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Symmetry-adapted moving mesh schemes for the nonlinear Schrödinger equation

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Abstract

In this paper we consider symmetry-preserving difference schemes for the nonlinear Schrödinger equation

$$\mathrm{i}\frac{\partial u}{\partial t} + \frac{\partial^2 u}{\partial r^2} + \frac{n-1}{r}\frac{\partial u}{\partial r} + u|u|^2 = 0$$

where n is the number of space dimensions.

This equation describes one-dimensional waves in n space dimensions in many physical situations, including phenomena in plasma physics and nonlinear optics. We will consider the nonintegrable case $n \geqslant 2$ for which the equation admits solutions that blow up in a finite time, and construct discretizations based upon moving mesh schemes that have the same Lie group properties and Lagrangian structures as the continuous counterpart.

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1. Introduction

Lie group theory started out as a theory of transformations of solutions of sets of differential equations. Over the years it has developed into a powerful tool for classifying differential equations and for solving them. These aspects of Lie group theory have been described in many books and lecture notes [1–5].

Applications of Lie group theory to difference equations are much more recent [6–25] with important recent work by Hydon [26] on continuous symmetries of discrete systems. The main point in this area which distinguishes different approaches is the transformation of the independent variables. One approach [6, 7, 13–15] deals with transformations of dependent variables only, while the independent variables are fixed, and consequently so is the lattice. This restriction is very strong and excludes most of the symmetries of the physical problems. The second approach is to consider a difference, or differential-difference equation, together with a fixed lattice, on which the discrete variables take their values, to be given. One then develops techniques for finding symmetries of these equations [22, 23]. In this approach it is necessary to go beyond point symmetries and to consider Lie group actions at different points of the lattice simultaneously. That way leads to the deformations of the admitted Lie algebra with certain losses in some useful properties, and is applicable mainly to linear, linearizable, or integrable equations.

The third approach is to start with symmetries of a differential equation and to introduce a difference equation together with a symmetry-adapted mesh in such a way that all the symmetries of the original differential equation are preserved [8–12, 16–21, 24]. In general it is not possible to discretize a differential equation on a simple regular and orthogonal mesh while preserving all of the point symmetries. It is either necessary to give up their point character [22, 23], or to construct a symmetry-adapted mesh which can be nonregular and nonorthogonal [16–21, 24]. In this article we follow the last procedure.

Our point of view is to pose the question: how does one discretize a differential equation while preserving all of its Lie point symmetries? Here one starts from a differential equation and finds its Lie point symmetries, using well known techniques [1–4]. Thus a symmetry group and its Lie algebra are *a priori* given. One then looks for a difference scheme, i.e. a difference equation and a spatial mesh that have the same symmetry group and the same symmetry algebra L. In particular the Lie algebra L is realized by the same vector fields in the continuous and in the discrete case. The use of symmetry group methods thus leads to a natural, and powerful technique for deriving moving mesh discretizations of partial differential equations. Such moving meshes are especially important when studying problems (such as the nonlinear Schrödinger equation (NLS) in higher dimensions) which develop singular structures.

The structure of the symmetry group essentially effects the construction of equations and meshes. Group transformations can distort the geometric structure of a mesh that influences the approximation and other properties of the difference equations. For earlier work on the construction of the difference grids based on the symmetries of the initial differential equation see references [8–12, 16, 17].

In this work we will follow the moving mesh idea combined with the conservation of Lie point symmetries and the Lagrangian structure. The object of our study is an investigation of methods for determining the local structure of the blow-up of the radial solutions of the NLS. In one dimension this equation is integrable and there exist many numerical schemes—see for example [27–30]—which are either based upon preserving this integrability (often through a direct discretization of the underlying Lagrangian) and/or preserving the mass or Hamiltonian energy of the solution. When studying blow-up phenomena in higher dimensions it is much less clear whether this is a good idea. In particular it can lead to meshes which have a relatively sparse number of points in the blow-up region [21]. An alternative approach, which is described in [20, 21], which has proved effective for a number of blow-up problems is to construct (moving mesh) numerical methods which preserve the scaling symmetries close to the blow-up point. Whilst these may not strictly conserve mass or energy, they have proved effective in resolving the blow-up structure. A key test of this is whether they can accurately reproduce the self-similar evolutionary behaviour which is known [31] to describe the asymptotic behaviour of the blow-up in dimensions greater than 2. The purpose of this current study is to determine how feasible it is to combine these two approaches, namely a discretization of the Lagrangian, together with conserving the scaling symmetries.

The structure of the remainder of this paper is as follows. In section 2 we review the symmetries and conservation laws of the NLS. In sections 3 and 4 we introduce new Lagrangian coordinate systems which will eventually form the basis of the moving mesh discretization. In section 5 we study the conservation laws of the original problem when viewed in these new coordinates. In section 6 we introduce a first invariant discretization of the NLS based upon a fixed mesh. In section 7 we then extend this to a moving mesh discretization and in section 8 study the conservation laws associated with this. Finally in section 9 we consider the problem with blow-up.

2. The cubic nonlinear Schrödinger equation: symmetry, Lagrangian structure and conservation laws

We now turn our attention to considering the singular solutions of the radially symmetric cubic NLS given by

$$\mathrm{i}\frac{\partial u}{\partial t}+\frac{\partial^2 u}{\partial r^2}+\frac{n-1}{r}\frac{\partial u}{\partial r}+u|u|^2=0 \tag{1}$$

where n is the number of space dimensions.

This equation describes many physical situations, including phenomena in plasma physics and nonlinear optics, and a review of these is given in [31]. For the case of $n=1$, the equation is integrable and a solution exists globally. For the remainder of this paper we will consider the nonintegrable case $n \geqslant 2$ in which singularities are observed to develop given suitable initial data. A motivation for considering the radially symmetric form of the NLS is that it has been observed in numerical experiments reported in [31] that singularities in the NLS when posed as a problem in three dimensions are highly symmetric close to the singular point.

Let us substitute the polar representation

$$u(r,t)=A\mathrm{e}^{\mathrm{i}\Phi} \tag{2}$$

(where $A=A(r,t)$, $\Phi=\Phi(r,t)$ are real functions) into equation (1); we then get the following two equations:

$$A_t+A\Phi_{rr}+2A_r\Phi_r+\frac{n-1}{r}A\Phi_r=0 \tag{3}$$

$$A\Phi_t+A\Phi_r^2-A_{rr}-\frac{n-1}{r}A_r-A^3=0. \tag{4}$$

Standard Lie group analysis methods yield the symmetries of the system (3), (4), and for the case $n \geqslant 2$ the admitted Lie algebra of generators is the following which describes translations in time and phase and a rescaling of the solution:

$$\begin{aligned} X_1&=\frac{\partial}{\partial t} \qquad X_2=\frac{\partial}{\partial \Phi}\\ X_3&=2t\frac{\partial}{\partial t}+r\frac{\partial}{\partial r}-A\frac{\partial}{\partial A}. \end{aligned} \tag{5}$$

Now consider the following functional:

$$L=\int_\Omega \mathcal{L}(t,r,u,u_t,u_r)r^{n-1}\,\mathrm{d}r\,\mathrm{d}t \tag{6}$$

where $\mathcal{L}$ is some Lagrangian function.

The invariance of $\mathcal{L}$ under the action of a symmetry group is connected through Noether's theorem with existence of conservation laws for the Euler equations, which yield the stationary value of functional (6).

To apply Noether's theorem for (3), (4) we have generalized the Noether-type identity (see [4]) to the case of radially symmetric solutions in dimension n so that the variation in L

may be expressed in the following manner:

$$
\begin{aligned}
&\xi^t \frac{\partial \mathcal{L}}{\partial t} + \xi^r \frac{\partial \mathcal{L}}{\partial r} + \eta \frac{\partial \mathcal{L}}{\partial u} + [D_t(\eta) - u_t D_t(\xi^t) - u_r D_t(\xi^r)] \frac{\partial \mathcal{L}}{\partial u_t} \\
&\qquad + [D_r(\eta) - u_t D_r(\xi^t) - u_r D_r(\xi^r)] \frac{\partial \mathcal{L}}{\partial u_r} + \mathcal{L}[D_t(\xi^t) + D_r(\xi^r)] + \left(\frac{n-1}{r}\right) \xi^r \mathcal{L} \\
&\qquad \equiv (\eta - \xi^t u_t - \xi^r u_r) \left[\frac{\partial \mathcal{L}}{\partial u} - D_t \left(\frac{\partial \mathcal{L}}{\partial u_t} \right) - \frac{1}{r^{n-1}} D_r \left(r^{n-1} \frac{\partial \mathcal{L}}{\partial u_r} \right) \right] \\
&\qquad + D_t \left[\xi^t \mathcal{L} + (\eta - \xi^t u_t - \xi^r u_r) \frac{\partial \mathcal{L}}{\partial u_t} \right] \\
&\qquad + \frac{1}{r^{(n-1)}} D_r \left[r^{n-1} \left(\xi^r \mathcal{L} + (\eta - \xi^t u_t - \xi^r u_r) \frac{\partial \mathcal{L}}{\partial u_r} \right) \right] \qquad (7)
\end{aligned}
$$

where

$$
D_t = \frac{\partial}{\partial t} + u_t \frac{\partial}{\partial u} + \cdots \qquad D_r = \frac{\partial}{\partial r} + u_r \frac{\partial}{\partial u} + \cdots \qquad u = (A, \Phi). \qquad (8)
$$

The operator identity (7) makes evident the connection of the invariance of functional (6):

$$
\begin{aligned}
&\xi^t \frac{\partial \mathcal{L}}{\partial t} + \xi^r \frac{\partial \mathcal{L}}{\partial r} + \eta \frac{\partial \mathcal{L}}{\partial u} + [D_t(\eta) - u_t D_t(\xi^t) - u_r D_t(\xi^r)] \frac{\partial \mathcal{L}}{\partial u_t} \\
&\qquad + [D_r(\eta) - u_t D_r(\xi^t) - u_r D_r(\xi^r)] \frac{\partial \mathcal{L}}{\partial u_r} + \mathcal{L}[D_t(\xi^t) + D_r(\xi^r)] \\
&\qquad + \left(\frac{n-1}{r}\right) \xi^r \mathcal{L} = 0
\end{aligned}
$$

with conservation law

$$
D_t \left[\xi^t \mathcal{L} + (\eta - \xi^t u_t - \xi^r u_r) \frac{\partial \mathcal{L}}{\partial u_t} \right] + \frac{1}{r^{(n-1)}} D_r \left[r^{n-1} \left(\xi^r \mathcal{L} + (\eta - \xi^t u_t - \xi^r u_r) \frac{\partial \mathcal{L}}{\partial u_r} \right) \right] = 0
$$

for any solution of the Euler equations

$$
\frac{\partial \mathcal{L}}{\partial u} - D_t \left(\frac{\partial \mathcal{L}}{\partial u_t} \right) - \frac{1}{r^{n-1}} D_r \left(r^{n-1} \frac{\partial \mathcal{L}}{\partial u_r} \right) = 0.
$$

For the NLS problem, it is easy to check that the Lagrangian

$$
\mathcal{L} = A_r^2 + A^2 \Phi_r^2 + A^2 \Phi_t - \tfrac{1}{2} A^4 \qquad (9)
$$

yields the NLS system (3), (4) as Euler's equations. This Lagrangian (9) is invariant with respect to X_1 and X_2, and according to the Noether thereom (see the identity (7) with $u = (A, \Phi)$) provides the system (3), (4) with the following conservation laws:

$$
\begin{aligned}
&D_t\{A^2\} + \frac{1}{r^{n-1}} D_r\{r^{n-1} 2A^2 \Phi_r\} = 0 \\
&D_t \left\{ \frac{A^4}{2} - A_r^2 - A^2 \Phi_r^2 \right\} + \frac{1}{r^{n-1}} D_r\{r^{n-1}(2A_t A_r + 2A^2 \Phi_t \Phi_r)\} = 0
\end{aligned} \qquad (10)
$$

which are the well known laws of conservation of mass and Hamiltonian for the NLS system.

3. Intermediate Lagrange coordinate system

Now we will change the coordinate system to allow for the potential movement of points in the mesh that we will analyse in section 7. Let us prolong the symmetry operators (5) to the subspace

$$
\{t, r, A, \Phi; \mathrm{d}t; \mathrm{d}r; \mathrm{d}A; \mathrm{d}\Phi\}
$$

which contains differentials $\mathrm{d}t$, $\mathrm{d}r$, $\mathrm{d}A$, $\mathrm{d}\Phi$ so that

$$X_1 = \frac{\partial}{\partial t} \qquad X_2 = \frac{\partial}{\partial \Phi}$$
$$X_3 = 2t\frac{\partial}{\partial t} + r\frac{\partial}{\partial r} - A\frac{\partial}{\partial A} + 2\,\mathrm{d}t\,\frac{\partial}{\partial(\mathrm{d}t)} + \mathrm{d}r\,\frac{\partial}{\partial(\mathrm{d}r)} - \mathrm{d}A\,\frac{\partial}{\partial(\mathrm{d}A)}. \tag{11}$$

By solving the system of linear differential equations with partial derivatives

$$X_i(J_k) = 0$$

where $i = 1, 2, 3$; $k = 1, 2, 3, 4, 5$, we get the following complete set of differential invariants:

$$J_1 = rA \qquad J_2 = \mathrm{d}t\,(\mathrm{d}A)^2 \qquad J_3 = \frac{(\mathrm{d}r)^2}{\mathrm{d}t} \qquad J_4 = \mathrm{d}\Phi \qquad J_5 = A\,\mathrm{d}r. \tag{12}$$

This set gives us the possibility of finding the most general form for the evolution of r, which also conserves the scaling symmetry (11):

$$\frac{\mathrm{d}r}{\mathrm{d}t} = \frac{1}{\mathrm{d}r}F(A\,\mathrm{d}r;\,\mathrm{d}t\,(\mathrm{d}A)^2;\,\mathrm{d}\Phi;\,rA). \tag{13}$$

This result gives a means of evolving a computational mesh. If $F = 0$, then we get an orthogonal coordinate system (on a fixed mesh); If $F \neq 0$, then we have a moving coordinate system with an invariant evolution of r.

For simplicity we choose the following invariant evolution of r:

$$F = k(\mathrm{d}\Phi) \qquad \frac{\mathrm{d}r}{\mathrm{d}t} = k\Phi_r$$

where $k > 0$ is a control parameter (depending upon n), which can be chosen to control the form of mesh obtained in the numerical calculations. For example it can prevent the mesh becoming too sparse in certain regions.

As r varies we must extend the time derivative to involve the following Lagrangian derivative:

$$\frac{\mathrm{d}}{\mathrm{d}t} = D_t + k\Phi_r D_r. \tag{14}$$

Significantly, this operation does not commute with D_r:

$$\left[\frac{\mathrm{d}}{\mathrm{d}t}, D_r\right] \neq 0. \tag{15}$$

Rewriting the system (3), (4) in the Lagrangian coordinates then gives

$$\begin{aligned} &\frac{\mathrm{d}r}{\mathrm{d}t} = k\Phi_r \\ &\frac{\mathrm{d}A}{\mathrm{d}t} = -A\Phi_{rr} + (k-2)\Phi_r A_r - \frac{n-1}{r}A\Phi_r \\ &A\frac{\mathrm{d}\Phi}{\mathrm{d}t} = A_{rr} + \frac{n-1}{r}A_r + (k-1)A\Phi_r^2 + A^3. \end{aligned} \tag{16}$$

It is easy to show that the extended system (16) admits the symmetry operators (11) prolonged for the partial derivatives Φ_r, Φ_{rr}, A_r, A_{rr}, $\mathrm{d}r/\mathrm{d}t$, $\mathrm{d}A/\mathrm{d}t$, $\mathrm{d}\Phi/\mathrm{d}t$:

$$X_1 = \frac{\partial}{\partial t} \qquad X_2 = \frac{\partial}{\partial \Phi}$$
$$\begin{aligned} X_3 = 2t\frac{\partial}{\partial t} &+ r\frac{\partial}{\partial r} - A\frac{\partial}{\partial A} - 2A_r\frac{\partial}{\partial A_r} - 3A_{rr}\frac{\partial}{\partial A_{rr}} - \Phi_r\frac{\partial}{\partial \Phi_r} - 2\Phi_{rr}\frac{\partial}{\partial \Phi_{rr}} \\ &- \frac{\mathrm{d}r}{\mathrm{d}t}\frac{\partial}{\partial(\mathrm{d}r/\mathrm{d}t)} - 3\frac{\mathrm{d}A}{\mathrm{d}t}\frac{\partial}{\partial(\mathrm{d}A/\mathrm{d}t)} - 2\frac{\mathrm{d}\Phi}{\mathrm{d}t}\frac{\partial}{\partial(\mathrm{d}\Phi/\mathrm{d}t)}. \end{aligned}$$

4. The 'mass' Lagrange coordinate system

Now we will rewrite the system (16) in an orthogonal coordinate system by changing independent variables (t, r) to (t, s) and involving the new dependent variable ρ as follows:

$$D_s = \frac{1}{\rho r^{n-1}} D_r. \tag{17}$$

The purpose of this procedure is to recover the orthogonal differentiation property satisfied by a fixed coordinate mesh, so that in the revised coordinate system

$$\left[\frac{\mathrm{d}}{\mathrm{d}t}, D_s\right] = 0 \tag{18}$$

where

$$\frac{\mathrm{d}}{\mathrm{d}t} = D_t + k\Phi_r D_r.$$

From (18) we have the following equation for ρ:

$$\rho_t + (k\rho\Phi_r)_r + k\frac{n-1}{r}\rho\Phi_r = 0. \tag{19}$$

From (19) and

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = \rho_t + k\Phi_r\rho_r$$

we get one more equation, which yields an evolution for ρ of the form

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -k\frac{\rho}{r^{n-1}}(r^{n-1}\Phi_r)_r. \tag{20}$$

Let us find the connection between s and t, r. From (17) we have

$$s_r = \rho r^{n-1}.$$

From the orthogonality of the coordinates (t, s):

$$\frac{\mathrm{d}s}{\mathrm{d}t} = 0$$

we get

$$s_t = -k\rho\Phi_r r^{n-1}.$$

Thus, we have a nonpoint transformation of the independent variables from (t, r) to (t, s):

$$\begin{aligned} \mathrm{d}s &= \rho r^{n-1}\,\mathrm{d}r - k\rho r^{n-1}\Phi_r\,\mathrm{d}t \\ \bar{t} &= t. \end{aligned} \tag{21}$$

We also should add to (21)

$$\rho > 0$$

which implies the absence of a 'vacuum gap' in the Lagrange coordinate system. It is worth drawing a link at this stage between this approach and the theory of equidistributed meshes—see [20]. In this procedure a time-independent *computational variable* s is used for all calculations and r is expressed in terms of s. To determine r a *monitor* function M is used such that $\partial s/\partial r = M$. It is plain that this approach is equivalent to the orthogonal Lagrangian approach that we consider provided that we set $M = \rho r^{n-1}$.

Remark. We notice that the differential form (21) is total (complete); moreover it possible to start from the differential form ds as

$$\mathrm{d}s = \rho r^{n-1}\,\mathrm{d}r - k\rho r^{n-1}\Phi_r\,\mathrm{d}t$$

and then to demand the completeness of it, i.e.

$$D_t(\rho r^{n-1}) = -D_r(k\rho r^{n-1}\Phi_r)$$

which is equivalent to (19).

Now, rewriting the system (16)–(20) in terms of the orthogonal Lagrange coordinates (t, s) we obtain the system

$$\begin{aligned}
&\frac{\mathrm{d}r}{\mathrm{d}t} = k\rho r^{n-1}\Phi_s,\\
&\frac{\mathrm{d}A}{\mathrm{d}t} = r^{n-1}\left(-A\rho(\rho r^{n-1}\Phi_s)_s + (k-2)\rho^2 r^{n-1}\Phi_s A_s - \frac{n-1}{r}A\rho\Phi_s\right)\\
&A\frac{\mathrm{d}\Phi}{\mathrm{d}t} = \rho r^{n-1}(\rho r^{n-1}A_s)_s + \frac{n-1}{r}r^{n-1}\rho A_s + (k-1)A\rho^2\Phi_s^2 r^{2(n-1)} + A^3\\
&\frac{\mathrm{d}\rho}{\mathrm{d}t} = -k\rho^2(\rho r^{2(n-1)}\Phi_s)_s.
\end{aligned} \tag{22}$$

5. Conservation laws in the Lagrangian coordinate system

We can now derive the conservation laws for the system (22), by using the conservation of differential forms. We denote conservation laws for the system (3), (4) as

$$D_t\{A_0\} + D_r\{B_0\} = 0 \tag{23}$$

where A_0, for instance, for the first (mass) conservation law is

$$A_0 = r^{n-1}A^2.$$

The equation (23) is equivalent to the existence of the differential form

$$\mathrm{d}\Omega = A_0\,\mathrm{d}r - B_0\,\mathrm{d}t. \tag{24}$$

If we now transform the differential form (24) to the new set of independent variables (21) we have

$$\mathrm{d}\Omega = A_1\,\mathrm{d}s - B_1\,\mathrm{d}t = A_1(\rho r^{n-1}\,\mathrm{d}r - k\rho r^{n-1}\Phi_r\,\mathrm{d}t) - B_1\,\mathrm{d}t.$$

It follows that

$$A_1 = \frac{A_0}{\rho r^{n-1}} \qquad B_1 = B_0 - kA_0\Phi_r. \tag{25}$$

This we may rewrite as a conservation law in the new coordinate system to give

$$\frac{\mathrm{d}}{\mathrm{d}t}\{A_1\} + D_s\{B_1\} = 0. \tag{26}$$

In accordance with (25), the system (22) then has the following conservation laws:

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}t}\left\{\frac{A^2}{\rho}\right\} + D_s\{r^{2(n-1)}A^2\rho\Phi_s(2-k)\} = 0\\
&\frac{\mathrm{d}}{\mathrm{d}t}\left\{\frac{1}{\rho}\left(\frac{A^4}{2} - \rho^2 A_s^2 r^{2(n-1)} - \rho^2 A^2 r^{2(n-1)}\Phi_s^2\right)\right\}\\
&\qquad + D_s\left\{\rho r^{2(n-1)}\left[2A_s(\dot{A} - k\rho^2 r^{2(n-1)}A_s\Phi_s) + 2A^2\Phi_s(\dot{\Phi} - k\rho^2 r^{2(n-1)}\Phi_s^2)\right.\right.\\
&\qquad \left.\left. - k\Phi_s\left(\frac{A^4}{2} - \rho^2 r^{2(n-1)}A_s^2 - A^2\rho^2 r^{2(n-1)}\Phi_s^2\right)\right]\right\} = 0
\end{aligned} \tag{27}$$

where

$$\dot{A} = \frac{\mathrm{d}A}{\mathrm{d}t} \qquad \dot{\Phi} = \frac{\mathrm{d}\Phi}{\mathrm{d}t}.$$

Interestingly, the system (22) has one additional conservation law:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\{\frac{1}{\rho}\right\} + D_s\{-k\rho r^{2(n-1)}\Phi_s\} = 0 \tag{28}$$

which does not spring from the invariant Lagrange structure and is a continuity equation for the mesh density.

Transforming into the space (s, t, A, Φ, ρ, r) the symmetry operators (5) become

$$\begin{aligned} X_1 &= \frac{\partial}{\partial t} \qquad X_2 = \frac{\partial}{\partial \Phi} \\ X_3 &= 2t\frac{\partial}{\partial t} + r\frac{\partial}{\partial r} - A\frac{\partial}{\partial A} + s\frac{\partial}{\partial s} + (1-n)\rho\frac{\partial}{\partial \rho}. \end{aligned} \tag{29}$$

The system (22) allows an infinite-dimensional symmetry algebra. Indeed, in addition to the algebra (29) it allows the symmetries generated by

$$X_4 = f(s)\frac{\partial}{\partial s} + \rho f_s\frac{\partial}{\partial \rho} \tag{30}$$

where $f = f(s)$ is an arbitrary function.

6. The discretization procedure

Having considered various coordinate transformations of the NLS we now turn our attention to discretizations of this system in terms of these coordinates. We start our study of such discretizations by considering the NLS in the original variables (3), (4) and will proceed to construct an invariant difference scheme with all of the appropriate conservation laws. The first question that we need to address is finding the geometry of a mesh appropriate to the discretization procedure. In [9–12] the criterion of the invariance of an orthogonal mesh under the action of a symmetry operator was developed and led to the system

$$\underset{+h}{D}(\xi^t) = -\underset{+\tau}{D}(\xi^r). \tag{31}$$

Here h is the mesh spacing in the r-direction and τ in the t-direction. The equation (31) is true for all of the symmetry operators (5), so we can consider using an orthogonal mesh. The following criterion provides with the invariance of regularity of a mesh in both the r- and t-directions:

$$\underset{+\tau}{D}\,\underset{-\tau}{D}(\xi^t) = 0 \qquad \underset{+h}{D}\,\underset{-h}{D}(\xi^r) = 0 \tag{32}$$

where

$$\underset{+h}{D} = \frac{\underset{+h}{S} - 1}{h} \qquad \underset{-h}{D} = \frac{1 - \underset{-h}{S}}{h} \qquad \underset{+\tau}{D} = \frac{\underset{+\tau}{S} - 1}{\tau} \qquad \underset{-\tau}{D} = \frac{1 - \underset{-\tau}{S}}{\tau}$$

are the right and left difference differentiation in the x- and t-directions; $\underset{+h}{S}, \underset{-h}{S}, \underset{+\tau}{S}, \underset{-\tau}{S}$ are corresponding shift operators. Thus we will initially use the simplest invariant mesh which is orthogonal and regular in both directions (see figure 1), with the constant steps h and τ. We note at this stage that whilst this mesh has good symmetry properties it is not necessarily ideal for problems with associated small scales of time and length—this leads to the discretizations on regular meshes in the Lagrangian variables that we consider in subsequent sections.

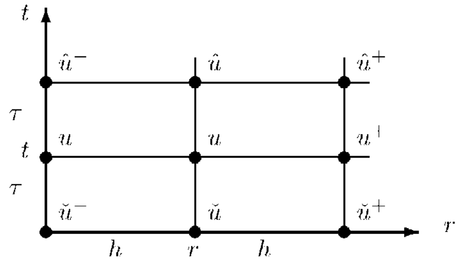

Figure 1. The orthogonal mesh in the original variables.

On this mesh we can consider the discrete version of the Lagrangian functional given by

$$L = \sum_i \mathcal{L}_i(A, A_r, \Phi_r, \Phi_t) h\tau \tag{33}$$

derived over an appropriate domain Ω. As a discrete Lagrangian we choose the following:

$$\mathcal{L} = A_r^2 + A^2\Phi_r^2 + A^2\Phi_t - \tfrac{1}{2}A^4 \tag{34}$$

where

$$A_r = \frac{A^+ - A}{h} = \underset{+h}{D}(A) \qquad \Phi_r = \frac{\Phi^+ - \Phi}{h} = \underset{+h}{D}(\Phi) \qquad \Phi_t = \frac{\hat{\Phi} - \Phi}{\tau} = \underset{+\tau}{D}(\Phi) \tag{35}$$

are the corresponding right difference derivatives. Our motivation is now to use this to derive discretization schemes with the correct conservation laws. To apply the difference analogue of the Noether theorem for (34) we have generalized the Noether-type operator identity (see [8–12]) to give

$$\begin{aligned}
&\xi^t \frac{\partial \mathcal{L}}{\partial t} + \xi^r \frac{\partial \mathcal{L}}{\partial r} + \eta \frac{\partial \mathcal{L}}{\partial u} + [\underset{+\tau}{D}(\eta) - u_t \underset{+\tau}{D}(\xi^t) - u_r \underset{+\tau}{D}(\xi^r)] \frac{\partial \mathcal{L}}{\partial u_t} \\
&\qquad + [\underset{+h}{D}(\eta) - u_t \underset{+h}{D}(\xi^t) - u_r \underset{+h}{D}(\xi^r)] \frac{\partial \mathcal{L}}{\partial u_r} + \mathcal{L}[\underset{+\tau}{D}(\xi^t) + \underset{+h}{D}(\xi^r)] + \left(\frac{n-1}{r}\right)\xi^r \mathcal{L} \\
&\quad \equiv \xi^t \left\{ \frac{\partial \mathcal{L}}{\partial t} + \underset{-\tau}{D}\left(u_t \frac{\partial \mathcal{L}}{\partial u_t} - \mathcal{L}\right) + \frac{1}{r^{n-1}} \underset{-h}{D}\left(r^{n-1} u_t \frac{\partial \mathcal{L}}{\partial u_r}\right)\right\} \\
&\qquad + \xi^r \left\{ \frac{\partial \mathcal{L}}{\partial r} + \underset{+\tau}{D}\left(\check{u}_r \left(\widecheck{\frac{\partial \mathcal{L}}{\partial u_t}}\right)\right)\right\} + \frac{1}{r^{(n-1)}} \underset{+h}{D}\left\{(r^-)^{n-1}\left[u_r^- \left(\frac{\partial \mathcal{L}}{\partial u_r}\right)^- - \mathcal{L}^-\right]\right. \\
&\qquad \left. + \left(\frac{n-1}{r}\right)\mathcal{L}\right\} + \eta \left\{ \frac{\partial \mathcal{L}}{\partial u} - \underset{-\tau}{D}\left(\frac{\partial \mathcal{L}}{\partial u_t}\right) - \frac{1}{r^{n-1}} \underset{-h}{D}\left(r^{n-1}\frac{\partial \mathcal{L}}{\partial u_r}\right)\right\} \\
&\qquad + \underset{+\tau}{D}\left\{\xi^t \check{\mathcal{L}} + (\eta - \xi^t \check{u}_t - \xi^r \check{u}_r)\left(\widecheck{\frac{\partial \mathcal{L}}{\partial u_t}}\right)\right\} \\
&\qquad + \frac{1}{r^{(n-1)}} \underset{+h}{D}\left\{(r^-)^{n-1}\left[\xi^r \mathcal{L}^- + (\eta - \xi^t u_t^- - \xi^r u_r^-)\left(\frac{\partial \mathcal{L}}{\partial u_r}\right)^-\right]\right\}
\end{aligned} \tag{36}$$

where $u = (A, \Phi)$, and all derivatives are difference derivatives. The identity (36) can be proved by direct calculations by applying a specific difference Leibnitz rule which is given in [9–12].

From the identity (36) we have the difference Euler equation

$$\frac{\partial \mathcal{L}}{\partial u} - \underset{-\tau}{D}\left(\frac{\partial \mathcal{L}}{\partial u_t}\right) - \frac{1}{r^{n-1}} \underset{-h}{D}\left(r^{n-1}\frac{\partial \mathcal{L}}{\partial u_r}\right) = 0 \tag{37}$$

but this equation possesses conservation laws only if $\xi^t = \xi^r = 0$.

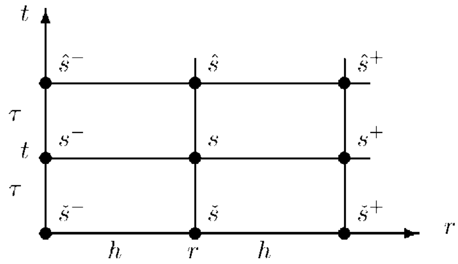

Figure 2. The orthogonal mesh in the computational variables.

If the left-hand side of the equation (36) equals 0, then some other equation

$$\begin{aligned}\xi^t&\left\{\frac{\partial\mathcal{L}}{\partial t}+\underset{-\tau}{D}\left(u_t\frac{\partial\mathcal{L}}{\partial u_t}-\mathcal{L}\right)+\frac{1}{r^{n-1}}\underset{-h}{D}\left(r^{n-1}u_t\frac{\partial\mathcal{L}}{\partial u_r}\right)\right\}\\&+\xi^r\left\{\frac{\partial\mathcal{L}}{\partial r}+\underset{+\tau}{D}\left(\check{u}_r\left(\frac{\partial\check{\mathcal{L}}}{\partial u_t}\right)\right)\right\}+\frac{1}{r^{(n-1)}}\underset{+h}{D}\left\{(r^-)^{n-1}\left[u_r^-\left(\frac{\partial\mathcal{L}}{\partial u_r}\right)^- -\mathcal{L}^-\right]\right.\\&\left.+\left(\frac{n-1}{r}\right)\mathcal{L}\right\}+\eta\left\{\frac{\partial\mathcal{L}}{\partial u}-\underset{-\tau}{D}\left(\frac{\partial\mathcal{L}}{\partial u_t}\right)-\frac{1}{r^{n-1}}\underset{-h}{D}\left(r^{n-1}\frac{\partial\mathcal{L}}{\partial u_r}\right)\right\}=0\end{aligned}\tag{38}$$

possesses the conservation law

$$\begin{aligned}&\underset{+\tau}{D}\left\{\xi^t\check{\mathcal{L}}+(\eta-\xi^t\check{u}_t-\xi^r\check{u}_r)\left(\frac{\partial\check{\mathcal{L}}}{\partial u_t}\right)\right\}\\&\quad+\frac{1}{r^{(n-1)}}\underset{+h}{D}\left\{(r^-)^{n-1}\left[\xi^r\mathcal{L}^-+(\eta-\xi^t u_t^- -\xi^r u_r^-)\left(\frac{\partial\mathcal{L}}{\partial u_r}\right)^-\right]\right\}=0.\end{aligned}\tag{39}$$

Now, let us apply this Noether-type identity for the Lagrangian (34). The Lagrangian (34) is invariant under the actions of X_1 and X_2. This immediately leads to the following conservation laws:

$$\underset{-\tau}{D}\{A^2\}+\frac{1}{r^{(n-1)}}\underset{-h}{D}\{2r^{n-1}A^2\Phi_r\}=0\tag{40}$$

$$\underset{-\tau}{D}\left\{\frac{A^4}{2}-A^2\Phi_r^2-A_r^2\right\}+\frac{1}{r^{(n-1)}}\underset{-h}{D}\{2r^{n-1}[A_rA_t+A^2\Phi_t\Phi_r]\}=0.\tag{41}$$

So, the difference equations (40), (41) form an invariant scheme on an orthogonal regular mesh and thus coincide with the difference conservation laws.

Notice, that this model is not unique, as some other equations can be obtained by the same procedure starting from some other invariant Lagrangian.

7. The total difference form

Now let us consider the difference analogue of a total differential form on the orthogonal difference mesh in the computational variable s, in accordance with the following picture (figure 2).

By doing this we may derive discretizations of the NLS more appropriate to problems with increasingly small length scales. In the upper right box we consider the following difference form:

$$\Delta s=s_rh+s_t^+\tau=\hat{s}_rh+s_t\tau\tag{42}$$

where the difference operators on s are as follows:

$$s_r = \frac{s^+ - s}{h} \qquad \hat{s}_r = \frac{\hat{s}^+ - \hat{s}}{h} \qquad s_t = \frac{\hat{s} - s}{\tau} \qquad s_t^+ = \frac{\hat{s}^+ - s^+}{\tau}.$$

It follows from (42) that

$$\underset{+h}{D}(s_t) = \underset{+\tau}{D}(s_r) \tag{43}$$

leading to the completeness of the difference form (42).

Let us restate the following difference derivatives of the computational variable s:

$$s_r = \rho r^{n-1} \qquad s_t = -k\rho r^{n-1}\Phi_r.$$

The completeness condition (43) then yields:

$$\underset{+\tau}{D}(\rho r^{n-1}) = -k\underset{+h}{D}(\rho r^{n-1}\Phi_r). \tag{44}$$

Relation (44) can be easily shifted to any needed mesh point.

Now we introduce the new difference differentiation operators of Lagrange type:

$$\frac{\mathrm{d}}{\mathrm{d}t_+} = \underset{+\tau}{D} + k\Phi_r \underset{+h}{D} \qquad \frac{\mathrm{d}}{\mathrm{d}t_-} = \underset{-\tau}{D} + k\check{\Phi}_r \underset{+h}{\check{D}} \tag{45}$$

where

$$\underset{+h}{\check{D}} = \underset{-\tau}{S}\underset{+h}{D} = \underset{+h}{D}\underset{-\tau}{S} \qquad \check{\Phi}_r = \underset{-\tau}{S}\Phi_r.$$

We also invoke a couple of difference operators corresponding to right and left differentiation in the s-direction as follows:

$$\rho r^{n-1}\underset{+h}{D}s = \underset{+h}{D} \qquad \rho^-(r^-)^{n-1}\underset{-h}{D}s = \underset{-h}{D}. \tag{46}$$

It is easy to check that the above-stated definitions give the orthogonality of a new mesh in the 'computational' (t, s) coordinate system:

$$\frac{\mathrm{d}s}{\mathrm{d}t_+} = 0 \qquad \frac{\mathrm{d}s}{\mathrm{d}t_-} = 0. \tag{47}$$

8. Difference conservation laws in the Lagrange coordinate system

To study discretizations in the new coordinate system we transform the difference conservation laws (40), (41) for the Lagrange coordinate system in the same manner as was followed in the continuous case using the conservation of differential forms.

We denote the conservation law (40), (41) as

$$\underset{+\tau}{D}\{A_0\} + \underset{+h}{D}\{B_0\} = 0 \tag{48}$$

which is equivalent to the existence of the difference form

$$\Delta_0 = A_0 h - B_0^+\tau = \hat{A}_0 h - B_0\tau. \tag{49}$$

Now transform the differential form (49) by the change of independent variables:

$$\bar{t} = t \qquad \Delta s = \rho r^{(n-1)}h - k\rho^+(r^+)^{(n-1)}\Phi_r^+\tau = \hat{\rho}\hat{r}^{(n-1)}h - k\rho r^{(n-1)}\Phi_r\tau. \tag{50}$$

In this derivation we have a 'new' spatial step $h_s = \Delta s$ in the computational variable.

The difference form (49) can be represented in the (t, s) coordinate system by

$$\begin{aligned}\Delta_0 &= A_1 h_s - B_1^+\tau = \hat{A}_1 h_s - B_1\tau = A_1(\rho r^{(n-1)}h - k\rho^+(r^+)^{n-1}\Phi_r^+\tau) - B_1^+\tau \\ &= \hat{A}_1(\hat{\rho}\hat{r}^{n-1}h - k\rho r^{n-1}\Phi_r\tau) - B_1\tau.\end{aligned} \tag{51}$$

Then we have

$$A_1 = \frac{A_0}{\rho r^{n-1}} \qquad B_1 = B_0 - kA_0\Phi_r \frac{\rho r^{n-1}}{\hat{\rho}\hat{r}^{n-1}} \tag{52}$$

which we may rewrite as a difference conservation law in a new coordinate system:

$$\underset{+\tau}{D}\{A_1\} + \underset{+h}{D}s\{B_1\} = 0. \tag{53}$$

In accordance with (52), (53) we can finally rewrite the conservation laws in the following form:

$$\frac{\mathrm{d}}{\mathrm{d}t_+}\left(\check{A}^2 \frac{\check{r}^{n-1}}{\rho r^{n-1}}\right) + \underset{+h}{D}s\left(2(r^-)^{2(n-1)}(A^-)^2\rho^-\Phi_s^- - kA^2\frac{\rho^2 r^{3(n-1)}}{\hat{\rho}\hat{r}^{n-1}}\Phi_s\right) = 0 \tag{54}$$

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}t_+}\left(\frac{\check{r}^{n-1}}{\rho r^{n-1}}\left[\frac{\check{A}^4}{2} - \check{\rho}^2\check{A}^2\check{\Phi}_s^2\check{r}^{2(n-1)} - \check{\rho}^2\check{r}^{2(n-1)}\check{A}_s^2\right]\right)\\
&\quad + \underset{+h}{D}s\Big(2(r^-)^{2(n-1)}\rho^-[A_s^-(\dot{A}^- - k(\rho^-)^2(r^-)^{2(n-1)}A_s^-\Phi_s^-)\\
&\quad + (A^-)^2\Phi_s^-(\dot{\Phi}^- - k(\rho^-)^2(r^-)^{2(n-1)}(\Phi_s^-)^2)]\\
&\quad - k\Phi_s\frac{\rho^2 r^{3(n-1)}}{\hat{\rho}\hat{r}^{n-1}}\left[\frac{A^4}{2} - \rho^2A^2\Phi_s^2r^{2(n-1)} - \rho^2r^{2(n-1)}A_s^2\right]\Big) = 0.
\end{aligned} \tag{55}$$

This system allows us to evolve the discrete solution. We must also allow for the evolution of the mesh points given by the following two equations for the evolution of r and ρ:

$$\frac{\mathrm{d}r}{\mathrm{d}t_+} = k\rho r^{n-1}\Phi_s \tag{56}$$

$$\frac{\mathrm{d}}{\mathrm{d}t_+}\left(\rho r^{n-1}\right) = -k\rho^+(r^+)^{n-1}\rho r^{n-1}(\rho r^{n-1}\Phi_s)_s. \tag{57}$$

Thus, equations (54)–(57) form an invariant difference scheme on the orthogonal mesh in the (t, s) plane which can be implemented to calculate solutions of the NLS as it evolves toward a singularity.

9. The blow-up invariant solution

Finally we consider the application of the discretization (54) in the context of solutions with developing singularities.

Let us first transform the symmetry operators (5) into the space (s, t, A, Φ, ρ, r):

$$\begin{aligned}
&X_1 = \frac{\partial}{\partial t} \qquad X_2 = \frac{\partial}{\partial \Phi}\\
&X_3 = 2t\frac{\partial}{\partial t} + r\frac{\partial}{\partial r} - A\frac{\partial}{\partial A} + s\frac{\partial}{\partial s} + (1-n)\rho\frac{\partial}{\partial \rho}.
\end{aligned} \tag{58}$$

We showed that the system (22) together with (58) has one more additional symmetry

$$X^* = f(s)\frac{\partial}{\partial s} + \rho f_s\frac{\partial}{\partial \rho} \tag{59}$$

where $f = f(s)$ is an arbitrary function.

The system (54)–(57) possesses the same symmetries (58) and has the additional symmetry

$$X^* = f(s)\frac{\partial}{\partial s} + \rho\underset{+h}{D}s(f)\frac{\partial}{\partial \rho}. \tag{60}$$

Now, let us now consider the symmetry subalgebra

$$X = -2T_0X_1 + X_3 = 2(T_0 - t)\frac{\partial}{\partial(T_0 - t)} + r\frac{\partial}{\partial r} - A\frac{\partial}{\partial A} + s\frac{\partial}{\partial s} + (1 - n)\rho\frac{\partial}{\partial \rho} \tag{61}$$

where T_0 is some positive constant. Then we add to (61) the special case of operator (59), (60):

$$X^{**} = \gamma\left(s\frac{\partial}{\partial s} + \rho\frac{\partial}{\partial \rho}\right) \tag{62}$$

that yields the subalgebra

$$\hat{X} = 2(T_0 - t)\frac{\partial}{\partial(T_0 - t)} + r\frac{\partial}{\partial r} - A\frac{\partial}{\partial A} + s(1 + \gamma)\frac{\partial}{\partial s} + (1 - n + \gamma)\rho\frac{\partial}{\partial \rho} \tag{63}$$

where γ is some 'monitoring' parameter. It is easy to see that $\gamma = -1$ corresponds to the situation when s is an invariant of subalgebra (63). The corresponding symmetry operator is the following:

$$\hat{X}^{*} = 2(T_0 - t)\frac{\partial}{\partial(T_0 - t)} + r\frac{\partial}{\partial r} - A\frac{\partial}{\partial A} - n\rho\frac{\partial}{\partial \rho}. \tag{64}$$

Let us write down the invariant representation of the solution in that case:

$$\begin{aligned} &A = \bar{A}(\lambda)(T_0 - t)^{-1/2} \qquad && \Phi = \bar{\Phi}(\lambda) \\ &\rho = \bar{\rho}(\lambda)(T_0 - t)^{-n/2} && s = \bar{s}(\lambda) \\ &\lambda = r(T_0 - t)^{-1/2}. \end{aligned} \tag{65}$$

This solution has the desired property of having a self-similar form and of becoming singular in a finite time T_0 with amplitude proportional to $(T_0 - t)^{-1/2}$ whilst evolving on a length scale proportional to $(T_0 - t)^{1/2}$. Thus, if such a solution exists for the underlying problem, it is admitted by the discretization. As remarked earlier, this is a significant feature of such a method, as it is known [31] that if $n > 2$ then the stable form of singularity evolution is that of a monotone decreasing self-similar solution.

Remark. We should emphasize at this stage that whilst a solution of the form (65) may formally be admitted, there is no *a priori* guarantee that the appropriate function $\bar{A}(\lambda)$ (which usually has to satisfy certain regularity conditions at infinity) will exist. The evidence [32] is that such a function does exist if n is slightly greater than 2 but it does not exist if $n = 2$.

As s is an invariant of this solution, there is no movement of waves in the s-direction for the invariant solution of the form (65) and any distinctive point of the solution (65) in the λ (gradient maximum or zero point for example) does not move in the s-direction. Thus s is a true computational variable, in the sense that a 'difficult' problem computationally when expressed in terms of r has been transformed into a more 'regular' problem in s allowing for a more straightforward discretization.

The ordinary differential system and corresponding ordinary difference system can be easily obtained by substitution of the invariant representation (65) into the system (22) and (54)–(57).

References

[1] Ovsiannikov L V 1982 *Group Analysis of Differential Equations* (New York: Academic)
[2] Olver P J 1986 *Applications of Lie Groups to Differential Equations* (Berlin: Springer)
[3] Bluman G W and Kumei S 1989 *Symmetries and Differential Equations* (Berlin: Springer)
[4] Ibragimov N H 1985 *Transformation Groups Applied to Mathematical Physics* (Boston, MA: Reidel)

[5] Hydon P 1999 *Symmetry Methods for Ordinary Differential Equations* (Cambridge: Cambridge University Press)

[6] Maeda S 1980 Canonical structure and symmetries for discrete systems *Math. Japan* **25** 405

[7] Maeda S 1987 The similarity method for difference equations *J. Inst. Math. Appl.* **38** 129

[8] Dorodnitsyn V A 1989 Transformation groups in a space of difference variables *VINITI Acad. Sci. USSR, Itogi Nauk. Tekh.* **34** 149 (Engl. transl. 1991 *J. Sov. Math.* **55** 1490)

[9] Dorodnitsyn V 1993 Finite-difference models entirely inheriting symmetry of original differential equations *Modern Group Analysis: Advanced Analytical and Computational Methods in Mathematical Physics* (Dordrecht: Kluwer Academic) p 191

[10] Ames W F, Anderson R L, Dorodnitsyn V A, Ferapontov E V, Gazizov R K, Ibragimov N H and Svirshchevskii S R 1994 *Symmetries, Exact Solutions and Conservation Laws (CRC Handbook of Lie Group Analysis of Differential Equations vol 1)* (Boca Raton, FL: Chemical Rubber Company)

[11] Dorodnitsyn V A 1993 Finite-difference analogue of the Noether theorem *Dokl. Akad. Nauk* **328** 678 (in Russian)
Dorodnitsyn V 1998 Noether-type theorems for difference equation *Report* IHES/M/98/27, Bures-sur-Yvette

[12] Dorodnitsyn V A 1994 Finite-difference models entirely inheriting continuous symmetry of original differential equations *Int. J. Mod. Phys.* **5** 723

[13] Levi D and Winternitz P 1991 Continuous symmetries of discrete equations *Phys. Lett.* A **152** 335

[14] Quispel G R W, Capel H W and Sahadevan R 1992 Continuous symmetries of difference equations; the Kac–van Moerbeke equation and Painleve reduction *Phys. Lett.* A **170** 379

[15] Quispel G R W and Sahadevan R 1993 Lie symmetries and integration of difference equations *Phys. Lett.* A **184** 64

[16] Dorodnitsyn V 1996 Continuous symmetries of finite-difference evolution equations and grids *Symmetries and Integrability of Difference Equations (CRM Proceedings and Lecture Notes vol 9)* (Providence, RI: American Mathematical Society) pp 103–12
See also Dorodnitsyn V 1994 Invariant discrete model for the Korteweg–de Vries equation *Preprint* CRM-2187, Montreal

[17] Bakirova M, Dorodnitsyn V and Kozlov R 1997 Invariant difference schemes for heat transfer equations with a source *J. Phys. A: Math. Gen.* **30** 8139
See also Dorodnitsyn V and Kozlov R 1997 The complete set of symmetry preserving discrete versions of a heat transfer equation with a source *Preprint* NTNU, NUMERICS No 4/1997, Trondheim, Norway

[18] Budd C and Collins G J 1997 Symmetry based numerical methods for partial differential equations *1997 Dundee Conf. on Numerical Analysis* ed D Griffiths, D Higham and G Watson (Harlow: Addison Wesley, Longman)

[19] Budd C and Collins G 1998 An invariant moving mesh scheme for the nonlinear diffusion equation *Appl. Numer. Math.* **26** 23

[20] Budd C, Huang W and Russell R 1996 Moving mesh methods for problems with blow-up *SIAM J. Sci. Comput.* **17** 305

[21] Budd C, Chen S and Russell R 1999 New self-similar solutions of the nonlinear Schrödinger equation, with moving mesh computations *J. Comput. Phys.* **152** 756

[22] Levi D and Winternitz P 1996 Symmetries of discrete dynamical systems *J. Math. Phys.* **37** 5551

[23] Hernandez Heredero R, Levi D and Winternitz P Symmetries of the discrete Burgers equation *J. Phys. A: Math. Gen.* **32** 2685

[24] Dorodnitsyn V and Winternitz P 1999 Lie point symmetry preserving discretizations for variable coefficient Korteweg–de Vries equations *Preprint* CRM-2607, Université de Montreal

[25] Dorodnitsyn V, Kozlov R and Winternitz P 2000 Lie group classification of second-order difference equations *J. Math. Phys.* **41** 480

[26] Hydon P 2000 Symmetries and first integrals of ordinary difference equations *Proc. R. Soc.* A **456** 2835

[27] Ablowitz M and Herbst B 1990 On homoclinic structure and numerically induced chaos for the nonlinear Schrödinger equation *SIAM J. Appl. Math.* **50** 339

[28] MacLachlan R 1994 Symplectic integration of Hamiltonian wave equations *Numer. Math.* **66** 465

[29] Akrivas G, Dougalis V and Karakashian O 1993 On fully discrete Galerkin methods of second order temporal accuracy for the nonlinear Schrödinger equation *Numer. Math.* **59** 31

[30] Tourigny Y and Sanz Serna J M 1992 The numerical study of blowup with application to the nonlinear Schrödinger equation *J. Comput. Phys.* **102** 407

[31] Sulem C and Sulem P-L 1999 *The Nonlinear Schrödinger Equation (Springer Series in Applied Mathematical Sciences vol 139)* (Berlin: Springer)

[32] Koppel N and Landman M 1995 Spatial structure of the focussing singularity of the nonlinear Schrödinger equation: a geometrical analysis *SIAM J. Appl. Math.* **55** 1297