SIAM J. NUMER. ANAL.
Vol. 38, No. 1, pp. 129–148

NONLINEAR STABILITY ANALYSIS OF AREA-PRESERVING INTEGRATORS*

ROBERT D. SKEEL† AND K. SRINIVAS‡

Abstract. Linear stability analysis is inadequate for integrators designed for nondissipative systems such as Hamiltonian systems in which nonlinear effects are often decisive. Mathematical theory exists (KAM theory) for rigorous analysis of small perturbations from equilibria, but it needs to be expressed in a form that is more easily applicable to the study of area-preserving maps. We have pursued this, obtaining a completely rigorous nonlinear stability analysis for elliptic equilibria based on the Moser twist theorem and a result of Cabral and Meyer [*Nonlinearity*, 12 (1999), pp. 1351–1362], together with the theory of normal forms for Hamiltonian systems. The result is a determination of necessary and sufficient conditions for stability. These conditions are sharpened for the case of reversible maps and applied to the symplectic members of the Newmark family of integrators, which includes the leapfrog, the implicit midpoint, and the Störmer–Cowell methods. Nonlinear stability limits are more severe than those of linear theory. As an example, the leapfrog scheme actually has a step-size limitation of 71% of that predicted by linear analysis.

Key words. symplectic, stability, nonlinear, Hamiltonian, twist map, integrator

AMS subject classifications. 65L20, 39A11

PII. S0036142998349527

1. Introduction.

The application of a numerical integrator to a dynamical system can introduce spurious instabilities. For most systems these can be explained by means of a linearized analysis. However, for a neutrally stable dynamical system integrated by a scheme that does not introduce artificial damping, a linearized analysis is usually indeterminate. Limited nonlinear analysis is possible: mathematical theory exists for analyzing rigorously small perturbations from equilibria for a single second order ordinary differential equation (ODE). Instabilities in this situation arise from resonance artifacts due to the integration step size being one-third or one-quarter, or—rarely—some other rational fraction, of the period of a normal mode of the discrete dynamics [9]. That these instabilities are relevant to large multidimensional simulations far from dynamical equilibrium is shown in [15]. Resonance artifacts might also explain instabilities observed for the implicit midpoint rule in structural mechanics simulations [18]. In this paper we outline a rigorous and nearly complete nonlinear stability analysis for elliptic equilibria, which is based on the Moser twist theorem [11] and a theorem of Cabral and Meyer [6]. The result is a determination of necessary and sufficient conditions for stability, including the case of third and fourth order resonance, which is readily applicable to the study of symplectic integrators. These conditions are sharpened for the case of reversible symplectic integrators. Limits on step size imposed by nonlinear stability are more severe than those imposed by linear stability. As an example, the leapfrog scheme actually has a step-size limitation of 71% of that predicted by linear analysis. It is envisioned that this analysis will offer (i) advice in the choice of a step size for an existing integrator and (ii) guidance for

*Received by the editors December 21, 1998; accepted for publication (in revised form) December 10, 1999; published electronically June 20, 2000. This work was supported in part by NSF grants DMS-9600088/9971830, NSF grant BIR-9318159, and NIH grant P41RR05969.

http://www.siam.org/journals/sinum/38-1/34952.html

†Department of Computer Science (and Beckman Institute), University of Illinois, Urbana, IL 61801-2987 (skeel@uiuc.edu).

‡Microsoft Corporation, One Microsoft Way, Redmond, WA 98052 (ksrini@microsoft.com).

the construction of integrators that can take longer step sizes.

An early nonlinear stability analysis appears in [14], where the Moser twist theorem is used to show stability for small enough step sizes for the leapfrog scheme applied to pendulum dynamics. Later work [13] showed stability under the assumption that the step size is not equal to one-third or one-quarter of the period of the discrete map. Also interesting is the article [10], which shows that a stable resonance produces an oscillation with an amplitude that depends on the order of the resonance.

Not all nonlinear instabilities are due to resonances, e.g., [7, 3]. And in the case of molecular dynamics, it seems that discontinuous approximations such as truncated multipole expansions can produce instability [5].

In section 2 we consider a general area-preserving (and hence two-dimensional) map $y_{n+1} = M(y_n)$ which has a fixed point $y^* = M(y^*)$. The map M is said to be stable at equilibrium y^* if for any $\epsilon > 0$ there exists $\delta > 0$ such that

$$\|y_0 - y^*\| < \delta \quad \Rightarrow \quad \|y_n - y^*\| < \epsilon \quad \text{for} \quad n = 0, 1, 2, \dots, \tag{1.1}$$

where y_n, $n = 0, 1, 2, \dots$ are the successive iterates. We write the recurrence in abbreviated style as

$$y_1 = M(y). \tag{1.2}$$

Linearized stability analysis imposes the following requirement on the Jacobian matrix of the map at the equilibrium point:

$$M'(y^*) \text{ is similar to } \mathrm{diag}(\lambda, \bar{\lambda}) \text{ for some } \lambda = \mathrm{e}^{\mathrm{i}\phi}. \tag{1.3}$$

If, in addition, $\lambda \neq \pm 1$, we call y^* an *elliptic* fixed point. Resonance of order r occurs if $\lambda^r = 1$. We change to a representation in terms of complex variables,

$$y = \left(\frac{z + \bar{z}}{2}, \frac{z - \bar{z}}{2\mathrm{i}} \right), \tag{1.4}$$

and transform the map to a simpler form using the theory of normal forms for Hamiltonian systems. This changes the map $z_1 = M_{\mathrm{z}}(z, \bar{z})$ to one of the following three forms:

$$\lambda^3 = 1 : z_1 = \lambda(z + c_{02}\bar{z}^2 + O(|z|^3)), \tag{1.5}$$
$$\lambda^4 = 1 : z_1 = \lambda(z + c'_{21}z^2\bar{z} + c'_{03}\bar{z}^3 + O(|z|^4)), \tag{1.6}$$
$$z_1 = \lambda(z + c'_{21}z^2\bar{z} + O(|z|^4)). \tag{1.7}$$

The resulting map is used in section 3 to demonstrate instability under certain conditions and to prove stability under other conditions. Instability in the case of $\lambda = 1$ can be determined using the Cabral–Meyer result [6] given in section 3. We do not consider this case because it does not occur for the Newmark family of integrators we analyze in section 5.

In section 3 we show instability in the following cases:

$$\lambda^3 = 1 : \qquad c_{02} \neq 0, \tag{1.8}$$
$$\lambda^4 = 1 : \qquad |c'_{03}| > |c'_{21}|. \tag{1.9}$$

In the same section we obtain sufficient conditions for stability at elliptic equilibria using the Moser twist theorem, together with a sharpened result of Cabral and

Meyer [6] to justify neglect of higher order terms. We show stability in the following cases:

$$\lambda^3 = 1: \qquad c_{02} = 0 \text{ and } c'_{21} \neq 0, \tag{1.10}$$

$$\lambda^4 = 1: \qquad |c'_{03}| < |c'_{21}|, \tag{1.11}$$

$$\lambda^3 \neq 1, \lambda^4 \neq 1: \qquad c_{02} \neq 0. \tag{1.12}$$

The other cases not covered by the theorems are very special in the sense that at least two equality conditions must hold. This is discussed further in section 3.

In practice the instabilities are most important for their implications when λ is close to satisfying an unstable resonance condition. What happens then is that the stability basin around the equilibrium point is small, or more specifically, the δ in the definition of stability is small [1, p. 392].

The analysis has several limitations; for example, it is restricted to some neighborhood of an equilibrium, and it applies only to two-dimensional maps. Hence, we can depend on it only to give *necessary* conditions for stability, which are, of course, still very useful. At the same time, the stability results generalize somewhat to higher dimensional maps in the form of KAM theory [1, p. 411]. Consider a $2d$-dimensional symplectic map whose Jacobian matrix at equilibrium is diagonalizable with eigenvalues λ_1, $\bar{\lambda}_1$, λ_2, $\bar{\lambda}_2$, $\ldots$, λ_d, $\bar{\lambda}_d$ all of unit modulus. If there are integers r_1, r_2, $\ldots$, r_d such that

$$\lambda_1^{r_1}\lambda_2^{r_2}\cdots\lambda_d^{r_d} = 1, \tag{1.13}$$

we have resonance of order $r = r_1 + r_2 + \cdots + r_d$. Unfortunately, instability is possible in higher dimensions, even if unstable resonances are avoided, through a phenomenon known as Arnol'd diffusion. A third limitation of the analysis is neglect of the effects of finite precision. It is shown in [19] that with minor adjustments in the implementation of the integrator the symplectic property is preserved in floating-point arithmetic; the effect on stability may be equally benign.

The detailed stability conditions simplify considerably if we restrict ourselves to a "reversible" area-preserving map with a fixed point $y^* = (q^*, 0)$. The map (1.2) is reversible if $RM(RM(y)) = y$ where $R = \operatorname{diag}(1, -1)$. These simplified conditions are obtained in section 4.

In section 5 these conditions are applied to the symplectic members [20] of the Newmark family of numerical integrators [12]. This is a one-parameter family of integrators for Hamiltonian systems, and it includes the leapfrog/Störmer/Verlet, Störmer-Cowell/Numerov, and implicit midpoint/trapezoid methods. We consider a Hamiltonian system with Hamiltonian

$$H(q,p) = \frac{1}{2}p^2 + V(q), \tag{1.14}$$

where we assume unit mass for simplicity and potential energy function

$$V(q) = \frac{1}{2}\omega^2 q^2 + \frac{1}{3}Bq^3 + \frac{1}{4}Cq^4 + O(q^5), \tag{1.15}$$

where $\omega > 0$. The family of symplectic integrators depending on the parameter α is defined as follows:

$$q_{n+1/2} = q_n + \frac{h}{2}p_n, \tag{1.16}$$

$$F_{n+1/2} = -V'(q_{n+1/2} + \alpha h^2 F_{n+1/2}), \tag{1.17}$$
$$p_{n+1} = p_n + hF_{n+1/2}, \tag{1.18}$$
$$q_{n+1} = q_{n+1/2} + \frac{h}{2} p_{n+1}, \tag{1.19}$$

where h is the step size. Resonance of order 3 and 4 occurs for a step size h_3 and h_4, respectively, given by

$$h_3 = \frac{1}{\omega}\sqrt{3/(1-3\alpha)}, \qquad h_4 = \frac{1}{\omega}\sqrt{2/(1-2\alpha)} \tag{1.20}$$

if $\alpha < \frac{1}{3}$, $\alpha < \frac{1}{2}$, respectively. Theorem 5.1 determines the stability of the integrator for the two cases of resonance given below:

(1) for $h = h_3$ (third order resonance):
   (a) If $B = 0$ and $C \neq 0$, the integrator is stable at equilibrium.
   (b) If $B \neq 0$, the integrator is not stable at equilibrium.

(2) for $h = h_4$ (fourth order resonance):
   (a) If $(\omega^2 C - 4\alpha B^2)(\omega^2 C - 2B^2) > 0$, the integrator is stable at equilibrium.
   (b) If $(\omega^2 C - 4\alpha B^2)(\omega^2 C - 2B^2) < 0$, the integrator is not stable at equilibrium.

The choice $\alpha = \frac{1}{2}$, which is the method LIM2 [21], avoids resonances of orders 3 and 4. The choice $\alpha = \frac{1}{3}$, which is the method EW [20], avoids the generally unstable resonance of order 3. As examples, the analysis is applied to the case of a Morse oscillator and a Lennard–Jones potential. The fourth order resonance is stable in the case of the Morse oscillator if $\alpha > \frac{7}{54}$ and is stable for the Lennard–Jones oscillator if $\alpha > \frac{106}{567}$. These conditions are independent of the parameters of the oscillator. For both potentials the implicit midpoint method ($\alpha = \frac{1}{4}$) is stable for fourth order resonances but the Störmer–Cowell method ($\alpha = \frac{1}{12}$) is not. This is consistent with the experimental findings in [15].

Precise statements of the results are given in the remainder of the paper. Most of the proofs are separated from the statements of the results making the proofs easy to avoid.

2. Reduction of a map to a normal form.

The objective is to analyze the stability of the area-preserving map (1.2) at a fixed point $y^* = M(y^*)$. The map is assumed to be real analytic in some neighborhood of y^*. The first part of the analysis is to construct symplectic transformations $y = T(Y)$ which are invertible and real analytic in a neighborhood of the fixed point and which simplify the form of the map. The transformed map retains both the area-preserving and stability properties of the original map M, but its simpler form facilitates stability analysis. The area-preserving property implies that $|\det M'(y)| \equiv 1$. We will assume that

$$\det M'(y) \equiv 1, \tag{2.1}$$

which is the case for an area-preserving integrator that is consistent and depends continuously on the step size. If not, we can consider instead the sequence $(q_n, (-1)^n p_n)$. In two dimensions a map M is *symplectic* if it satisfies (2.1). For certain facts relating to symplectic transformations, the reader is referred to [1, Chapter 9],[8, Chapter 7].

Note. The Moser twist theorem, which we invoke to prove stability, actually requires only that the map possess the following intersection property: if Γ is a nearly circular closed curve around the equilibrium point, then its image curve $M(\Gamma)$ must intersect itself. This property is satisfied by an area-preserving map (and by a reversible map [4]). To preserve this property, it would be sufficient to use transformations T that are merely real analytic. However, it is not a significant encumbrance to make use only of symplectic transformations T, and it serves to limit the number of free parameters in the maps. Also, many versions of the twist theorem do not require the map to be analytic but only to be C^ℓ for some $\ell > 3$.

First and foremost, the map will not be stable at equilibrium unless the Jacobian matrix $M'(y^*)$ is power-bounded. Property (2.1) implies that the product of the eigenvalues is 1. Hence, the linear stability requirement is violated unless both roots are of unit modulus, and the equilibrium will be stable only if $M'(y^*)$ is similar to $\mathrm{diag}(\lambda, \bar{\lambda})$ for some $|\lambda| = 1$. Henceforth, assume that $M'(y^*)$ is similar to $\mathrm{diag}(\lambda, \bar{\lambda})$ for some $\lambda = \mathrm{e}^{\mathrm{i}\phi}$.

The first step of the reduction to normal form is to reduce the constant and linear part of the mapping to a pure rotation. The matrix $\mathrm{diag}(\lambda, \bar{\lambda})$ is similar to

$$\begin{bmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{bmatrix}. \tag{2.2}$$

Therefore, there exists a nonsingular matrix X such that

$$X^{-1}M'(y^*)X = \begin{bmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{bmatrix}. \tag{2.3}$$

The matrix X can be scaled so that $|\det X| = 1$. Perform the area-preserving affine transformation $y = y^* + XY$, and the map (1.2) becomes

$$Y_1 = X^{-1}(M(y^* + XY) - y^*) \tag{2.4}$$

$$= \begin{bmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{bmatrix} Y + O(\|Y\|^2). \tag{2.5}$$

For algebraic convenience [1, p. 391] we introduce a complex variable z by writing

$$Y = \left(\frac{z+\bar{z}}{2}, \frac{z-\bar{z}}{2\mathrm{i}}\right) \tag{2.6}$$

and the map takes the form

$$z_1 = \lambda z + \lambda \sum_{N=2}^{\infty} \sum_{m=0}^{N} c_{m,N-m} z^m \bar{z}^{N-m}. \tag{2.7}$$

LEMMA 2.1. *Let $N \geq 2$. Then*

$$z_1 = \lambda z + \lambda \sum_{m=0}^{N} c_m z^m \bar{z}^{N-m} + O(|z|^{N+1}) \tag{2.8}$$

is a symplectic map only if the coefficients c_m satisfy

$$m c_m + (N+1-m)\bar{c}_{N+1-m} = 0, \qquad m = 1, 2, \ldots, N. \tag{2.9}$$

Proof. Let

$$M_z(z, \bar{z}) = \lambda z + \lambda q_N(z, \bar{z}) + O(|z|^{N+1}), \tag{2.10}$$

where

$$q_N(z,\bar z) = \sum_{m=0}^{N} c_m z^m \bar z^{N-m}. \tag{2.11}$$

It is straightforward to show that being symplectic is equivalent to

$$|\partial_1 M_{\rm z}(z,\bar z)|^2 - |\partial_2 M_{\rm z}(z,\bar z)|^2 = 1. \tag{2.12}$$

For the assumed form of $M_{\rm z}(z,\bar z)$ this reduces to

$$\partial_1 q_N(z,\bar z) + \overline{\partial_1 q_N(z,\bar z)} = 0, \tag{2.13}$$

which becomes

$$\sum_{m=1}^{N} (mc_m + (N+1-m)\bar c_{N+1-m}) z^{m-1}\bar z^{N-m} = 0, \tag{2.14}$$

from which we conclude (2.9). ∎

A consequence of the lemma is that the map takes the slightly more special form

$$z_1 = \lambda z + \lambda(c_{20}z^2 - 2\bar c_{20} z\bar z + c_{02}\bar z^2) + \lambda \sum_{N=3}^{\infty}\sum_{m=0}^{N} c_{m,N-m} z^m \bar z^{N-m}. \tag{2.15}$$

LEMMA 2.2. *Let $N \ge 2$, and let σ_m, $m = 0, 1, \ldots, N$, be complex numbers satisfying*

$$m\sigma_m + (N+1-m)\bar\sigma_{N+1-m} = 0, \qquad m = 1, 2, \ldots, N. \tag{2.16}$$

Then there exists an analytic symplectic transformation $(q,p) \mapsto (Q,P)$ of the form

$$z = Z + \sum_{m=0}^{N} \sigma_m Z^m \bar Z^{N-m} + O(|Z|^{N+1}), \tag{2.17}$$

where $z = q + \mathrm{i}p$ and $Z = Q + \mathrm{i}P$.

Proof. Let $s_m := \sigma_m/(2\mathrm{i}(N+1-m))$, $m = 0, 1, \ldots, N$, and let $s_{N+1} := \bar s_0$. From the relation $\bar s_m = s_{N+1-m}$ it follows that

$$S(Q,P) := \sum_{m=0}^{N+1} s_m Z^m \bar Z^{N+1-m} \tag{2.18}$$

is a real function of Q and P. An analytic symplectic transformation can be defined by using $qP + S(q,P)$ as a generating function of the second kind. It is well known (and is straightforward to verify) that the following implicitly defined transformation from (q,p) to (Q,P) is symplectic:

$$Q = q + \partial_2 S(q,P), \tag{2.19}$$

$$p = P + \partial_1 S(q,P). \tag{2.20}$$

The explicit form is

$$q = Q - \partial_2 S(Q,P) + O(|Z|^{2N-1}), \tag{2.21}$$

$$p = P + \partial_1 S(Q,P) + O(|Z|^{2N-1}). \tag{2.22}$$

In complex form

$$q + \mathrm{i}p = Q + \mathrm{i}P + (-\partial_P + \mathrm{i}\partial_Q) \sum_{m=0}^{N+1} s_m (Q + \mathrm{i}P)^m (Q - \mathrm{i}P)^{N+1-m} + O(|Z|^{N+1}) \tag{2.23}$$

$$= Q + \mathrm{i}P + 2\mathrm{i} \sum_{m=0}^{N} s_m (N + 1 - m)(Q + \mathrm{i}P)^m (Q - \mathrm{i}P)^{N-m} + O(|Z|^{N+1}). \tag{2.24}$$ ∎

Next a lemma follows, which we use for transforming a map.

LEMMA 2.3. *Let $N \geq 2$. Let M_{z} be the map*

$$z_1 = \lambda(z + q_N(z, \bar{z}) + s_{N+1}(z, \bar{z})), \tag{2.25}$$

where q_N is a homogeneous polynomial of degree N and $s_{N+1}(z, \bar{z}) = O(|z|^{N+1})$ and let T_{N+1} be a transformation

$$z = Z + r_N(Z, \bar{Z}) + t_{N+1}(Z, \bar{Z}), \tag{2.26}$$

where r_N is a homogeneous polynomial of degree N and $t_{N+1}(Z, \bar{Z}) = O(|Z|^{N+1})$. Then the map M_{z} under the transformation T_{N+1} transforms to a map of the following form:

$$Z_1 = \lambda(Z + r_N(Z, \bar{Z}) - \bar{\lambda} r_N(\lambda Z, \bar{\lambda}\bar{Z}) + q_N(Z, \bar{Z}) + O(|Z|^{N+1})). \tag{2.27}$$

If the terms of degree N vanish, then the transformed map is

$$\begin{aligned} Z_1 = \lambda(Z &+ \partial_1 q_N(Z, \bar{Z}) r_N(Z, \bar{Z}) + \partial_2 q_N(Z, \bar{Z}) \overline{r_N(Z, \bar{Z})} \\ &+ s_{N+1}(Z, \bar{Z}) + t_{N+1}(Z, \bar{Z}) - \bar{\lambda} t_{N+1}(\lambda Z, \bar{\lambda}\bar{Z}) + O(|Z|^{2N})). \end{aligned} \tag{2.28}$$

Proof. Substituting the transformation T_{N+1} into M_{z} we get

$$\begin{aligned} Z_1 + r_N(Z_1, \bar{Z}_1) + t_{N+1}(Z_1, \bar{Z}_1) = \lambda(Z &+ r_N(Z, \bar{Z}) + t_{N+1}(Z, \bar{Z}) \\ &+ q_N(Z + r_N(Z, \bar{Z}), \bar{Z} + \overline{r_N(Z, \bar{Z})}) \\ &+ s_{N+1}(Z, \bar{Z}) + O(|Z|^{2N})). \end{aligned} \tag{2.29}$$

This implies $Z_1 = \lambda Z + O(|Z|^N)$, whence

$$Z_1 + r_N(\lambda Z, \bar{\lambda}\bar{Z}) = \lambda(Z + r_N(Z, \bar{Z}) + q_N(Z, \bar{Z}) + O(|Z|^{N+1})). \tag{2.30}$$

If the terms of degree N vanish, we have

$$Z_1 = \lambda Z + O(|Z|^{N+1}). \tag{2.31}$$

Substituting this into (2.29), expanding $q_N(\ldots, \ldots)$, and using again the vanishing of terms of degree N gives the stated result. ∎

The following theorem [2, p. 306]. is useful for reducing a map to a normal form.

THEOREM 2.4. *Let $z_1 = M_{\mathrm{z}}(z, \bar{z})$ be a symplectic map where*

$$M_{\mathrm{z}}(z, \bar{z}) = \lambda \left(z + \sum_{m=0}^{N} c_m z^m \bar{z}^{N-m} + O(|z|^{N+1}) \right). \tag{2.32}$$

Then there is a symplectic transformation

$$z = Z + \sum_{m=0}^{N} \sigma_m Z^m \bar{Z}^{N-m} + O(|Z|^{N+1}) \tag{2.33}$$

that zeros coefficients of all terms $c_m Z^m \bar{Z}^{N-m}$ *with the following exceptions:*

(1) *the term* $c_{(N+1)/2} Z^{(N+1)/2} \bar{Z}^{(N-1)/2}$ *if* N *is odd, and*

(2) *those terms* $c_m Z^m \bar{Z}^{N-m}$ *where* $(2m - N - 1)/r$ *is a nonzero integer if* $\lambda^r = 1$ *(resonance of order* r*). These terms* $c_m Z^m \bar{Z}^{N-m}$ *are called resonant terms of order* r.

The coefficients of any exceptional terms are left unchanged. Moreover, $\sigma_m = 0$ *for* m *such that* $\lambda^{2m-N-1} = 1$ *and otherwise*

$$\sigma_m = -\frac{c_m}{1 - \lambda^{2m-N-1}}. \tag{2.34}$$

Proof. From Lemma 2.1 the coefficients c_m satisfy

$$m c_m + (N + 1 - m)\bar{c}_{N+1-m} = 0, \qquad m = 1, 2, \ldots, N. \tag{2.35}$$

From this it can be shown that the given choice for $\sigma_m = 0$ satisfies $m\sigma_m + (N + 1 - m)\bar{\sigma}_{N+1-m} = 0$, $m = 1, 2, \ldots, N$, so by Lemma 2.2 there exists a suitable symplectic transformation. Then by the use of Lemma 2.3 with

$$r_N(Z, \bar{Z}) = \sum_{m=0}^{N} \sigma_m Z^m \bar{Z}^{N-m} \tag{2.36}$$

and

$$q_N(z, \bar{z}) = \sum_{m=0}^{N} c_m z^m \bar{z}^{N-m}, \tag{2.37}$$

we get

$$Z_1 = \lambda \left(Z + \sum_{m=0}^{N} \left(c_m + \sigma_m(1 - \lambda^{2m-N-1})\right) Z^m \bar{Z}^{N-m} + O(|Z|^{N+1}) \right). \qquad \square \tag{2.38}$$

For $N = 2$ in Theorem 2.4, only third order resonance is possible, with resonant term $\bar{Z}^2$. For $N = 3$, only fourth order resonance is possible, with resonant term $\bar{Z}^3$.

The following result will be useful in the next section for proving instability in the case $\lambda^3 = 1$.

THEOREM 2.5. *If* $\lambda \neq 1$, *there exists a symplectic transformation of map* (2.7) *such that the transformed map satisfies*

$$Z_1 = \lambda(Z + c_{02}\bar{Z}^2 + O(|Z|^3)). \tag{2.39}$$

Proof. Use Theorem 2.4 to eliminate all terms other than third order resonant terms. $\square$

The following result will be useful in the two next sections for all other cases.

THEOREM 2.6. *If* $\lambda^3 \neq 1$ *or if* $c_{02} = 0$ *and* $\lambda \neq 1$, *there exists a symplectic transformation of map* (2.7) *such that the transformed map satisfies*

$$Z_1 = \lambda(Z + c'_{21} Z^2 \bar{Z} + \mathrm{i}|c'_{03}|\bar{Z}^3 + O(|Z|^4)), \tag{2.40}$$

where

$$c'_{21} = \begin{cases} c_{21} + \dfrac{4|c_{20}|^2}{1-\lambda^{-1}} - \dfrac{2|c_{20}|^2}{1-\lambda} - \dfrac{2|c_{02}|^2}{1-\lambda^3}, & \lambda^3 \neq 1, \\ c_{21} + \dfrac{4|c_{20}|^2}{1-\lambda^{-1}} - \dfrac{2|c_{20}|^2}{1-\lambda}, & \lambda^3 = 1, c_{02} = 0 \end{cases} \tag{2.41}$$

and

$$c'_{03} = \begin{cases} 0, & \lambda^4 \neq 1, \\ c_{03} + \dfrac{2\bar{c}_{20}c_{02}}{1-\lambda^{-3}} - \dfrac{2\bar{c}_{20}c_{02}}{1-\lambda^{-1}}, & \lambda^4 = 1. \end{cases} \tag{2.42}$$

Moreover, $c'_{21} = \mathrm{i}F$ *for some real number* F.

Proof. Express the map given by (2.7) as $z_1 = \lambda(z + q_2(z,\bar{z}) + s_3(z,\bar{z}))$ where $q_2(z,\bar{z}) = c_{20}z^2 + c_{11}z\bar{z} + c_{02}\bar{z}^2$ and $s_3(z,\bar{z})$ is the $O(|z|^3)$ part. Let T_3 be a symplectic transformation given by Theorem 2.4 that eliminates all quadratic terms in this map. For $\lambda^3 \neq 1$ the symplectic transformation T_3 can be expressed as

$$z = Z + r_2(Z,\bar{Z}) + t_3(Z,\bar{Z}), \tag{2.43}$$

where

$$r_2(Z,\bar{Z}) = -\frac{c_{20}Z^2}{1-\lambda} - \frac{c_{11}Z\bar{Z}}{1-\lambda^{-1}} - \frac{c_{02}\bar{Z}^2}{1-\lambda^{-3}} \tag{2.44}$$

and $t_3(Z,\bar{Z})$ is the $O(|Z|^3)$ part of T_3. Applying Lemma 2.3, we obtain

$$\begin{aligned} Z_1 = \lambda(Z &+ (2c_{20}Z + c_{11}\bar{Z})r_2(Z,\bar{Z}) + (c_{11}Z + 2c_{02}\bar{Z})\overline{r_2(Z,\bar{Z})} \\ &+ s_3(Z,\bar{Z}) + t_3(Z,\bar{Z}) - \bar{\lambda}t_3(\lambda Z, \bar{\lambda}\bar{Z}) + O(|Z|^4)). \end{aligned} \tag{2.45}$$

The coefficient of the $Z^2\bar{Z}$ term is

$$c'_{21} = -\frac{2c_{11}c_{20}}{1-\lambda^{-1}} - \frac{c_{11}c_{20}}{1-\lambda} - \frac{c_{11}\bar{c}_{11}}{1-\lambda} - \frac{2c_{02}\bar{c}_{02}}{1-\lambda^3} + c_{21}. \tag{2.46}$$

This simplifies to the expression given by (2.41) due to the relation $c_{11} = -2\bar{c}_{20}$ arising from the symplectic property (2.9). The forgoing also holds for $\lambda^3 = 1$, but $c_{02} \neq 0$ if we omit the last term from the choice of $r_2(Z,\bar{Z})$. With the quadratic terms removed we turn our attention to the cubic terms. If $\lambda^4 \neq 1$, we perform a symplectic transformation to wipe out all cubic terms other than the $Z^2\bar{Z}$ term to obtain the normal form of the map given by Theorem 2.4. If $\lambda^4 = 1$, we perform a symplectic transformation that retains both the $Z^2\bar{Z}$ and $\bar{Z}^3$ terms. A simple calculation shows that the $Z^2\bar{Z}$ and $\bar{Z}^3$ terms are absent from

$$t_3(Z,\bar{Z}) - \bar{\lambda}t_3(\lambda Z, \bar{\lambda}\bar{Z}). \tag{2.47}$$

This implies that the $\bar{Z}^3$ term has coefficient

$$c'_{03} = -\frac{c_{11}c_{02}}{1-\lambda^{-3}} - \frac{2c_{02}\bar{c}_{20}}{1-\lambda^{-1}} + c_{03}, \tag{2.48}$$

which simplifies to the expression given by (2.42) again due to the relation $c_{11} = -2\bar{c}_{20}$. We write $c'_{03} = \mathrm{i}G\mathrm{e}^{\mathrm{i}\gamma}$ where G is real. Equation (2.40) follows by performing the symplectic transformation $Z = \mathrm{e}^{\mathrm{i}\gamma/4}w$ and changing w back to Z. Finally, in all cases the symplecticness of the transformed map (2.40) and property (2.9) of symplectic maps implies that c'_{21} is a pure imaginary number. ∎

3. Determining stability and instability of a map. Stability for the general case is addressed by the following result.

THEOREM 3.1 (Moser). *Let $N \geq 3$ be an odd integer. A real analytic area-preserving map of the form*

$$Z_1 = \lambda Z(1 + \mathrm{i}F|Z|^{N-1} + O(|Z|^N)), \tag{3.1}$$

$\lambda = \mathrm{e}^{\mathrm{i}\phi}$, *is stable at $Z = 0$ if $\lambda^k \neq 1$ for $k = 1, 2, \dots, N+1$ and if F is real and nonzero.*

Proof. This is a variation of Theorem 2.13 of [11, p. 56], in which we have chosen N to be such that $\alpha_1 = \alpha_2 = \cdots = \alpha_{(N-3)/2} = 0$ and have chosen $q = N+1$. See also [6, p. 1355]. ∎

To prove stability for cases of low order resonance, we need a stronger result.

THEOREM 3.2 (Cabral–Meyer). *Consider a real analytic area-preserving map of the form*

$$Z_1 = \lambda Z(1 + (rf'(r\theta) - \mathrm{i}(N+1)f(r\theta))|Z|^{N-1} + O(|Z|^N)), \qquad Z = |Z|\mathrm{e}^{\mathrm{i}\theta}, \tag{3.2}$$

where $\lambda = \mathrm{e}^{\mathrm{i}\phi}$, $\lambda^k \neq 1$ for $k = 1, 2, \dots, r-1$, $\lambda^r = 1$, $N \geq 2$, and $f(\cdot)$ is a real 2π-periodic trigonometric polynomial. Then

(1) *if f is never zero, the fixed point is stable;*

(2) *if f has a simple zero, the fixed point is unstable.*

Proof. This is a restatement of Corollary 3.1 in [6, p. 1355], which uses symplectic polar coordinates $Z = \sqrt{2I}\exp(\mathrm{i}\theta)$. Transforming map (3.2) to such coordinates gives

$$\sqrt{2I_1}\mathrm{e}^{\mathrm{i}\theta_1} = \sqrt{2I}\mathrm{e}^{\mathrm{i}(\theta+\phi)}(1 + (rf'(r\theta) - \mathrm{i}(N+1)f(r\theta))(2I)^{(N-1)/2} + O(I^{N/2})), \tag{3.3}$$

whence

$$I_1 = I + 2^{(N+1)/2} rf'(r\theta) I^{(N+1)/2} + O(I^{(N+2)/2}), \tag{3.4}$$

$$\theta_1 = \theta + \phi - (N+1)2^{(N-1)/2} f(r\theta) I^{(N-1)/2} + O(I^{N/2}). \tag{3.5}$$

The stated theorem follows by applying Corollary 3.1 in [6, p. 1355] with $\Psi(\cdot) = 2^{(N+1)/2} f(\cdot)$, $b = r$, $2\pi a/b = \phi$, and $m = (N+1)/2$. ∎

Remarks. In the important case when f is a nonzero constant, the Cabral–Meyer result overlaps with Theorem 3.1. The Cabral–Meyer result does not address the case where all zeros of f have multiplicity > 1.

The special form that is assumed for the degree N terms of map (3.2) is a consequence of the area-preserving property (see Lemma 2.1). The fact that these terms can be made to be $2\pi/r$-periodic is a consequence of Theorem 2.4.

THEOREM 3.3. *Let c'_{03} and F be defined as in Theorem 2.6 when appropriate.*

(1) *For $\lambda^3 = 1$, $\lambda \neq 1$ (third order resonance) the map (2.7)*

  (a) *is stable at equilibrium if $c_{02} = 0$ and $F \neq 0$,*

  (b) *is not stable at equilibrium if $c_{02} \neq 0$.*

(2) *For $\lambda^4 = 1$, $\lambda \neq 1$ (fourth order resonance) the map (2.7)*

  (a) *is stable at equilibrium if $|c'_{03}| < |F|$,*

  (b) *is not stable at equilibrium if $|c'_{03}| > |F|$.*

(3) *For $\lambda^3 \neq 1$, $\lambda^4 \neq 1$, the map (2.7) is stable at equilibrium if $F \neq 0$.*

Proof. If $\lambda^3 = 1$ and $c_{02} \neq 0$, it follows from [16, p. 222] (or Theorem 3.2) that map (2.39) is not stable. Now consider the cases with either $\lambda^3 \neq 1$ or $c_{02} = 0$.

From (2.40) of Theorem 2.6 there exists a symplectic transformation such that the transformed map satisfies

$$Z_1 = \lambda(Z + \mathrm{i}FZ^2\bar{Z} + \mathrm{i}C\bar{Z}^3 + O(|Z|^4)), \tag{3.6}$$

where $C = |c'_{03}|$. This can be expressed as

$$Z_1 = \lambda Z(1 + (C\sin 4\theta + \mathrm{i}(F + C\cos 4\theta))|Z|^2 + O(|Z|^3)). \tag{3.7}$$

For case (1)(a), for which $C = 0$, stability follows from Theorem 3.2 with $N = 3$, $r = 3$, and $f(3\theta) = -\frac{1}{4}F$. For case (2), where $\lambda^4 = 1$, stability/instability follows from Theorem 3.2 with $N = 3$, $r = 4$, and $f(4\theta) = -\frac{1}{4}(F + C\cos 4\theta)$. For case (3), apply Theorem 2.6, and stability follows from Theorem 3.1 because $F \neq 0$. ∎

Now consider the cases, other than $\lambda = 1$, not covered by the preceding theorem. Some of these, such as the case $\lambda^3 = 1$, $c_{02} = 0$, $F = 0$, can be further analyzed with the help of the Cabral–Meyer result. Others, such as the case $\lambda^4 = 1$, $|c'_{03}| = |F|$, cannot. Both of these cases are very special. The remaining case to consider is $\lambda^3 \neq 1$, $\lambda^4 \neq 1$, $F = 0$. In this case it is possible (see Theorem 2.4), except for the very special case of fifth or sixth order resonance, to eliminate all but one term of degree 4 or 5 to get

$$Z_1 = \lambda(Z + c''_{32}Z^3\bar{Z}^2 + O(|Z|^6)). \tag{3.8}$$

Except for the very special case $c''_{32} = 0$ we can apply Theorem 3.2 to infer stability. The possibility of instability becomes even more special as we consider yet higher order resonances. And in the case where λ is not a root of unity there is no possibility of instability unless all the coefficients in the normal form vanish.

4. Application to reversible integrators. The remainder of the paper considers the important special case where the area-preserving mapping (1.2) is reversible, meaning that

$$RM(RM(y)) = y, \tag{4.1}$$

where $R = \mathrm{diag}(1, -1)$. It is further assumed that the fixed point $y^* = (q^*, 0)$. We continue to assume that mapping (1.2) is real analytic in some neighborhood of y^* and that y^* is an elliptic fixed point.

In the reduction of the linear part to a pure rotation given by (2.4), (2.5) the reversibility property is generally not preserved. It is straightforward to show that it is preserved if the linear transformation matrix X is a diagonal. And the following lemma shows that a diagonal transformation is sufficient for the reduction of the linear part.

LEMMA 4.1. *Let $y_1 = M(y)$ be a reversible area-preserving map with an elliptic fixed point y^*. There exists $\nu > 0$ such that the transformation $y = y^* + \mathrm{diag}(\nu, 1/\nu)Y$, converts the map* (1.2) *to the form*

$$Y_1 = \begin{bmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{bmatrix} Y + O(\|Y\|^2) \tag{4.2}$$

for some real ϕ. The new map is reversible and area-preserving.

Proof. Forming the Jacobian matrices for each side of (4.1) gives

$$RM'(y^*)RM'(y^*) = I, \tag{4.3}$$

which implies that the eigenvalues of $RM'(y^*)$ are 1 and/or -1. We have $\det(RM'(y^*)) = \det(R)\det(M'(y^*)) = (-1)(1) = -1$, so $RM'(y^*)$ has eigenvalues 1, -1. Therefore, the trace of $RM'(y^*)$ is 0 and the matrix has the form

$$RM'(y^*) = \begin{bmatrix} c & a \\ b & -c \end{bmatrix}, \qquad \text{which implies} \quad M'(y^*) = \begin{bmatrix} c & a \\ -b & c \end{bmatrix}. \tag{4.4}$$

We know that $M'(y^*)$ has eigenvalues λ, $\bar\lambda$ of unit modulus and hence $|\mathrm{trace} M'(y^*)| \le 2$. This together with $\det(M'(y^*)) = 1$ implies that $ab \ge 0$. If $ab = 0$, then the matrix is triangular with two equal eigenvalues. Because it is diagonalizable, it must, in fact, be diagonal, in which case the lemma follows with $\nu = 1$. If $ab > 0$, the transformed Jacobian matrix $\mathrm{diag}(\nu, 1/\nu)^{-1}M'(y^*)\mathrm{diag}(\nu, 1/\nu)$ has the required from with $\nu^2 = \sqrt{a/b}$. □

Introduce a complex variable w as in (2.6) by writing

$$Y = \left(\frac{w+\bar w}{2}, \frac{w-\bar w}{2\mathrm{i}}\right), \tag{4.5}$$

and the mapping (4.2) can be expressed $w_1 = M_{\mathrm{w}}(w, \bar w)$. Being reversible means that

$$\overline{M_{\mathrm{w}}(\overline{M_{\mathrm{w}}(w,\bar w)}, M_{\mathrm{w}}(w,\bar w))} = w. \tag{4.6}$$

Reversibility restricts the map to a form described by the following lemma. Only the forms of those terms of greatest interest in stability analysis are given.

LEMMA 4.2. *The map* (4.2) *has the form*

$$w_1 = \lambda w + \mathrm{i}\lambda^{1/2} L(\lambda^{1/2} w, \bar\lambda^{1/2}\bar w), \tag{4.7}$$

where

$$\begin{aligned} L(w,\bar w) = {} & aw^2 + 2aw\bar w + c\bar w^2 + \mathrm{i}c_{30}w^3 + (f + \mathrm{i}(a^2 - c^2))w^2\bar w + \mathrm{i}c_{12}w\bar w^2 + g\bar w^3 \\ & + O(|w|^4) \end{aligned} \tag{4.8}$$

and a, c, f, g *are real.*

Proof. Without loss of generality we can express the map $w_1 = M_{\mathrm{w}}(w, \bar w)$ as

$$w_1 = \lambda w + \mathrm{i}\lambda^{1/2} L(\lambda^{1/2} w, \bar\lambda^{1/2}\bar w). \tag{4.9}$$

The reversibility property (4.6) works out to be

$$L(w - \mathrm{i}\overline{L(\bar w, w)}, \bar w + \mathrm{i}L(\bar w, w)) - \overline{L(\bar w, w)} = 0. \tag{4.10}$$

Expanding this gives

$$L(w,\bar w) - \overline{L(\bar w, w)} = \mathrm{i}(\partial_1 L(w,\bar w)\overline{L(\bar w, w)} - \partial_2 L(w,\bar w)L(\bar w, w)) + O(|w|^4). \tag{4.11}$$

Write

$$L(w,\bar w) = aw^2 + bw\bar w + c\bar w^2 + \mathrm{i}v_2(w,\bar w) + u_3(w,\bar w) + \mathrm{i}v_3(w,\bar w) + O(|w|^4) \tag{4.12}$$

where a, b, c are real, $v_2(w, \bar w)$ is a homogeneous quadratic polynomial with real coefficients, and $u_3(w, \bar w)$ and $v_3(w, \bar w)$ are homogeneous cubic polynomials with real coefficients. Substituting this into (4.11) implies

$$v_2(w,\bar w) \equiv 0. \tag{4.13}$$

According to Lemma 2.1, the symplectic property implies $b = 2a$. Therefore, we have the simplification

$$L(w, \bar{w}) = aw^2 + 2aw\bar{w} + c\bar{w}^2 + u_3(w, \bar{w}) + \mathrm{i}v_3(w, \bar{w}) + O(|w|^4). \tag{4.14}$$

Substituting this into (4.11) implies

$$v_3(w, \bar{w}) = (a^2 - ac)w^3 + (a^2 - c^2)w^2\bar{w} + (a^2 - ac)w\bar{w}^2. \tag{4.15}$$

Define f and g to be the coefficients of the $w^2\bar{w}$ and $\bar{w}^3$ terms, respectively, in $u_3(w, \bar{w})$, and define $\mathrm{i}c_{30}$ and $\mathrm{i}c_{12}$ to be the coefficients of the w^3 and $w\bar{w}^2$ terms, respectively, in $u_3(w, \bar{w}) + \mathrm{i}v_3(w, \bar{w})$. ∎

Now that the reversibility property has been exploited, we make the symplectic change of variables

$$w = -\mathrm{i}\lambda^{-1/2} z, \tag{4.16}$$

and the map becomes

$$z_1 = \lambda(z - L(-\mathrm{i}z, \mathrm{i}\bar{z})) \tag{4.17}$$

$$= \lambda\left(z + az^2 - 2az\bar{z} + c\bar{z}^2 + c_{30}z^3 + (c^2 - a^2 + \mathrm{i}f)z^2\bar{z} + c_{12}z\bar{z}^2 + \mathrm{i}g\bar{z}^3) + O(|z|^4)\right). \tag{4.18}$$

The following theorem specializes the stability results of sections 3 and 4 to the map (4.18).

THEOREM 4.3. *Assume* $\lambda \neq 1$.

(1) *For* $\lambda^3 = 1$ *(third order resonance) the map* (4.7)
  (a) *is stable at equilibrium if* $c = 0$ *and* $F \neq 0$,
  (b) *is not stable at equilibrium if* $c \neq 0$,

where

$$F := f - 3a^2 \cot\frac{\phi}{2}. \tag{4.19}$$

(2) *For* $\lambda^4 = 1$ *(fourth order resonance) the map* (4.7)
  (a) *is stable at equilibrium if* $|G| < |F|$,
  (b) *is not stable at equilibrium if* $|G| > |F|$,

where

$$F := f - 3a^2 \cot\frac{\phi}{2} - c^2 \cot\frac{3\phi}{2} \quad \textit{and} \quad G := g + 2ac\frac{\cos\frac{1}{2}\phi}{\sin\frac{3}{2}\phi}. \tag{4.20}$$

(3) *For* $\lambda^3 \neq 1$, $\lambda^4 \neq 1$ *the map* (4.7) *is stable at equilibrium if* $F \neq 0$ *where*

$$F := f - 3a^2 \cot\frac{\phi}{2} - c^2 \cot\frac{3\phi}{2}. \tag{4.21}$$

Proof. Comparing (4.18) and (2.7), we make the identification

$$c_{20} = a, \qquad c_{02} = c, \qquad c_{21} = c^2 - a^2 + \mathrm{i}f, \qquad c_{03} = \mathrm{i}g. \tag{4.22}$$

From Theorem 3.3 follows part (1)(b) of the result. Assume now that either $\lambda^3 \neq 1$ or $c_{02} = 0$ and apply Theorem 2.6 to obtain a symplectic transformation of the original map such that the transformed map satisfies

$$Z_1 = \lambda(Z + c'_{21} Z^2 \bar{Z} + c'_{03} \bar{Z}^3 + O(|Z|^4)), \tag{4.23}$$

where

$$c'_{21} = \begin{cases} \mathrm{i}f - 3a^2 \dfrac{1+\lambda}{1-\lambda} - c^2 \dfrac{1+\lambda^3}{1-\lambda^3}, & \lambda^3 \neq 1, \\ \mathrm{i}f - 3a^2 \dfrac{1+\lambda}{1-\lambda}, & \lambda^3 = 1, c = 0 \end{cases} \tag{4.24}$$

and

$$c'_{03} = \begin{cases} 0, & \lambda^4 \neq 1, \\ \mathrm{i}g + 2ac \dfrac{\lambda + \lambda^2}{1-\lambda^3}, & \lambda^4 = 1. \end{cases} \tag{4.25}$$

Parts (1)(a), (2), and (3) of the result follow from Theorem 3.3. $\square$

5. Application to the symplectic Newmark integrators. We consider a Hamiltonian system with Hamiltonian $H(q,p) = \frac{1}{2}p^2 + V(q)$ where

$$V(q) = \frac{1}{2}\omega^2 q^2 + \frac{1}{3}Bq^3 + \frac{1}{4}Cq^4 + O(q^5) \tag{5.1}$$

is assumed to be real analytic at $q = 0$.

We consider the one-parameter family of symplectic numerical integrators defined in the article [20], which includes the leapfrog/Störmer/Verlet, Störmer–Cowell/Numerov, and implicit midpoint/trapezoid methods. An integration step, depending on the parameter α, is defined as follows:

$$q_{n+1/2} = q_n + \frac{h}{2} p_n, \tag{5.2}$$

$$F_{n+1/2} = -V'(q_{n+1/2} + \alpha h^2 F_{n+1/2}), \tag{5.3}$$

$$p_{n+1} = p_n + h F_{n+1/2}, \tag{5.4}$$

$$q_{n+1} = q_{n+1/2} + \frac{h}{2} p_{n+1}, \tag{5.5}$$

where h is the step size and the value $F_{n+1/2}$ is defined implicitly as the solution of (5.3) if $\alpha \neq 0$. This is the symplectic subfamily of the Newmark [12] family of methods. In the notation of [17, Equation (2.14)] $\gamma = \frac{1}{2}$ gives the subfamily of symplectic methods and β corresponds to α above. We impose the restriction that

$$h < h_2 \quad \text{where } h_2 = \begin{cases} 2(1-4\alpha)^{-1/2}/\omega & \text{if } \alpha < \frac{1}{4}, \\ +\infty & \text{if } \alpha \geq \frac{1}{4}. \end{cases} \tag{5.6}$$

This will be shown to be necessary for stability. The reason for the subscript 2 will become apparent later, in (5.32).

The goal is to obtain an expansion for (q_{n+1}, p_{n+1}) in powers of q_n and p_n. As the first step we seek an expansion for $F_{n+1/2}$ about $q_{n+1/2} = 0$ using (5.3) and the expansion

$$-V'(q) = -\omega^2 q - Bq^2 - Cq^3 + O(q^4). \tag{5.7}$$

We apply the implicit function theorem to the solution $(q, F) = (0, 0)$ of $F + V'(q + \alpha h^2 F) = 0$, and existence and uniqueness is guaranteed for sufficiently small $q_{n+1/2}$ if

$$\partial_F (F + V'(q + \alpha h^2 F))|_{(q,F)=(0,0)} \neq 0, \tag{5.8}$$

which simplifies to $1 + \alpha h^2 \omega^2 \neq 0$, and this holds because of assumption (5.6). Write

$$F_{n+1/2} = k_1 q_{n+1/2} + k_2 q_{n+1/2}^2 + k_3 q_{n+1/2}^3 + O(q_{n+1/2}^4). \tag{5.9}$$

Substituting this into (5.3) and equating the coefficients of powers of $q_{n+1/2}$, we get

$$k_1 = -\omega^2 \theta, \qquad k_2 = -B\theta^3, \qquad k_3 = -C\theta^4 + 2\alpha B^2 h^2 \theta^5, \tag{5.10}$$

where

$$\theta = \frac{1}{1 + \alpha h^2 \omega^2}. \tag{5.11}$$

Eliminate the $q_{n+1/2}$ stage of the integrator (5.2)–(5.5), and it becomes

$$p_{n+1} = p_n + hF_{n+1/2}, \tag{5.12}$$

$$q_{n+1} = q_n + hp_n + \frac{h^2}{2} F_{n+1/2}. \tag{5.13}$$

Substituting for $F_{n+1/2}$ and using $q_{n+1/2} = q_n + \frac{h}{2} p_n$ we get

(5.14)
$$q_{n+1} = \left(1 - \frac{h^2 \omega^2 \theta}{2}\right) q_n + h \left(1 - \frac{h^2 \omega^2 \theta}{4}\right) p_n + \frac{h^2}{2} k_2 q_{n+1/2}^2 + \frac{h^2}{2} k_3 q_{n+1/2}^3 + O(q_{n+1/2}^4),$$

(5.15)
$$p_{n+1} = -h\omega^2 \theta q_n + \left(1 - \frac{h^2 \omega^2 \theta}{2}\right) p_n + hk_2 q_{n+1/2}^2 + hk_3 q_{n+1/2}^3 + O(q_{n+1/2}^4).$$

The determinant of the linear part of the map is 1. We require for linear stability the condition

$$h^2 \omega^2 \theta < 4, \tag{5.16}$$

which is equivalent to assumption (5.6).

We make the following symplectic transformation so that in the new coordinates, the linear part of the map is a pure rotation:

$$q_n = \nu Q_n, \tag{5.17}$$

$$p_n = \frac{1}{\nu} P_n. \tag{5.18}$$

In the (Q, P) coordinates, we get the map

(5.19)
$$Q_{n+1} = \left(1 - \frac{h^2 \omega^2 \theta}{2}\right) Q_n + \frac{h}{\nu^2} \left(1 - \frac{h^2 \omega^2 \theta}{4}\right) P_n + \frac{h^2}{2\nu} k_2 l_n^2 + \frac{h^2}{2\nu} k_3 l_n^3 + O(l_n^4),$$

(5.20)
$$P_{n+1} = -\nu^2 h \omega^2 \theta Q_n + \left(1 - \frac{h^2 \omega^2 \theta}{2}\right) P_n + \nu h k_2 l_n^2 + \nu h k_3 l_n^3 + O(l_n^4),$$

where $l_n = \nu Q_n + \frac{h}{2\nu} P_n$. For the linear part of the map in the (Q, P) coordinates to be a pure rotation, we must have

$$-\nu^2 h\omega^2\theta = -\frac{h}{\nu^2}\left(1 - \frac{h^2\omega^2\theta}{4}\right). \tag{5.21}$$

This implies that

$$\nu^2 = \frac{1}{\omega\sqrt{\theta}}\sqrt{1 - \frac{h^2\omega^2\theta}{4}}. \tag{5.22}$$

For the rotation to be counterclockwise by angle ϕ, we must have

$$1 - \frac{h^2\omega^2\theta}{2} = \cos\phi, \qquad -\nu^2 h\omega^2\theta = \sin\phi. \tag{5.23}$$

LEMMA 5.1. *Letting*

$$w_n = Q_n + \mathrm{i}P_n, \tag{5.24}$$

we have the form given by Lemma 4.2 *with*

$$a = c, \qquad c = \frac{1}{4}hk_2\rho^3, \qquad f = 3g, \qquad g = \frac{1}{8}hk_3\rho^4, \tag{5.25}$$

where

$$\rho = \left(\nu\omega\sqrt{\theta}\right)^{-1}. \tag{5.26}$$

Proof. Transforming (5.19), (5.20) to the complex plane, we have

$$w_{n+1} = \lambda w_n + \delta hk_2\left(\frac{\delta w_n - \bar{\delta}\bar{w}_n}{2\mathrm{i}}\right)^2 + \delta hk_3\left(\frac{\delta w_n - \bar{\delta}\bar{w}_n}{2\mathrm{i}}\right)^3 + O(|w_n|^4), \tag{5.27}$$

where

$$\delta = \frac{h}{2\nu} + \mathrm{i}\nu. \tag{5.28}$$

It can be shown using first (5.22) and then (5.23) that

$$\nu^2\omega^2\theta\delta^2 = \frac{h^2\omega^2\theta}{4} - \nu^4\omega^2\theta + \mathrm{i}h\nu^2\omega^2\theta = \frac{h^2\omega^2\theta}{2} - 1 + \mathrm{i}h\nu^2\omega^2\theta = -\mathrm{e}^{\mathrm{i}\phi}. \tag{5.29}$$

Therefore $\delta = \mathrm{i}\rho\lambda^{1/2}$ with ρ is given by (5.26). Substituting for δ in (5.27) gives the form

$$w_{n+1} = \lambda w_n + \mathrm{i}\lambda^{1/2}L(\lambda^{1/2}w_n, \bar{\lambda}^{1/2}\bar{w}_n), \tag{5.30}$$

where

$$L(w, \bar{w}) = \frac{hk_2}{4}\rho^3(w + \bar{w})^2 + \frac{hk_3}{8}\rho^4(w + \bar{w})^3 + O(|w|^4). \qquad \square \tag{5.31}$$

Resonance of order r occurs when $\phi = -\frac{2\pi}{r}$. This happens for a step size h_r given by

$$h_r = \begin{cases} \frac{2}{\omega}\sin\frac{\pi}{r}(1-4\alpha\sin^2\frac{\pi}{r})^{-1/2} & \text{if } \alpha < (2\sin\frac{\pi}{r})^{-2}, \\ +\infty & \text{otherwise.} \end{cases} \tag{5.32}$$

In particular

$$h_3 = \frac{1}{\omega}\sqrt{3/(1-3\alpha)}, \qquad h_4 = \frac{1}{\omega}\sqrt{2/(1-2\alpha)} \tag{5.33}$$

if $\alpha < \frac{1}{3}$, $\alpha < \frac{1}{2}$, respectively.

The following theorem gives the stability of the integrator for most cases.

THEOREM 5.2. *Assume $h < h_2$.*

(1) *For $h = h_3$ (third order resonance) the integrator*
   (a) *is stable at equilibrium if $B = 0$ and $C \neq 0$,*
   (b) *is not stable at equilibrium if $B \neq 0$.*

(2) *For $h = h_4$ (fourth order resonance) the integrator*
   (a) *is stable at equilibrium if $(\omega^2 C - 4\alpha B^2)(\omega^2 C - 2B^2) > 0$,*
   (b) *is not stable at equilibrium if $(\omega^2 C - 4\alpha B^2)(\omega^2 C - 2B^2) < 0$.*

(3) *For $h \neq h_3$, $h \neq h_4$ the integrator is stable at equilibrium if*

$$-2\alpha B^2(h^2\omega^2\theta)^2 + (3\omega^2 C + (8\alpha - 4)B^2)h^2\omega^2\theta + 10B^2 - 9\omega^2 C \neq 0. \tag{5.34}$$

Not all cases are covered by the theorem. Some cases not covered depend on higher than fourth derivatives of the potential $V(q)$.

Proof of case (1). We have $c = \frac{1}{4}hk_2\rho^3 = 0$ if and only if $B = 0$. Suppose $B = 0$. Then $a = 0$, and $F = f = \frac{3}{8}hk_3\rho^4 \neq 0$ if and only if $C \neq 0$. ∎

Proof of case (2). It is enough to show that

$$\operatorname{sign}(|F| - |G|) = \operatorname{sign}\left(\left(\omega^2 C - 4\alpha B^2\right)\left(\omega^2 C - 2B^2\right)\right), \tag{5.35}$$

where $\operatorname{sign}(x)$ is -1, 0, or 1 depending on whether x is negative, zero, or positive. Note that $\phi = -\pi/2$. We have, using (5.25),

$$\operatorname{sign}(|F| - |G|) = \operatorname{sign}(F^2 - G^2) \tag{5.36}$$

$$= \operatorname{sign}((3g + 2c^2)^2 - (g - 2c^2)^2) \tag{5.37}$$

$$= \operatorname{sign}(8g^2 + 16gc^2) = \operatorname{sign}(g(g + 2c^2)) \tag{5.38}$$

$$= \operatorname{sign}\left(\frac{1}{8}hk_3\rho^4\left(\frac{1}{8}hk_3\rho^4 + 2\left(\frac{1}{4}hk_2\rho^3\right)^2\right)\right). \tag{5.39}$$

Using (5.10),

$$\operatorname{sign}(|F| - |G|) = \operatorname{sign}(k_3(k_3 + h\rho^2 k_2^2)) \tag{5.40}$$

$$= \operatorname{sign}((2h^2\alpha\theta B^2 - C)(2h^2\alpha\theta B^2 - C + h\rho^2\theta^2 B^2)). \tag{5.41}$$

From the discussion at the beginning of section 5, we know that $h = h_4$ is possible only if $\alpha < \frac{1}{2}$ in which case

$$h^2\omega^2 = \frac{2}{1-2\alpha}, \qquad \theta = 1 - 2\alpha > 0. \tag{5.42}$$

From (5.26) and (5.22)

$$\rho^{-1} = \nu\omega\sqrt{\theta}, \qquad \nu^2 = \sqrt{\frac{1}{\omega^2\theta} - \frac{h^2}{4}}, \tag{5.43}$$

and hence,

$$\rho^2\omega = \sqrt{\frac{2}{1-2\alpha}}. \tag{5.44}$$

The condition becomes

$$\text{sign}(|F| - |G|) = \text{sign}((C\omega^2 - 2h^2\alpha\theta\omega^2B^2)(C\omega^2 - 2h^2\alpha\theta\omega^2B^2 - h\omega\rho^2\omega\theta^2B^2)) \tag{5.45}$$

$$= \text{sign}((C\omega^2 - 4\alpha B^2)(C\omega^2 - 2B^2)). \qquad \square \tag{5.46}$$

Proof of case (3). Let us determine F in terms of the integrator parameters h, α and the problem parameters ω, B, C. We have

$$F = 3g - 3c^2\cot\frac{\phi}{2} - c^2\cot\frac{3\phi}{2} = 3g - 2c^2\cot\frac{\phi}{2}\cdot\frac{1+4\cos\phi}{1+2\cos\phi}$$

$$= \frac{3}{8}hk_3\rho^4 - 2\cot\frac{\phi}{2}\left(\frac{1}{4}hk_2\rho^3\right)^2\frac{1+4\cos\phi}{1+2\cos\phi}. \tag{5.47}$$

Using (5.23), we have

$$\cot\frac{\phi}{2} = \frac{\sin\phi}{1-\cos\phi} = \frac{-\nu^2h\omega^2\theta}{\frac{1}{2}h^2\omega^2\theta} = \frac{-2\nu^2}{h}. \tag{5.48}$$

Substituting this and (5.26) into (5.47) yields

$$F = \frac{h}{8\nu^4\omega^6\theta^2}\left(3\omega^2k_3 + 2\theta^{-1}k_2^2\frac{1+4\cos\phi}{1+2\cos\phi}\right). \tag{5.49}$$

Substituting (5.23) and (5.10) into this yields

$$F = \frac{h\theta^2}{8\nu^4\omega^6(1+2\cos\phi)}\left(3\omega^2(-C + 2\alpha h^2\theta B^2)(3 - h^2\omega^2\theta) + 2\theta B^2(5 - 2h^2\omega^2\theta)\right). \tag{5.50}$$

Replacing the one occurrence of "2θ" by "$2(1-\alpha h^2\omega^2\theta)$" gives the result

$$F = \frac{h\theta^2}{8\nu^4\omega^6(1+2\cos\phi)}\left(-2\alpha B^2(h^2\omega^2\theta)^2 + (3\omega^2C + (8\alpha-4)B^2)h^2\omega^2\theta + 10B^2 - 9\omega^2C\right). \qquad \square \tag{5.51}$$

Example 1: *Morse oscillator.* The potential for the Morse oscillator [15] is

$$V(q) = D(1 - \exp(-S(q-q^*))^2 \tag{5.52}$$

$$= DS^2(q-q^*)^2 - DS^3(q-q^*)^3 + \frac{7}{12}DS^4(q-q^*)^4 + O((q-q^*)^5), \tag{5.53}$$

where D, S, and q^* are positive numbers. Hence,

$$\omega^2 = 2DS^2, \qquad B = -3DS^3, \qquad C = \frac{7}{3}DS^4. \tag{5.54}$$

Hence, third order resonances are not stable, and fourth order resonances are not stable if

$$\alpha < \frac{\omega^2 C}{4B^2} = \frac{7}{54} \tag{5.55}$$

but stable for α greater than the given value.

Example 2: *Lennard–Jones oscillator.* The Lennard–Jones potential [15] is

$$V(q) = \epsilon(1 - 2(\sigma/q)^6)^2 \tag{5.56}$$

$$= \frac{72\epsilon}{(q^*)^2}(q - q^*)^2 - \frac{1512\epsilon}{(q^*)^3}(q - q^*)^3 + \frac{26712\epsilon}{(q^*)^4}S(q - q^*)^4 + O((q - q^*)^5), \tag{5.57}$$

where ϵ and σ are positive numbers and $q^* = 2^{1/6}\sigma$. Hence,

$$\omega^2 = 144\epsilon(q^*)^{-2}, \qquad B = -4536\epsilon(q^*)^{-3}, \qquad C = 106848\epsilon(q^*)^{-4}. \tag{5.58}$$

Hence, third order resonances are not stable, and fourth order resonances are not stable if

$$\alpha < \frac{\omega^2 C}{4B^2} = \frac{106}{567} \tag{5.59}$$

but are stable for α greater than the given value.

For both potentials the implicit midpoint method ($\alpha = \frac{1}{4}$) is stable for fourth order resonances but the Störmer–Cowell method ($\alpha = \frac{1}{12}$) is not. This is consistent with the experimental findings of [15].

Acknowledgments. We are indebted to an anonymous referee and Sebastian Reich for bringing our attention to the work of K.R. Meyer and H.E. Cabral, which both strengthened and shortened this paper.

REFERENCES

[1] V. I. Arnol'd, *Mathematical Methods of Classical Mechanics*, 2nd ed., Springer-Verlag, New York, 1989.

[2] D. K. Arrowsmith and C. M. Place, *An Introduction to Dynamical Systems*, Cambridge University Press, Cambridge, UK, 1990.

[3] U. M. Ascher and S. Reich, *The midpoint scheme and variants for Hamiltonian systems: Advantages and pitfalls*, SIAM J. Sci. Comput., 21 (1999), pp. 1045–1065.

[4] G. D. Birkhoff, *Dynamical Systems*, AMS, Providence, RI, 1927, rev. ed. 1966.

[5] T. Bishop, R. D. Skeel, and K. Schulten, *Difficulties with multiple timestepping and the fast multipole algorithm in molecular dynamics*, J. Comput. Chem., 18 (1997), pp. 1785–1791.

[6] H. E. Cabral and K. R. Meyer, *Stability of equilibria and fixed points of conservative systems*, Nonlinearity, 12 (1999), pp. 1351–1362.

[7] O. Gonzalez and J. Simo, *On the stability of symplectic and energy-momentum algorithms for nonlinear Hamiltonian systems with symmetry*, Comput. Methods Appl. Mech. Engrg., 134 (1996), pp. 197–222.

[8] C. Lanczos, *The Variational Principles of Mechanics*, 4th ed., Dover, New York, 1986.

[9] M. Mandziuk and T. Schlick, *Resonance in the dynamics of chemical systems simulated by the implicit midpoint scheme*, Chem. Phys. Lett., 237 (1995), pp. 525–535.

[10] R. I. McLachlan and P. Atela, *The accuracy of symplectic integrators*, Nonlinearity, 5 (1992), pp. 541–562.

[11] J. Moser, *Stable and Random Motions in Dynamical Systems*, Princeton University Press, Princeton, NJ, 1973.

[12] N. M. Newmark, *A method of computation for structural dynamics*, ASCE J. Engrg. Mech. Division, 85 (1959), pp. 67–94.

[13] J. M. Sanz-Serna, *Two topics in nonlinear stability*, in Advances in Numerical Analysis, W. Light, ed., Clarendon Press, Oxford, 1991, pp. 147–174.

[14] J. M. Sanz-Serna and F. Vadillo, *Nonlinear instability, the dynamic approach*, in Numerical Analysis, D. F. Griffiths and G. A. Watson, eds., Pitman Res. Notes Math. Ser. 140, Longman Scientific and Technical, Harlow, UK, 1986, pp. 187–199.

[15] T. Schlick, M. Mandziuk, R. D. Skeel, and K. Srinivas, *Nonlinear resonance artifacts in molecular dynamics simulations*, J. Comput. Phys., 139 (1998), pp. 1–29.

[16] C. L. Siegel and J. K. Moser, *Lectures on Celestial Mechanics*, Springer-Verlag, New York, Heidelberg, 1971.

[17] J. Simo, N. Tarnow, and K. Wong, *Exact energy-momentum conserving algorithms and symplectic schemes for nonlinear dynamics*, Comput. Methods Appl. Mech. Engrg., 100 (1992), pp. 63–116.

[18] J. C. Simo and N. Tarnow, *A Review of Conserving Algorithms for Nonlinear Dynamics*, Tech. Rep. SUDAM Report 92-7, Department of Mechanical Engineering, Stanford University, Stanford, CA, 1992.

[19] R. D. Skeel, *Symplectic integration with floating-point arithmetic and other approximations*, Appl. Numer. Math., 29 (1999), pp. 3–18.

[20] R. D. Skeel, G. Zhang, and T. Schlick, *A family of symplectic integrators: Stability, accuracy, and molecular dynamics applications*, SIAM J. Sci. Comput., 18 (1997), pp. 203–222.

[21] G. Zhang and T. Schlick, *Implicit discretization schemes for Langevin dynamics*, Molecular Phys., 84 (1995), pp. 1077–1098.