

# On the Hamiltonian Interpolation of Near-to-the-Identity Symplectic Mappings with Application to Symplectic Integration Algorithms

Giancarlo Benettin<sup>1</sup> and Antonio Giorgilli<sup>2</sup>

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We reconsider the problem of the Hamiltonian interpolation of symplectic mappings. Following Moser's scheme, we prove that for any mapping  $\Psi_\epsilon$ , analytic and  $\epsilon$ -close to the identity, there exists an analytic autonomous Hamiltonian system,  $H_\epsilon$  such that its time-one mapping  $\Phi_{H_\epsilon}$  differs from  $\Psi_\epsilon$  by a quantity exponentially small in  $1/\epsilon$ . This result is applied, in particular, to the problem of numerical integration of Hamiltonian systems by symplectic algorithms; it turns out that, when using an analytic symplectic algorithm of order  $s$  to integrate a Hamiltonian system  $K$ , one actually follows "exactly," namely within the computer roundoff error, the trajectories of the interpolating Hamiltonian  $H_\epsilon$ , or equivalently of the rescaled Hamiltonian  $K_\epsilon = \epsilon^{-1}H_\epsilon$ , which differs from  $K$ , but turns out to be  $\epsilon^s$  close to it. Special attention is devoted to numerical integration for scattering problems.

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**KEY WORDS:** Hamiltonian systems; symplectic mappings; symplectic integration algorithms; perturbation theory.

## 1. INTRODUCTION

Let us consider a smooth symplectic mapping  $\Psi: \mathcal{D} \rightarrow \mathcal{D}$ , where  $\mathcal{D}$  is a domain in  $\mathbb{R}^{2n}$  (or a symplectic manifold of dimension  $2n$ ), endowed with canonical coordinates  $(p, q) = (p^1, \dots, p^n, q^1, \dots, q^n)$ . A classical problem is the search for an (autonomous) interpolating Hamiltonian, namely a Hamiltonian  $H$  such that its flow  $\Phi_H^t$  at time  $t = 1$ , or time-one mapping,

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<sup>1</sup> Università di Padova, Dipartimento di Matematica Pura e Applicata, GNFM (CNR) and INFN, 35131 Padova, Italy. Benettin @ padova. infn. it.

<sup>2</sup> Università di Milano, Dipartimento di Matematica and GNFM (CNR), 20133 Milano, Italy.

coincides with  $\Psi$ . Let us notice that, if  $H$  exists, then the mapping  $\Psi$  admits an integral of motion, namely  $H$  itself, and this is not trivial.

A special case is that of mappings which are near the identity, more precisely mappings  $\Psi_\varepsilon$  smoothly depending on a (small) parameter  $\varepsilon$ , such that  $\Psi_0(p, q) = (p, q)$ . For such mappings a formal solution was provided by Moser,<sup>(1)</sup> who proved that<sup>3</sup> one can construct a formal, i.e., possibly nonconverging, series  $H_\varepsilon = \varepsilon h_1 + \varepsilon^2 h_2 + \dots$ , such that its (formal) time-one flow agrees, order by order, with  $\Psi_\varepsilon$ . Moser's construction follows a "direct" method: namely, without any change of variables, one directly constructs each term of the Hamiltonian (more precisely, of its vector field). Formal results related to Moser's can be found in ref. 2 and 3.

Later, Neishtadt<sup>(4)</sup> provided for this problem an exponential estimate, namely (in the analytic case) he proved that there exists a Hamiltonian  $H_\varepsilon$ , small with  $\varepsilon$ , such that, denoting by  $\Phi_{H_\varepsilon} = \Phi_{H_\varepsilon}^1$  its time-one flow, one has

$$\|\Phi_{H_\varepsilon} - \Psi_\varepsilon\| \leq C\varepsilon e^{-\varepsilon^*/\varepsilon} \quad (1.1)$$

with  $C, \varepsilon^* > 0$ . Neishtadt's construction is instead "indirect": indeed, there one preliminarily introduces a nonautonomous Hamiltonian  $\tilde{H}_\varepsilon(p, q, t)$ , which interpolates  $\psi_\varepsilon$  exactly (such Hamiltonian is known to exist; see, for example, ref. 5) and then, by a suitable canonical transformation, one eliminates from  $\tilde{H}_\varepsilon$  the variable  $t$ , which for small  $\varepsilon$  turns out to be a "fast variable"; practically, the exponential estimate (1.1) comes out as a byproduct of a more general estimate on adiabatic invariants.

The purpose of the present paper is twofold. On one hand, we reconsider the interpolation problem, and show that Moser's scheme leads in a very simple and direct way to the exponential estimate (1.1); in particular (at variance with the indirect method) one easily gets in this way quite reasonable (although not optimal) expressions for the constants entering the estimate. On the other hand, we aim to stress some consequences of the exponential estimate (1.1), in particular in connection with the use of symplectic mappings for the numerical integration of Hamiltonian systems.

Let us quickly examine some elementary consequences of the estimate (1.1); more precise statements will be found in Section 2.

(i) The mapping  $\Psi_\varepsilon$  admits an almost-integral of motion, up to an exponentially large number of iterations. Precisely, with a suitable constant  $C' > 0$  one deduces

$$|H_\varepsilon(\Psi_\varepsilon^k(p, q)) - H_\varepsilon(p, q)| \leq kC'\varepsilon e^{-\varepsilon^*/\varepsilon} \quad (1.2)$$

<sup>3</sup> Properly speaking, in ref. 1 one does not refer to a small parameter  $\varepsilon$ ; equivalently, series expansions in  $(p, q)$  are introduced.

so that, in particular, for any  $s \geq 1$  one obtains estimates of the form

$$|H_\varepsilon(\Psi_\varepsilon^k(p, q)) - H_\varepsilon(p, q)| \leq C'\varepsilon^s \quad \text{for } k \leq \varepsilon^{s-1}e^{+\varepsilon^*/\varepsilon} \quad (1.3)$$

(ii) The distance

$$d_k = \|\Psi_\varepsilon^k - \Phi_{H_\varepsilon}^k\|$$

between the  $k$ th iterate of  $\Psi_\varepsilon$  and the flow of  $\Phi_{H_\varepsilon}$  at time  $k$  grows slowly with  $k$ , even if the mapping admits exponential divergence of nearby trajectories: precisely, with suitable constant  $\mu > 0$  [in fact, the Lipschitz constant of  $\psi_\varepsilon(p, q) = \varepsilon^{-1}(\Psi_\varepsilon(p, q) - (p, q))$ ], one gets

$$d_k < C \frac{e^{k\mu\varepsilon} - 1}{\mu} e^{-\varepsilon^*/\varepsilon} \quad (1.4)$$

so that for  $k = \mathcal{O}(\varepsilon^{-1})$ , corresponding to  $|\Psi_\varepsilon^k(p, q) - (p, q)| = \mathcal{O}(1)$ , one gets  $d_k = \mathcal{O}(e^{-\varepsilon^*/\varepsilon})$ , and only for much larger  $k = \mathcal{O}(\varepsilon^{-2})$  does divergence possibly occur.

Let us stress here the relevance of these properties for the problem of the integration of Hamiltonian systems by means of symplectic algorithms (a comment on the general case is deferred to the end of the conclusions). This problem has attracted attention in the recent literature (see, for example, refs. 6–8); in fact, it is a common experience among people working numerically in dynamical systems or in molecular dynamics that even very simple symplectic algorithms, like the so-called leap-frog algorithm (also called central differences method; Verlet algorithm, in the literature on molecular dynamics), often behave better than other more sophisticated or higher-order nonsymplectic schemes (see, for example, ref. 9 for a comparison).

Suppose one is given a Hamiltonian system  $K$ . Integrating numerically its equations of motion means precisely replacing its time- $\varepsilon$  mapping  $\Phi_K^\varepsilon$  by a mapping  $\Psi_\varepsilon$  close in some sense to  $\Phi_K^\varepsilon$ : for example, such that

$$\|\Phi_K^\varepsilon - \Psi_\varepsilon\| = \mathcal{O}(\varepsilon^{s+1}), \quad s \geq 1 \quad (1.5)$$

( $s$  is called the order of the algorithm). Now, assume the algorithm  $\Psi_\varepsilon$  is symplectic; let  $H_\varepsilon$  be its interpolating Hamiltonian, and denote  $K_\varepsilon = \varepsilon^{-1}H_\varepsilon$ . For any  $t$  one has clearly  $\Phi_{H_\varepsilon}^t = \Phi_{K_\varepsilon}^t$ ;  $K_\varepsilon$  is thus a time- $\varepsilon$  interpolating Hamiltonian, and the estimate (1.1) can be rewritten in the form

$$\|\Phi_{K_\varepsilon}^\varepsilon - \Psi_\varepsilon\| \leq C\varepsilon e^{-\varepsilon^*/\varepsilon} \quad (1.6)$$

By comparison of (1.5) and (1.6), one then deduces that  $K_\varepsilon$  is close to the original Hamiltonian  $K$ . In fact, with suitable  $C'' > 0$ , one finds

$$\|K_\varepsilon - K\| \leq C'' \varepsilon^s \quad (1.7)$$

(see Section 4 for details). On the other hand, as remarked above, the algorithm  $\mathcal{P}_\varepsilon$  follows the orbits of the interpolating Hamiltonian  $K_\varepsilon$  up to  $k = \mathcal{O}(\varepsilon^{-1})$  with exponentially small error: in particular, with very reasonable values of  $\varepsilon$ , the error at  $t = 1$  can be easily made (much) smaller than the computer roundoff error. It is then clear, in our opinion, what one really does when integrating numerically the equations of motion of a Hamiltonian system by means of a symplectic algorithm: indeed, one simply replaces the "true" Hamiltonian  $K$  by a different autonomous Hamiltonian  $K_\varepsilon$ ,  $\varepsilon^s$ -close to it, and then computes "exactly" (namely, within the roundoff error) the time-one mapping of  $K_\varepsilon$ .

This is a fact. Whether it implies something for the accuracy of the numerical integration is a delicate point. In our opinion, the question crucially depends on the structural stability of the problem at hand: namely, if a small change of the Hamiltonian is expected to influence deeply the results, then replacing  $K$  by  $K_\varepsilon$  makes indeed a big difference: in this case, however, we sincerely doubt that a numerical computation with any integration method can be of any interest. On the contrary, if small changes in the Hamiltonian are expected to be not really relevant, at least for the quantities one is looking at, then according to the above analysis, the numerical computation should be considered as essentially reliable. Some further comments on this point, including an example, are deferred to the final section.

In particular, one easily explains in this way why symplectic algorithms give rise to a good energy conservation, with essentially no accumulation of errors in time: indeed, according to (1.3) and (1.7), one gets [using the short notation  $K(t) \equiv K(p(t), q(t))$ , and so on]

$$|K(t) - K(0)| \leq |K(t) - K_\varepsilon(t)| + |K_\varepsilon(t) - K_\varepsilon(0)| + |K_\varepsilon(0) - K(0)| \leq C''' \varepsilon^s \quad (1.8)$$

with suitable  $C''' > 0$ , almost uniformly in  $t$ , namely up to times exponentially long in  $\varepsilon^{-1}$ .

In fact, we became interested in trying to understand this problem for the purpose of understanding in a rigorous framework the apparently "too accurate" numerical results reported in ref. 10. That paper studied numerically the scattering of a plane rotator from a fixed obstacle, in order to measure the energy exchange between the translational and the rotational degrees of freedom produced by the collision; the accuracy of the results

found there, in particular for the overall energy conservation, is apparently “too high” (as a matter of fact, the relative error in energy conservation, at the end of each scattering process, is *almost as small as the computer roundoff error*), and apparently not compatible with the precision of the algorithm used in the numerical computation: thus, an explanation is needed. As already remarked in ref. 10, the existence of a Hamiltonian which almost exactly interpolates the integration algorithm does provide the required explanation. This particular problem will be studied in detail in Section 4, by suitably adapting the general results to the case of scattering.

The paper is organized as follows: Section 2 is devoted to general results, which are then proved in Section 3; Section 4 is devoted to numerical integration algorithms, with special attention to the scattering case; a short conclusion follows in Section 5.

## 2. RESULTS

As in ref. 1, we find it more convenient to study the general case of a mapping  $\Psi_\varepsilon: \mathbb{R}^m \rightarrow \mathbb{R}^m$ , and treat the symplectic case as a particular one. We shall consider mappings  $\Psi_\varepsilon$  which are near the identity, and can be written as power series in  $\varepsilon$ , namely

$$\Psi_\varepsilon(x) = x + \varepsilon\psi_1(x) + \varepsilon^2\psi_2(x) + \dots \tag{2.1}$$

Each  $\psi_k$ ,  $k \geq 1$ , will be assumed to be real analytic in a suitable complex neighborhood  $\mathcal{D}_\rho$  of a real set  $\mathcal{D} \subset \mathbb{R}^m$ , defined as follows: given an “extension vector”  $\rho = (\rho^1, \dots, \rho^m)$  with positive entries, one denotes

$$\begin{aligned} \mathcal{D}_\rho &= \bigcup_{x \in \mathcal{D}} \Delta_\rho \\ \Delta_\rho &= \{y \in \mathbb{C}^m; |y^i - x^i| \leq \rho^i, 1 \leq i \leq m\} \end{aligned} \tag{2.2}$$

Let us now introduce convenient norms. For a function  $w$  real analytic in  $\mathcal{D}_{\rho'}$ , with  $\rho' \leq \rho$  (the inequality is intended to work separately in all components), one denotes

$$\|w\|_{\rho'} = \sup_{x \in \mathcal{D}_{\rho'}} |w(x)| \tag{2.3}$$

while for any vector-valued function  $W = (W^1, \dots, W^m)$ , with  $W^1, \dots, W^m$  real analytic in  $\mathcal{D}_{\rho'}$ , we denote

$$\|W\|_{\rho'} = \max_{1 \leq i \leq m} \frac{\|W^i\|_{\rho'}}{\rho^i} \tag{2.4}$$

Given any vector field  $f = (f^1, \dots, f^m)$ , we denote by  $L_f$  the differential operator acting on scalar functions according to the usual rule

$$L_f w = \sum_{i=1}^m f^i \frac{\partial w}{\partial x^i} \tag{2.5}$$

For vector-valued functions, it will be convenient to denote (at variance with a more common use of the same notation)

$$L_f W = (L_f W^1, \dots, L_f W^m) \tag{2.6}$$

The flow associated with the differential equation  $\dot{x} = f(x)$  will be denoted by  $\Phi_f$ ; if  $f$  is Hamiltonian, with Hamiltonian  $h$ , the equivalent notation  $\Phi_h$  is used. For the time-one map, we shall simply denote  $\Phi_f$  or  $\Phi_h$ . Denoting by  $\xi = (\xi^1, \dots, \xi^m)$  the identity function in  $\mathbb{R}^n$ , namely

$$\xi(x) = x, \quad \xi^i(x) = x^i$$

one has clearly  $\Phi_f = e^{L_f \xi}$ . Finally, in the proposition below we shall also deal with a formal series of vector fields

$$F_\varepsilon^x = \varepsilon f_1 + \varepsilon^2 f_2 + \dots, \quad f_k: \mathcal{D}_\rho \rightarrow \mathbb{C}^m$$

It is worthwhile to notice that its exponential  $\exp L_{F_\varepsilon^x}$  is formally well defined, since at each finite order in  $\varepsilon$  one gets only a finite number of contributions.

We can now state our basic proposition.

**Proposition 1.** Consider the mapping

$$\Psi_\varepsilon(x) = x + \sum_{k=1}^{\infty} \varepsilon^k \psi_k(x), \quad \varepsilon \geq 0 \tag{2.7}$$

Assume the functions  $\psi_k$ ,  $k \geq 1$ , are real analytic in  $\mathcal{D}_\rho$ , and satisfy there the estimates

$$\|\psi_k\|_\rho \leq \gamma^{k-1} \Gamma \tag{2.8}$$

for some positive constants  $\gamma$ ,  $\Gamma$ .

Then there exists a formal series of vector fields

$$F_\varepsilon^x = \varepsilon f_1 + \varepsilon^2 f_2 + \dots \tag{2.9}$$

analytic in  $\mathcal{D}_\rho$ , such that

(i) One has formally

$$(\exp L_{F_\varepsilon^x}) \xi = \Psi_\varepsilon \tag{2.10}$$

(ii) The vector fields  $f_k$ ,  $k \geq 1$ , satisfy the estimates

$$\begin{aligned} \|f_1\|_\rho &\leq \Gamma \\ \|f_k\|_{\rho/2} &< \frac{1}{2}k^{k-1}\beta^{k-1}\Gamma, \quad k \geq 2 \end{aligned} \tag{2.11}$$

with

$$\beta = 4 \max(\gamma, \Gamma) \tag{2.12}$$

moreover, as long as  $1 \leq r \leq (2\beta\epsilon)^{-1}$ , the finite sum

$$F_\epsilon^r = \epsilon f_1 + \dots + \epsilon^r f_r \tag{2.13}$$

satisfies the estimates

$$\|F_\epsilon^r\|_{\rho/2} \leq \frac{3}{2}\epsilon\Gamma \tag{2.14a}$$

$$\|\Phi_{F_\epsilon^r} - \Psi_\epsilon\|_{\rho/4} < 3\epsilon\Gamma(2r\beta\epsilon)^r \tag{2.14b}$$

(iii) If  $\Psi_\epsilon$  is symplectic, then all vector fields  $f_1, f_2, \dots$ , are locally Hamiltonian.

*Remark.* In the symplectic case, the global existence of a Hamilton function  $H_\epsilon^r$ , corresponding to the vector field  $F_\epsilon^r$ , requires additional assumptions (unless the domain is simply connected). For instance, a (globally defined) symplectic mapping, such that its interpolating vector field is only locally Hamiltonian, is  $\Psi_\epsilon: (I, \varphi) \mapsto (I + \epsilon, \varphi)$ , for  $I \in \mathbb{R}$ ,  $\varphi \in S^1$ : indeed, one has  $F_\epsilon^r(I, \varphi) = (\epsilon, 0)$ , constant and independent of  $r$ , and correspondingly  $H(I, \varphi) = -\epsilon\varphi$ , which, however, is not globally defined on  $\mathbb{R} \times S^1$ . On the other hand, as we shall see, it is quite crucial in the applications to know whether or not the interpolation is global. This is a delicate question whose general discussion goes beyond the purpose of this paper. However, we remark that the global existence of the interpolating Hamiltonian is guaranteed at least for a relevant class of symplectic mappings, including the more common integration schemes. Indeed, one can prove that, if a mapping  $\Psi_\epsilon$  admits a mixed-variables generating function of the form  $S_\epsilon(p', q) = p' \cdot q + \tilde{S}_\epsilon(p', q)$ , where  $\tilde{S}_\epsilon$  is globally defined, then all of our vector fields  $f_k$  turn out to be globally Hamiltonian. An indirect proof of such a claim makes use of two previous results. On one hand, it is well known that the mapping  $\Psi_\epsilon$  can be represented by the time- $\epsilon$  flow of a time-dependent Hamiltonian  $\tilde{H}_\epsilon$ ; explicit formulas relating  $\tilde{S}_\epsilon$  to  $\tilde{H}_\epsilon$  are produced in ref. 2. On the other hand, according to ref. 3, the flow of  $\tilde{H}_\epsilon$  can be formally approximated at any order in  $\epsilon$  by the flow of a time-independent Hamiltonian  $H_\epsilon$ ; explicit formulas relating  $\tilde{H}_\epsilon$  to  $H_\epsilon$  are given in ref. 3. In the following, we shall refer to this case as the global symplectic case.

Deferring to the next section the proof of Proposition 1, we state and prove here two simple corollaries, corresponding to the results announced in the Introduction.

**Corollary 1.** Under the above assumptions, there exists an autonomous interpolating vector field  $F_\varepsilon$  such that

$$\|\Phi_{F_\varepsilon} - \Psi_\varepsilon\|_{\rho/4} \leq 3\varepsilon\Gamma e^{-[\varepsilon^*/\varepsilon]}, \quad \varepsilon^* = \frac{1}{2e\beta} \tag{2.15}$$

for any  $\varepsilon \leq \varepsilon^*$ , where  $[\cdot]$  denotes the integer part; in the (global) symplectic case,  $F_\varepsilon$  is (globally) Hamiltonian.

*Proof.* One simply makes use of (2.14b), taking  $r$  to be a function of  $\varepsilon$ , in such a way to get the best result, i.e., the minimum of  $(2r\beta\varepsilon)^r$ . The best value of  $r$  turns out to be  $r = [\varepsilon^*/\varepsilon]$ . QED

The next corollary concerns the relation between the iterates  $\Psi_\varepsilon^k$  of  $\Psi_\varepsilon$  and the flow  $\Phi_{F_\varepsilon}^j$  of the above best interpolating vector field  $F_\varepsilon$ . We here need that  $\Psi_\varepsilon^k(x)$  is well defined; to this purpose, we restrict ourselves to the set  $\mathcal{D}^{(k)} \subset \mathcal{D}$ , such that  $\Psi_\varepsilon^j(x) \in \mathcal{D}$  for  $0 \leq j \leq k-1$ , and denote

$$d_j = \sup_{x \in \mathcal{D}^{(k)}} \max_{1 \leq i \leq m} \frac{|[\Phi_{F_\varepsilon}^j(x) - \Psi_\varepsilon^j(x)]^i|}{\rho^i} \tag{2.16}$$

(the mapping  $\Phi_{F_\varepsilon}^j$  will also turn out to be well defined in  $\mathcal{D}^{(k)}$ , for  $0 \leq j \leq k$ ). The latter statement in the corollary concerns the accuracy of energy conservation by  $\Psi_\varepsilon^k$  in the symplectic case. Let, with notation adapted to this case,  $\rho = (\sigma_1, \dots, \sigma_n, \tau_1, \dots, \tau_n)$ ; with no possibility of confusion, we also denote by  $\rho$  the positive number defined by

$$\rho^2 = \max_{1 \leq i \leq n} \sigma_i \tau_i \tag{2.17}$$

**Corollary 2.** Let  $\mu$  denote the supremum for  $\varepsilon \leq \varepsilon^*$  of the Lipschitz constant of the (order-one) mapping  $\varepsilon^{-1}(\Psi_\varepsilon - \xi)$ . If  $k \leq (\mu\varepsilon)^{-1}$ , then one has

$$d_k \leq 3\Gamma \frac{(1 + \mu\varepsilon)^k - 1}{\mu} e^{-[\varepsilon^*/\varepsilon]} < 6 \frac{\Gamma}{\mu} e^{-[\varepsilon^*/\varepsilon]} \tag{2.18}$$

Moreover, in the global symplectic case, denoting by  $H_\varepsilon$  the Hamiltonian corresponding to the best interpolating vector field  $F_\varepsilon$ , for  $x \in \mathcal{D}^{(k)}$  one has

$$|H_\varepsilon(\Psi_\varepsilon^k(x)) - H_\varepsilon(x)| \leq 3nk\rho^2\Gamma\varepsilon e^{-[\varepsilon^*/\varepsilon]} \tag{2.19}$$



*Remark.* This corollary is meaningful as long as there are initial data which do not escape  $\mathcal{D}$  for a large number of iterations, i.e., as long as  $\mathcal{D}^{(k)}$ , for large  $k$ , is not empty. In the global symplectic case, this is typically guaranteed by the conservation of energy: indeed, if a surface of constant energy is contained in  $\mathcal{D}$ , and is not too close to the border, then (2.19) guarantees *a priori* that for  $x$  on that surface  $\Psi_\varepsilon^k(x)$  cannot escape  $\mathcal{D}$ , up to very large  $k$ . This is the usual case of symplectic mappings which are introduced to numerically integrate Hamiltonian systems.

*Proof.* Assume provisionally that  $\Phi_{F_\varepsilon}^j(x)$  does not escape  $\mathcal{D}_{\rho/4}$  for  $0 \leq j \leq k-1$  and  $x \in \mathcal{D}^{(k)}$ . From the trivial inequality

$$\begin{aligned} |\Psi_\varepsilon^j(x) - \Phi_{F_\varepsilon}^j(x)| &\leq |\Psi_\varepsilon(\Psi_\varepsilon^{j-1}(x)) - \Psi_\varepsilon(\Phi_{F_\varepsilon}^{j-1}(x))| \\ &\quad + |\Psi_\varepsilon(\Phi_{F_\varepsilon}^{k-1}(x)) - \Phi_{F_\varepsilon}(\Phi_{F_\varepsilon}^{k-1}(x))| \end{aligned} \tag{2.20}$$

and using the definition of  $\mu$  and the previous corollary, one immediately finds the recurrent estimate

$$d_j \leq (1 + \mu\varepsilon) d_{j-1} + 3\Gamma\varepsilon e^{-[e^*/\varepsilon]} \quad \text{for } 0 < j \leq k \tag{2.21}$$

(with  $d_0 = 0$ ), which in turn gives

$$d_j \leq 3\Gamma \frac{(1 + \mu\varepsilon)^j - 1}{\mu\varepsilon} \varepsilon e^{-[e^*/\varepsilon]}, \quad 0 \leq j \leq k \tag{2.22}$$

as claimed in (2.18). The above provisional assumption is easily removed: indeed, by recurrence, one immediately recognizes that if  $\Phi_{F_\varepsilon}, \dots, \Phi_{F_\varepsilon}^{j-1}(x) \in \mathcal{D}_{\rho/4}$ , then, just because of (2.22),  $\Phi_{F_\varepsilon}^j(x)$  also belongs to  $\mathcal{D}_{\rho/4}$ .

Finally, to prove (2.19), let us write

$$\begin{aligned} |H_\varepsilon(\Psi_\varepsilon^k(x)) - H_\varepsilon(x)| &\leq \sum_{j=0}^{k-1} |H_\varepsilon(\Psi_\varepsilon^{j+1}(x)) - H_\varepsilon(\Psi_\varepsilon^j(x))| \\ &= \sum_{j=0}^{k-1} |H_\varepsilon(\Psi_\varepsilon(\Psi_\varepsilon^j(x))) - H_\varepsilon(\Phi_{H_\varepsilon}(\Psi_\varepsilon^j(x)))| \\ &\leq k\lambda_\varepsilon \|\Psi_\varepsilon - \Phi_{H_\varepsilon}\|_{\rho/4} \end{aligned} \tag{2.23}$$

where  $\lambda_\varepsilon$  denotes the Lipschitz constant of  $H_\varepsilon$ ; recalling the definition of norms, as well as (2.14a), one easily gets  $\lambda_\varepsilon \leq 2n\rho^2 \|F_\varepsilon\|_{\rho/4} \leq 3n\rho^2\varepsilon\Gamma$ . Using inequality (2.15) to estimate  $\|\Psi_\varepsilon - \Phi_{H_\varepsilon}\|_{\rho/4}$ , (2.19) immediately follows. QED

### 3. PROOF OF PROPOSITION 1

#### 3.1. The Recursive Scheme

Let us use the short notation  $L_k = L_{fk}$ . By formally expanding the exponential of  $L_{F_\epsilon^\alpha}$ , one gets

$$\exp L_{F_\epsilon^\alpha} = \mathbb{1} + \sum_{j \geq 1} \frac{1}{j!} \left( \sum_{k \geq 1} \epsilon^k L_k \right)^j = \mathbb{1} + \sum_{l \geq 1} \epsilon^l \sum_{j=1}^l \frac{1}{j!} A_{j,l} \quad (3.1)$$

with

$$A_{j,l} = \sum_{\substack{k_1, \dots, k_j \geq 1 \\ k_1 + \dots + k_j = l}} L_{k_1} \cdots L_{k_j}, \quad 1 \leq j \leq l \quad (3.2)$$

From this definition, one easily gets for  $A_{j,l}$ ,  $l \geq 1$ , the recursive relations

$$A_{1,l} = L_l \quad (3.3a)$$

$$A_{j,l} = \sum_{k=1}^{l-j+1} L_k A_{j-1, l-k}, \quad 2 \leq j \leq l \quad (3.3b)$$

By comparing expression (3.1) for  $\exp L_{F_\epsilon^\alpha}$  with the series (2.7) of  $\Psi_\epsilon$ , it is not difficult to get the further recursive relations

$$f_1 = \psi_1 \quad (3.4a)$$

$$f_l = \psi_l - \sum_{j=2}^l \frac{1}{j!} A_{j,l} \xi, \quad l \geq 2 \quad (3.4b)$$

Indeed, the former equality is trivial, while for any  $l \geq 2$  one has

$$\psi_l = A_{1,l} \xi + \sum_{j=2}^l \frac{1}{j!} A_{j,l} \xi \quad (3.5)$$

and (3.4b) is immediate, since  $A_{1,l} \xi = L_l \xi = f_l$ .

The recursive scheme defined by (3.3), (3.4) provides a way of calculating the vector fields  $f_k$ ,  $1 \leq k < \infty$ , in such a way that  $\exp L_{F_\epsilon^\alpha}$  coincides with  $\Psi_\epsilon$  at any order in  $\epsilon$ . To better understand the recursion, one may refer to the triangular diagram

$$\begin{array}{cccccc} f_1 & f_2 & f_3 & f_4 & \cdots & \\ & A_{2,2} & A_{2,3} & A_{2,4} & \cdots & \\ & & A_{3,3} & A_{3,4} & \cdots & \\ & & & A_{4,4} & \cdots & \\ & & & & \cdots & \end{array} \quad (3.6)$$

where the  $A_{1,k}$  do not appear, but in fact, in virtue of (3.3a), are implicitly contained in the first row. The recursion proceeds as follows: assume one has already defined the first  $l-1$  columns of the array; then, using (3.3), one defines all the elements of the next column  $l$  but the first one, while later, using (3.4), one also defines  $f_l$  and  $A_{1,l}$ . One should notice that all functions appearing in (3.6) are well defined in a finite number of operations, without any inversion or convergence problem, so all of them are analytic in  $\mathcal{D}_\rho$ , regardless of the value of  $\varepsilon$ .

**3.2. The Estimate (2.11) of  $f_k$**

Let

$$\delta = \frac{\rho}{2k}, \quad \mathcal{B} = k\beta = 4k \max(\gamma, \Gamma) \tag{3.7}$$

We prove recursively that the following estimates hold:

$$\begin{aligned} (a_1) \quad & \|f_1\|_\rho < \Gamma \\ (a_l) \quad & \|f_l\|_{\rho - (l + \eta - 1)\delta} < \frac{\mathcal{B}^{l-1}}{1 + \eta} \Gamma \quad \begin{cases} 2 \leq l \leq k \\ \eta \geq 0, l + \eta - 1 \leq k \end{cases} \\ (b_{1,1}) \quad & \|A_{1,1}\xi\|_\rho < \Gamma \\ (b_{j,l}) \quad & \|A_{j,l}\xi\|_{\rho - (l + \eta - 1)\delta} < \frac{\mathcal{B}^{l-1}}{1 + \eta} \Gamma \quad \begin{cases} 2 \leq l \leq k, 1 \leq j \leq l \\ \eta \geq 0, l + \eta - 1 \leq k \end{cases} \end{aligned} \tag{3.8}$$

In particular, for  $l=k$  and  $\eta=1$ , one gets the required estimate on  $f_k$ ,  $k \geq 2$ . Also notice that the estimates (a<sub>1</sub>) and (b<sub>1,1</sub>) are exceptional, and, unfortunately, worse, because they do not contain the free parameter  $\eta$ .

The estimates (a<sub>1</sub>) and (b<sub>1,1</sub>) follow immediately from  $A_{1,1}\xi = f_1 = \psi_1$ . We then assume that the above inequalities are satisfied up to a given value of  $l$ , for  $1 \leq j \leq l$ , and show (in the order, according to the recursive scheme) that (b<sub>*j,l+1*</sub>) for  $2 \leq j \leq l+1$ , then (a<sub>*l+1*</sub>), and finally (b<sub>1,*l+1*</sub>), are also satisfied.

In the estimates, we shall frequently use the following elementary result.

**Lemma 1.** Let  $\delta$  be as in (3.7), and consider any positive constants  $\theta, \theta'$ , with  $\theta + \theta' < 2k$ . If the vector field  $f$  is analytic in  $\mathcal{D}_{\rho - (\theta + \theta')\delta}$ , and the scalar- or vector-valued function  $w$  is analytic in  $\mathcal{D}_{\rho - \theta\delta}$ , one has

$$\|L_f w\|_{\rho - (\theta + \theta')\delta} \leq \frac{2k}{\theta'} \|f\|_{\rho - (\theta + \theta')\delta} \|w\|_{\rho - \theta\delta} \tag{3.9}$$

*Proof.* Let  $w$  be a scalar function and, for any  $x \in \mathcal{D}_{\rho - (\theta + \theta')\delta}$ , denote

$$w_x(z) = w(x + zf(x)) \tag{3.10}$$

One has clearly

$$(L_f w)(x) = \frac{dw_x}{dz}(0)$$

Now, as long as  $|z| \leq \zeta$ ,

$$\zeta = \min_{1 \leq i \leq m} \frac{\theta' \delta^i}{|f^i(x)|} \tag{3.11}$$

one has  $x + zf(x) \in \mathcal{D}_{\rho - \theta\delta}$ ; a Cauchy estimate gives then

$$\left| \frac{dw_x}{dz}(0) \right| \leq \frac{1}{\zeta} \sup_{|z| \leq \zeta} |w_x(z)| \leq \frac{2k}{\theta'} \|f\|_{\rho - (\theta + \theta')\delta} \|w\|_{\rho - \theta\delta} \tag{3.12}$$

and (3.9) is immediate. The case of a vector-valued function is treated in a similar way. QED

Let us then prove  $(b_{j,l+1})$ ,  $2 \leq j \leq l + 1$ . Forget for a moment the case  $j = 2$ , which needs special considerations. From very definition of  $A_{j,l+1}$ , using Lemma 1, one gets

$$\begin{aligned} \|A_{j,l+1} \xi\|_{\rho - (l+\eta)\delta} &\leq \|L_1 A_{j-1,l} \xi\|_{\rho - (l+\eta)\delta} + \sum_{s=2}^{l-j+2} \|L_s A_{j-1,l+1-s} \xi\|_{\rho - (l+\eta)\delta} \\ &\leq 2k \|f_1\|_{\rho} \|A_{j-1,l} \xi\|_{\rho - (l+\eta-1)\delta} \\ &\quad + \frac{2k}{s} \sum_{s=2}^{l-j+2} \|f_s\|_{\rho - (l+\eta)\delta} \|A_{j-1,l+1-s} \xi\|_{\rho - (l+\eta-s)\delta} \end{aligned} \tag{3.13}$$

(the sum is intended to vanish if  $j = l + 1$ ). By the inductive hypothesis, one finds

$$\|A_{j,l+1} \xi\|_{\rho - (l+\eta)\delta} \leq 2k\Gamma^2 \frac{\mathcal{B}^{l-1}}{1+\eta} \left[ 1 + \sum_{s=2}^{l-j+2} \frac{1}{s(1+\eta+k-s)} \right] \tag{3.14}$$

and the conclusion is immediate: indeed, one easily recognizes that each of the  $l-j$  terms of the sum does not exceed  $l^{-1}$ , so that

$$\|A_{j,l+1} \xi\|_{\rho - (l+\eta)\delta} < 4k\Gamma^2 \frac{\mathcal{B}^{l-1}}{1+\eta} \tag{3.15}$$

Inequality  $(b_{j,l+1})$ ,  $2 < j \leq l$ , is then guaranteed by the choice (3.7) of  $\mathcal{B}$ .

Let us now consider the case  $j = 2$ ; this is a special case, because the last term of the sum, namely  $L_l A_{1,1} \xi$ , contains  $A_{1,1}$ , whose estimate is known only in  $\mathcal{D}_\rho$ . In fact, for  $l + 1 = 2$  this is the only term, and one finds

$$\|A_{2,2} \xi\|_{\rho - (1 + \eta)\delta} \leq \frac{2k}{1 + \eta} \|f_l\|_\rho \|A_{1,1} \xi\|_\rho \leq \frac{2k}{1 + \eta} \Gamma^2 \quad (3.16)$$

For the choice of  $\mathcal{B}$ , the required estimate is immediate. For  $l + 1 > 2$ , one finds instead

$$\begin{aligned} \|L_l A_{1,1} \xi\|_{\rho - (l + \eta)\delta} &\leq \frac{2k}{l + \eta} \|f_l\|_{\rho - (l + \eta)\delta} \|A_{1,1} \xi\|_\rho \\ &\leq \frac{2k}{l + \eta} \Gamma \frac{\mathcal{B}^{l-1}}{2 + \eta} \\ &< \frac{1}{l} 2k \Gamma^2 \frac{\mathcal{B}^{l-1}}{1 + \eta} \end{aligned} \quad (3.17)$$

Thus, in this case, too, one gets (3.15), and  $(b_{2,l+1})$  is proven.

Let us now come to  $(a_{l+1})$ . Using the recursive definition (3.4) of  $f_{l+1}$ , as well as the assumption (2.8) on  $\psi_l$  and the previously obtained inequalities  $(b_{j,l+1})$ , we can write

$$\|f_{l+1}\|_{\rho - (l + \eta)\delta} \leq \gamma^l \Gamma + \frac{\mathcal{B}^l \Gamma}{1 + \eta} \sum_{j=2}^{l+1} \frac{1}{j!} < \frac{\mathcal{B}^l \Gamma}{1 + \eta} \left[ (1 + \eta) \frac{\gamma^l}{\mathcal{B}^l} + e - 2 \right] \quad (3.18)$$

Since  $1 + \eta \leq k$ , using (3.7) [in fact,  $\mathcal{B} > k\gamma/(3 - e)$  would be enough], one immediately gets  $(1 + \eta) \gamma^l / \mathcal{B}^l \leq k\gamma / \mathcal{B} < 3 - e$ , and  $(a_{l+1})$  is achieved.

Finally, the last inequality, namely  $(b_{1,l+1})$ , is a direct consequence of  $(a_{l+1})$ , since, according to (3.3b), one has  $A_{1,l+1} \xi = L_{l+1} \xi = f_{l+1}$ .

### 3.3. The Estimates (2.14a), (2.14b)

Inequality (2.14a) is trivial for  $r = 1$ . For  $1 < r \leq (2\beta\epsilon)^{-1}$ , according to (2.11), one can write

$$\|F_\epsilon^r\|_{\rho/2} \leq \epsilon \Gamma + \frac{\Gamma}{2} \sum_{k=2}^r \epsilon^k k^{k-1} \beta^{k-1} \leq \frac{1}{2} \epsilon \Gamma \left[ 1 + \sum_{k=1}^r \left( \frac{k}{2r} \right)^{k-1} \right] \quad (3.19)$$

Since the sum does not exceed 2, (2.14a) is certainly satisfied. Concerning (2.14b), one proceeds as follows: let

$$A_\epsilon^r(x) = \Phi_{F_\epsilon^r}(x) - \Psi_\epsilon(x) \quad (3.20)$$

From the formal part, we already know that  $\mathcal{A}'_\varepsilon(x)$ , as a function of  $\varepsilon$ , is analytic and divisible by  $\varepsilon^{r+1}$ : by a well-known property of analytic functions, one then gets for any positive  $\zeta$

$$|\mathcal{A}'_\varepsilon(x)| \leq \left(\frac{\varepsilon}{\zeta}\right)^{r+1} \max_{z \in \mathbb{C}, |z| \leq \zeta} |\mathcal{A}'_\varepsilon(x)| \tag{3.21}$$

Now, a trivial generalization of the estimate (2.14a) for  $F'_\varepsilon$  gives

$$\|F'_\varepsilon\|_{\rho/2} \leq \frac{3}{2} |z| \Gamma \tag{3.22}$$

and the estimate holds for  $r \leq (2\beta |z|)^{-1}$ , i.e., for  $|z| \leq \zeta = (2\beta r)^{-1}$ . If this condition is satisfied, then for  $x \in \mathcal{D}_{\rho/4}$  one has certainly  $\Phi_{F'_\varepsilon}(x) \in \mathcal{D}_{\rho/2}$ , and

$$\|\Phi_{F'_\varepsilon} - \xi\|_{\rho/4} \leq \frac{3}{2} \zeta \Gamma \tag{3.23}$$

On the other hand, for  $|z| \leq \zeta$  one has in particular  $|z| < 1/(4\gamma)$ , and thus, from (2.7), (2.8),

$$\|\Psi_\varepsilon - \xi\|_\rho \leq \frac{|z| \Gamma}{1 - |z| \gamma} < \frac{3}{2} \zeta \Gamma \tag{3.24}$$

For  $|z| \leq \zeta$  one has then

$$\|\mathcal{A}'_\varepsilon\|_{\rho/4} \leq \|\Phi_{F'_\varepsilon} - \xi\|_{\rho/2} + \|\Psi_\varepsilon - \xi\|_{\rho/4} \leq 3\zeta \Gamma \tag{3.25}$$

and consequently

$$\|\mathcal{A}'_\varepsilon\|_{\rho/4} \leq 3\zeta \Gamma \left(\frac{\varepsilon}{\zeta}\right)^{r+1} \leq 3\varepsilon \Gamma (2r\beta\varepsilon)^r \tag{3.26}$$

as claimed.

### 3.4. The Symplectic Case

Point (iii) of Proposition 1 practically reduces to the following purely algebraic result.

**Lemma 2.** If a vector field

$$F'_\varepsilon = \varepsilon f_1 + \dots + \varepsilon^r f_r$$

satisfies the relation

$$\{(\exp L_{F'_\varepsilon}) \xi^i, (\exp L_{F'_\varepsilon}) \xi^j\} - \{\xi^i, \xi^j\} = \mathcal{O}(\varepsilon^{r+1}) \tag{3.27}$$

where  $\{\cdot, \cdot\}$  denotes the Poisson bracket, then the vector fields  $f_1, \dots, f_r$  are locally Hamiltonian [and consequently, the rhs of (3.27) actually vanishes].

*Proof.* At first order in  $\varepsilon$ , (3.27) gives

$$\{L_1 \xi^i, \xi^j\} + \{\xi^i, L_1 \xi^j\} = 0 \tag{3.28}$$

that is,

$$\{f_1^i, \xi^j\} + \{\xi^i, f_1^j\} = 0 \tag{3.29}$$

This is a well-known necessary and sufficient condition in order for  $f_1$  to be locally Hamiltonian.

Proceeding by induction, assume that  $f_1, \dots, f_k$ ,  $k < r$ , are locally Hamiltonian. One has clearly

$$\exp L_{F'_\varepsilon} = \exp(\varepsilon L_1 + \dots + \varepsilon^k L_k) + \varepsilon^{k+1} L_{k+1} + \mathcal{O}(\varepsilon^{k+2}) \tag{3.30}$$

and thus, from (3.27),

$$\begin{aligned} & \{(e^{\varepsilon L_1 + \dots + \varepsilon^k L_k} + \varepsilon^{k+1} L_{k+1}) \xi^i, (e^{\varepsilon L_1 + \dots + \varepsilon^k L_k} + \varepsilon^{k+1} L_{k+1}) \xi^j\} \\ & - \{\xi^i, \xi^j\} = \mathcal{O}(\varepsilon^{k+2}) \end{aligned} \tag{3.31}$$

Now, according to the inductive hypothesis, one has

$$\{e^{\varepsilon L_1 + \dots + \varepsilon^k L_k} \xi^i, e^{\varepsilon L_1 + \dots + \varepsilon^k L_k} \xi^j\} = \{\xi^i, \xi^j\}$$

It follows that

$$\{L_{k+1} \xi^i, \xi^j\} + \{\xi^i, L_{k+1} \xi^j\} = 0$$

so that  $f_{k+1}$  is locally Hamiltonian. The lemma is thus proven. QED

Point (iii) of Proposition 1 is now immediate: indeed, from the formal part one has

$$(\exp L_{F'_\varepsilon}) \xi - \Psi_\varepsilon = \mathcal{O}(\varepsilon^{r+1})$$

so that, for symplectic  $\Psi_\varepsilon$ , (3.27) is guaranteed. This concludes the proof of Proposition 1. QED

#### 4. ON SYMPLECTIC INTEGRATION ALGORITHMS

This section is devoted to the problem of numerical integration of Hamiltonian systems by means of symplectic algorithms. To be definite, we consider the particular class of Hamiltonian systems

$$K(p, q) = \frac{1}{2} \sum_{i=1}^n (p^i)^2 + V(q^1, \dots, q^n) \tag{4.1}$$

and the most elementary symplectic integration scheme, namely

$$\Psi_\varepsilon(p, q) = (p + \varepsilon u(q), q + \varepsilon p + \varepsilon^2 u(q)) \tag{4.2}$$

where

$$u = (u^1, \dots, u^n), \quad u^i = -\frac{\partial V}{\partial q^i} \tag{4.3}$$

The algorithm is immediately recognized to be globally symplectic. Then one has  $\Psi_\varepsilon = \varepsilon\psi_1 + \varepsilon^2\psi_2$ , with

$$\psi_1 = (u, \pi), \quad \psi_2 = (0, u) \tag{4.4}$$

$\pi$  is the projector defined by  $\pi(p, q) = p$ . Special attention will be devoted to the case of scattering, namely the case in which one or more of the  $q^i$  run over the whole real line, and the potential vanishes if any of these goes to infinity; the Hamiltonian system considered in the already quoted ref. 10, namely

$$K(p, q, I, \varphi) = \frac{I^2}{2C} + \frac{p^2}{2m} + V(q, \varphi), \quad I, p, q \in \mathbb{R}, \quad \varphi \in S^1 \tag{4.5}$$

belongs in particular (after a rescaling) to this class. Another common situation we shall consider is the case of motion in a bounded region; such a situation typically occurs when the constant-energy surfaces of Hamiltonian (4.1) are compact.

To be definite, let us assume that the domain  $\mathcal{D}$  of the Hamiltonian  $K$  (and of the mapping  $\Psi_\varepsilon$ ) is given by  $|p^i| \leq P, i = 1, \dots, n$ , and  $q \in D \subset \mathbb{R}^n$ . Denoting by  $\rho = (\sigma^1, \dots, \sigma^n, \tau^1, \dots, \tau^n)$  the extension vector, we introduce the extended domains

$$D_\tau = \bigcup_{q \in D} \{ \tilde{q} \in \mathbb{C}^n : |\tilde{q}^i - q^i| \leq \tau^i, 1 \leq i \leq n \} \tag{4.6}$$

$$\mathcal{D}_\rho = \{ (p, q) \in \mathbb{C}^{2n} : q \in D_\tau; |\text{Im } p^i| \leq \sigma^i \}$$

For notational simplicity, we assume the extensions be independent of  $i$ , namely  $\sigma^i = \sigma, \tau^i = \tau$ . The quantity  $\rho^2$  introduced in Section 2 is then the product  $\sigma\tau$ . It is worthwhile to notice that, while  $\tau$  depends in general on  $V$ ,  $\sigma$  is instead arbitrary. One could simply take  $\sigma = P$ , or profit from this arbitrariness to (slightly) optimize the results; in the following, to clarify our procedure, we keep  $\sigma$  free.

Denote

$$\mathcal{U}^* = \max_{1 \leq i \leq n} \sup_{q \in D_i} |u^i(q)| \tag{4.7}$$



Then one has

$$\|\psi_1\|_\rho = \max\left(\frac{\mathcal{U}^*}{\sigma}, \frac{P + \sigma}{\tau}\right), \quad \|\psi_2\|_\rho = \frac{\mathcal{U}^*}{\tau} \tag{4.8}$$

and consequently the constants  $\Gamma$ ,  $\gamma$ , and  $\beta$  entering Proposition 1 are given by

$$\Gamma = \max\left(\frac{\mathcal{U}^*}{\sigma}, \frac{P + \sigma}{\tau}\right), \quad \gamma = \frac{\mathcal{U}^*}{\tau\Gamma} < \Gamma, \quad \beta = 4\Gamma \tag{4.9}$$

One could also see that the Lipschitz constant  $\mu$  entering Corollary 2 satisfies the simple estimate

$$\mu \leq \Gamma \tag{4.10}$$

in the real domain  $\mathcal{D}_0 = \mathcal{D}$  (the estimate requires some tedious work, but is not difficult). For convenience, in place of the best time-one interpolating Hamiltonian  $H_\varepsilon$ , we refer here to the time- $\varepsilon$  interpolating Hamiltonian  $K_\varepsilon = \varepsilon^{-1}H_\varepsilon$ , for which one has  $\Phi_{K_\varepsilon}^{\varepsilon t} = \Phi_{H_\varepsilon}^t$ .

#### 4.1. The Case of Motion in a Bounded Region

Let us first consider the easier case of motion in a bounded region; the (more interesting) case of scattering requires further considerations, and will be considered later. From Corollary 2, using the above estimate of  $\mu$ , one gets that, up to time  $k\varepsilon \leq \Gamma^{-1}$  (notice that  $\Gamma^{-1}$  is a quite natural time unit in the problem at hand), one has

$$|\Phi_{K_\varepsilon}^{k\varepsilon}(x) - \Psi_\varepsilon^k(x)| < 6e^{-[\varepsilon^*/\varepsilon]}, \quad x \in \mathcal{D}^{(k)} \tag{4.11}$$

i.e., the algorithm  $\Psi_\varepsilon$  follows the trajectories of the interpolating Hamiltonian  $K_\varepsilon$  up to times of order one, with exponentially small error. Using quite reasonable values of the timestep  $\varepsilon$ , this error is easily made (much) smaller than roundoff errors, in any reasonable precision; as remarked in the Introduction, this means that the essential effect of the discretization introduced by the algorithm is to replace the original Hamiltonian  $K$  by  $K_\varepsilon$ , and then to proceed “exactly,” as for the case of iterated maps.

The problem then arises of knowing the relation between  $K$  and  $K_\varepsilon$ . To this purpose, one has the following elementary corollary, which makes precise some considerations already anticipated in the Introduction.

**Corollary 3.** Let  $H_\varepsilon$  be the best time-one interpolating Hamiltonian introduced in Corollary 2, and consider the time- $\varepsilon$  interpolating Hamilto-

nian  $K_\varepsilon = \varepsilon^{-1}H_\varepsilon$ ; let  $X$  and  $X_\varepsilon$  denote the Hamiltonian vector fields of  $K$  and  $K_\varepsilon$ , respectively. If  $\varepsilon \leq \frac{1}{2}\varepsilon^*$ , with  $\varepsilon^*$  as in Corollary 1, then one has

$$\|X_\varepsilon - X\|_{\rho/2} \leq 8\varepsilon\Gamma^2 \tag{4.12}$$

Moreover, if  $K_\varepsilon(0, \bar{q}) = K(0, \bar{q})$  for some given  $\bar{q} \in D$ , then one has

$$\|K_\varepsilon - K\|_{\rho/2} \leq nB\sigma\tau\Gamma^2\varepsilon, \quad B = 16 \left( \frac{P}{\sigma} + \frac{d}{\tau} \right) \tag{4.13}$$

with

$$d = \max_{1 \leq i \leq n} \sup_{q \in D} |q^i - \bar{q}^i| \tag{4.14}$$

Finally, the algorithm preserves both  $K$  and  $K_\varepsilon$  up to an exponentially large time, namely one has

$$\begin{aligned} |K_\varepsilon(p_k, q_k) - K_\varepsilon(p_0, q_0)| &\leq 4n\sigma\tau\Gamma^2\varepsilon \\ |K(p_k, q_k) - K(p_0, q_0)| &\leq (3 + 2B)n\sigma\tau\Gamma^2\varepsilon \end{aligned} \tag{4.15}$$

for

$$k \leq \varepsilon\Gamma e^{+[\varepsilon^*/\varepsilon]} \tag{4.16}$$

*Proof.* One has  $X = \psi_1 = f_1$ , and  $X_\varepsilon = \varepsilon^{-1}F'_\varepsilon$ ,  $r = [\varepsilon^*/\varepsilon]$ . Using (2.11), one then gets

$$\begin{aligned} \|X_\varepsilon - X\|_{\rho/2} &\leq \varepsilon^{-1} \|F'_\varepsilon - \varepsilon f_1\|_{\rho/2} \leq \frac{1}{2}\varepsilon\beta\Gamma \sum_{k=2}^r k(\varepsilon\beta k)^{k-2} \\ &\leq \frac{1}{2}\varepsilon\beta\Gamma \sum_{k=2}^r 2^{k-1}(\varepsilon\beta k)^{k-2} \leq 2\varepsilon\beta\Gamma = 8\varepsilon\Gamma^2 \end{aligned} \tag{4.17}$$

as claimed in (4.12). Inequality (4.13) is also easily achieved: indeed, for any  $(p, q) \in \mathcal{D}$  one has clearly

$$K_\varepsilon(p, q) - K(p, q) = \int_{(0, \bar{q})}^{(p, q)} (\nabla K_\varepsilon - \nabla K) \cdot dl \tag{4.18}$$

where  $\nabla$  denotes the gradient, and the line integral is independent of the path in  $\mathcal{D}$ ; on the other hand, from (4.12) one has

$$\left| \frac{\partial K_\varepsilon}{\partial p^i} - \frac{\partial K}{\partial p^i} \right| \leq 8\varepsilon\Gamma^2\tau, \quad \left| \frac{\partial K_\varepsilon}{\partial q^i} - \frac{\partial K}{\partial q^i} \right| \leq 8\varepsilon\Gamma^2\sigma \tag{4.19}$$

and (4.13) immediately follows. Finally, the former of (4.15) is a trivial consequence of (2.19), after the choice (4.16) of  $k$ , while the latter immediately follows from

$$\begin{aligned}
 |K(p_k, q_k) - K(p_0, q_0)| &\leq |K(p_k, q_k) - K_\varepsilon(p_k, q_k)| \\
 &\quad + |K_\varepsilon(p_k, q_k) - K_\varepsilon(p_0, q_0)| \\
 &\quad + |K_\varepsilon(p_0, q_0) - K(p_0, q_0)| \\
 &\leq (3 + 2B) n\sigma\tau\Gamma^2\varepsilon \quad \text{QED} \tag{4.20}
 \end{aligned}$$

### 4.2. The Case of Scattering

Let us now come to the problem of scattering. The uniform estimates (4.9) are of course correct, but definitely rough for the problem at hand, since one misses the essential property that, asymptotically,  $u$  vanishes, and, correspondingly, as is clear from (4.2), the algorithm  $\Psi_\varepsilon$  becomes exact.

To take this crucial fact into consideration, we introduce the following more detailed, “local” estimate of  $u$ :

$$\mathcal{U}(q) = \max_{1 \leq i \leq n} \sup_{|q' - q| < \tau} |u^i(q')|, \quad \mathcal{U}(q) \leq \mathcal{U}^* \tag{4.21}$$

For any function  $w: \mathcal{D} \rightarrow \mathbb{C}$ , it is then convenient to introduce, besides the usual norm, the “local norm”

$$\|w; q\|_{\rho'} = \sup_{|Im p| \leq \sigma; |q' - q| < \tau} |w(p, q')|, \quad q \in \mathbb{R}^n \tag{4.22}$$

and also define, by analogy, the local norm  $\|W; q\|_{\rho'}$  for vector-valued functions  $W: \mathcal{D} \rightarrow \mathbb{C}^{2n}$ . Let us notice that one has

$$\|\psi_2; q\|_{\rho} = \frac{\mathcal{U}(q)}{\tau} \tag{4.23}$$

Instead, because of the  $q$ -component,  $\|\psi_1; q\|_{\rho}$  does not vanish for vanishing  $u$ .

In the following Proposition 1' we adapt to the particular problem at hand the estimates of Proposition 1; the essential difference is that norms are here replaced by local norms, while the constant  $\Gamma$  on the rhs of each estimate is replaced by the function

$$\mathcal{G}(q) = \frac{\mathcal{U}(q)}{\sigma} \leq \Gamma \tag{4.24}$$

**Proposition 1'.** Let  $K$  and  $\Psi_\varepsilon$  be as above, and let  $F_\varepsilon^\infty = \varepsilon f_1 + \varepsilon^2 f_2 + \dots$  be the formal interpolating vector field of  $\Psi_\varepsilon$ , as in Proposition 1. With reference to the constants  $\gamma$ ,  $\Gamma$ , and  $\beta$  and to the function  $\mathcal{G}$  defined above, one has

$$\begin{aligned} \|f_1\|_\rho &\leq \Gamma \\ \|f_k; q\|_{\rho/2} &\leq \frac{1}{2} k^{k-1} \beta^{k-1} \mathcal{G}(q), \quad k \geq 2 \end{aligned} \tag{4.25}$$

Moreover, for any  $r \leq (2\beta\varepsilon)^{-1}$  the finite sum  $F_\varepsilon^r = \varepsilon f_1 + \dots + \varepsilon^r f_r$  satisfies the estimates

$$\|F_\varepsilon^r - \varepsilon f_1; q\|_{\rho/2} \leq \frac{1}{2} \varepsilon \mathcal{G}(q) \tag{4.26a}$$

$$\|\Phi_{F_\varepsilon^r} - \Psi_\varepsilon; q\|_{\rho/16} \leq 3\varepsilon(2r\beta\varepsilon)^r \mathcal{G}(q) \tag{4.26b}$$

*Proof.* The proof of (4.25) is straightforward. Indeed, the recurrent assumptions (a<sub>l</sub>) and (b<sub>l,i</sub>) are replaced by

$$\|f_l; q\|_{\rho-(l+\eta-1)\delta} < \frac{\mathcal{B}^{l-1}}{1+\eta} \mathcal{G}(q), \quad \|A_{l,i}\xi; q\|_{\rho-(l+\eta-1)\delta} < \frac{\mathcal{B}^{l-1}}{1+\eta} \mathcal{G}(q) \tag{4.27}$$

and the proof of the recurrence runs smoothly, exactly as for Proposition 1, with the only exception of the estimate of  $A_{2,2}\xi = L_1 f_1 = L_{\psi_1} \psi_1$ , which requires some care because, as remarked above, the local norm of  $\psi_1$  does not vanish for vanishing  $u$ . Nevertheless, a direct computation shows that one has  $L_{\psi_1} \psi_1 = (\pi \partial u / \partial q, u)$ , and a Cauchy estimate for  $\partial u / \partial q$  easily leads to

$$\|A_{2,2}; q\|_{\rho-(1+\eta)\delta} \leq \frac{k}{1+\eta} \frac{P+\sigma}{\tau} \mathcal{G}(q) < \frac{\mathcal{B}}{1+\eta} \mathcal{G}(q) \tag{4.28}$$

as required.

Let us come to the inequalities (4.26). The former immediately follows from (4.25); the latter requires instead some work, which we simply sketch. Denote, as in Proposition 1,

$$\Delta_\varepsilon^r(p, q) = \Phi_{F_\varepsilon^r}(p, q) - \Psi_\varepsilon(p, q) \tag{4.29}$$

Proceeding as there, we replace  $\varepsilon$  by the complex variable  $z$ , and work out a local estimate of  $\Delta_z^r$ , for  $|z|$  up to some convenient  $\zeta$ . To this purpose, let us write

$$\begin{aligned} \Delta_z^r &= \Delta' + \Delta'' \\ \Delta' &= \Phi_{F_\varepsilon^r} - \xi - L_{F_\varepsilon^r} \xi, \quad \Delta'' = L_{F_\varepsilon^r} \xi - (\Psi_z - \xi) \end{aligned} \tag{4.30}$$

We claim that, for  $|z| \leq \zeta = (2\beta r)^{-1}$ , the two terms are estimated by

$$\|A'; q\|_{\rho/16} \leq \frac{5}{8}\zeta\mathcal{G}(q), \quad \|A''; q\|_{\rho/2} < \frac{2}{16}\zeta\mathcal{G}(q) \tag{4.31}$$

The latter estimate is quite simple: indeed, recalling  $\psi_1 = f_1$ , one has  $\Psi_z - \xi = zf_1 + z^2\psi_2$ , and thus

$$\begin{aligned} \|L_{F'_z}\xi - \Psi_z; q\|_{\rho/2} &\leq \|F'_z - zf_1; q\|_{\rho/2} + |z|^2 \|\psi_2; q\|_{\rho/2} \\ &\leq \frac{1}{2}\zeta\mathcal{G}(q) + \zeta^2 \frac{\sigma}{\tau} \mathcal{G}(q) \end{aligned} \tag{4.32}$$

Using then  $\sigma/\tau \leq \Gamma = \frac{1}{4}\beta$ ,  $\zeta\beta \leq \frac{1}{2}$ , the estimate is immediate. Concerning  $A'$ , there is instead some work. Let  $(\hat{p}, \hat{q})$  be such that

$$|\text{Im } \hat{p}| \leq \frac{1}{16}\sigma, \quad |\hat{q} - q| \leq \frac{1}{16}\tau \tag{4.33}$$

and denote

$$\Phi'_{F'_z}(\hat{p}, \hat{q}) = (P(t, \hat{p}, \hat{q}), Q(t, \hat{p}, \hat{q}))$$

One has clearly

$$\begin{aligned} A'(\hat{p}, \hat{q}) &= \int_0^1 dt \int_0^t (\ddot{P}(t, \hat{p}, \hat{q}), \ddot{Q}(t, \hat{p}, \hat{q})) ds \\ &= \int_0^1 dt \int_0^t (L_{F'_z}F'_z)(P(t, \hat{p}, \hat{q}), Q(t, \hat{p}, \hat{q})) ds \end{aligned} \tag{4.34}$$

and thus

$$\begin{aligned} |A'(\hat{p}, \hat{q})| &\leq \frac{1}{2} \sup_{0 \leq t \leq 1} |(L_{F'_z}F'_z)(P(t, \hat{p}, \hat{q}), Q(t, \hat{p}, \hat{q}))| \\ &\leq \frac{1}{2} \|L_{F'_z}F'_z; q\|_{\rho/4} \end{aligned} \tag{4.35}$$

provided

$$|\text{Im } P(t, \hat{p}, \hat{q})| \leq \frac{1}{4}\sigma, \quad |Q(t, \hat{p}, \hat{q}) - q| \leq \frac{1}{4}\tau \quad \text{for } 0 \leq t \leq 1$$

One can see that, for  $\hat{p}, \hat{q}$  as in (4.33), such a condition is guaranteed by

$$\|F'_z\|_{\rho/2} \leq \frac{3}{2}\zeta\Gamma \leq \frac{3}{16} \tag{4.36}$$

which in turn follows from (4.26a). After some elementary work, based on the trivial decomposition  $F'_z = zf_1 + (F'_z - zf_1)$ , one finds

$$\|L_{F'_z}F'_z; q\|_{\rho/4} \leq 5 |z|^2 \Gamma\mathcal{G}(q) \leq \frac{5}{4}\zeta\beta\mathcal{G}(q) \tag{4.37}$$

and the estimate for  $\Delta'$  is immediate. From (4.31) one has  $\|\Delta'_\varepsilon; q\|_{\rho/16} < \frac{3}{2}\varepsilon\mathcal{G}(q)$ , and (4.26b) follows. This concludes the proof of Proposition 1'. QED

In the next corollary we adapt to the problem at hand the relevant results of Corollaries 1–3.

**Corollary 4.** Within the above assumptions and notations, if  $|q| \mathcal{G}(q) \rightarrow 0$  for  $|q| \rightarrow \infty$ , then:

(i) There exists a Hamiltonian  $K_\varepsilon$  such that, denoting by  $\Phi_{K_\varepsilon}^\varepsilon$  its time- $\varepsilon$  flow, one has

$$\|\Phi_{K_\varepsilon}^\varepsilon - \Psi_\varepsilon; q\|_{\rho/16} \leq \varepsilon e^{-[\varepsilon^*/\varepsilon]}\mathcal{G}(q), \quad \varepsilon^* = \frac{1}{2e\beta} \tag{4.38}$$

(ii) For any initial datum  $(p, q) \in \mathcal{D}^{(k)}$ , denoting by  $Q(k, p, q)$  the  $q$ -component of  $\Psi_\varepsilon^k(p, q)$ , one has

$$|K_\varepsilon(\Psi_\varepsilon^k(p, q)) - K_\varepsilon(p, q)| \leq 4n\varepsilon\Gamma e^{-[\varepsilon^*/\varepsilon]} \sum_{j=0}^k \mathcal{G}(Q(j, p, q)) \tag{4.39}$$

(iii) The vector fields  $X$  and  $X_\varepsilon$  are related by

$$\|X_\varepsilon - X; q\|_{\rho/16} \leq 8\varepsilon^2\Gamma\mathcal{G}(q) \tag{4.40}$$

(iv) With appropriate choice of the additive constant in  $K$ , the Hamiltonians  $K_\varepsilon$  and  $K$  turn out to coincide everywhere at infinity,

$$\lim_{|q| \rightarrow \infty} |K_\varepsilon(p, q) - K(p, q)| = 0 \tag{4.41}$$

while for any  $(p, q) \in \mathcal{D}$  one has

$$|K_\varepsilon(p, q) - K(p, q)| \leq \varepsilon\mathcal{F}(q) \tag{4.42}$$

with

$$\mathcal{F}(q) = 8\Gamma\sigma \inf_{l_q} \int_{l_q} \mathcal{G}(q) \|dq\| \xrightarrow{|q| \rightarrow \infty} 0 \tag{4.43}$$

$l_q$  denotes a path in  $D$  from  $q$  to infinity.

(v) The algorithm  $\Psi_\varepsilon$  preserves  $K_\varepsilon$ , uniformly in time, up to an exponentially small quantity, namely for any  $k > 0$  one has

$$|K_\varepsilon(\Psi_\varepsilon^k(p, q)) - K_\varepsilon(p, q)| \leq C\varepsilon e^{-[\varepsilon^*/\varepsilon]} \tag{4.44}$$

$$C = 4n \sum_{i=0}^{\infty} \mathcal{G}(Q(j, p, q)) < \infty$$

Concerning  $K$ , one has instead

$$|K(p_k, q_k) - K(p_0, q_0)| \leq \varepsilon[\mathcal{F}(q_k) + \mathcal{F}(q_0)] + \varepsilon e^{-[\varepsilon^*/\varepsilon]} \tag{4.45}$$

**Remark.** The last statement (4.45) shows that the error in the energy conservation is bounded uniformly in time, and small with  $\varepsilon$ ; moreover, according to (4.43), *asymptotically for  $|q_0|, |q_k| \rightarrow \infty$ , the overall error in energy conservation is exponentially small.*

*Proof.* The proof of (4.38) directly follows from (4.26b), by simply proceeding as in Corollary 1; in a similar way, following the last part of Corollary 2, one gets (4.39). Concerning instead inequality (4.40), one proceeds as follows: from (4.25), one easily gets [besides the already used estimate (4.26a)]

$$\|F'_\varepsilon - \varepsilon f_1; q\|_{\rho/2} \leq 2\varepsilon^2 \beta \mathcal{G}(q) \quad \text{for } \varepsilon \leq 1/(4r\beta) \tag{4.46}$$

Indeed, from (4.25) one can write

$$\begin{aligned} \|F'_\varepsilon - \varepsilon f_1; q\|_{\rho/2} &\leq \frac{1}{2} \varepsilon^2 \beta \mathcal{G}(q) \sum_{k=2}^r k(\varepsilon \beta k)^{k-2} \\ &\leq \frac{1}{2} \varepsilon^2 \beta \mathcal{G}(q) \sum_{k=2}^r 2^{k-1} (\varepsilon \beta k)^{k-2} \end{aligned} \tag{4.47}$$

and the estimate is immediate. Proceeding as in (4.17), inequality (4.40) directly follows.

Concerning point (iv), let  $K_\varepsilon(0, \bar{q}) = K_\varepsilon(0, \bar{q})$  for some arbitrarily fixed point  $\bar{q} \in D$ ; for any  $(p, q) \in \mathcal{D}$  one has then

$$K_\varepsilon(p, q) - K(0, q) = \int_{(\bar{p}, \bar{q})}^{(p, q)} (\nabla K_\varepsilon - \nabla K) \cdot dl \tag{4.48}$$

Moving first  $p$  at fixed  $\bar{q}$  and then  $q$ , and proceeding as in Corollary 3, one then obtains

$$|K_\varepsilon(p, q) - K(p, q)| \leq 8n\varepsilon\Gamma\tau \|p - \bar{p}\| \mathcal{G}(\bar{q}) + 8\varepsilon\Gamma\sigma \int_{l_{\bar{q}, q}} \mathcal{G}(q) \|dq\| \tag{4.49}$$

$l_{\bar{q}, q}$  is any path from  $\bar{q}$  to  $q$  in  $\mathbb{R}^n$ . Taking the reference point  $\bar{q} \rightarrow \infty$ , the first term of (4.49) vanishes, and one gets

$$|K_\varepsilon(p, q) - K(p, q)| \leq 8\varepsilon\Gamma\sigma \int_{l_q} \mathcal{G}(q) \|dq\| \tag{4.50}$$

$l_q$  is any path from  $q$  to the given "point" at infinity. The limit (4.41) is then immediately achieved, by simply taking a path at infinity<sup>4</sup> [one uses here the assumption  $|q| \mathcal{G}(q) \rightarrow 0$  for  $|q| \rightarrow \infty$ ]; moreover, this shows that the particular choice of  $|\bar{q}|$  at infinity is irrelevant, and (4.43) immediately follows. Finally, (4.44) and (4.45) trivially follow from (4.39), and this completes the proof of the corollary. QED

Figure 1 shows the asymptotic error in the energy conservation, as a function of the inverse timestep  $\varepsilon^{-1}$  (in semilogarithmic scale), for a very simple scattering problem in two dimensions; with obvious meaning of the symbols, the Hamiltonian has the form

$$K(p_x, p_y, x, y) = \frac{p_x^2 + p_y^2}{2m} + V(x, y) \quad (4.51)$$

$$V(x, y) = V_0 \frac{e^{-(x^2 + y^2)/d^2}}{(1 + x^2/\tau^2)(1 + y^2/\tau^2)}$$

We used  $m$ ,  $d$ , and  $V_0$ , respectively, as units of mass, length, and energy; computations were performed in quadruple precision (approximately 33 decimal digits). The initial point was taken at a distance  $r \simeq 10d$  from the origin; at such a distance, within the computer precision, both the potential energy and the forces are negligible, i.e., the point is practically at infinity. Each run is stopped when the final point is again at a distance  $r$  from the origin. The quantity plotted in Fig. 1 is the relative error  $\delta E = |\Delta E|/E_0$ , where  $\Delta E$  is the difference between the initial and final values of  $K$ , and  $E_0$  is the initial energy. The initial data are (in the above units)  $x^0 = -10$ ,  $y^0 = 0.1$ ,  $p_x^0 = 0$ ; we set  $\tau = 0.5$ . As one can see, at least for small  $\varepsilon$ , the asymptotic error follows, with good accuracy, an exponential law  $\delta E \sim e^{-\lambda/\varepsilon}$ , and even relatively large timesteps lead to quite small final errors. Let us stress that only at the end of the collision is the error  $\delta E$  so small: on the contrary, at the middle of the collision, the error is simply of order  $\varepsilon$ ,<sup>5</sup> and thus much larger, for several orders of magnitude.

<sup>4</sup> It may appear that this argument fails for systems in which only one coordinate can go to infinity (for example, one-dimensional systems) if the asymptotic states lie at opposite sides of zero, and thus cannot be joined by a path at infinity. However, it is not difficult to add to the system a fictitious degree of freedom in such a way as to overcome this topological difficulty.

<sup>5</sup> In fact, according to the usual prescription of the leap-frog algorithm, before using  $p$  in the computation of energy, one introduces a correction (the so-called "half step" of the algorithm). This correction vanishes asymptotically where the forces vanish and the algorithm is exact, and is of order  $\varepsilon$  during the collision; its effect is a reduction of  $\delta E$  from order  $\varepsilon$  to order  $\varepsilon^2$ . This fact, although significant in practical computations, is quite irrelevant in the present discussion.



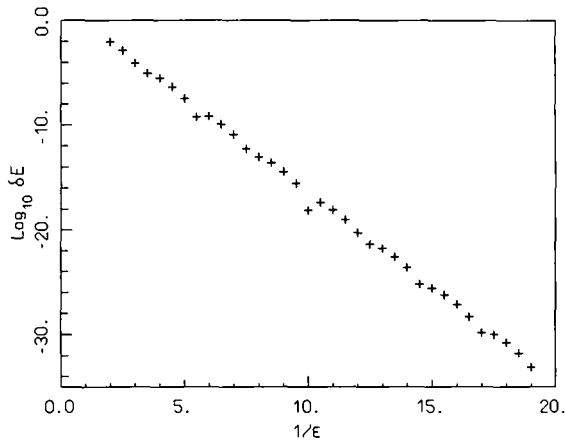


Fig. 1. The asymptotic error in energy conservation,  $\delta E$ , as function of the inverse timestep  $1/\epsilon$ , in semilogarithmic scale, for an elementary scattering problem (quadruple precision, approximately 33 significant digits).

Essentially the same results are obtained in more complicated scattering problems, in particular for systems like (4.5), where the scattering object has an internal degree of freedom; in fact, according to the above theoretical analysis, one only needs that asymptotically, when the scattering object moves freely, the algorithm is exact. Notice that, in the case of an internal vibrational degree of freedom, it is necessary to use for the oscillator the action-angle variables (as is not common in numerical studies).

## 5. CONCLUSIONS

In this paper we reconsidered the problem of the Hamiltonian interpolation of symplectic mappings. More precisely, we introduced quantitative estimates in Moser's formal scheme, and proved that, if a mapping  $\Psi_\epsilon$  is analytic and  $\epsilon$ -close to the identity, then there exists an analytic autonomous Hamiltonian system  $H_\epsilon$  such that its time-one flow  $\Phi_{H_\epsilon}$  differs from  $\Psi_\epsilon$  by a quantity exponentially small in  $1/\epsilon$ . This result has been applied, in particular, to the problem of numerical integration of Hamiltonian systems by symplectic algorithms; the conclusion is that, when using an analytic algorithm of order  $s$  to integrate a Hamiltonian system  $K$ , one actually follows "exactly," namely within the computer roundoff error, the trajectories of the interpolating Hamiltonian  $H_\epsilon$ , or equivalently of the order-one Hamiltonian  $K_\epsilon = \epsilon^{-1}H_\epsilon$ , which differs from  $K$ , but turns out to be  $\epsilon^s$  close to it.

Now, a typical motivation for numerical studies on Hamiltonian systems concerns the presence and the behavior of the integrals of motion: in the simplest case, one deals with a nearly integrable Hamiltonian system of the form

$$K_\alpha(I, \varphi) = K_0(I) + \alpha f(I, \varphi), \quad I \in \mathbb{R}^n, \quad \varphi \in \mathbb{T}^n$$

( $\alpha$  is here a small parameter), and questions, for example, the number of actions which are practically conserved, or the time scale on which they are allowed to change significantly. For such a problem, one clearly expects that the use of a numerical algorithm does modify the system, but in an inessential way: indeed, the original Hamiltonian  $K_\alpha$  is simply replaced by

$$K_{\alpha,\varepsilon}(I, \varphi) = K_0(I) + \alpha f(I, \varphi) + \varepsilon^s g(I, \varphi)$$

with  $g$  bounded and essentially as regular as  $f$ . Unless  $f$  is chosen in a class with very special properties, for small  $\varepsilon$  one expects, on the basis of the typical results of perturbation theory, that the two Hamiltonians behave practically in the same way: so, studying  $K_\alpha$  or  $K_{\alpha,\varepsilon}$  makes no essential difference. This is an example of a situation of structural stability to which remark (ii) in the Introduction applies. Let us stress that here both the symplectic character of the integration scheme and the globality of the interpolating Hamiltonian are essential: otherwise we could not interpret the effect of the algorithm simply as a small additional perturbation in the Hamiltonian, and the results, namely the long-time behavior of the approximate integrals of motion, could drastically change.

Another point that we consider to be relevant for the numerical integration of Hamiltonian systems is the problem of energy conservation in “asymptotically free” systems, say in numerical studies of scattering processes. As we have seen, in this case  $K$  and  $K_\varepsilon$  asymptotically coincide, and the final error in energy conservation turns out to be totally negligible. As a matter of fact, this allows one to measure relevant quantities, like the energy exchanges among different degrees of freedom at the end of a scattering process, with very high accuracy: this is important, because these quantities are known to be, in some cases, so small that they risk getting completely lost by numerical errors; actually, they typically decrease exponentially with the frequency of the vibrational or rotational degrees of freedom involved in the process (see, for example, refs. 4 and 11–14). In simple examples, as shown in refs. 10 and 15, one can appreciate quite small energy exchanges—even smaller than one part over  $10^{30}$ , in ref. 15—and confidently follow the exponential laws governing the energy exchanges over many decades.

A final question one could be interested in is whether our results have

some consequences for the reliability of numerical integration schemes in the general non-Hamiltonian case. In fact, we made use of the Hamiltonian structure only in the applications, while the basic results, namely the existence of an interpolating flow close to the one to be studied, is clearly independent of it. In particular, remark (ii) in the Introduction applies to this case, too. Nevertheless it is not clear to us whether this is relevant for the accuracy of numerical integrators. In fact, we could not produce significant examples of non-Hamiltonian flows which are interesting for numerical study and at the same time exhibit some kind of structural stability which can be used to guarantee the reliability of results.

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