EXPLICIT ADAPTIVE SYMPLECTIC (EASY) INTEGRATORS: A SCALING INVARIANT GENERALISATION OF THE LEVI-CIVITA AND KS REGULARISATIONS

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Abstract. We present a generalisation of the Levi-Civita and Kustaanheimo–Stiefel regularisation. This allows the use of more general time rescalings. In particular, it is possible to find a regularisation which removes the singularity of the equations and preserves scaling invariance. In addition, these equations can, in certain cases, be integrated with explicit symplectic Runge–Kutta–Nyström methods. The combination of both techniques gives an explicit adaptive symplectic (EASY) integrator. We apply those methods to some perturbations of the Kepler problem and illustrate, by means of some numerical examples, when scaling invariant regularisations are more efficient that the LC/KS regularisation.

Key words: canonical transformations, Levi-Civita, regularisation, scaling invariance

1. Introduction

The Levi-Civita (LC) regularisation for the planar motion of two body problems (Levi-Civita, 1920), or its extension to the spatial case given by Kustaanheimo and Stiefel (KS) (Kustaanheimo and Stiefel, 1965; Stiefel and Scheifele, 1971) is a standard technique for the numerical integration of eccentric orbits in the Kepler problem. It combines a time regularisation with a canonical transformation. The time regularisation removes the singularity in the potential terms, but it has the disadvantage of making the system (or Hamiltonian) more complicated. However, by using a proper canonical transformation the system becomes a regular Hamiltonian problem (a harmonic oscillator), making its numerical integration very efficient. This technique has been used as a tool for treating two-body close encounters because it reduces the accumulation of numerical error in highly eccentric orbits. The long-term behaviour of the resulting integration errors of the orbital motions has been studied in (Arakida and Fukushima, 2000), and these show that the regularised method is also superior to non regularised methods even when the orbit is far from a close encounter.


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On the other hand, it has also been shown that for systems with singularities, the use of methods which inherit natural scalings (scale-invariant methods) can lead to low errors (Barenblatt, 1996, Budd et al., 1996, 2001; Budd and Piggott, 2001, Blanes and Budd, 2004). Numerical integrators preserving (or nearly preserving) this property have proved to be superior to other regularisations for a number of problems. Although the Kepler problem is invariant under changes of scale in space and time (a result encapsulated in Kepler's third law) the LC/KS regularisation does not exploit this scaling invariance. The performance of numerical methods based on this regularisation can then considerably decrease when some perturbations to the Kepler problem are considered for which the transformed problem is no longer a simple harmonic oscillator, as shown in Blanes and Budd (2004) for a particular example. Alternatively, the performance of integrators which inherit natural scalings is not degraded by such perturbations.

In order to preserve scaling invariance, the monitor function controlling the time-transformation has to be chosen properly. The monitor function for the LC/KS transformation is simply the radial distance r. In this paper we generalise the LC/KS regularisation for two- and three-dimensional problems so, more general monitor functions can be used. The approach we describe contains the LC/KS regularisation as a particular case. It also contains another regularisation which removes the singularity of the Kepler problem, preserving at the same time its scaling invariance. The resulting system is, in general, suitable to be numerically integrated with high order symplectic Rung–Kutta–Nyström (RKN) integrators, and in certain cases this integration can be performed by using explicit methods. As a result, we have in these cases an explicit adaptive symplectic (EASY) method which preserves the scaling invariance of the Kepler problem.

We study some circumstances under which a scaling invariant transformation is superior to other time regularisations. In particular, we consider the collision problem and several perturbations to the Kepler problem. We find that for the pure Kepler problem (with no collision) and for regular polynomial perturbations to it, the LC/KS regularisation is the most efficient method. However, for the collision problem and for near collisions where perturbations with higher singularities are included, the scaling invariant transformation is the most efficient technique giving the lowest errors for a given computational cost. A particular example being computations of perturbed, highly eccentric orbits. Since the LC/KS regularisation has been widely used for the numerical integration of the N-body problem both with gravitational and Coulombic interactions (Waldvogel, 1972; Mikkola, 1997b; Leimkuhler, 1999), we propose that the new scale-invariant regularisation could be very useful for the accurate integration of these problems. Scale invariant regularisations can be seen as complimentary to LC/KS as they

work well for non-integrable problems, where the high eccentricity and/or singularities in the orbits make scaling effects important.

The plan of the remainder of this paper is as follows. In Section 2 the Levi-Civita regularisation and the KS generalisation of two and three-dimensional problems is presented. These transformations are generalised in Section 3 to allow for the use of different regularisation functions. In Section 4 we relate the regularisation function to scaling structures in the original system. Numerical examples are presented in Section 5, and Section 6 gives some conclusions.

2. Levi-Civita and Kustaanheimo–Stiefel Regularisations

Let us denote by $\mathbf{q} = (q_1 \ldots, q_k)^{\mathrm{T}}$, $\mathbf{p} = (p_1 \ldots, p_k)^{\mathrm{T}}$, $k = 2, 3$ the coordinates and associated momenta of a system in a $2\,k$ -dimensional phase space with Hamiltonian

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

This system can be integrated numerically using explicit symplectic integrators with constant time steps (Yoshida, 1990; Kinoshita et al., 1991; Wisdom and Holman, 1991; Yoshida, 1993; Blanes et al., 2000; Hairer et al., 2002). These methods are very efficient for the long time integration of such Hamiltonian systems (for non-eccentric trajectories). In addition, since T is quadratic in momenta then the more efficient symplectic RKN integrators can be used (Sanz-Serna and Calvo, 1994; McLachlan and Quispel, 2002). However, if the potential has singularities, the numerical integration of the system of differential equations derived from (1) can produce large errors when the particle approaches the singularity (Gladman et al., 1991; Calvo and Sanz-Serna, 1993). A standard technique to reduce such errors is to regularise the equations through a time rescaling in order to remove or reduce the strength of the singularity. This can be achieved if a fictive time, τ, is introduced through the ordinary differential equation,

$$\frac{\mathrm{d}t}{\mathrm{d}\tau} = g(\mathbf{q}, \mathbf{p}), \tag{2}$$

defining a *Sundman transformation* (Leimkuhler, 1999, and references therein). Here g is a positive scalar monitor function which is taken to be small if the solution is evolving rapidly and τ is the fictive time which is used for all computations. Next, we introduce two new conjugate coordinates[1]

[1] It is usual in the literature to take $q^t = t$ and $p^t = -H(\mathbf{q}_0, \mathbf{p}_0)$. However, to obtain a more natural splitting of the extended Hamiltonian, in this paper we take p^t to be the time.

$$q^t = H(\mathbf{q}_0, \mathbf{p}_0) \quad \text{and} \quad p^t = t.$$

To preserve the Hamiltonian structure of the system after rescaling in terms of τ, we apply a Poincaré transformation (Waldvogel, 1972; Mikkola, 1997a). With this transformation the whole system $(\mathbf{q}, q^t, \mathbf{p}, p^t)$ is Hamiltonian and evolves in the fictive time, τ, with Hamiltonian

$$K(\mathbf{q}, q^t, \mathbf{p}, p^t) = g(\mathbf{q}, \mathbf{p})(H(\mathbf{q}, \mathbf{p}) - q^t). \tag{3}$$

Observe that with this choice of q^t and p^t the evolution of the system of ordinary differential equations corresponding to the Hamiltonian (1) is equivalent to the evolution of the extended system with Hamiltonian (3), where the effect of the time transformation is included automatically.

With this transformation it is possible to remove the singularity of the potential with a careful choice of the monitor function $g(\mathbf{q}, \mathbf{p})$ but, usually this leads to a more complicated system to be solved numerically and it may not be possible to use explicit symplectic integrators. This problem can be simplified if a canonical transformation is found such that the Hamiltonian, in the new coordinates, recovers a simple structure. For the Kepler problem, this can be achieved using the LC or KS regularisation.

2.1. THE KUSTAANHEIMO–STIEFEL REGULARISATION

Given the Hamiltonian (1) with $k = 3$, the Kustaanheimo–Stiefel regularisation of the Kepler problem uses the Poincaré transformation (3) together with the monitor function

$$g(\mathbf{q}) = r \equiv \sqrt{q_1^2 + q_2^2 + q_3^2}.$$

This leads to the following Hamiltonian

$$K(\mathbf{q}, q^t, \mathbf{p}, p^t) = \frac{1}{2} r \mathbf{p}^{\mathrm{T}} \mathbf{p} + r(V(\mathbf{q}) - q^t). \tag{4}$$

This transformation is especially suitable for the analysis of eccentric orbits in the Kepler problem under the usual gravitational potential, $V = c/r$, with c a constant, because the singularity in the potential is removed. As mentioned, the original Hamiltonian H is separable, but the transformed Hamiltonian K is not as it contains the term $\frac{1}{2} r \mathbf{p}^{\mathrm{T}} \mathbf{p}$. Although the Hamiltonian $H = \frac{1}{2} r \mathbf{p}^{\mathrm{T}} \mathbf{p}$ is exactly solvable using, for example, the KS transformation that we show below, it is necessary to compute both the transformation and its inverse at each stage of the computation. This makes the exploitation of such separability expensive, and the benefits of using, for example, an explicit symplectic integrator in this case are not clear.

Fortunately, there is a simple solution which allows the use of an efficient numerical method on the transformed problem. It is possible to find an

invertible canonical transformation (CT) to a new set of coordinates $(\mathbf{Q}, Q^t, \mathbf{P}, P^t)$ which allows us to rewrite K as a simple and separable Hamiltonian in the new coordinates. This is the KS canonical transformation (with $(Q^t, P^t) = (q^t, p^t)$)

$$\begin{cases} \mathbf{q} = \widehat{Q}\mathbf{Q}, \\ \mathbf{p} = \frac{1}{2R^2}\widehat{Q}\mathbf{P}, \end{cases} \tag{5}$$

where now $\mathbf{q} = (q_1, q_2, q_3, 0)^{\mathrm{T}}$, $\mathbf{p} = (p_1, p_2, p_3, 0)^{\mathrm{T}}$ are four-dimensional vectors, $\mathbf{Q} = (Q_1, Q_2, Q_3, Q_4)^{\mathrm{T}}$, $\mathbf{P} = (P_1, P_2, P_3, P_4)^{\mathrm{T}}$ are the four-dimensional KS-variables, $R = \sqrt{Q_1^2 + \cdots + Q_4^2}$ and

$$\widehat{Q} = \begin{pmatrix} Q_1 & -Q_2 & -Q_3 & Q_4 \\ Q_2 & Q_1 & -Q_4 & -Q_3 \\ Q_3 & Q_4 & Q_1 & Q_2 \\ Q_4 & -Q_3 & Q_2 & -Q_1 \end{pmatrix}, \tag{6}$$

is the KS matrix which has the property

$$\widehat{Q}^{\mathrm{T}}\widehat{Q} = \widehat{Q}\widehat{Q}^{\mathrm{T}} = R^2 I, \tag{7}$$

where I is the identity matrix.

If we consider this canonical transformation, it follows that

$$r = \sqrt{\mathbf{q}^{\mathrm{T}}\mathbf{q}} = \sqrt{\mathbf{Q}^{\mathrm{T}}\widehat{Q}^{\mathrm{T}}\widehat{Q}\mathbf{Q}} = R^2, \quad \frac{1}{2}r\mathbf{p}^{\mathrm{T}}\mathbf{p} = \frac{1}{8}\mathbf{P}^{\mathrm{T}}\mathbf{P}. \tag{8}$$

The Hamiltonian K in the new coordinates then takes the form

$$K = \frac{1}{8}\mathbf{P}^{\mathrm{T}}\mathbf{P} + R^2 V(\mathbf{Q}) - R^2 Q^t, \tag{9}$$

which is separable in two trivially solvable parts, $K = \widetilde{T}(\mathbf{P}) + \widetilde{V}(\mathbf{Q}, Q^t)$ with $\widetilde{T}$ again quadratic in momenta. For the Kepler problem ($V = -1/r = -1/R^2$) we then have

$$K = \frac{1}{8}\mathbf{P}^{\mathrm{T}}\mathbf{P} - 1 - R^2 Q^t. \tag{10}$$

Since $Q^t < 0$ for bounded trajectories, this corresponds to a harmonic oscillator which can be integrated to high accuracy.

The two-dimensional Levi-Civita regularisations corresponds to the particular case where $q_i = p_i = Q_i = P_i = 0$, $i > 2$. The LC/KS regularisation has been used during the last decades as a very efficient technique for numerically solving the Kepler problem as well as for some perturbations to it (Arakida and Fukushima, 2000; Celletti, 2002). However, we must keep in mind that this CT is only valid for one particular regularisation function ($g = r$) which, as we will see, does not preserve the scaling invariance for the Kepler problem. On the other hand, for different potentials or for some perturbations to the Kepler problem other regularisation functions can give

better performances (Janin, 1974). For this reason, it seems interesting to look for different CTs for more appropriate monitor functions, g . An additional bonus is obtained if the final Hamiltonian is still separable taking the same form as (9), with the kinetic energy quadratic in momenta, being then suitable to be integrated with explicit symplectic RKN integrators.

3. Generalisations of the LC/KS Transformation

We now consider more general CTs which can be applied to a variety of scaling functions $g(\mathbf{q})$, depending only on the coordinates. At this stage it is convenient to consider the following result (Marsden, 1992)

THEOREM 1. *The transformation*

$$\begin{cases} \mathbf{q} = \Phi(\mathbf{Q}), \\ \Phi'(\mathbf{Q})^{\mathrm{T}}\mathbf{p} = \mathbf{P}, \end{cases} \tag{11}$$

where Φ *is a diffeomorphism of* $\mathbb{R}^{2k}$ *and* $\Phi'_{ij} \equiv \partial\Phi_i/\partial\mathbf{Q}_j$, *is canonical.*

We want to generalise the CT (5) with the goal that for a family of regularisation functions, $g(\mathbf{q})$, the following conditions are satisfied

$$\mathbf{q} = \Phi(\mathbf{Q}), \quad g(\mathbf{q})\frac{1}{2}\mathbf{p}^{\mathrm{T}}\mathbf{p} = a\mathbf{P}^{\mathrm{T}}\mathbf{P}, \tag{12}$$

with a being a constant and Φ a given function. If a CT satisfying (12) is found, the Hamiltonian (3), which takes the form

$$K = \frac{1}{2}g(\mathbf{q})\mathbf{p}^{\mathrm{T}}\mathbf{p} + g(\mathbf{q})(V(\mathbf{q}) - q^t) \tag{13}$$

transforms to the separable Hamiltonian

$$K = a\mathbf{P}^{\mathrm{T}}\mathbf{P} + \widetilde{V}(\mathbf{Q}, Q^t). \tag{14}$$

If g is properly chosen then $a\mathbf{P}^{\mathrm{T}}\mathbf{P}$ and $\widetilde{V}(\mathbf{Q}, Q^t)$ should both be reasonably small, and explicit symplectic RKN methods with constant time step, $\Delta\tau$, will be computationally stable and very efficient.

We present a procedure to find one family of such CTs. Suppose we have determined a function $\Phi(\mathbf{Q})$ such that

$$\Phi(\mathbf{Q})^{\mathrm{T}}\Phi(\mathbf{Q}) = R^{\alpha} \tag{15}$$

$\alpha \neq 0$, and

$$\Phi'(\mathbf{Q})\Phi'(\mathbf{Q})^{\mathrm{T}} = cR^{\beta}I, \tag{16}$$

with α, β and c constants. If this function is used to define the CT given in (11), then $r = (\mathbf{q}^{\mathrm{T}}\mathbf{q})^{1/2} = (\Phi^{\mathrm{T}}\Phi)^{1/2} = R^{\alpha/2}$ or $R = r^{2/\alpha}$. On the other hand,

since $\mathbf{P}^{\mathrm{T}}\mathbf{P} = \mathbf{p}^{\mathrm{T}}\Phi'\Phi'^{\mathrm{T}}\mathbf{p} = cR^{\beta}\mathbf{p}^{\mathrm{T}}\mathbf{p} = cr^{2\beta/\alpha}\mathbf{p}^{\mathrm{T}}\mathbf{p}$, then conditions (12) are satisfied for the case

$$g = r^{\gamma} \quad \text{with} \quad \gamma = 2\beta/\alpha,$$

and the separable Hamiltonian (14) is obtained. Observe that for the LC/KS transformation (5) we have $\Phi(\mathbf{Q}) = \widehat{Q}\mathbf{Q}$ (then $\Phi^{\mathrm{T}}\Phi = R^4$ and $\alpha = 4$) and $\Phi'(\mathbf{Q}) = 2\widehat{Q}$ (then $\Phi'\Phi'^{\mathrm{T}} = 4R^2$ and $\beta = 2$) so that in this case $\gamma = 1$. Note that the unscaled problem corresponds to taking $\gamma = 0$.

We follow this procedure to generalise (5) so that the LC/KS transformation can be generalised to different values for γ than unity. Since the performance of a numerical integrator can be highly dependent on the choice of γ with choices of $\gamma \neq 1$ sometimes leading to much smaller error than either $\gamma = 0$ or $\gamma = 1$ (Blanes and Budd, 2004), this generalisation allows us to take a more appropriate regularisation function for each particular problem studied.

Let us now consider the following permutations

$$\begin{aligned} &\mathcal{P}^{(1)}\mathbf{Q} = \mathbf{Q}, \quad \mathcal{P}^{(3)}\mathbf{Q} = (-Q_3, -Q_4, Q_1, Q_2)^{\mathrm{T}}, \\ &\mathcal{P}^{(2)}\mathbf{Q} = (-Q_2, Q_1, Q_4, -Q_3)^{\mathrm{T}}, \quad \mathcal{P}^{(4)}\mathbf{Q} = (Q_4, -Q_3, Q_2, -Q_1)^{\mathrm{T}}. \end{aligned} \tag{17}$$

With these vectors we can write the matrix, $\widehat{Q}$, in (6) as

$$\widehat{Q} = (\mathcal{P}^{(1)}\mathbf{Q}, \mathcal{P}^{(2)}\mathbf{Q}, \mathcal{P}^{(3)}\mathbf{Q}, \mathcal{P}^{(4)}\mathbf{Q}).$$

Next, we define the following sequence of vectors and matrices

$$\begin{aligned} &\mathbf{Q}^{(i)} = \widehat{Q}_{i-1}\mathbf{Q}, \\ &\widehat{Q}_i = (\mathcal{P}^{(1)}\mathbf{Q}^{(i)}, \mathcal{P}^{(2)}\mathbf{Q}^{(i)}, \mathcal{P}^{(3)}\mathbf{Q}^{(i)}, \mathcal{P}^{(4)}\mathbf{Q}^{(i)}), \quad i \geqslant 1 \end{aligned} \tag{18}$$

with $\widehat{Q}_0 = I$ which have the following properties.

LEMMA 1. *The matrices* $\widehat{Q}_i$ *defined in* (18) *with* $\mathcal{P}^{(j)}$ *given in* (17) *satisfy*

$$\widehat{Q}_i\widehat{Q}_i^{\mathrm{T}} = \widehat{Q}_i^{\mathrm{T}}\widehat{Q}_i = R^{2i}I. \tag{19}$$

Proof. From (17) we have

$$(\mathcal{P}^{(l)}\mathbf{Q}^{(k)})^{\mathrm{T}}(\mathcal{P}^{(m)}\mathbf{Q}^{(k)}) = \delta_{lm}(\mathbf{Q}^{(k)})^{\mathrm{T}}\mathbf{Q}^{(k)} \quad \forall \mathbf{Q}^{(k)} \in \mathbb{R}^4$$

so,

$$\widehat{Q}_i\widehat{Q}_i^{\mathrm{T}} = \widehat{Q}_i^{\mathrm{T}}\widehat{Q}_i = (\mathbf{Q}^{(i)})^{\mathrm{T}}\mathbf{Q}^{(i)}I = \mathbf{Q}^{\mathrm{T}}(\widehat{Q}_{i-1}^{\mathrm{T}}\widehat{Q}_{i-1})\mathbf{Q}I, \tag{20}$$

and by simple induction the lemma is proved. □

This is a generalisation of property (7). The relation between the vectors and matrices given in (18) is as follows.

LEMMA 2. *Given the vectors* $\mathbf{Q}^{(i)}$ *and matrices* $\widehat{Q}_i$ *defined according to* (18), *then*

$$(\mathbf{Q}^{(m+1)})' = (m+1)\widehat{Q}_m. \tag{21}$$

Proof. We proceed by induction. It is immediate that

$$(\mathbf{Q}^{(2)})' = 2\widehat{Q}_1, \tag{22}$$

and from (18) we have

$$\begin{aligned}
(\mathbf{Q}^{(m+1)})'_{ij} &= \frac{\partial \mathbf{Q}_i^{(m+1)}}{\partial \mathbf{Q}_j} = \frac{\partial}{\partial \mathbf{Q}_j}(\widehat{Q}_m\mathbf{Q})_i = \frac{\partial}{\partial \mathbf{Q}_j}\left(\sum_k \mathbf{Q}_k \mathcal{P}^{(k)}\mathbf{Q}^{(m)}\right)_i \\
&= (\mathcal{P}^{(j)}\mathbf{Q}^{(m)})_i + \left(\sum_k \mathbf{Q}_k \mathcal{P}^{(k)} \frac{\partial \mathbf{Q}^{(m)}}{\partial Q_j}\right)_i \\
&= (\mathcal{P}^{(j)}\mathbf{Q}^{(m)})_i + \left(\sum_k \mathbf{Q}_k \mathcal{P}^{(k)} (m\mathcal{P}^{(j)}\mathbf{Q}^{(m-1)})\right)_i \\
&= (\mathcal{P}^{(j)}\mathbf{Q}^{(m)})_i + \left(m\mathcal{P}^{(j)} \underbrace{\sum_k \mathbf{Q}\mathcal{P}^{(k)}\mathbf{Q}^{(m-1)}}_{\mathbf{Q}^{(m)}}\right)_i \\
&= (m+1)(\mathcal{P}^{(j)}\mathbf{Q}^{(m)})_i = (m+1)(\widehat{Q}_m)_{ij}.
\end{aligned}$$

□

Next, we generalise the CT (5) as follows

THEOREM 2. *The following family of transformations*

$$\begin{cases} \mathbf{q} = \widehat{Q}_m\mathbf{Q}, \\ \mathbf{p} = \frac{1}{(m+1)R^{2m}}\widehat{Q}_m\mathbf{P}, \end{cases} \tag{23}$$

for $m = 0, 1, 2, \ldots$, *is canonical.*

Proof. From Theorem 1, the following transformation

$$\begin{cases} \mathbf{q} = \mathbf{Q}^{(m+1)}, \\ (\mathbf{Q}^{(m+1)})'^{\mathrm{T}}\mathbf{p} = \mathbf{P}, \end{cases} \tag{24}$$

with $\mathbf{Q}^{(m+1)} = \widehat{Q}_m\mathbf{Q}$ is canonical, and from Lemma 2 it is equivalent to

$$\begin{cases} \mathbf{q} = \mathbf{Q}^{(m+1)}, \\ (m+1)\widehat{Q}_m^{\mathrm{T}}\mathbf{p} = \mathbf{P}. \end{cases} \tag{25}$$

Multiplying the second equation by $\widehat{Q}_m$ and using Lemma 1, the transformation (23) is obtained and hence is canonical. □

Notice that $m = 0$ corresponds to the identity transformation and the LC/KS transformation corresponds to the particular case of taking $m = 1$ in (23). The two-dimensional case corresponds to the generalisation of LC where the transformation (23) can also be written using complex notation as

$$\begin{cases} q_1 + \mathrm{i}q_2 = (Q_1 + \mathrm{i}Q_2)^{m+1}, \\ p_1 + \mathrm{i}p_2 = \frac{P_1 + \mathrm{i}P_2}{(m+1)(Q_1 - \mathrm{i}Q_2)^m}. \end{cases} \tag{26}$$

Observe that if we define $\Phi = \widehat{Q}_m \mathbf{Q}$ then

$$\Phi^{\mathrm{T}}\Phi = \mathbf{Q}^{\mathrm{T}}\widehat{Q}_m^{\mathrm{T}}\widehat{Q}_m\mathbf{Q} = R^{2m}\mathbf{Q}^{\mathrm{T}}I\mathbf{Q} = R^{2(m+1)}$$

so $r = (\Phi^{\mathrm{T}}\Phi)^{1/2} = R^{m+1}$ and

$$\Phi'\Phi'^{\mathrm{T}} = (m+1)^2\widehat{Q}_m\widehat{Q}_m^{\mathrm{T}} = (m+1)^2R^{2m}I.$$

If we compare with (15) and (16) we have that $\alpha = 2(m+1)$ and $\beta = 2m$. This implies that for the family of regularisation functions

$$g(\mathbf{q}) = r^{\gamma} \quad \text{with} \quad \gamma = \frac{2m}{m+1}, \tag{27}$$

the conditions of (12) are satisfied using the previous CT. Substituting in (13) we get

$$K = \frac{1}{2(m+1)^2}\mathbf{P}^{\mathrm{T}}\mathbf{P} + R^{2m}V(\mathbf{Q}) - R^{2m}Q^t. \tag{28}$$

This regularisation removes the singularity for the following family of Potentials

$$V(r) = \frac{c}{R^{2m}} = \frac{c}{r^{\frac{2m}{m+1}}}, \tag{29}$$

as well as for $V = c/r^{\alpha}$ with $\alpha < 2m/(m+1)$, and with c a constant. Although a number of potentials can be considered, we still have the constraint that $0 \leq 2m/(m+1) < 2$. Other potentials can also be regularised following a different technique to get CTs. For example, in (Blanes and Budd, in press) a CT in two and three dimensions is presented for the regularisation function $g = r^4$ (removing the singularity for the potential $V(r) = c/r^4$) and it is shown that for the one-dimensional potentials $V = c/q^{\alpha}$ the regularisation function $g = q^{\alpha}$ removes the singularity and the CT $(q,p) = (Q^{\frac{2}{2-\alpha}}, \frac{2-\alpha}{2}Q^{\frac{\alpha}{\alpha-2}}P)$ transforms the Hamiltonian into a separable system as (28).

On the other hand, the inverse of (23), $(\mathbf{Q},\mathbf{P}) = \mathcal{C}^{-1}(\mathbf{q},\mathbf{p})$, can be numerically expensive to compute. Fortunately, it has to be evaluated only once for starting the computation, which then proceeds to use the transformed coordinates. For the output we have to compute the transformation (23), $(\mathbf{q},\mathbf{p}) = \mathcal{C}(\mathbf{Q},\mathbf{P})$, which involves only a few and simple arithmetic operations, in general they are not required at each step, and they can also be computed in parallel.

This new technique can also be useful for potentials with no singularities. For example, suppose we find a function, g, and a CT such that the new potential $\widetilde{V}(\mathbf{Q}, Q^t)$ and the transformation $(\mathbf{q}, \mathbf{p}) = \mathcal{C}(\mathbf{Q}, \mathbf{P})$ are easy and cheap to compute, or the equations in the new coordinates have better properties. In other words, the complexity of the original potential, $V(\mathbf{q})$, moves to the CT, $(\mathbf{Q}, \mathbf{P}) = \mathcal{C}^{-1}(\mathbf{q}, \mathbf{p})$, which, as previously mentioned, is only required once for starting the computation, and has not to be computed at each step. Then, the new algorithm for the integration will be faster and can be more efficient even for smooth trajectories, where the variable time-step technique seems not appropriate. This is also the case of the Kepler problem, which requires the computation of a square root at each stage in a numerical integration. However, if the previous regularisation is considered with m odd (remember that $m = 1$ corresponds to LC/KS) one square root appears in the computation of the initial conditions $(\mathbf{Q}_0, \mathbf{P}_0)$, and the remainder of the integration can then be done only with simple arithmetic operations.

4. EASY Integrators

The evolution of the Hamiltonian (1) in the real time, t, and coordinates $(\mathbf{q}, \mathbf{p})$ is equivalent to the evolution of the Hamiltonian (28) in the fictive time, τ, introduced through (2) and (27), and coordinates $(\mathbf{Q}, \mathbf{P})$ related to $(\mathbf{q}, \mathbf{p})$ through (23). Since (28) is also separable into very simple parts then splitting and explicit symplectic integrators, which we briefly introduce, can be used. As a result, we can solve numerically the system (1) with explicit adaptive symplectic (EASY) integrators.

Given the Hamiltonian $H = T(\mathbf{p}) + V(\mathbf{q})$ we have that T and V are exactly solvable and the second order symmetric and symplectic Störmer/leapfrog/Verlet method, for one time step h, is

$$S_2(h) = \mathrm{e}^{(-h/2)L_V} \mathrm{e}^{-hL_T} \mathrm{e}^{(-h/2)L_V} = \mathrm{e}^{-hL_H} + \mathrm{O}(h^3) \tag{30}$$

with $L_F := \{F, \cdot\}$, where $\{\cdot, \cdot\}$ denotes the usual Poisson bracket so, the algorithm for one step is given by

$$\begin{aligned} \mathbf{p}_{n+1/2} &= \mathbf{p}_n - \frac{h}{2} \nabla_{\mathbf{q}} V(\mathbf{q}_n), \\ \mathbf{q}_{n+1} &= \mathbf{q}_n + h\mathbf{p}_{n+1/2}, \\ \mathbf{p}_{n+1} &= \mathbf{p}_{n+1/2} - \frac{h}{2} \nabla_{\mathbf{q}} V(\mathbf{q}_{n+1}), \end{aligned} \tag{31}$$

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 $\nabla_q V(\mathbf{q}_{n+1})$ at each step can be reused in the next step, and only one evaluation of $\nabla_{\mathbf{q}} V$ per step is required.

Higher order symplectic methods can be obtained by composition of this method (Creutz and Gocksch, 1989; Suzuki, 1990; Yoshida, 1990). For example, a well known symmetric fourth order method is given by

$$\begin{aligned} S_4(h) &= S_2(x_1)S_2(x_0)S_2(x_1) \\ &= \mathrm{e}^{(-x_1/2)/L_V}\mathrm{e}^{-x_1 L_T}\mathrm{e}^{-((x_1+x_0)/2)L_V}\mathrm{e}^{-x_0 L_T}\mathrm{e}^{((x_1+x_0)/2)L_V}\mathrm{e}^{-x_1 L_T}\mathrm{e}^{-h(x_1/2)L_V} \end{aligned} \tag{32}$$

with $x_1 = h/(2-2^{1/3})$, $x_0 = h - 2x_1$. Higher order methods are also presented in Yoshida (1990). These methods have become very well known due to their good behaviour for long time integration (Yoshida, 1993; Sanz-Serna and Calvo, 1994; Hairer et al., 2002; McLachlan and Quispel, 2002; Budd and Piggott, 2003). Recently, a number of new splitting methods have appeared which are more efficient (McLachlan, 1995; Blanes and Moan, 2002; McLachlan and Quispel, 2002). In addition, for Hamiltonians like (1), which are quadratic in momenta, more efficient symplectic RKN methods in the more general form

$$\Phi_h = \prod_{i=0}^{k} \mathrm{e}^{-a_i h L_T}\mathrm{e}^{-b_i h L_V} \tag{33}$$

can be used. In particular, fourth- and sixth-order methods are presented in Blanes and Moan (2002), being the methods used in this paper, and referred hereafter as RKN_4 and RKN_6. Methods up to order eight, using the processing technique and modified potentials, are presented in Blanes et al. (2001).

5. Scaling Invariance

5.1. PURE SCALE INVARIANCE

The main motivation for the previous generalisation of the LC/KS regularisation comes from the fact that by using them we can use different scaling functions g. In particular, these can be chosen to exploit natural scaling laws obeyed by the solution. Many systems of ODEs are invariant under changes of scale. A given differential equation

$$\mathrm{d}z_i/\mathrm{d}t = f_i(z_1, \ldots, z_N), \quad i = 1, \ldots, N, \tag{34}$$

is *scale invariant* if it is unchanged under the scaling transformation of the form

$$t \to \lambda t, \quad z_i \to \lambda^{\alpha_i} z_i, \tag{35}$$

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 it is also invariant under this change so that

$$z_i(\lambda t) = \lambda^{\alpha_i} z_i(t).$$

Whilst most of the solutions of (34) are not self-similar (for example, periodic orbits), the self-similar solutions are often attractors and/or describe interesting behaviour such as the formation of singularities. Applying the Sundman transformation (2) to the system (34) we have

$$\mathrm{d}z_i/\mathrm{d}\tau = g(\mathbf{z}) f_i(\mathbf{z}).$$

With a careful choice of g we can construct an scaling invariant system which has the desirable property that two solutions mapped into each other by the scaling relation (35) evolve at the same fictive time and the resulting numerical method has a relative local truncations error which is independent of the scale of the solution (Budd et al., 2001). It is also possible to compute self-similar solutions with uniformly bounded relative errors on all fictive times. To achieve scale invariance the function g must satisfy the functional equation

$$g(\lambda^{\alpha_1} z_1, \lambda^{\alpha_2} z_2, \ldots, \lambda^{\alpha_N} z_N) = \lambda g(z_1, z_2, \ldots, z_N). \tag{36}$$

Given the potential $V = c/r^{\alpha}$ and the regularisation function $g = r^{\gamma}$, it is easy to see that the Hamiltonian equations are scaling invariant for the choice $\gamma = \gamma_{\mathrm{sc}} \equiv 1 + \alpha/2$. From (27), if we choose $\gamma_{\mathrm{sc}} = 2m/(m+1)$ we have: (i) For $\alpha < 2$, the singularity is removed because $\gamma > \alpha$; (ii) for the family of potentials ($\gamma_{\mathrm{sc}} = 2m/(m+1) = 1 + \alpha_m/2$)

$$V(r) = \frac{c}{r^{\alpha_m}}, \quad \alpha_m = \frac{2(m+1)}{m+1} \tag{37}$$

the scaling invariance is preserved, a CT is known, and condition (i) is satisfied. In addition, this class contains (29) as a particular case ($\alpha_{2k+1} = 2k/(k+1)$). From (37) we observe that the Kepler potential ($\alpha_m = 1$) corresponds to the case $m = 3$ for which

$$\gamma_{\mathrm{sc}} = 3/2,$$

and the regularisation for this value of m preserves the scaling invariance. Then, it is important to know under which conditions this scaling invariant regularisation is superior to the LC/KS regularisation $m = 1 (\gamma = 1)$.

5.2. NEAR SCALING INVARIANCE

Whereas most problems are not exactly scale invariant they are often closely approximated by scale invariant systems. For example, the equations for the Kepler problem are scaling invariant, but for most perturbations to the Kepler problem they are only close to scale invariant. Suppose the perturbation is conservative and the system is described by the Hamiltonian

$H = H_{\text{Kep}} + H_{\text{pert}}$, where H_{Kep} corresponds to the pure Kepler problem and H_{pert} is the perturbation. Two classes of perturbations are considered:

(i) A perturbation which vanishes, or can be neglected at the singularity, i.e. $|H_{\text{pert}}/H_{\text{Kep}}| \to 0$ as $r \to 0$. In this case, close to a collision the system can be considered as purely Keplerian, and the analysis for the pure Kepler problem should apply.
(ii) A perturbation with a higher singularity. Suppose that close to the singularity $H_{\text{pert}} \simeq 1/r^{\delta}$, $\delta > 1$. Some examples are: the oblateness perturbation, the perturbation due to relativistic effects, or the angular momentum term of the evolutionary equation for r in polar or spherical coordinates.

In the last case, for those initial conditions which allow close approaches to the origin the perturbation have an important contribution in those regions where $1/r \sim 1/r^{\delta}$. In such a case, it seems difficult to know in advance which regularisation function $g(\mathbf{q})$ gives the best performance. A preliminary analysis (Blanes and Budd, 2004) for the one-dimensional problem with the potential $V = -1/q^{\alpha} + \varepsilon/q^{\beta}$ for different values of ε, α, β, with $\beta > \alpha$, suggested that when using a regularisation function of the form $g = q^{\gamma}$ there was a value $\gamma = \gamma_*$ for which optimal results were obtained. In particular, as the order of the method increased it was found that $\gamma_* \to \gamma_{\text{sc}} = 1 + \alpha/2$ which gave a regularisation function exactly preserving scaling invariance for the unperturbed part $-1/q^{\alpha}$. Since these results also apply to near scale invariant higher dimensional systems then, $g = r^{3/2}$ preserving the scale invariance for the pure Kepler problem, will be very close to the optimal choice for most perturbations with singularities at the origin if the trajectory is near self-similar (i.e. close to a collision or for a high eccentricity).

6. Numerical Examples

In this section we will look at a series of problems in which there is an orbit with a singularity or high eccentricity. We will consider both integrable and perturbations of integrable problems. Our conclusions from these calculations are that if we perturb a nearly singular integrable problem, then the scale invariant method performs better than the LC/KS methods in terms of accuracy versus computational cost. In contrast if the problem is integrable or not especially singular or eccentric then LC/KS gives more accurate answers. Hence these two rescalings can be seen as complimentary to each other.

6.1. THE COLLISION PROBLEM

As a first test, we consider a collapse in finite time, T, in the Kepler problem, so that $q \to 0$, $p \to \infty$ as $t \to T$. This is a problem with a singularity, which can be described by a self-similar solution. This corresponds to the one-dimensional Hamiltonian

$$H = \frac{1}{2}p^2 - \frac{1}{q}. \tag{38}$$

We take as initial conditions $(q(0), p(0)) = (1, 0)$, (so $q^t = -1$) which has a solution which collapses at the finite time $p^t = T = \frac{\pi}{2\sqrt{2}} = 1.11072\ldots$ (Such a solution is asymptotically self-similar). If we consider the regularisation function (27) and the CT (23) for the one-dimensional problem: $q = Q^{m+1}$, $p = P/((m+1)Q^m)$ (which corresponds to (26) with $q_2 = p_2 = Q_2 = P_2 = 0$) then the transformed Hamiltonian system is $(Q^t = -1)$

$$K = \frac{1}{2(m+1)^2}P^2 - Q^{m-1} - Q^{2m}Q^t. \tag{39}$$

In Figure 1 we show the curves obtained taking $m = 1, 2, 3, 4$ for $\tau \in [0, 10]$. We observe that if $m \geqslant 3$ then the singularity in finite time becomes an asymptotic limit of a smooth solution in the fictive time τ as $\tau \to \infty$. If $m = 1, 2$ then the numerical method instead gives a periodic solution. This fact is due to the regularisation considered and not to the numerical integrator used. Observe that for the LC regularisation ($m = 1$) the Hamiltonian (39) is equivalent to $K = P^2/8 - Q^tQ^2$, with initial conditions $(Q(0), P(0)) = (1, 0)$, giving oscillatory solutions, and then crossing the singularity because this Hamiltonian allows the value $Q = 0$ (q takes positive values because $q = Q^2$). If we want to study how the system approaches the singular point asymptotically, this method needs a variable time step strategy on the fictive time τ in order not to cross through this point. However, with the scaling invariant regularisation ($m = 3$, $\gamma_s = 3/2$), the Hamiltonian to be solved is $K = P^2/32 - Q^2 - Q^tQ^6$, with initial conditions $(Q(0), P(0)) = (1, 0)$.

The solution of the numerical discretisation with a constant time step $\Delta\tau$ then approaches the origin asymptotically as $\tau \to \infty$, as does the exact solution, although the numerically computed and actual collapse times differ. In order to know how accurately the methods approach this collapsing time, in Figure 2 we present $|q^t(\tau) - T|$ for $m \geqslant 3$ at $\tau = 10$ and $\tau = 20$ respectively, taking different values of $\Delta\tau$ and using always RKN_4 as the symplectic numerical integrator. Here, $p^t(\tau)$ is used as an estimate of the collapse time. It seems clear that for this particular problem the choice $m = 3$, preserving scaling invariance, is optimal to study how the solution approaches the collision as well as in approximating T.

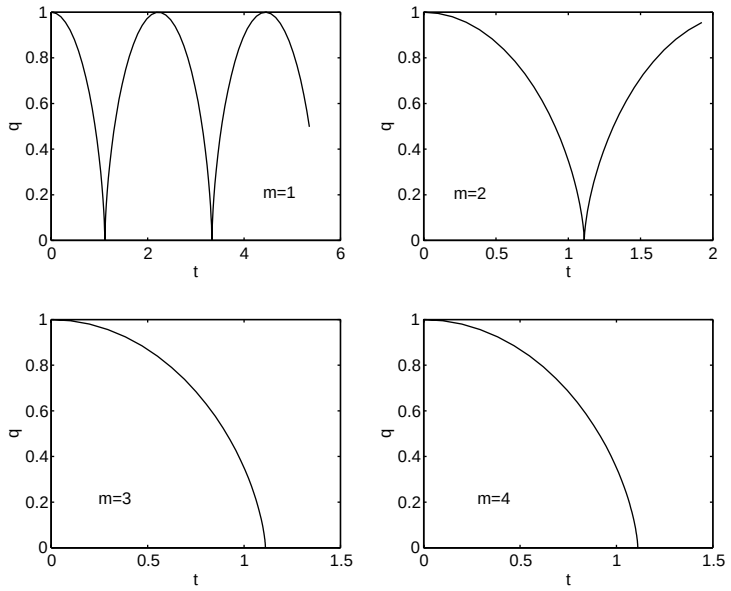

Figure 1. Trajectories obtained for the collapsing problem taking different values of m in the generalisation of the LC/KS regularisation. The case $m = 1$ corresponds to LC/KS.

6.2. OBLATENESS PERTURBATION

In the previous section we have seen that the scale invariant method works very well for a singular problem. We now consider the related problem of a highly eccentric, periodic, orbit. In the computation of highly eccentric satellite orbits, the oblateness perturbation is the dominant perturbation (Janin, 1974). In first approximation, the dynamics of a satellite moving into the gravitational field produced by a slightly oblate spherical planet is described by the following Hamiltonian (Stiefel and Scheifele, 1971)

$$H + \frac{1}{2}(p_1^2 + p_2^2) - \frac{1}{r} + \frac{\varepsilon}{2r^3}\left(1 - \alpha\frac{3q_1^2}{r^2}\right). \tag{40}$$

The motion takes place in a plane containing the symmetry axis of the planet when $\alpha = 1$, whereas $\alpha = 0$ corresponds to a plane perpendicular to that axis. Taking the general regularisation function "g^γ with $\gamma = \frac{2m}{r^{m+1}}$" and the generalised transformation (23), the Hamiltonian (40) becomes

$$\begin{aligned} K &= \widetilde{T}(\mathbf{P}) + \widetilde{V}(\mathbf{Q}, Q^t) \\ &= \frac{P_1^2 + P_2^2}{2(m+1)^2} - R^{m-1} + \frac{\varepsilon}{2R^{m+3}}\left(1 - \alpha\frac{q_1^2(\mathbf{Q})}{R^{2(m+1)}}\right) - Q^t R^{2m}, \end{aligned} \tag{41}$$

where the function $q_1(\mathbf{Q})$ can easily be obtained from (26).

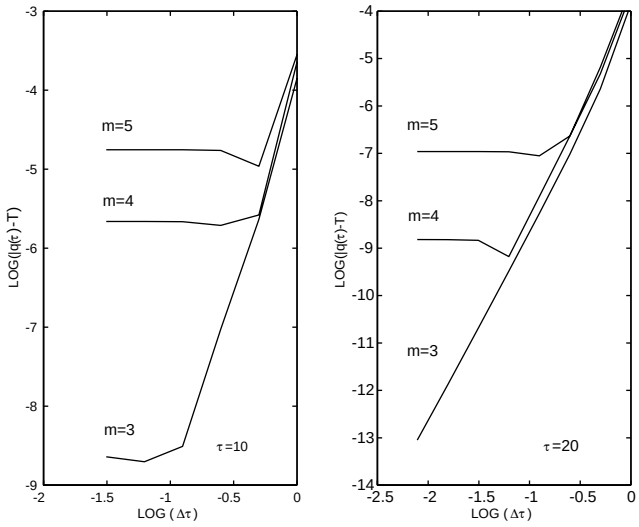

Figure 2. Log–log curves for the error in the collision time, T, for different values of the fictive time step, taking as the final fictive time $\tau = 10$ and 20. Only values of $m \geq 3$ are considered since the resulting trajectories then approach the collision asymptotically.

We study the performance of the methods taking $\alpha = 1$ and different values of m (similar results are obtained with $\alpha = 0$). This problem is neither integrable nor scaling invariant, although it does have an approximate scaling symmetry if ε/r^3 is small in which case it approximates the Kepler problem. 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 a periodic orbit with eccentricity e and energy $-1/2$. We integrated the resulting system of ODEs using RKN_6 until $t_f = 20\pi$ for different values of $e \in (0, e^*)$, where e^* is the largest value for e which gives apparently bounded trajectories, and measured the average relative error in energy. The fictive time step is adjusted such that t_f is reached with approximately 200 steps. We considered three values of m: (i) $m = 0$ (non-regularisation); $m = 1$ (the standard Levi-Civita regularisation), and (iii) $m = 3$ (the scaling invariant regularisation for the unperturbed Kepler problem).

*Case (*a*)*: $\varepsilon = 0$ (unperturbed problem). The results of this experiment are shown in Figure 3. Three important facts can be deduced: (i) For the regularised schemes ($m = 1, 3$), the error is nearly independent of the eccentricity in contrast to the case $m = 0$ where the errors became very large as $e \to 1$. The error for the case $m = 3$ increases when e is very close to 1 because a large fictive time step is necessary to reach the final time t_f with the fixed number of steps, and the numerical integrator is unstable for these time steps. (ii) The performance of the regularised schemes is clearly superior to the non regularised method, even for small eccentricities, as already observed in

Arakida and Fukushima (2000). (iii) LC is more accurate than the optimal scaling invariant scheme.

*Case (*b*)*: $\varepsilon = 10^{-8}$, $\varepsilon = 10^{-6}$ and $\varepsilon = 10^{-4}$ (small perturbations). We now make the following observations from Figure 3: (i) The accuracy for $m = 3$ is apparently not reduced; (ii) the high performance of LC is retained for most eccentricities, but it is severely deteriorated for high eccentricities and then it is out performed by the scaling invariant regularisation; and (iii) this effect is magnified with ε. We conclude that the scaling invariant method works best for large eccentricities and moderately large perturbations.

In Figure 4 we show the results of the experiment for $\varepsilon = 10^{-8}$ and taking $m = 1, 2, 3, 4, 5$. We clearly observe that for high eccentricities the nearly scaling invariant regularisation, $m = 3$, gives the most accurate results.

The reason for the good performance of the Levi-Civita regularisation on the unperturbed problem comes because, if $\varepsilon = 0$ and $m = 1$ in (41), the Hamiltonian to be solved is (10) which is exactly solvable. This is possible because the original system is also integrable. However, if $\varepsilon \neq 0$, integrability is lost and the LC method gives markedly worst results when the perturbation is strong (i.e. for high eccentricities). In contrast, the scaling invariant method does not rely on integrability. The symplectic integrators used on the pure

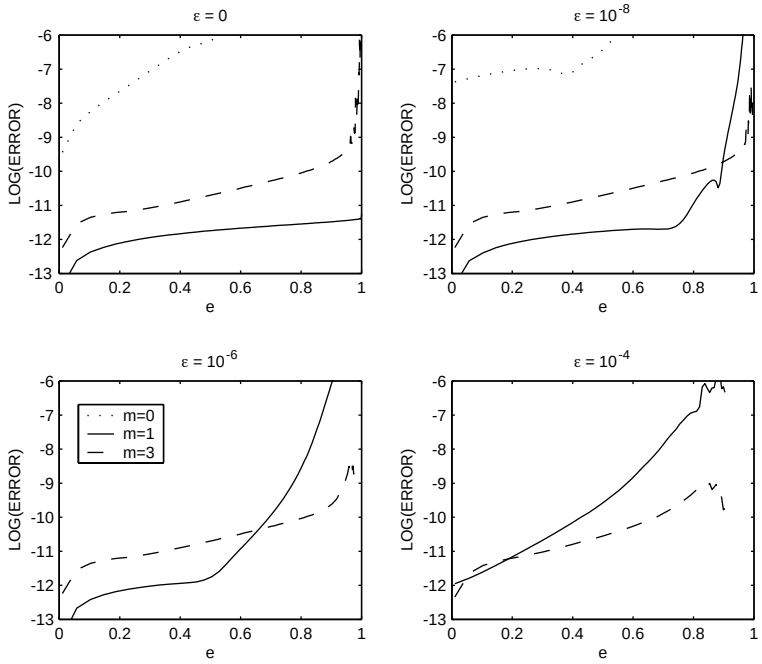

Figure 3. Average relative error in energy as a function of the eccentricity for $m = 0, 1, 3$, and for different values of ε. Only values of e giving bounded trajectories are considered.

Kepler problem with the LC regularisation solve exactly a slightly perturbed harmonic oscillator or, equivalently, they solve exactly a Kepler problem, with slightly different parameters, giving also a closed trajectory (Mikkola and Tanikawa, 1999; Preto and Tremaine, 1999). 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. We illustrate this fact in Figure 5. First, we consider the pure Kepler problem with $e = 0.999$ and we integrate for three periods with a time step requiring approximately 50 steps per period. We consider the LC/KS regularisation (stars) and the scaling invariant regularisation with $m = 3$ (circles). The numerical integrator used was the second order method described in (30) and (31). Each star in the figure corresponds to three different points (to drawing accuracy they look the same) staying in a closed trajectory very near the exact one (solid line). However, the solution for $m = 3$ shows the typical precession of a symplectic integrator applied to the Kepler problem. Next, we repeat the experiment for $\varepsilon = 10^{-4}$ and $e = 0.9$. We integrate until $t_f = 20\pi$ choosing a time step such that the whole integration is done with approximately 100 steps. Now, the exact solution (obtained numerically with a very small time step) has a precession which is better approximated with the scaling invariant regularisation.

On the other hand, the previous good behaviour for the LC/KS regularisation only happens when solving the pure Kepler problem in Cartesian coordinates, but not in polar coordinates for the one-dimensional Hamiltonian $H = \frac{1}{2}p^2 - \frac{1}{p} + \frac{l^2}{q^2}$ with l the angular momentum, and the one-dimen-

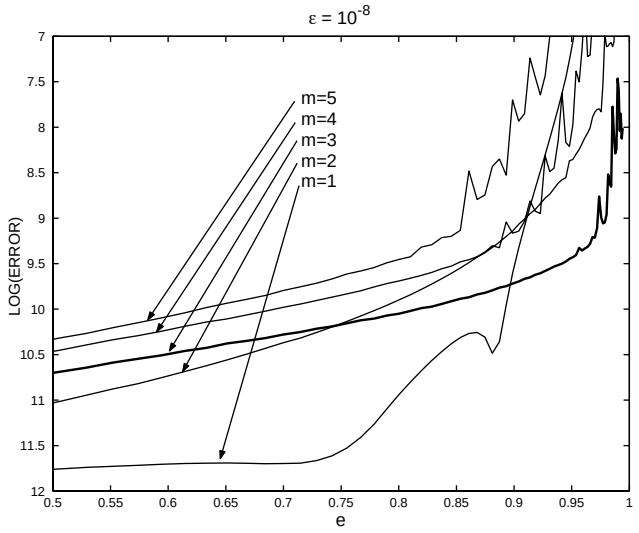

Figure 4. Average relative error in energy for $\varepsilon = 10^{-8}$ as a function of the eccentricity for $m = 1, 2, 3, 4, 5$.

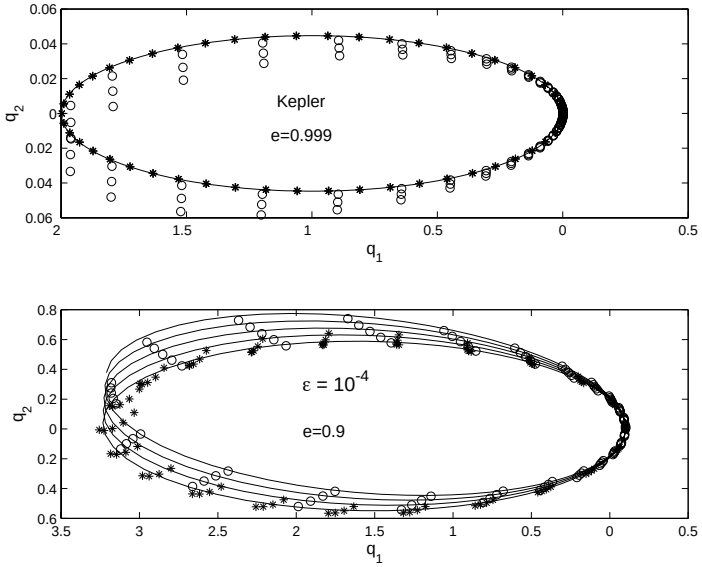

Figure 5. Numerical approximations for the oblateness perturbation (40) using the symplectic integrator (30) with the LC/KS regularisation (stars) and the scaling invariant regularisation with $m = 3$ (circles): (i) for $\varepsilon = 0$ (pure Kepler problem) with $e = 0.999$ and (ii) for $\varepsilon = 10^{-4}$ with $e = 0.9$. The solid line represents a near exact solution obtained by using a very small step-size.

sional LC transformation $(q, p) = (Q^2, P/(2Q))$, as observed in (Blanes and Budd, 2004). This is because the singularity in $\frac{L^2}{q^2}$ can not be removed with the regularisation function $g = q$. The choice $m = 3$ (or $g = r^{3/2}$) resulting a nearly scaling invariant scheme, gives a much better performance for high eccentricities for this *perturbed*, Kepler problem.

To illustrate the performance of the methods at high eccentricities, we consider again (40) with: (i) $\varepsilon = 0$ and $e = 0.999$; (ii) $\varepsilon = 10^{-8}$ and $e = 0.98$. The EASY integrators use the following RKN integrators: the second order method (30), RKN_4 and RKN_6. We compare the results when the numerical integrators are used with the LC regularisation (LCn, $n = 2, 4, 6$) and with the nearly scaling invariant $(m = 3)$ regularisation (EASYn, $n = 2, 4, 6$). We measure the average relative error in energy versus the number of force evaluations. Figure 6 shows the results obtained. For the pure Kepler problem with $\varepsilon = 0$, the LC regularisation gives more accurate results for each integrator. However the relative performance of the two regularisations completely change when the small perturbation is introduced. Observe that the difference between EASYn and LCn increases with n in agreement with the general results obtained for the one-dimensional problem studied in (Blanes and Budd, 2004).

Finally, several examples such as the Hill's lunar problem, a perturbation due to a constant electric and magnetic field or the Stark problem (which correspond to a regular perturbation to the Kepler problem in the sense that $H_{\text{pert}}/H_{\text{Kep}} \to 0$ as $r \to 0$) have been considered. During a near-collision these systems can be considered as purely Keplerian. For this reason, the LC/KS regularisation works more efficiently than the scaling invariant regularisation. This has been observed on several numerical experiments carried out by us but not reported in this paper. However, if in these problems a perturbation with a singularity which cannot be removed with the LC/KS regularisation is introduced, the performance of LC/KS deteriorates as happened in the oblateness perturbation, and the scaling invariant regularisation works, in general, more efficiently for high eccentricities.

7. Conclusions

The Levi-Civita and Kustaanheimo–Stiefel regularisation have been revisited. With a time transformation and a canonical transformation the unstable differential equation with a singularity, associated to the Kepler problem, is

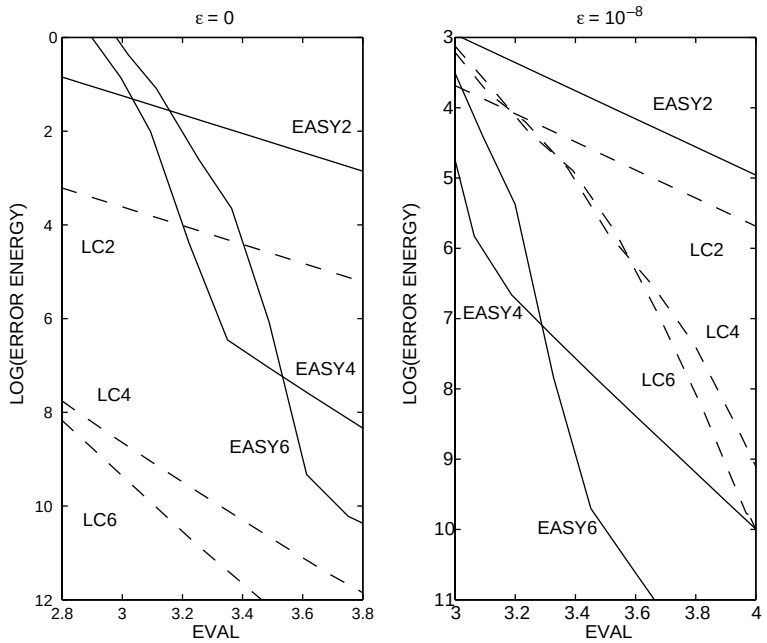

Figure 6. Average relative error in energy versus the number of potential evaluations for the LC regularisation (LCn, $n = 2, 4, 6$) and the nearly scaling invariant ($m = 3$) regularisation (En, $n = 2, 4, 6$).

transformed into a stable differential equation with no singularities. However, the equations for the Kepler problem are scaling invariant, and this property is not preserved by the LC/KS regularisation, reducing its performance on a number of problems. Then, a generalisation of the LC/KS regularisation is presented which removes the singularity and preserves the scaling invariance for a family of potentials including the Kepler potential as a particular case.

From the theoretical analysis and the numerical experiments carried out for several perturbations to the Kepler problem it seems clear that for the numerical integration of the pure Kepler problem or some polynomial perturbations to it, the LC/KS regularisation, in general, gives the most efficient technique. However, for collision problems as well as if the perturbation has an important contribution close to the singularity, the scaling invariant regularisation is more efficient for eccentric orbits. We reiterate the observation that scale invariant methods seem to be complimentary to LC/KS working best (for high eccentricty, near singular and non-integrable behaviour) precisely where LC/KS has certain difficulties.

Acknowledgements

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