Resonances and instabilities in symmetric multistep methods

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Abstract

The symmetric multistep methods developed by Quinlan and Tremaine (1990) are shown to suffer from resonances and instabilities at special stepsizes when used to integrate nonlinear equations. This property of symmetric multistep methods was missed in previous studies that considered only the linear stability of the methods. The resonances and instabilities are worse for high-order methods than for low-order methods, and the number of bad stepsizes increases with the number frequencies present in the solution. Symmetric methods are still recommended for some problems, including long-term integrations of planetary orbits, but the high-order methods must be used with caution.

1 Introduction

In many physical problems one has to solve second-order differential equations of the type

\[ x''(t) = f(x, t), \]  

where \( x(t) \) is the position at time \( t \) and \( f(x, t) \) is the force, assumed to be independent of the velocity. Such an equation or set of equations can be solved efficiently by a multistep method

\[ \alpha_k x_{n+k} + \cdots + \alpha_0 x_n = h^2 (\beta_k f_{n+k} + \cdots + \beta_0 f_n), \]  

where \( x_n \) is the computed position at time step \( n \) and \( h \) is the stepsize. A popular class of such methods is the the Störmer-Cowell class, for which \( \alpha_k = 1, \alpha_{k-1} = -2, \alpha_{k-2} = 1, \) and \( \alpha_{k-3} = \cdots = \alpha_0 = 0, \) with the Störmer method being explicit (\( \beta_k = 0 \)) and the Cowell method implicit (\( \beta_k \neq 0 \)). Störmer-Cowell methods have often been used for long-term integrations of planetary orbits (see Quinlan and Tremaine 1990 and references therein). But the Störmer-Cowell methods suffer from a defect, sometimes called an orbital instability, when the stepnumber \( k \) exceeds 2: if a Störmer-Cowell method with \( k > 2 \) is used to integrate a circular orbit, the radius does not remain constant, and the orbit spirals either inwards or outwards (the direction depends on \( k \)). This defect was recognized by Gautschi (1961) and Stiefel and Bettis (1969), who proposed modified multistep methods for orbital integrations. Their methods require a priori knowledge of the frequency of the solution, however, which is usually unknown or, at best, known only approximately.

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Lambert and Watson (1976) showed that the orbital instability of the Störmer-Cowell methods can be avoided by choosing the coefficients of a multistep method to be symmetric, so that

\[ \alpha_i = \alpha_{k-i}, \quad \beta_i = \beta_{k-i}, \quad i = 0, \ldots, k. \]  

Lambert and Watson analysed in detail the application of symmetric methods to the linear test equation

\[ x''(t) = -\omega^2 x(t), \]  

and showed that if \( \omega^2 h^2 \) lies within an interval \((0, H_0^2)\), which they called the interval of periodicity, the solution is guaranteed to be periodic. Quinlan and Tremaine (1990) extended the work of Lambert and Watson (1976) to derive high-order explicit symmetric methods suitable for the integration of planetary orbits, and compared these with high-order Störmer methods. The symmetric methods gave energy errors that did not grow with time, and position errors that grew only linearly with time, whereas the Störmer methods gave energy errors that grew linearly with time, and position errors that grew as the time squared.

Soon after Quinlan and Tremaine’s methods were published, however, Alar Toomre discovered a disturbing feature of the methods, an example of which is shown in Figure 1. Panel (a) shows the maximum error in the energy of a circular Kepler orbit integrated with the 8th-order symmetric method of Quinlan and Tremaine and with the 8th-order Störmer method, plotted versus the stepsize used in the integration. The energy error decreases with the stepsize as \( \sim h^9 \), as expected for an 8th-order method, and at most stepsizes the error from the symmetric method is much smaller than the error from the Störmer method. But there is a startling spike in the energy error from the symmetric method near a stepsize corresponding to 60 steps per orbit, a stepsize that is well within this method’s interval of periodicity. Figure 2 shows the time development of the instability for a circular orbit integrated with 60 steps per orbit. The energy error grows exponentially for about the first 400 periods until it reaches a maximum value of about 0.25. It decreases over the next few hundred periods to a minimum value of about \( 10^{-7} \), and then oscillates between these extremes with a period of roughly 550 orbital periods. The longitude error (not shown in the figure) grows exponentially until it reaches a value of order unity and then stays at that level.

The problems are worse for eccentric orbits, as shown in panel (b) of Figure 1 for an orbit with \( e = 0.2 \). The symmetric method is still much better than the Störmer method at most stepsizes, but now there are spikes in the energy error at a number of stepsizes. The spikes that appear at the stepnumbers (the number of steps per orbit) 90, 120, 150, etc. are similar to the spike at 60 steps per orbit: they are instabilities at which the error grows exponentially with time. The smaller spikes at stepnumbers that are multiples of 5 or 6 (54, 55, 65, 66, 70, 72, etc.) are resonances, and not instabilities, since at these stepsizes the energy error grows linearly with time, as shown in panel (b) of Figure 2.

The resonances and instabilities do not occur for the linear test equation (4) that has been used in previous discussions of symmetric multistep methods. The present paper is written to explain their origin, to see if anything can be done to reduce their severity, and to decide if they render the methods unsuitable for problems like the long-term planetary integrations considered by Quinlan and Tremaine (1990).

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1The value of the energy error at the instability depends on the formula used to compute the velocities. If the multistep equation is written in summed form (Henrici 1962; Quinlan 1994) and the velocities are computed from the summed accelerations, the maximum error is about 10 times smaller than shown in Figure 2, but apart from this difference the instability remains the same. In this paper the summed form was used only for the planetary integrations described in Section 1.
Figure 1: Maximum fractional energy error during integrations of a Kepler orbit for 25000 periods using the method SY8 (solid lines) and the 8th-order Störmer method (dashed lines), plotted as a function of the number of steps per orbit: (a) circular orbit; (b) eccentric orbit ($e = 0.2$).

2 Symmetric multistep methods

We start by reviewing symmetric multistep methods and some properties of them that are needed for explaining the resonances and instabilities. These properties are described in more detail by
Figure 2: Time dependence of the fractional energy error with the 8th-order symmetric method SY8. Panels (a) and (b) plot the maximum error observed in the previous period during integrations of Kepler orbits with (a) a circular orbit using 60 steps per period and (b) an eccentric orbit ($e = 0.2$) using 54.03 steps per period.

Henrici (1962) and Lambert and Watson (1976). A survey of multistep methods and other methods for integrating second-order differential equations is given by Coleman (1993). Practical techniques for reducing roundoff error in long multistep integrations are described by Quinlan (1994).

We consider $k$-step multistep methods of the type $\bar{\beta}$, where without loss of generality we assume
\( \alpha_k = 1 \) and \(|\alpha_0| + |\beta_0| > 0\). With the multistep method we associate the linear difference operator

\[
L [x(t); h] = \sum_{j=0}^{k} \left[ \alpha_j x(t + j \cdot h) - h^2 \beta_j x''(t + j \cdot h) \right].
\]  

(5)

If \( x(t) \) has continuous derivatives of sufficiently high order then

\[
L [x(t); h] = C_0 x(t) + C_1 x'(t) h + \cdots + C_q x^{(q)}(t) h^q + \cdots,
\]  

(6)

where

\[
C_q = \frac{1}{q!} (0^q \alpha_0 + \cdots + k^q \alpha_k) - \frac{1}{(q - 2)!} (0^q - 2 \beta_0 + \cdots + k^q - 2 \beta_k)
\]  

(7)

(the second term on the right is absent if \( q < 2 \)). The order \( p \) is the integer for which \( C_0 = \cdots = C_{p+1} = 0, C_{p+2} \neq 0 \). A method is said to be consistent if its order is at least 1, i.e., if \( C_0 = C_1 = C_2 = 0 \).

To discuss the stability of multistep methods we introduce the polynomials

\[
\rho(z) = \alpha_k z^k + \alpha_{k-1} z^{k-1} + \cdots + \alpha_0,
\]  

(8)

\[
\sigma(z) = \beta_k z^k + \beta_{k-1} z^{k-1} + \cdots + \beta_0.
\]  

(9)

A method is said to be zero-stable if no root of \( \rho(z) \) has modulus greater than one and if every root of modulus one has multiplicity not greater than two. A consistent method has \( \rho(1) = \rho'(1) = 0 \), so for zero-stability \( \rho(z) \) must have a double root at \( z = 1 \). This is called the principal root; the other roots are called spurious. A method is convergent if and only if it is consistent and zero-stable (convergence means essentially that \( x_n \rightarrow x(t) \) as \( h \rightarrow 0 \) with \( nh = t \)). The order of a convergent \( k \)-step method cannot be higher than \( k + 2 \).

The orbital instability of the Störmer-Cowell methods can be explained by a simple example (Lambert and Watson 1976). Consider equation (4), whose general solution is the periodic function

\[
x(t) = A \cos(\omega t) + B \sin(\omega t).
\]

Applying the multistep method (2) to this equation we obtain the difference equation

\[
\sum_{i=0}^{k} (\alpha_i + H^2 \beta_i) x_{n+i} = 0, \quad H = h \omega,
\]  

(10)

whose general solution is

\[
x_n = \sum_{j=1}^{k} A_j Z_j^n,
\]  

(11)

where the \( Z_j (j = 1, 2, \ldots, k) \) are the roots, assumed distinct, of the polynomial

\[
\Omega(Z; H^2) = \rho(Z) + H^2 \sigma(Z).
\]  

(12)

The roots \( Z_j \) of \( \Omega \) are perturbations of the roots \( z_j \) of \( \rho \); let \( Z_1 \) and \( Z_2 \) be the perturbations of the principal roots. The problem with the Störmer-Cowell methods is that, if \( k > 2 \), the roots \( Z_1 \) and \( Z_2 \) do not lie on the unit circle. No matter how small \( H^2 \) is the orbit grows or shrinks, and the energy error increases linearly with time.

Lambert and Watson (1976) showed that this orbital instability can be avoided if the multistep coefficients are chosen to be symmetric, as in equation (3). A multistep method is said to have an interval of periodicity \((0, H_0^2)\) if for all \( 0 < H < H_0 \) the roots of \( \Omega(Z; H^2) \) satisfy

\[
|Z_1| = |Z_2| = 1, \quad |Z_j| \leq 1 \quad (j = 3, \ldots, k).
\]  

(13)
Lambert and Watson proved that a convergent multistep method with a non-zero interval of periodicity must be a symmetric method and must have an even order. For a symmetric method the ≤ in (3) can be replaced by =, and hence inside the interval of periodicity the roots all lie on the unit circle. The solution (11) of equation (4) is then guaranteed to be periodic (or quasi-periodic).

The requirement that a $k$-step symmetric multistep method have order $k$ (for an explicit method) or $k + 2$ (for an implicit method) does not determine the $\alpha$ and $\beta$ coefficients uniquely when $k > 2$, because for a symmetric method the equations $C_j = 0$ with $j$ odd are not independent of the equations with $j$ even. There are thus some free coefficients that can be chosen by the user, although their range is restricted by the requirement of zero-stability. Lambert and Watson (1976) gave examples of explicit methods with orders 2, 4, and 6, and implicit methods with orders 4, 6, and 8. Quinlan and Tremaine (1990) gave examples of explicit methods with orders 8, 10, 12, and 14. Table 1 lists the coefficients of five explicit methods that will be discussed in what follows. The methods SY8, SY10, and SY12 are the 8th-, 10th-, and 12th-order methods of Quinlan and Tremaine; SY8A and SY8B are 8th-order methods that have not previously been published. Table 2 lists the spurious roots of $\rho(z)$ for these five methods.

| Method | $z = \exp(\pm 2\pi i/n)$ | $\max_{j \neq i} 2n_j n_i$ |
|--------|-------------------------|--------------------------|
| SY8    | $n = 2.500, 5.000, 6.000$ | 60.00                    |
| SY8A   | $n = 2.667, 4.000, 8.000$ | 16.00                    |
| SY8B   | $n = 2.278, 3.353, 4.678$ | 23.67                    |
| SY10   | $n = 2.333, 3.500, 6.000, 7.000$ | 84.00                    |
| SY12   | $n = 2.250, 3.000, 4.500, 6.000, 9.000$ | 36.00                    |

Table 2: Spurious Roots of $\rho(z)$ for the methods in Table 1.

3 Origin of the resonances and instabilities

The origin of the resonances and instabilities will be explained using a Kepler orbit as an example. The resonances and instabilities occur for all nonlinear oscillatory problems, not just for the Kepler problem; other examples will be given later.
3.1 A simple explanation for the instabilities

We start with a simple explanation for the instability that occurs when a circular orbit is integrated with the method SY8 using 60 steps per orbit. The spurious roots of $\rho(z)$ for the method SY8 are located on the unit circle at angles $\pm 4\pi/5$, $\pm 2\pi/5$, and $\pm 2\pi/6$ (i.e., at $\pm 144^\circ$, $\pm 72^\circ$, and $\pm 60^\circ$). At 60 steps per orbit the spurious roots of $\Omega(Z;\omega^2h^2)$ differ little from those of $\rho(z)$; the difference will be ignored here. It is the roots at $2\pi/5$ and $2\pi/6$ (or $-2\pi/5$ and $-2\pi/6$) that cause the trouble. The root at $2\pi/5$ allows a 5-step oscillation: in the absence of any forces, equation (2) admits a solution $x_n = \exp(2\pi in/5)$. Similarly, the root at $2\pi/6$ allows a 6-step oscillation. By themselves the oscillations would be harmless for this problem as long as the start-up routine is accurate. The trouble arises when the 5- and 6-step oscillations can resonate.

Consider first the 5-step oscillation. The perturbations to the $x$ and $y$ coordinates can both oscillate with a 5-step period. If the $y$ oscillation is $90^\circ$ ahead of the $x$ oscillation, the perturbation goes around in a counter-clockwise sense with a 5-step period. Assume that the orbit also moves in a counter-clockwise sense. During one orbital period the perturbation goes around $60/5 = 12$ times. Because the perturbation goes around in the same sense as the orbit, however, the perturbation to the orbital radius completes only $12 - 1 = 11$ oscillations. Now consider the 6-step oscillation. This time assume that the $y$ oscillation is $90^\circ$ behind the $x$ oscillation, so that the perturbation goes around in a clockwise sense with a period of 6 steps. During one orbital period the perturbation goes around $60/6 = 10$ times, but the radial perturbation completes $10 + 1 = 11$ oscillations. This leads to the resonance: the radial perturbations from both the 5-step and 6-step oscillations can go around 11 times in one orbital period. The perturbation analysis given below shows that the resonance causes an instability.

The explanation was verified by checking that the instability can be enhanced by adding noise to the initial conditions with the right frequency and phase. When noise was added with a 5-step component polarized in a counter-clockwise sense and a 6-step component polarized in clockwise sense, the instability became obvious sooner, but when the polarizations were reversed, so that the 5-step component was clockwise and the 6-step component counter-clockwise, the instability was delayed.

The explanation predicts that instabilities will occur for other symmetric multistep methods at stepsizes at which the number of steps per orbit $N$ satisfies

$$\frac{N}{2\pi/\theta_l} + 1 = \frac{N}{2\pi/\theta_j} - 1,$$

where $\exp(i\theta_l)$ and $\exp(i\theta_j)$ are spurious roots of $\rho(z)$. The order of the method must be at least six for an instability of this type to occur, since the polynomial $\rho(z)$ must have at least four spurious roots. According to the prediction the method SY10 of Quinlan and Tremaine should be unstable for circular orbits at 84 steps per orbit, and the method SY12 should be stable as long as the number of steps per orbit is at least 36; both predictions were verified, along with similar predictions for other symmetric multistep methods.

For eccentric Kepler orbits equation (14) must be generalized to allow for the different frequency components present in the motion. The forces in an eccentric Kepler orbit (with unit major axis) can be expanded as (Kovalevsky 1967)

$$\frac{x(t)}{r(t)^3} = \sum_{q=1}^{\infty} q [J_{q+1}(qe) - J_{q-1}(qe)] \cos(q\omega t),$$

$$\frac{y(t)}{r(t)^3} = -\sqrt{1-e^2} \sum_{q=1}^{\infty} q [J_{q+1}(qe) + J_{q-1}(qe)] \sin(q\omega t),$$

considering the perturbations to the $x$ and $y$ coordinates in an eccentric Kepler orbit (with unit major axis) can be expanded as (Kovalevsky 1967)
where the $J_q$ are Bessel functions of the first kind. The forces can be built up from components with frequencies that are integral multiples of the fundamental frequency $\omega$. The “1” on the left-hand side of equation (14) must therefore be allowed to take on the integer values 1, 2, 3, …, corresponding to the fundamental frequency and the higher harmonics, and similarly the “1” on the right-hand side must be allowed to take on the same values, independently of the value assumed on the left-hand side. This leads to the prediction of instabilities at $N = 60, 90, 120, 150$, etc. The width of the instability at small eccentricities (when plotted as in Figure 1) is found to vary with the eccentricity as $\sim e^0$ at $N = 60$, as $\sim e^1$ at $N = 90$, as $\sim e^2$ at $N = 120$, and so on, as expected since the different frequency components have amplitudes that vary as powers of the eccentricity.

3.2 Perturbation analysis for a circular orbit

A perturbation analysis can be used to show that circular orbits are unstable when the condition (14) is satisfied. Consider a circular orbit of radius $R$ in a two-dimensional axisymmetric potential $\phi(r)$. The circular frequency $\omega$ is

$$\omega(r)^2 = \frac{\phi'(r)}{r}. \quad (17)$$

Let $x_n$ and $y_n$ be the $x$ and $y$ coordinates at the $n$th time step. Define $z = x + iy$, $r = |z|$, and write equation (2) as

$$k \sum_{j=0}^{k} \alpha_j z_{n+j} = h^2 \sum_{j=0}^{k} \beta_j F_{n+j}, \quad (18)$$

where the complex force $F$ is

$$F = f_x + if_y = -\frac{z}{r} \phi'(r). \quad (19)$$

Provided that the stepsize $h$ lies within the interval of periodicity, and that the radius is assumed to be fixed, so that equation (18) is linear in $z$, the principal roots $Z_p^{\pm 1}$ (in fact all the roots) of (18) will lie on the unit circle, and the numerical solution will have the form

$$z_n = R Z_p^n, \quad Z_p \simeq e^{i\omega h}, \quad (20)$$

where $Z_p$ is the principal root of $\Omega(Z; \omega^2 h^2)$ corresponding to the assumed counter-clockwise rotation.

Now consider a perturbed circular orbit

$$z_n = R Z_p^n (1 + u_n), \quad (21)$$

where $R Z_p^n u_n$ is a small perturbation at time step $n$. The perturbed radius is

$$R_n = (z_n z_n^*)^{1/2} \simeq R[1 + (u_n + u_n^*)/2], \quad (22)$$

where the * denotes complex conjugation. Substituting (21) into equation (18) and linearizing the resulting equation we find

$$\sum_{j=0}^{k} \alpha_j Z_p^{n+j} u_{n+j} = -h^2 \sum_{j=0}^{k} \beta_j Z_p^j \left(\omega_1 u_{n+j} - \omega_2 u_{n+j}^*\right), \quad (23)$$

where

$$\omega_1 = \frac{1}{2} \left[ \frac{1}{r} \phi'(r) + \phi''(r) \right] = \frac{1}{2} (\kappa^2 - 2\omega^2), \quad (24)$$

$$\omega_2 = \frac{1}{2} \left[ \frac{1}{r} \phi'(r) - \phi''(r) \right] = \frac{1}{2} (4\omega^2 - \kappa^2), \quad (25)$$
and where $\kappa$ is the epicyclic frequency, given by (Binney and Tremaine 1987)

$$\kappa^2(r) = r \frac{d\omega^2}{dr} + 4 \omega^2 = \phi''(r) + \frac{3}{r} \phi'(r).$$

(26)

A trial perturbation of the form

$$u_n = A_1 S^n + A_2 S^{2n}$$

(27)

leads to a solution for $S$ that is independent of the step number $n$ if the following two equations are satisfied:

$$A_1 \sum_{j=0}^{k} \left( \alpha_j Z_p^j S^j + \omega_1 h^2 \beta_j Z_p^j S^j \right) = A_2 \sum_{j=0}^{k} \omega_2 h^2 \beta_j Z_p^j S^j;$$

(28)

$$A_2 \sum_{j=0}^{k} \left( \alpha_j Z_p^j S^{2j} + \omega_1 h^2 \beta_j Z_p^j S^{2j} \right) = A_1 \sum_{j=0}^{k} \omega_2 h^2 \beta_j Z_p^j S^{2j}. $$

(29)

Taking the complex conjugate of the second equation, we get two equations for the two unknowns $A_1$ and $A_2$. The determinant of the system must vanish, which gives (using $H = \omega h$)

$$D(S) = \Omega(SZ_p; H^2)\Omega(S/Z_p; H^2) - \omega_2 h^2 \left[ \Omega(SZ_p; H^2)\sigma(S/Z_p) + \Omega(S/Z_p; H^2)\sigma(SZ_p) \right] = 0.$$

(30)

$D(S)$ is a symmetric polynomial of degree $2k$ in $S$, with real coefficients. There are several things to note about the roots of this polynomial. If $S$ is a root then so are $S^*$, $1/S$, and $1/S^*$. $S = 1$ is always a root, since $\Omega(Z_p; H^2) = \Omega(1/Z_p; H^2) = 0$. The root $S = 1$ corresponds to unperturbed motion, because for this root $A_1 = -A_2^*$ and hence the linearized perturbation to the radius is zero. If $h = 0$ then $D(S) = \rho(S)^2$, whose roots are the same as those of $\rho(z)$, with each root $S_i$ having twice the multiplicity of the corresponding root $z_i$ of $\rho(z)$. Thus when $h = 0$ the spurious roots of $\rho(z)$ (assumed to be distinct) are double roots of $D(S)$, and $S = 1$ is a root of multiplicity four. If $h$ is small but nonzero the roots that were double roots of $D(S)$ when $h = 0$ split, and are approximately $Z_j Z_p^{\pm 1}$ ($j = 3, \ldots, k$), where the $Z_j$ are the spurious roots of $\Omega(Z; H^2)$. The root $S = 1$ is a double root when $h \neq 0$, and two new roots appear at approximately $Z_p^{\pm \kappa/\omega}$, corresponding to the usual epicyclic oscillations with frequency $\omega \pm \kappa$.

As $h$ increases away from 0 the roots of $D(S)$ move around the unit circle as just described. Problems arise, however, near stepsizes where $Z_p^2 Z_l/Z_j = 1$ for some spurious roots $Z_l$ and $Z_j$. When this happens the approximate solutions for two of the roots coincide, $Z_l Z_p = Z_j/Z_p$, and a more careful analysis is needed. The troublesome stepsizes can be estimated by replacing $Z_p$ by $\exp(i\omega h)$ and $Z_l$ and $Z_j$ by the corresponding roots of $\rho(z)$, which we write as $z_l = \exp(i\theta_l)$ and $z_j = \exp(i\theta_j)$. The troublesome stepsizes then occur when

$$\theta_j - \theta_l = 2 \omega h = 4\pi/N,$$

(31)

where $N$ is the number of steps per orbit. This is the instability criterion (4) that was given earlier.

Figure 3 shows the maximum magnitude of the roots of $D(S)$ for the method SY8 used near 60 steps per orbit with a Kepler potential $\phi(r) = -1/r$. The solid line is the exact solution found by numerical calculation of the roots. The dashed line is an approximate solution found by simplifying $D(S)$ by writing

$$\Omega(SZ_p^{\pm 1}; H^2) \simeq \prod_{m=1}^{8} (SZ_p^{\pm 1} - Z_{m,r}),$$

(32)

where the $Z_{m,r}$ are the roots of $\Omega$ at the resonant stepsizes ($N \approx 60.455$), and by replacing $SZ_p$ by $Z_{l,r}$ and $S/Z_p$ by $Z_{j,r}$ everywhere except in the terms $(SZ_p - Z_{l,r})$ and $(S/Z_p - Z_{j,r})$; the same
Figure 3: Maximum value of $|S_i|$ ($i = 1, \ldots, 16$) for the roots of $D(S)$ using the method SY8 with a Kepler potential $\phi(r) = -1/r$. The solid line is the exact result from a numerical calculation of the roots; the long-dashed line is the approximate solution described in the text. The short-dashed line marks the value $N \approx 60.455$ at which $Z_i^2 Z_l/Z_j = 1$ for two of the spurious roots of $\Omega$.

replacements are made in the $\sigma$ functions. We thus obtain from $D(S) = 0$ a quadratic equation in $S$, whose roots are easily found. The exact and approximate solutions both show that there are roots of $D(S)$ that lie off the unit circle when $N$ is in the range 59.2–60.4. The amount by which the roots move off the unit circle depends on the value of $\kappa^2 - 4\omega^2$. For a harmonic oscillator potential
$\phi(r) \sim r^2$ the roots of $D(S)$ do not move off the unit circle, since $\kappa^2 - 4\omega^2 = 0$, and the instability does not occur.

### 3.3 Location of the resonances

The resonances in Figure 1 are easier to predict than the instabilities. Since the force acting on an eccentric Kepler orbit is a superposition of components with frequencies that are integral multiples of the fundamental frequency $\omega$, the resonances occur when the principal root $Z_p \simeq \exp(i\omega h)$ raised to some integral power $q$ coincides with one of the spurious roots $Z_j$, i.e., when

$$N \simeq \frac{2\pi q}{\theta_j}, \quad q = 1, 2, 3, \ldots,$$

(33)

where $z_j = \exp(i\theta_j)$ is a spurious root of $\rho(z)$. This correctly predicts the resonances for the method SY8 at stepnumbers that are multiples of 5 and 6 (and also 2.5, although these resonances are usually too weak to be seen). The amplitude and growth rate of the resonance decrease as $q$ increases, because for small eccentricities the Bessel functions in equations (15) and (16) decrease rapidly with $q$.

### 4 Further examples

Three more examples will be given to show how the resonance and instability locations depend on the multistep method and on the equation being integrated.

#### 4.1 Kepler orbits with a 12th-order symmetric method

The 12th-order symmetric method SY12 is expected to be better than the 8th-order method SY8 for circular Kepler orbits, since the 12th-order method is free of instabilities for these orbits as long as the integration takes at least 36 steps per orbit. This is confirmed in panel (a) of Figure 1 (the energy error of the symmetric method is caused by roundoff error at most stepsizes in this panel). For eccentric orbits, however, the 12th-order method can be as troublesome as the 8th-order method, if not more so, because the extra spurious roots allow more opportunities for resonances and instabilities to occur, and because the spurious root at $2\pi/9$ on the unit circle leads to a resonance that can be excited even at low eccentricities. Panel (b) of Figure 1 shows resonances at stepnumbers that are multiples of 4.5, 6, and 9, and instabilities at stepnumbers that are multiples of 36, although these are not the only instabilities; there are others in the figure, and more would be present if the stepsizes had been sampled more finely.

#### 4.2 Orbits in a logarithmic potential

The Kepler potential is special in that all bound orbits are closed and have $\omega = \kappa$, i.e., the azimuthal period $T_a = 2\pi/\omega$ is equal to the radial period $T_r = 2\pi/\kappa$ (equation (26) gives $\kappa$ for a circular orbit). For most potentials $T_a \neq T_r$, and the analysis given previously must be modified. Consider an eccentric orbit in a logarithmic potential $\phi(r) = \log(r)$, for which (in the limit of a circular orbit) $\kappa = \sqrt{2} \omega$. A Fourier analysis of the motion contains frequencies $\omega + q\kappa$ (where $q$ is an integer), and hence the prediction (33) for the resonant stepsizes must be modified to read

$$N \simeq \frac{2\pi q}{\theta_j} \left(1 + \frac{q\kappa}{\omega}\right) = \frac{2\pi}{\theta_j} \left(1 + \frac{qT_a}{T_r}\right), \quad q = 0, 1, 2, \ldots,$$

(34)
Figure 4: Maximum fractional energy error during integrations of a Kepler orbit for 25000 periods using
the method SY12 (solid lines) and the 12th-order Störmer method (dashed lines) with about 1600 different
stepsizes, plotted as a function of the number of steps per orbit: (a) circular orbit; (b) eccentric orbit ($e = 0.2$).

where $N = T_a/h$ is the number of steps per azimuthal period. This prediction is verified for the
method SY8 in Figure 5, which shows results from integrating an orbit with initial conditions $x_0 = 1,$
$y_0 = 0,$ $x'_0 = 0,$ $y'_0 = 1.1,$ for which $T_a/T_r = 1.41536,$ close to the value $\sqrt{2}$ for a circular orbit (the
stepsizes were not sampled as finely in this figure as in the other figures). There is an instability

Figure 5: Maximum fractional energy error during integrations of an eccentric orbit in a logarithmic potential for 10000 periods with the method SY8, using 500 equally-spaced stepsizes (see text).

at 60 steps per azimuthal period, just as with the Kepler potential, and resonances at the $N$ values predicted by equation (34), taking $\theta_j$ to be $2\pi/5$ (the short dashed lines in Figure 5) or $2\pi/6$ (the long dashed lines).
4.3 The one-dimensional hard spring

As a final example we consider the one-dimensional hard-spring equation

$$x''(t) = -x(t)^3.$$  

(35)

While this is not an orbital equation, the motion is similar to an eccentric orbit in that it is periodic and contains frequencies that are integral multiples of the fundamental frequency, although in this case only the odd multiples are present. Figure 6 shows the errors obtained by integrating this equation with the method SY8. As expected, there are resonances at stepnumbers that are odd multiples of 5 or 6, such as 65, 66, 75, 78, etc.; the even multiples are missing because of the missing frequencies in the motion. There are instabilities at 60 steps per orbit and at integer multiples of this number: 120, 180, etc.; the instabilities at 90, 150, etc., are missing, again because of the missing frequencies.

5 A search for better symmetric methods

A question that naturally arises is whether Quinlan and Tremaine (1990) could have chosen better multistep coefficients to reduce the resonance and instability problems. The answer is yes for the 8th- and 10th-order methods, but probably no for the 12th-order method.

There are three properties that we would like a symmetric multistep method to have:

1. The method should have a large interval of periodicity.
2. To avoid instabilities the spurious roots of $\rho(z)$ should be well spread out on the unit circle.
3. To avoid resonances the spurious roots of $\rho(z)$ should be far from $z = 1$.

Fukushima (1998) has searched for multistep methods with large intervals of periodicity. It is properties 2 and 3 that concern us here. Unfortunately these properties are not compatible: the spurious roots cannot be well spread out on the unit circle and at the same time be far from $z = 1$.

A compromise must be made, which becomes more difficult the more spurious roots there are, i.e., the higher the order of the method.

A systematic search was made through symmetric multistep methods with $\alpha$ coefficients drawn from the set $\{0, \pm 1/8, \pm 2/8, \ldots, \pm 7/8, \pm 1, \pm 2, \pm 4\}$ (with $\alpha_k = 1$). This set was chosen because the integration method suffers less from roundoff error if the $\alpha$'s are integral powers of 2; it is unlikely that much better methods would have been found by letting the $\alpha$'s take on arbitrary values. For each set of coefficients the roots of $\rho(z)$ were computed and checked to see if and where they lie on the unit circle. The most promising methods (based on the three properties given above) were compared in integrations of eccentric Kepler orbits.

Consider first the 8th-order methods. For any even integration order $k$, the choice $1, -2, +2, -2, +2, \ldots$, for the $\alpha$ coefficients spreads the spurious roots on the unit circle as evenly as possible, and tends to minimize the instabilities. That choice was made for the method SY8A listed in Table 1, which has the largest interval of periodicity of the 8th-order methods that were tested. This method is much more stable than the method SY8; the integration results in Figure 7 show no signs of instabilities even for an orbit with an eccentricity $e = 0.3$. The drawback of the method SY8A, however, is the spurious root at $2\pi/8$, or 45°, which leads to resonances (at stepnumbers $N$ that are multiples of 8) that are stronger than for SY8. The method SY8A is certainly an improvement over SY8, but the resonances are annoying.

The resonances can be reduced by picking a method whose spurious roots are farther from $z = 1$. An example is the method SY8B, whose spurious root closest to $z = 1$ is at 76.96°. (It is easy
to find methods whose resonances are weaker than those of SY8B, but these methods have much poorer stability properties.) Figure 6 shows that the resonances are much weaker with this method than with SY8A and SY8: they fall off faster as the number of steps per orbit is increased, being almost unnoticeable when the $e = 0.15$ orbit is integrated with more than 75 steps per orbit, and the

Figure 6: Maximum energy error measured during integrations of the hard-spring equation (35) for 50000 periods starting from the initial conditions $x_0 = 0$ and $x'_0 = 1/\sqrt{2}$, using the method SY8 with 1600 different stepsizes.
Figure 7: Error versus stepsize during integrations of Kepler orbits for 25000 periods with the 8th-order symmetric methods SY8A and SY8B, using 1500 different stepsizes.

$e = 0.30$ orbit with more than 120 steps per orbit. But the price we pay for this gain is a decrease in stability, as revealed by the spikes in the error plot, especially at the higher eccentricity, $e = 0.3$. The instabilities can be avoided if the stepsize is chosen small enough, however, and are not as bad as with the method SY8. The method SY8B is the most promising of the 8th-order methods that were tested.
The search for better 10th- and 12th-order symmetric methods was not as successful. The method SY10 of Quinlan and Tremaine (1990) is unstable at 84 steps per orbit, even for a circular orbit. The method SY10A (like SY8A, with the spurious roots spread out evenly on the unit circle) is much more stable, but has an annoying resonance at stepnumbers \( N \) that are multiples of 10. None of the other 10th-order methods tested was much better than SY10A. For the 12th-order methods none was found to be better than SY12. The method SY12A (again, with the spurious roots spread out evenly on the unit circle) has an annoying resonance at stepnumbers that are multiples of 12, and its stability properties are no better than those of SY12.

Fukushima (1999) has tested some implicit symmetric methods to see if they are affected by the resonance and instability problems as badly as the explicit methods. The disadvantage of implicit symmetric methods is that the corrector step must be applied at least twice for the benefits of the symmetry to be realized, so that for the same stepsize an implicit method requires at least three times the number of force evaluations required by an explicit method. Unless implicit methods can be found with much weaker resonances and instabilities than the explicit methods, this extra work would be better spent using an explicit method with a smaller stepsize.

6 The use of symmetric methods for integrating planetary orbits

The examples considered so far have been chosen for their simplicity and pedagogical value. We now test the method SY12 on a more complex example, typical of those encountered in research problems, to get a better idea of how the method compares with a high-order Størmer method and how its effectiveness is reduced by the resonances and instabilities. The example is the long-term integration of a planetary system, the problem that was the motivation for the high-order symmetric multistep methods of Quinlan and Tremaine (1990), and a research problem on which the method SY12 has been used (the 3 Myr integration of all nine planets by Quinn, Tremaine, and Duncan 1991). We consider an idealized solar system containing only two planets, Jupiter and Saturn, as this is sufficiently complex to suggest how the method will work for a system with more than two planets.

The initial conditions for Jupiter and Saturn are taken from Standish (1990). The initial major axes are \( a_J \approx 5.203 \) AU and \( a_S \approx 19.280 \) AU, giving orbital periods \( P_J \approx 4332.8 \) and \( P_S \approx 30905 \) (in days, the unit of time in this discussion). The initial eccentricities are \( e_J \approx 0.048 \) and \( e_S \approx 0.051 \). The orbits were integrated for 1 Myr using 1000 different stepizes \( h \) spaced equally in \( 1/h \) between \( h = 50 \) and \( h = 81 \), corresponding to approximately 86.6 and 53.5 steps per orbit for Jupiter. To speed the calculations the energy error was measured every 5th integration step, rather than every step. Jupiter’s longitude at the end of the integration was compared with an accurate value determined by an integration with a much smaller stepsize (\( h = 10 \)). The integration errors are plotted versus stepsize in Figure 8.

The two planets were first integrated separately, with no gravitational interaction between them. The maximum energy errors are shown in panel (a). The errors for Saturn in this panel are caused by roundoff error and are not interesting. The Størmer method is unstable if it is used for Jupiter’s orbit with a stepsize larger than \( h \approx 57 \). The symmetric method is stable for Jupiter’s orbit with stepsizes as large as \( h \approx 80 \), although the effects of resonances are seen when the number of steps per orbit is a multiple of 9 (near the \( h \) values 53.5, 60.2, and 68.8, corresponding to 81, 72, and 63 steps per orbit), and also, to a lesser extent, a multiple of 6 (near \( h = 72.2 \), or 60 steps per orbit). The spike in the error near \( h = 80 \) (54 steps per orbit) is an instability, not a resonance, as there is a sudden growth in the error to a large value early in the integration. Away from the resonances the maximum energy error is more than 100 times smaller with the symmetric method than with the Størmer method.
Figure 8: Error versus stepsize for 1 Myr integrations of the Jupiter-Saturn system using the 12th-order symmetric method SY12 (solid lines) and 13th-order Störmer method (dashed lines). The ordinate gives the common logarithm of the error. Panel (a) shows the maximum energy error in the orbits of Jupiter (upper lines) and Saturn (lower lines) when the planets are integrated separately, with no interaction between them. The other three panels include the gravitational attraction between Jupiter and Saturn, and show the maximum (b) and average (c) energy errors during the integration, and (d) the longitude error for Jupiter at the end of the integration.
The planets were then integrated together including their gravitational interaction, in the hope that it might detune the resonances and remove the spikes from the error plot. This is not what happened. Panel (b) shows a profusion of new resonances resulting from the high-frequency perturbation terms in the Jupiter-Saturn interaction. There is still the instability near $h = 80$ that was present for Jupiter alone, plus a narrow instability near $h = 78.55$ that was not present for Jupiter alone, but it is hard to identify the resonances at 60, 63, 72, and 81 steps per Jupiter orbit, as they are lost in the other resonances.

With the symmetric method the maximum energy error away from the resonance peaks is noticeably larger for the Jupiter-Saturn system than for the single-planet (Jupiter) system, whereas for the Störmer method the errors for the two systems are comparable. At first this suggests that the symmetric method is not much better than the Störmer method for the two planet system. But panels (c) and (d) suggest the opposite conclusion. With the symmetric method the average energy error is several orders of magnitude smaller than the maximum error, whereas with the Störmer method the average and maximum errors are comparable. The error in Jupiter’s longitude at the end of the integration is much smaller with the symmetric method than with the Störmer method. Even at the resonance peaks the longitude error is more than an order of magnitude smaller with the symmetric method than with the Störmer method, and away from the resonances the difference is more than three orders of magnitude. The narrowness of the resonances is difficult to appreciate from the figure. Out of the 310 stepsizes that were tested in the range $h = 60–70$, only 16 (or 8) resulted in longitude errors larger than $10^{-5}$ (or $10^{-4}$).

These results show that the maximum energy error can be an unduly strict criterion to use for evaluating the performance of a symmetric method. In a planetary integration the position errors are determined by the average energy error, which for the symmetric methods is much smaller than the maximum error. The maximum error is important for calculations of instantaneous orbital elements that depend on the velocity, such as the major axis, eccentricity, and inclination. In the 3 Myr integration of the solar system by Quinn et al. (1991) these elements were digitally filtered to remove oscillations with periods smaller than 500 yr; the filtering probably removed any spurious oscillations caused by the symmetric method, and the errors in the output elements were probably closer to the average errors than to the maximum errors. The comparison that Quinn et al. made of their results with the results of a shorter but more accurate Störmer integration (with a smaller stepsize) showed satisfactory agreement.

Despite the resonances and instabilities, then, symmetric methods can still be a better choice than Störmer methods for long integrations of planetary orbits provided that the user is aware of the dangers.

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