq \Delta_1$ and for $t \in [0, \delta_6]$ with a smaller positive number δ_6 which depends also on Δ_1, so that $\widetilde{G}^{\mathrm{t}}_{K_\varepsilon} : (p, q) \to (\hat{p}, \hat{q})$ can be expressed as follows

(4.4)
$$\hat{p} = p - \frac{\partial h^{\varepsilon,t}}{\partial q}(\hat{p}, q), \quad \hat{q} = q + t\omega(\hat{p}) + \frac{\partial h^{\varepsilon,t}}{\partial \hat{p}}(\hat{p}, q).$$

Moreover, by a similar argument to that below Lemma 3.3, the function $h^{\varepsilon,t}(\hat{p}, q)$ may be chosen to obey the estimate

(4.5)
$$\|h^{\varepsilon,t}\|_{\frac{r_0}{4}, \frac{\rho_0}{4}} \leq 2nM_3L(t^{s+1} + |\varepsilon t|), \quad t \in [0, \delta_6], \quad |\varepsilon| \leq \Delta_1.$$

We can prove a result, which can be stated in a parallel form to Theorem 1 but here we omit, by applying Theorem 2 and choosing

$$\gamma = \gamma_{\varepsilon,t} =: \Gamma_3(|\varepsilon| + t^s)^d,$$
$$\text{with } 0 < d \leq 1/2 \text{ and } \Gamma_3 = \sqrt{\frac{2nM_3L}{\delta_0}}\theta^{-1}\Theta^{3/2}, \tag{(4.6)}$$

where θ and Θ are nondegeneracy parameters of the frequency map ω of the integrable part. The detailed argument is parallel to the proof of Theorem 1 with the only notice that corresponding to the estimates for mD_t, $\Psi_t - \Psi$ and $\omega_t - \omega$ there, here we have

$$mD_{\varepsilon,t} \geq \left(1 - c'\Gamma_3\left(\theta\Theta^{-1}\right)^{-n}(|\varepsilon| + t^s)^d\right)mD,$$
$$\|\Psi_{\varepsilon,t} - \Psi\|_{\beta,\beta\lambda;B_{\varepsilon,t}\times \boldsymbol{T}^n} \leq c_8'\theta^{2+\beta}\Theta^{-(2+\beta/2)} \cdot (|\varepsilon| + t^s)^{1-(2+\beta)d},$$
$$\|\omega_{\varepsilon,t} - \omega\|_{\beta+1;B_{\varepsilon,t}} \leq c_8'\theta^{2+\beta}\Theta^{-(1+\beta/2)} \cdot (|\varepsilon| + t^s)^{1-(2+\beta)d}.$$

$D_{\varepsilon,t}, \Psi_{\varepsilon,t}$, etc. are used to replace D_t, Ψ_t, etc. because everything in the nearly integrable case depends also on the perturbation parameter ε. Therefore the convergence of $\Psi_{\varepsilon,t}$ to Ψ in the class $C^{\beta,\beta\lambda}$ as well as $\omega_{\varepsilon,t}$ to ω in the class $C^{\beta+1}$ is guaranteed for any given $\beta \geq 0$ if $0 < d < 1/(2+\beta)$. We have also a more quantitative result similar to that of Sect. 3.1 if we fix in advance the diophantine parameter γ sufficiently small and not depending on ε and t only but in all the estimates of Sect. 3.1, t^s is replaced by $|\varepsilon| + t^s$.

We note, however, that such a result is of less interest. As the referees pointed out, the interesting situation is when ε is constant (and sufficiently small) and when t tends to zero, and accordingly, the proper assertions should be that

$$mD_{\varepsilon,t} \to mD_\varepsilon,\ \Psi_{\varepsilon,t} \to \Psi_\varepsilon,\ \omega_{\varepsilon,t} \to \omega_\varepsilon,\ B_{\varepsilon,t} \to B_\varepsilon$$

as $t \to 0$, with the corresponding quantitative estimates, here D_ε is the Cantor set filled out by the invariant tori of the nearly integrable system, $B_\varepsilon \times \boldsymbol{T}^n$ is the action-angle representation of D_ε, Ψ_ε is the coordinate transformation from $B_\varepsilon \times \boldsymbol{T}^n$ onto D_ε, and ω_ε is the corresponding frequency map, well-defined on the Cantor set B_ε, of the nearly integrable system when the system is restricted to D_ε. I believe that such a more relevant result is true but its proof requires an improved version of Theorem 2. We do not discuss this problem in this paper.

J.C. Yoccoz (1995) remarked that the goal of the theory of dynamical systems is to understand *most* of the dynamics of *most* systems. Correspondingly, one may say that the goal of the theory of numerical algorithms should be to design “proper” algorithms to preserve *most* of the dynamics of *most* systems. On the other hand, according to Poincaré ([2], Appendix 8), the problem of studying quasi-periodic motions of nearly integrable Hamiltonian systems is the fundamental problem of dynamics. In this sense, the results of this paper suggest, at least partially, that symplectic algorithms are proper for Hamiltonian systems.

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