Hamiltonian Approximants for Symplectic Integrators

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Abstract

Symplectic integrators do not, in general, reproduce all the features of the dynamics of the Hamiltonian systems which they approximate. For example, energy conservation is lost, and global features such as separatrices can be destroyed. We study these effects for a Hamiltonian system with a single degree of freedom and the simplest possible symplectic integrator. We look at a sequence of Hamiltonian systems of higher and higher dimension, that interpolate between the original Hamiltonian system and the symplectic integrator. In these intermediate Hamiltonian systems we can make concrete statements about energy conservation and separatrix splitting. The qualitative dynamics of the symplectic integrator seems to be inherited from these intermediate systems, and in some cases we can even deduce quantitative results for the symplectic integrator from those of the intermediate systems.

1 Introduction

Hamiltonian problems are of particular interest to physicists, mathematicians, and numerical analysts. The computer simulation of such problems, particularly over long times, presents a special challenge, since it is essential that the discrete methods employed reproduce both qualitatively and quantitatively the underlying dynamics of the continuous system they are supposed to approximate. During the last decade, many investigators have adopted *symplectic methods*. A useful tool, often invoked in the study of symplectic methods, is the construction by Lie series techniques of a sequence of Hamiltonian systems, whose exact solutions give higher and higher order approximations to the results of a given symplectic method—we review this construction below. The existence of this construction has given rise to the myth, despite copious evidence to the contrary, that using a symplectic integrator on a Hamiltonian system is equivalent to *exactly* solving a modified Hamiltonian system, the putative limit of the sequence of approximants which unfortunately in general does not exist. In this paper we present a different method to build a sequence of Hamiltonian systems, of higher and higher dimension, approximating a given symplectic integrator. We will see that unlike the Hamiltonian approximants from the Lie series method, these approximants *do* offer accurate insight into the qualitative behavior of the symplectic integrator. In particular we study energy conservation and separatrix splitting for the symplectic integrator; the Hamiltonian approximants from the Lie series method give the false impression that symplectic integrators do have a conserved energy function and do not break separatrices, while our new approximants give the correct picture.

As a simple yet easily generalizable prototype, we work with the (unit-mass) Hamiltonian in the spatial coordinate q and momentum p

$$H(q,p) = \frac{p^2}{2} + V(q) \tag{1}$$

which yields the 1 degree of freedom Hamiltonian system of autonomous equations

$$\dot{q} = p, \quad \dot{p} = -\frac{\partial V(q)}{\partial q} \tag{2}$$

corresponding to Newton's second law

$$\ddot{q} = -\frac{\partial V(q)}{\partial q} \quad . \tag{3}$$

A one–step numerical method for (2)

$$q_{n+1} = Q(q_n, p_n) \ , \quad p_{n+1} = P(q_n, p_n) \ , \tag{4}$$

is *symplectic* if the map $(q,p) \rightarrow (Q(q,p), P(q,p))$ satisfies a set of derivative-based relationships, known as the "direct conditions," and has Jacobian 1 [1], i.e. is area preserving. The direct conditions are local and do not reflect any global conservation laws—the reader is encouraged to consult Goldstein [1] for a derivation of what is meant by a symplectic transformation. Thus it can be verified that the first order Euler method [2]

$$q_{n+1} = q_n + hp_n \ , \qquad p_{n+1} = p_n - h \left. \frac{\partial V(q)}{\partial q} \right|_{q=q_n} \tag{5}$$

is not symplectic, while the method

$$q_{n+1} = q_n + hp_n \ , \qquad p_{n+1} = p_n - h \left. \frac{\partial V(q)}{\partial q} \right|_{q=q_{n+1}=q_n+hp_n} \tag{6}$$

is. This latter method, which is known as the (lowest-order) Forest-Ruth method [3], is similar to the Euler method except that the updated momentum variable p_{n+1} is obtained using the updated position variable q_{n+1}. Using the Euler method, the phase trajectory around a center with $\partial^2 V/\partial q^2 > 0$, will spiral away in a non-physical manner, while the Forest-Ruth method produces a trajectory that is neither repelled by nor attracted to the center. We will study the Forest-Ruth method in the current paper.

The rationale for preferring symplectic maps for the numerical work on a Hamiltonian system is that the exact time evolution of a Hamiltonian system is symplectic [1, 4]. Having chosen to use the method (6) to integrate (2), it is natural to ask whether there is a different Hamiltonian problem, with a "modified Hamiltonian" H_m, for which (6) is the exact time evolution map. Wisdom and Holman [5] devised a time-dependent Hamiltonian, incorporating an infinite number of δ-functions, that can produce the map (6), generalizing a result due to Lichtenberg and Lieberman [6]. However, since their Hamiltonian is neither autonomous nor bounded, we will not consider their methodology further. Instead, we will review the methodology of Dragt and Finn [7], which is otherwise universally employed, for generating a series representation for H_m.

We begin by noting that for any function $\eta\,(q,p)$

$$\frac{d\eta}{dt} = \dot{q}\frac{\partial \eta}{\partial q} + \dot{p}\frac{\partial \eta}{\partial p} = \frac{\partial H_m}{\partial p}\frac{\partial \eta}{\partial q} - \frac{\partial H_m}{\partial q}\frac{\partial \eta}{\partial p} \equiv -\left[H_m, \eta\right] \tag{7}$$

where we have employed Hamilton's equations of motion—for the modified Hamiltonian H_m, assuming that it exists—and the Poisson bracket notation, defined, for 1 degree of freedom, by

$$[A,B] \equiv \frac{\partial A}{\partial q}\frac{\partial B}{\partial p} - \frac{\partial A}{\partial p}\frac{\partial B}{\partial q} \ . \tag{8}$$

For convenience, we introduce an operator $\hat{H}_m$ defined by

$$\hat{H}_m \eta \equiv [H_m, \eta] \ . \tag{9}$$

We can then write a Lie series

$$q_{n+1} = q_n + h \left.\frac{dq}{dt}\right|_{t=t_n} + \frac{h^2}{2!} \left.\frac{d^2q}{dt^2}\right|_{t=t_n} + ... = q_n - h\hat{H}_m \, q|_{t=t_n} + \frac{h^2}{2}\hat{H}_m^2 \, q|_{t=t_n} \mp ... \quad , \tag{10}$$

and analogously for p_{n+1}. We want the latter equation, together with its counterpart for p_{n+1}, to reproduce the mapping (6). This is the criterion we use to determine H_m. We write H_m as a series

$$H_m \left(q, p, h\right) = H_0 \left(q, p\right) + hH_1 \left(q, p\right) + h^2 H_2 \left(q, p\right) + ... \, . \tag{11}$$

Inserting the latter into (10) and its equivalent for p_{n+1}, keeping only terms of order h, and requiring equality, up to order h with the RHS of (6) gives

$$\frac{\partial H_0 \left(q, p\right)}{\partial p} = p \ , \quad \frac{\partial H_0 \left(q, p\right)}{\partial q} = \frac{\partial V \left(q\right)}{\partial q} \ . \tag{12}$$

Solving the first of these equations yields

$$H_0 \left(q, p\right) = \frac{p^2}{2} + \mathcal{F} \left(q\right) \ , \tag{13}$$

where $\mathcal{F}\left(q\right)$ is any function of q, solving the second gives

$$H_0 \left(q, p\right) = V \left(q\right) + \mathcal{G} \left(p\right) \ , \tag{14}$$

where $\mathcal{G}\left(p\right)$ is any function of p. Combining the latter two expressions gives

$$H_0 \left(q, p\right) = \frac{p^2}{2} + V \left(q\right) \ , \tag{15}$$

up to an unimportant additive constant. Once H_0 has been determined in this way, we return to (10), insert (11) and require equality with the RHS of (6) up to order h^2, and thus obtain expressions for $\frac{\partial H_1(q,p)}{\partial q}$ and $\frac{\partial H_1(q,p)}{\partial p}$, which can be solved for H_1. Continuing this procedure a few steps we obtain

$$H_1 \left(q, p\right) = \tfrac{1}{2} p \frac{\partial V}{\partial q} \ , \quad H_2 \left(q, p\right) = \tfrac{1}{12} \left[p^2 \frac{\partial^2 V}{\partial q^2} + \left(\frac{\partial V}{\partial q}\right)^2 \right] \ , \quad H_3 \left(q, p\right) = \tfrac{1}{12} p \frac{\partial^2 V}{\partial q^2} \frac{\partial V}{\partial q} \ , \ \ldots \tag{16}$$

It rapidly becomes clear that the recursive procedure for computing terms in H_m—which is intimately related to the Baker-Campbell-Hausdorff (BCH) algorithm—is algebraically intensive, and is best left to a symbolic manipulator such as Maple or Mathematica; the reader is referred to Sanz-Serna and Calvo [4] for details, as well as a rich discussion of symplectic integration methods and their properties. The $H_m \left(q, p\right)$ terms become systematically more complicated as m increases.

The upshoot of the above construction is that we have a sequence of Hamiltonians (obtained by taking an increasing number of terms in the series representation for H_m), that apparently give better and better approximations to the dynamics of the symplectic integrator. The only problem is that relatively little is known about the convergence properties of the series (11). Varadarajan [8] is one of the few investigators to develop a theorem regarding the convergence of Lie series, but here it appears to be applicable only to the special case of the simple harmonic oscillator, i.e., $V(q) \propto q^2$ which corresponds to a linear force law. See Lessnick [9] for a treatment of the summation of the Lie series. On the other hand, ample evidence is now available showing that the radius of convergence (in h) of the series (11) is at best small. For nonlinear problems, Sanz-Serna [10] showed that in general the series does not converge and it is impossible to find an autonomous differential system so that the computed points exactly lie on trajectories of the system. Iserles *et al.* [11] and Newman *et al* [12], among others, also have confirmed that the modified Hamiltonian does not, as a rule, exist. Moreover, Lichtenberg and Lieberman's [6] now classic textbook on regular and chaotic dynamics contains a dramatic refutation of the existence of a modified Hamiltonian. They employed (6) applied to the simple pendulum $V(q) = 1 - \cos q$, a transformation commonly known as the "standard map," The phase plane representations that they obtained do not in general show points residing on closed curves or level sets. Instead, their Figure 4.3 reveals island chains and global stochasticity. Thus, in summary, we see there is a wide gap between the qualitative dynamics of the Hamiltonian approximants computed by the Lie series approach and that of the symplectic integrator.

In this paper, we propose an alternate approach to deriving a sequence of Hamiltonian systems which approximate (6). Using the first equation in (6) to eliminate the momentum variable from the second equation, we obtain the recursion

$$\frac{q_{n+1} - 2q_n + q_{n-1}}{h^2} = -\frac{\partial V(q_n)}{\partial q_n} \ . \tag{17}$$

This expression, first proposed by Störmer (1907) [13], is the simplest member of a family of "multistep methods"—see the textbooks by Henrici [2] and Hairer *et al.* [14]. This class of methods has a venerable history in celestial mechanics, beginning with the apparition of Halley's comet at the beginning of the previous century, since it makes use of previously determined estimates of the acceleration in order to (implicitly) establish the time-variability in the forcing term. Its stability and error properties have been explored in depth recently by Goldstein [15], while Grazier *et al.* [16] recently employed a high order version of this methodology—structured to minimize computational roundoff error while keeping the truncation error of the method below machine precision—in applications to the outer solar system. As a practical matter, symplectic methods—especially those of higher order—tend

to be more complex than such non-symplectic methods and, as a result, can be less efficient and/or accurate than simpler schemes.

Our key observation is the following: if the Störmer method is a good approximation for equation (3), we would expect it to be an even better approximation for the series of equations

$$\ddot{q} + \frac{h^2}{12}\,\ddddot{q} = -\frac{\partial V(q)}{\partial q}\ , \tag{18}$$

$$\ddot{q} + \frac{h^2}{12}\,\ddddot{q} + \frac{h^4}{360}\,\dddddddot{q} = -\frac{\partial V(q)}{\partial q}\ , \tag{19}$$

$$\vdots \qquad .$$

Thus our proposal is to study what wse will now call—for abvious reasons—the Forest-Ruth-Störmer method by looking at the sequence of continuous systems

$$\sum_{i=0}^{r} \frac{2q^{(2i+2)}h^{2i}}{(2i+2)!} = -\frac{\partial V(q)}{\partial q} \qquad r = 1, 2, \ldots \quad , \tag{20}$$

and in particular to derive useful information about the symplectic scheme (6) from these systems.

At this stage it is not clear the systems (20) are Hamiltonian. Section 2 is devoted to their variational and Hamiltonian formulation, thus justifying the title of this paper. The systems are of higher and higher dimension. From both the variational and Hamiltonian approaches we deduce that the systems (20) have a conserved quantity, which is critical in the sequel.

In Section 3 we show how to partially integrate each of the systems (20), reducing each one to an integro-differential system in a 2-dimensional phase space. This allows immediate comparison of (20) with (3) in its Hamiltonian form (2). Herein lies the strength of our approach. By increasing r we can make the system (20) as good an approximation as we want to the Forest-Ruth-Störmer method. But at the same time it is rather easier to compare the dynamics of (20) and (3) than to directly compare the dynamics of (17) and (3).

In Sections 4 and 5 we use our approach to look at some of the more subtle aspects of the dynamics of symplectic integrators. In Section 4 we reconsider the question of energy conservation for the map (6). As we have explained at length above, (6) does not admit a conserved energy function. But in practice symplectic integrators do display remarkably "good" energy-conservation properties (see [4] section 10.1.2 or [17] section 1.4 for existing explanations). In our approach, the symplectic scheme (6) arises as the limit of the continuous systems (20), each of which are Hamiltonian and have a conserved energy in a suitable

higher dimensional phase space. On the reduction to a 2-dimensional phase space the conserved energy becomes non-local and time-dependent, but is still sufficient to guarantee that most orbits are highly concentrated around the level set of a suitable function (the function depending on the orbit, thus allowing for the crossing of orbits). It seems that (6) inherits precisely these properties.

Section 5 deals with separatrix splitting from our approach. For the case of the simple pendulum, $V(q) = 1 - \cos q$, the Forest-Ruth-Störmer method is equivalent to the standard map, for which exponentially small separatrix splitting has been observed [18]. In the setting of (6) this means that the stable manifold of the fixed point $(\pi, 0)$ and the unstable manifold of the fixed point $(-\pi, 0)$ do not coincide, as is the case for the continuum system (3), but instead intersect transversally at an angle that is exponentially small in h. This is an example of the crossing of orbits of (6) mentioned above. We show that separatrix splitting happens in all the systems (20), and provide an easy way to show exponential smallness.

Section 6 contains some conclusions and suggestions for further work.

2 Variational and Hamiltonian Structure of (20)

In this section we show that the systems (20) can be obtained both from a variational principle and as Hamilton's equations for a suitable Hamiltonian. In fact the same is true for all equations of the form

$$\sum_{i=0}^{r} a_i q^{(2i+2)} = -\frac{\partial V(q)}{\partial q} \ , \tag{21}$$

where $a_1, \ldots, a_r$ are constants, so we work with this more general system. We assume $a_r \neq 0$ without loss of generality. For the special case of the Forest-Ruth-Störmer method, $q_i = 2\,h^{2i}/\,(2i+2)!$.

Proposition 1. Equation (21) is the Euler-Lagrange equation for the Lagrangian

$$L = \tfrac{1}{2} \sum_{i=0}^{r} (-1)^i a_i \left(q^{(i+1)}\right)^2 - V(q) \tag{22}$$

which makes $\int dt\, L\left(q, \dot{q}, ..., q^{(r+1)}\right)\, dt$ an extremum.

Proof. A trivial calculation. •

Proposition 2. The system (21) has a conserved quantity

$$K = \sum_{i=0}^{r} a_i \left(\sum_{j=0}^{i-1} (-1)^j q^{(j+1)} q^{(2i+1-j)} + (-1)^i \frac{1}{2} \left(q^{(i+1)}\right)^2 \right) + V(q) \ . \tag{23}$$

Proof. A trivial calculation. Or, if you want, you can apply Noether's theorem [19] to the Lagrangian (22), which is invariant under time translation. •

Proposition 3. Equation (21) is equivalent to Hamilton's equations for the Hamiltonian

$$H(q_0,\dots,q_r,p_0,\dots,p_r) = \frac{(-1)^r}{2a_r}p_r^2 + \sum_{i=0}^{r-1} p_i q_{i+1} + \frac{1}{2}\sum_{i=1}^{r}(-1)^i a_{i-1}q_i^2 + V(q_0) \ . \tag{24}$$

Proof. Hamilton's equations

$$\dot{q}_i = \frac{\partial H}{\partial p_i} \ , \qquad \dot{p}_i = -\frac{\partial H}{\partial q_i} \ , \tag{25}$$

yield

$$\begin{aligned}
\dot{q}_i &= q_{i+1} \ , \qquad i = 0,\dots,r-1 \ , && (26)\\
\dot{q}_r &= (-1)^r \frac{p_r}{a_r} \ , && (27)\\
\dot{p}_0 &= -\frac{\partial V(q_0)}{\partial q_0} \ , && (28)\\
\dot{p}_i &= -p_{i-1} - (-1)^i a_{i-1} q_i \ , \qquad i = 1,\dots,r \ . && (29)
\end{aligned}$$

From (26)

$$q_i = q_0^{(i)} \ , \qquad i = 1,\dots,r \ , \tag{30}$$

and from (27)

$$p_r = (-1)^r a_r q_0^{(r+1)} \ . \tag{31}$$

Writing (29) in the form

$$p_{i-1} = -\dot{p}_i - (-1)^i a_{i-1} q_i \ , \qquad i = 1,\dots,r \ , \tag{32}$$

we can recursively find $p_{r-1}, p_{r-2}, \dots, p_0$ in terms of q_0. The result takes the simple form

$$p_i = (-1)^i \sum_{j=0}^{r-i} a_{i+j} q_0^{(i+2j+1)} \ , \qquad i = 0,\dots,r \ . \tag{33}$$

In particular we have

$$p_0 = \sum_{j=0}^{r} a_j q_0^{(2j+1)} \ , \tag{34}$$

and thus from (28) we see q_0 must satisfy (21). Thus from a solution of Hamilton's equations for the Hamiltonian (24) we recover a solution of (21), and conversely, given a solution of (21) we recover a solution of (26)-(29) using (30) and (33). •

Notes: 1. Since

$$\det\left(\frac{\partial^2 H}{\partial p_i \partial p_j}\right) = 0 \ , \tag{35}$$

our Hamiltonian is degenerate, in the sense of classical mechanics, and it is not clear in what way the variational principle for (21) and the Hamiltonian formulation of (21) are related. The usual proof of equivalence of Lagrangian and Hamiltonian formulations in classical mechanics requires nondegeneracy.

2. H of course is a conserved quantity. Substituting (30) and (33) in H we recover the conserved quantity K defined in (23).

3. A useful alternate form of the Hamiltonian H, if $a_0, \ldots, a_{r-1}$ are all positive, is

$$H = \frac{1}{2}\sum_{i=0}^{r}(-1)^i\frac{p_i^2}{a_i} + \frac{1}{2}\sum_{i=1}^{r}(-1)^i\left(\sqrt{a_{i-1}}q_i + \frac{(-1)^i p_{i-1}}{\sqrt{a_{i-1}}}\right)^2 + V(q_0)\ . \tag{36}$$

If $a_i = (-1)^i\alpha_i$, $i = 0, \ldots, r$, where all the α_i are positive, then we can write

$$H = \frac{1}{2}\sum_{i=0}^{r}\frac{p_i^2}{\alpha_i} - \frac{1}{2}\sum_{i=1}^{r}\left(\sqrt{\alpha_{i-1}}q_i - \frac{p_{i-1}}{\sqrt{\alpha_{i-1}}}\right)^2 + V(q_0)\ . \tag{37}$$

4. The Hamiltonian (24) is certainly not unique, and we have the freedom to make canonical changes of coordinates. In light of this, the identification of the q_i as positions and the p_i as momenta is, at least for $i \geq 1$, arbitrary. Equations (36) and (37) would arguably look better if for all odd i we were to "switch" q_i and p_i (by which we mean replace q_i by p_i and p_i by $-q_i$). This would prevent the need for linear combinations of q's and p's in the second sum, but on the other hand it complicates the first sum. Likewise, this change complicates the proof of proposition 3. Equations (39), (41) and (42)-(43) below, however, are all made a little cleaner by switching q_1 and p_1, and the reader is asked to mentally make this cosmetic change if he/she finds it helpful.

Examples: 1. Equation (18). $r = 1$, $a_0 = 1$, $a_1 = h^2/12$.

$$\begin{aligned} H &= -\frac{6}{h^2}p_1^2 + p_0q_1 - \frac{1}{2}q_1^2 + V(q_0) &(38)\\ &= \frac{1}{2}p_0^2 + V(q_0) - \frac{6}{h^2}p_1^2 - \frac{1}{2}(p_0 - q_1)^2\ . &(39)\end{aligned}$$

Note this has the form of the Hamiltonian for (2) minus a sum of nonnegative terms. It becomes useful to think of q_1 and p_1 as "hidden variables." In particular, we observe that the trajectory for q_0 and p_0 lies on an outside a level surface. The rapid oscillations—to be described below—of the hidden variables renders the orbit "thick" or "fuzzy" and established a conceptual link to critical ingredients in KAM theory.

2. Equation (19). $r = 2$, $a_0 = 1$, $a_1 = h^2/12$, $a_2 = h^4/360$.

$$\begin{aligned} H &= \frac{180}{h^4}p_2^2 + p_0q_1 + p_1q_2 - \frac{1}{2}q_1^2 + \frac{h^2}{24}q_2^2 + V(q_0) &(40)\\ &= \frac{1}{2}p_0^2 + V(q_0) - \frac{6}{h^2}p_1^2 - \frac{1}{2}(p_0 - q_1)^2 + \frac{180}{h^4}p_2^2 + \frac{1}{2}\left(\frac{h}{\sqrt{12}}q_2 + \frac{\sqrt{12}}{h}p_1\right)^2\ . &(41)\end{aligned}$$

Note this has the form of the Hamiltonian (39) for (18) plus a sum of nonnegative terms. The role of hidden variables and of "thickness" or "fuzziness" becomes especially clear.

3 The dynamics of (20) as a perturbation of (3)

The aim in this section is to compare the dynamics of (20) and (3). To do this we show that (20) can be written in a manner very similar to the Hamiltonian formulation (2) of (3).

The starting point is the $\dot{q}_0$ and $\dot{p}_0$ equations in the Hamiltonian formulation given for (20) in Section 2. These are

$$\dot{q_0} = q_1 \ , \qquad \dot{p_0} = -\frac{\partial V(q_0)}{\partial q_0} \ , \tag{42}$$

where now q_1 is not quite p_0, but instead

$$p_0 = q_1 + \frac{h^2}{12}\ddot{q_1} + \ldots + \frac{2h^{2r}}{(2r+2)!}q_1^{(2r)} \ . \tag{43}$$

To write an analog of (2) we need to invert this last equation to write q_1 in terms of p_0. Let $\lambda_1, \ldots, \lambda_{2r}$ denote the $2r$ roots of the equation

$$1 + \frac{z^2}{12} + \frac{z^4}{360} \ldots + \frac{2z^{2r}}{(2r+2)!} = 0 \ . \tag{44}$$

On the basis of numerical evidence we have, we will assume the roots of this equation to be distinct, for any r (see the appendix for more information). The roots λ_i evidently come in complex–conjugate plus–minus quadruples, except for roots on the imaginary axis, which come in plus–minus pairs (there are clearly no real roots). Assuming that the roots are distinct[1], we can use the method of variation of constants to obtain the general solution of (43),

$$q_1 = \sum_{i=1}^{2r} A_i e^{\lambda_i t/h} + \frac{1}{h}\int_0^t \left(\sum_{i=1}^{2r} V_i e^{\lambda_i (t-s)/h} \right) p_0(s) ds \ , \tag{45}$$

where the A_i, $i = 1, \ldots, 2r$, are arbitrary constants, and the V_i, $i = 1, \ldots, 2r$, are constants satisfying

$$\sum_{i=1}^{2r} V_i = \sum_{i=1}^{2r} V_i \lambda_i = \sum_{i=1}^{2r} V_i \lambda_i^2 = \ldots = \sum_{i=1}^{2r} V_i \lambda_i^{2r-2} = 0 \ , \tag{46}$$

$$\sum_{i=1}^{2r} V_i \lambda_i^{2r-1} = \frac{(2r+2)!}{2} \ . \tag{47}$$

[1]If the roots are not distinct—although we believe that they are—then we can employ a simple variant of the method of variation of constants, simply by altering the relevant basis set. Suppose that a root $\hat{\lambda}$ has multiplicity M. then, $t^i e^{\hat{\lambda} t}$ for $i = 0, ..., M-1$ are also solutions of (43) an can be employed in lieu of $e^{\lambda_i t}$ for M values of i.

Note that the condition for the existence of a unique solution V_i of equations (46)-(47) is the nonvanishing of a Vandermonde determinant, which is automatically nonzero if the λ_i are distinct [20].

Proposition 4.

$$(1) \qquad \sum_{i=1}^{2r} V_i \lambda_i^{2n} = 0 \ , \qquad n \in \mathbf{Z} \ . \tag{48}$$

$$(2) \qquad \sum_{i=1}^{2r} \frac{V_i}{\lambda_i} = -1 \ , \qquad \sum_{i=1}^{2r} \frac{V_i}{\lambda_i^3} = \frac{1}{12} \ , \qquad \sum_{i=1}^{2r} \frac{V_i}{\lambda_i^5} = \begin{cases} -\frac{1}{144} & r = 1 \\ -\frac{1}{240} & r \geq 2 \end{cases} \ . \tag{49}$$

$$(3) \qquad \text{For } r \geq n \ , \ n \in \mathbf{N} \ , \ \sum_{i=1}^{2r} \frac{V_i}{\lambda_i^{2n+1}} \ \text{ is independent of } r \ .$$

Proof. (1) Without loss of generality we assume $\lambda_i = -\lambda_{r+i}$, $i = 1, \ldots, r$. We then have $V_i = -V_{r+i}$, $i = 1, \ldots, r$ and the identity follows trivially.

(2) For each $i = 1, \ldots, 2r$ we have

$$1 + \frac{\lambda_i^2}{12} + \frac{\lambda_i^4}{360} \ldots + \frac{2\lambda_i^{2r}}{(2r+2)!} = 0 \ , \tag{50}$$

and so

$$\frac{1}{\lambda_i} + \frac{\lambda_i}{12} + \frac{\lambda_i^3}{360} \ldots + \frac{2\lambda_i^{2r-1}}{(2r+2)!} = 0 \ . \tag{51}$$

Multiplying by V_i, summing over i and using (46)-(47) we have

$$\sum_{i=1}^{2r} \frac{V_i}{\lambda_i} + 1 = 0, \tag{52}$$

proving the first identity. Similarly, starting with

$$\frac{1}{\lambda_i^3} + \frac{1}{12\lambda_i} + \frac{\lambda_i}{360} \ldots + \frac{2\lambda_i^{2r-3}}{(2r+2)!} = 0 \ , \tag{53}$$

multiplying by V_i, summing over i and using (46) and (52) gives

$$\sum_{i=1}^{2r} \frac{V_i}{\lambda_i^3} - \frac{1}{12} = 0, \tag{54}$$

the second identity. For the third identity, we start with

$$\frac{1}{\lambda_i^5} + \frac{1}{12\lambda_i^3} + \frac{1}{360\lambda_i} \ldots + \frac{2\lambda_i^{2r-5}}{(2r+2)!} = 0 \ , \tag{55}$$

multiply by V_i, sum over i and use (46) to get

$$\sum_{i=1}^{2r} \frac{V_i}{\lambda_i^5} + \frac{1}{12} \sum_{i=1}^{2r} \frac{V_i}{\lambda_i^3} + \frac{1}{360} \sum_{i=1}^{2r} \frac{V_i}{\lambda_i^1} = 0 \tag{56}$$

if $r \geq 2$, but

$$\sum_{i=1}^{2r} \frac{V_i}{\lambda_i^5} + \frac{1}{12} \sum_{i=1}^{2r} \frac{V_i}{\lambda_i^3} = 0 \tag{57}$$

if $r = 1$. The result follows.

(3) follows by an obvious extension of the arguments used to prove (2). •

The first identity in part (2) of the above proposition allows us to integrate (45) by parts to obtain

$$q_1(t) = p_0(t) + \sum_{i=1}^{2r} B_i e^{\lambda_i t/h} + \int_0^t \left(\sum_{i=1}^{2r} V_i \frac{e^{\lambda_i (t-s)/h}}{\lambda_i} \right) \dot{p}_0(s) ds \ , \tag{58}$$

where the B_i, $i = 1, \ldots, 2r$, are new arbitrary constants. Thus we have our final result:

Proposition 5. For each $r = 1, 2, \ldots$, (20) can be written as a perturbation of (2) as:

$$\dot{q}(t) = p(t) + \sum_{i=1}^{2r} B_i e^{\lambda_i t/h} - \int_0^t \left(\sum_{i=1}^{2r} V_i \frac{e^{\lambda_i (t-s)/h}}{\lambda_i} \right) \frac{\partial V(q(s))}{\partial q(s)} ds \ , \tag{59}$$

$$\dot{p}(t) = -\frac{\partial V(q(t))}{\partial q(t)} \ , \tag{60}$$

where the B_i are arbitrary constants.

Here (and henceforth) we have dropped the suffix on q_0, p_0, which should cause no confusion.

Example. In the case $r = 1$, $\lambda_1 = -\lambda_2 = i\sqrt{12}$, $V_1/\lambda_1 = V_2/\lambda_2 = -1/2$, and the system (59)-(60) becomes

$$\dot{q}(t) = p(t) + A \sin\left(\frac{\sqrt{12}}{h} t \right) + B \cos\left(\frac{\sqrt{12}}{h} t \right) + \int_0^t \cos\left(\frac{\sqrt{12}}{h} (t-s) \right) \frac{\partial V(q(s))}{\partial q(s)} ds, \tag{61}$$

$$\dot{p}(t) = -\frac{\partial V(q(t))}{\partial q(t)} \ , \tag{62}$$

where A, B are constants.

Comparison of (59)-(60) and (2). In the passage from (3) to (20) we see we have added two terms to the first equation in (2). To understand the first extra term, we start by supposing that the λ_i are pure imaginary (which is only actually true in the case $r = 1$, but we will describe the necessary modification below). Then the extra first term in (59) is simply a high frequency oscillatory forcing term. For small B_i the orbit will be a low-amplitude, high-frequency oscillation around an orbit determined by the other terms in the equation. The reason the constants B_i are there is because the in passing from (3) to (20) we have passed from a 2nd order system to a $(2r + 2)$th order system. Thus instead of a single orbit through each point in the (q, p) plane there is now $2r$-dimensional family of orbits, all oscillating around some fundamental orbit. In other words, the first extra term in (59) describes a "thickening" "fuzziness" of the underlying orbit.

In fact unless $r = 1$, some of the λ_i do have nonzero real part (see the appendix), which for sufficiently large positive or negative times will have a substantial effect. As we will see later, it seems that in the limit $r \to \infty$ it is the pure imaginary λ_i that are of greatest significance. For finite r, though, the effect of the nonzero real parts of some of the λ_i is that our picture of a "thickening" of orbits is only valid for finite time intervals.

Moving now to the second extra term in (59), we integrate repeatedly by parts, always integrating the exponential factors, thus developing an asymptotic expansion in h. A single integration by parts gives

$$\dot{q}(t) = p(t) + \sum_{i=1}^{2r} \tilde{B}_i e^{\lambda_i t/h} - h \int_0^t \sum_{i=1}^{2r} \frac{V_i}{\lambda_i^2} e^{\lambda_i (t-s)/h} \frac{\partial^2 V(q(s))}{\partial q(s)^2} \dot{q}(s) ds \ , \tag{63}$$

where

$$\tilde{B}_i = B_i - h \frac{V_i}{\lambda_i^2} \frac{\partial V(q(0))}{\partial q(0)} \tag{64}$$

are new constants, and we have used (1) in Proposition 4. (63) functions as a bootstrap equation: if we know $\dot{q}$ to order h^n we can insert on the RHS to find $\dot{q}$ to order h^{n+1}. Also we see from (63) that

$$\dot{q}(t) = p(t) + \sum_{i=1}^{2r} \tilde{B}_i e^{\lambda_i t/h} + O(h) \ , \tag{65}$$

telling us how to start the bootstrap procedure. Substituting (65) into (63) and integrating by parts gives us the result to the next order which is just

$$\dot{q}(t) = p(t) + \sum_{i=1}^{2r} \tilde{B}_i e^{\lambda_i t/h} - h \sum_{i=1}^{2r} \frac{V_i \tilde{B}_i}{\lambda_i^2} e^{\lambda_i t/h} \int_0^t \frac{\partial^2 V(q(s))}{\partial q(s)^2} ds + O(h^2) \ . \tag{66}$$

The only correction at this order is addition of a new oscillatory term. At the next order a large number of new oscillatory terms enter, but so does a single other term. The result can be written

$$\dot{q}(t) = p(t) + \sum_{i=1}^{2r} B_i(t) e^{\lambda_i t/h} + \frac{h^2}{12} p(t) \frac{\partial^2 V(q(t))}{\partial q(t)^2} + O(h^3) \ . \tag{67}$$

The appearance of a nonoscillatory term at order h^2 is no surprise. (20) is an order h^2 perturbation of (3), and so in addition to the "thickening the orbits", we expect to see order h^2 corrections in the passage from (2) to (59)-(60) . Continuing the bootstrap procedure it is possible to see that the content of the second extra term in (59) is a series of corrections to the "underlying dynamics" at orders $h^2, h^4, \ldots$, and a menagerie of oscillatory terms. It is possible to determine the nonoscillatory terms without calculating the oscillatory terms. If the nonoscillatory terms in $\dot{q}$ are of the form $\sum_{n=0}^{\infty} h^{2n} A_n(q,p)$, consistency with (63) requires

$$\sum_{n=0}^{\infty} h^{2n} A_n(q,p) = p + \sum_{s=1}^{\infty} h^{2s} \left(\sum_{i=1}^{2r} \frac{V_i}{\lambda_i^{2s+1}} \right) \left(-\frac{\partial V}{\partial q} \frac{\partial}{\partial p} + \left(\sum_{m=0}^{\infty} h^{2m} A_m \right) \frac{\partial}{\partial q} \right)^s \frac{\partial V}{\partial q} \ . \tag{68}$$

The infinite series here are formal, not convergent. The sums $\sum_{i=1}^{2r} V_i/\lambda_i^{2s+1}$ can be computed as in Proposition 4.

Thus we have the full picture of the corrections in the passage from (2) to (59)-(60) . The orbits undergo $O(h^2)$ corrections, and "thickening" due to the arbitrary constants and the oscillatory forcing terms. In fact this is all standard from regarding (20) as a singular perturbation of (3). The standard approach of singular perturbation theory (see for example [21]) would have as solve (20) by first looking for a formal solution in powers of h^2, with leading term a solution of (3), and then adding a rapidly changing correction term to account for initial or boundary conditions. We are fortunate in having the exact formula (59)-(60) , and that we do not need to rely on asymptotic, but divergent, pertrubation series in h^2.

4 Do Symplectic Integrators Have a Conserved Energy Function?

In this section we wish to look at the question whether there is a function on phase space conserved under the map (6). We now have an obvious candidate for this. The systems (20) are closer and closer approximations to (17) which is equivalent to (6). But in Section 2 we have seen that each of the systems (20) has a conserved quantity. However, as noted earlier, this does *not* mean that the orbit of q_0 and p_0 lies on a level surface of the true (i.e., original) Hamiltonian. What happens to this as $r \to \infty$?

We need to write the conserved quantity of (20)—which we have in a variety of forms (23),(24),(36)—in terms of just the q and p variables used in (59)-(60) . This is a rather arduous procedure, but the answer is simple to check once you have it, so we just state the result. We start with the case $r = 1$.

Proposition 6a. The quantity

$$\begin{aligned}\tilde{H} &= \frac{1}{2}p^2 + V(q) - \frac{1}{2}\left(A + \int_0^t \sin\left(\frac{\sqrt{12}s}{h}\right)\frac{\partial V(q(s))}{\partial q(s)}ds\right)^2 \\ &\quad -\frac{1}{2}\left(B + \int_0^t \cos\left(\frac{\sqrt{12}s}{h}\right)\frac{\partial V(q(s))}{\partial q(s)}ds\right)^2 \end{aligned} \tag{69}$$

is a conserved quantity for the flow (61)-(62).

For the general case, using the fact that the λ_i come in plus-minus pairs, we assume without loss of generality that $\lambda_i = -\lambda_{r+i}$, $i = 1, \ldots, r$ and thus $V_i = -V_{r+i}$, $i = 1, \ldots, r$. With this choice it is straightforward to verify the following:

Proposition 6. The quantity

$$\begin{aligned}\tilde{H} &= \frac{1}{2}p^2 + V(q) \\ &+ \sum_{i=1}^{r} \frac{V_i}{\lambda_i}\left(B_i + \int_0^t e^{-\lambda_i s/h}\frac{\partial V(q(s))}{\partial q(s)}ds\right)\left(B_{i+r} + \int_0^t e^{\lambda_i s/h}\frac{\partial V(q(s))}{\partial q(s)}ds\right) \end{aligned} \tag{70}$$

is a conserved quantity for the flow (59)-(60). This reduces to (69) in the case $r = 1$. Not surprisingly, this Hamiltonian is reminiscent of that obtained in canonical perturbation theory, using the Von Zeipel procedure [22], for transformations of the Hamilton-Jacobi equation.

Comments on $\tilde{H}$: This is not a conserved quantity in the usual sense. It is nonlocal, explicitly t-dependent and depends on the constants B_i.

The dependence on the B_i is expected, and reflects the fact that there are multiple orbits, labelled by the B_i, through each point in the (q, p) plane. Ignoring for a moment the other complications in $\tilde{H}$ (nonlocality and time-dependence), the existence of a conserved quantity depending on constants in this manner is an interesting notion, which means that each individual orbit has the property that it lies on the level set of some function, but nevertheless orbits can cross, because the constants change from orbit to orbit.

The nonlocality and expicit t-dependence of $\tilde{H}$ can be dealt with as follows. Using the integration by parts procedure from Section 3 we can compute $\tilde{H}$ to any finite order in h. The result will be a sum of terms local in q, p and oscillatory terms (as in Section 3 we ignore the real parts of the λ_i for our initial discussion). The local terms alone must provide a conserved quantity of the relevant order (i.e. a quantity whose derivative vanishes modulo terms of higher order). It is possible to write a formula for the local terms in $\tilde{H}$ in terms of the local terms $A_n(p, q))$ in $\dot{q}$ (see (68)):

$$\bar{H} = \frac{1}{2}p^2 + V(q) - \frac{1}{2}\sum_{n=0}^{\infty} h^{2n+2}\left[\sum_{i=1}^{2r}\frac{V_i}{\lambda_i^{2n+3}}\right]\left[\sum_{s=0}^{2n}(-1)^s D^s\left(\frac{\partial V}{\partial q}\right)\cdot D^{2n-s}\left(\frac{\partial V}{\partial q}\right)\right], \tag{71}$$

where

$$D = -\frac{\partial V}{\partial q}\frac{\partial}{\partial p} + \left(\sum_{m=0}^{\infty} h^{2m}A_m\right)\frac{\partial}{\partial q}. \tag{72}$$

In particular for the first few terms we have

$$\bar{H} = \frac{1}{2}p^2 + V(q) - \frac{h^2}{24}\left(\frac{\partial V}{\partial q}\right)^2 + \frac{h^4}{96c}\left[2p^2\frac{\partial V}{\partial q}\frac{\partial^3 V}{\partial q^3} - p^2\left(\frac{\partial^2 V}{\partial q^2}\right)^2 - 2\left(\frac{\partial V}{\partial q}\right)^2\frac{\partial^2 V}{\partial q^2}\right] + \dots, \tag{73}$$

where $c = 3$ if $r = 1$ and $c = 5$ if $r \geq 2$. The reader is invited to check that $\dot{\bar{H}} = O(h^6)$ using just the equations of motion $\dot{q} = q_1$, $\dot{p} = -\partial V/\partial q$, where $p = q_1 + h^2\ddot{q}_1/12$ if $r = 1$

and $p = q_1 + h^2\ddot{q}_1/12 + h^4\,\dddot{q}_1\,/360$ if $r \geq 2$. We once again emphasize that the perturbative conserved quantity $\bar{H}$ is a formal power series in h, and is asymptotic, but not convergent.

Returning now to the full conserved quantity $\tilde{H}$: as explained in the last paragraph, after a sufficient number of integrations by parts $\tilde{H}$ is the sum of some local terms, some oscillatory terms, and terms of higher order in h. Assuming that the constants B_i are chosen so the amplitude of the oscillatory terms is not too high, and that we have reached an order where the "higher order term" can genuinely be neglected, we can conclude that orbits will be highly concentrated around a level set of the function given by the local terms. This picture is on the (false) assumption that the λ_i are pure imaginary. Reintroducing their real parts means that the picture will change for sufficiently large positive or negative t, when what we have called the oscillatory terms in fact become large.

The limit $r \to \infty$. We are now ready to discuss the limit $r \to \infty$. In this limit the equation (20) becomes the Forest-Ruth-Störmer method (17). Our first observation is that in the perturbative series $\bar{H}$ defined in (71), the term of order h^{2n} does not change for $r > n$. Thus the $r \to \infty$ limit of this series is well-defined, and gives rise to the perturbative conserved quantity for the Forest-Ruth-Störmer method. We say "gives rise to" as opposed to "is", because the usage of p in (71) differs from the usage of p in equations (11), (15), and (16) in which we gave the first few terms of the perturbative conserved quantity for the Forest-Ruth-Störmer method. In (71), for large r, p and q satisfy by $\dot{q} = q_1$, $\dot{p} = -\frac{\partial V}{\partial q}$, $p = q_1 + h^2\ddot{q}_1/12 + h^4\,\dddot{q}_1\,/360 + \ldots$ In (11),(15),(16), the relation of p and q is from the first equation of (6), $p = (q(t_n + h) - q(t_n))/h = \dot{q} + h\ddot{q}/2 + h^2\,\ddot{q}\,/6 + \ldots$. A brief calculation shows that to obtain (11) from (71) it is necessary to replace p in (71) by

$$p + \frac{h}{2}\frac{\partial V}{\partial q} + \frac{h^2}{12}p\frac{\partial^2 V}{\partial q^2} + \frac{h^3}{24}p\frac{\partial V}{\partial q}\frac{\partial^2 V}{\partial q^2} + \ldots \ . \tag{74}$$

Our second observation is that since the systems (20) approximate (17) to arbitrary accuracy, and since for the systems (20) we have seen that orbits are concentrated around level sets of the perturbative conserved quantity, this should hold true for (17) too, giving the expected behavior for a symplectic integrator. However, it is difficult to say if this is the case only for long, finite times, or for all time. In the limit $r \to \infty$ the equation (44) becomes

$$\frac{\cosh z - 1}{z^2} = 0 \ , \tag{75}$$

with double roots at $z = 2\pi i n$ for every nonzero integer n. This suggests that in the limit $r \to \infty$ the real parts of the λ_i may not be significant. There are several subtleties here though, as for fixed r only a fraction of the λ_i are close to the limit points $2\pi i n$, and also

because in the limit the roots are double, while we have been assuming they are single (see the appendix describing the behavior of the λ_i).

We are hopeful that further detailed study of the implications of the conserved quantity (70) for the systems (20) will yield the r dependence of the time for which orbits remain close to orbits of the perturbative conserved quantity, which will allow us to take the $r \to \infty$ limit. It is even possible that we might be able to make sense of the explicit expression $\tilde{H}$ in the limit $r \to \infty$. This requires information on the limit of the constants V_i/λ_i, which we do not as of yet have. We emphasize that even if it is possible to make sense of $\tilde{H}$ in the limit $r \to \infty$, it of course will not yield a standard conserved quantity for the symplectic integrator, this is prohibited by the classic results of Ge and Marsden [23].

To summarize: For the systems (20) we have presented a nonlocal, time-dependent, constant-dependent conserved quantity, from which we can derive the formal perturbative conserved quantity, and which keeps orbits close to the level sets of the perturbative conserved quantity for long finite times. In the $r \to \infty$ limit we recover the perturbative conserved quantity of the symplectic integrator (6), and see an origin for the known "almost energy conserving" properties of the symplectic integrator.

5 Separatrix Splitting

In this section we take $V(q) = 1 - \cos q$, i.e. we restrict to the case of the simple pendulum, and our aim is to study separtrix splitting for the systems (20), or equivalently (59)-(60). We start by looking at the case $r = 1$, i.e. the system (18) or equivalently (61)-(62).

The system (61)-(62) has fixed points at $(q_0, p_0) = (0, 0), (\pm\pi, 0)$ (take $A = B = 0$). Let us look for solutions with $(q(t), p(t)) \to (\pi, 0)$ as $t \to \infty$. Expanding the cosine in the integral in (61) we have

$$\begin{aligned} \dot{q}(t) &= p(t) + \sin\left(\frac{\sqrt{12}}{h}t\right)\left[A + \int_0^t \sin\left(\frac{\sqrt{12}}{h}s\right)\sin q(s) ds\right] \\ &\quad + \cos\left(\frac{\sqrt{12}}{h}t\right)\left[B + \int_0^t \cos\left(\frac{\sqrt{12}}{h}s\right)\sin q(s) ds\right] \ . \end{aligned} \tag{76}$$

If we want a solution with $\dot{q}(t) \to 0$ as $t \to \infty$ we clearly need to choose

$$A = -\int_0^\infty \sin\left(\frac{\sqrt{12}}{h}s\right)\sin q(s) ds \ , \qquad B = \int_0^\infty \cos\left(\frac{\sqrt{12}}{h}s\right)\sin q(s) ds \ . \tag{77}$$

With this choice (76) becomes

$$\dot{q}(t) = p(t) - \int_t^\infty \cos\left(\frac{\sqrt{12}}{h}(t-s)\right)\sin q(s) ds \ , \tag{78}$$

and we of course still have

$$\dot{p}(t) = -\sin q(t) \ . \tag{79}$$

Consider the solution of (78)-(79) such that $(q(t), p(t)) \to (\pi, 0)$ as $t \to \infty$, the stable manifold of the point $(\pi, 0)$. To fix the time translation invariance let us specify $q(0) = 0$. From (79), $\dot{p}(0) = 0$, so if we look at this orbit in the (q, p) plane, it has zero gradient when it crosses $q = 0$, just like the stable manifold of $(\pi, 0)$ for the unperturbed pendulum (2). However $p \neq \dot{q}$!! Suppose we look at the orbit in the $(q, \dot{q})$ plane. Then the gradient as it crosses $q = 0$ is just $\ddot{q}(0)/\dot{q}(0)$. Differentiating (78) and using (79) we have

$$\ddot{q}(t) = \frac{\sqrt{12}}{h} \int_t^\infty \sin\left(\frac{\sqrt{12}}{h}(t-s)\right) \sin\left(q(s)\right) ds \ . \tag{80}$$

Thus we arrive at

Proposition 7a. The gradient at $q = 0$ of the stable manifold of $(\pi, 0)$ in the $(q, \dot{q})$ plane is

$$-\frac{\sqrt{12}}{h\dot{q}(0)} \int_0^\infty \sin\left(\frac{\sqrt{12}}{h}s\right) \sin\left(q(s)\right) ds \ , \tag{81}$$

where $q(t)$ is the solution of (18) corresponding to the stable manifold.

At first glance this proposition does not look at all useful: If we know $q(t)$ then we can compute $\ddot{q}(0)/\dot{q}(0)$ directly and have no need for (81)! The utility of the proposition lies in the fact that inserting the perturbative approximation for $q(t)$ in (81) gives a much better approximation to the true gradient than inserting it in the naive formula $\ddot{q}(0)/\dot{q}(0)$ (which gives 0). In fact a first approximation to the gradient can be obtained by inserting in (81) the $q(t)$ corresponding to the stable manifold of $(\pi, 0)$ for the *unperturbed* pendulum (2),

$$q(t) = 2\mathrm{arctan}(\sinh t) \ . \tag{82}$$

Using this gives an approximation for the gradient of

$$-\frac{\sqrt{12}}{h} \int_0^\infty \sin\left(\frac{\sqrt{12}}{h}s\right) \frac{\sinh s}{\cosh^2 s} ds = -\frac{\sqrt{3}}{hi} \int_{-\infty}^\infty \exp\left(i\frac{\sqrt{12}}{h}s\right) \frac{\sinh s}{\cosh^2 s} ds \ . \tag{83}$$

This last integral is straightforward to find by contour integration techniques. The dominant contribution is from the double pole of the integrand at $s = i\pi/2$, and evaluating this gives an approximation for the gradient of

$$-\frac{12\pi}{h^2} e^{-\sqrt{3}\pi/h} \approx -\frac{37.7}{h^2} e^{-\sqrt{3}\pi/h} \ . \tag{84}$$

Some careful numerical work gives the correct formula for the gradient to be approximately

$$-\frac{78.2}{h^2} e^{-\sqrt{3}\pi/h} \ . \tag{85}$$

In the next paragraph we explain how to improve the theoretical prediction by using the $q(t)$ obtained from perturbation theory, not simply that of the unperturbed pendulum; but we note that use of the unperturbed $q(t)$ already suffices to give the general form of the gradient, and particularly that it is exponentially small.

Using a symbolic manipulator it is straightforward to obtain the first few terms in the perturbation series for the stable manifold of $(\pi, 0)$ for the perturbed pendulum (18):

$$\begin{aligned} q(t) &= 2\arctan(\sinh t) + \frac{h^2}{12}\left(-\frac{t}{\cosh t} + 3\frac{\sinh t}{\cosh^2 t}\right) + \frac{h^4}{144}\left(\frac{13}{4}\frac{t}{\cosh t} - \frac{1}{4}\frac{(t^2+31)\sinh t}{\cosh^2 t}\right. \\ &\quad \left. -\frac{3t}{\cosh^3 t} + \frac{41}{2}\frac{\sinh t}{\cosh^4 t}\right) + \frac{h^6}{1728}\left(-\frac{255t + t^3}{24\cosh t} + \frac{(1287 + 50t^2)\sinh t}{40\cosh^2 t}\right. \\ &\quad \left. + \frac{(525t + t^3)}{12\cosh^3 t} - \frac{(5502 + 45t^2)\sinh t}{20\cosh^4 t} - \frac{41t}{\cosh^5 t} + \frac{2169\sinh t}{5\cosh^6 t}\right) + \dots \ . \end{aligned} \tag{86}$$

To all orders in h^2 the perturbation series solution is an odd function of t (and thus to all orders $\ddot{q}(0) = 0$). It follows that we can replace (81) by

$$-\frac{\sqrt{3}}{ih\dot{q}(0)}\int_{-\infty}^{\infty} \exp\left(i\frac{\sqrt{12}}{h}s\right)\sin(q(s)ds \ . \tag{87}$$

The integral can be evaluated by completing the contour in the upper half plane, and is dominated by contributions from the pole at $s = i\pi/2$. The leading term in the series in h^2 for $\sin q(s)$ has a double pole at $s = i\pi/2$, the $O(h^2)$ term has a fourth order pole, the $O(h^4)$ term a sixth order pole and so on. Thus there will be $O(e^{-\sqrt{3}\pi/h}/h^2)$ contributions to the gradient from every order in the perturbation series of $q(t)$. Table 1 shows the coefficient multiplying $-e^{-\sqrt{3}\pi/h}/h^2$ as a function of the maximal power of h^2 retained. By fitting a curve of the form $a + b/n + c/n^2$ to the last 6 data points (a, b, c are coefficients to be fitted, n is the power of h^2) we find a limit as $n \to \infty$ of the coefficient of 78.2, in agreement with the numerical result (85).

Before leaving this section, we note that it is also possible to predict exponentially small separatrix splitting for (18) using the power series methods of [24].

Separatrix splitting for (20) for arbitrary r.

For general r the stable manifold of $(\pi, 0)$ for the system (59)-(60) is more than one dimensional. Because some of the λ_i have nonzero real part, not all the B_i are fixed uniquely by the requirement that the system admit a solution tending to $(\pi, 0)$. We focus on a one-dimensional submanifold of the stable manifold given by the system

$$\dot{q}(t) = p(t) + \int_t^{\infty} \sum_{i=1}^{2r} \frac{V_i}{\lambda_i} e^{\lambda_i(t-s)/h} \sin q(s) ds \ , \tag{88}$$

$$\dot{p}(t) = -\sin q(t) \ . \tag{89}$$

highest power of h^2 used	coefficient (exact)	coefficient (5 s.f.)
1	18π	56.549
2	$\frac{41}{2}\pi$	64.403
3	$\frac{2169}{100}\pi$	68.141
4	$\frac{2630051}{117600}\pi$	70.260
5	$\frac{48261629}{2116800}\pi$	71.626
6	$\frac{161396252183}{6985440000}\pi$	72.585
7	$\frac{55087526993651}{2361078720000}\pi$	73.298
8	$\frac{130540216171272433}{5553257149440000}\pi$	73.849
9	$\frac{1897530085396862066083}{80244565809408000000}\pi$	74.289
10	$\frac{24779363408224296282104087}{10428583772590663680000000}\pi$	74.647
11	$\frac{16419754034984973727950224 87}{6882865289909838028800000 0}\pi$	74.946
12	$\frac{19709932099706514602144907492855 07}{82343423621424420712857600000000}\pi$	75.198
13	$\frac{51392984861216591921592831818657033}{21409290141570349385342976000000000}\pi$	75.414
14	$\frac{17413905764397482368236689753508185557 1}{72363400678507780922459258880000000 00}\pi$	75.601
15	$\frac{29720470376110857838299627957443887005906553 07}{12323668044051571360547117935411200000000000 0}\pi$	75.764

Table 1: The coefficient multiplying $-e^{-\sqrt{3}\pi/h}/h^2$ in (87) as a function of the maximal power of h^2 retained in the perturbative solution $q(t)$.

The full stable manifold of $(\pi, 0)$ is obtained by addding terms of the form $e^{-at}(C\cos bt + D\sin bt)$ to the RHS in (88), where $a+bi$ is any root with positive real part of (44) and C, D are constants. As we have explained, we do not expect the roots of (44) with nonzero real part to play a role in the $r \to \infty$ limit, which is why we ignore such terms. From here on we refer to the solution of (88)-(89) as "the stable manifold" without further qualification. Arguing as in the $r = 1$ case we have:

Proposition 7. The gradient at $q = 0$ of the stable manifold of $(\pi, 0)$ in the $(q, \dot{q})$ plane is

$$\frac{1}{h\dot{q}(0)} \int_0^\infty \sum_{i=1}^{2r} V_i e^{-\lambda_i s/h} \sin q(s) ds \ , \tag{90}$$

where $q(t)$ is the solution of (88)-(89) corresponding to the stable manifold.

As before we choose the λ_i so that $\lambda_{i+r} = -\lambda_i$, $V_{i+r} = -V_i$, $i = 1, \ldots, r$. Our plan is to compute the gradient by substituting the perturbative solution for $q(s)$ into (90). Since the perturbative solution is odd, the gradient formula becomes

$$-\frac{1}{h\dot{q}(0)} \int_{-\infty}^\infty \sum_{i=1}^{r} V_i e^{\lambda_i s/h} \sin q(s) ds \ . \tag{91}$$

Without loss of generality we can assume the λ_i for $i = 1, \ldots, r$ have positive imaginary part. Then the integral can be computed by closing the contour in the upper half plane, and is clearly dominated by contributions from the pole at $s = i\pi/2$ and (for large r) by the two of the λ_i that are close to $2\pi i$ (see the appendix). Thus at once we see the gradient for large r is of order $O(e^{-\pi^2/h}/h^2)$, in agreement with the results of [18].

We do not deal here with the computation of the coefficient multiplying $e^{-\pi^2/h}/h^2$. Computing the perturbative solution of (20) is just as easy as computing the perturbative solution of (18). However for large r it becomes increasingly difficult to accurately computate the coefficients V_i. Since for large r pairs of roots of (44) coallesce, the system (46)-(47) becomes more and more ill-conditioned. We hope to deal with the question of the limit of the V_i in a later work.

6 Conclusions and Further Directions

We have studied the systems (20) as a "bridge" between the continuum system (3) and its discretization (17); we have seen in what sense the systems (20) conserve energy and in what sense not, and that they exhibit separatrix splitting. Although some doubt remains over the long time behavior, it is fair to say that the critical differences in qualitative dynamics

between (3) and (17) can be seen when comparing (3) to any of the systems (20). In particular, the simplest perturbed system (18) can be usefully used to study the qualitative dynamics of the discrete map (17). We expect such an approach to discrete dynamical systems (approximating by a continuum system, but retaining the lowest order correction in h) might be a useful tool in many other problems. It also immediately shows us that we should think of discretization of a continuum system as a singular perturbation: and thus we should not be surprised to uncover effects, like separatrix splitting in our problem, that are not analytic in h.

As explained in section 4 there remains some work to be done to see if any sense can be made of the full conserved quantity $\tilde{H}$ in the limit $r \to \infty$. This requires rigorous results on the λ_i and the V_i (solutions of (44) and (46)-(47)). Even numerical computation of the V_i for large r is very difficult. We note that once this problem has been overcome, it should be straightforward to use the methods of section 5 to compute the full asymptotic formula for separatrix splitting, as given in [18].

It is reasonable to suspect that the symplecticity of (17) is what is responsible for the smallness of the separatrix splitting, and we are currently looking at this phenomenon for general symplectic methods, of the form

$$q_n = q_{n-1} + h\frac{\partial S(p_{n-1}, q_n, h)}{\partial p_{n-1}} \ , \qquad p_n = p_{n-1} - h\frac{\partial S(p_{n-1}, q_n, h)}{\partial q_n} \ , \tag{92}$$

as well as for nonsymplectic methods. Of course, it is to be hoped that we will be able to make statements for systems more general than the simple pendulum.

Finally, we wonder if there may be a physical interpretation of the basic tool we have used in this paper, that a discrete dynamic system can be viewed as a limit of a sequence of higher and higher dimensional (but degenerate) continuum systems.

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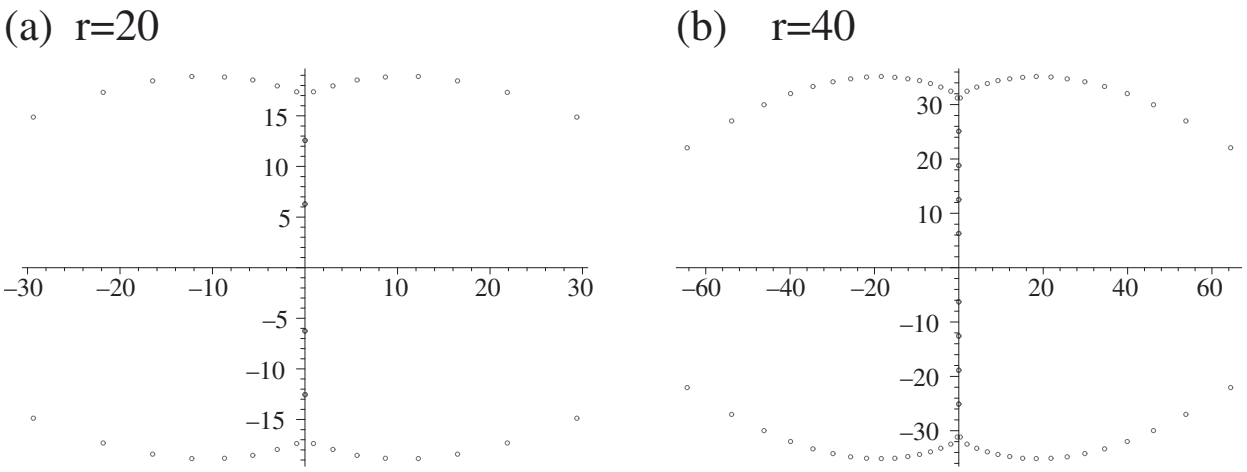

Figure 1: Solutions of characteristic polynomial (44) for $r = 20$ and $r = 40$

Appendix: The Solutions of (44)

We briefly outline what we know about the roots of (44). We have looked at the roots of (44) numerically for values of r up to 60. In all these cases we have found (44) has distinct roots. For large r, a little less than a quarter of these roots lie on, or very close to, the imaginary axis. More precisely, for each integer n with $|n| < r/\pi e$ it seems there is a pair of roots close to $2\pi in$, and if r is odd there are also single roots on the imaginary axis close to $\pm 2\pi in$, where n is the smallest integer greater than $r/\pi e$. In figure 1 we show the roots when $r = 20$ and $r = 40$. The points on the imaginary axis are in fact pairs of roots lying very close to the axis, one on each side (for r odd the pairs are on the axis). The rest of the roots lie on 4 arcs well away from the real axis.

One of the implications of the above results is that for any positive integer n, for $r < (n\pi e) - 1$ there is no root of (44) close to $2\pi in$, but for $r > n\pi e$ there is a pair of nearby roots, and in fact these roots converge to $2\pi in$ *exponentially fast* as r increases. To illustrate this we list below the imaginary part of the roots closest to the real axis for small even r:

r	2	4	6	8
imaginary part	4.12150858067	5.23349005117	6.01489826089	6.27265462330
r	10	12	14	16
imaginary part	6.28310259934	6.28318499591	6.28318530653	6.28318530718

By $r = 16$ the imaginary part is already 2π to 12 figure accuracy.

Results very similar to these for the roots of (44) have been observed for the roots of Bernoulli polynomials in [25].

In the body of the paper we have assumed that the roots of (44) are indeed distinct, for

all r, and we have also assumed that the patterns established above are correct in general, namely that as r increases we have more and more roots closer and closer to the points $2\pi in$, and that the roots with signifcant real part get further from the origin.

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