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STUDIES IN NUMERICAL NONLINEAR INSTABILITY III: AUGMENTED HAMILTONIAN SYSTEMS*

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Abstract. Leap-frog (explicit mid-point) discretizations of Hamiltonian systems are considered. It is proved that the discrete evolution preserves the symplectic structure of the phase space. The Kolmogorov-Arnold-Moser (KAM) theory is applied to guarantee the boundedness of the computed points under suitable restrictions of the time-step. The general ideas introduced are employed to provide an extensive analysis of the leap-frog discretization of the complex equation $iz_t + |z|^2 z = 0$, which describes the nonlinear selfinteraction of a Fourier mode. The paper emphasizes the relations between Numerical Analysis and Classical Mechanics/Dynamical Systems.

Key words. dynamical systems, nonlinear instability, Hamiltonian systems, leap-frog discretization

AMS(MOS) subject classifications. 65L07, 65M10, 58F05, 58F27, 70H05, 70H15

1. Introduction. The cubic Schrödinger equation

$$iz_t + z_{xx} + |z|^2 z = 0, \qquad i^2 = -1, \quad z \text{ complex} \tag{1.1}$$

is well known to play a very important role in modelling a number of physical phenomena (see e.g. [23]). Its importance partly stems from the fact that it combines the dispersive behaviour of its linearization

$$iz_t + z_{xx} = 0 \tag{1.2}$$

with the simplest odd nonlinearity of

$$iz_t + |z|^2 z = 0. \tag{1.3}$$

The ODE (1.3) not only describes the x-independent solutions of (1.1) but also, more generally, the nonlinear self-interaction of a Fourier mode, leading to the Stokes effect in the corresponding frequency [23, p. 529].

It was found in [17] that, when numerically integrating (1.1) with a standard leap-frog scheme, it is possible for the numerical solution to remain bounded for a considerable number of steps and then to explode violently. Leap-frog schemes are notorious for this kind of unwelcome behaviour, that can be avoided by odd-even averaging and/or artificial viscosity [15].

In [15] one of the present authors described a means for investigating the dynamics of leap-frog discretizations which basically consists of the analysis of a differential system larger than the one actually being integrated. One of our purposes in this article is to apply that general technique to discretizations of (1.1) or (1.3). The treatment relies on the theory of *dynamical systems*, a tool that is becoming increasingly more popular in the analysis of numerical methods for evolutionary equations, see [2], [8], [13], [14], [15], [18], [21], [22] and their references. Of particular significance here are the KAM *theory*, which sometimes can be applied to *guarantee rigorously the boundedness* of the computed points, and the use of *action/angle variables*. The role played by the latter in numerical work was perhaps first noticed by Newell [12]. General background references are [3], [9], [11].

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The study of (1.1)-(1.3) is carried out in § 4. Some of our findings possess a wider scope and may be useful in other contexts. We have therefore chosen to state them separately in § 3. The second section is devoted to the introduction of the necessary notation and also recalls from [15] a number of results crucial in the understanding of the subsequent material. Some conclusions are presented in § 5.

It should be mentioned that other aspects of the numerical nonlinear stability of (1.1) have been investigated by Herbst et al. [6]. In their paper and in [10], [17], [19] the interested reader can find additional references to the numerical treatment of nonlinear Schrödinger equations.

2. Augmented systems. We consider an s-dimensional system of differential equations

$$dp/dt = f(p), \qquad p \in \mathbb{R}^s, \tag{2.1}$$

where the function $\mathbf{f}$ is smooth. In the sequel (2.1) will be referred to as the *original system.* When numerically integrating (2.1), the leap-frog discretization with step-length k

$$\begin{aligned} &\mathbf{P}^0, \mathbf{P}^1 \quad \text{given}, \\ &\mathbf{P}^{n+1} = \mathbf{P}^{n-1} + 2k\mathbf{f}(\mathbf{P}^n), \qquad n = 1, 2, 3, \cdots \end{aligned} \tag{2.2}$$

provides a convergent approximation [5], [7], [10], [16], i.e., if a particular solution $\mathbf{p}(t)$ of (2.1) has been chosen and a family $\mathbf{P}^0 = \mathbf{P}^0(k)$, $\mathbf{P}^1 = \mathbf{P}^1(k)$ of starting vectors is considered such that

$$\lim_{k \to 0} \mathbf{P}^0 = \lim_{k \to 0} \mathbf{P}^1 = \mathbf{p}(0), \tag{2.3}$$

then, for nk fixed, $k \to 0$

$$\lim \mathbf{P}^n = \mathbf{p}(nk). \tag{2.4}$$

However, it is well known [7], [14], [15], [18] that, as n increases with k fixed, the sequences

$$\mathbf{p}(0), \mathbf{p}(k), \mathbf{p}(2k), \cdots, \mathbf{p}(nk), \cdots, \tag{2.5}$$

$$\mathbf{P}^0, \mathbf{P}^1, \mathbf{P}^2, \cdots, \mathbf{P}^n, \cdots \tag{2.6}$$

may possess widely different behaviours, even if k is small and the original system is linear. (Note that in this paper solutions of differential equations are represented by small-case letters, while capital letters denote the corresponding discrete approximations.)

The recursion (2.2) can be rewritten in the form

$$\mathbf{P}^{2n} = \mathbf{P}^{2n-2} + 2k\mathbf{f}(\mathbf{P}^{2n-1}), \qquad \mathbf{P}^{2n+1} = \mathbf{P}^{2n-1} + 2k\mathbf{f}(\mathbf{P}^{2n}), \tag{2.7}$$

$n = 1, 2, \cdots$, where we have simply displayed two consecutive steps. With the notation $\mathbf{P}^{2n} = \mathbf{U}^n$, $\mathbf{P}^{2n+1} = \mathbf{U}^{*n}$, $n = 0, 1, \cdots$, (2.7) becomes

$$\mathbf{U}^n = \mathbf{U}^{n-1} + 2k\mathbf{f}(\mathbf{U}^{*n-1}), \qquad \mathbf{U}^{*n} = \mathbf{U}^{*n-1} + 2k\mathbf{f}(\mathbf{U}^n), \tag{2.8}$$

$n = 1, 2, \cdots$, a recursion that can clearly be regarded as a consistent, one-step discretization (with step-length $2k$) of the system of $2s$ differential equations

$$\frac{d\mathbf{u}}{dt} = \mathbf{f}(\mathbf{u}^*), \qquad \frac{d\mathbf{u}^*}{dt} = \mathbf{f}(\mathbf{u}), \tag{2.9}$$

where $\mathbf{u}(n2k) \simeq \mathbf{U}^n = \mathbf{P}^{2n}$, $\mathbf{u}^*(n2k) \simeq \mathbf{U}^{*n} = \mathbf{P}^{2n+1}$. Thus the even-numbered $\mathbf{P}^n$ computed in (2.2) approximate the component $\mathbf{u}(t)$ of the solutions $[\mathbf{u}(t), \mathbf{u}^*(t)]$ of the so-called *augmented system* (2.9), while odd-numbered $\mathbf{P}^n$ approximate the component $\mathbf{u}^*(t)$. More precisely, one-step discretizations of ordinary differential equations are always 0-stable [5] and this implies that, if we fix a solution $[\mathbf{u}(t), \mathbf{u}^*(t)]$ of (2.9) and introduce a family of starting vectors $\mathbf{P}^0 = \mathbf{U}^0 = \mathbf{U}^0(k)$, $\mathbf{P}^1 = \mathbf{U}^{*0} = \mathbf{U}^{*0}(\mathbf{k})$, such that

$$(2.10) \qquad \lim_k \mathbf{P}^0 = \lim_k \mathbf{U}^0 = \mathbf{u}(0), \qquad \lim_k \mathbf{P}^1 = \lim_k \mathbf{U}^{*0} = \mathbf{u}^*(0),$$

then, for nk fixed, $k \to 0$

$$(2.11) \qquad \lim \mathbf{P}^{2n} = \lim \mathbf{U}^n = \mathbf{u}(2nk), \qquad \lim \mathbf{P}^{2n+1} = \lim \mathbf{U}^{*n} = \mathbf{u}^*(2nk).$$

Of importance is that the convergence property (2.11) does not contradict the convergence previously noted in (2.4). In fact, if (2.3) holds, then in (2.10), $\mathbf{u}(0) = \mathbf{u}^*(0) = \mathbf{p}(0)$. This clearly forces in (2.1), (2.9) that, for all values of t, $\mathbf{u}(t) = \mathbf{u}^*(t) = \mathbf{p}(t)$ and then the convergence statements (2.4), (2.11) are obviously equivalent. Note that there is a one-to-one correspondence between solutions $\mathbf{p}(t)$ of the original system (2.1) and the solutions $[\mathbf{u}(t), \mathbf{u}^*(t)]$ of (2.9) that satisfy $\mathbf{u}(t) \equiv \mathbf{u}^*(t)$. Augmented solutions of this form are called *diagonal solutions* and their dynamics replicates that of the original system.

Thus when studying the $k \to 0$ behaviour of the leap-frog points when (2.3) holds, nothing is gained by the introduction of the augmented system because (2.3) effectively restricts the attention to the diagonal solutions of (2.9). However, for *fixed k*, (2.9) provides a very useful tool for the investigation of the behaviour of (2.6) (see [15]). Also the leap-frog discretization possesses a number of properties which mimic properties of the augmented system (2.9) rather than properties of the original system (2.1) [15]. An instance is provided by the conservation of volume: for *any* function $\mathbf{f}$ the mapping $(\mathbf{U}^{n-1}, \mathbf{U}^{*n-1}) \to (\mathbf{U}^n, \mathbf{U}^{*n})$ in (2.8) is a diffeomorphism (one-to-one and onto smooth mapping) in $\mathbb{R}^s \times \mathbb{R}^s$ which conserves volume. This parallels the fact that the differential system (2.9) is divergence-free which entails [3] that the oriented volume in $\mathbb{R}^s \times \mathbb{R}^s$ is preserved by the $2k$-flow of (2.9), i.e., the mapping in $\mathbb{R}^s \times \mathbb{R}^s$ which advances solutions of (2.9) by $2k$ units of time. It should be emphasized that the present conservation of volume is analogous to that in steady incompressible flows, and accordingly solutions of (2.9) behave like streamlines in such a flow: they attract their neighbours in regions where the flow accelerates. In [22] we have discussed some practical implications of this attraction. Other consequences of the conservation of volume of (2.8)-(2.9) are: (i) that the corresponding dynamics cannot possess asymptotically stable equilibria or asymptotically stable limit cycles; (ii) the appearance of phenomena linked to the Poincaré recurrence theorem [3]. This theorem explains the recurrence found in [24].

Finally, note that in the terminology of differential forms [3], conservation of volume is the conservation of the $2s$-form (subscripts denote components):

$$(2.12) \qquad du_1 \wedge du_2 \wedge \cdots \wedge du_s \wedge du_1^* \wedge du_2^* \wedge \cdots \wedge du_s^*.$$

3. Augmented Hamiltonian systems. We now examine the particular situation where the s-dimensional original system (2.1) is Hamiltonian with g degrees of freedom ($s = 2g$). Namely

$$(3.1) \qquad \frac{dp_i}{dt} = -D_{g+i}H(\mathbf{p}, \mathbf{q}), \qquad \frac{dq_i}{dt} = D_iH(\mathbf{p}, \mathbf{q}),$$

$i = 1, 2, \cdots, g$, where $\mathbf{p} = [p_1, p_2, \cdots, p_g]$, $\mathbf{q} = [q_1, q_2, \cdots, q_g]$, H is the Hamiltonian function and D_j denotes partial differentiation with respect to the jth argument $j = 1, \cdots, s$. The augmented system (2.9), with $2s$ or $4g$ scalar components takes the form

(3.2a) $$\frac{du_i}{dt} = -D_{g+i}H(\mathbf{u}^*, \mathbf{v}^*),$$

(3.2b) $$\frac{dv_i}{dt} = D_iH(\mathbf{u}^*, \mathbf{v}^*),$$

(3.2c) $$\frac{du_i^*}{dt} = -D_{g+i}H(\mathbf{u}, \mathbf{v}),$$

(3.2d) $$\frac{dv_i^*}{dt} = D_iH(\mathbf{u}, \mathbf{v}),$$

$i = 1, 2, \cdots, g$. Here the augmented variables $\mathbf{v}$, $\mathbf{v}^*$ play with respect to the original variables $\mathbf{q}$ (positions), the role played by the augmented variables $\mathbf{u}$, $\mathbf{u}^*$ in connection with the original variables $\mathbf{p}$ (momenta).

We use the following terminology. If $\mathbf{y}' = \mathbf{g}(\mathbf{y})$ is a differential system, its k-flow (k a real number) is the mapping $\mathbf{y}_0 \to \mathbf{y}(k, \mathbf{y}_0)$, where $\mathbf{y}(\cdot, \mathbf{y}_0)$ denotes the solution of the system that at $t = 0$ takes the value $\mathbf{y}(0, \mathbf{y}_0) = \mathbf{y}_0$.

PROPOSITION 1. (i) *The system* (3.2) *is Hamiltonian, with the Hamiltonian function*

(3.3) $$\mathcal{H}(\mathbf{u}, \mathbf{v}, \mathbf{u}^*, \mathbf{v}^*) = H(\mathbf{u}, \mathbf{v}) + H(\mathbf{u}^*, \mathbf{v}^*).$$

The variables $\mathbf{u}$ *act as conjugated momenta of the positions* $\mathbf{v}^*$ *and the variables* $\mathbf{u}^*$ *provide the momenta conjugated to the positions* $\mathbf{v}$.

(ii) *The* $2k$*-flow of* (3.2) *preserves the standard* 2*-form in* $\mathbb{R}^{2s} = \mathbb{R}^{4g}$

(3.4) $$\omega^2 = \sum_{i=1}^{g} (du_i \wedge dv_i^* + du_i^* \wedge dv_i)$$

and its exterior powers ω^{2j}, $j = 1, 2, \cdots, s$.

(iii) *The function* $\mathcal{H}$ *in* (3.3) *is an invariant of the solutions of* (3.2).

Proof. (i) is a trivial observation and (ii)-(iii) are general properties of Hamiltonian systems [3]. Note that the conservation of ω^{2s} in (ii) is the conservation of volume (2.12), which takes place even if the augmented system (2.9) is not Hamiltonian.

It is perhaps useful to notice that augmented systems are Hamiltonian not only if the corresponding original system is Hamiltonian (i.e. in the case just considered) but also if the original system is a *gradient* system (see [15, Thm. 3 (iii)] and also [20]).

For the benefit of numerical analysts we recall that the form (3.4) defines the so-called standard *symplectic* structure in R^{2s} (just as the quadratic form $(dx)^2 + (dy)^2 + (dz)^2$ defines the standard metric structure in R^3). Changes of variables which preserve the symplectic structure (i.e., the form (3.4)) are crucial in mechanics and referred to as *canonical*. In particular a canonical change of variables preserves the Hamiltonian form of the equations of motion [3, p. 241].

Turning now to the discrete approximation, the leap-frog scheme for (3.1) is given by

(3.5) $$P_i^{n+1} = P_i^{n-1} - 2kD_{g+i}H(\mathbf{P}^n, \mathbf{Q}^n), \qquad Q_i^{n+1} = Q_i^{n-1} + 2kD_iH(\mathbf{P}^n, \mathbf{Q}^n),$$

$i=1,2,\cdots,g$; $n=1,2,\cdots$ or with the notation $\mathbf{P}^{2n}=\mathbf{U}^n$, $\mathbf{P}^{2n+1}=\mathbf{U}^{*n}$, $\mathbf{Q}^{2n}=\mathbf{V}^n$, $\mathbf{Q}^{2n+1}=\mathbf{V}^{*n}$, $n=0,1,2,\cdots$

$$U_i^n = U_i^{n-1} - 2kD_{g+i}H(\mathbf{U}^{*n-1},\mathbf{V}^{*n-1}), \tag{3.6a}$$

$$V_i^n = V_i^{n-1} + 2kD_iH(\mathbf{U}^{*n-1},\mathbf{V}^{*n-1}), \tag{3.6b}$$

$$U_i^{*n} = U_i^{*n-1} - 2kD_{g+i}H(\mathbf{U}^n,\mathbf{V}^n), \tag{3.6c}$$

$$V_i^{*n} = V_i^{*n-1} + 2kD_iH(\mathbf{U}^n,\mathbf{V}^n). \tag{3.6d}$$

PROPOSITION 2. *The mapping* $(\mathbf{U}^{n-1},\mathbf{V}^{n-1},\mathbf{U}^{*n-1},\mathbf{V}^{*n-1})\to(\mathbf{U}^n,\mathbf{V}^n,\mathbf{U}^{*n},\mathbf{V}^{*n})$ *in* (3.6) *is a canonical diffeomorphism, i.e. it preserves the standard form* (3.4).

Proof. In (3.6) we transfer to the left-hand side all terms with a superscript n and to the right-hand side all terms with a superscript $n-1$. Next we differentiate, take exterior products and sum to arrive at

$$\sum_{i=1}^{g}\{dU_i\wedge[dV_i^*-2k\,dD_iH(\mathbf{U},\mathbf{V})]+[dU_i^*+2k\,dD_{g+i}H(\mathbf{U},\mathbf{V})]\wedge dV_i\}^{(n)}$$

$$= \sum_{i=1}^{g}\{[dU_i-2k\,dD_{g+i}H(\mathbf{U}^*,\mathbf{V}^*)]\wedge dV_i^* + dU_i^*\wedge[dV_i+2k\,D_iH(\mathbf{U}^*,\mathbf{V}^*)]\}^{(n-1)}. \tag{3.7}$$

Now in the left-hand side, with an obvious simplified notation

$$\sum_i\{dU_i\wedge dD_i + dV_i\wedge dD_{g+i}\}$$
$$=\sum_{i,j} D^2_{i,j}(dU_i\wedge dU_j)+D^2_{i,g+j}(dU_i\wedge dV_j)+D^2_{g+i,j}(dV_i\wedge dU_j)$$
$$+D^2_{g+i,g+j}(dV_i\wedge dV_j) = d\sum_i(D_i\,dU_i + D_{g+i}\,dV_i) = ddH = 0.$$

A similar cancellation takes place in the right-hand side of (3.7) and then the proof is complete.

The general properties discussed so far possess some important implications. We successively consider the two most simple cases:

(A) The original Hamiltonian $H(\mathbf{p},\mathbf{q})$ takes the form

$$H(\mathbf{p},\mathbf{q}) = T(\mathbf{p}) + V(\mathbf{q}),$$

i.e., the kinetic energy only depends on the momenta and the potential energy only depends on the positions. Then (3.2a)-(3.2d) are uncoupled from (3.2b)-(3.2c) and the augmented system is just the direct product or juxtaposition of the two systems (3.2a)-(3.2d) and (3.2b)-(3.2c) which are replicas of the original system (3.1). Analogously in (3.6) there is no coupling between $\mathbf{U}$, $\mathbf{V}^*$ on the one hand and $\mathbf{U}^*$, $\mathbf{V}$ on the other. In terms of (3.5) this means that even-numbered momenta $\mathbf{P}^{2n}$ and odd-numbered positions $\mathbf{Q}^{2n+1}$ approximate the motions of (3.2a)-(3.2b), and are uncoupled from odd-numbered momenta $\mathbf{P}^{2n+1}$ and even-numbered positions $\mathbf{Q}^{2n}$ that in turn approximate the motions of (3.2b)-(3.2c). An example of this sort of behaviour has been discussed in detail in [18].

(B) The augmented Hamiltonian system is *completely integrable* [3] and nondegenerate. We recall that for this to be the case (3.2) must in particular possess s independent conserved quantities. In this situation s variables of action $\mathbf{I}$ and s variables of angle $\boldsymbol{\phi}$ can be introduced to replace $(\mathbf{u}, \mathbf{v}, \mathbf{u}^*, \mathbf{v}^*)$ so that in the new variables the $2k$-flow of (3.2) is simply given by the multidimensional *twist mapping* [11]

$$\boldsymbol{\phi} \to \boldsymbol{\phi} + 2k\boldsymbol{\nu}(\mathbf{I}), \quad \mathbf{I} \text{ constant}, \tag{3.8}$$

where $\boldsymbol{\nu} = \partial\mathcal{H}/\partial\mathbf{I}$. Each surface $\mathbf{I} = \text{constant}$ in $\mathbb{R}^{2s}$ is an s-dimensional torus, parameterized by the s angles $\boldsymbol{\phi}$. These tori are left invariant by the flow of (3.2). Now the mapping in (3.6) is *canonical* (Proposition 2) and, due to the consistency of the discretization, differs from (3.8) by $O(k^2)$ terms. The KAM (Kolmogorov–Arnold–Moser) theorem can then be applied to conclude that to each torus $\mathbf{I} = \text{constant}$ on which the s angular frequencies $\boldsymbol{\nu}(\mathbf{I})$ are far from being resonant there corresponds, for small values of k, a neighbouring, slightly distorted torus invariant for the leap-frog mapping (3.6).

A full, rigorous statement of the KAM theorem is too long to be given here and can be seen in [18] or [21] together with more details of its application to leap-frog discretizations. We emphasize that the canonical character of the discretization proved in Proposition 2 is essential. It should also be noted that before the theorem can be applied to concrete examples one has to check that the augmented system is completely integrable (i.e., possesses s independent conserved quantities in involution) and nondegenerate (i.e., the s frequencies $\boldsymbol{\phi}$ are functionally independent).

Also note that a function $u = u(\phi_1, \phi_2)$ of two periodic functions $\phi_1 = \phi_1(t)$, $\phi_2 = \phi_2(t)$ is not itself a periodic function of t (unless the corresponding periods T_1 and T_2 are rationally dependent $mT_1 = nT_2$, m, n integers). For this reason the motions of a completely integrable Hamiltonian system are not in general periodic, even though they can be expressed in terms of s periodic functions. Motions of this kind are sometimes called *conditionally periodic*.

In the particular case where the KAM theorem applies, $g = 1$ and the 4-dimensional mapping (3.6) possesses a *conserved quantity*, the iterates $(\mathbf{U}^n, \mathbf{V}^n, \mathbf{U}^{*n}, \mathbf{V}^{*n})$, i.e. $(\mathbf{P}^{2n}, \mathbf{Q}^{2n}, \mathbf{P}^{2n+1}, \mathbf{Q}^{2n+1})$, lie in a 3-dimensional manifold that for small k contains 2-dimensional invariant tori and accordingly the iterates must remain in the "interior" of the tori. In particular they must remain bounded as n increases so that blow-ups like those mentioned in the introduction cannot take place.

In more general circumstances the existence of invariant tori does not ensure the boundedness of the leap-frog solutions, because in higher dimensions a torus does not divide the space into an interior and an exterior part. It is possible for the points to escape to infinity (Arnold's diffusion) but this is a very slow process, completely different from the typical nonlinear explosion often encountered in leap-frog discretizations.

Before we close this section some remarks should be made in connection with the general case where complete integrability of the augmented Hamiltonian does not hold. Generically, in the neighbourhood of an equilibrium, Hamiltonian systems can readily be approximated by completely integrable systems, via Birkhoff's normal forms [3]. Unfortunately the leap-frog technique is only useful if the original equilibrium is a *centre* with eigenvalues $\pm\lambda i$, λ real [15]. These equilibria induce [15] in the corresponding augmented system equilibria with *double* eigenvalues $\pm\lambda i$ and the reduction to Birkhoff's normal form cannot be accomplished in the presence of this resonance. The discussion becomes then rather involved [21].

4. Schrödinger equations.

4.1. Original system. On introducing the real and imaginary parts p, q of $z = p + iq$, the complex equation (1.3) is transformed into

$$\frac{dp}{dt} = -(p^2+q^2)q, \qquad \frac{dq}{dt} = (p^2+q^2)p, \tag{4.1}$$

a Hamiltonian system with the quartic Hamiltonian function

$$H(p, q) = \tfrac{1}{4}(p^2+q^2)^2. \tag{4.2}$$

Any function $F(H(p, q))$ is then a conserved quantity of (4.1). In particular the quadratic invariant

$$r^2 = p^2 + q^2 \tag{4.3}$$

shows that in the (p, q)-plane the motions of (4.1) correspond to circumferences $r = \text{constant}$. On each circumference the polar angle α varies with a constant rate

$$\frac{d\alpha}{dt} = r^2$$

and therefore the period of the movement is given by

$$T = \frac{2\pi}{r^2}. \tag{4.4}$$

Of course the period of a Hamiltonian movement with one degree of freedom can be obtained without integrating the motion, via the formula

$$T = \frac{dA(h)}{dh}, \tag{4.5}$$

where $A(h)$ is the area of the (p, q)-region bounded by the curve $H(p, q) = h$.

4.2. Augmented system. This is given by

$$\frac{du}{dt} = -(u^{*2} + v^{*2})v^*, \tag{4.6a}$$

$$\frac{dv}{dt} = (u^{*2} + v^{*2})u^*, \tag{4.6b}$$

$$\frac{du^*}{dt} = -(u^2 + v^2)v, \tag{4.6c}$$

$$\frac{dv^*}{dt} = (u^2 + v^2)u, \tag{4.6d}$$

and according to Proposition 1 (i) is Hamiltonian. The Hamiltonian function is given by (see (3.3), (4.2))

$$\mathscr{H} = \tfrac{1}{4}[(u^2+v^2)^2 + (u^{*2}+v^{*2})^2]. \tag{4.7}$$

The conservation of (4.7) implies that the solutions of (4.6) remain bounded and therefore exist for all values of t.

Each quadratic original invariant gives rise to a quadratic augmented invariant [15]. Here (4.3) generates the invariant

$$e = uu^* + vv^*. \tag{4.8}$$

The conservation of e is obviously independent from the conservation of (4.7) and therefore we are dealing with a *completely integrable* system [3].

We now discuss the features of the motions of (4.6) which are helpful in describing the dynamics of the leap-frog discretization.

It is expedient to introduce the (noncanonical) polar coordinates

$$u=\rho\cos\theta,\qquad v=\rho\sin\theta,$$
$$u^*=\rho^*\cos\theta^*,\qquad v^*=\rho^*\sin\theta^*.$$

With these new variables (4.6) can be written

$$\frac{d\rho}{dt}=\rho^{*3}\sin(\theta-\theta^*),\tag{4.9a}$$

$$\frac{\rho d\theta}{dt}=\rho^{*3}\cos(\theta-\theta^*),\tag{4.9b}$$

$$\frac{d\rho^*}{dt}=-\rho^3\sin(\theta-\theta^*),\tag{4.9c}$$

$$\frac{\rho^*\,d\theta^*}{dt}=\rho^3\cos(\theta-\theta^*).\tag{4.9d}$$

Clearly (4.9) possesses the one-parameter group of transformations $\theta\to\theta+\beta$, $\theta^*\to\theta^*+\beta$. In fact these transformations are easily seen to be the flow generated by the function $e(u, v, u^*, v^*)$, so that e is the conserved quantity stemming from the group [3, Chap. 8, Cor. 9]. In polar coordinates the invariants (4.7), (4.8) become

$$\mathcal{H}=\tfrac{1}{4}(\rho^4+\rho^{*4}),\tag{4.10}$$

$$e=\rho\rho^*\cos(\theta-\theta^*).\tag{4.11}$$

(i) We first *fix* a value $e\neq 0$. The constraint (4.11) implies that ρ, ρ^* do not vanish in the motion and then the following equation for $\psi=\theta-\theta^*$ is a consequence of (4.9b)-(4.9d) and (4.11)

$$\frac{d\psi}{dt}=\left[\frac{\rho^{*4}-\rho^4}{\rho\rho^*}\right]\cos\psi=e^{-1}(\rho^{*4}-\rho^4)\cos^2\psi.\tag{4.12}$$

Also, from (4.9) and (4.11)

$$\frac{d}{dt}(\rho^{*4}-\rho^4)=-8e^3\tan\psi\cos^{-2}\psi.\tag{4.13}$$

The two equations (4.12)-(4.13) together with the constraint (4.11) provide a full set of relations for the functions $\rho(t)$, $\rho^*(t)$, $\psi(t)=\theta(t)-\theta^*(t)$. It is advisable to consider the variables

$$\mu=\rho^{*4}-\rho^4,\qquad \gamma=\operatorname{tg}\psi,$$

as with them (4.12)-(4.13) adopt the Hamiltonian form

$$\frac{d\mu}{dt}=-8e^3(\gamma+\gamma^3),\qquad \frac{d\gamma}{dt}=\frac{\mu}{e}.\tag{4.14}$$

Here μ, γ play respectively the roles of momentum and Lagrangian coordinate and the Hamiltonian is

$$J=\frac{\mu^2}{2e}+e^3(4\gamma^2+2\gamma^4)=8e^{-1}\mathcal{H}^2-2e^3.\tag{4.15}$$

The period of the solutions can be obtained by means of the formula (4.5). After a certain amount of manipulation in the resulting integral, we find the expression

$$\mathcal{H}^{-1/2}K\left(\frac{1}{2}-\frac{e^2}{4\mathcal{H}}\right), \tag{4.16}$$

where $K(m)$ denotes the complete elliptic integral of the first kind with parameter m [1]. To sum up, for solutions of (4.6) with $e \neq 0$, ρ, ρ^*, $\theta-\theta^*$ *vary periodically with the period* (4.16).

For a given nonzero value of e, it is easily proved from (4.10)-(4.11) that $\mathcal{H}$ cannot be smaller than $e^2/2$. When $\mathcal{H}$ has the minimum value $e^2/2$, we find in (4.15) that $J=0$, so that $\mu(t)\equiv 0$, $\gamma(t)\equiv 0$ or $\rho(t)\equiv\rho^*(t)$, $\theta(t)\equiv\theta^*(t)$ and therefore we are dealing with a diagonal solution of (4.6) with $\rho(t)=\rho^*(t)=r=\text{constant}$ and $d\theta/dt=d\theta^*/dt=d\alpha/dt=r^2$.

For $\mathcal{H}>e^2/2$ it may be concluded from (4.10)-(4.11) that the functions $\rho(t)$, $\rho^*(t)$ oscillate between the values

$$\begin{aligned}\rho_{\min}=\rho^*_{\min}&=(2\mathcal{H}-(4\mathcal{H}^2-e^4)^{1/2})^{1/4}<(2\mathcal{H}+(4\mathcal{H}^2-e^4)^{1/2})^{1/4}\\&=\rho_{\max}=\rho^*_{\max},\end{aligned} \tag{4.17}$$

and ψ between

$$-\pi/2<\psi_{\min}=-\arccos(e/\sqrt{2\mathcal{H}})<\arccos(e/\sqrt{2\mathcal{H}})=\psi_{\max}<\pi/2,$$

if $e>0$, or between

$$\pi/2<\psi_{\min}=\arccos(e/\sqrt{2\mathcal{H}})<\pi+\arccos-(e/\sqrt{2\mathcal{H}})=\psi_{\max}<3\pi/2,$$

if $e<0$. Here arc cos takes values in $[0,\pi]$ and it is assumed that, at $t=0$, the branches of arc tg giving $\theta=\operatorname{arc\,tg}(v/u)$, $\theta^*=\operatorname{arc\,tg}(v^*/u^*)$ are chosen so that $-\pi/2\leqq\psi(0)<3\pi/2$. As $\mathcal{H}$ approaches $e^2/2$ (near diagonal behaviour) the period of the oscillation tends to

$$\mathcal{H}^{-1/2}K(0)=\pi/(2\mathcal{H}^{1/2})=\pi/(\sqrt{2}r^2). \tag{4.18}$$

On the other hand, as $\mathcal{H}\uparrow\infty$ the period behaves like

$$K(\tfrac{1}{2})/\mathcal{H}^{1/2}\cong 1.854/\mathcal{H}^{1/2}, \tag{4.19}$$

so that the variations of ρ, ρ^* become increasingly rapid, and

$$\rho_{\min}=\rho^*_{\min}\sim e(4\mathcal{H})^{-1/4},$$
$$\rho_{\max}=\rho^*_{\max}\sim(4\mathcal{H})^{1/4},$$

leading to large amplitude oscillations in ρ, ρ^*. Finally

$$\lim\psi_{\max}=\pi/2,\quad \lim\psi_{\min}=-\pi/2\quad(\mathcal{H}\to\infty,\ e>0)$$

or

$$\lim\psi_{\max}=3\pi/2,\quad \lim\psi_{\min}=\pi/2\quad(\mathcal{H}\to\infty,\ e<0).$$

Thus, in the motion, the plane vectors (u, v), (u^*, v^*) (which are *collinear* in diagonal solutions) *may become nearly orthogonal.*

(ii) So far the analysis has been centered in the evolution of ρ, ρ^*, ψ given by (4.14). It is in principle possible to solve (4.14) by quadratures and in fact $\rho(t)$, $\rho^*(t)$, $\psi(t)$ can be expressed in terms of elliptic integrals. These expressions can in turn be taken into (4.9b) and (4.9d) and then a final quadrature yields $\theta(t)$, $\theta^*(t)$. However it is more advantageous to compute the action/angle variables of (4.6) which in particular allows a direct investigation of the periods similar to that in (4.5). The corresponding algebraic details become nevertheless rather heavy and can be seen in [21]. Here we just quote that (4.6) possesses, for $e \neq 0$, periods of the form

$$T_1 = \mathcal{H}^{-1/2} K\left(\frac{1}{2} - \frac{e^2}{4\mathcal{H}}\right), \qquad T_2 = T_1 \Phi\left(\frac{\mathcal{H}}{e^2}\right), \tag{4.20}$$

where Φ is a decreasing function of its argument. When $\mathcal{H}/e^2$ takes its minimum value $\frac{1}{2}$, $\Phi = 2\sqrt{2}$, while as $\mathcal{H}/e^2 \uparrow \infty$, Φ tends to 2. We *first* note that one of these periods is identical to (4.16) as could have been anticipated. *Secondly* (4.20) shows that (4.6) is *nondegenerate*, i.e. possesses two independent frequencies. Next for diagonal solutions with $\mathcal{H} = e^2/2$ and $\rho = \rho^* = r =$ constant, $\theta(t) = \theta^*(t) = \alpha(t)$, the formulas (4.18) prove that the periods T_1 and T_2 in (4.20) take respectively the values

$$\pi/(\sqrt{2}r^2), \qquad (\pi/(\sqrt{2}r^2))\Phi(\tfrac{1}{2}) = 2\pi/r^2. \tag{4.21}$$

In the second of these we recover the amount of time needed by $\theta = \theta^* = \alpha$ to describe a full cycle (see (4.4)), while the first provides the limit as $\mathcal{H}/e^2 \to \frac{1}{2}$ of the period of the evolution of ρ, ρ^*, $\theta - \theta^*$. *Finally* as $\mathcal{H}/e^2 \uparrow \infty$, the behaviour of T_1 is given by (4.19) whereas T_2/T_1 tends to 2. In particular, motions with $e = 0$ are *periodic* with the period

$$T_2 = 2T_1 \simeq 3.708\,\mathcal{H}^{-1/2}. \tag{4.22}$$

(iii) The solutions of (4.6) for which $e = 0$, excluded in (i), play an important role in the sequel. As $e \to 0$, (4.17) shows that $\rho_{\min} = \rho^*_{\min}$ tends to 0 and then polar coordinates are not suitable for the case $e = 0$, as they would introduce a fictitious singularity in the problem. We rather note in (4.8) that $e = 0$ implies that, as t varies, the plane vectors $(u(t), v(t))$, $(u^*(t), v^*(t))$ are constantly orthogonal. Then (4.6a)-(4.6b) show that the vectors $(du/dt, dv/dt)$ and (u, v) are parallel and thus the direction of (u, v) remains constant in the motion. The same remark applies of course to (u^*, v^*), which must constantly lie in a direction perpendicular to (u, v). We conclude that

$$u = w\cos\beta, \qquad v = w\sin\beta,$$
$$u^* = -w^*\sin\beta, \qquad v^* = w^*\cos\beta,$$

β constant $-\pi/2 < \beta \leqq \pi/2$, provides a suitable parameterization. This differs from polar coordinates in that now w, w^* may become negative. From (4.6a)-(4.6c) the equations for w, w^* are

$$\frac{dw}{dt} = -w^{*3}, \qquad \frac{dw^*}{dt} = w^3, \tag{4.23}$$

a system which is again Hamiltonian for the Hamiltonian function

$$\tfrac{1}{4}(w^4 + w^{*4}) = \tfrac{1}{4}[(u^2+v^2)^2 + (u^{*2}+v^{*2})^2] = \mathcal{H}.$$

The formula (4.5) for the period yields now

$$T = 4\mathcal{I}\mathcal{H}^{-1/2}, \tag{4.24}$$

where $\mathcal{I}$ is the integral

$$\mathcal{I} = \int_0^1 (1-\xi^4)^{1/4}\, d\xi = \tfrac{1}{4}B(\tfrac{5}{4}, \tfrac{1}{4}) \cong .927$$

(B denotes the standard Eulerian beta function [1]). Therefore solutions of (4.6) with $e = 0$ are *periodic* with the period (4.24) in agreement with our earlier findings in (4.22).

4.3. Leap-frog points.

(i) *Conditionally periodic character of the computed points.* In a Numerical Analysis context, an initial value problem given by the *original* system (4.1) along with initial conditions $p(0)$, $q(0)$ is numerically integrated by means of the leap-frog scheme with step-length k. The missing starting values P^1, Q^1 must be provided as approximations to $p(k)$, $q(k)$ and then the scheme generates points P^n, Q^n which are meant to approximate $p(nk)$, $q(nk)$. However, we noted in § 2 that the behaviour of P^n, Q^n can best be predicted from the *augmented* system, which therefore acts as a *modified* system in the sense of [4].

Here solutions of the original system have $r=\text{constant}$, while near-diagonal augmented solutions have ρ, ρ^* periodic with the period (4.18). We integrated numerically (4.1) with $k=.1$, $p(0)=1$, $q(0)=0$ and the missing P^1, Q^1 computed by Euler's rule. (Note that this yields a point $(P^0, Q^0, P^1, Q^1)=(U^0, V^0, U^{*0}, V^{*0})$ near the diagonal $U=U^*$, $V=V^*$.) The period (4.18) is then $\pi/\sqrt{2}\sim 2.22$. In Table 1 we have displayed against the time the modulus $|R^n-R^0|$, with $(R^n)^2=(U^n)^2+(V^n)^2=(P^{2n})^2+(Q^{2n})^2$. It is clear that when t approximately equals a whole number of periods then R^n assumes its initial value. We conclude that the computed leap-frog points exhibit a *conditionally periodic* behaviour analogous to that of solutions of the augmented system. (The value of k is not crucial in the experiment: other small values of k with starting point near the diagonal lead to the same period 2.22.)

(ii) *Conserved quantities, invariant tori, stability.* The invariant e in (4.8) is *quadratic* and therefore inherited by the leap-frog discretization [15]. Namely

$$e=U^nU^{*n}+V^nV^{*n}=P^{2n}P^{2n+1}+Q^{2n}Q^{2n+1}=\text{constant},\qquad n=0,1,\cdots. \tag{4.25}$$

This conservation is not strong enough to ensure the boundedness of the computed points, for the surfaces $e=\text{constant}$ are unbounded in $\mathbb{R}^4$.

The augmented system has been proved to be completely integrable and nondegenerate and then, as discussed in § 3, to each torus $e=\text{constant}$, $\mathcal{H}=\text{constant}$, invariant by the augmented flow, on which the periods (4.20) are far from resonant, there corresponds, for small k, a neighbouring, slightly distorted torus, invariant by the leap-frog mapping $(P^{2n}, Q^{2n}, P^{2n+1}, Q^{2n+1})\rightarrow(P^{2n+2}, Q^{2n+2}, P^{2n+3}, Q^{2n+3})$. In Fig. 1 we have plotted the even points (P^{2n}, Q^{2n}), $0\leqq n\leqq 2{,}500$, with $k=0.4$, $(p(0), q(0))$ randomly generated in $[0,1]\times[0,1]$ (uniform distribution), $P^0=p(0)$, $Q^0=q(0)$ and P^1, Q^1 computed from Euler's rule. The conditionally periodic character of the leap-frog points is noticeable and the whole picture has the appearance of a plane projection of a conditionally periodic flow on a bidimensional torus.

Figure 2 differs from Fig. 1 in that now both $(p(0), q(0))$ and (P^1, Q^1) were generated randomly. While this does not make much sense from the numerical analysis point of view (where (P^1, Q^1) must be close to $(p(0), q(0))$) it has the merit of showing the behaviour of the leap-frog points away from the diagonal. As expected from § 4.2 the oscillations in polar radius are now more pronounced and the ratio T_2/T_1 is smaller than it was near the diagonal.

The largest value of k for which an invariant torus of the augmented flow gives rise to an invariant leap-frog torus depends of course on the particular torus being considered [11], [18], [21]. In the present case the discussion is made simpler by the fact that in (3.5) or (3.6) the partial derivatives D_jH are homogeneous of degree 3, which entails that in the new scaled variables $\hat{P}=Pk^{1/2}$, $\hat{Q}=Qk^{1/2}$ the parameter k disappears from the formulae. We conclude that division by a factor of 4 of the

TABLE 1

n	t	t/T	$\lvert R^n - R^0 \rvert$
0	0.0	0.00	0.0
1	0.2	0.09	4.0×10^{-4}
2	0.4	0.18	1.4×10^{-3}
3	0.6	0.27	2.9×10^{-3}
4	0.8	0.36	4.2×10^{-3}
5	1.0	0.45	4.9×10^{-3}
6	1.2	0.54	4.9×10^{-3}
7	1.4	0.63	4.2×10^{-3}
8	1.6	0.72	2.9×10^{-3}
9	1.8	0.81	1.5×10^{-3}
10	2.0	0.90	4.1×10^{-3}
11	2.2	0.99	7.4×10^{-7}
12	2.4	1.08	3.9×10^{-4}
21	4.2	1.89	4.2×10^{-4}
22	4.4	1.98	2.9×10^{-7}
23	4.6	2.07	3.8×10^{-4}
32	6.4	2.88	4.3×10^{-4}
33	6.6	2.97	6.6×10^{-7}
34	6.8	3.06	3.7×10^{-4}
54	10.8	4.86	4.6×10^{-4}
55	11.0	4.95	1.8×10^{-6}
56	11.2	5.04	3.5×10^{-4}

step-length k doubles the diameter of the region in (U, U^*, V, V^*)-space where invariant tori exist.

When k is so *small* that the starting values (P^0, Q^0, P^1, Q^1) lie within an invariant torus, subsequent values $(P^{2n}, Q^{2n}, P^{2n+1}, Q^{2n+1})$, which lie in a 3-dimensional manifold $e = \text{constant}$, cannot leave the "interior" of the torus and therefore the leap-frog points remain bounded as n increases. However, numerical experiments, and/or a theoretical analysis of the behaviour at infinity, show that for k *large* (relative to the magnitude of the starting values) it is possible for P^n, Q^n to approach infinity in a very quick manner. The dynamics of this escape will be investigated next. We mention that such blow-ups are possible because the conservation of the positive-definite, quartic quantity (4.7) is not inherited by the leap-frog discretization.

(iii) ***Blow-ups.*** We first note that if a sequence (P^n, Q^n) of computed points blows up then (4.25) holds with a value of e that, as n increases, becomes negligible relatively both to the magnitude of the 4-dimensional vector $(P^{2n}, Q^{2n}, P^{2n+1}, Q^{2n+1}) = (U^n, V^n, U^{*n}, V^{*n})$ and to the value of $\mathcal{H}$. This implies that the parameter $\mathcal{H}/e^2$ which measures the amount of "nondiagonality" in the solutions of (4.6) increases. Also the magnitude of the gradient

$$\left(\frac{\partial}{\partial u}, \frac{\partial}{\partial v}, \frac{\partial}{\partial u^*}, \frac{\partial}{\partial v^*}\right) e = (u^*, v^*, u, v)$$

grows with the magnitude of the vector (u, v, u^*, v^*) and therefore the hypersurfaces $e = \text{constant}$ become closer in $\mathbb{R}^4$ as they approach infinity. This shows that if the sequence (P^n, Q^n) tends to infinity then the points (P^n, Q^n), while remaining in the original surface (4.25), become closer to the hypersurface $e = 0$. We conclude that the

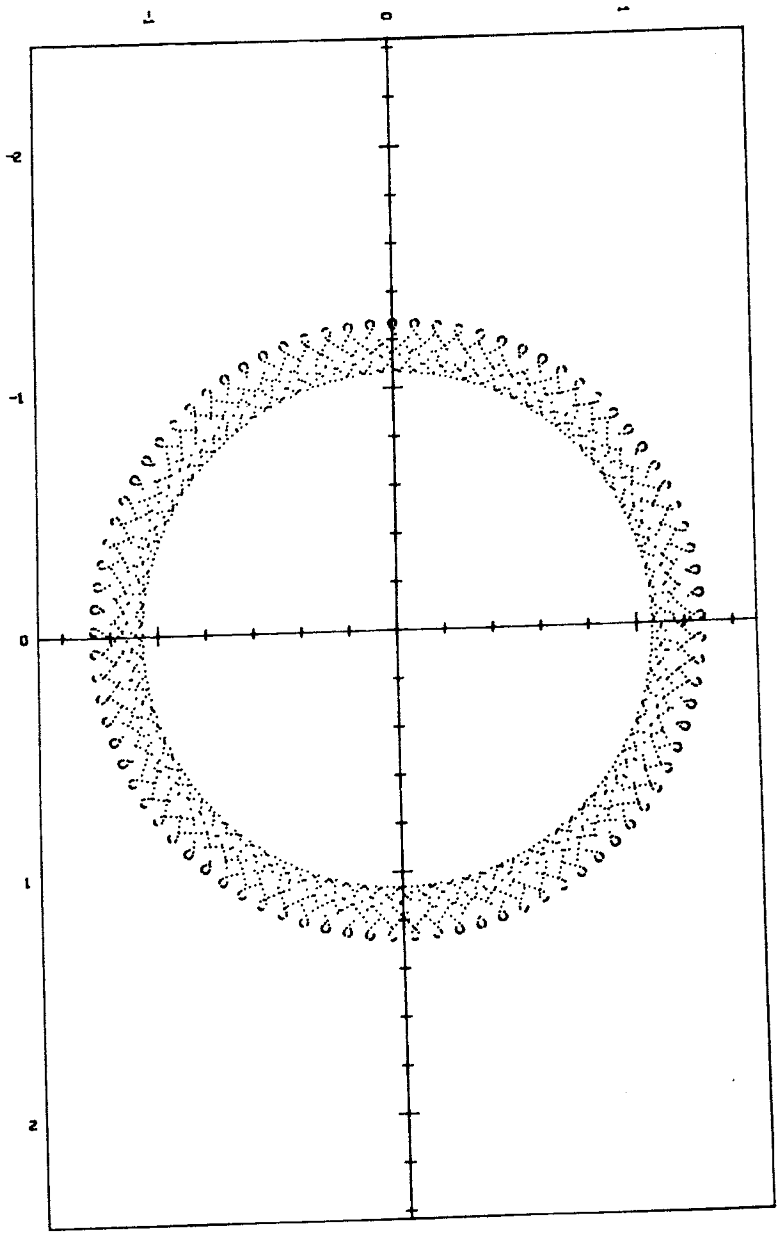

FIG. 1

large n behaviour of blowing-up solutions can be approximately described by the behaviour of leap-frog solutions with $e=0$. Note that this sort of solution with the vectors (P^{2n}, Q^{2n}), (P^{2n+1}, Q^{2n+1}) orthogonal to each other is the farthest away from the diagonal behaviour.

Considerations similar to those in § 4.2(iii) show that when $e=0$ we may write

$$P^{2n}=U^n=W^n\cos\beta, \qquad Q^{2n}=V^n=W^n\sin\beta,$$
$$P^{2n+1}=U^{*n}=-W^{*n}\sin\beta, \qquad Q^{2n+1}=V^{*n}=W^{*n}\cos\beta, \tag{4.26}$$

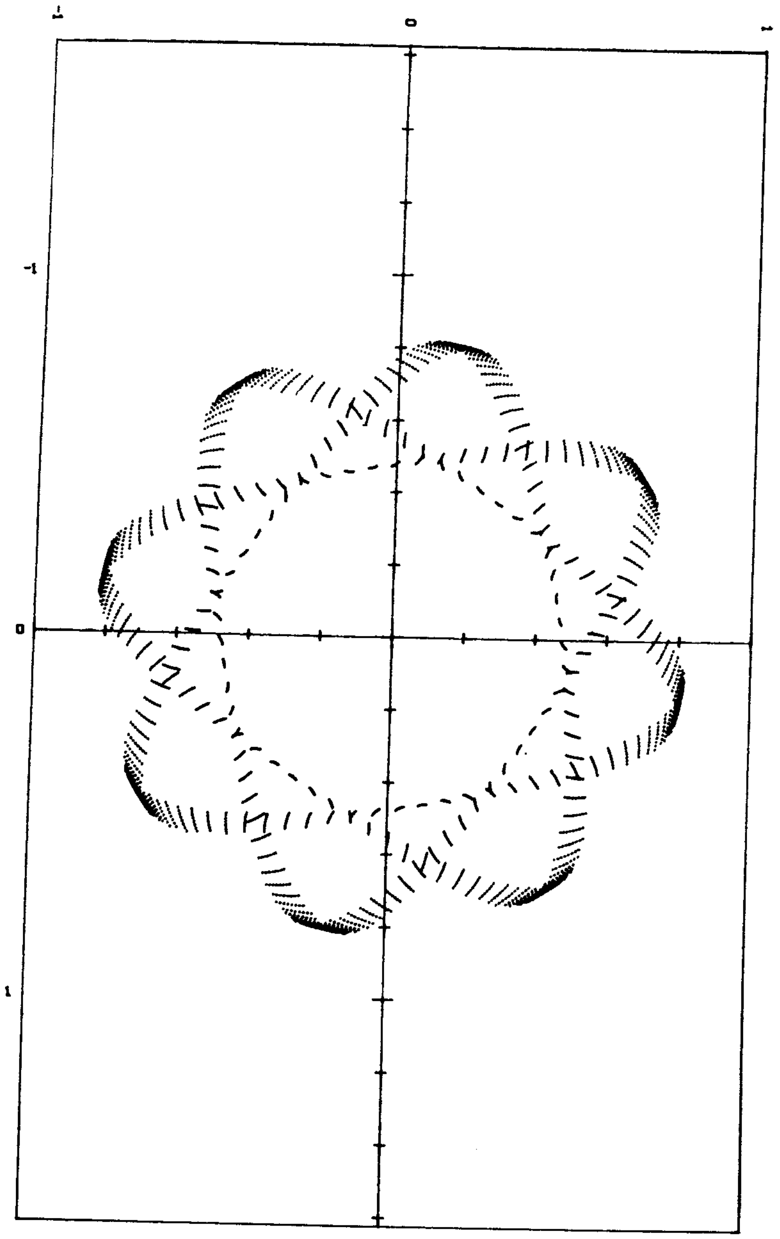

FIG. 2

where β is fixed, $-\pi/2 < \beta \leqq \pi/2$ and W^n, W^{*n} satisfy for $n = 0, 1, \cdots$

$$W^{n+1} = W^n - 2k(W^{*n})^3, \qquad W^{*n+1} = W^{*n} + 2k(W^{n+1})^3. \tag{4.27}$$

Clearly (4.27) is a one-step consistent discretization of the one-degree of freedom Hamiltonian system (4.23). It is easily checked that (4.27) preserves area and therefore the KAM theory applies once more, so that for *small* values of k there will be invariant curves surrounding the origin in (W, W^*)-space and guaranteeing boundedness. Note that now with $e = 0$ the KAM theory is applied to (4.27) as an approximation to the flow of (4.23), while before it was applied to (4.6) and its leap-frog discretization. In this respect note that the hypotheses of the KAM theorem for (4.6) were only checked for the case of $e \neq 0$ and that for $e = 0$ the two periods of (4.6) are rationally dependent $T_2 = 2T_1$.

In a numerical experiment we took $\hat{W}^{*0} = 0$ and left the nondimensional quantity $\hat{W}^0 = \hat{W}^0(2k)^{1/2} = \lambda$ as a free parameter. By bisecting λ intervals, we found that $\lambda = .6321$ is the smallest value for which an overflow takes place before 5,000 points (W^n, W^{*n}) can be computed. Figure 3 depicts a thousand points of each of the orbits $\lambda = .4, .5, .6, .632$. The values $\lambda = .4, .5$ lead, as far as the graph can tell, to KAM invariant curves. The value .6 corresponds, very approximately, to a 10-periodic point and $\lambda = .632$ generates the typical islands around this periodic point. The orbit of the overflow value .6321 (not plotted) lies in a stochastic region. The existence of periodic points and invariant curves can of course be more accurately investigated by studying the corresponding rotation numbers.

Finally we scale out k in (4.27) to get

$$\hat{W}^{n+1} = \hat{W}^n - (\hat{W}^{*n})^3, \qquad \hat{W}^{*n+1} = \hat{W}^{*n} + (\hat{W}^{n+1})^3. \tag{4.28}$$

If W^{*n} is considerably larger in magnitude than W^n, then

$$\hat{W}^{n+1} \cong -(\hat{W}^{*n})^3, \qquad \hat{W}^{*n+1} \cong (\hat{W}^{n+1})^3, \tag{4.29}$$

so that

$$\hat{W}^{*n+1} \cong -(\hat{W}^{*n})^9. \tag{4.30}$$

Thus at the new time-step $n+1$ the assumption $|\hat{W}^*| \gg |\hat{W}|$ leading from the exact (4.28) to the approximation (4.29) certainly remains valid and in the step $n+1 \to n+2$ a new substantial increase like (4.30) will take place. These violently growing solutions of (4.28) actually describe, via the scaling and (4.26), growing leap-frog solutions (P^n, Q^n) lying on the hypersurface $e = 0$. It was found experimentally that for any $e \neq 0$ unbounded leap-frog sequences were attracted by the violently growing solutions just mentioned. This agrees with our former discussion and with the material in [22].

4.4. The cubic Schrödinger equation. Experiments were conducted in order to examine blow-ups like the one reported in [17]. The time-step k was always taken to satisfy the stability condition for the linear equation (1.2). It turns out that the spatial (dispersive) term z_{xx} plays little or no role in the dynamics of the blow-up, which is governed by the nonlinearity $|z|^2 z$ and confined to a very narrow section of the x-axis. Thus the details of the blow-up are very similar to those for (1.3) we have extensively discussed. Further details can be seen in [21].

5. Conclusions. The concept of augmented system was introduced in [15] as a means to describe the behaviour of leap-frog discretizations of (original) differential systems. In the present paper we have considered the particular case of Hamiltonian original systems. It has been shown that the corresponding augmented system is also Hamiltonian and that the leap-frog discretization induces a canonical transformation in the augmented phase space. These results lead to the possibility of applying the KAM theory which in turn may rigorously guarantee that, as the time increases without bound, the numerical approximations remain bounded.

The general results of the paper (§ 3) have been applied (§ 4) to the study of the stability of x-independent solutions of the cubic Schrödinger equation. It has been

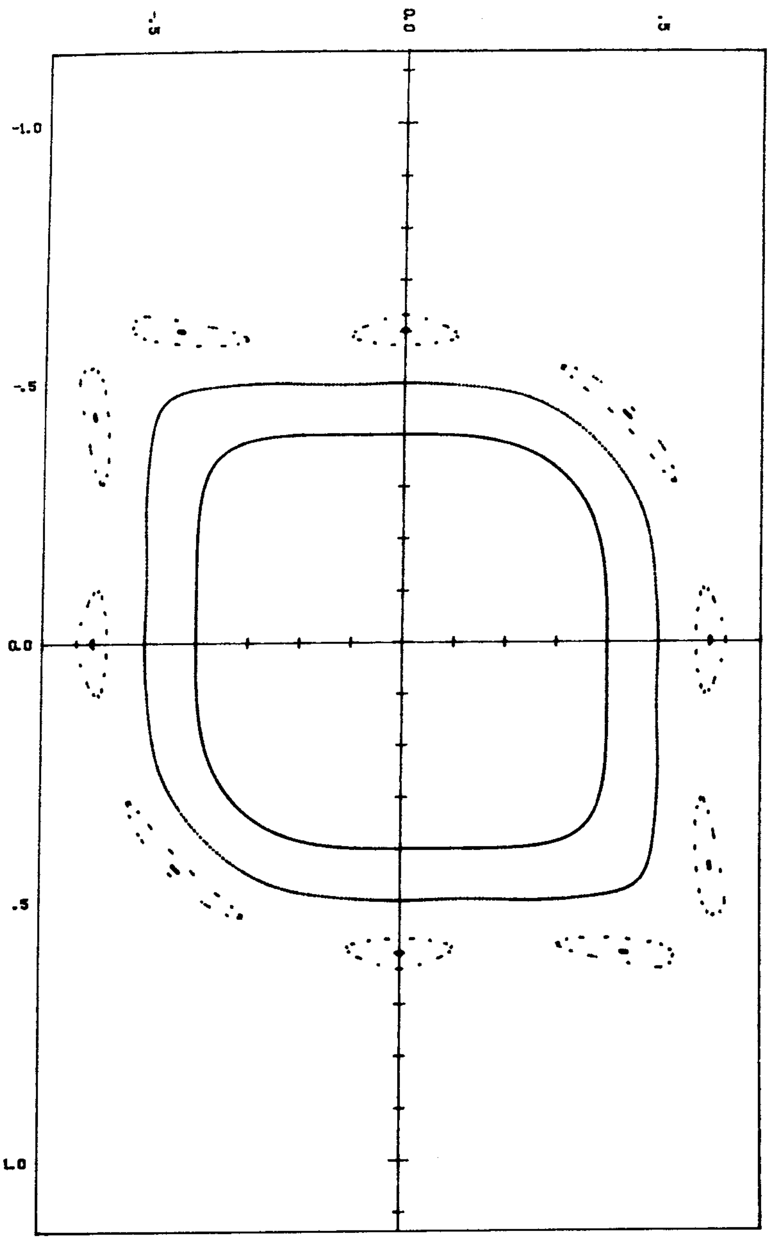

FIG. 3

shown that if the time-step k is small (relative to the magnitude of the starting point) then, as the time increases, the computed points remain bounded, while if k is large the numerical solution will blow up. This behaviour is quite different from that investigated in [22]. There, the leap-frog blow-up takes place for any k, no matter how small: a smaller value of k delays but not precludes the occurrence of the blow-up. Although our findings restore to some extent our faith in leap-frog schemes (cf. [17]) we fear that the techniques used in this paper are not powerful enough to show a priori how to choose k to avoid blow-ups in a practical computation.

The dynamics of the blow-up of x-independent solutions of the cubic Schrödinger equation has been described in detail. Experiments suggest that the blow-up of more general solutions strongly resembles that of the x-independent case.

The augmented system has also been successfully applied to predict a number of features of the leap-frog points, such as the periodic behaviour of their polar radius.

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