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Authors

Romero, Ignacio
Armero, Francisco

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DISCRETE RELATIVE EQUILIBRIA OF TIME-STEPPING ALGORITHMS FOR A MODEL PROBLEM OF NONLINEAR DYNAMICS

BY

I. ROMERO

AND

F. ARMERO

DEPARTMENT OF CIVIL AND ENVIRONMENTAL ENGINEERING
UNIVERSITY OF CALIFORNIA
BERKELEY, CALIFORNIA

Discrete relative equilibria of time-stepping algorithms for a model problem of nonlinear dynamics

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I. ROMERO AND F. ARMERO

Structural Engineering, Mechanics and Materials

Department of Civil and Environmental Engineering

University of California, Berkeley CA 94720, USA

iromero@ce.berkeley.edu

armero@ce.berkeley.edu

Abstract

We present a simple analysis that highlights the behaviour of commonly used time-integration schemes when applied to mechanical systems that possess relative equilibria. Using a spring/mass nonlinear system, we study the discrete solutions to relative equilibrium conditions of the trapezoidal rule, a one-parameter family of dissipative Newmark methods, the midpoint rule, the Energy-Momentum and a new method developed by the authors, the Energy-Dissipating Momentum-Conserving (EDMC) scheme. The simplicity of the mechanical model allows to find explicit conditions on the discrete dynamics generated by each of the schemes which either prohibit or assure the existence of discrete motions that accurately approximate relative equilibria.

1. Introduction

The dynamical system resulting from the time solution of nonlinear elastodynamics has important qualitative features and it is desirable that the numerical schemes devised to obtain approximate solutions capture these properties as accurately as possible. For example, if there are no external forces to the system, the total energy or Hamiltonian as well as the symplectic form are conserved. If the mechanical problem possesses additional symmetries, conservation of momenta and the existence of relative equilibria are also of relevance. These properties contain important information about the dynamics of the system.

Many papers have addressed the issue of conservation laws, and in particular the energy and momentum conserving method of Simo and co-workers was developed so that energy and momenta conservation were enforced algorithmically (see e.g. SIMO & WONG [1991], SIMO & TARNOW [1992]). But not much attention has been devoted to the study of numerical methods for nonlinear elastodynamics in the presence of relative equilibria (ARMERO & ROMERO [1999]). The motivation for this paper is to analyze in the simplest possible setting how well some of the popular integration schemes employed for time-integrating nonlinear elastodynamics solve relative equilibria. More specifically, we will analyze the trapezoidal rule, a dissipative family of Newmark methods, the midpoint rule, the energy-momentum conserving and the energy-dissipating momentum-conserving method (EDMC from now on) recently introduced by the authors.

Relative equilibria play an important role in stability analysis of nonlinear dynamics of Hamiltonian systems with symmetry and give important information about the long term solution of systems with some mechanism of energy dissipation. The mathematical analysis of a general case is complex, thus we must restrict ourselves to the example indicated previously, the spring/mass system. The analysis of the solution to this problem by the different methods can illustrate the behavior of these schemes in more complex situations.

Of particular interest is the long term solution of schemes with algorithmic dissipation. Numerical dissipation is normally introduced to damp out spurious high frequency noise which in some cases may turn the computations unstable. Commonly used methods of this type (see e.g. HILBER, HUGHES & TAYLOR [1977], BAZZI & ANDERHEGGEN [1982] and CHUNG & HULBERT [1993]) couple group motions and elastic deformations hence energy is dissipated from the system arbitrarily and conservation laws are violated . The EDMC method effectively decouples group and internal motions and is able to conserve momenta. Energy is only dissipated only from internal motions resulting on the *first dissipative scheme able to conserve relative equilibria* if initial conditions are those of an relative equilibrium. Moreover, energy is *strictly* dissipated when the system is not in a relative equilibrium, and hence, *the long term solutions for this method are always the relative equilibria corresponding to the initial values of momenta*. The limit solutions are the ones corresponding to physically dissipative mechanical systems.

A previous numerical analysis of relative equilibria can be found in GONZÁLEZ & SIMO [1996] for the same spring/mass problem. They studied the stability of midpoint rule and the energy-momentum method near the relative equilibrium. Their approach was completely different to the one we follow: making use of the momentum conservation of the two methods, they analyzed the relative equilibria in the reduced space, the phase space modulo rotations. The reduction process is rather elaborated and the results can not be extended to other commonly used integration schemes as we present.

The rest of the paper is as follows: in section 2 we will describe the physical problem of the spring/mass system and the conservation laws arising from its Hamiltonian formulation. In section 3 we define the notion of *discrete relative equilibrium* and analyze the

trapezoidal rule, a family of dissipative Newmark methods, the midpoint rule, the energy-momentum and the EDMC. In section 4 we show numerical examples to illustrate the results of section 3. Finally in section 5 we summarize the results and present conclusions.

2. Problem definition

This section examines the mathematical formulation of the equations of motion of an elastic spring with a mass at its end. From the analysis of these equations we extract qualitative information about the dynamics of the problem. Of most interest it is the issue of conservation laws and relative equilibria, which we identify and prove.

2.1. The spring and mass system

Consider an elastic spring moving on 3-dimensional Euclidean space with one end fixed to a point O and the opposite end attached to a particle of mass m. The linear spring has elastic constant k and natural length L_0. Initial conditions on position and momenta must be given to complete the description of the dynamical system.

Let $q(t)$ and $p(t) = m\dot{q}(t)$ be the position and momenta of the mass m at time t. The phase space P for this problem is $P = \{z(t) = (q(t), p(t)) \in \mathbb{R}^3 \times \mathbb{R}^3, t \in \mathbb{R}\}$. This system is Hamiltonian, and we define the potential energy V, the kinetic energy K and the total energy (or Hamiltonian) H as:

$$\begin{cases} V(\boldsymbol{q}) = \hat{V}(\|\boldsymbol{q}\|) \\ K(\boldsymbol{p}) = \hat{K}(\|\boldsymbol{p}\|) = \frac{1}{2}m^{-1}\|\boldsymbol{p}\|^2 \\ H(\boldsymbol{q}, \boldsymbol{p}) = V(\boldsymbol{q}) + K(\boldsymbol{p}) \end{cases} \tag{2.1}$$

where $\|\cdot\|$ is the standard Euclidean norm.

Remark 2.1.

Note that the kinetic and potential energies (and hence the Hamiltonian) depend on their arguments only through their moduli. This in a requirement of frame invariance. It is a key property and we will use it throughout the whole analysis. □

The equations of motion of the spring/mass system are Hamilton's equations with Hamiltonian (2.1.3).

$$\begin{cases} \dot{\boldsymbol{q}} = \dfrac{\partial H}{\partial \boldsymbol{p}} = \dfrac{1}{m}\boldsymbol{p} \\ \dot{\boldsymbol{p}} = -\dfrac{\partial H}{\partial \boldsymbol{q}} = -\dfrac{\hat{V}'(\boldsymbol{q})}{\|\boldsymbol{q}\|}\boldsymbol{q} \end{cases} \tag{2.2}$$

2.2. Conservation laws of the motion

A consequence of the structure of equations (2.2) is the existence of first integrals of the motion, quantities that are conserved in time.

Conservation of energy

Conservation of energy is a direct consequence of Hamilton's equations for problems with no external forces:

$$\frac{dH}{dt} = \frac{\partial H}{\partial q}\dot{q} + \frac{\partial H}{\partial p}\dot{p} = \frac{\partial H}{\partial q}\frac{\partial H}{\partial p} - \frac{\partial H}{\partial p}\frac{\partial H}{\partial q} = 0 \tag{2.3}$$

Conservation of angular momentum

Define $\boldsymbol{J} = \boldsymbol{q} \times \boldsymbol{p}$ the angular momentum of the spring/mass system. To verify that $\boldsymbol{J}$ is constant along a motion we use equations (2.2) as follows

$$\frac{d\boldsymbol{J}}{dt} = \dot{\boldsymbol{q}} \times \boldsymbol{p} + \boldsymbol{q} \times \dot{\boldsymbol{p}} = \frac{1}{m}\boldsymbol{p} \times \boldsymbol{p} - \boldsymbol{q} \times \frac{\hat{V}'(\boldsymbol{q})}{\|\boldsymbol{q}\|}\boldsymbol{q} = \boldsymbol{0} \tag{2.4}$$

Remarks 2.2.

1. From the definition of angular momentum we deduce that $\boldsymbol{q}$ and $\boldsymbol{p}$ are perpendicular to $\boldsymbol{J}$ at any instant. Because of conservation of angular momentum, $\boldsymbol{J}$ is a constant vector, hence $\boldsymbol{q}$ and $\boldsymbol{p}$ must lie inside a fixed plane Π normal to $\boldsymbol{J}$. We conclude that the motion of the mass is restricted to that plane.

2. Conservation of angular momentum is a particular case of Noether's theorem (see ARNOLD [1989]) which states that for every symmetry of the Hamiltonian system there exists a first integral of the motion. For the spring/mass system, the symmetry group S is the special orthogonal group $SO2$, the set of rotations about an axis perpendicular to Π.

Conservation of symplectic form

The spring/mass system conserves the symplectic 2-form. This property is not so important for our analysis and we refer to GONZÁLEZ & SIMO [1996] for a proof of the statement.

2.3. Relative equilibria

Another consequence of the symmetry of the system is the existence of relative equilibria. These are solutions of (2.2) which are orbits of a one-parameter subgroup of $SO2$, the

symmetry group of the system. A solution of Hamilton's equations (2.2), $z(t) : \mathbb{R}^+ \to P$, is a relative equilibrium of the spring/mass system if it can be expressed in the form

$$\boxed{\Big(q(t), p(t)\Big) = \Big(Q(t)q_e, Q(t)p_e\Big)} \tag{2.5}$$

Where $z_e = (q_e, p_e) \in P$ is a solution of (2.2) for $t = t_e$ and $Q(t) : \mathbb{R}^+ \to SO2, Q(0) = 1$ is a C^1 one-parameter subgroup of planar rotations. As noted in remark 2.2.1 both $q(t)$ and $p(t)$ must always remain perpendicular to J, so $Q(t)$ can only be a rotation about an axis parallel to J. We can redefine the symmetry group S as a subgroup of $SO3$, the group of rotations over $\mathbb{R}^3$, as follows

$$S = \{Q_t \mid Q_t \in SO3, \ Q_t J = J\} \tag{2.6}$$

Let $\{e_1, e_2, e_3\}$ be an orthonormal basis of fixed vectors with e_3 normal to Π and e_1 in the direction of q_e. With that choice of basis,

$$J = Je_3$$

$$q_e = q_e e_1$$

$$Q_t = \begin{pmatrix} \cos\theta_t & -\sin\theta_t & 0 \\ \sin\theta_t & \cos\theta_t & 0 \\ 0 & 0 & 1 \end{pmatrix}, \ \theta_t : R^+ \to (-2\pi, 2\pi], \theta_0 = 1 \tag{2.7}$$

Remarks 2.3.

1. The symmetry group S is commutative.

$$\forall Q_1, Q_2 \in S, \ Q_1 Q_2 = Q_2 Q_1 \tag{2.8}$$

2. The norms of the position and momenta are conserved along a relative equilibrium,

$$\|q(t)\| = \|Q(t)q_e\| = \|q_e\| \quad \text{and} \quad \|p(t)\| = \|Q(t)p_e\| = \|p_e\|, \ \forall Q(t) \in S \tag{2.9}$$

3. Because the relative equilibrium is a solution of (2.2), energy is conserved. But furthermore, due to special form of K and V, which depend on q and p only through their moduli, the kinetic and potential energies are also constant along a relative equilibrium

$$V(q(t)) = \hat{V}(\|Q(t)q_e\|) = \hat{V}(\|q_e\|) = V(q_e)$$
$$K(p(t)) = \hat{K}(\|Q(t)p_e\|) = \hat{K}(\|p_e\|) = K(p_e) \tag{2.10}$$

4. If (q^*, p^*) is any solution of the orbit, then any other solution of the relative equilibrium can be expressed as $(q(t), p(t)) = (Q^*(t)q^*, Q^*(t)p^*)$.

$$q(t) = Q(t)q_e, \ q^* = Q(t^*)q_e \Rightarrow q(t) = Q(t)Q(t^*)^{-1}q_e = Q^*(t)q^*$$
$$p(t) = Q(t)p_e, \ p^* = Q(t^*)p_e \Rightarrow p(t) = Q(t)Q(t^*)^{-1}p_e = Q^*(t)p^* \tag{2.11}$$

These properties will play an important role is the development that follows. □

2.3.1. Relative equilibria of the spring/mass system

We now find the expression of the position and momenta in a relative equilibrium of angular momentum J. If suffices to find a particular solution (q_e, p_e) to (2.5). To find these values we substitute (2.5) in (2.2). The time derivatives are computed as follows:

$$\frac{dq(t)}{dt} = \frac{d}{dt}(Q(t)q_e) = \dot{Q}(t)q_e = W(t)Q(t)q_e = Q(t)W(t)q_e = Q(t)\Omega(t) \times q_e$$
$$\frac{dp(t)}{dt} = \frac{d}{dt}(Q(t)p_e) = \dot{Q}(t)p_e = W(t)Q(t)p_e = Q(t)W(t)p_e = Q(t)\Omega(t) \times p_e$$

(2.12)

where $W(t)$ is a skew-symmetric tensor, $W = -W^T$, and $\Omega = \Omega e_3$ is the angular velocity of the system. Using these results and eliminating $Q(t)$ from the equations, Hamilton's equations (2.2) in the relative equilibria are

$$\begin{cases} \Omega \times q_e = \dfrac{1}{m} p_e \\[2mm] \Omega \times p_e = -\dfrac{\hat{V}'(\|q_e\|)}{\|q_e\|} q_e \end{cases}$$

(2.13)

From either of this two equations we deduce that q_e, p_e and Ω must be orthogonal. In the basis $\{e_1, e_2, e_3\}$ we have

$$q_e = \|q_e\| e_1$$
$$p_e = \|p_e\| e_2$$
$$J = \|J\| e_3$$

(2.14)

After a straightforward manipulation we obtain an implicit formula for q_e in terms of the potential energy function $\hat{V}$ and explicit expressions for Ω and p_e.

$$\|J\|^2 = \|q_e\|^3 \hat{V}'(\|q_e\|)$$
$$q_e = \|q_e\| e_1$$
$$\Omega = \frac{1}{m} \frac{\|J\|}{\|q_e\|^2} e_3$$
$$p_e = \frac{\|J\|}{\|q_e\|} e_2$$

(2.15)

Because the relative equilibrium is of the form (2.5), we know that the value of the Hamiltonian at any time is

$$H(q(t), p(t)) = \hat{V}(\|q_e\|) + \hat{K}(\|p_e\|);$$

(2.16)

3. Discrete solutions for the relative equilibria

Once the exact relative equilibria of the spring/mass system have been identified, we consider six numerical methods and determine how accurately they can represent those particular solutions. These numerical schemes are: the trapezoidal rule, a one-parameter family of dissipative Newmark's methods, the HHT method, the midpoint rule, the energy-momentum conserving method and the EDMC method. The second, third and last methods have some kind of high frequency numerical dissipation.

We study if the equations resulting from the time discretization of (2.2) by each of the numerical methods admit solutions that are one parameter orbits of a discrete symmetry group. If this type of solutions exist, we also verify if the discrete orbits lie inside the exact ones. For methods that include high frequency numerical dissipation we investigate how does this dissipation affect a motion of a relative equilibrium.

3.1. Discrete relative equilibria

Consider $\{(q_n, p_n), n \in \mathbb{N}, (q_n, p_n) \in P\}$, the solution of a numerical method to problem (2.2). We define a *discrete relative equilibria* as numerical solutions of the problem (2.2) that satisfy the discrete equivalent of (2.5), namely

$$\boxed{(q_n, p_n) = \left(Q_n q_e, Q_n p_e \right)} \tag{3.1}$$

where q_n and p_n are the numerical approximations for the position and momentum at time $t_n = n\Delta t$, Δt is the time step and $Q_n \in \hat{S}$, the discrete symmetry group. We define this group as a subgroup of S

$$\hat{S} = \{Q_n \in S, \ n \in \mathbb{N}\} \tag{3.2}$$

Remarks 3.1.

Every remark in 2.3 must have a discrete equivalent:

1. $\|q_n\| = \|Q_n q_e\| = \|q_e\|, \quad \|p_n\| = \|Q_n p_e\| = \|p_e\|$
2. $V(q_n) = \hat{V}(\|q_n\|) = \hat{V}(\|q_e\|), \quad K(p_n) = \hat{K}(\|p_e\|) = \hat{K}(\|p_e\|)$

We introduce a discrete incremental rotation $\hat{Q} \in \hat{S}$ that relates the position and momenta in two consecutive time steps.

$$\begin{aligned} q_{n+1} &= \hat{Q} q_n \\ p_{n+1} &= \hat{Q} p_n \end{aligned} \tag{3.3}$$

For an interpolated vector $q_{n+\alpha} = (1 - \alpha)q_n + \alpha q_{n+1}$ there is also an interpolating tensor G defined as $G = (1 - \alpha)\hat{Q}^T + \alpha \mathbf{1}$ such that

$$\begin{aligned} q_{n+\alpha} &= G q_{n+1} = G\hat{Q} q_n \\ p_{n+\alpha} &= G p_{n+1} = G\hat{Q} p_n \end{aligned} \tag{3.4}$$

Remarks 3.2.

1. G is not a rotation, except when α is 0 or 1. Nevertheless, it commutes with the discrete symmetry group.

2. $Q_n = \widehat{Q}^n$

3. $\|q_{n+\alpha}\| = \|G\widehat{Q}q_n\| = \|G\widehat{Q}^n q_e\| = \|Gq_e\|$

3. If $\hat{\theta}$ is the angle between q_n and q_{n+1} then $\widehat{Q}$ is of the form

$$\widehat{Q} = \begin{pmatrix} \cos\hat{\theta} & -\sin\hat{\theta} & 0 \\ \sin\hat{\theta} & \cos\hat{\theta} & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{3.5}$$

3.2. The generalized α-method

This 3-parameter family of methods generalizes the HHTα−method, in a way that includes Newmark's method and therefore the trapezoidal rule as particular cases. We will develop the analysis in this general form and later on particularize for each of those methods. The discrete equations of the generalized α−method for the motion of the mass are:

$$\boxed{\begin{aligned} & 0 = ma_{n+1} + N[q_{n+\alpha}] \\ & q_{n+1} = q_n + \Delta t m^{-1} p_n + \frac{\Delta t^2}{2}\Big[(1-2\beta)a_n + 2\beta a_{n+1}\Big] \\ & p_{n+1} = p_n + m\Delta t\Big[(1-\gamma)a_n + \gamma a_{n+1}\Big] \end{aligned}} \tag{3.6}$$

Where a_n is the algorithmic approximation to the acceleration of the mass m at time t_n, $q_{n+\alpha} = (1-\alpha)q_n + \alpha q_{n+1}$ and

$$N[q_{n+\alpha}] = V'(q_{n+\alpha})q_{n+\alpha} = \frac{\hat{V}'(\|q_{n+\alpha}\|)}{\|q_{n+\alpha}\|}q_{n+\alpha} \tag{3.7}$$

Defining

$$\nu = \frac{\Delta t^2}{m}\frac{\hat{V}'(\|q_{n+\alpha}\|)}{\|q_{n+\alpha}\|} = \frac{\Delta t^2}{m}\frac{\hat{V}'(\|Gq_e\|)}{\|Gq_e\|} \tag{3.8}$$

and evaluating (3.6.1) at times t_n and t_{n+1} we obtain

$$N[q_{n+\alpha}] = \frac{m\nu}{\Delta t^2}q_{n+\alpha}$$

$$N[q_{n-1+\alpha}] = \frac{m\nu}{\Delta t^2}q_{n-1+\alpha}$$

$$a_{n+1} = -\nu\Delta t^2 G\widehat{Q}q_n \tag{3.9}$$

$$a_n = -\nu\Delta t^2 Gq_n$$

.

With the last two equations we can eliminate the acceleration field from (3.6)

$$(\widehat{Q} - 1)q_n = m^{-1}p_n\Delta t - m\nu\left[(\tfrac{1}{2} - \beta)1 + \beta\widehat{Q}\right]Gq_n$$
$$(\widehat{Q} - 1)m^{-1}p_n\Delta t = -m\nu\left[(1 - \gamma)1 + \gamma\widehat{Q}\right]Gq_n$$

(3.10)

Using relations (3.1), the commutativity property of rotations in $\widehat{S}$ and inserting (3.10.1) in (3.10.2) we obtain the equations of the position and momenta along the relative equilibria.

$$\boxed{\begin{aligned} p_e &= m/\Delta t\left[\widehat{Q} - 1 + \nu(\tfrac{1}{2} - \beta)G + \nu\beta\widehat{Q}G\right]q_e \\ (\widehat{Q} - 1)^2 q_e &+ \nu(\widehat{Q} - 1)\left[(\tfrac{1}{2} - \beta)1 + \beta\widehat{Q}\right]Gq_e + \nu\left[(1 - \gamma)1 + \gamma\widehat{Q}\right]Gq_e = 0 \end{aligned}}$$

(3.11)

Defining the factors $\kappa_2, \kappa_1, \kappa_T, \kappa_0$

$$\boxed{\begin{aligned} \kappa_0 &= 1 + \nu(\tfrac{1}{2} - 2\beta + 3\alpha\beta + \gamma - 2\alpha\gamma) \\ \kappa_1 &= -2 + \nu(-3\alpha\beta + \beta + \frac{\alpha}{2} + \alpha\gamma) \\ \kappa_2 &= 1 + \alpha\beta\nu \\ \kappa_T &= \nu\left[(\beta - \tfrac{1}{2})(1 - \alpha) + (1 - \gamma)(1 - \alpha)\right] \end{aligned}}$$

(3.12)

equation (3.11.2) becomes

$$\left[\kappa_2\widehat{Q}^2 + \kappa_1\widehat{Q} + \kappa_T\widehat{Q}^T + \kappa_0 1\right]Q_n q_e = 0$$

(3.13)

Q_n commutes with $\widehat{Q}, \widehat{Q}^T$ and $\widehat{Q}^2$. Moreover, a rotation is never singular so we can multiply (3.13) from the left by Q_n^{-1} and (3.13) becomes

$$\left[\kappa_2\widehat{Q}^2 + \kappa_1\widehat{Q} + \kappa_T\widehat{Q}^T + \kappa_0 1\right]q_e = 0$$

(3.14)

Replacing q_e by $\|q_e\|e_1$ and dividing by $\|q_e\|$ we finally obtain

$$\boxed{\left[\kappa_2\widehat{Q}^2 + \kappa_1\widehat{Q} + \kappa_T\widehat{Q}^T + \kappa_0 1\right]e_1 = 0}$$

(3.15)

Remarks 3.3.

1. $\widehat{Q} = 1, \nu = 0$ is a solution for every combination (α, β, γ). This is the trivial solution, when the mass is at rest and every consistent method should have it.
2. If a given combination (α, β, γ) allows the existence of a numerical relative equilibrium, then equation (3.15) must have a real solutions for $\widehat{Q}$ and κ_i. Using that solution in (3.11) and (3.8) we obtain the values of q and p.
3. Equation (3.15) can be interpreted as the sum of 4 vectors $e_1, \widehat{Q}e_1, \widehat{Q}^2 e_1, \widehat{Q}^T e_1$ each one scaled by a factor $\kappa_0, \kappa_1, \kappa_2, \kappa_T$ respectively. $\square$
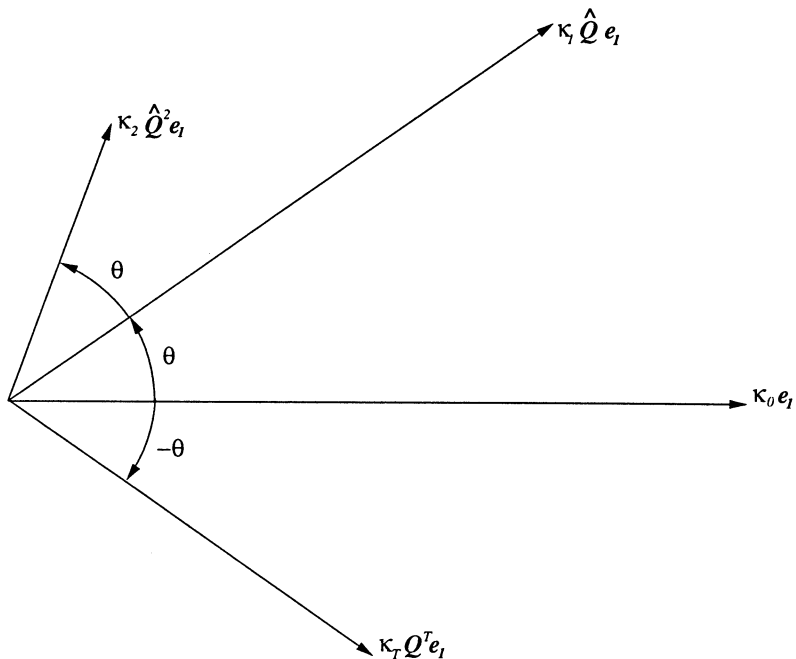
FIGURE 3.1. Graphical interpretation of equation (3.15). Each term of the equation can be viewed as a vector their vectorial sum must vanish.

3.3. The trapezoidal rule

The trapezoidal rule corresponds to the choice $(\alpha, \beta, \gamma) = (1, \frac{1}{4}, \frac{1}{2})$ in (3.6). Substituting these values in (3.12) and (3.15) we obtain

$$
\begin{aligned}
\kappa_0 &= \ 1 + \frac{\nu}{4} \\
\kappa_1 &= -2 + \frac{\nu}{2} \\
\kappa_2 &= \ 1 + \frac{\nu}{4} \\
\kappa_T &= \ 0
\end{aligned}
\tag{3.16}
$$

$$
0 = \left[(1 + \frac{\nu}{4})\widehat{Q}^2 + (\frac{\nu}{2} - 2)\widehat{Q} + (1 + \frac{\nu}{4})\mathbf{1} \right] e_1
$$

$\nu > 0$ so we can divide (3.16.4) by $1 + \frac{\nu}{4}$ and defining $\eta = \frac{\frac{\nu}{2} - 2}{1 + \frac{\nu}{4}}$ obtain the simplified equation

$$
\left[\widehat{Q}^2 + \eta \widehat{Q} + \mathbf{1} \right] e_1 = \mathbf{0}
\tag{3.17}
$$

As in the general case, (3.17) admits a graphical interpretation of three vectors of sum **0**
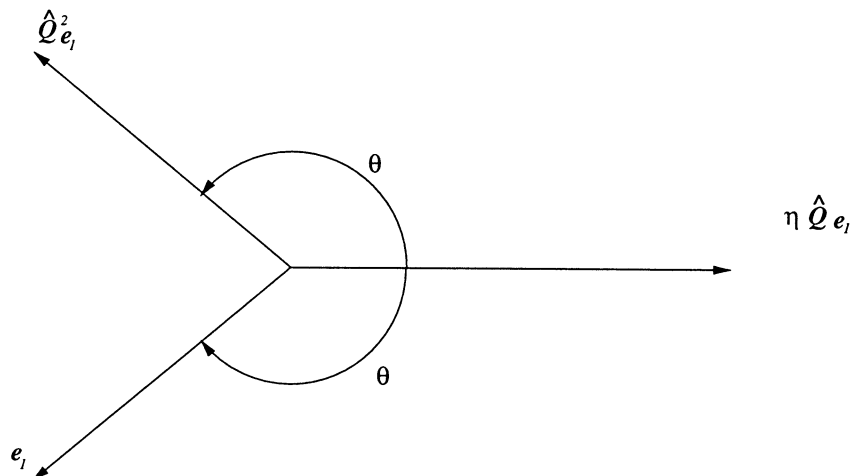
FIGURE 3.2. Graphical interpretation of equation (3.17). We identify each term of (3.17) as a vector, and their sum must be equal to 0.

$\widehat{Q}$ is of the form (3.5), so equation (3.17) is equivalent to the system of equations

$$\begin{cases} \cos 2\hat{\theta} + \eta \cos \hat{\theta} = -1 \\ \sin 2\hat{\theta} + \eta \sin \hat{\theta} = 0 \end{cases} \tag{3.18}$$

Equations (3.18) have a nontrivial solution $\eta = -2\cos\hat{\theta}$, and this implies that *the trapezoidal rule admits solutions which are discrete relative equilibria of the spring/mass problem.* For a given q_e, the corresponding p_e is recovered from (3.11), using $\eta = \frac{\frac{\nu}{2}-2}{1+\frac{\nu}{4}} = -2\cos\hat{\theta}$:

$$p_e = \frac{m}{\Delta t} \begin{pmatrix} 0 & \frac{2\sin\hat{\theta}}{1+\cos\hat{\theta}} & 0 \\ -\frac{2\sin\hat{\theta}}{1+\cos\hat{\theta}} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} q_e = \frac{m}{\Delta t}\sqrt{\nu} \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} q_e \tag{3.19}$$

Proposition 3.1 *The discrete relative equilibria of the trapezoidal rule lie on the exact ones*

PROOF: We now show that the motion generated as a one-parameter group orbit of the form (3.1) with a given q_e and a p_e as in (3.19), has the same angular momentum and energy as the exact relative equilibrium.

First note that we have already proven that for q_e and p_e of the form (3.19) the solution is of the form (3.1). A consequence of this is that momentum and energy are

conserved along this motion. The Hamiltonian has the value

$$H(\boldsymbol{q}_n, \boldsymbol{p}_n) = \hat{V}(\|\boldsymbol{q}_n\|) + \hat{K}(\|\boldsymbol{p}_n\|) = \hat{V}(\|\boldsymbol{q}_e\|) + \hat{K}(\|\boldsymbol{p}_e\|) \tag{3.20}$$

We now calculate the angular momentum. If $\boldsymbol{q}_e = \|\boldsymbol{q}_e\|\boldsymbol{e}_1$, using (3.19) and (3.8),

$$\boldsymbol{p}_e = \frac{m}{\Delta t}\sqrt{\nu}\|\boldsymbol{q}_e\|\boldsymbol{e}_2$$

$$\boldsymbol{J} = \boldsymbol{q}_e \times \boldsymbol{p}_e = \frac{m}{\Delta t}\sqrt{\nu}\|\boldsymbol{q}_e\|^2\boldsymbol{e}_3 \tag{3.21}$$

$$\|\boldsymbol{J}\|^2 = \frac{m^2}{\Delta t^2}\nu\|\boldsymbol{q}_e\|^4 = m\hat{V}'(\|\boldsymbol{q}_e\|)\|\boldsymbol{q}_e\|^3$$

Comparing (3.20) with (2.16) and (3.21) with (2.15.3) we conclude that the points of the discrete relative equilibria of the trapezoidal rule lie over points of the exact orbit with same energy and momentum. ∎

3.4. A dissipative Newmark scheme

Newmark's method corresponds to the generalized α−method with parameters $\alpha = 1$ and $0 \leq \beta, \gamma \leq 1$. The trapezoidal rule was a particular case of this method, but now we are interested in a more general class, namely the one with

$$\tfrac{1}{2} < \gamma \leq 1, \quad \beta = (\gamma + \tfrac{1}{2})^2/4 \tag{3.22}$$

For linear problems of elastodynamics, this 1-parameter family of methods is first order accurate, unconditionally stable and has artificial numerical dissipation in the high frequencies, controlled by the parameter γ. Substituting $\alpha = 1$ in (3.12) we obtain

$$\begin{aligned}
\kappa_0 &= \ \ 1 + \nu(\tfrac{1}{2} + \beta - \gamma) \\
\kappa_1 &= -2 + \nu(-2\beta + \tfrac{1}{2} + \gamma) \\
\kappa_2 &= \ \ 1 + \nu\beta \\
\kappa_T &= 0
\end{aligned} \tag{3.23}$$

Inserting this parameters in (3.15) and dividing by $1 + \nu(\beta - \gamma + \tfrac{1}{2})$ (which is always positive if $\beta = (\gamma + \tfrac{1}{2})^2/4$, $\tfrac{1}{2} < \gamma \leq 1$) we get

$$\eta_1 = \frac{-2 + \nu(\tfrac{1}{2} + \gamma - 2\beta)}{1 + \nu(\beta - \gamma + \tfrac{1}{2})}$$

$$\eta_2 = \frac{(1 + \beta\nu)}{1 + \nu(\beta - \gamma + \tfrac{1}{2})} \tag{3.24}$$

$$\left[\eta_2\widehat{Q}^2 + \eta_1\widehat{Q} + 1\right]\boldsymbol{e}_1 = 0$$
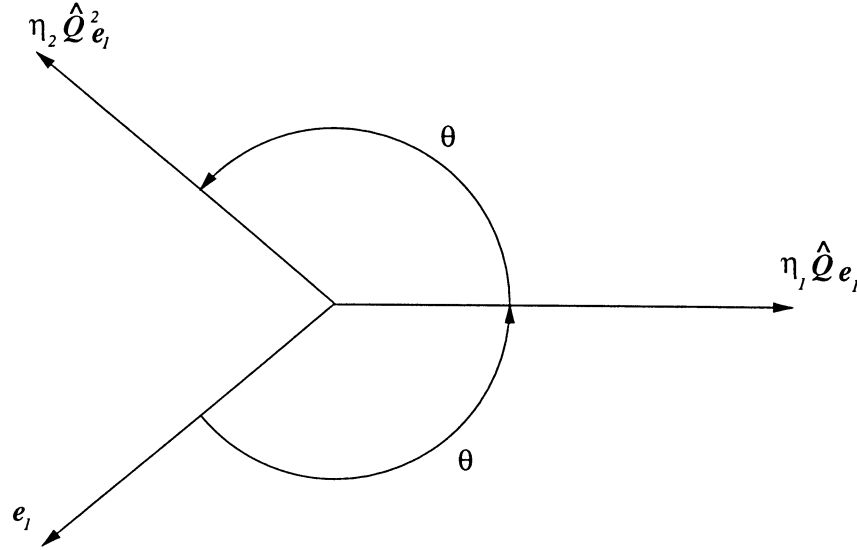
FIGURE 3.3. Graphical interpretation of equation $(3.24._3)$. Each of the terms represented by a vector. A necessary condition for their sum to be zero is that the vertical components of e_1 and $\alpha_2 \widehat{Q} e_1$ are equal and opposite. This implies $\alpha_2 = 1$.

From figure 3.3 we deduce that a necessary condition for (3.24) to have solution is that $\eta_2 = 1$. But defining $\epsilon = \gamma - \frac{1}{2}$, $\epsilon > 0$ it is easy to see that η_2 is strictly greater than 1 for every $\nu > 0$

$$\eta_2 = \frac{1 + \beta\nu}{1 + \beta\nu - \nu\epsilon} > 1 \tag{3.25}$$

This implies that (3.24) does not have a solution and hence, *this dissipative family of Newmark's method can not have solutions which are relative equilibria of the problem.*

3.5. The Hilber-Hughes-Taylor method

The HHT methods correspond to equations (3.6) with parameters

$$(\alpha, \beta, \gamma) = \left(\alpha, \frac{(2-\alpha)^2}{4}, \frac{(3-2\alpha)}{2}\right), \quad 0.7 \leq \alpha \leq 1 \tag{3.26}$$

It is a second order accurate method very widely used in linear structural dynamics for its good dissipative properties. To see if it can have solutions which are *discrete relative equilibria*, we do as before, substituting the values of (α, β, γ) in (3.12) and trying to solve
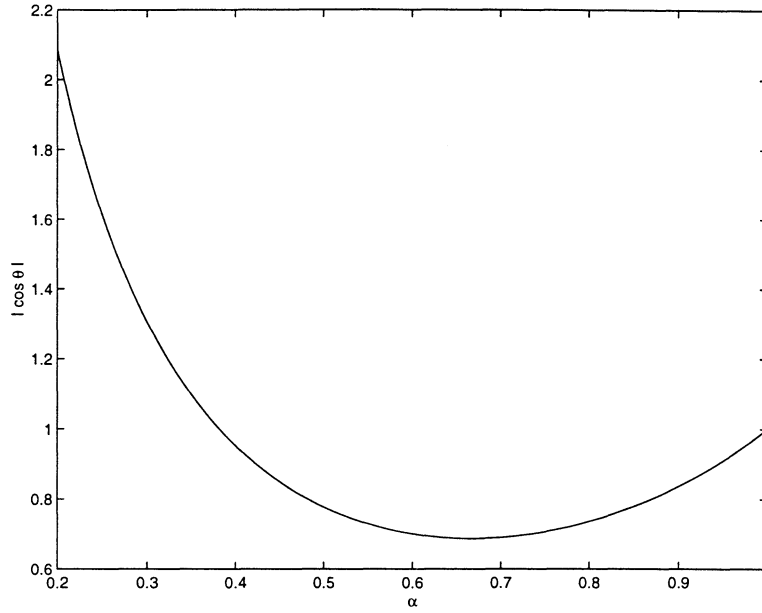
FIGURE 3.4. HHT method. $\max_\nu |\cos\hat\theta|$ for $0.2 \le \alpha \le 1$. If $|\cos\hat\theta| \le 1$, we must restrict α to $0.35 \le \alpha \le 1$

(3.15). The values of the parameters κ_i are

$$
\begin{aligned}
\kappa_0 &= 1 + \frac{\nu}{4}\alpha(3\alpha^2 - 6\alpha + 4) \\
\kappa_1 &= -2 + \frac{\nu}{4}(-3\alpha^3 + 9\alpha^2 - 8\alpha + 4) \\
\kappa_2 &= 1 + \frac{\nu}{4}\alpha(2 - \alpha)^2 \\
\kappa_T &= \frac{\nu}{4}\alpha^2(1 - \alpha)
\end{aligned}
\tag{3.27}
$$

If we introduce (3.27) in (3.15), where $\widehat{Q}$ is of the form (3.5), we obtain the following system of equations:

$$
\begin{cases}
\kappa_2 \cos(2\hat\theta) + (\kappa_1 + \kappa_T)\cos\hat\theta + \kappa_0 = 0 \\
\kappa_2 \sin(2\hat\theta) + (\kappa_1 - \kappa_T)\sin\hat\theta = 0
\end{cases}
\tag{3.28}
$$

From (3.28.2) we get

$$
\cos\hat\theta = \frac{\kappa_T - \kappa_1}{2\kappa_2}
\tag{3.29}
$$

In figure 3.4 we have plotted the maximum $\cos\hat\theta$ as a function of α. For a given α this maximum is attained as $\nu \to \infty$. In order to have $\left|\frac{\kappa_T - \kappa_1}{2\kappa_2}\right| \le 1$ for any value of ν, we must restrict $\alpha > 0.35$. But the HHT only considers $\alpha > 0.7$. Introducing (3.29) in (3.28.1) we

obtain

$$\kappa_T(\kappa_T - \kappa_1) + \kappa_2(\kappa_0 - \kappa_2) = 0 \Leftrightarrow \frac{1}{4}(\alpha - 1)\alpha^2\nu^2 = 0 \qquad (3.30)$$

This equation is satisfied in three cases: when $\nu = 0$ (the mass is stopped), $\alpha = 1$ (in this case the HHT method reduces to the trapezoidal rule) and $\alpha = 0$. This last case can not be taken into account because we have the restriction $\alpha > 0.7$. We conclude that *there is no dissipative HHT scheme able to represent a discrete relative equilibrium of the spring/mass system.*

3.6. The midpoint rule

The midpoint rule can be put into the form (3.6) by selecting the parameters $(\alpha, \beta, \gamma) = (\frac{1}{2}, \frac{1}{2}, 1)$. After reordering we obtain the usual form for this method:

$$\begin{cases} \dfrac{q_{n+1} - q_n}{\Delta t} = \dfrac{1}{m} p_{n+\frac{1}{2}} \\[2ex] \dfrac{p_{n+1} - p_n}{\Delta t} = -N[q_{n+\frac{1}{2}}] \end{cases} \qquad (3.31)$$

With this choice of parameters, and defining as for the trapezoidal rule $\eta = \frac{\frac{\nu}{2} - 2}{1 + \frac{\nu}{4}}$, equations (3.12) and (3.15) become

$$\begin{aligned} \kappa_0 &= 1 + \nu(\tfrac{1}{2} + \beta - \gamma) \\ \kappa_1 &= -2 + \nu(-2\beta + \tfrac{1}{2} + \gamma) \\ \kappa_2 &= 1 + \nu\beta \\ \kappa_T &= 0 \end{aligned} \qquad (3.32)$$

$$\left[\widehat{Q}^2 + \eta\widehat{Q} + 1\right] e_1 = 0$$

which is precisely (3.17). We have already showed that this equation has a solution $\eta = -2\cos\widehat{\theta}$ and hence *the midpoint rule has solutions which are discrete relative equilibria.*

Remark 3.4.

Even though equations (3.32) and (3.17) are the same, their solutions are different because the numerical value of η in each case is different. In both cases $\eta = \frac{\frac{\nu}{2} - 2}{\frac{\nu}{4} + 1}$ but the definition of ν is different in the two methods. Recall their definitions

$$\nu_{\text{trapez}} = \frac{\Delta t^2}{m} \frac{\widehat{V}'(\|q_n\|)}{\|q_n\|}$$

$$\nu_{\text{midpoint}} = \frac{\Delta t^2}{m} \frac{\widehat{V}'(\|q_{n+\frac{1}{2}}\|)}{\|q_{n+\frac{1}{2}}\|} \qquad (3.33)$$

that difference turns out to be important as we now show.

Proposition 3.2 *The discrete relative equilibria of the midpoint rule depend on the time step.*

PROOF: Because (3.32) is identical to (3.17) we can use the same arguments as in the proof of Proposition 3.1, with the appropriate redefinition of the parameter ν. For a given angular momentum $\boldsymbol{J}$ there exists a unique discrete relative equilibria of the form (3.1) satisfying:

$$
\begin{aligned}
H(\boldsymbol{q}_n, \boldsymbol{p}_n) &= \hat{V}(\|\boldsymbol{q}_e\|) + \hat{K}(\|\boldsymbol{p}_e\|) \\
\boldsymbol{q}_e &= \|\boldsymbol{q}_e\| \boldsymbol{e}_1 \\
\boldsymbol{p}_e &= \frac{m}{\Delta t}\sqrt{\nu}\|\boldsymbol{e}\|_2 \\
\boldsymbol{J} &= \boldsymbol{q}_e \times \boldsymbol{p}_e = \frac{m}{\Delta t}\sqrt{\nu}\|\boldsymbol{q}_e\|^2 \boldsymbol{e}_3 \\
\|\boldsymbol{J}\| &= \frac{m^2}{\Delta t}\nu\|\boldsymbol{q}_e\|^4 = m\frac{\hat{V}'(\|\boldsymbol{G}\boldsymbol{q}_e\|)}{\|\boldsymbol{G}\boldsymbol{q}_e\|}\|\boldsymbol{q}_e\|^4
\end{aligned}
\tag{3.34}
$$

Note the difference between (3.34.5) and (3.21.3). In the expression of the midpoint rule the matrix $\boldsymbol{G}$ enters the definition of the relative equilibria. This matrix depends on the time step Δt and

$$
\|\boldsymbol{G}\boldsymbol{q}_e\| = \frac{q_e}{\sqrt{2}}\sqrt{1 + \cos\hat{\theta}}
\tag{3.35}
$$

where $\hat{\theta}$ is the angle between two consecutive positions $\boldsymbol{q}_n$ and $\boldsymbol{q}_{n+1}$. The larger the time step we pick for our calculations, the larger $\hat{\theta}$ will be. We conclude that the relative equilibria depend on the time step we select for the calculations.

3.7. The energy-momentum method

The equations of the energy-momentum conserving method for the problem at hand are

$$
\begin{cases}
\dfrac{\boldsymbol{q}_{n+1} - \boldsymbol{q}_n}{\Delta t} = \dfrac{1}{m}\boldsymbol{p}_{n+\frac{1}{2}} \\[2ex]
\dfrac{\boldsymbol{p}_{n+1} - \boldsymbol{p}_n}{\Delta t} = -\dfrac{\hat{V}(\|\boldsymbol{q}_{n+1}\|) - \hat{V}(\|\boldsymbol{q}_n\|)}{\|\boldsymbol{q}_{n+1}\| - \|\boldsymbol{q}_n\|}\dfrac{\boldsymbol{q}_{n+1} + \boldsymbol{q}_n}{\|\boldsymbol{q}_{n+1}\| + \|\boldsymbol{q}_n\|}
\end{cases}
\tag{3.36}
$$

For the limit $\|\boldsymbol{q}_{n+1}\| \to \|\boldsymbol{q}_n\|$ equation (3.36) is well defined

$$
\frac{\boldsymbol{p}_{n+1} - \boldsymbol{p}_n}{\Delta t} = -\hat{V}'\left(\frac{\|\boldsymbol{q}_{n+1}\| + \|\boldsymbol{q}_n\|}{2}\right)\frac{\boldsymbol{q}_{n+1} + \boldsymbol{q}_n}{\|\boldsymbol{q}_{n+1}\| + \|\boldsymbol{q}_n\|}
\tag{3.37}
$$

It is this last equation the one we should use for our analysis because in relative equilibrium $\|\boldsymbol{q}_{n+1}\| = \|\boldsymbol{q}_n\|$. We proceed as with the midpoint rule obtaining the same equations as

(3.31)

$$\begin{cases} (\widehat{Q} - 1)q_n = \dfrac{\Delta t}{m} G p_{n+1} \\ (\widehat{Q} - 1)p_n = -\dfrac{m\nu}{\Delta t} G q_{n+1} \end{cases} \qquad (3.38)$$

Once more, the definition of the parameter δ is crucial. For this method

$$\nu = \frac{\Delta t^2}{m} \frac{\widehat{V}'(\frac{1}{2}(\|q_n\| + \|q_{n+1}\|))}{\frac{1}{2}(\|q_n\| + \|q_{n+1}\|)} \qquad (3.39)$$

which for the case of a relative equilibrium simplifies to

$$\nu = \frac{\Delta t^2}{m} \frac{\widehat{V}'(\|q_e\|)}{\|q_e\|} \qquad (3.40)$$

If we proceed with the analysis, as in the case of the midpoint rule, equations (3.38) will lead to (3.32) but now δ has the same value as in the trapezoidal rule, so equations (3.38) have solutions which are the exact relative equilibrium.

Remark 3.5.

The equations of the trapezoidal rule and the energy-momentum method are the same if the motion of the spring/mass system is a relative equilibria, and moreover, their solution lies on the exact trajectory. This means that if the initial conditions of position and momenta are such that the exact motion of the system is in relative equilibrium, both numerical methods will give the same result, coinciding in the discrete points on the exact trajectory. But if the initial conditions are not of this kind the solutions of both methods would be different. This two methods are only equal in the relative equilibria and in the trivial case. $\qquad \square$

3.8. Energy dissipative, momentum conserving method

The same authors have recently presented a new method for nonlinear elastodynamics with controllable numerical dissipation in the high frequency range. The equations of the EDMC scheme for our problem are:

$$\begin{cases} \dfrac{q_{n+1} - q_n}{\Delta t} = \dfrac{1}{m}\left(1 + \dfrac{\chi}{4}\dfrac{\|p_{n+1}\| - \|p_n\|}{\|p_{n+1}\| + \|p_n\|}\right) p_{n+\frac{1}{2}} \\ \dfrac{p_{n+1} - p_n}{\Delta t} = -\dfrac{\widehat{V}(\|q_{n+1}\|) - \widehat{V}(\|q_n\|) + \chi \mathcal{DV}}{\|q_{n+1}\| - \|q_n\|} \dfrac{q_{n+1} + q_n}{\|q_{n+1}\| + \|q_n\|} \\ \mathcal{DV} = \frac{1}{2}(\widehat{V}(\|q_{n+1}\|) + \widehat{V}(\|q_n\|)) - \widehat{V}(\frac{1}{2}(\|q_{n+1}\| + \|q_n\|)) \end{cases} \qquad (3.41)$$

with χ a parameter that controls the amount of numerical dissipation. For the relative equilibrium case, $\mathcal{DV} = 0$, the method reduces to the energy-momentum and has no

numerical dissipation. *The dissipative energy-momentum is the only dissipative method that has solutions which are discrete relative equilibria.*

4. Numerical simulations

In this section we show numerical examples to illustrate the results of section 3. Consider a spring/mass system with point mass $m = 1$, spring of natural length $L_0 = 10$ and quadratic potential energy:

$$\hat{V}(\|\boldsymbol{q}\|) = k(\|\boldsymbol{q}\| - L_0)^2 \tag{4.1}$$

where $k = 2$ is the elastic constant. We choose the following initial conditions:

$$\begin{aligned} \boldsymbol{q}(0) &= 10.18907153978086 \\ \boldsymbol{p}(0) &= 1.96288738595216 \end{aligned} \tag{4.2}$$

One can verify that (4.2) correspond to the solution of (2.15) with angular momentum $J = 20$ and Hamiltonian $H = 1.9622115$ and hence the motion of the mass would be a relative equilibrium.

In the following plots we show the solutions to this problem using the trapezoidal rule, a dissipative Newmark of the type (3.22) with $\gamma = 0.51$, the HHT with $\alpha = 0.8$, the midpoint rule, the energy momentum and the EDMC with $\chi = 0.05$. For all the examples we have used a time increment of $\Delta t = 1$ and we have run 1000 time steps. From the plots it is easy to see which methods conserve the relative equilibria: those whose solutions have constant energy, momentum and radius.

5. Summary and conclusions

We have analyzed the numerical solutions to the spring and mass system by several commonly used time integration schemes. We started by defining a *discrete relative equilibrium*, a discrete motion along which relative distance between points on the moving solid remain constant. The results obtained show that the HHT and dissipative Newmark schemes can not have discrete relative equilibrium solutions. The trapezoidal rule, the energy-momentum conserving and the EDMC method have identical solutions when the initial conditions correspond to a relative equilibria. This solution is a discrete relative equilibria and lies inside the exact trajectory of a relative equilibrium. Finally, the midpoint rule has discrete relative equilibria but they do not lie inside the exact trajectory.

We confirmed numerically the analytical results and observed that, given initial conditions in relative equilibrium, the long term solution of all the dissipative algorithms except the EDMC is the static solution. The solution for this last method is the relative equilibrium orbit.
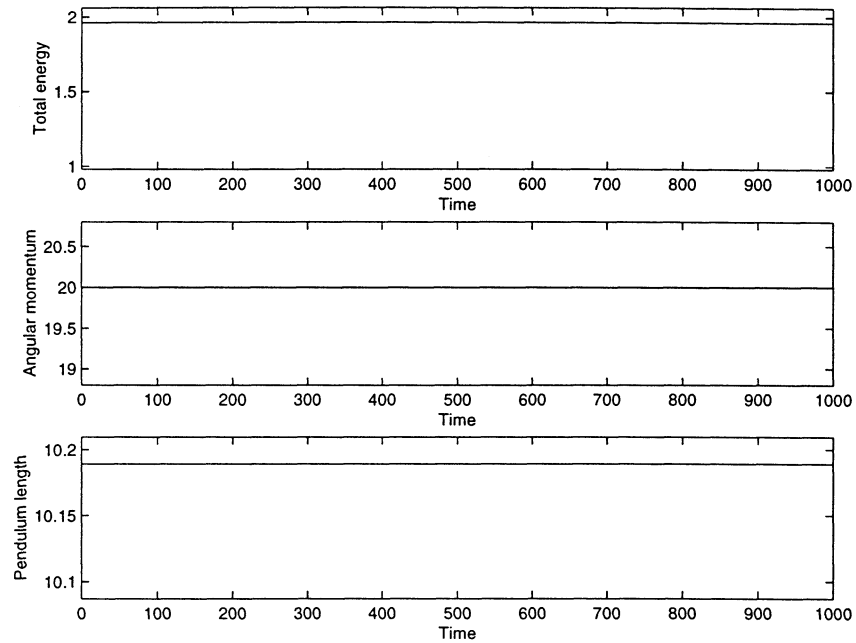
FIGURE 4.1. Trapezoidal rule solution for initial conditions on relative equilibrium. Momentum and energy are conserved and the length of the spring is constant.
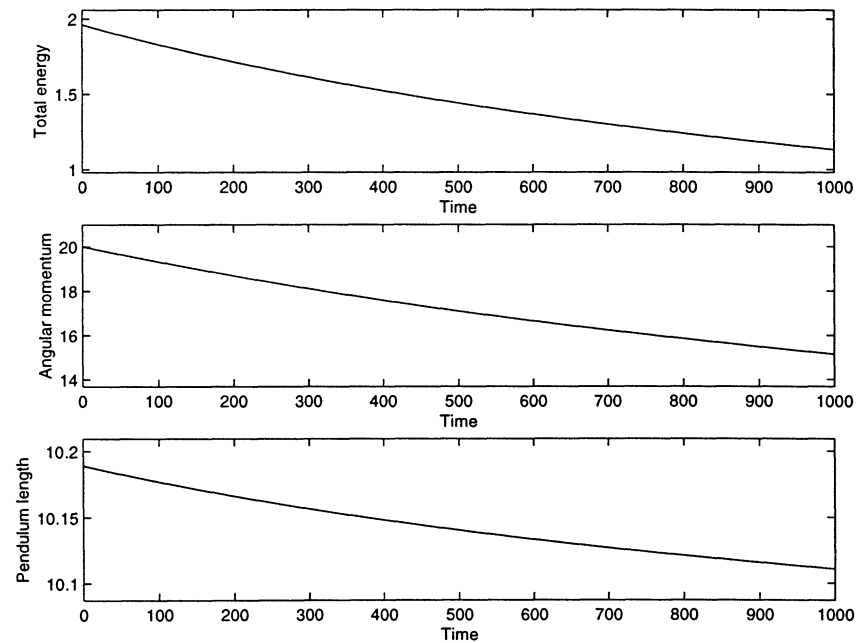

FIGURE 4.2. Dissipative Newmark method solution for initial conditions on relative equilibrium. Energy is dissipated, angular momentum and spring length decrease. The limit solution is the static solution.
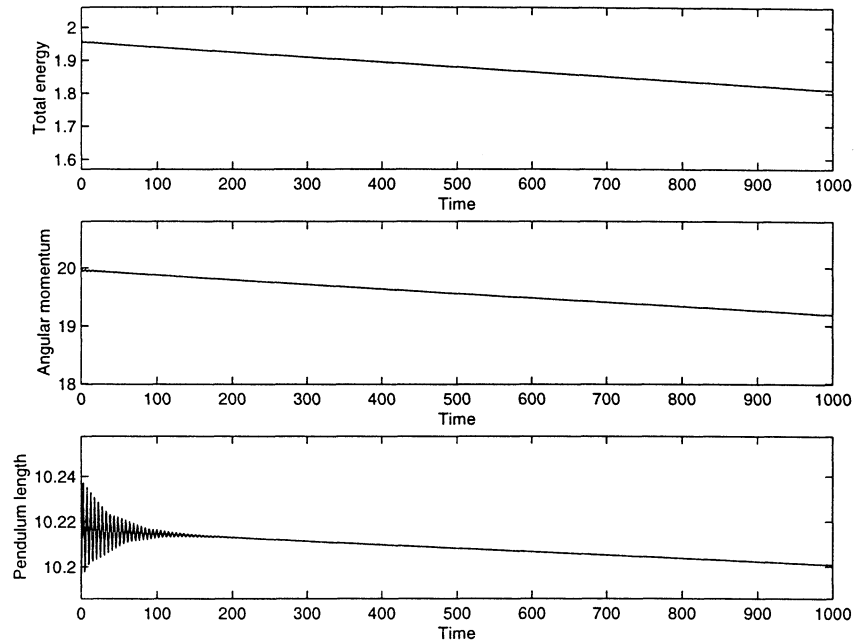
FIGURE 4.3. HHT solution for initial conditions on relative equilibrium. The dissipation is smaller than for the dissipative Newmark scheme, nevertheless still the limit solution is the static one.
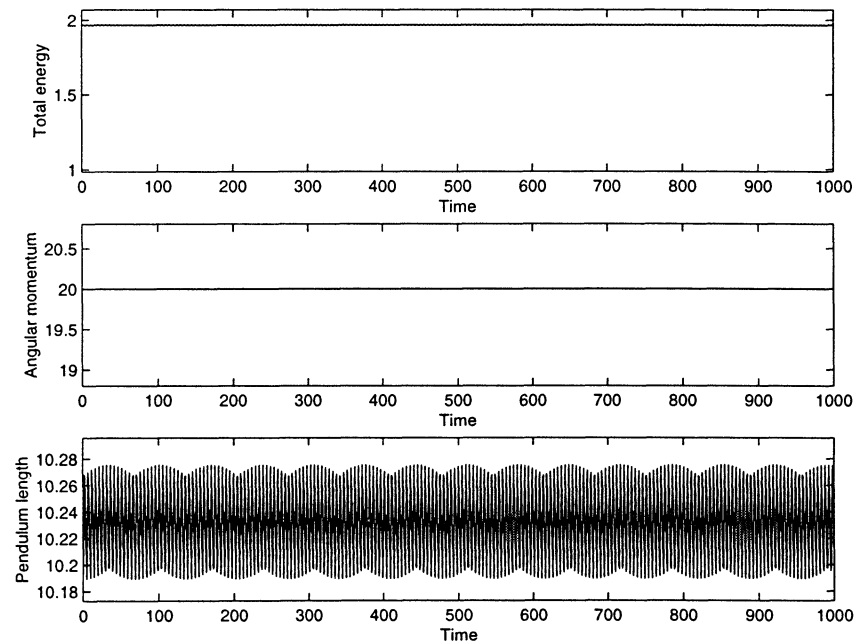

FIGURE 4.4. Midpoint rule for initial conditions on relative equilibrium. Note that the exact conditions of a relative equilibrium do not correspond to a discrete relative equilibrium for this method. Small variations on the energy can be observed.
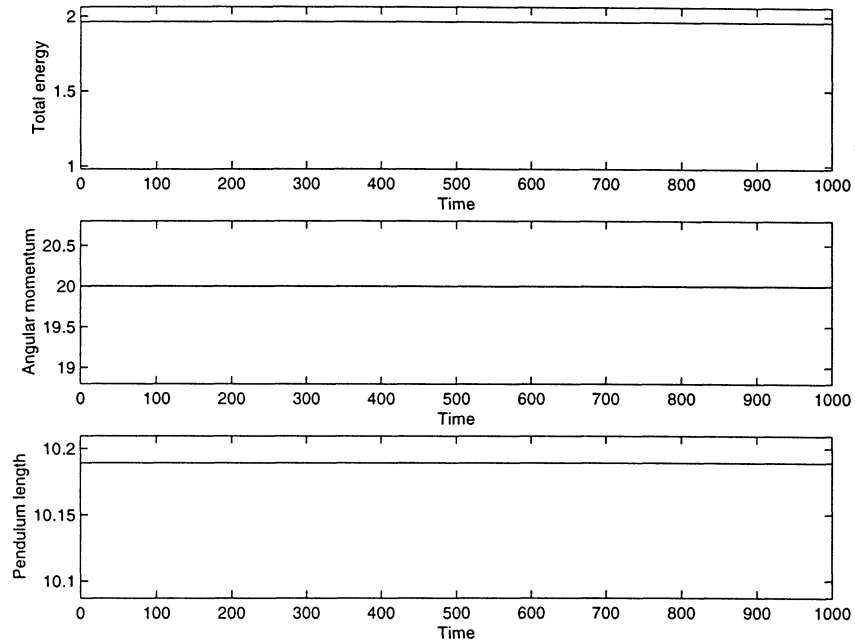
FIGURE 4.5. Energy-momentum method for initial conditions on relative equilibrium. Momentum and energy are conserved and the length of the spring is constant. The method has a discrete relative equilibrium that lies on the exact one.
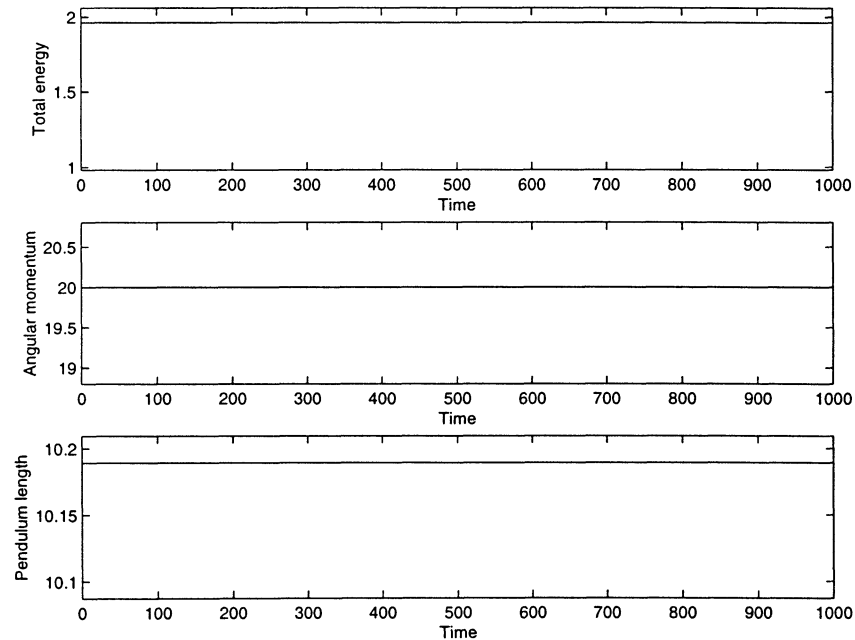

FIGURE 4.6. Energy-momentum dissipative for initial conditions on relative equilibrium. Momentum and energy are conserved and the length of the spring is constant. The discrete trajectory lies on the exact relative equilibrium.

The conclusions obtained here are not definitive because of the simplicity of the system analyzed. Nevertheless, the analysis gives some insight into the numerical properties of commonly used time integration schemes and identifies desirable properties for nonlinear dynamics integrators. In this sense, the recently proposed scheme EDMC seems a valuable tool for the solution of nonlinear elastodynamics. In ARMERO & ROMERO [1999] most of this aspects are further analyzed in more general settings.

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