The Numerical Integration of Hamiltonian Systems

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1 Introduction

We study methods for the numerical integration of ordinary differential equations specifically aimed at the important family of Hamiltonian systems. Algorithms are presented which preserve all Poincaré integral invariants and therefore mimic relevant qualitative properties of the theoretical solutions. The emphasis is on Runge–Kutta schemes. Numerical illustrations are provided.

In ordinary differential equations (ODEs), the most general initial value problem (IVP) can be easily written down in the form

$$dy/dt = \phi(y), \qquad y(0) = \eta, \tag{1.1}$$

with ϕ a given R^d-valued function and η a given vector in R^d. This is in sharp contrast with the situation in partial differential equations, where the problem specification is necessarily involved (domain, boundary conditions, differential operator, etc....). The simplicity of the format above has made it possible to formulate, analyse and implement numerical methods aimed at the 'general problem' (1.1). On the one hand, such a generality should be viewed positively. In the analysis of numerical methods for (1.1) a few simple and comprehensive hypotheses can be made under which powerful and elegant results are possible (see e.g. [8]). General purpose, versatile codes have been developed (e.g. [21]) where each IVP in ODEs can be accommodated by simply providing η and a subroutine for the evaluation of the right hand side function ϕ. On the other hand, it is clear that generality is not a feature without drawbacks. A 'general method' cannot possibly be optimal when applied to all individual cases. Stiff problems [2] provide a well-known instance of an important family of IVPs which cannot be integrated (or at least cannot be integrated efficiently) with a general method. The goal of the present contribution is to consider numerical ODE methods specifically aimed at the class of Hamiltonian systems of ODEs

that so frequently arise in the mathematical description of nondissipative problems.

2 Hamiltonian Systems

Hamiltonian systems are of the form (see e.g. [1])

$$dp/dt = f(p,q), \qquad dq/dt = g(p,q), \tag{2.1}$$

where p, q are vectors, $p = (p^{(1)}, \ldots, p^{(g)})$, $q = (q^{(1)}, \ldots, q^{(g)})$,($g$ is the number of degrees of freedom) and the components $f^{(i)}, g^{(i)}$ of the vector valued functions f and g are given by

$$f^{(i)} = -\partial H/\partial q^{(i)}, \qquad g^{(i)} = \partial H/\partial p^{(i)}, \qquad 1 \le i \le g, \tag{2.2}$$

with $H = H(p^{(1)}, \ldots, p^{(g)}; q^{(1)}, \ldots, q^{(g)})$ a real function of $2g$ real variables (the Hamiltonian function). Clearly (2.1) is a particular case of the system in (1.1) with $y = (p,q), d = 2g, \phi = (f,g)$. Non-autonomous Hamiltonian systems, where H, f, g depend explicitly on t, also arise in applications. While most of the contents of this paper may easily be extended to the non-autonomous case, we have chosen to stay within the autonomous case in order to simplify the presentation. The system (2.1) may arise either directly in the modelling of a physical system with a finite number of degrees of freedom or as a spatial discretization of an infinite-dimensional Hamiltonian system [7]. In applications H often corresponds to the physical energy of the system.

Throughout the paper we assume that q (the vector of coordinates) takes values in an open subset Ω of R^g, that p takes values in the whole of R^g and that H is a smooth function defined in $X = R^g \times \Omega$, the *phase space*. For real t, we denote by F_t the t-flow of (2.1), i.e. F_t is the mapping in X that transforms each point (p_0, q_0) into the point $(p,q) = F_t(p_0, q_0)$ where (p,q) is the value at time t of the solution of (2.1) with initial value (p_0, q_0) at $t = 0$. For a given (p_0, q_0), $F_1(p_0, q_0)$ is well defined at least for small values of $|t|$.

Hamiltonian systems possess a number of features that are not shared by the 'general problem' (1.1). It has become increasingly clear that all such specific features derive from a single geometric property, namely from the conservation by the Hamiltonian flow F_t of the *symplectic structure* [1] of the phase space X. Some appreciation of the meaning of this conservation is essential in what follows and, accordingly, indications in this connection will now be presented.

We first consider the one degree of freedom case $g = 1$. Then the phase space X is a subset of the two-dimensional plane (p,q) and each open, bounded subset Y of X has a well-defined area $S(Y)$. Conservation of the

symplectic structure means that F_t preserves the orientation of the plane and that $S(Y) = S(F_t(Y))$ for each open, bounded subset Y of X, and for each real t (more precisely, for each real t small enough for $F_t(Y)$ to be defined). Upon writing the area as an integral, it is easily seen that an equivalent formulation states that the determinant of the Jacobian ∂F_t of F_t with respect to (p,q) is identically 1. Note that, in particular, this implies that if F_t is linearized near an equilibrium of (2.1) then the eigenvalues λ_1, λ_2 of the linearization satisfy $\lambda_1\lambda_2 = 1$, which in turn guarantees that, generically, the equilibrium is a centre (λ_1, λ_2 complex conjugate with unit modulus) or a saddle (real eigenvalues with $|\lambda_1| < 1 < |\lambda_2|$). Thus, the stable spiral equilibria found in dissipative systems are ruled out here.

Before leaving the case $g = 1$, it is convenient to note that the property of conservation of area, i.e. the property $\det(\partial F_t) = 1$, can be expressed in a third alternative manner. In fact, the oriented area of Y is nothing but the integral over Y of the differential form $dp \wedge dq$, so that conservation of oriented area is equivalent to the property that F_t leaves invariant the form $dp \wedge dq$. In geometric terms the form $dp \wedge dq$ introduces a symplectic structure in X, just as $((dp)^2 + (dq)^2)^{1/2}$ defines a metric or Riemannian structure. In symplectic geometry, the capability of measuring two-dimensional areas plays the role that is played by the measurement of lengths in metric geometry.

In the case $g > 2$, conservation of the symplectic structure means that F_t preserves the differential form

$$\omega = dp \wedge dq = dp^{(1)} \wedge dq^{(1)} + \cdots + dp^{(g)} \wedge dq^{(g)} \tag{2.3}$$

Thus, if for each bounded, open subset Y of X, we denote by $S^*(Y)$ the result of adding the oriented two-dimensional areas of the g projections of Y onto the planes $(p^{(1)}, q^{(1)})$, ..., $(p^{(g)}, q^{(g)})$, then $S^*(Y) = S^*(F_t(Y))$ for each Y. This property can also be expressed in terms of the Jacobian matrix of F_t (not just in terms of the Jacobian determinant); for the details see e.g. [6].

The conservation of ω entails the conservation of the exterior powers $\omega^2 = \omega \wedge \omega, \omega^3 = \omega \wedge \omega \wedge \omega, \ldots$ whose integrals are the classical Poincaré invariants [1]. In particular, the invariance of ω^g under the Hamiltonian flow means that the ($2g$-dimensional) oriented element of volume in the phase space X is an invariant. This is the well-known Liouville theorem [1] which leads to the Poincaré recurrence property.

3 Canonical Integration Methods

A transformation $\Phi : X \to X$ is said to be *canonical* if it preserves the differential form ω in (2.3). With this terminology, the main property of the Hamiltonian flow may be expressed by saying that, for each t, F_t is a

canonical mapping. Each one-step method for the numerical integration of (2.1) is given by a mapping $(p,q) = G_h(p_0,q_0)$ that advances the solution over a time step of length h. For a p-th order method, G_h differs from the flow F_h in terms $O(h^{p+1})$. Since the structure of the Hamiltonian flow F_h is determined by its canonical character, it may seem advisable to use numerical methods for which G_h is also a canonical mapping (for each real step h and each Hamiltonian function H). Such numerical methods are called canonical or symplectic [6], [11]. Unfortunately, standard numerical methods, such as explicit Runge–Kutta methods, are *not* canonical. A survey of the available canonical methods will be given in Sections 5–7 below and we now examine the benefits that may be expected from switching from standard integration methods to their canonical counterparts.

In short time computations, that G_h approximates F_h ensures, via the classical error bound [8], that the computed points $G_h(p_0,q_0)$, $G_h(G_h(p_0,q_0)),\ldots$ will remain close to the exact points $F_h(p_0,q_0)$, $F_h(F_h(p_0,q_0)),\ldots$. In this sort of computation, switching to a canonical scheme is likely to be of secondary importance when compared with the advantages to be gained by using higher order standard methods or smaller values of h. However in situations where a very high number of steps must be computed, the accuracy of any method necessarily drops. If a canonical method is used, the numerical solution will retain some qualitative features possessed by the exact solution. If a non-canonical method is used, the computed solution is likely to be meaningless, since the dynamics of F_h and G_h may be entirely different.

An alternative wording of the previous observation may be given. A Hamiltonian system S_{Ham} is a mathematical model for the physics of a (nondissipative) system S_{Ph}. When using a numerical method, S_{Ham} is in turn replaced by a system S_{Num}. If the method is canonical, S_{Num} may be viewed (backward error analysis) as an *exact* model of a physical system in the neighbourhood of S_{Ph}. For noncanonical methods such an interpretation is not possible as S_{Num} does not possess a number of features that are always present in actual physical problems. This issue is discussed further in [3].

In a different vein, F. Vadillo and the present author [17], [18] have shown how the canonical character of a discretization can be used, in conjunction with the Kolmogorov–Arnold–Moser theory [1], to derive useful stability results.

4 Conservation of Energy

For autonomous Hamiltonian systems (2.1), the Hamiltonian or energy H is a conserved quantity i.e. $H(F_t(p_0,q_0)) = H(p_0,q_0)$. It has often been argued in the literature that exact conservation of energy $H(G_h(p_0,q_0)) = H(p_0,q_0)$ is a desirable feature for a numerical method to possess. Claims in that direction were made by the present author in [12], [13], [16]. Before we critically discuss this issue, we would like to observe that, if we fix an *individual* initial point (p_0,q_0) and advance it in time by a numerical method to get $G_h(p_0,q_0)$, then it is possible to compare the energy $H(G_h(p_0,q_0))$, after the step with the initial energy $H(p_0,q_0)$ to see whether conservation has occurred. This is not the case for the conservation of ω, whose checking involves the knowledge of the *transformation* G_h rather than the mere knowledge of the transformed point $G_h(p_0,q_0)$. This is in line with a deeper remark: the conservation of a symplectic structure imposes strong constraints on the dynamics of a system; conservation of energy only restricts the dynamics by forcing the orbits to be in the $(2g-1)$-dimensional surface $E_0 = \{(p,q) : H(p,q) = H(p_0,q_0)\}$, while leaving them entirely free within this surface. Thus energy-preserving schemes cannot be expected to capture all the relevant qualitative properties of the continuous system.

Numerical experimentation [15],[19] has now convinced the author that the fact that a scheme preserves energy exactly is neither necessary nor sufficient in order to guarantee a good practical performance. Furthermore, a surprising result of Ge and Marsden [23] ensures that for a *general* Hamiltonian system, if a mapping G_h is symplectic and conserves H exactly, then G_h coincides with F_h after a suitable reparametrization of time. Thus energy conservation and canonicity cannot hold simultaneously. Further references on conservation of energy are [14] and [20].

5 Constructing Canonical Integration Methods

The history of the development of canonical integration methods is surveyed in [3]. For our purposes, it is enough to note that the first occurrences of symplectic schemes in the open literature are due to Ruth in 1983 [11] and Feng in 1985–1986 [5], [6]. Most available methods (see [3]) have been constructed from the point of view of Classical Mechanics by using generating functions. In fact, every canonical transformation G_h of the phase space X can be obtained via a corresponding scalar-valued generating function S_h. The $2g$ scalar components of the vector-valued mapping G_h are simple linear combinations of the $2g$ partial derivatives of S_h with respect to its arguments [6]. Feng and his co-workers have obtained symplectic methods of arbitraily high order of accuracy. Unfortunately these methods employ higher and higher derivatives of the functions f and g in (2.1), a feature that makes them not very useful in the development of a code aimed at arbitrary Hamiltonians. The paper [3] by Channell and Scovel gives further examples of the construction of symplectic schemes via generating functions. Often, the methods in [3] are not completely numerical and symbolic manipulation has to be resorted to in order to generate

the actual algorithm. Again, it is clear that such techniques are not very appealing in connection with the design of a general Hamiltonian code.

In the course of a visit to Prof. Feng's institute in Beijing in 1987, the present author was led to consider the question of whether the familiar class of (implicit) Runge–Kutta (RK) methods contains symplectic schemes. Recall that an s-stage RK method, as applied to the 'general problem' (1.1), can be described as follows. Let y_n be the approximation at the current step. Compute s internal vectors $Y_1, \ldots, Y_s$ by solving the system

$$Y_i = y_n + \sum_{j=1}^{s} a_{ij} h\phi(Y_j), \qquad 1 \le i \le s. \tag{5.1}$$

Then compute the approximation y_{n+1} at the advanced time level as

$$y_{n+1} = y_n + \sum_{i=1}^{s} b_i h\phi(Y_i). \tag{5.2}$$

The coefficients a_{ij}, b_i define the method. Here and later h may depend on n.

Theorem 5.1. [14] If for each $i, j = 1, \ldots, s$

$$b_i a_{ij} + b_j a_{ji} - b_i b_j = 0, \tag{5.3}$$

then the RK method (5.1-5.2) is symplectic.

Classes of RK methods for which (5.3) holds had been studied by Cooper [4]. In particular, for each s, the method based on Gauss–Legendre quadrature with maximal order $2s$, due to Butcher, is symplectic. Theorem 5.1 has also been discovered by Lasagni [10] and Suris [22].

6 Partitioned Canonical Runge–Kutta Methods

The fact that the equations (2.1) fall naturally into two groups leads to the consideration of partitioned RK methods [8], where the p and q equations are treated with different coefficients. With a self-explanatory notation

$$Y_i = p_n + \sum_{j=1}^{s} a_{ij} h f_j; \;\; Z_i = q_n + \sum_{j=1}^{s} A_{ij} h g_j, \;\; 1 \le i \le s. \tag{6.1}$$

$$p_{n+1} = p_n + \sum_{i=1}^{s} b_i h f(Y_i, Z_i), \qquad q_{n+1} = q_n + \sum_{i=1}^{s} B_i h g(Y_i, Z_i). \tag{6.2}$$

In the remainder of this section we shall always assume that we are dealing with *separable* Hamiltonians, i.e. the case where $H(p,q)$ is of the form

$T(p) + V(q)$. Separable Hamiltonians arise very frequently, with T, V representing the kinetic and potential energies respectively. The next result, which is given for the first time in this paper, can be established by following the techniques of the proof of Theorem 1 in [14].

Theorem 6.1 Assume that in (2.1) the Hamiltonian H is separable. Then, if for $1 \le i, j \le s$

$$b_i A_{ij} + B_j a_{ji} - b_i B_j = 0 \tag{6.3}$$

(cf. (5.3)), the method (6.1) - (6.2) is canonical when applied to (2.1).

Particular canonical partitioned RK schemes were constructed by Ruth [11]. This author works with generating functions and does not employ the Runge–Kutta formalism. He considers a family of three stage methods of the form (6.1) - (6.2), with *six* free parameters $b_i, B_i, 1 \le i \le 3$, and

$$\begin{aligned} a_{11} = a_{21} = a_{31} = b_1, \qquad & A_{21} = A_{31} = B_1, \\ a_{22} = a_{32} = b_2, \qquad & A_{32} = B_2, \\ a_{33} = b_3, \qquad & \\ a_{ij} = 0, \text{ if } i < j, \qquad & A_{ij} = 0, \text{ if } i \le j, \end{aligned} \tag{6.4}$$

and shows canonicity for separable Hamiltonians. Furthermore (6.4) has third order of accuracy under the *five* order conditions

$$b_1 + b_2 + b_3 = B_1 + B_2 + B_3 = 1, b_2 B_1 + b_3(B_1 + B_2) = 1/2, \tag{6.5}$$

$$b_2 B_1^2 + b_3(B_1 + B_2)^2 = B_1 b_1^2 + B_2(b_1 + b_2)^2 + B_3(b_1 + b_2 + b_3)^2 = 1/3.$$

Of importance is the fact that, even though $a_{ii} \neq 0$, the algorithm (6.4) is *explicit* since for separable Hamiltonians Y_i is not an argument of $f_i = f(Z_i)$ in (6.1).

Ruth points out that the choice $B_1 = 2/3$ leads in (6.5) to a particularly simple solution for the remaining parameters. We prefer to choose the free parameter as follows. A separable Hamiltonian system is left invariant by simultaneously interchanging the roles of kinetic and potential energies, coordinates and momenta and reversing the direction of t. It is easy to see (cf. [8] pp. 214–215) that the same invariance will be true for the numerical method (6.4) if

$$b_1 = B_3, b_2 = B_2, b_3 = B_1. \tag{6.6}$$

The system (6.5)–(6.6) (8 equations for six unknowns) is compatible and yields

$$B_1 = 0.91966152 \tag{6.7}$$

a root of $12z^4 - 24z^2 + 16z - 3 = 0$.

Furthermore, the present author employs (6.4) so as to have to have canonical integrations with *fourth order* accuracy. In fact, it is enough to use before each step of the method one step (of the same length h)

of the adjoint method ([8] pp.214–215). It is easy to see that, since the combination of the two steps is symmetric, the combined method must have fourth order of global accuracy at each step. (This enhancement of the order does not depend on the specific choice of the free parameter B_1.) Over two-steps the composite scheme can be written as

$$\begin{aligned} Y_1 &= q_{2n} + B_3 hg(p_{2n}), & Z_2 &= p_{2n} + b_3 hf(Y_1), \\ Y_2 &= Y_1 + B_2 hg(Z_2), & Z_3 &= Z_2 + b_2 hf(Y_2), \\ q_{2n+1} &= Y_2 + B_1 hg(Z_3), & p_{2n+1} &= p_{2n} + b_1 hf(q_{2n+1}), \end{aligned} \tag{6.8}$$

$$\begin{aligned} Z_1^* &= p_{2n+1} + b_1 hf(q_{2n+1}), & Y_2^* &= q_{2n} + B_1 hg(Z_1^*), \\ Z_2^* &= Z_1^* + b_2 hf(Y_2^*), & Y_3^* &= Y_2^* + B_2 hg(Z_2^*), \\ p_{2n+2} &= Z_2^* + b_3 hf(Y_3^*), & q_{2n+2} &= Y_3^* + B_3 hg(p_{2n+2}). \end{aligned} \tag{6.9}$$

The whole algorithm is explicit. Furthermore only five evaluations of f are needed over the two steps. This is important since in many applications the evaluation of f (the forces) in (2.1) is far more expensive than the evaluation of g, for instance $g(p)$ is simply p if

$$T = \frac{1}{2}(p_1^2 + \cdots + p_g^2), \tag{6.10}$$

the most frequently occurring kinetic energy. Incidentally, it should be noted that for separable Hamiltonians with kinetic energy (6.10) the system (2.1), after elimination of $p = dq/dt$, can be reduced to the second order form $d^2q/dt^2 = f(q)$ and then treated with a Runge–Kutta–Nyström (RKN) method [8]. Suris [22] studies conditions for RKN algorithms to be symplectic in the case (6.10) and suggests a three-stage, third order method, which turns out to be equivalent to the method (6.4), with Ruth's choice of the free parameter $B_1 = 2/3$. Suris does not appear to be aware of Ruth's work.

7 Numerical illustrations

Clearly, extensive numerical experimentation is needed to assess the advantages, if any, to be gained by the use of canonical integration techniques and to identify the best canonical schemes. Here we only report two experiments that illustrate the preceding material. Of course, the canonical methods described above would only be competitive with available software if implemented in a code with variable time-steps, something which as yet has not been done. Therefore our experiments refer to fixed-h implementations. Nevertheless, we have chosen the test problems in such a way that, as the integration proceeds, the time-scale of the solutions does not change significantly, so that variable time-steps are not crucial. As a reference noncanonical method we have used the 'classical' fourth-order

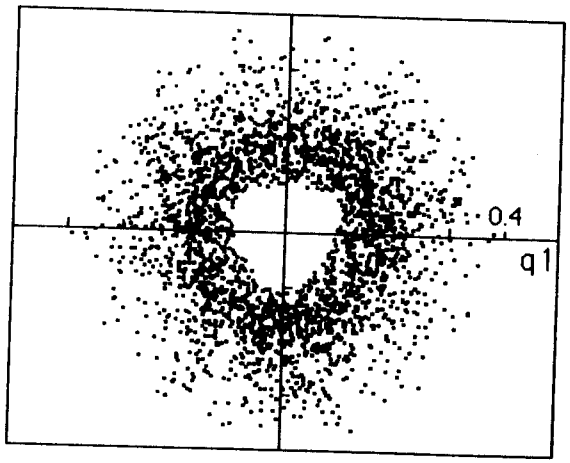

Figure 1. Hénon–Heiles problem. Standard method.

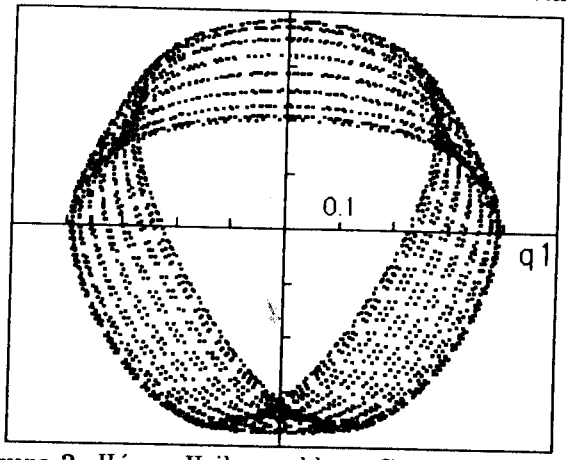

Figure 2. Hénon–Heiles problem. Canonical method.

RK scheme, while as an example of a canonical integrator we have used the fourth-order method (6.5) – (6.9).

(i) **Hénon–Heiles Hamiltonian**. This is given by

$$H = (1/2)(p_1^2 + p_2^2 + q_1^2 + q_2^2) + q_1^2 q_2 - (1/3)q_2^3. \tag{7.1}$$

For solutions near the origin the Hamiltonian is close to that of the double harmonic oscillator

$$(1/2)(p_1^2 + p_2^2 + q_1^2 + q_2^2), \tag{7.2}$$

whose solutions are 2π-periodic. It is of interest to ascertain whether orbits of (7.1) away from the origin retain the regular character of the orbits of

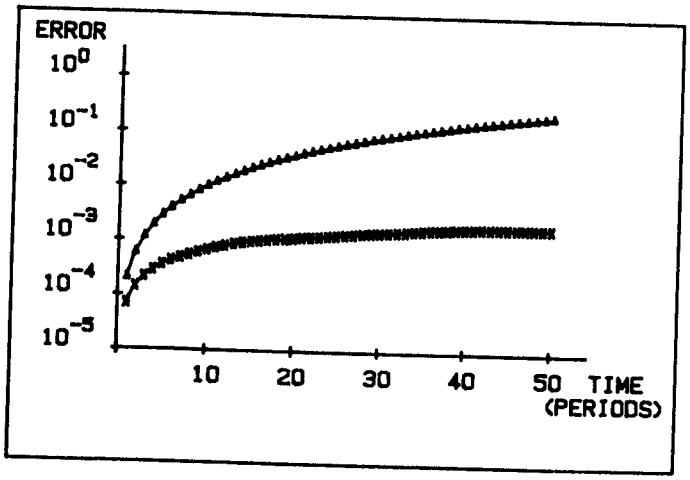

Figure 3. Kepler problem. Standard method (triangles) and canonical method (stars).

(7.2). As in [3], we use the initial condition $p_2 = 0, q_1 = 0, q_2 = 0.2$, with p_1 chosen so as to have an energy $H = 0.117835$. The number of steps is 5000 with a step-length $h = 0.5$. For the neighbouring Hamiltonian (7.2) this would mean that the solution is being sampled about 12 times per period of length 2π, so that, in a short-time computation, the chosen value of h is expected to guarantee, at least, a moderate accuracy.

Figures 1 and 2 correspond to the noncanonical and canonical schemes respectively and depict the q_1 and q_2 components of the solution at the even-numbered time-steps. The differences are obvious. The symplectic scheme has identified that the solution lies on an invariant torus, while the classical Runge–Kutta method gives meaningless results. The final energies are $H = 0.1181911$ for the canonical method (with an error of 0.3 per cent) and $H = 1.7E-2$ for the classical scheme. We emphasize that, as discussed previously, the symplectic scheme is *not* (cannot be) energy-preserving. Of course the 'nice' appearance of Figure 2 does not guarantee that the computed points are close to the corresponding values of the theoretical solution, which probably is not true. However the canonical scheme has identified the right qualitative behaviour and this was the point of interest in the study of (7.1).

(ii) **Kepler's problem**. The Hamiltonian is given by the well-known expression

$$H = (1/2)(p_1^2 + p_2^2) - 1/r, \qquad r^2 = q_1^2 + q_2^2. \tag{7.3}$$

The solutions are, of course, available analytically [1]. However many important problems in celestial mechanics require the *numerical* integration of problems where the potential energy $-1/r$ is subjected to small perturbations. Typically, these problems demand computations over very long time intervals (say many revolutions of an artificial satellite) [9].

We have chosen the initial conditions $p_1 = 0, p_2 = 0.95, q_1 = 1, q_2 = 0$ leading to a low-eccentricity elliptic motion with period $T = 5.464783$, energy $H = -0.5487500$ and angular momentum $M = 0.9500000$. We have integrated over fifty revolutions of the satellite.

For the classical method h was taken to be $T/40$ (i.e. forty steps per revolution), while for the canonical method we set $h = T/64$, so that both runs employ the same number of evaluations of the force. The errors in the q_2 component at the end of each revolution have been plotted in Figure 3. While after one or two periods both schemes exhibit the same performance (recall that the canonical method is operating with a smaller value of h), the differences between the methods grow markedly as the integration proceeds. The error growth is much faster in the noncanonical method, and at the end of the experiment the difference in the size of the error is almost three orders of magnitude. At the end of the integration, the canonical scheme yields $H = -0.5487541, M = 0.9499964$, so that the error in the approximation of the conserved quantities is indeed much lower than the error in the individual solution components. But then the same is true for the classical method, which results in $H = -0.5493714, M = 0.9495119$.

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