EXPLICIT, ADAPTIVE, SYMPLECTIC (EASY) INTEGRATORS USING SCALE INVARIANT REGULARISATIONS AND CANONICAL TRANSFORMATIONS

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Abstract. We present explicit, adaptive symplectic (EASY) integrators for the numerical integration of Hamiltonian systems with greatly varying time-scales. A time regularisation is considered using the Poincaré transformation. This gives a new Hamiltonian which is usually not separable, and to recover the original separability a canonical transformation is considered. A backward error analysis for the numerical integration with a splitting symplectic integrator is presented. For a one-dimensional near singular problem, this analysis reveals a strong dependence of the performance of the method with the choice of the regularisation function, g, and the order of the method. The optimal choice corresponds to the function g which nearly preserves the scaling invariance of the system. Numerical examples supporting this result are presented. Finally, an EASY method for the two- and three-dimensional Lennard-Jones problem, nearly preserving scaling invariance is also presented.

Key words. Hamiltonian systems, symplectic integrators, variable time-step, scaling invariance, canonical transformations

AMS subject classifications. 34A26; 65L05; 65P10; 70F16; 70H15

1. Introduction. When solving Hamiltonian systems of ordinary differential equations, certain qualitative properties of the evolution are important and symplectic integrators have largely shown during the last decade to be superior to standard integrators [36, 10, 20] when used with constant time step. In contrast adaptive variable time step methods are often superior to fixed time step methods when applied to problems with varying evolutionary time scales. They lead to more regular problems with reduced local errors and with the effects of rounding error minimised. The results presented in the paper [8] demonstrate that adaptive methods can be especially effective when the underlying problem has a scaling structure. However, adaptive and symplectic methods have tended to sit uncomfortably together, with adaptivity often corrupting the powerful long time error estimates which can be obtained for fixed time step symplectic methods [36]. Attempts to rectify this problem, which will describe, have tended to either result in complex and hard to use algorithms or to low order methods. It is also not clear in many of these methods, what choice should be made of the adaptive procedure. We present in this paper a technique for both identifying an natural adaptive procedure based upon identifying the evolutionary scalings of the system, and then implementing this, by using a combination of a Sundman and a Poincaré transform, for Hamiltonian problems with up to six degrees of freedom. This procedure is seen to be appropriate for both problems with an exact scaling

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Email: sblanes@mat.uji.es This work has been partially supported by the Ministerio de Ciencia y Tecnología through a contract from the program Ramón y Cajal (2001).
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law and for others where the scaling law applies approximately at points where the solution is changing most rapidly. A certain canonical transformation of the rescaled problem is made which leads to a separable Hamiltonian in the transformed coordinates. Applying a symplectic splitting method to this transformed problem leads to an explicit, adaptive, symplectic (EASY) method of arbitrary order, which is also invariant under changes of scale. We show that the EASY method using a scale invariant adaptive strategy for time stepping out performs many other similar methods for a wide variety of (central force type) problems, including the central orbit problem with a Lennard-Jones potential.

1.1. Symplectic methods. Given the Hamiltonian $H(\mathbf{q},\mathbf{p})$, an n-th order symplectic integrator (SI) used with a *fixed* time step h, solves a discrete system which corresponds exactly (up to exponentially small terms in h) to the solutions of a perturbed Hamiltonian system with constant Hamiltonian $H(\mathbf{q},\mathbf{p})+\delta H(\mathbf{q},\mathbf{p},h)$, where $\delta H = \mathcal{O}(h^n)$. If δH is small enough, we can expect that both systems will share the same qualitative properties and their solutions (with the same initial conditions) will stay very close to each other for a long time, and accurate approximations can also be obtained. This observation explains, in part, the success of symplectic methods and their wide use in simulating celestial and molecular dynamics. Since the appearance of the papers by Yoshida [44] and Suzuki [40] [1], a considerable effort has been put into obtaining more efficient, explicit, constant time step based symplectic integrators. Particularly interesting are: symplectic partitioned Runge–Kutta (PRK) methods [29, 3, 6] for *separable systems* like $H = T(\mathbf{p}) + V(\mathbf{q})$; symplectic Runge–Kutta–Nyström (RKN) methods [14, 29, 5, 6] in case, for example, T is quadratic in momenta; and near-integrable systems, $H = H_0 + \epsilon H_1$, where both H_0 and H_1 are exactly solvable or easy to approximate, and ϵ is a small parameter [43, 30, 4]. Crucial to these methods is the separability of the Hamiltonian which allows the use of explicit methods. These integrators have proved to be highly competitive for each family of problems, being cheap to use (as they are explicit) and having excellent error bounds over long integration times.

1.2. Variable time step methods. If a dynamical system can evolve either rapidly or slowly along different regions of its trajectory, a standard technique for optimising the performance of an integrator is, for traditional methods, to introduce a variable time stepping strategy into the algorithm. The choice of time step is often dictated by an estimate of the local truncation error of the method given, for example by the Milne device or the Zadunaisky estimate [23]. As an example of where such methods are needed for a Hamiltonian problem, consider the many body problem, in which near collisions lead to rapid changes in the solution over small time scales. Adaptivity can markedly increase the integration accuracy of a numerical procedure over a short time-scale, although they may not improve its accuracy over long time intervals. In an attempt to overcome the latter problem, it is desirable to combine the short term accuracy of an adaptive method with the long time accuracy of a Hamiltonian method. However, this synthesis of techniques has proved difficult to

[1]Similar results were previously published in [16], but this paper has not been much cited in the *Geometric Integration* community.

achieve. When standard techniques for changing the time step were included in a symplectic integrator, it was found [36] (see also [13, 17, 37]) that several of the good properties of symplectic methods were lost. These integrators still preserve symplecticity, but now, roughly speaking, they are exactly solving a perturbed time-dependent Hamiltonian, $H(\mathbf{q},\mathbf{p})+\delta\tilde{H}(\mathbf{q},\mathbf{p},t)$. If the time step is not changed properly, secular terms will appear, $\delta\tilde{H}$ will grow with t, and the error in energy and positions will grow similarly to standard non symplectic integrators. More recently, this problem has been reconsidered, and integrators with variable time step and non secular terms have been obtained. The key behind these methods is to introduce a regularisation of the time (often by using a Sundman transformation). This technique has been successfully used for many years in celestial mechanics for solving the Kepler problem [42]. The drawback is that separable systems usually turn into non separable (or not easily separable), and the highly efficient explicit methods previously mentioned can not be used any longer. Several alternatives have been recently considered in the literature and some of them will be described in more detail in section 2. However, it is important to look for more efficient methods for a number of important problems.

1.3. Scaling Invariance. Many problems, such as the Kepler problem are invariant up to changes in the scale of both time and of the solution. Whilst many other systems are not scaling invariant, close to (hard to compute) near singular events such as near collisions they are approximately scaling invariant. Exploiting scaling invariance through a suitably chosen adaptive time stepping strategy has proved to be a very useful property for numerically solving both partial and ordinary differential equations [1, 11, 8, 9, 33]. For certain initial conditions, scaling invariant systems admit self-similar solutions (i.e. solutions which map to themselves under a change of scale) which can be attractors for many other solutions starting from more general boundary conditions. It has been shown [8] that multi-step and Runge-Kutta integrators for scale invariant ODEs admit discrete self-similar solutions obtained by group reductions of the discretisation of the original problem. These discrete self-similar solutions have the very desirable properties of (i) uniformly approximating the true self-similar solution for *all* times, (ii) retaining the stability of the underlying self-similar solution and hence describing correctly the asymptotic evolution of the whole ODE system. In a sense, such performance of an adaptive method is optimal for this particular class of solutions. The principle drawback of the methods implemented in [8] is that they involve enlarging the original system, they can be implicit and they are not necessarily symplectic. Furthermore, there are many problems which are unchanged under scaling but which posses solutions which are not self-similar. A good example is the Kepler problem which admits non self-similar periodic solutions which can be transformed into other periodic solutions through the action of Kepler's third law.

1.4. Canonical transformations. Many Hamiltonian problems are not easy to solve numerically with a SI because they are not separable in a simple form. This is the usual situation when time-regularization is included. However, some times, it is possible to find a *canonical transformation* (CT) such that the final system has a simple structure, suitable to be integrated easily and efficiently with constant time step SIs. Provided that a reasonable splitting method is used which retains the scaling structure (most splittings have this property) then the resulting methods will capture the properties of the scaling invariant system, such as the uniform approximation of self similar solutions over all time and admitting scaling transformations from one discrete solution to another. These are particularly appropriate for scale invariant problems in which periodic solutions are important, with adaptivity allowing for highly eccentric orbits to be computed accurately. When all this is possible, we end up with an integrator which is explicit, keep the good behaviour for long time integration, have the benefits of a variable time step algorithm and can accept scaling invariant solution with a constant relative error.

The techniques we describe can be considered a generalisation of the Levi-Civita (LC) [27] or Kustaanheimo-Stiefel (KS) [24, 38] regularisation of the equations. They combine a regularisation with a canonical transformation, and they are standard methods in celestial mechanics. We derive and then test a new tool, showing that, for a number of important problems it can be used, giving very efficient explicit integrators. Consequently we restrict our discussions to Hamiltonian problems of one, two and three degrees of freedom.

1.5. An example. All of the above discussion, and indeed the remainder of this paper can be both summarised and motivated through the following example. As remarked above, we hope to achieve, by combining adaptive, symplectic and explicit methods with a choice of time-step based on scaling invariance, a method which is accurate on both short and long time-scales and which is also computationally cheap. A problem in which all of these features are desirable is the Kepler problem which possesses periodic orbits with close approaches. An orbit with a small angular momentum has a radial coordinate q with associated momentum p which evolve according to the Hamiltonian

$$H = \frac{1}{2}p^2 - \frac{1}{q} + \frac{\varepsilon}{q^2}, \tag{1.1}$$

where $\sqrt{\varepsilon}$ is the angular momentum. We integrate the system taking as initial conditions $(q_0, p_0) = (1, 0)$, in the case of $\varepsilon = 0.1$ over 40 periods using four different methods, namely the Matlab integrators `ode45, ode113`, an explicit $6th$-order RKN symplectic method with constant time step, and the same method included as part of an EASY integrator in which a scale invariant time transformation is employed. In each case the step size of each method was chosen so that approximately the same number of evaluations of the potential was made during the integration. Since the value of H is constant, we compute its numerical value at each step and measure its relative error with respect to the original value. Figure 1.1 shows the results obtained, which neatly illustrates all that we have said. The adaptive, non-symplectic methods out perform the classical SI integrator over the initial integration period, but both have errors that grow linearly , which is not the case of the the SI integrator. The EASY method outperforms all of them, having low errors initially which hardly grow at all during the integration. More details of this example, together with other calculations are given in Section 4.

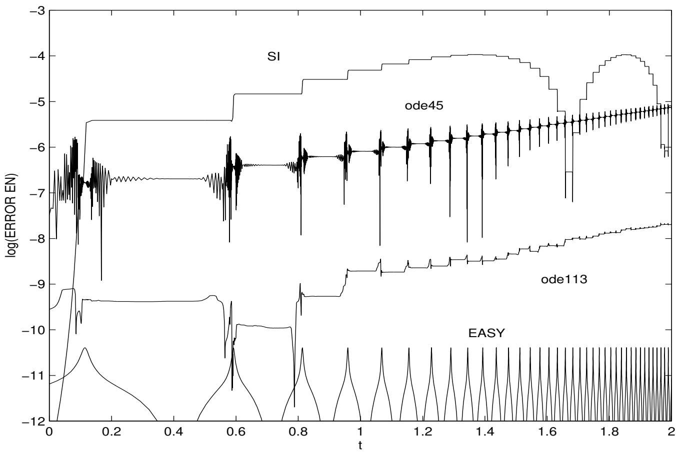

FIG. 1.1. *Evolution of the error in energy for the Hamiltonian (1.1) using different integrators. The time step and tolerances are chosen such that all methods require approximately the same number of potential evaluations. For a better illustration, SI has been computed with twice the number of evaluations.*

1.6. Summary. The remainder of this paper is set out as follows. The class of (scale invariant) Hamiltonian problems to be studied is presented in Section 2. The analysis of the scaling function is carried out in Section 3. In Section 4 we consider problems with one degree of freedom. Section 5 reviews the LC and KS transformations in two- and three-dimensions, respectively. This is generalised to the Lennard-Jones potential, making the resulting Hamiltonian system both scaling invariant and separable. The new method is numerically tested in in Section 6.

2. Adaptive and symplectic methods for Hamiltonian problems.

2.1. Hamiltonian problem and symplectic methods. Let us consider the following Hamiltonian

$$H = T(\mathbf{p}) + V(\mathbf{q}) = \frac{1}{2}\mathbf{p}^T\mathbf{p} + V(\mathbf{q}) \tag{2.1}$$

with $\mathbf{q} = (q_1, \ldots, q_k)^T$, $\mathbf{p} = (p_1, \ldots, p_k)^T$. If $\hat{H}$ is the Lie operator associated to the Hamiltonian[2] and t is the time, the Lie transformation, $e^{-t\hat{H}}$, acting on $(\mathbf{q}, \mathbf{p})$ gives the evolution, which is a canonical or symplectic transformation. Since T and V are exactly solvable, the second order explicit, symmetric and symplectic Störmer/leapfrog/Verlet method, for one time step h, is

$$S_2(h) = e^{-\frac{h}{2}\hat{V}}\, e^{-h\hat{T}}\, e^{-\frac{h}{2}\hat{V}} = e^{-h\hat{H}} + O(h^3) \tag{2.2}$$

giving the algorithm

$$\begin{aligned} \mathbf{p}_{n+1/2} &= \mathbf{p}_n - \tfrac{h}{2}\nabla_{\mathbf{q}} V(\mathbf{q}_n) \\ \mathbf{q}_{n+1} &= \mathbf{q}_n + h\mathbf{p}_{n+1/2} \\ \mathbf{p}_{n+1} &= \mathbf{p}_{n+1/2} - \tfrac{h}{2}\nabla_{\mathbf{q}} V(\mathbf{q}_{n+1}), \end{aligned} \tag{2.3}$$

[2]It is defined by its action on a differentiable function, $f(\mathbf{q}, \mathbf{p})$, as $\hat{H}f = \{H, f\}$, being $\{\cdot, \cdot\}$ the usual Poisson bracket.

where $(\mathbf{q}_n, \mathbf{p}_n) \simeq (\mathbf{q}(t_n), \mathbf{p}(t_n))$ with $t_n = t_0 + nh$. For N steps, the last computation of $\nabla_{\mathbf{q}} V(\mathbf{q}_{n+1})$ at each step can be reused in the next step, and only one evaluation of $\nabla_{\mathbf{q}} V$ per step is required. Fourth-order symplectic methods can be obtained by composition of this method [40, 44]. For example, a well known symmetric fourth order method is given by

$$S_4(h) = S_2(x_1 h) S_2(x_0 h) S_2(x_1 h) \tag{2.4}$$

with $x_1 = 1/(2 - 2^{1/3})$, $x_0 = 1 - 2x_1$. Higher order methods are also presented in [44]. These methods have become very well known due to their good behaviour for long time integration but, they are not very accurate. Recently, a number of new splitting methods have appeared which are more efficient. For Hamiltonians like (2.1), which are quadratic in momenta, more efficient symplectic RKN composition methods like

$$\Phi_h = \prod_{i=0}^{k} e^{-a_i h \hat{T}} \, e^{-b_i h \hat{V}} \tag{2.5}$$

with appropriate coefficients a_i, b_i can be used. We denote by RKN_4 the 6-stages fourth-order integrator and by RKN_6 the 11-stages sixth-order integrator presented in [6]. Methods up to order eight, using the processing technique, are presented in [3, 5].

2.2. The Sundman and Poincaré regularisations.
A standard a-priori adaptive technique for an ODE integration method is based on a time-regularisation so that the solution evolves on a *fictive time* τ which is used for all computations. Ideally rapid variations in t should correspond to moderate variations in τ. This fictive time is introduced through the ordinary differential equation defining a *Sundman transformation*

$$\frac{dt}{d\tau} = g(\mathbf{q}, \mathbf{p}). \tag{2.6}$$

Here g is a positive scalar function which is taken to be small if the solution is evolving rapidly. This transformation leads to the system

$$\frac{d\mathbf{p}}{d\tau} = -g \nabla_{\mathbf{q}} H = -g \nabla_{\mathbf{q}} V, \qquad \frac{d\mathbf{q}}{d\tau} = g \nabla_{\mathbf{p}} H = g \mathbf{p}. \tag{2.7}$$

In general, this system is no longer Hamiltonian. To recover a Hamiltonian structure we introduce two new conjugate coordinates[3] $q^t = H(\mathbf{q}_0, \mathbf{p}_0)$ and $p^t = t$, which satisfy the differential equations

$$\frac{dq^t}{d\tau} = 0 \quad \text{and} \quad \frac{dp^t}{d\tau} = g.$$

As the Hamiltonian H of the original system is constant we have that $H(\mathbf{p}, \mathbf{q}) - q^t \equiv 0$ for all time. The whole system $(\mathbf{q}, q^t, \mathbf{p}, p^t)$ then evolves in the fictive time, τ, and is Hamiltonian with Hamiltonian

$$K = g(\mathbf{q}, \mathbf{p})(H(\mathbf{q}, \mathbf{p}) - q^t). \tag{2.8}$$

[3]In the literature it is usual to take $q^t = t$ and $p^t = -H(\mathbf{q}_0, \mathbf{p}_0)$, but to get a more natural splitting of the extended Hamiltonian, in this paper we prefer to consider p^t as the time.

The extended system of ordinary differential equations that we now require to solve are

$$\frac{d\mathbf{q}}{d\tau} = g\mathbf{p} + \nabla_{\mathbf{p}} g(H - q^t), \qquad \frac{dq^t}{d\tau} = 0, \tag{2.9}$$
$$\frac{d\mathbf{p}}{d\tau} = -g\nabla_{\mathbf{q}} V - \nabla_{\mathbf{q}} g(H - q^t), \qquad \frac{dp^t}{d\tau} = g.$$

This system is a Poincaré transformation of the original [19, 35, 42]. Observe that with this choice of q^t and p^t the evolution of the ordinary differential equation system corresponding to the Hamiltonian (2.1) is equivalent to the evolution of the extended system with corresponding Hamiltonian (2.8), where the effect of the time transformation is now included automatically.

2.3. Canonical transformations. We study for which functions g it is possible to find a set of coordinates derived from those used in the Poincaré transformation, so that the Hamiltonian (2.8), in the transformed coordinates, has a separable form like the Hamiltonian (2.1). We can then apply a splitting Nyström method, such as given in Section 2.1, to this new system. To perform this analysis we consider the case in which g only depends on the coordinates, $g \equiv g(\mathbf{q})$. This is a natural condition for the central force examples that we consider later in this paper, and at the same time the system simplifies slightly. Then, the Hamiltonian (2.8) can be written as

$$K = \tilde{T}(\mathbf{q}, \mathbf{p}) + \tilde{V}(\mathbf{q}, q^t) = g(\mathbf{q})\frac{1}{2}\mathbf{p}^T\mathbf{p} + g(\mathbf{q})\left(V(\mathbf{q}) - q^t\right). \tag{2.10}$$

Describing the evolution of a system using Hamiltonian equations has the advantage that $\mathbf{q}$ and $\mathbf{p}$ are independent coordinates which play symmetric roles in the equations. This allow us to choose the most appropriate coordinates and momenta to describe a particular system. In the numerical integration of separable systems, it is important to take into account how easy and fast it is to compute each part of the system (or each part of the Hamiltonian). If new coordinates and momenta $\mathbf{Q}, \mathbf{P}$ are found, giving a simpler and faster to compute Hamiltonian, then the performance of the integrators can improve. If the transformation $(\mathbf{q}, \mathbf{p}) = \mathcal{C}(\mathbf{Q}, \mathbf{P})$ is canonical, the Hamiltonian which describes the evolution on the new coordinates is $H(\mathbf{Q}, \mathbf{P}) = H(\mathbf{q}(\mathbf{Q}, \mathbf{P}), \mathbf{p}(\mathbf{Q}, \mathbf{P}))$. The problem we then face is to find the CT which transform a complicated Hamiltonian into a simpler one, for example one which takes a non-separable Hamiltonian into a separable one. For this purpose, the following theorem is very useful

THEOREM 2.1. *The transformation*

$$\left\{ \begin{array}{rl} \mathbf{q} & = \Phi(\mathbf{Q}) \\ \Phi'(\mathbf{Q})^T\mathbf{p} & = \mathbf{P}, \end{array} \right. \tag{2.11}$$

where Φ is a diffeomorphism of $\mathbb{R}^{2k}$, is canonical.

Proof. A well known technique for building canonical transformations is by using generating functions. Let us consider the following generating function depending on the new coordinates and old momenta

$$F(\mathbf{Q},\mathbf{p}) = -\Phi(\mathbf{Q})^T\mathbf{p} \tag{2.12}$$

then, the following equations define a canonical transformation [18, 28]

$$\mathbf{q} = -\frac{\partial F}{\partial \mathbf{p}} = \Phi(\mathbf{Q}), \qquad \mathbf{P} = -\frac{\partial F}{\partial \mathbf{Q}} = \Phi'(\mathbf{Q})^T\mathbf{p} \tag{2.13}$$

□

2.3.1. Example. In order to illustrate the benefits of using a CT for the numerical integration of a Hamiltonian system, let us consider the Hamiltonian (1.1) with the regularisation function $g = q^{3/2}$. The motivation for this particular choice will come later when we consider scaling symmetries. Now, (2.10) takes the form

$$K = \tilde{T}(q,p) + \tilde{V}(q,q^t) = \frac{1}{2}q^{3/2}p^2 + \left(-q^{1/2} + \frac{\varepsilon}{q^{1/2}} - q^t q^{3/2}\right), \tag{2.14}$$

where both $\tilde{T}$ and $\tilde{V}$ are exactly solvable (the Hamiltonian $H = q^\alpha p^\beta$, with α,β constants, is exactly solvable), and, because $\{\tilde{V},\{\tilde{V},\{\tilde{V},\tilde{T}\}\}\} = 0$, symplectic RKN integrators can be used. However, $\tilde{T}$ can be relatively expensive to compute. If the same problem is considered using new coordinates (Q,P), related to the old coordinates through the CT

$$q = Q^4, \quad p = P/(4Q^3), \quad p^t = P^t, \quad q^t = Q^t,$$

the Hamiltonian to be solved is

$$K = \frac{1}{32}P^2 + \left(-Q^2 + \frac{\varepsilon}{Q^2} - Q^t Q^6\right). \tag{2.15}$$

If a splitting method is used in (2.14), at least one square root per stage is needed. However, if the same splitting method is applied to (2.15) no square root is required as well as a small number of arithmetic operations is required. The only root needed is for starting the computation. In addition, if at a given instant the output is desired in the old coordinates, this can also be cheaply computed.

2.4. Other Explicit Adaptive Integrators. In the following we present in more detail some of the most important explicit adaptive integrators for Hamiltonian systems. Some implicit adaptive symplectic integrators have also been constructed [19, 13, 12], but these are usually expensive and they are not considered in this paper.

2.4.1. Symmetric non-symplectic methods. Reversible integration methods have desirable properties [39], and, from the Verlet algorithm (2.3), the following second order symmetric non-symplectic *adaptive Verlet method* is presented in [22, 7, 21]

$$\mathbf{p}_{n+1/2} = \mathbf{p}_n - \frac{h}{2\rho_n}\nabla_{\mathbf{q}}V(\mathbf{q}_n)$$
$$\mathbf{q}_{n+1/2} = \mathbf{q}_n + \frac{h}{2\rho_n}\mathbf{p}_{n+1/2}$$

$$\begin{aligned}\rho_{n+1}+\rho_n &= 2/g(\mathbf{q}_{n+1/2},\mathbf{p}_{n+1/2})\\ \mathbf{q}_{n+1} &= \mathbf{q}_{n+1/2}+\frac{h}{2\rho_{n+1}}\mathbf{p}_{n+1/2}\\ \mathbf{p}_{n+1} &= \mathbf{p}_{n+1/2}-\frac{h}{2\rho_{n+1}}\nabla_{\mathbf{q}}V(\mathbf{q}_{n+1}).\end{aligned} \tag{2.16}$$

To start the integration one can use $\rho_0 = 1/g(x_0)$ but, this choice might lead to *oscillations* in the numerically computed ρ_n's, which can be avoided choosing a modified initialization [15]. By composition it is possible to build higher order methods but, only general compositions like (2.4) can be used, being less efficient than using Nyström methods for problems with quadratic kinetic energy. In addition, choosing the previous value for ρ_0 introduces some new error terms in the algorithm (backward error analysis [15]) which can not be cancelled by composition to get methods of order higher than four. This problem can be avoided choosing a slightly different basic method, and it is in this moment under investigation [41].

2.4.2. Generalised logarithmic Hamiltonian methods. Suppose that for solving the Hamiltonian problem (2.9) we consider [34]

$$g = \frac{f(T(\mathbf{p})-q^t)-f(-V(\mathbf{q}))}{H(\mathbf{q},\mathbf{p})-q^t} \tag{2.17}$$

with $f(u)$ an analytic function. Since numerically $T(\mathbf{p})-q^t \simeq -V(\mathbf{q})$ then $g \simeq f'(-V(\mathbf{q}))$, where $f(u)$ has to be a function such that $f'(u)>0$, and with no singularities in the region of interest. Substituting into (2.8), the Hamiltonian to solve is

$$K = f(T(\mathbf{p})-q^t)-f(-V(\mathbf{q})) \tag{2.18}$$

which is again separable. The particular case $f(u)=\log(u)$ has been considered in [31, 32]. Now, $f(T(\mathbf{p})-q^t)$ is not quadratic in momenta and RKN methods can not be used.

3. Choice of the scaling function $g(u)$. Before we consider the canonical changes of coordinates for a general function $g(u)$ we investigate optimal rescalings which can be used for certain classes of problems. Since the performance of the numerical integration is highly dependent on the function g, it is very important to have a simple criterion to find a very good regularization function for a given problem. This criterion seems to be closely related with the scaling invariance of the dominant part of the potential in those regions where the system evolves rapidly. We see this by looking at a particular example.

Example We consider the Hamiltonian (1.1) with $\varepsilon = 0.001$ and integrate the system until $t=20$ for different values of γ. The trajectories of this problem are periodic orbits with close approaches to the origin where the particle moves rapidly and adaptivity is necessary. To compare methods we measure the average error in the energy (Hamiltonian) using a time step, $\Delta\,\tau$, such that the final time is always reached with approximately 12000 potential evaluations. Figure 3.1 shows the results obtained when using: the second order, S_2, and the fourth order, S_4, methods given in (2.2)

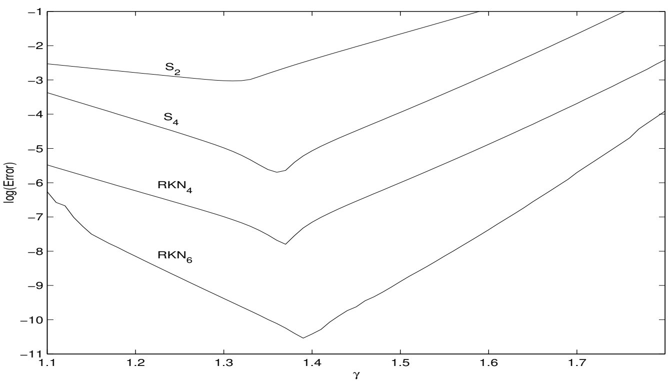

FIG. 3.1. *Average error in energy in the integration of (1.1). The system is integrated until the final real time $t = 20$. All integrations require, approximately, the same number of potential evaluations for each value of γ.*

and (2.4), respectively, and using RKN_4 and RKN_6. For each method, these graphs of the error plotted against γ have a sharp minimum. It is clear that to obtain a low error it is important to choose γ carefully. Comparing the results of S_4 and RKN_4 we can also appreciate the benefits of using a Nyström method versus a more general integrator.
The optimal value of γ as seen on these graphs is quite different from $\gamma = 0$ (constant time step), $\gamma = 1$ (the Levi-Civita scaling) or $\gamma = 2$ (arc-length parametrisation), but lies close to the scale invariant value of $\gamma = 1.5$. In section 4 we return to give a more detailed analysis of this example using backward error analysis, and show that $\gamma \to 1.5$ as the order of the method increases.

3.1. Computational cost and backward error analysis. Backward error analysis [20] implies that a symplectic integrator for a Hamiltonian system with Hamiltonian K used with a *fixed* time step $\Delta\tau$, solves a discrete system which corresponds exactly (up to exponentially small terms in $\Delta\tau$) to the solutions of a perturbed Hamiltonian system $K + \Delta\tau K_2 + \Delta\tau^2 K_3 + \ldots$. If the integrator is a splitting method the functions K_i are linear combinations of nested commutators of the parts of the Hamiltonian [44]. In particular we have that

$$K_2 = k_{21}\{\tilde{T},\tilde{V}\}, \quad K_3 = k_{31}\{\tilde{V},\{\tilde{V},\tilde{T}\}\} + k_{32}\{\tilde{T},\{\tilde{V},\tilde{T}\}\}, \quad \ldots$$

where the coefficients k_{ij} depend only on the particular integrator used. For instance, $k_{ij} = 0, \; i = 2,\ldots,n, \; j = 1,\ldots$ if the integrator is of order n. For simplicity, let us consider the one dimensional problem with $\tilde{T} = \frac{1}{2}g(q)p^2$ and $\tilde{V} = g(q)(V(q) - q^t)$ then

$$K_2 = k_{21} g\tilde{V}'p, \qquad K_3 = k_{31} g\left(\tilde{V}'\right)^2 - \frac{k_{32}}{2} g\left(\tilde{V}'g' + 2g\tilde{V}''\right)p^2, \quad \ldots$$

To obtain a realistic error analysis we look at the error in the unscaled Hamiltonian H where, up to a constant $H = K/g$. Thus, H is perturbed to $H + \Delta\tau H_2 + \Delta\tau^2 H_3 + \ldots$ where $H_i = K_i/g$. We aim to choose the scaling function g for an nth-order method by so that the average of $\Delta\tau^n H_{n+1}$ over an orbit is minimised for a fixed computational cost. In general, this calculation will be very hard and more detailed information on the problem is needed to find the optimal g. This analysis will be described in section 4.4.

3.2. Scale invariance. A further motivation of our choice of the function g is the phenomenon of scale invariance. Adaptive methods for scale invariant problems which themselves inherit the invariance, shadow self-similar solutions with a uniform error and inherit any conservation properties of the original problem which are linked to symmetries. Moreover, it is relatively easy to identify functions $g(\mathbf{q})$ which lead to scale invariant discretisations. Suppose that we consider the (not necessarily Hamiltonian) ODE system $du_i/dt = f_i(u_1, ..., u_N), \quad i = 1, \dots, N$. This system is *scale invariant* if it is unchanged under the transformation

$$t \to \lambda t, \quad u_i \to \lambda^{\alpha_i} u_i \tag{3.1}$$

where $\lambda > 0$ is an arbitrary real number and the α_i depend on the problem. A solution of such a system is *self-similar* if $u_i(\lambda t) = \lambda^{\alpha_i} u_i(t)$. Such solutions have the general form $u_i = t^{\alpha_i} v_i$ where the constants v_i satisfy an algebraic equation. The Kepler problem admits (both regular and singular) self-similar solutions with zero angular momentum, as well as non self-similar periodic solutions with non-zero angular momentum. Applying the Sundman transformation to this system we have

$$dt/d\tau = g(\mathbf{u}) \quad \text{and} \quad du_i/d\tau = g(\mathbf{u}) f_i(\mathbf{u}).$$

Unless g is chosen appropriately, this system is no longer scale invariant. However, with a careful choice of g we can construct a system which has the desirable property that two solutions mapped into each other by the scaling relation (3.1) evolve at the same fictive time. This is a desirable property for an adaptive method which can use a constant step size $\Delta\tau$ for two solutions evolving on different spatial scales. To achieve scale invariance the function g must satisfy the functional equation

$$g(\lambda^{\alpha_1} u_1, \lambda^{\alpha_2} u_2, \dots, \lambda^{\alpha_N} u_N) = \lambda g(u_1, u_2, \dots, u_N). \tag{3.2}$$

In general, functions $g(u)$ which satisfy such scaling laws are either multi-variable polynomials or are functions of groupings of the variables u_i which scale in a similar manner. For the two-dimensional Kepler problem ($V = -1/r$ with $r = (q_1^2 + q_2^2)^{1/2}$ in (2.1)) we have $g(\mathbf{q}) = r^{3/2}$.

Suppose that we now discretise the transformed system with a multi-step or Runge-Kutta method with a constant step size $\Delta\tau$, so that $U_i^n \approx u_i(n\Delta\tau)$ is a discrete approximation of $u(\tau)$ at time t_n. If the underlying ODE admits a self-similar solution then the following result is proved in [8]

THEOREM 3.1. *(i) If $\Delta\tau$ is sufficiently small then the discrete problem admits a discrete self-similar solution of the form $U_i^n = z^{\alpha_i n} V_i, \quad t_n = z^n$,*
(ii) if $u(t)$ is the true self-similar solution then $\|U_i^n - u_i(t_n)\| = u_i(t_n)(1 + \mathcal{O}(\Delta\tau^p))$ where the implied constant in the order relationship does not depend upon n,

(iii) if the true self-similar solution is an attractor, then so is the discrete self-similar solution.

This theorem only applies for problems which are scale invariant. In practice most problems arising in applications are not truly scale invariant, but are approximately so (for example close to a collision). This is true for the Hamiltonian (1.1) when $\varepsilon \neq 0$. In this case the choice of $g(u)$ may not be optimal, but should still give reasonable results, and we explore this in the next section.

4. Regularisation and error analysis for problems with one degree of freedom.

4.1. The canonical transformation. The previous section has described certain forms of the function g that might be desirable for an adaptive problem, and has also indicated the sort of errors that might arise in the application of the Poincaré transformation. We now look at the difficult problem of finding a canonical transformation which leads to a separable Hamiltonian problem for which we may apply splitting methods and which can be applied to the general types of function g determined in Section 3. To motivate our derivation of suitable canonical transformations, we firstly look at problems with one degree of freedom where the issues are reasonably transparent. We then extend our analysis to problems with 2 and 3 degrees of freedom. Accordingly, let us consider (2.1) for the 1-dimensional problem in a 2-dimensional phase space. Once the regularisation function, $g(q)$, has been introduced and the phase space enlarged with (q^t, p^t), the Hamiltonian (2.10) for the extended system is now

$$K(p,q,p^t,q^t) = \frac{1}{2}p^2 g(q) + g(q)(V(q) - q^t). \tag{4.1}$$

We now combine the regularisation of the system with the following transformation

$$\left\{ \begin{array}{rlrl} Q & = G(q), & \qquad Q^t & = q^t \\ G'(q)P & = p, & \qquad P^t & = p^t. \end{array} \right. \tag{4.2}$$

Here the function $G(q)$ is defined via the differential equation $G'(q) = 1/(a\sqrt{g})$, where a is a suitable constant. The most important feature of this transformation is that it is *canonical* (from a direct application of Theorem 2.1) and leads to a new Hamiltonian problem evolving on the fictive time τ.

The Hamiltonian (4.1) in the new coordinates takes the form

$$K(P,Q,P^t,Q^t) = \frac{1}{2a^2}P^2 + \tilde{V}(Q,Q^t), \tag{4.3}$$

so that $K = \tilde{T}(P,P^t) + \tilde{V}(Q,Q^t)$, with $\tilde{T}$ quadratic in momenta, and hence we can now apply the explicit splitting bases symplectic RKN integrators described in Section 2 to this problem directly to give an EASY method. Observe that we have not imposed any special structure on the function $g(q)$ to derive this transformation.

4.2. Preserving scaling invariance for the one-dimensional problem. Suppose that the Hamilton equations obtained from (2.1) are invariant under a linear scaling

$$(t,q,p) \to (\lambda t, \lambda^{\alpha_1} q, \lambda^{\alpha_2} p) \tag{4.4}$$

then, this leads to certain restrictions on the scaling function $g(q)$ which in turn is reflected in the nature of the CT. We consider this question in the context of a central force type of equation. Suppose the potential is given by $V(q) = C/q^r$ then, the Hamiltonian equations are invariant when

$$(\alpha_1, \alpha_2) = \left(\frac{2}{2+r}, \frac{-r}{2+r} \right). \tag{4.5}$$

Consider now a rescaling function of the form $g(q) = q^\gamma$ then, taking $a = 2/(2-\gamma)$ (for simplicity in (4.2)) the CT becomes

$$\left\{ \begin{array}{l} Q = q^{\frac{2-\gamma}{2}} \\ P = \frac{2}{2-\gamma} q^{\frac{\gamma}{2}} p \end{array} \right. \quad \Leftrightarrow \quad \left\{ \begin{array}{l} q = Q^{\frac{2}{2-\gamma}} \\ p = \frac{2-\gamma}{2} Q^{\frac{\gamma}{\gamma-2}} P. \end{array} \right. \tag{4.6}$$

The Hamiltonian in the new coordinates is given by

$$K = \frac{(2-\gamma)^2}{8} P^2 + C Q^{\frac{2(\gamma-r)}{2-\gamma}} - Q^t Q^{\frac{2\gamma}{2-\gamma}}, \tag{4.7}$$

and the corresponding differential equations are

$$\begin{array}{ll} \dfrac{dQ}{d\tau} = \dfrac{(2-\gamma)}{4} P, & \dfrac{dQ^t}{d\tau} = 0, \\ \dfrac{dP}{d\tau} = -2C \dfrac{\gamma - r}{2-\gamma} Q^{\frac{2(\gamma-r)}{2-\gamma}-1} + \dfrac{2\gamma}{2-\gamma} Q^t Q^{\frac{3\gamma-2}{2-\gamma}}, & \dfrac{dP^t}{d\tau} = Q^{\frac{2\gamma}{2-\gamma}}. \end{array} \tag{4.8}$$

Now consider the scalings of this transformed equation of the form $(Q, Q^t, P, P^t, \tau) \to (\lambda^{\beta_1} Q, \lambda^{\beta_2} Q^t, \lambda^{\beta_3} P, \lambda^{\beta_4} P^t, \lambda^{\beta_5} \tau)$. As the original system is scale invariant it is important that the system in the canonical coordinates should also have this property. Furthermore, we require that all solutions, at all scales, should evolve with the same fictive time, so that $\beta_5 = 0$. Inspection of the equation for dQ/dt shows that $\beta_1 = \beta_3$. Making this substitution in the equation for dP/dt implies that we have scale invariance ($\beta_5 = 0$) only if

$$\gamma = \gamma_s = 1 + r/2.$$

This forces our choice of the scaling function $g(q)$. We may also, without loss of generality, and in keeping with $P_t = t$ set $\beta_4 = 1$. This then implies that $2\gamma\beta_3/(2-\gamma) = 1$ so that $\beta_3 = (2-\gamma)/2\gamma = (2-r)/(2(2+r))$. The resulting Hamiltonian is then

$$K = \frac{(2-r)^2}{32} P^2 + C Q^2 - Q^t Q^{\frac{4+2r}{2-r}}. \tag{4.9}$$

The canonical transformation then has a singularity when $\gamma = r = 2$ and this procedure fails, but it can be solved with the CT: $Q = \log(q)$, $P = qp$, with $g = q^2$.

4.3. Example. We consider again the 1-dimensional Hamiltonian

$$H = \frac{1}{2}p^2 - \frac{1}{q^r} + \frac{\varepsilon}{q^{2r}} \tag{4.10}$$

with $\varepsilon \geq 0$. In this problem q is the radial coordinate of a particle moving under a central force, and ε is a measure of the angular momentum of the particle or the intensity of the repulsive part of the force. If $H < 0$ and $\varepsilon > 0$ then the solution is bounded and periodic, and it has very close approaches to the origin when $\varepsilon \ll 1$. If $\varepsilon = 0$ and $H \leq 0$, then $q \to 0$ and $|p| \to \infty$ in a finite time T (gravitational collapse). In either case the solution evolves on small time-scales and hence small time-steps must be used for these parts of the motion, whilst longer time steps are desirable when q is not small. Taking $g = q^\gamma$ and the CT (4.6), the Hamiltonian to be solved becomes

$$K = \frac{(2-\gamma)^2}{8}P^2 - Q^{\frac{2(\gamma-r)}{2-\gamma}} + \varepsilon Q^{\frac{2(\gamma-2r)}{2-\gamma}} - Q^t Q^{\frac{2\gamma}{2-\gamma}}. \tag{4.11}$$

When $\varepsilon = 0$ the differential equations derived from this Hamiltonian are *exactly* invariant under the change of scale given by (4.4) and (4.5). There is an exact (singular) self-similar solution of the form

$$q(t) = C(T-t)^\alpha, \qquad p(t) = C\alpha(T-t)^{\alpha-1}, \tag{4.12}$$

where $\alpha = 2/(r+2)$, $C = (2/\alpha^2)^{1/(r+2)}$, which acts as an attractor [8]. Here T is a finite time at which the singularity occurs. In this case a scale invariant numerical method is a natural choice for integrating the differential equation.

If $\varepsilon > 0$ then the differential equations are not precisely invariant under this change of scale, but are close to being so provided that $q > \varepsilon^{1/r}$, and in this case the corresponding solutions are close to the self-similar solution.

4.4. Error analysis. We now combine the backward error analysis of section 3.1 with the scaling ideas to give an explanation of the distinctive form of the graphs in Fig. 3.1, and to estimate the error for the more general Hamiltonian (4.10).
Suppose that we consider a periodic orbit with initial values of $(q,p) = (1,0)$ so that $H = \varepsilon - 1$. If $\varepsilon > 0$ is small then the orbit has a close approach so that the minimum value of q is given by $q_{min} \simeq \varepsilon^{1/r}$ with $d^2q/dt^2 \approx 1/\varepsilon^{(r+1)/r}$ at this point. Similarly, the maximum value of p is given by $p_{max} \approx \varepsilon^{-1/2}$ and occurs when $q = (2\varepsilon)^{1/r}$. Thus this orbit is close to being singular at this point. We identify two regions of the orbit, the *outer region* in which $q > (2\varepsilon)^{1/r}$ and $|p|$ increases to $\varepsilon^{-1/2}$ and an *inner region* in which $q_{min} < q < (2\varepsilon)^{1/r}$ and $0 < p < \varepsilon^{-1/2}$. A simple estimate, using the approximation of $d^2q/dt^2 \approx 1/\varepsilon^{(r+1)/r}$, implies that the timescale T_2 of the inner region is proportional to $T_2 = \varepsilon^{(1+2/r)/2}$. Using the scaling function $g = q^\gamma$, the time-step Δt selected for this part of the motion (over which the scaling symmetry of the problem does not apply, as $1/q^r$ is comparable to ε/q^{2r}) is approximately uniform at $\Delta t \approx \varepsilon^{\gamma/r}\Delta\tau$. The outer region exists for times increasing from zero until the time $T - T_2$ close to the collapse time T for the unperturbed problem. The equation is close to being scaling invariant in the outer region, and the solution lies close to the

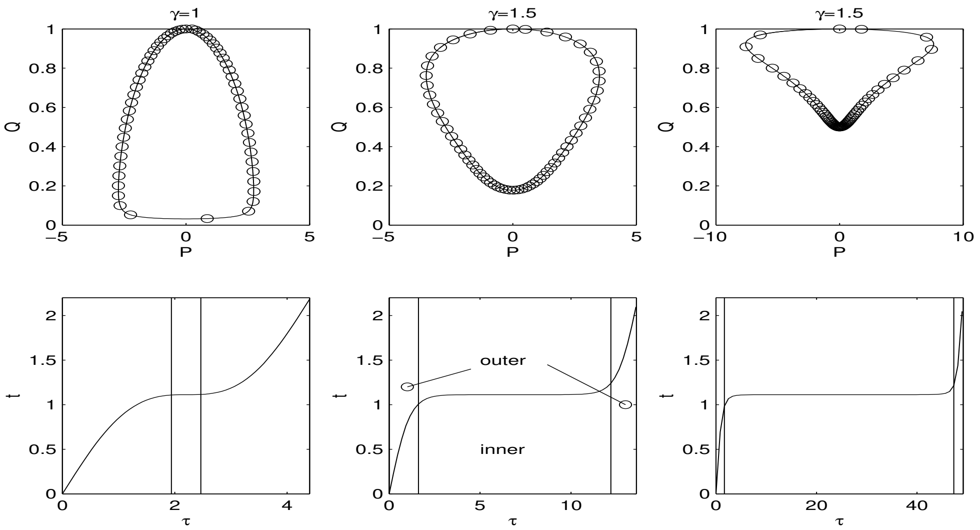

FIG. 4.1. *Top figures: Rescaled phase space trajectories for $r = 1$, $\varepsilon = 0.001$, $N = 60$, and $\gamma = 1, 1.5, 1.8$. Bottom figures: plots of t versus computational time. The vertical lines separate the inner from the outer regions*

singular self-similar solution (4.12) for which $p^2 = 2/q^r$. From the previous analysis we know that this self-similar solution is approximated optimally well if we use a scale invariant discretisation in this region. If a monitor function of the form $g(u) = q^\gamma$ is used, then the following heuristic argument explains the errors that we observe. If γ is too small then too large a time step is chosen and the motion in the inner region is poorly approximated leading to large errors. Conversely, if γ is too large then a small time step is chosen and a large number of calculations are made in the inner region. If the overall computational cost is to be held constant, then fewer calculations are made in the outer region and the error here is large. It is only when it is close to the scaling invariance value that we achieve the right balance between computational cost and accuracy. We now show that the optimal value is

$$\gamma \simeq \frac{r+2}{2} + \frac{r-2}{2n} = \gamma_s + \frac{r-2}{2n}, \tag{4.13}$$

where n is the order of the method.

Computational cost: We presume that all calculations are made in the computational τ space, that $\Delta\tau$ is uniform and we make N calculations overall. A computational time τ_1 is spent in the outer region and a time τ_2 in the inner region. This is illustrated by the Figure 4.1, were we present the phase space trajectories in the $Q - P$ phase space for $r = 1$, $\varepsilon = 0.001$, and $\gamma = 1$, 1.5, 1.8, taking $N = 60$ and also show how the true time varies as a function of the computational time.

The true time T_2 spent in the inner region is proportional to $\varepsilon^{(1+2/r)/2}$ so that, as $g(q) \approx \varepsilon^{\gamma/r}$ in this region we have

$$\tau_2 = \mathcal{O}(\varepsilon^{(1+\frac{r}{2}-\gamma)/r}). \tag{4.14}$$

Note that τ_2 is small if $\gamma < 1 + \frac{r}{2}$ and large if $\gamma > 1 + \frac{r}{2}$. In the outer region $q(t)$ approximates the self-similar solution which is proportional to $(T-t)^{2/(2+r)}$ close to the point of singularity. We can make an order of magnitude estimate of τ_1 by assuming that the true time interval for the outer region is given by $t \in [0, T - \varepsilon^{(1+r/2)/r}]$. From the identity $dt/d\tau = g(u)$ we have that

$$\tau_1 \approx \int_0^{T-\varepsilon^{(1+r/2)/r}} (T-t)^{-2\gamma/(2+r)} dt = \begin{cases} \mathcal{O}(1) & \text{if} \quad \gamma < 1 + \frac{r}{2}, \\ \mathcal{O}(\log(\varepsilon)) & \text{if} \quad \gamma = 1 + \frac{r}{2}, \\ \mathcal{O}(\varepsilon^{(1+\frac{r}{2}-\gamma)/r}) & \text{if} \quad \gamma > 1 + \frac{r}{2}. \end{cases}$$

As N calculations are made in the computational time space, we have $\Delta\tau = (\tau_1 + \tau_2)/N$, so that

$$\begin{array}{lll} \Delta\tau = \mathcal{O}(1/N) & \text{if} & \gamma < 1 + \frac{r}{2}, \\ \Delta\tau = \mathcal{O}(\log(\varepsilon)/N) & \text{if} & \gamma = 1 + \frac{r}{2}, \\ \Delta\tau = \mathcal{O}(\varepsilon^{(1+\frac{r}{2}-\gamma)/r}/N) & \text{if} & \gamma > 1 + \frac{r}{2}. \end{array} \tag{4.15}$$

Backward error analysis. To apply the backward error analysis of section 3.1 we make estimates of the terms H_i for the orbit we are considering. Here the scaling structure of the problem works strongly to our advantage as the various dominant commutator terms involved in H_i all scale in a similar manner and the precise values of the coefficients k_{ij} do not matter. In particular we have that $\tilde{T} = q^\gamma p^2/2$ and $\tilde{V} = -q^{\gamma-r} + \varepsilon q^{\gamma-2r} - q^t q^\gamma$. As we are interested in the dominant contributions to the error, expressions involving $q^t q^\gamma$ can be neglected so that the dominant terms in H_2 take the form $pq^{\gamma-r-1}$, $\varepsilon pq^{\gamma-2r-1}$, the dominant terms in H_3 take the form $q^{2\gamma-2r-2}$, $p^2 q^{2\gamma-r-2}$, $\varepsilon q^{2\gamma-3r-2}$, $\varepsilon p^2 q^{2\gamma-2r-2}$, and $\varepsilon^2 q^{2\gamma-4r-2}$, etc. In the inner region, p is bounded above by $\varepsilon^{-1/2}$ and q is bounded below by $\varepsilon^{1/r}$. Thus, all dominant terms in H_i scale in the same way with H_2 bounded by $\varepsilon^{(\gamma-1)/r-3/2}$, H_3 by $\varepsilon^{2(\gamma-1)/r-2}$, H_4 by $\varepsilon^{3(\gamma-1)/r-5/2}$, etc. Continuing this calculation inductively, it follows that in the inner region

$$H_{i+1} < C\varepsilon^{[i(\gamma-1-r/2)-r]/r}. \tag{4.16}$$

In the outer region we exploit the fact that ε is small and that (q,p) are close to the self-similar solution (4.12). Again, all terms scale similarly and we have

$$H_{i+1} \sim (T-t)^{[i(\gamma-1-r/2)-r]/(1+r/2)}. \tag{4.17}$$

Using (4.16) and (4.17) we may now determine the average contribution, E, to the error over one period for a method of order n. This is given by combining the estimate over the inner and outer regions so that

$$\begin{aligned} E = \Delta\tau^n \int_0^T H_{n+1}(t) dt \simeq \Delta\tau^n \int_{T-\varepsilon^{\frac{1}{2}(1+\frac{2}{r})}}^T C\varepsilon^{\frac{1}{r}[n(\gamma-1-\frac{r}{2})-r]} dt \\ + \Delta\tau^n \int_0^{T-\varepsilon^{\frac{1}{2}(1+\frac{2}{r})}} (T-t)^{[n(\gamma-1-\frac{r}{2})-r]/(1+r/2)} dt \end{aligned} \tag{4.18}$$

so

$$E = C\varepsilon^{\frac{1}{r}[n(\gamma-1-\frac{r}{2})+1-\frac{r}{2}]}\Delta\tau^n + \begin{cases} \mathcal{O}(\varepsilon^{\frac{1}{r}[n(\gamma-1-\frac{r}{2})+1-\frac{r}{2}]}\Delta\tau^n), & \text{if} \quad \gamma < \gamma^* \\ \mathcal{O}(\Delta\tau^n), & \text{if} \quad \gamma > \gamma^*. \end{cases} \tag{4.19}$$

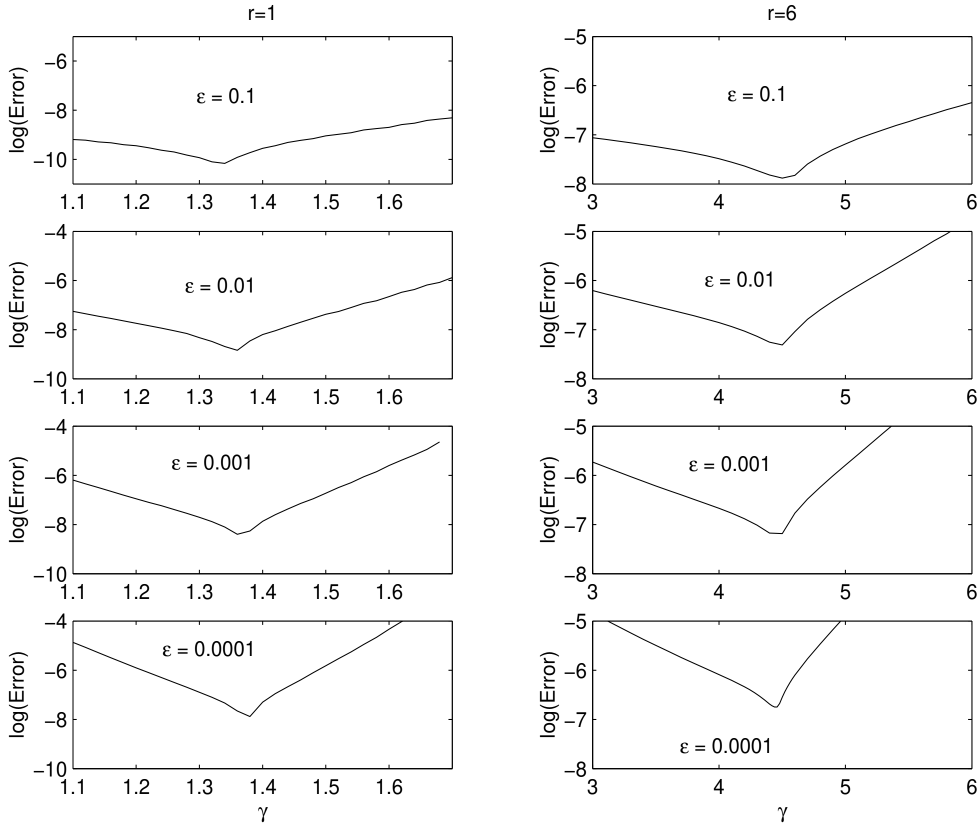

FIG. 4.2. *Average error in energy in the integration of (4.10). The system is integrated until the final real time $t = 20$ for $r = 1$ (left column), and until $t = 10$ for $r = 6$ (right column). For each particular value of ε all integrations require, approximately, the same number of potential evaluations.*

Here γ^* is the critical exponent for which both $[n(\gamma - 1 - \frac{r}{2}) - r]/(1 + r/2) = -1$ and $\frac{1}{r}[n(\gamma - 1 - \frac{r}{2}) + 1 - \frac{r}{2}] = 0$ so that γ^* is given by (4.13).

The value of $\Delta\tau$ above depends upon γ from the previous analysis, so that $\Delta\tau$ is $\mathcal{O}(1/N)$ if $\gamma < 1 + r/2$ and $\Delta\tau$ is $\mathcal{O}(\varepsilon^{(1+\frac{r}{2}-\gamma)/r}/N)$ if $\gamma > 1 + r/2$. Substituting these estimates into (4.19) and extracting the dominant error contribution we have that

$$E = \begin{cases} \mathcal{O}(\varepsilon^{\frac{1}{r}[n(\gamma-1-r/2)+1-r/2]}/N^n), & \text{if} \quad \gamma < \gamma^* \\ \mathcal{O}(\varepsilon^{\frac{1}{r}[n(1+r/2-\gamma)+1-r/2]}/N^n), & \text{if} \quad \gamma^* < \gamma. \end{cases} \tag{4.20}$$

Thus E has a minimum at $\gamma = \gamma^*$ and it is clear that γ^* approaches the scaling invariant value of $1 + \frac{r}{2}$ as $n \to \infty$.

Numerical experiments. In the limit $\varepsilon \to 0$ the evolution of the orbit becomes more nearly singular and we can study if the choice (4.13), which nearly preserves scaling invariance in the fictive time, approaches the numerically observed optimal value. To find the optimal choice of γ numerically, we consider problems with $\varepsilon =$

0.1, 0.01, 0.001, 0.0001 and a range of values of γ, on the following two cases:

Case 1: The Kepler problem ($r = 1$). We integrated the system until $t = 20$ for different values of γ and measured the average error in energy using a time step, $\Delta\,\tau$, such that the final time, $t = 20$, is reached in approximately 1000 ($\varepsilon = 0.1$), 1500 ($\varepsilon = 0.01$), 3000 ($\varepsilon = 0.001$) and 5000 ($\varepsilon = 0.0001$) steps, respectively. The fourth-order RKN_4 integrator is used for the numerical experiments. The results obtained are presented in the left column of Figure 4.2 (which is similar to Figure 3.1).

Case 2: The Lennard-Jones potential ($r = 6$). In this case, we integrated until $t = 10$ using, approximately, 500 ($\varepsilon = 0.1$), 1000 ($\varepsilon = 0.01$), 2000 ($\varepsilon = 0.001$) and 3000 ($\varepsilon = 0.0001$) steps, respectively. See the right column of Figure 4.2.

The error formula (4.20) describes certain features of the graphs in Figs. 3.1 and 4.2. In particular, the minimum of the error when $\gamma = \gamma^*$ is well approximated. In the two cases considered we have that

$$\gamma^* = \frac{3}{2} - \frac{1}{2n} < \frac{3}{2} \quad \text{if} \quad r = 1; \qquad\qquad \gamma^* = 4 + \frac{2}{n} > 4 \quad \text{if} \quad r = 6,$$

so that in both cases γ^* approaches the scaling invariant values of 3/2 and 4 respectively as n increases. The results also predicts that $\log(E)$ should have a linear dependence on $\gamma - \gamma^*$, n and $\log(\varepsilon)$ which is as observed. If $\gamma > \gamma^*$ the predicted slope is $\log(E) \sim \log(\varepsilon)\frac{n}{r}(1 + \frac{r}{2} - \gamma)$ which is very close to that observed. If $\gamma < \gamma^*$ the slope observed is smaller. A possible explanation for this is that the approximation we have used for the outer region is valid for $t \in [T - \tilde{\varepsilon}^{\frac{1}{2}(1+\frac{2}{r})}, T]$ with $\tilde{\varepsilon} \geq \varepsilon$. Then, $\log(\varepsilon)$ has to be changed by $\log(\tilde{\varepsilon}) = \alpha \log(\varepsilon)$ with $\alpha \leq 1$.

4.5. Other adaptive methods. The previous examples show the importance of a good choice of a scaling function g. Now, we study the benefits of using the EASY methods described in this paper versus other explicit adaptive geometric (GI) and non-geometric (NGI) integrators, using related scaling functions.

(NGI). First, to show the benefits of using the EASY method versus other standard adaptive non symplectic algorithms and SI with constant time step, we consider the case $r = 1$, which corresponds to (1.1). We take as initial conditions $(q_0, p_0) = (1, 0)$, $\varepsilon = 0.1$, and integrate until $t = 100$ (40 periods, approximately). The following integrators are considered:

1. The variable time-step non symplectic **ode45** from Matlab with RelTol= 10^{-7} and AbsTol= 10^{-10} applied to (4.10) (18685 potential evaluations).
2. The variable time-step variable order non symplectic **ode113** from Matlab with RelTol= 10^{-10} and AbsTol= 10^{-12} applied to (4.10) (18361 evaluations).
3. RKN_6 applied to (4.10) with $h = \frac{1}{35}$ (38489 evaluations).
4. RKN_6 applied to (4.11) with $\gamma = 1.5$ and $\Delta\tau = \frac{1}{6}$ (19019 evaluations).

All methods involve approximately the same number of potential evaluations except SI, which requires twice this number. The results were shown in Fig. 1.1, where the benefits of combining adaptivity and symplecticity are clear.

(GI). Now consider the symmetric second order scheme (2.16) as the basic method (EAV2) to get a fourth order method (EAV4) using the best 5 stages fourth-order composition given in [29]. (This is more efficient than using the 3 stage fourth order

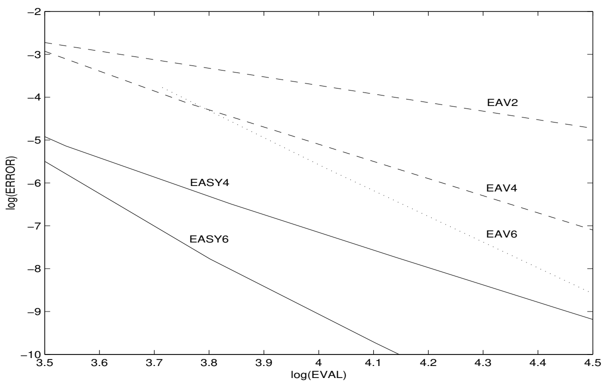

FIG. 4.3. *Relative error in energy versus number of evaluations for second- fourth- (dashed lines) and sixth-order (dotted line) symmetric methods using (2.16) as the basic method, and fourth- and sixth-order RKN EASY methods (solid lines).*

method (2.4)). To get a sixth-order method (EAV6) we take as the basic method two steps of (2.16) [41], and consider the composition of nine basic methods given in [29] (requiring 18 potential evaluations per step). We compare the results with those obtained with the EASY methods implemented with RKN_4 (EASY4) and RKN_6 (EASY6). We consider $r = 1$, $\varepsilon = 0.01$ and $\gamma = 1.5$, and the average relative error in energy is measured for different time steps. Figure 4.3 shows the results obtained. The superiority of the EASY methods is apparent from these graphs and comes from the fact that they can be implemented with more efficient symplectic integrators than the other methods considered. For this one-dimensional problem, (2.17) gives similar results to the non regularised problem. This is because at the pericenter and apocenter of the orbit, we find that $T(p) = 0$ and the time step for the numerical algorithm is the same in those points. This method is not recommended for one dimensional non-symmetric problems.

5. Two and three dimensional problems. To extend the previous analysis to problems in two- and three-dimensions is more complicated. To find a good regularisation function to preserve (or nearly preserve) scaling invariance is still relatively easy. However, in contrast to the one dimensional problem, there is not a systematic procedure to find a CT such that the new Hamiltonian is still easily separable. For this reason, it is natural to consider important physical problems and to analyse if it is possible to apply this technique case by case. If this happens, a very efficient method should be obtained. Indeed, this technique of combining regularisation with a CT is a standard technique in celestial mechanics for numerically solving the Kepler problem for eccentric orbits, and it is described in the following section.

5.1. The Levi-Civita/Kustaanheimo-Stiefel regularisation and transformation. The Levi-Civita (LC) regularisation and transformation [27] applies to the two-dimensional problem, and its generalisation to the three-dimensional space is due to Kustaanheimo-Stiefel (KS) [24, 38]. It corresponds to the Hamiltonian (2.10) with the following regularisation function, $g(\mathbf{q}) = r$, with $r = (\mathbf{q}^T\mathbf{q})^{1/2}$. This transformation is specially suitable for the numerical analysis of highly eccentric orbits in the Kepler problem (for which $V = -1/r$) as the singularity in the potential is removed. As in the one-dimensional problem, the original Hamiltonian H is separable, but the transformed Hamiltonian K contains the term $\frac{1}{2}r\mathbf{p}^T\mathbf{p}$ which is exactly solvable. However, it is computationally expensive, and the benefits of using splitting methods breaks down. However, there is a simple solution. Kustaanheimo and Stiefel [24, 38] proposed the following transformation.

$$\left\{ \begin{array}{l} \mathbf{q} = \hat{Q}\mathbf{Q}, \\ \mathbf{p} = \dfrac{1}{2R^2}\hat{Q}\mathbf{P}. \end{array} \right. \tag{5.1}$$

Here, the three-dimensional system has been enlarged with another dimension, using the vectors $\mathbf{q} = (q_1, q_2, q_3, 0)^T$ and $\mathbf{p} = (p_1, p_2, p_3, 0)^T$. Now $\mathbf{Q} = (Q_1, Q_2, Q_3, Q_4)^T$, $\mathbf{P} = (P_1, P_2, P_3, P_4)^T$ are the KS-variables, $R = (\mathbf{Q}^T\mathbf{Q})^{1/2}$ and $\hat{Q}$ is the KS-matrix

$$\hat{Q} = \begin{pmatrix} Q_1 & -Q_2 & -Q_3 & Q_4 \\ Q_2 & Q_1 & -Q_4 & -Q_3 \\ Q_3 & Q_4 & Q_1 & Q_2 \\ Q_4 & -Q_3 & Q_2 & -Q_1 \end{pmatrix}.$$

This includes the Levi-Civita transformation, which corresponds to the particular case $q_3 = p_3 = Q_3 = Q_4 = P_3 = P_4 = 0$.

COROLLARY 5.1. *The transformation (5.1) is canonical.*

Proof. Let us consider $\Phi(\mathbf{Q}) = \hat{Q}\mathbf{Q}$ then, it is immediate to check that

$$\Phi'(\mathbf{Q}) = 2\hat{Q}. \tag{5.2}$$

Substituting Φ and Φ' in (2.11) and considering that

$$\hat{Q}^T\hat{Q} = \hat{Q}\hat{Q}^T = R^2 I, \tag{5.3}$$

where I is the identity matrix, we get (5.1), and the transformation is canonical. □

Now, we substitute this transformation into the Hamiltonian (2.10). If we consider that

$$\frac{1}{2}\mathbf{p}^T\mathbf{p} = \frac{1}{8R^4}\mathbf{P}^T\hat{Q}^T\hat{Q}\mathbf{P} = \frac{1}{8R^2}\mathbf{P}^T\mathbf{P}, \qquad r = \sqrt{\mathbf{q}^T\mathbf{q}} = \sqrt{\mathbf{Q}^T\hat{Q}^T\hat{Q}\mathbf{Q}} = R^2,$$

the Hamiltonian K in the new coordinates takes the form

$$K = \frac{1}{8}\mathbf{P}^T\mathbf{P} + R^2V(\mathbf{Q}) - R^2Q^t, \tag{5.4}$$

which is separable in two trivially solvable parts, $K = \tilde{T}(\mathbf{P}) + \tilde{V}(\mathbf{Q}, Q^t)$ with $\tilde{T}$ still quadratic in momenta. For the Kepler problem ($V = 1/r = 1/R^2$) it gives

$$K = \frac{1}{8}\mathbf{P}^T\mathbf{P} + 1 - R^2Q^t. \tag{5.5}$$

Since $Q^t = H_0$ is constant, this is an harmonic oscillator which is easy and cheap to integrate even for highly eccentric orbits. One problem for this regularisation is that it does not preserve the scaling invariance of the Kepler problem. From the one-dimensional problem we know the influence of the regularisation function on the performance of a numerical integrator as well as its close relation with the scaling invariance. Then, as we will show in one example, the performance of the LC/KS regularisation deteriorates for some problems. For this reason, it is important to generalise the LC/KS transformation in order to allow the use of a regularisation function which both removes the singularity of the Kepler problem and still preserves its scaling invariance. This is studied in [2].

5.2. The Lennard-Jones potential. The Lennard-Jones potential is one of the most important potentials in molecular dynamics. The system is described by the Hamiltonian

$$H = \frac{1}{2}\mathbf{p}^T\mathbf{p} - \frac{a}{r^6} + \frac{b}{r^{12}}, \tag{5.6}$$

with $a = c\beta^6$, $b = c\beta^{12}$ and c, β constants. The term $-a/r^6$ gives usually the dominant contribution for most evolution region, and a regularization function which makes this part scaling invariant is $g = r^4$. Unlike in the previous case, we present a CT which works for this important potential and function g. Let us consider the coordinate transformation $\mathbf{q} = \Phi(\mathbf{Q})$ with

$$\Phi(\mathbf{Q}) = \frac{1}{R^{2m}}\mathbf{Q} \tag{5.7}$$

then

$$\Phi'(\mathbf{Q})_{i,j} = \frac{1}{R^{2(m+1)}}\left(R^2\delta_{ij} - 2mQ_iQ_j\right). \tag{5.8}$$

A simple inspection of (5.8) indicates that Φ' is orthogonal only for $m = 1$, and this is the only case we consider, where

$$\Phi'\Phi'^T = \frac{1}{R^4}I. \tag{5.9}$$

Let us denote $\hat{Q}_{ij} = \left(R^2\delta_{ij} - 2Q_iQ_j\right)$, $\hat{q}_{ij} = \left(r^2\delta_{ij} - 2q_iq_j\right)$, where $r = 1/R$, $\hat{Q}^T\hat{Q} = R^4I$, $\hat{q}^T\hat{q} = r^4I$. Then, from Theorem 2.1 and (5.7)-(5.9) with $m = 1$ it is immediate to show that the following transformation

$$\left\{\begin{array}{l} \mathbf{q} = \frac{1}{R^2}\mathbf{Q} \\ \mathbf{p} = \hat{Q}\mathbf{P} \end{array}\right. \quad \Leftrightarrow \quad \left\{\begin{array}{l} \mathbf{Q} = \frac{1}{r^2}\mathbf{q} \\ \mathbf{P} = \hat{q}\mathbf{p} \end{array}\right. \tag{5.10}$$

is canonical, both for the two and three dimensional problem (it is not necessary to introduce a new coordinate for the three dimensional problem, as in the KS transformation). In addition, since $r^4\mathbf{p}^T\mathbf{p} = \mathbf{P}^T\mathbf{P}$, this CT makes separable the Lennard-Jones Hamiltonian with $g = r^4$ (which makes the system nearly scaling invariant), and the Hamiltonian to solve is

$$K_{sc} = \frac{1}{2}\mathbf{P}^T\mathbf{P} - aR^2 + bR^8 + \frac{Q^t}{R^4}. \tag{5.11}$$

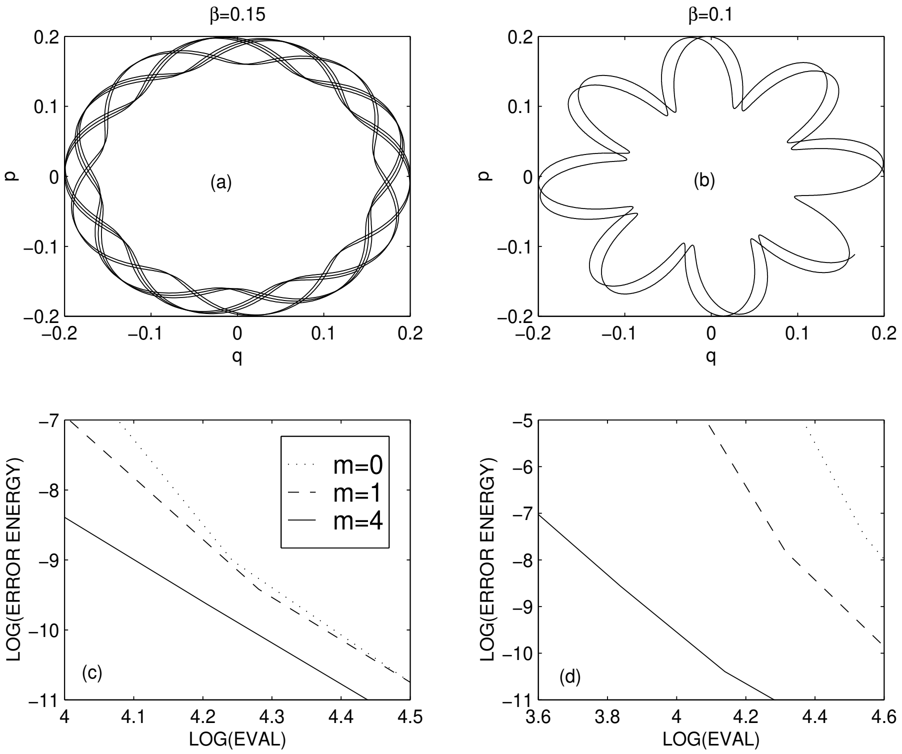

FIG. 6.1. *(a), (b): trajectories for the Lennard-Jones problem. (c), (d): average relative error in energy versus number of evaluations when non regularisation is considered ($m = 0$), when considering the LC regularisation ($m = 1$) and when considering the scaling invariant regularisation ($m = 4$).*

If the LC/KS regularisation is considered, the resulting Hamiltonian is

$$K_{LC} = \frac{1}{8}\mathbf{P}^T\mathbf{P} - \frac{a}{R^{10}} + \frac{b}{R^{22}} + Q^t R^2. \tag{5.12}$$

whch contains singularities of higher order.

In [2] we present a generalisation of the LC/KS transformation which can be used in a number of different potentials. However, there is no simple generalization of (5.10) to be used with more general potentials, this being an interesting subject for investigation.

6. Numerical Examples of two-dimensional problems.

6.1. The two-dimensional Lennard-Jones problem. We consider (5.6) with initial conditions $q_1 = 1/5$, $q_2 = 0$, $p_1 = 0$, $p_2 = \sqrt{2(H_0 - V(r))}$, for $H_0 - V(r) \geq 0$, which corresponds to a system with energy H_0. We take $c = 20$, $\beta = 0.15, 0.1$ and $H_0 = -0.1$, and we integrated until $t = 5$. We study the performance of the schemes taking $g = r^m$ in the following cases: I- non regularisation ($m = 0$); II- LC regularisation ($m = 1$); and III- scaling invariant regularisation ($m = 4$). We measured the average relative error in energy versus the number of potential evaluations for

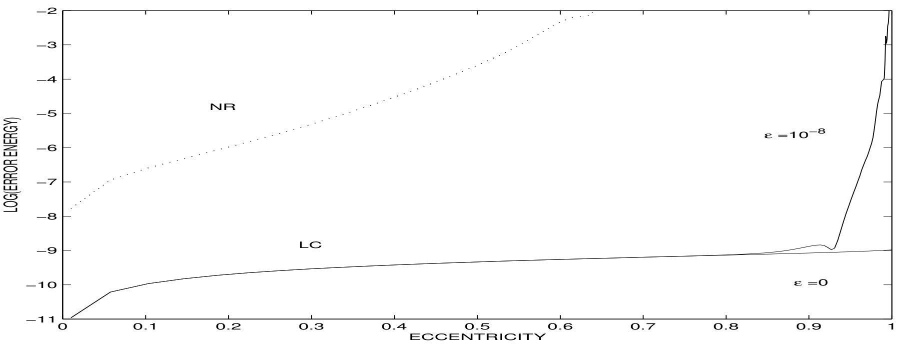

FIG. 6.2. *Average relative error in energy as a function of the eccentricity for the non-regularised system and for the LC regularisation using the same fictive time-step. This is done for* $\varepsilon = 0$ *and* $\varepsilon = 10^{-8}$.

different time steps $\Delta\tau$. In all cases, we integrated the systems using the symplectic RKN_6 integrator. Fig. 6.1 shows the trajectory of the orbits and the average relative error in energy of the methods versus the number of evaluations. We observe that for $\beta = 0.1$ the trajectory approaches closer to the origin and the scaling invariant scheme is much superior. We clearly observe that the case $m = 1$ does not play any special role as in the Kepler problem, giving less efficient results. Then, for this problem the choice $m = 4$ gives the most efficient algorithm, and the relative performance will increase in the limit $\beta \to 0$.

6.2. Perturbed Kepler problem. Let us now consider the following two-dimensional perturbed Kepler problem

$$H = \frac{1}{2}(p_1^2 + p_2^2) - \frac{1}{r} + \frac{\varepsilon}{r^3}. \tag{6.1}$$

This problem is neither integrable or scaling invariant, although it does have an approximate scaling symmetry if ε/r^3 is small. We take as initial conditions $q_1 = 1 - e$, $q_2 = 0$, $p_1 = 0$, $p_2 = \sqrt{(1+e)/(1-e)}$ which, for the unperturbed problem, would correspond to an orbit of period 2π, eccentricity e and energy $-1/2$. We integrated until $t = 10\pi$ for different values of e using the RKN_4 integrator, and measured the average relative error in energy choosing a fictive time steps such that the whole integration is carried out with approximately 100 steps. We considered two cases: (i) the non regularised case (NR); and (ii) the Levi-Civita regularisation (LC). We started the experiments with $\varepsilon = 0$ (unperturbed problem) and repeated the experiment with $\varepsilon = 10^{-8}$. The results are shown in Fig. 6.2 where three important facts can be deduced: (i) when using LC regularisation the error does not deteriorates at high eccentricities if $\varepsilon = 0$; (ii) the performance of the regularised scheme is considerably superior, to the constant step size integrator, even for small eccentricities; (iii) even for a very small perturbation the performance of LC is severely deteriorated for high eccentricities.

The reason for the good performance of the Levi-Civita regularisation on the unperturbed Kepler ($\varepsilon = 0$) problem comes because, the Hamiltonian to be solved is (5.5) which is exactly solvable. This is possible because the original system is also integrable. The symplectic integrators used solve exactly a perturbed harmonic oscillator or, equivalently, they solve exactly a Kepler problem, with slightly different parameters, giving also a closed trajectory (this is a surprising fact since it is well known that most symplectic integrators, when applied to the Kepler problem give trajectories with a precession of the orbit). However, if some perturbations are introduced making the system not integrable, the performance of the LC/KS regularisation can seriously deteriorated for high eccentricities. The main reason is because the fictive time is not (nearly) scaling invariant. In addition, we must remember that this excellent performance for the LC/KS regularisation only happens when solving the Kepler problem in Cartesian coordinates, but not in polar coordinates as shown in the one-dimensional example of Section 4.

7. Conclusions. In this paper we have presented a procedure to build explicit adaptive symplectic (EASY) integrators. This technique combines the Poincaré transformation with a canonical transformation, to recover the separability of the original system. It can be considered as a generalisation of the LC/KS regularisation. For the one-dimensional problem, a backward error analysis for a family of problems is presented and an explicit dependence of the error with the regularisation function, g (at constant work) is obtained. The error and the optimal function, g, depend on the order of the method used and, most importantly, on the value which makes the regularised system scaling invariant (for the dominant part of the potential). These results perfectly agree with those obtained from the numerical experiments and can be extrapolated to other higher dimensional problems. As an example, an EASY method for the two- and three-dimensional Lennard-Jones potential is presented, showing its superiority versus other regularisations. We have also shown how the well known LC/KS regularisation (which does not preserves scaling invariance for the Kepler problem) looses its efficiency on some problems. This is studied in more detail in [2], where a generalisation of the LC/KS regularisation is presented in order to preserve the scaling invariance of the Kepler problem.

Obviously, it not always possible to find a CT for each function, g. In such a case, several alternatives can be considered. For example: (i) to considerer the function g and its corresponding CT which are closer to the optimal g obtained from the error analysis; (ii) to choose this optimal function and to use an alternative method, for example, the explicit adaptive Verlet method (2.16), or to consider it as the basic method to higher orders composition integrators. In the last case, the previous backward error analysis does not apply, but we expect the results obtained are still approximately valid.

REFERENCES

[1] G.I. Barenblat, *Scaling, self-similarity and intermediate asymptotics.* CUP, (1996).

[2] S. Blanes and C.J. Budd, *A generalisation of the Levi-Civita/Kustaanheimo-Stiefel regularisation: Scaling invariance.* Work in progress.

[3] S. Blanes, F. Casas, and J. Ros, *Symplectic integrators with processing: a general study*, SIAM J. Sci. Comput., **21** (1999), pp. 711–727.

[4] S. Blanes, F. Casas, and J. Ros, *Processing symplectic methods for near-integrable Hamiltonian systems*, Celest. Mech. & Dyn. Astr., **77** (2000), pp. 17–35.

[5] S. Blanes, F. Casas, and J. Ros, *High-order Runge-Kutta-Nyström geometric integrators with processing*, Appl. Numer. Math., **39** (2001), pp. 245–259.

[6] S. Blanes and P.C. Moan, *Practical Symplectic Partitioned Runge–Kutta and Runge–Kutta–Nyström Methods*, J. Comp. Appl. Math. In press.

[7] S.D. Bond and B. Leimkuhler, *Time-transformations for reversible variable step-size integration*, Numerical Algorithms, **19** (1998), pp. 55–71.

[8] C.J. Budd, B. Leimkuhler, and M.D. Piggot, *Scaling invariance and adaptivity*, Appl. Numer. Math., **39** (2001), pp. 261–288.

[9] C.J. Budd and M.D. Piggot, *The geometric integration of scale invariant ordinary and partial differential equations*, J. Comp. Appl. Math., **128** (2001), pp. 399–422.

[10] C.J. Budd and M.D. Piggot, *Geometric integration and its applications*, to appear in 'Foundations of Computational Mathematics', a volume of the 'Handbook of Numerical Analysis', ed. F. Cucker.

[11] C.J. Budd, W. Huang, and R.D. Russell, *Moving mesh for problems with blow-up*, SIAM J. Sci. Comput., **17** (1997), pp. 305–327.

[12] M.P. Calvo, *High order starting iterates for implicit Runge–Kutta methods: an improvement for variable-step symplectic integrators*, IMA Jour. Num. Anal., **22** (2002), pp. 153–166.

[13] M.P. Calvo, J.M. Sanz-Serna, and M.A. López-Marcos, *Variable step implementations of geometric integrators*, Appl. Numer. Math., **28** (1998), pp. 1–16.

[14] M.P. Calvo and J.M. Sanz-Serna, *The development of variable-step symplectic integrators, with applications to the two-body problem*, SIAM J. Sci. Comput., **14** (1993), pp. 936–952.

[15] S. Cirilli, E. Hairer, and B. Leimkuhler, *Asymptotic error analysis of the adaptive Verlet method*, BIT, **39**, (1999), pp. 25–33.

[16] M. Creutz and A. Gocksch, *Higher-order hybrid Monte Carlo Algorithms*, Phys. Rev. Lett., **63** (1989), pp. 9–12.

[17] B. Gladman, M. Duncan, and J.Candy, *Symplectic integrators for long-term integrations in celestial mechanics*, Celest. Mech., **52** (1991) 221–240

[18] H. Goldstein, *Classical Mechanics*, Addison-Wesley, Reading, 1980.

[19] E. Hairer, *Variable time step integration with symplectic methods*, Appl. Numer. Math., **25** (1997), pp. 219–227.

[20] E. Hairer, Ch. Lubich, and G. Wanner, *Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations*, Springer Series in Computational Mathematics **31**, Springer-Verlag, 2002.

[21] T. Holder, B. Leimkuhler, and S. Reich, *Explicit variable step-size and time-reversible integration*, Appl. Numer. Math., **39** (2001), pp. 367–377.

[22] W. Huand and B. Leimkuhler, *The adaptive Verlet metho*, SIAM J. Sci. Comput., **18** (1997), pp. 239–256.

[23] A. Iserles, *A First Course in the Numerical Analysis of Differential Equations*, (1996), Cambridge University Press, Cambridge.

[24] P. Kustaanheimo and E. Stiefel, *Perturbation theory of Kepler motion based on spinor regularization*, J. Reine Angewande M., **218** (1965), pp. 204–219.

[25] B. Leimkuhler, *Reversible adaptive regularization: perturbed Kepler motion and classical atomic trajectories*, R. Soc. London Philos. Trans. Ser. A Maths. Phys. Engrg. Sci., 357 (1999), pp. 1101–1133.

[26] B. Leimkuhler, *Reversible adaptive regularization methods for atomic N-body problems in applied fields*, Appl. Numer. Math., **29** (1999), pp. 31–43.

[27] T. Levi-Civita, *Sur la regularisation du problème des trois corps*, Acta Math., **42** (1920), pp. 99–144.

[28] J.E. Marsden, *Lectures on mechanics*, (1992), Cambridge University Press.

[29] R.I. McLachlan, *On the numerical integration of ordinary differential equations by symmetric composition methods*, SIAM J. Sci. Comput., **16** (1995), pp. 151–168.

[30] R.I. McLachlan, *Composition methods in the presence of small parameters*, BIT, **35**, (1995), pp. 258–268.

[31] S. Mikkola,*Practical symplectic methods with time transformation for the few-body problem*, Celest. Mech. & Dyn. Astr., **67** (1997), pp. 145–165.

[32] S. Mikkola and K. Tanikawa, *Explicit symplectic algorithms for time-transformed Hamiltonians*, Celest. Mech. & Dyn. Astr., **74** (1999), pp. 287–295.

[33] M.D. Piggot, *Geometric integration ofdifferential equations*, Ph.D. Thesis, University of Bath, 2002.
[34] M. Preto and S. Tremaine, *A class of symplectic integrators with adaptive time step for separable Hamiltonian systems*, Astron. J., **118** (1999), pp. 2532–2541.
[35] S. Reich, *Bacward error analysis for numerical integrators*, SIAM J. Numer. Anal. **36** (1999), pp. 1549-1570.
[36] J.M. Sanz-Serna and M.P. Calvo, *Numerical Hamiltonian Problems*, (1994), Chapman and Hall.
[37] R. Skeel, *Variable step size destabilizes the Störmer/leapfrog/Verlet method*, BIT, **33** (1993), pp. 172–175.
[38] E.L. Stiefel and G. Scheifel, *Linear and regular celestial mechanics*, Springer, Berlin, 1971.
[39] D. Stoffer, *Variable steps for reversible integration methods*, Computing, **55** (1995), pp. 1–22.
[40] M. Suzuki, *Fractal decomposition of exponential operators with applications to many-body theories and Monte Carlo simulations*, Phys. Lett. A, **146** (1990) 319–323.
[41] C. Sweet and B. Leimkuhler, Private communication.
[42] J. Waldvogel, *A new regularization of the planar problem of three bodies*, Celest. Mech., **6** (1972), pp. 221–231.
[43] J. Wisdom and M. Holman, *Symplectic maps for the N-body problem*, Astron. J., **102** (1991), pp. 1528–1538.
[44] H. Yoshida, *Construction of higher order symplectic integrators*, Phys. Lett. A, **150** (1990) 262–268.