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Numerical Solution of Hamiltonian Systems in Reaction-Diffusion by Symplectic Difference Schemes

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Discrete models in time and space of Fishers equation, $\partial u/\partial t = \partial^2 u/\partial x^2 + f(u)$, in reaction diffusion are numerous in mathematical biology (Weinberger, *SIAM J. Math. Anal.* **13**, 353 (1982) and the references therein). For $f(u) = u(1-u)$ and no dissipation, May (*Nature* **261**, 459 (1976)), using the Euler discretization of the time derivative, found stable solutions (period 2 in time) provided the time step satisfies $2 < k \leqslant \sqrt{6}$, the linearized stability for period 1 solutions being $0 < k \leqslant 2$. When the dissipation term in discretised form is added to May's ordinary difference scheme, it is shown by Griffiths and Mitchell (*IMA J. Numer. Anal.* **8**, 435 (1988); *Numerical Analysis*, Pitman Res. Notes in Math., Vol. 140, Longman, Sci. Tech., Harlow, 1986), and Sleeman (*Proc. Roy. Soc. London Ser. A* **425**, 17 (1989)) that the stable period 2 in time solutions persist. Here it is shown (Sleeman, *op. cit.*), that when the dissipation term in continuous form is added to May's difference equation, solutions period 2 in time for each value of x satisfy a Hamiltonian system in space. The latter, being non integrable, is solved numerically by symplectic difference schemes constructed to maintain the values of the Hamiltonain energy up to large values of the space variable (Feng Kang and his co-authors (*J. Comput. Math.* **4**, 279 (1986); Lect. Notes in Math., Vol. 1297, Springer-Verlag, New York, 1987)). The shape of the solution, in calculations involving 200,000 space steps, is shown to depend crucially on the type and location of the fixed points of the Hamiltonian system in phase space at the position of the initial data at $x = 0$ relative to these fixed points.

1. INTRODUCTION

One of the outstanding problems in numerical analysis is the assessment of stability of numerical solutions of non-linear time-dependent partial difference equations which arise in the physical sciences and mathematical biology, either as models in their own right or as discretizations of non-linear partial differential equations. The problem is particularly severe when solutions are required for long periods of time and the standard Von Neumann-type stability analysis, although remaining a useful guide locally, is no longer adequate. Time-dependent problems can be classified broadly as dissipative or non-dissipative, it being possible in many cases to represent the latter by a Hamiltonian system the exact solution of which guarantees that the Hamiltonian energy remains constant with increasing time. Although near conservation of the Hamiltonian energy is necessary for obtaining an

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accurate numerical solution with increasing time, it is not sufficient. Nevertheless it is a useful guide, and Feng Kang and his co-workers [1, 2] have developed symplectic difference schemes as a means of obtaining accurate numerical solutions of Hamiltonian systems. One of these schemes is Leap frog which Sanz Serna and Vadillo [7] have shown preserves the symplectic structure of the phase space in numerical solutions of the complex equation,

$$i\frac{dz}{dt}+|z|^2 z=0.$$

Here we consider discretisations first in time and then in space of Fisher's equation

$$\frac{\partial u}{\partial t}=\frac{\partial^2 u}{\partial x^2}+u(1-u), \tag{1.1}$$

where the presence of the diffusion term presents severe problems as far as analytical studies of (1.1) are considered, Fife and McLeod [3], unless wave solutions of constant speed are assumed.

Already in the absence of diffusion, May [5] has shown that a discrete model in population dynamics

$$U^{n+1}(x)=U^n(x)+kU^n(x)(1-U^n(x)), \qquad n=0, 1, 2, ... \tag{1.2}$$

has stable solutions (period 2 in time) provided the time step satisfies $2<k\leqslant\sqrt{6}$, where (1.2) can be identified as the Euler discretisation of the logistic growth Riccati equation

$$\frac{du}{dt}=u(1-u).$$

An extension of May's results to a fully discretised model of (1.1) has been carried out by Griffiths and Mitchell [4, 6] and Sleeman [8], where periodic solutions in time and space are obtained for parameter values (grid sizes) beyond those required for linearised stability, suggesting that periodic solutions are basic to many discrete biological systems. Similar periodic behaviour, for discretisations of more general parabolic equations, has been analysed by Sleeman [9] and Stuart [10, 11].

In the present study, we look for solutions of discrete forms of (1.1), models in their own right, which are period 2 in time, but no longer necessarily periodic in space. This is achieved by first considering the discrete time model in population dynamics in the general form

$$U^{n+1}(x)=Q[U^n(x)], \qquad n=1, 2, ..., \tag{1.3}$$

where $U^n(x)$ represents the population density at time n at the point x of the habitat. In this model the population is measured from time to time, it being impossible to measure populations continuously at all times. The model (1.3), for various forms of the operator Q, is discussed at length in Weinberger [12] and other references therein.

The addition of a diffusion term to (1.2) at a location x leads to (1.3) in the form

$$U^{n+1}(x) = U^n(x) + k\left(\frac{d^2U^n(x)}{dx^2}\right) + kU^n(x)(1 - U^n(x)), \qquad n = 0, 1, 2, ..., \tag{1.4}$$

where multiplication of the dissipative term by a parameter $k(>0)$ is for convenience, since any positive factor of this term can be introduced (or removed) by making a suitable change in the x-variable.

The first aim of the paper is to show that solutions (period 2 in time) of (1.4) satisfy a continuous Hamiltonian system in *space*. The further aim is to solve the Hamiltonian system numerically for large values of x, the space variable, by symplectic difference schemes, the latter devised by Feng Kang and his co-workers [1, 2] to maintain a constant value of the Hamiltonian energy.

2. Derivation of Hamiltonian System

Following [8], we now consider solutions of (1.1) which are period 2 in time for each value of x, viz.,

$$U^n(x) = q_1(x) + (-1)^n q_2(x), \qquad n = 0, 1, 2, ... \tag{2.1}$$

Substitution of (2.1) into (1.4) leads to the 2-system,

$$\begin{aligned} q_1'' &= q_1^2 + q_2^2 - q_1 \\ q_2'' &= \left(2q_1 - \frac{2}{k} - 1\right) q_2, \end{aligned} \tag{2.2}$$

where the dash denotes differentiation with respect to x. This can be written in the first order form,

$$\begin{aligned} p_1' &= q_1^2 + q_2^2 - q_1 \\ p_2' &= \left(2q_1 - \frac{2}{k} - 1\right) q_2 \\ q_1' &= p_1 \\ q_2' &= p_2. \end{aligned} \tag{2.3}$$

Now the vector functions $\mathbf{p}(x)$, $\mathbf{q}(x) \in \Re^2$ form a Hamiltonian system of ordinary differential equations if there exists a function $H(\mathbf{p}(x), \mathbf{q}(x))$ such that

$$\frac{\partial H}{\partial p_i} = \frac{dq_i}{dx}, \qquad -\frac{\partial H}{\partial q_i} = \frac{dp_i}{dx} \qquad (i = 1, 2). \tag{2.4}$$

For the first order system (2.3), the conditions (2.4) are satisfied, provided

$$H(\mathbf{p}, \mathbf{q}) = \frac{1}{2}(p_1^2 + p_2^2) + \frac{1}{2}(q_1^2 + q_2^2) - \left(q_1 - \frac{1}{k}\right) q_2^2 - \frac{1}{3} q_1^3 \tag{2.5}$$

and, if we introduce

$$\mathbf{z} = (\mathbf{p}, \mathbf{q})^{\mathrm{T}} \in \Re^4,$$

(2.3) may be expressed in the form

$$\frac{d\mathbf{z}}{dx} = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix} \frac{\partial H}{\partial \mathbf{z}} = J^{-1} \frac{\partial H}{\partial \mathbf{z}}, \tag{2.6}$$

where

$$J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} = -J^{\mathrm{T}} = -J^{-1}$$

and $I \in \Re^2$ is the unit matrix. In (2.6), H is the sum of the kinetic and potential energies and so it is a *natural* Hamiltonian. In addition, the Hamiltonian system (2.3) (or 2.6)) is deemed to be integrable (possible to find an explicit solution) if two integrals of motion (the Hamiltonain and one other) are known. In this case, the other invariant integral,

$$\psi(z(t)) \equiv \psi(z(0)),$$

may be obtained from

$$\{\psi, H\} = 0,$$

where $\{\ \}$ is the Poisson bracket for the pair of differentiable functions ψ and H, provided, of course, it exists. In [8] it is proved that (2.5) is non-integrable in the sense that there is no analytic ψ satisfying $\{\psi, H\} = 0$.

Now, Hamiltonian formalism has the property of being area preserving (symplectic); i.e., the sum of the areas of canonical variable pairs, projected on any two-dimensional surface in phase space, is time invariant (Feng Kang *et al.* [1, 2]). Our aim in solving the Hamiltonian system numerically is to test the ability of area preserving (symplectic) difference schemes to preserve the Hamiltonian energy in long time calculation.

Prior to discretising in space, however, we analyse (2.3) in relation to its fixed points,

$$\begin{aligned} &\text{(i)} && (0,0,0,0)^{\mathrm{T}} \\ &\text{(ii)} && (0,0,1,0)^{\mathrm{T}} \\ &\text{(iii)} && \left(0,0,\frac{1}{2k}(k+2),\frac{1}{2k}\sqrt{k^2-4}\right)^{\mathrm{T}} \\ &\text{(iv)} && \left(0,0,\frac{1}{2k}(k+2),-\frac{1}{2k}\sqrt{k^2-4}\right)^{\mathrm{T}}, \end{aligned} \tag{2.7}$$

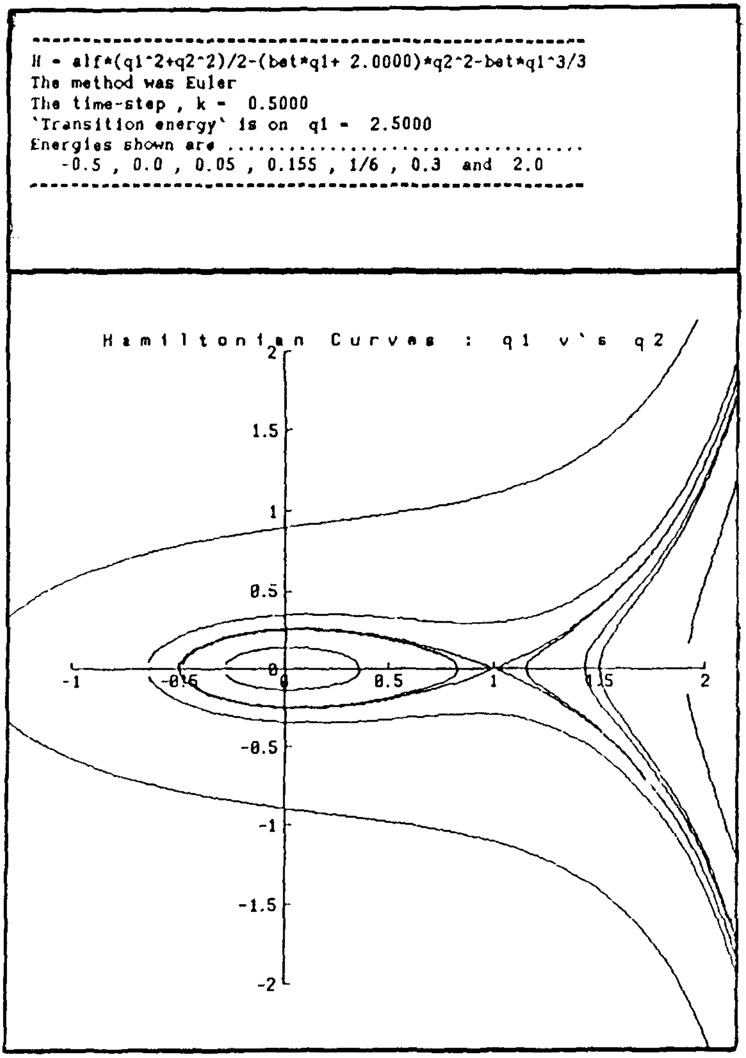

FIGURE 1

obtained by putting $p'_1 = p'_2 = q'_1 = q'_2 = 0$ in (2.3). Linearised stability about the fixed points is obtained by putting

$$(p_1, p_2, q_1, q_2)^{\mathrm{T}} \mapsto (p_1, p_2, q_1, q_2)^{\mathrm{T}} + (\varepsilon_1, \varepsilon_2, \varepsilon_3, \varepsilon_4)^{\mathrm{T}},$$

which leads to

$$\boldsymbol{\varepsilon}' = J\boldsymbol{\varepsilon} + O(\boldsymbol{\varepsilon}^2),$$

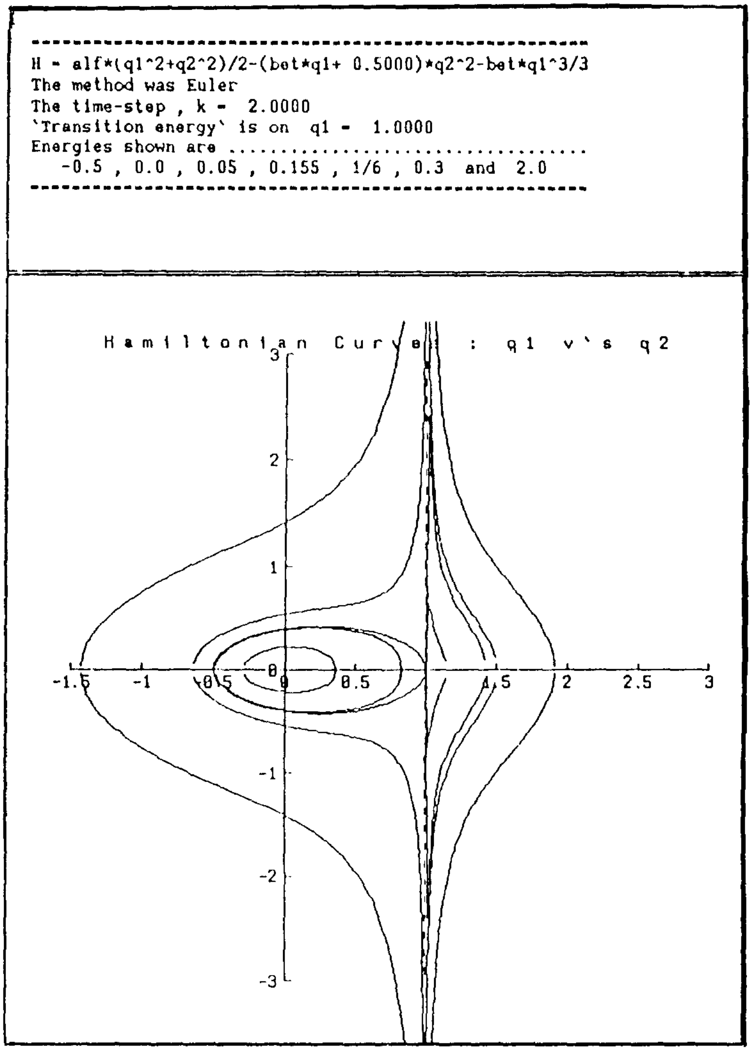

FIGURE 2

where the Jacobian is given by

$$J = \begin{pmatrix} 0 & 0 & 2q_1 - 1 & 2q_2 \\ 0 & 0 & 2q_2 & 2q_1 - 1 - (2/k) \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \tag{2.8}$$

and $\boldsymbol{\varepsilon} = (\varepsilon_1, \varepsilon_2, \varepsilon_3, \varepsilon_4)^{\mathrm{T}}$. We see from (2.7) that the fixed points (iii) and (iv) are

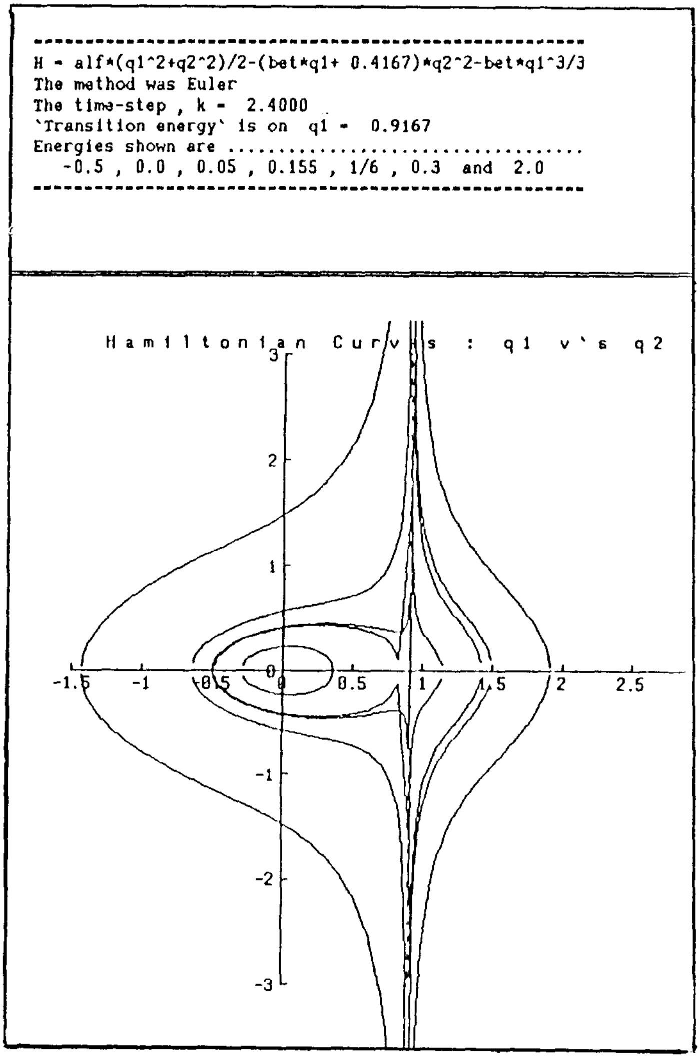

FIGURE 3

imaginary if $0<k<2$. Returning to the matrix J, given by (2.8), its eigenvalues satisfy the quartic equation,

$$\lambda^4-2\left(2q_1-1-\frac{1}{k}\right)\lambda^2+\left[4(q_1^2-q_2^2)-4\left(1+\frac{1}{k}\right)q_1+1+\frac{2}{k}\right]=0, \tag{2.9}$$

which, at the fixed points (2.7), become

$$\begin{aligned} &\text{(i)} && \pm i,\ \pm i\sqrt{1+\frac{2}{k}} \\ &\text{(ii)} && \pm 1,\ \pm i\sqrt{\frac{1}{k}(2-k)} \\ &\text{(iii), (iv)} && \pm\sqrt{\frac{1}{k}\pm\frac{1}{k}\sqrt{k^2-3}} \qquad (k\geqslant 2). \end{aligned} \tag{2.10}$$

Hence (i) is a centre, (ii) is a saddle point, and (iii) and (iv) exist and are saddle points if $k\geqslant 2$. This linear prediction appears to survive non-linear effects as can be seen from Sleeman [8], and Figs. 1, 2, and 3 where graphs of q_2 (vertical axis) against q_1 (horizontal axis) with $p_1\equiv 0\equiv p_2$ are plotted for constant Hamiltonian values and various values of k. These indicate the presence of a centre and saddle point(s) as given by (2.10). It should be remembered, however, that these diagrams are two-dimensional pictures of a problem in four dimensions. A significant energy value in (2.5) is $H=\frac{1}{6}$. For values of $H<\frac{1}{6}$, we can see the existence of closed periodic orbits.

3. Discretisations in Space

We now return to the task of discretising the Hamiltonian system (2.3) in space maintaining the area preservation property as far as possible; i.e., we look for symplectic difference representations of (2.3). A large selection of these are available, courtesy of Feng Kang and his fellow workers [1, 2], and for the purposes of comparison we choose

(I) Euler (not symplectic)

(II) A-II-1 (staggered Euler, symplectic)

(III) Leap frog (symplectic).

In order to derive these difference schemes for solving (2.3) numerically, we put $x=mh$ ($m=0, 1, 2, ...$), with h the grid size in space, and use the general difference replacement

$$f'_m=\frac{1}{h}(\phi\Delta_x+(1-\phi)\nabla_x)f_m, \qquad 0\leqslant\phi\leqslant 1,$$

where f is p_1, p_2, q_1, q_2 in turn. Euler is obtained when $\phi=1$ and Leap frog when $\phi=\frac{1}{2}$. Staggered Euler is obtained by updating the values of p_1 and p_2 in (2.3).

4. Stability about Fixed Points

I. *Euler*

The difference scheme is

$$\begin{bmatrix} p_1 \\ p_2 \\ q_1 \\ q_2 \end{bmatrix}^{m+1} = \begin{bmatrix} p_1 + h(q_1^2 + q_2^2 - q_1) \\ p_2 + h(2q_1 - (2/k) - 1)q_2 \\ q_1 + hp_1 \\ q_2 + hp_2 \end{bmatrix}^m, \qquad m = 0, 1, 2, ..., \tag{4.1}$$

where the eigenvalues, λ_i $(i = 1, 2, 3, 4)$, of the Jacobian of (4.1) are given by

$$(D^2 - h^2A)(D^2 - h^2B) - 4h^4C^2 = 0, \tag{4.2}$$

where $A = 2q_1 - 2/k - 1$, $B = 2q_1 - 1$, $C = q_2$, $D = 1 - \lambda$. The fixed points of (4.1) are obtained by solving the system of equations,

$$q_1^2 + q_2^2 - q_1 = 0$$

$$\left(2q_1 - \frac{2}{k} - 1\right) q_2 = 0$$

$$p_1 = p_2 = 0,$$

giving (p_1, p_2, q_1, q_2) the values

$$\begin{aligned} &\text{(i)} && (0, 0, 0, 0) \\ &\text{(ii)} && (0, 0, 1, 0) \\ &\text{(iii)} && \left(0, 0, \frac{1}{2} + \frac{1}{k}, \frac{1}{2k}\sqrt{k^2 - 4}\right) \\ &\text{(iv)} && \left(0, 0, \frac{1}{2} + \frac{1}{k}, -\frac{1}{2k}\sqrt{k^2 - 4}\right). \end{aligned} \tag{4.3}$$

Fixed points (iii) and (iv) are real if $k \geqslant 2$. Substitution of (4.3) in turn into (4.2) results in the eigenvalues,

$$\begin{aligned} &\text{(i)} && 1 \pm ih,\ 1 \pm ih\sqrt{1 + \frac{2}{k}} \\ &\text{(ii)} && 1 \pm h,\ 1 \pm ih\sqrt{\frac{1}{k}(2 - k)} \\ &\left.\begin{matrix}\text{(iii)} \\ \text{(iv)}\end{matrix}\right\} && 1 \pm h\sqrt{\frac{1}{k}(1 \pm \sqrt{k^2 - 3}} \qquad (k \geqslant 2). \end{aligned} \tag{4.4}$$

II. *Staggered Euler*

Updating the values of p_1 and p_2 in (2.3) leads to the difference system,

$$\begin{bmatrix} p_1 \\ p_2 \\ q_1 \\ q_2 \end{bmatrix}^{m+1} = \begin{bmatrix} p_1 + h(q_1^2 + q_2^2 - q_1) \\ p_2 + h(2q_1 - (2/k) - 1)q_2 \\ q_1 + h(p_1 + h(q_1^2 + q_2^2 - q_1)) \\ q_2 + h(p_2 + h(2q_1 - (2/k) - 1)q_2) \end{bmatrix}^m, \qquad m = 0, 1, 2, \ldots, \tag{4.5}$$

where the eigenvalues, μ_i ($i = 1, 2, 3, 4$), of the Jacobian of (4.5) are given by

$$(D^2 - h^2A(1-D))(D^2 - h^2B(1-D)) - 4h^4C^2(1-D)^2 = 0. \tag{4.6}$$

The fixed points of (4.5) are again given by (4.3). Substitution of (4.3) in turn into (4.6) gives the eigenvalues,

$$\begin{aligned} &\text{(i)} \quad \begin{cases} 1 - \dfrac{1}{2}h^2 \pm \dfrac{1}{2}ih\sqrt{4-h^2} \\[2ex] 1 - \dfrac{1}{2}\left(1 + \dfrac{2}{k}\right)h^2 \pm \dfrac{1}{2}ih\sqrt{\left(1+\dfrac{2}{k}\right)\left(4 - \left(1 + \dfrac{2}{k}\right)h^2\right)} \end{cases} \\ &\text{(ii)} \quad \begin{cases} 1 + \dfrac{1}{2}h^2 \pm \dfrac{1}{2}h\sqrt{4+h^2} \\[2ex] 1 - \dfrac{1}{2}\left(\dfrac{2-k}{k}\right)h^2 \pm \dfrac{1}{2}ih\sqrt{\left(\dfrac{2-k}{k}\right)\left[4 - \left(\dfrac{2-k}{k}\right)h^2\right]} \end{cases} \end{aligned} \tag{4.7}$$

together with extremely complicated expressions for the eigenvalues in the cases (iii) and (iv).

III. *Leap Frog*

The difference scheme is

$$\begin{bmatrix} p_1 \\ p_2 \\ q_1 \\ q_2 \end{bmatrix}^{m+1} = 2h\begin{bmatrix} q_1^2 + q_2^2 - q_1 \\ (2q_1 - (2/k) - 1)q_2 \\ p_1 \\ p_2 \end{bmatrix}^m + \begin{bmatrix} p_1 \\ p_2 \\ q_1 \\ q_2 \end{bmatrix}^{m-1}, \qquad m = 0, 1, 2, \ldots. \tag{4.8}$$

Writing (4.8) as a first-order system, we obtain the eigenvalues, λ_i ($i = 1, 2, \ldots, 8$), from the equation

$$((\lambda^2 - 1)^2 - 4h^2A\lambda^2)((\lambda^2 - 1)^2 - 4h^2B\lambda^2) - 64h^4C^2\lambda^4 = 0. \tag{4.9}$$

Substitution of the fixed points given by (4.3) into (4.9) gives the eigenvalues,

$$
\begin{aligned}
&\text{(i)} \quad \begin{cases} \pm\sqrt{1-h^2} \pm ih \\ \pm\sqrt{1-h^2\left(1+\dfrac{2}{k}\right)} \pm ih\sqrt{1+\dfrac{2}{k}} \end{cases} \\
&\text{(ii)} \quad \begin{cases} \pm\sqrt{1+h^2} \pm h \\ \pm\sqrt{1-h^2\left(\dfrac{2-k}{k}\right)} \pm ih\sqrt{\dfrac{2-k}{k}} \end{cases}
\end{aligned}
\tag{4.10}
$$

together with extremely complicated expressions for fixed points (iii) and (iv), the latter, of course, only existing if $k \geqslant 2$. It is interesting to compare the stability of the continuous and discrete systems, the latter restricted to $0 < k \leqslant 2$, about the fixed points given by (i) and (ii) of (2.7). The main conclusions from the comparisons which come from (2.10), (4.4), (4.7), and (4.10) are as follows:

Fixed point (i): In the continuous case, all four eigenvalues lie on the imaginary axis. With A-II-1 and Leap frog, all eigenvalues give $|\lambda| = 1$, leading to neutral stability, the property of a centre. Euler, however, gives $|\lambda| > 1$ for some of the eigenvalues irrespective of the values of k and h, and so is unstable.

Fixed point (ii): In the continuous case, two eigenvalues are on the imaginary axis and two on the real axis, the latter causing the instability associated with a saddle point. In the discrete case, A-II-1 and Leap frog mimic the continuous case by having $|\lambda| = 1$ for the eigenvalues corresponding to those on the imaginary axis for the continuous case, and $|\lambda| > 1$ for the remaining eigenvalues. Euler has $|\lambda| > 1$ for three of the eigenvalues and $|\lambda| < 1$ for the fourth eigenvalue and so it is unstable for all paths passing through the fixed point in the phase diagram.

5. Numerical Results

A preliminary conclusion from the previous section is that the symplectic schemes, A-II-1 and Leap frog, appear suitable schemes for the numerical solution of (2.3) whereas the non-symplectic Euler scheme appears very much in the doubtful category. To confirm this, and to see how well the symplectic schemes behave in a calculation for large x based on (2.3), we carry out numerical experiments for all three schemes, where the variable quantities are

(i) Initial values of $(p_1, p_2, q_1, q_2)^{\mathrm{T}}$,

(ii) Time step k,

(iii) Space step h.

Most of the numerical results quoted are for $k = \frac{1}{2}$, $h = 10^{-4}$ leaving the initial condition as the variable parameter. To limit the random nature of initial data, we

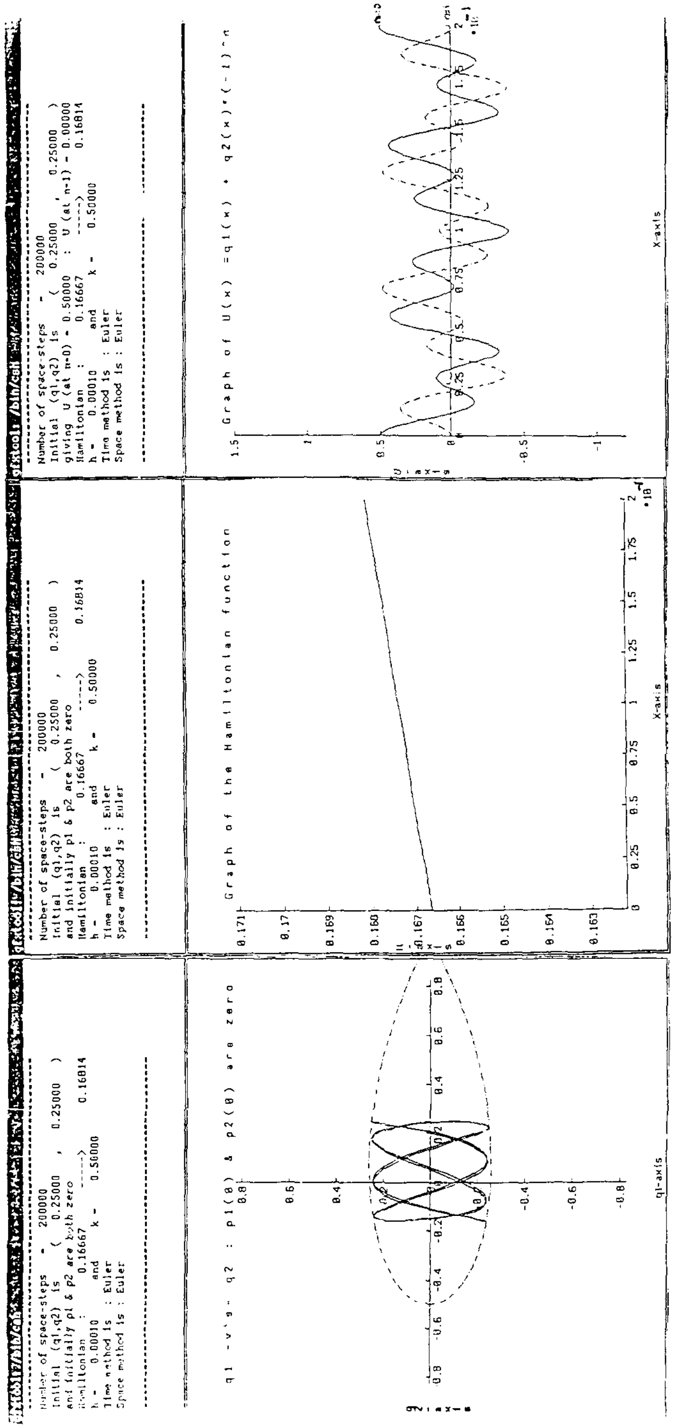

FIGURE 4

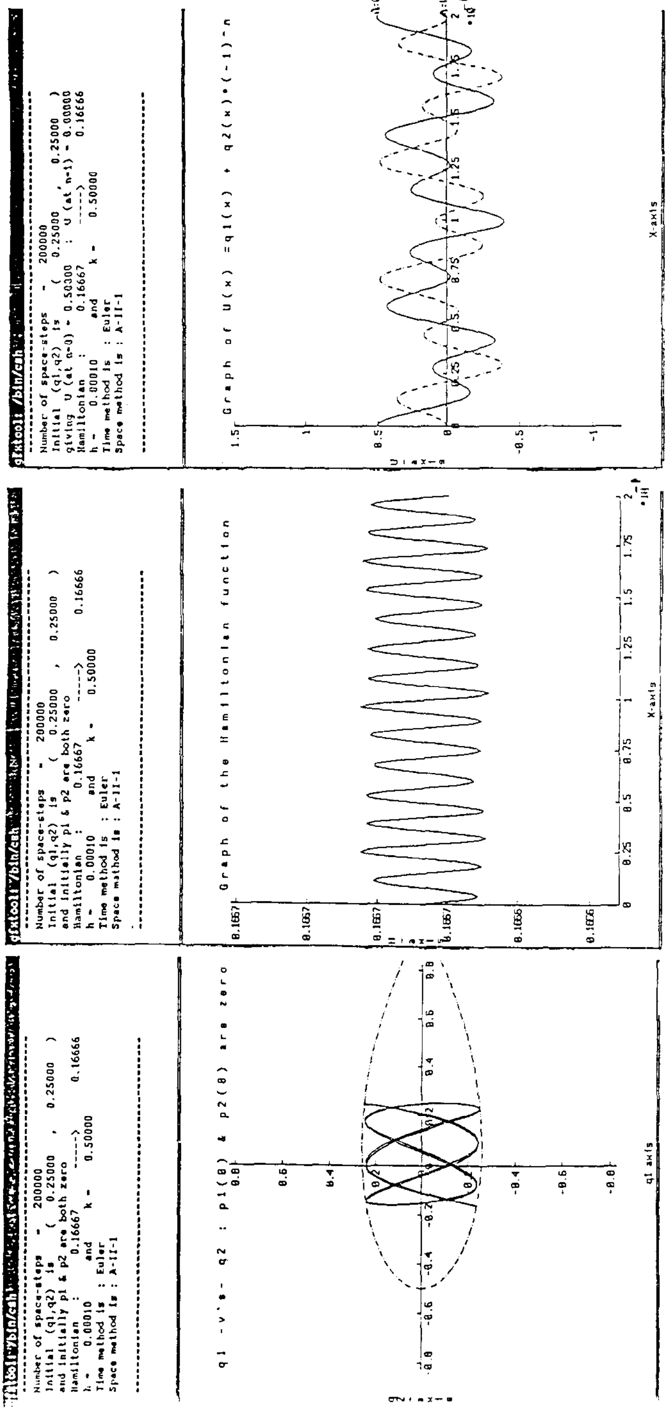
Number of space-steps = 200000
Initial (q1,q2) is (0.25000 , 0.25000)
and initially p1 & p2 are both zero
Hamiltonian : 0.16667 ----> 0.16666
h = 0.00010 and k = 0.50000
Time method is : Euler
Space method is : A-II-1
q1 -v's- q2 : p1(0) & p2(0) are zero
q1 axis
Graph of the Hamiltonian function
X-axis
giving U (at n-0) = 0.50000 : U (at n-1) = 0.00000
Graph of U(x) = q1(x) + q2(x)*(-1)^n
X-axis

FIGURE 5

choose the latter in the vicinity of one or another of the two real fixed points ($k \leqslant 2$) of the steady ($x \to \infty$) problem. Also the diagrams displaying the numerical results include $q_1(x)$ against $q_2(x)$ on the cross sectional plane $p_1(x) = p_2(x) = 0$, starting, in each case, from an initial point on this plane, giving an initial Hamiltonian value H_0. The zero p-values are, of course, not maintained for x-values other than zero, and so the curve in the (q_1, q_2) plane, on which the Hamiltonian has constant value H_0, is plotted (with a broken line) to show the expected envelope of the numerical results. In addition for each numerical run, the period 2

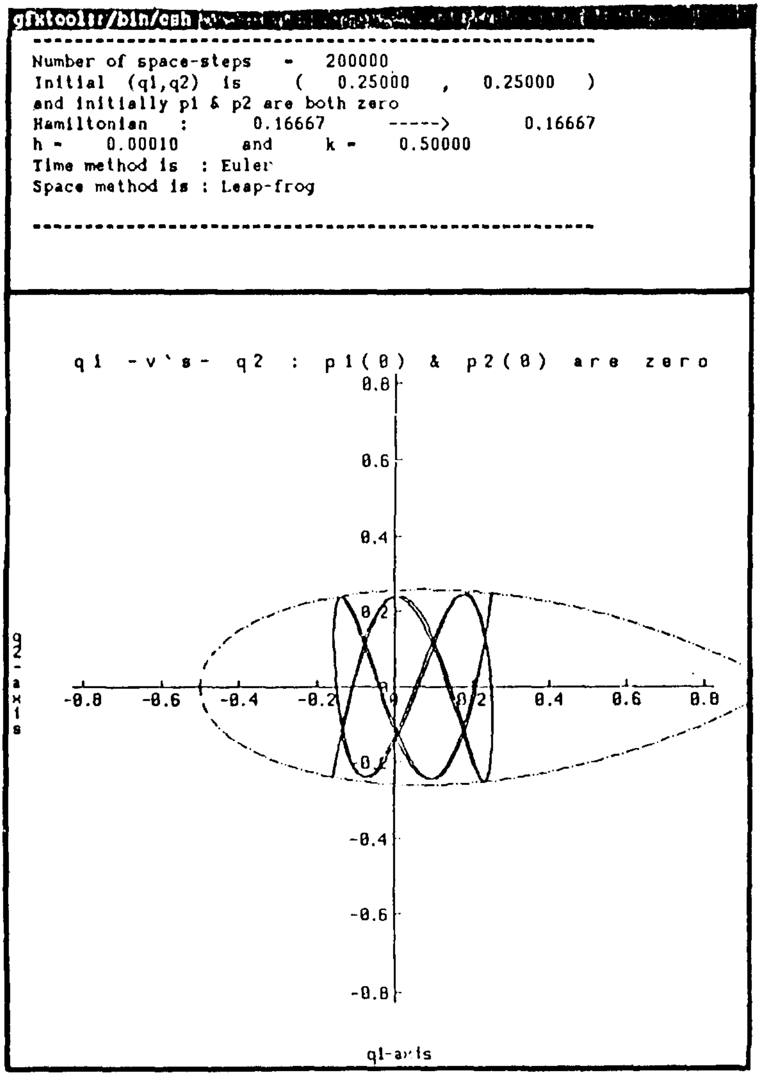

FIGURE 6

in time solution $U_n(x)$, $n=0$, 1 is plotted against x together with the value of the Hamiltonian.

(1) Initial data near the centre $(0,0,0,0)^T$. We start by comparing the trajectories of all three methods, Euler, staggered Euler (A-II-1), and Leap frog, with the initial point $(0, 0, \frac{1}{4}, \frac{1}{4})^T$. The results are shown in Figs. 4, 5, and 6, respectively. After 200,000 space steps, the three methods give similar results for $q_1(x)$ versus $q_2(x)$ and also for the period 2 solutions in time, $q_1(x) \pm q_2(x)$, but display different behaviour regarding conservation of the initial Hamiltonian value.

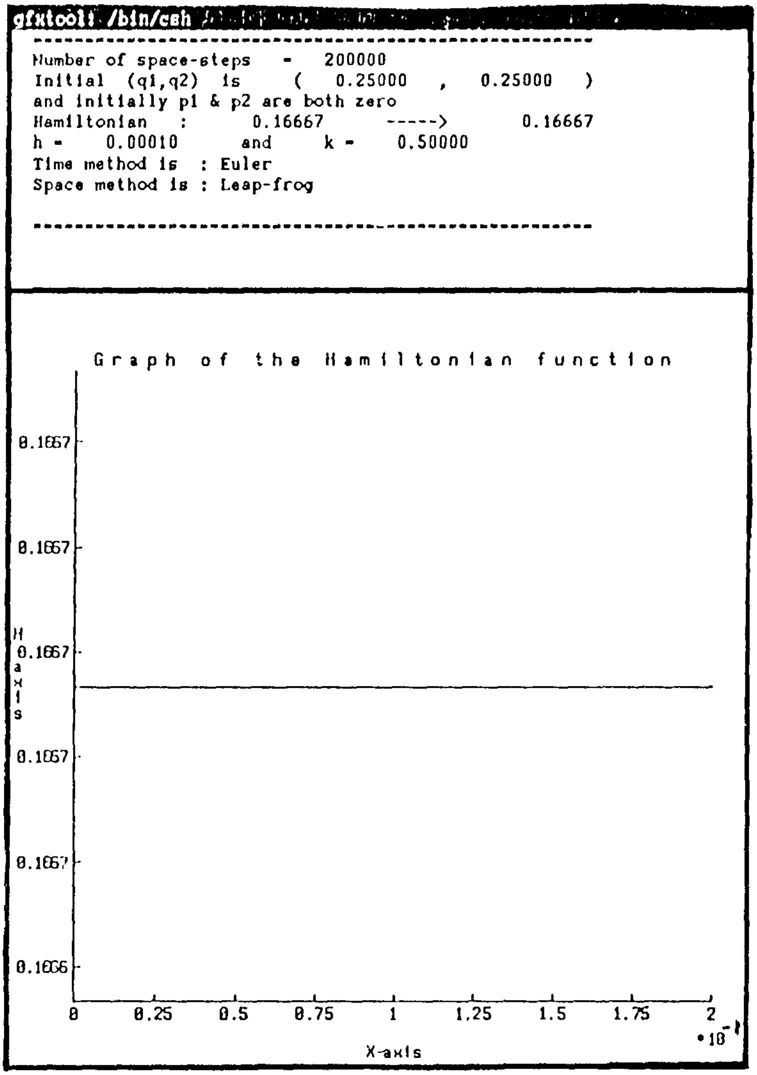

FIG. 6—*Continued*

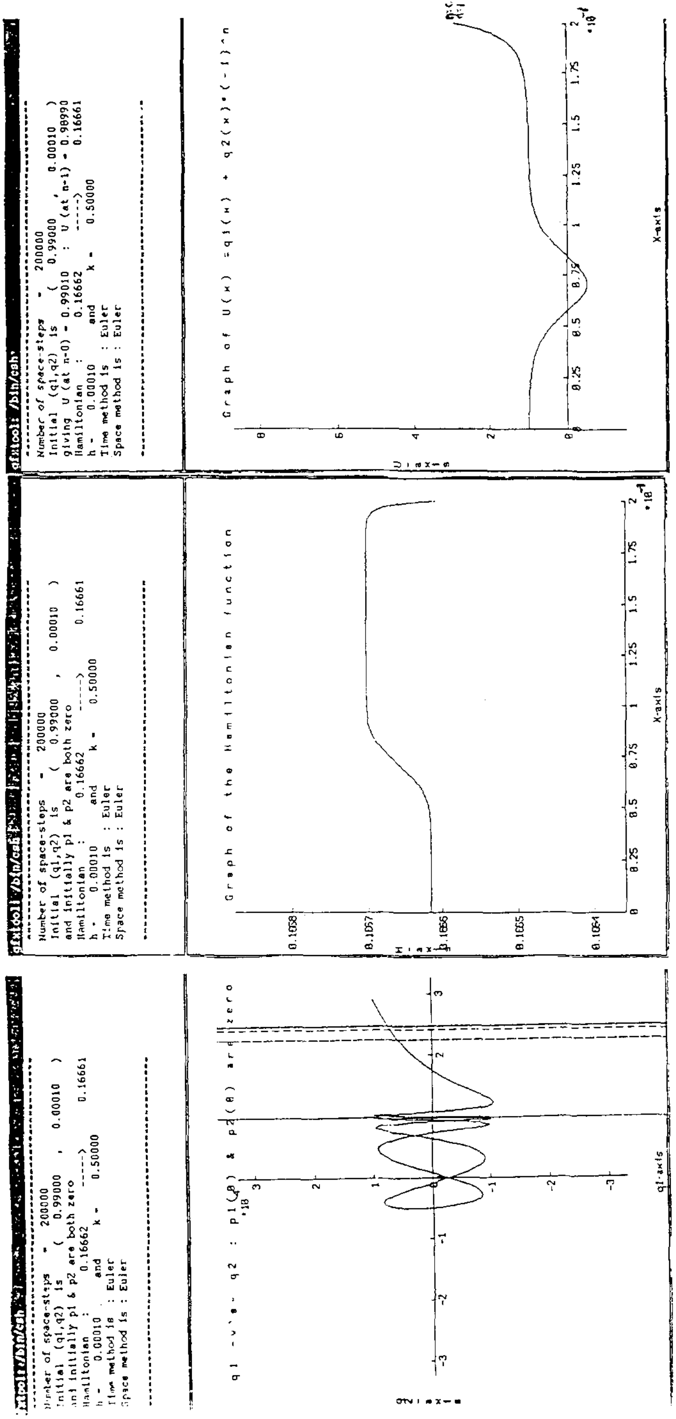
Number of space-steps = 200000
Initial (q1,q2) is (0.99000 , 0.00010)
and initially p1 & p2 are both zero
Hamiltonian : 0.16662 -----> 0.16661
h = 0.00010 and k = 0.50000
Time method is : Euler
Space method is : Euler
q1-axis
Graph of the Hamiltonian function
X-axis
giving U (at n=0) = 0.99010 : U (at n-1) = 0.98990
Graph of U(x) = q1(x) + q2(x)*(-1)^n

FIGURE 7

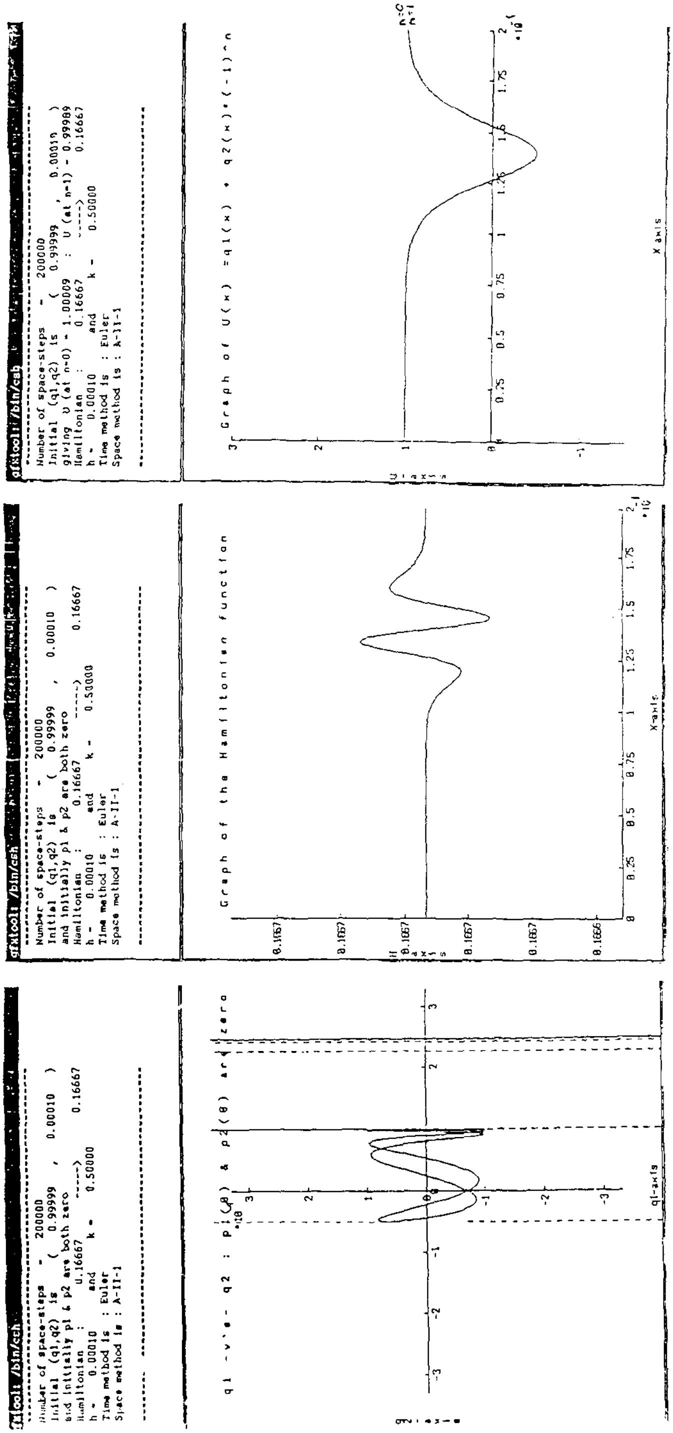
Number of space-steps = 200000
Initial (q1,q2) is (0.99999 , 0.00010)
and initially p1 & p2 are both zero
Hamiltonian : 0.16667 -----> 0.16667
h = 0.00010 and k = 0.50000
Time method is : Euler
Space method is : A-II-1
q1 -v's- q2 : p1(0) & p2(0) are zero
q1-axis
Graph of the Hamiltonian function
X-axis
Number of space-steps = 200000
Initial (q1,q2) is (0.99999 , 0.00019)
giving U (at n=0) = 1.00009 : U (at n=1) = 0.99989
Hamiltonian : 0.16667 -----> 0.16667
h = 0.00010 and k = 0.50000
Time method is : Euler
Space method is : A-II-1
Graph of U(x) = q1(x) + q2(x)*(-1)^n
X axis

FIGURE 8

The reasonable similarity regarding the solutions of all three methods illustrates the strong influence of the neutrally stable *centre* at $(0, 0, 0, 0)^{\mathrm{T}}$ on discretised problems with initial data close to this fixed point. Because the values of $q_1(x) \pm q_2(x)$ are similar in all three cases only the Euler and A-II-1 versions of the solution are given.

(2) Initial data near the saddle $(0, 0, 1, 0)^{\mathrm{T}}$. Once again we compare the performances of the three schemes, Euler, A-II-1, and Leap frog. With Euler,

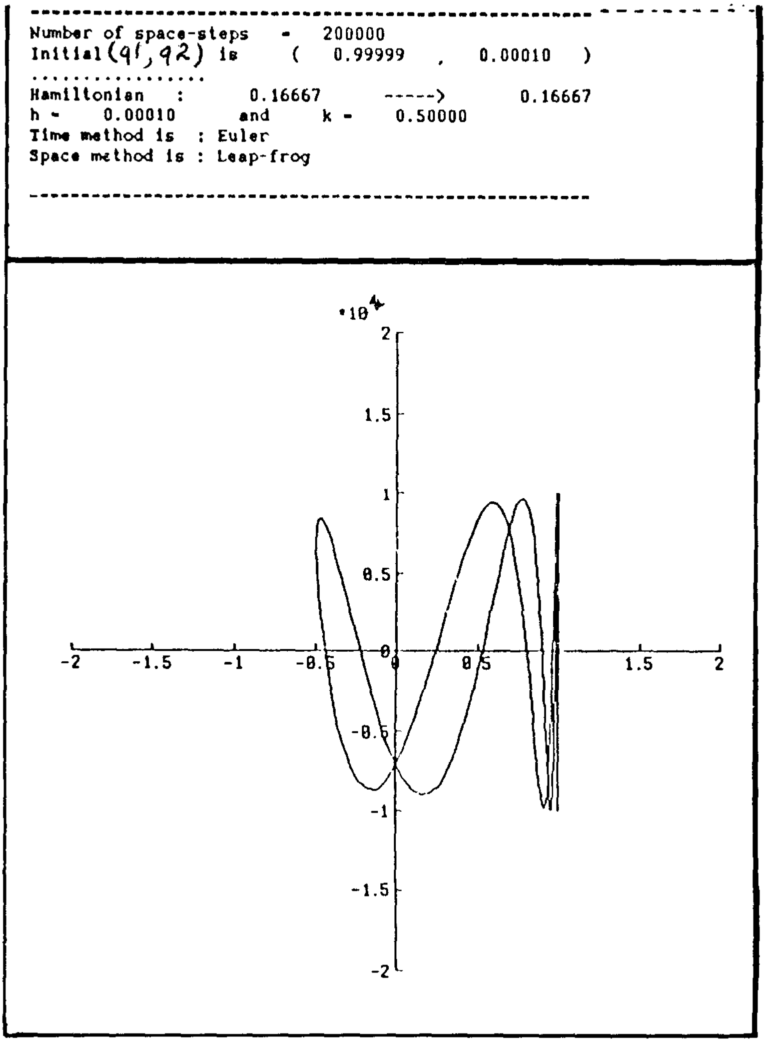

FIGURE 9

blowup occurs from an initial point $(0, 0, 0.99, 0.0001)^T$ with $q_1(x)$ versus $q_2(x)$, the Hamiltonian and the period 2 solutions in time given in Fig. 7. To the scale of the figure, $q_1(x)+q_2(x)$ is indiscernable from $q_1(x)-q_2(x)$, due to the small size of $q_2(x)$. Because of the symplectic nature of staggered Euler and Leap frog, we chose a starting point $(0, 0, 0.99999, 0.0001)^T$, closer to the saddle fixed point, for these schemes. The respective numerical results are shown in Figs. 8 and 9. Staggered Euler is beginning to disintegrate, whereas Leap frog maintains a constant value for the Hamiltonian for the duration in x of the numerical experiment.

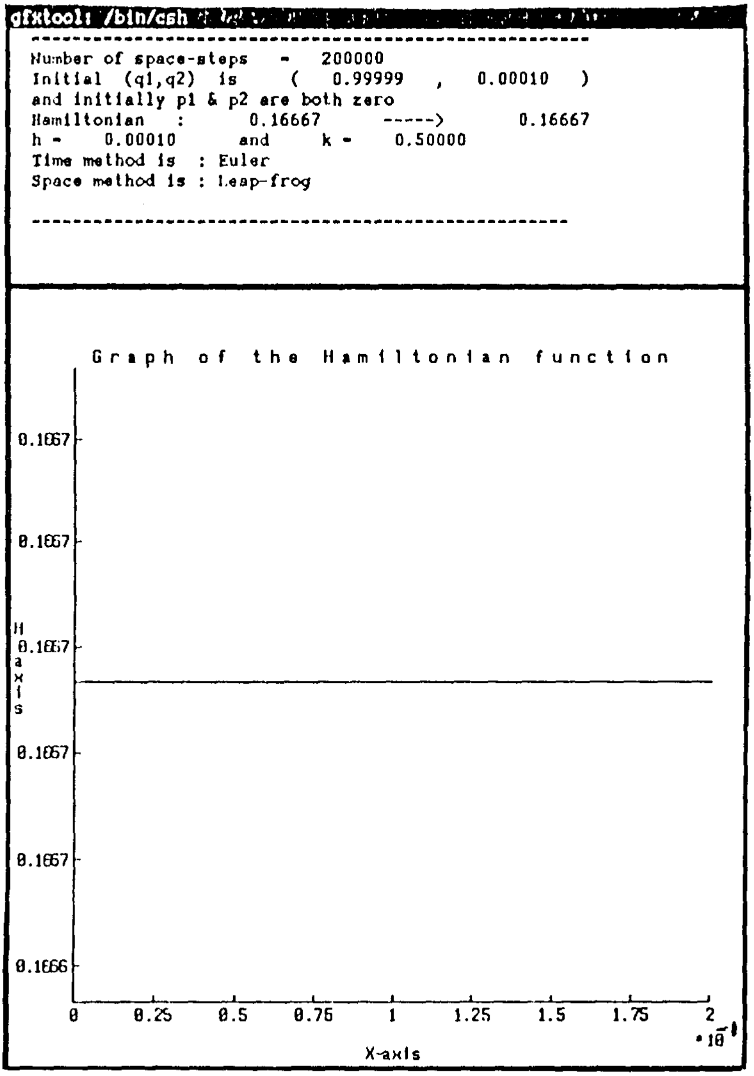

FIG. 9—*Continued*

6. Conclusions

In view of the many possible parameter values in the numerical experiments, viz. grid sizes k, h (>0), initial condition at $x=0$, and the location of the latter with respect to the fixed points, sufficient calculations only have been carried out to demonstrate main ideas of the paper. These are that:

(I) A time discretised model of a reaction diffusion equation satisfies a Hamiltonian system in space.

(II) Due to the non-integrability of the Hamiltonian system, symplectic difference schemes which preserve the Hamiltonian energy for $x \geqslant 0$ are employed to obtain numerical solutions up to large values of the space variable.

(III) Of the difference schemes in space that were tested, the symplectic schemes (Leap frog and A-II-1) behaved better than the non-symplectic scheme (Euler), with Leap frog behaving best overall.

(IV) Roud-off error did not seem to have a significant effect on the numerical results quoted, since accuracy to five decimal places was the same with single and double precision.

(V) In view of the large number of space steps (200,000) in each numerical experiment, simple explicit difference schemes were chosen, two symplectic and one non-symplectic, the latter for comparison purposes only.

Finally, the numerical solution of non-integrable Hamiltonian systems in general is without a doubt an important area for numerical analysis research in the future, with the many symplectic difference schemes devised by Fend Kang and his co-authors [1, 2] providing a useful starting point.

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