Journal of Computational Mathematics, Vol.20, No.6, 2002, 611–618.

VON NEUMANN STABILITY ANALYSIS OF SYMPLECTIC INTEGRATORS APPLIED TO HAMILTONIAN PDEs*[1)]

Helen M. Regan
(*Applied Biomathematics 100 North Country Road, Setauket, New York 11733, USA*)

Abstract

Symplectic integration of separable Hamiltonian ordinary and partial differential equations is discussed. A von Neumann analysis is performed to achieve general linear stability criteria for symplectic methods applied to a restricted class of Hamiltonian PDEs. In this treatment, the symplectic step is performed prior to the spatial step, as opposed to the standard approach of spatially discretising the PDE to form a system of Hamiltonian ODEs to which a symplectic integrator can be applied. In this way stability criteria are achieved by considering the spectra of linearised Hamiltonian PDEs rather than spatial step size.

Key words: symplectic integration, Hamiltonian PDEs, linear stability, von Neumann analysis.

1. Introduction

Symplectic integration schemes are numerical methods for solving Hamiltonian ordinary differential equations (ODEs). They differ from many other types of numerical integration schemes because they preserve the differential 2-form with each iteration (time step) of Hamiltonian ODEs. Symplectic schemes are the preferred method of numerical integration of Hamiltonian ODEs because they approximate the flow of the system. As a result, they inhibit artificial dissipation and other undesirable effects often introduced with the use of non-symplectic numerical methods (see [1]) and error growth is qualitatively and comparatively small [1, 2, 3].

Symplectic integration of Hamiltonian partial differential equations (PDEs) has traditionally been a matter of applying symplectic methods to a system of Hamiltonian ODEs resulting from a spatial discretisation of the PDE. This has been the case for applications to the sine-Gordon equation, the KdV equation, the "good" Boussinesq equation, Fisher's equation, the nonlinear Schrödinger equation and others [4, 5, 6, 7, 8, 9]. The usual procedures are to spatially discretise the Hamiltonian operator and the Hamiltonian separately, using a finite difference method or a spectral method, and then form the resultant ODEs, or to directly discretise the PDE in conservative form. This is followed by applying a symplectic integrator to the resultant system of ODEs.

In this paper we will investigate the linear stability of symplectic methods applied to Hamiltonian PDEs. We restrict consideration to separable Hamiltonian PDEs in canonical form. For these types of equations the Hamiltonian operator is linear and constant. Hence, the preservation of Hamiltonian structure is ensured when the Hamiltonian operator and the Hamiltonian are spatially discretised separately or when the PDE is discretised directly in conservative form [10].

In this paper, the symplectic integration scheme is applied directly to the PDEs in conservative form. The application of symplectic integrators to Hamiltonian PDEs in function space

* Received.

1) Current address: National Center for Ecological Analysis and Synthesis, University of California Santa Barbara, 735 State St., Suite 300, Santa Barbara, CA 93101, USA. Email: regan@nceas.ucsb.edu, Phone: (805) 892 2522, Fax: (805) 892 2510.

results in systems of equations which fit naturally into a von Neumann stability analysis. The result is a general method for determining stability criteria for symplectic methods applied directly to linearised Hamiltonian PDEs, independent of spatial discretisation.

2. Explicit and Implicit Symplectic Integrators

We first consider separable and autonomous Hamiltonian ODEs of the form $H(p,q) = T(p) + V(q)$, with Hamiltonian vector field $X_H = X_T + X_V$. Hamilton's equations are

$$\frac{d}{dt}\begin{pmatrix} p \\ q \end{pmatrix} = \begin{pmatrix} -\frac{\partial V}{\partial q} \\ \frac{\partial T}{\partial p} \end{pmatrix} = J\nabla H. \tag{1}$$

In this paper we will consider explicit and implicit symplectic integration schemes as constructed by the method of generating functions and composition [11, 12, 13, 14, 15], or by conditions imposed on Rung-Kutta schemes [2, 16, 17, 18, 19]). A general explicit symplectic method is

$$p_i = p_{i-1} - d_i\tau\frac{\partial V}{\partial q}(q_i), \qquad q_i = q_{i-1} + c_i\tau\frac{\partial T}{\partial p}(p_{i-1}), \tag{2}$$

where $i = 1, \ldots, k$, $(p_0, q_0) = (p(t_0), q(t_0))$ represent the initial conditions at time $t = t_0$ and $(p_k, q_k) = (p', q') = (p(t_0+\tau), q(t_0+\tau))$ is the approximation of the position and momentum after one time step of length τ. In terms of an exponential product, an explicit n-th order symplectic integrator can be expressed as

$$\begin{pmatrix} p' \\ q' \end{pmatrix} = \prod_{i=1}^{k} \mathrm{e}^{c_i\tau X_T}\mathrm{e}^{d_i\tau X_V}\begin{pmatrix} p_0 \\ q_0 \end{pmatrix} = S_n(\tau)\begin{pmatrix} p_0 \\ q_0 \end{pmatrix}. \tag{3}$$

Table 1 includes a selection of explicit symplectic methods constructed via a method of generating functions and composition (after [4]). Details of the calculation of the coefficients c_i and d_i can be found in [11, 12, 20, 13, 14, 15]. Table 2 contains 4th, 5th and 6th order Runge-Kutta-Nyström (RKN) methods constructed in [2, 19]. RKN methods are applicable only when the kinetic energy, $T(p)$, in the Hamiltonian is quadratic.

Implicit symplectic methods can be obtained by imposing conditions on already existing Runge-Kutta (RK) methods. When Hamilton's equations are of the form (1), an s-stage symplectic RK method can be expressed as

$$\begin{aligned} p' &= p_0 - \tau\sum_{i=1}^{s} b_i\frac{\partial V}{\partial q}(Q_i), \qquad q' = q_0 + \tau\sum_{i=1}^{s} b_i\frac{\partial T}{\partial p}(P_i), \\ P_i &= p_0 - \tau\sum_{j=1}^{s} a_{ij}\frac{\partial V}{\partial q}(Q_j), \qquad Q_i = q_0 + \tau\sum_{j=1}^{s} a_{ij}\frac{\partial T}{\partial p}(P_j). \end{aligned} \tag{4}$$

The necessary and sufficient conditions for an s-stage Runge-Kutta method to be symplectic [16, 21] are $b_ib_j - b_ia_{ij} - b_ja_{ji} = 0, i, j \leq s$. If $a_{ij} = 0$ for $i \leq j$ these methods are explicit, otherwise they are implicit.

Gaussian Runge-Kutta (GRK) methods are implicit even-order RK methods that are always symplectic [17]. Coefficients a_{ij}, b_j, are determined using methods specific to Gauss collocation, described in [17] and [18]. Coefficients for the 2nd order implicit midpoint rule (MP2), and the 4th, 6th, 8th and 10th order Gauss method (GRK4,6,8,10 respectively) appear in [17, 18, 22].

3. Linear Stability

3.1. Hamiltonian Ordinary Differential Equations

As an introduction to linear stability theory of symplectic maps we'll look at the stability of symplectic integrators applied to linear ODEs, as provided in [4] and [23], and then tackle the more complicated case of Hamiltonian PDEs.

Suppose we have a linear map resulting from the application of a symplectic integrator to an ODE over one time step, such that

$$\begin{pmatrix} p' \\ q' \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} p_0 \\ q_0 \end{pmatrix} = A \begin{pmatrix} p_0 \\ q_0 \end{pmatrix}. \tag{5}$$

Since A is a symplectic map one of its properties is that its determinant is equal to 1 (see [23]). The eigenvalues of A are solutions of $\lambda^2 - \mathrm{Tr}(A)\lambda + 1 = 0$. Following Arnold's treatment of the stability of symplectic maps [23], if the two roots, λ_1 and λ_2, of this equation are complex conjugates then

$$\lambda = \frac{\mathrm{Tr}(A)}{2} \pm i\sqrt{1 - \left(\frac{\mathrm{Tr}(A)}{2}\right)^2}$$

with $|\mathrm{Tr}(A)| < 2$ and $\lambda < 1$. For stability, $\lambda < 1$, and hence $|\mathrm{Tr}(A)| < 2$ is required. Since A depends explicitly on the step-size τ, it is necessary to take the least positive solution of $|\mathrm{Tr}(A)| = 2$ with respect to τ in the calculation of stability criteria.

Example: Linear Oscillator

Hamilton's equations for the linear oscillator are $\frac{dp}{dt} = -q$, $\frac{dq}{dt} = p$ with Hamiltonian $H = \frac{1}{2}p^2 + \frac{1}{2}q^2$. Applying a 2nd order explicit symplectic integrator (SI2) over one time step gives the following;

$$\begin{pmatrix} p' \\ q' \end{pmatrix} = \mathrm{e}^{\frac{1}{2}\tau X_T}\mathrm{e}^{\tau X_V}\mathrm{e}^{\frac{1}{2}\tau X_T} \begin{pmatrix} p_0 \\ q_0 \end{pmatrix} = \begin{pmatrix} 1 - \frac{1}{2}\tau^2 & -\tau \\ \tau - \frac{1}{4}\tau^3 & 1 - \frac{1}{2}\tau^2 \end{pmatrix} \begin{pmatrix} p_0 \\ q_0 \end{pmatrix} = A \begin{pmatrix} p_0 \\ q_0 \end{pmatrix}$$

where $\mathrm{Tr}(A) = 2 - \tau^2$. For stability we require $|\mathrm{Tr}(A)| = |2 - \tau^2| < 2$. Let $\tau^\star$ be the least positive root of the equation $|2 - \tau^2| = 2$. Hence, for stability we require $\tau < \tau^\star = 2$. For higher order methods $\mathrm{Tr}(A)$ will be higher order polynomials and a root finding algorithm is required to approximate $\tau^\star$. A table listing the stability criteria for various explicit symplectic methods applied to the linear oscillator is provided in [4].

Applying the 2nd order implicit midpoint rule (MP2) to the linear oscillator gives the equations

$$\begin{aligned} \begin{pmatrix} p' \\ q' \end{pmatrix} &= \begin{pmatrix} p_0 \\ q_0 \end{pmatrix} + \tau J \nabla H \left(\frac{p_0 + p'}{2}, \frac{q_0 + q'}{2}\right) \\ &= \frac{1}{1 + \frac{\tau^2}{4}} \begin{pmatrix} 1 - \frac{\tau^2}{4} & -\tau \\ \tau & 1 - \frac{\tau^2}{4} \end{pmatrix} \begin{pmatrix} p_0 \\ q_0 \end{pmatrix} = A \begin{pmatrix} p_0 \\ q_0 \end{pmatrix}. \end{aligned}$$

Here,

$$\mathrm{Tr}(A) = 2\left(\frac{1 - \frac{\tau^2}{4}}{1 + \frac{\tau^2}{4}}\right)$$

and so the stability criterion for MP2 applied to the linear oscillator becomes $\left|\frac{1 - \frac{\tau^2}{4}}{1 + \frac{\tau^2}{4}}\right| < 1$. This is true for any choice of τ, hence the method is unconditionally stable, as are all GRK methods applied to the linear oscillator.

3.2. Hamiltonian Partial Differential Equations

Here we will investigate the linear stability of maps that result from a symplectic temporal discretisation of Hamiltonian PDEs. In doing so, a von Neumann approach to examining the stability of symplectic methods is obtained that can be utilised in the stability analysis of symplectic methods to many types of Hamiltonian PDEs. In the approach taken here, it is not necessary to specify a spatial discretisation method. It suffices to know that there exists a spatial discretisation technique that can be applied to the resultant system of equations.

Let's consider the linear (or linearised) infinite dimensional Hamiltonian system $\mathcal{H} = \mathcal{T} + \mathcal{V} = \int T\,dx + \int V dx$ with the corresponding system of Hamiltonian evolution equations

$$\begin{pmatrix} \frac{\partial v}{\partial t} \\ \frac{\partial u}{\partial t} \end{pmatrix} = \begin{pmatrix} -\frac{\delta \mathcal{V}}{\delta u} \\ \frac{\delta \mathcal{T}}{\delta v} \end{pmatrix} = \begin{pmatrix} L_1(u) \\ L_2(v) \end{pmatrix} = \mathcal{D} \cdot \delta \mathcal{H} \tag{6}$$

where the Hamiltonian operator $\mathcal{D}$ is

$$\mathcal{D} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix},$$

L_1 and L_2 are linear operators, $u = u(x,t)$, $v = v(x,t)$, $\mathcal{H}$, $\mathcal{T}$ and $\mathcal{V}$ are functionals (i.e. $\mathcal{H} = \int H dx$ etc.), $\delta\mathcal{H} = \left(\frac{\delta\mathcal{H}}{\delta v}, \frac{\delta\mathcal{H}}{\delta u}\right)$ is the variational derivative of $\mathcal{H}$, and $\frac{\delta\mathcal{T}}{\delta v}$ and $\frac{\delta\mathcal{V}}{\delta u}$ are the variational derivatives of $\mathcal{T}$ and $\mathcal{V}$ (see [24] for a thorough formalism of Hamiltonian PDEs).

3.3. Linear Stability of Explicit Symplectic Methods

The direct application of a general explicit symplectic integrator such as those appearing in Tables 1 and 2 gives the following components:

$$\begin{aligned} \mathrm{e}^{d_i\tau X_{\mathcal{V}}} \begin{pmatrix} v_{i-1}(x) \\ u_{i-1}(x) \end{pmatrix} &= \begin{pmatrix} 1 & d_i\tau L_1 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} v_{i-1}(x) \\ u_{i-1}(x) \end{pmatrix} \\ \mathrm{e}^{c_i\tau X_{\mathcal{T}}} \begin{pmatrix} v_{i-1}(x) \\ u_{i-1}(x) \end{pmatrix} &= \begin{pmatrix} 1 & 0 \\ c_i\tau L_2 & 1 \end{pmatrix} \begin{pmatrix} v_{i-1}(x) \\ u_{i-1}(x) \end{pmatrix}, \end{aligned} \tag{7}$$

with $i = 1, \ldots, s$. The 2nd order explicit symplectic method (SI2) is now

$$\begin{pmatrix} v'(x) \\ u'(x) \end{pmatrix} = \begin{pmatrix} 1 + \frac{1}{2}\tau^2 L_2 L_1 & \tau L_1 \\ \tau L_2 + \frac{1}{4}\tau^3 L_2 L_1 L_2 & 1 + \frac{1}{2}\tau^2 L_1 L_2 \end{pmatrix} \begin{pmatrix} v_0(x) \\ u_0(x) \end{pmatrix} \tag{8}$$

where each element of the matrix is a polynomial in the linear operators L_1 and L_2, $v_0(x) = v(x,t_0)$ and $u_0(x) = u(x,t_0)$ are the temporal initial conditions, and $v'(x)$ and $u'(x)$ are the approximations of u and v in function space at time $t = t_0 + \tau$.

Suppose we have a linear map resulting from the application of an explicit symplectic integrator to the system (6) over one time step such that

$$\begin{pmatrix} v'(x) \\ u'(x) \end{pmatrix} = \begin{pmatrix} L_{11} & L_{12} \\ L_{21} & L_{22} \end{pmatrix} \begin{pmatrix} v_0(x) \\ u_0(x) \end{pmatrix} = A' \begin{pmatrix} v_0(x) \\ u_0(x) \end{pmatrix} \tag{9}$$

where A' is a matrix of linear operators, one example of which appears in equation (8). In section 3.1 the stability criterion for the analogous linear map was $|\mathrm{Tr}(A)| < 2$, however the treatment is not as straightforward here due to the presence of linear operators rather than scalars. In order to apply the stability theory appearing in section 3.1, A' must be manipulated into a matrix of scalars. This is done by taking Fourier transforms of (9) as would be done in a von Neumann stability analysis. We will restrict this discussion to linear operators that are either spatial derivatives of at least first order or the identity multiplied by real or complex scalars. This is not an unreasonable restriction considering that a large class of linear (or linearised) Hamiltonian wave equations take this form. Hence, composition of the exponential operators (7) produces polynomials in the differential operators. Given this restriction, applying a continuous Fourier transform to (9) according to the formula

$$\hat{u}(\omega) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \mathrm{e}^{-i\omega x} u(x)\, dx$$

will yield

$$\begin{pmatrix} \hat{v}'(\omega) \\ \hat{u}'(\omega) \end{pmatrix} = \begin{pmatrix} z_{11}(\omega) & z_{12}(\omega) \\ z_{21}(\omega) & z_{22}(\omega) \end{pmatrix} \begin{pmatrix} \hat{v}_0(\omega) \\ \hat{u}_0(\omega) \end{pmatrix} = A \begin{pmatrix} \hat{v}_0(\omega) \\ \hat{u}_0(\omega) \end{pmatrix} \tag{10}$$

where $z_{ij}(\omega)$ are complex scalars involving the frequency $\omega \in \mathbb{R}$.

Since the symplectic time step works identically in Fourier space and real space, the stability theory of section 3.1 can now be employed, i.e. for stability we require $|\mathrm{Tr}(A)| < 2$, where the modulus is now complex modulus. This gives stability criteria in terms of the spectral variable ω.

3.4. Applications

Sine-Gordon Equation

To avoid unwieldy equations we consider only 2nd order explicit methods in the present and following examples. Stability criteria for higher order methods can be obtained in exactly the same manner and often it is necessary to employ a numerical root finding method to determine $\tau^\star$.

Hamilton's equations for the sine-Gordon equation in 1 space dimension are

$$\frac{\partial}{\partial t}u(x,t) = v(x,t), \qquad \frac{\partial}{\partial t}v(x,t) = \frac{\partial^2}{\partial x^2}u(x,t) - \sin\left(u(x,t)\right).$$

A linearisation about the steady state $u = 0$ gives the equations

$$\begin{aligned}\frac{\partial}{\partial t}u(x,t) &= v(x,t) = L_2(v(x,t))\\ \frac{\partial}{\partial t}v(x,t) &= \frac{\partial^2}{\partial x^2}u(x,t) - u(x,t) = L_1(u(x,t)),\end{aligned}$$

where $L_2 = 1$ (the identity map), $L_1 = \partial_{xx} - 1$ and $\partial_{xx} = \frac{\partial^2}{\partial x^2}$.

Application of the 2nd order explicit method yields

$$\begin{pmatrix} v'(x) \\ u'(x) \end{pmatrix} = \begin{pmatrix} 1+\frac{1}{2}\tau^2(\partial_{xx}-1) & \tau(\partial_{xx}-1) \\ \tau+\frac{1}{4}\tau^3(\partial_{xx}-1) & 1+\frac{1}{2}\tau^2(\partial_{xx}-1) \end{pmatrix} \begin{pmatrix} v_0(x) \\ u_0(x) \end{pmatrix}.$$

Taking a Fourier transform of this gives

$$\begin{pmatrix} \hat{v}'(\omega) \\ \hat{u}'(\omega) \end{pmatrix} = \begin{pmatrix} 1-\frac{1}{2}\tau^2(\omega^2+1) & -\tau(\omega^2+1) \\ \tau-\frac{1}{4}\tau^3(\omega^2+1) & 1-\frac{1}{2}\tau^2(\omega^2+1) \end{pmatrix} \begin{pmatrix} \hat{v}_0(\omega) \\ \hat{u}_0(\omega) \end{pmatrix} = A \begin{pmatrix} \hat{v}_0(\omega) \\ \hat{u}_0(\omega) \end{pmatrix}.$$

For stability we require $|\mathrm{Tr(A)}| < 2 \Rightarrow \tau^2(\omega^2+1) < 4$.

3.5. Linear Stability of Implicit Symplectic Methods

For cases where the kinetic energy in the Hamiltonian PDE is quadratic (i.e. $\mathcal{T} = K\int v^2 dx$, with K constant) the general method for determining stability criteria is identical to that described above. The examples mentioned thus far have been of this type. The following example illustrates the technique and results for implicit methods applied to these types of Hamiltonian PDEs.

Hamilton's equations for the one dimensional linear wave are $\frac{\partial u(x,t)}{\partial t} = v(x,t)$, $\frac{\partial v(x,t)}{\partial t} = \frac{\partial^2 u(x,t)}{\partial x^2}$. The 2nd order implicit midpoint rule (MP2) applied to the linear wave equation is

$$\begin{pmatrix} v' \\ u' \end{pmatrix} = \begin{pmatrix} v_0 \\ u_0 \end{pmatrix} + \tau \begin{pmatrix} \frac{\partial^2}{\partial x^2}\left(\frac{u_0+u'}{2}\right) \\ \frac{v_0+v'}{2} \end{pmatrix}$$

or in Fourier space

$$\begin{pmatrix} \hat{v}' \\ \hat{u}' \end{pmatrix} = \frac{1}{1+\frac{\omega^2\tau^2}{4}} \begin{pmatrix} 1-\frac{\omega^2\tau^2}{4} & \tau \\ -\omega^2\tau & 1-\frac{\omega^2\tau^2}{4} \end{pmatrix} \begin{pmatrix} \hat{v}_0 \\ \hat{u}_0 \end{pmatrix} = A \begin{pmatrix} \hat{v}_0 \\ \hat{u}_0 \end{pmatrix}.$$

The stability criterion then becomes

$$\left|\frac{1-\omega^2\tau^2/4}{1+\omega^2\tau^2/4}\right| < 1,$$

however, this holds for any choice of ω and τ hence the method is unconditionally stable when applied to the linear wave equation. Similar results are obtained for all even order Gaussian-Runge-Kutta methods applied to separable systems of Hamilton's equations in canonical form.

Table 3 lists the stability criteria for some explicit symplectic methods applied to the linear wave equation and the sine-Gordon equation. The values appearing in Table 3 correlate with the stability criteria appearing in [4], obtained by a different method (see also [25]).

3.6. Higher Dimensions

Many Hamiltonian wave equations generalise to higher dimensions and so it is reasonable to consider how or if the linear stability results of the previous sections extend to higher dimensions. A Fourier transform in M dimensions of the function $u(\mathbf{x})$ where $\mathbf{x} \in \mathbb{R}^M$ is

$$\hat{u}(\vec{\omega}) = \frac{1}{(2\pi)^{\frac{M}{2}}}\int_{\mathbb{R}^M} \mathrm{e}^{-i\vec{\omega}\cdot\mathbf{x}} u(\mathbf{x})\, d\mathbf{x} \tag{11}$$

where $\vec{\omega} \in \mathbb{R}^M$. For example, the Laplacian, $\Delta = \frac{\partial^2}{\partial {x_1}^2} + \cdots + \frac{\partial^2}{\partial {x_M}^2}$, becomes a multiplication by $-(\omega_1^2 + \cdots + \omega_M^2) = -\|\vec{\omega}\|^2$ in Fourier space.

Consider the linear wave equation in three space dimensions to demonstrate the method for determining linear stability criteria for Hamiltonians in higher dimensions. The linear wave equation in three spatial dimensions is $\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = \Delta u$. Hamilton's equations are $\frac{\partial}{\partial t} u(\mathbf{x}, t) = v(\mathbf{x}, t)$, $\quad \frac{\partial}{\partial t} v(\mathbf{x}, t) = \Delta u(\mathbf{x}, t)$, where $\mathbf{x} = (x, y, z)$. Application of the explicit 2nd order method yields

$$\begin{pmatrix} v'(\mathbf{x}) \\ u'(\mathbf{x}) \end{pmatrix} = \begin{pmatrix} 1 + \frac{1}{2}\tau^2\Delta & \tau\Delta \\ \tau + \frac{1}{4}\tau^3\Delta & 1 + \frac{1}{2}\tau^2\Delta \end{pmatrix} \begin{pmatrix} v_0(\mathbf{x}) \\ u_0(\mathbf{x}) \end{pmatrix}.$$

Taking a 3-dimensional Fourier transform with wave numbers $\vec{\omega} = (\omega_1, \omega_2, \omega_3)$ gives

$$\begin{pmatrix} \hat{v}'(\vec{\omega}) \\ \hat{u}'(\vec{\omega}) \end{pmatrix} = \begin{pmatrix} 1 - \frac{1}{2}\tau^2(\omega_1^2 + \omega_2^2 + \omega_3^2) & -\tau(\omega_1^2 + \omega_2^2 + \omega_3^2) \\ \tau - \frac{1}{4}\tau^3(\omega_1^2 + \omega_2^2 + \omega_3^2) & 1 - \frac{1}{2}\tau^2(\omega_1^2 + \omega_2^2 + \omega_3^2) \end{pmatrix} \begin{pmatrix} \hat{v}_0(\vec{\omega}) \\ \hat{u}_0(\vec{\omega}) \end{pmatrix}.$$

The stability criterion, $|\mathrm{Tr}(A)| < 2$, can be applied to give $\tau^2(\omega_1^2 + \omega_2^2 + \omega_3^2) < 4$, implying $\tau\|\vec{\omega}\| < 2$ which is the same as for the 1+1-dimensional linear wave equation with $\vec{\omega} \in \mathbb{R}^3$ in the place of $\omega \in \mathbb{R}$. The stability criteria in Table 3 all follow through with ω replaced with $\vec{\omega}$.

Table 1. Explicit symplectic methods constructed via the method of generating functions and composition. The methods are attributed to [11, 12, 20, 13, 14, 15].

Explicit Symplectic Integrators			
Order	*Method*		
general even-order > 2	$S(\tau) = S_2(w_s\tau)\dots S_2(w_1\tau)S_2(w_0\tau)\dots S_2(w_1\tau)\dots S_2(w_s\tau)$ $= \prod_{j=1}^{k} \mathrm{e}^{c_j\tau X_T}\mathrm{e}^{d_j\tau X_V}$ $w_0 = 1 - 2(w_1 + \cdots + w_s)$ $k = 2s + 2$ $S_2(\tau) = \mathrm{e}^{\frac{1}{2}\tau X_T}\mathrm{e}^{\tau X_V}\mathrm{e}^{\frac{1}{2}\tau X_T}$		
2nd (SI2)	$S_2(\tau) = \mathrm{e}^{\frac{1}{2}\tau X_T}\mathrm{e}^{\tau X_V}\mathrm{e}^{\frac{1}{2}\tau X_T}$		
	s	$w_i,\ i = 1, \dots, s$	*coefficients*
4th a) (SI4a)	1	$w_1 = 1/(2 - 2^{\frac{1}{3}})$	$c_1 = c_4 = \frac{1}{2}w_1$ $c_2 = c_3 = \frac{1}{2}(w_0 + w_1)$ $d_1 = d_3 = w_1$
4th b) (SI4b)	2	$w_1 = 1/(4 - 4^{\frac{1}{3}})$ $w_2 = w_1$	$c_1 = c_{2s+2} = \frac{1}{2}w_s$ $c_2 = \frac{1}{2}(w_s + w_{s-1})$ $c_{2s+1} = c_2$ $c_{s+1} = \frac{1}{2}(w_1 + w_0)$ $c_{s+2} = c_{s+1}$ $d_1 = d_{2s+1} = w_s$ $d_2 = d_{2s} = w_{s-1}$ $d_s = d_{s+2} = w_1$ $d_{s+1} = w_0$
6th (SI6)	3	$w_1 = -1.17767998417887$ $w_2 = 0.235573213359357$ $w_3 = 0.784513610477560$	As above
8th (SI8)	7	$w_1 = 0.102799849391764e0$ $w_2 = -0.196061023297531e1$ $w_3 = 0.193813913762252e1$ $w_4 = -0.158240635368050e0$ $w_5 = -0.144485223686060e1$ $w_6 = 0.253693336566211e0$ $w_7 = 0.914844246229791e0$	As above

3.7. Conclusion

The merit of the temporal/spatial ordering of discretisation adopted in this paper, is that it simplifies the stability analysis of symplectic integration schemes applied to separable Hamiltonian PDEs in canonical form. Following the temporal discretisations, the equations are presented in a form such that von Neumann analysis can be easily applied. This is contrary to the more traditional spatial/temporal ordering where the resultant equations for finite difference approximations, are not naturally of a form appropriate for direct stability analysis—some manipulation is required at the outset. Furthermore, in the treatment presented here, the temporal discretisation is considered independently of the spatial discretisation. That is, the conditions under which symplectic integrators are linearly stable can be determined without explicitly taking into account the spatial discretisation. The results are stability criteria that are expressed in terms of the temporal step size, τ, and a frequency, ω.

Table 2. Runge-Kutta-Nyström methods. These methods are all explicit and are attributed to [2, 19].

Runge-Kutta-Nyström Methods			
Order	*Method*		
general	$S_n(\tau) = \prod_{j=s}^{1} \mathrm{e}^{c_j \tau X_T} \mathrm{e}^{d_j \tau X_V}$		
	s	c_j	d_j
1st (RKN1)	1	$c_1 = 1$	$d_1 = 1$
4th (RKN4)	4	$c_1 = 0.5153528374311229$ $c_2 = -0.0857820194129736$ $c_3 = 0.4415830236164665$ $c_4 = 0.1288461583653842$	$d_1 = 0.1344961992774311$ $d_2 = -0.2248198030794208$ $d_3 = 0.7563200005156683$ $d_4 = 0.3340036032863214$
6th (RKN6)	8	$c_1 = -1.0130879789881765$ $c_2 = 1.1874295738021426$ $c_3 = -0.0183358520956465$ $c_4 = 0.3439942572810803$ $c_j = c_{9-j}$, $j = 5, \ldots, 8$	$d_1 = 0$ $d_2 = 0.0001660069265094$ $d_3 = -0.3796242142744162$ $d_4 = 0.6891374118628093$ $d_5 = 0.3806415909701951$ $d_j = d_{10-j}$, $j = 6, 7, 8$

Table 3. The linear stability criteria of explicit symplectic integrators applied to two separable Hamiltonian wave equations.

Linear Stability Criteria for Explicit Methods		
Method	Linear wave	Sine-Gordon
	$\lvert\vec{\omega}\rvert\tau <$	$(\lvert\vec{\omega}\rvert^2 + 1)\tau^2 <$
SI2	2	4
SI4a	1.5734	2.4756
SI4b	2.7210	7.4038
SI6	2.2691	5.1486
SI8	1.2432	1.5456
RKN1	2	4
RKN4	3.0389	9.2349
RKN6	3.0674	9.4089

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