A note on the numerical integration of the KdV equation via isospectral deformations

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June 16, 2000

Abstract

The main purpose of this note is to test the performance of Lie group integrators as applied to a semi discrete version of the KdV equation.

1 Introduction

We consider the numerical approximation of the KdV equation

$$u_t + u_{xxx} - 3uu_x = 0. \tag{1.1}$$

In this manuscript we will focus our attention on the Lax formulation of the equation. Consider the Schroedinger operator

$$L = -D^2 + u, \tag{1.2}$$

where $D = \frac{d}{dx}$ represents differentiation with respect to the x variable. It is well known that if u evolves according to the KdV equation then the operator L is unitarily equivalent, i.e. L is such that

$$U^*(t)L(t)U(t) = L(0), \tag{1.3}$$

and $U(t)$ is a one-parameter family of unitary operators in $L_2(-\infty, \infty)$. The flow $L(t)$ is isospectral. This can otherwise be expressed by the following equation

$$L_t = [B, L], \tag{1.4}$$

where B is the infinitesimal generator of the family $U(t)$. For $B = D$ (skew-adjoint) (1.4) reduces to $u_t = u_x$ the infinitesimal generator of translations leaving L invariant. If we consider

$$B = -4D^3 + 2(qD + Dq), \tag{1.5}$$

(1.4) reduces to the KdV equation. There is a hierarchy of operators B defining non-linear evolutionary equations though (1.4), which leave the Schroedinger operator L invariant. The operators L and B are self and sew-adjoint respectively with respect to the inner product of $L_2(-\infty, \infty)$. In [2] Adler described the orbit symplectic structure of Konstant-Kirillov for the KdV equation. In his analysis, using the theory of pseudo-differential operators, the author identifies the formal Lie group G, the formal Lie algebra $\mathfrak{g}$ and the Lie coadjoint group action of G over $\mathfrak{g}^*$ necessary for defining the Konstant-Kirillov symplectic form. In this context we will be mostly concerned with the analogous adjoint action.

Several authors have been recently considering the use of Lie group actions in the numerical integration of ordinary differential equations on manifolds see [3] for an overview on the subject. The main idea of these methods is based on the assumption that the vector field of the given differential equation can be expressed in terms of a Lie group action on the manifold. Advancing in time the solution of a transformed problem in the Lie algebra using a Runge-Kutta method and then transforming back the result to the manifold it is possible to obtain approximations of the flow that preserve the orbits. More specifically in the case of isospectral flows the methods preserve the spectrum of the operators. In the case of the KdV equation (and other completely integrable systems) the Lax formulation of the equation involves infinite dimensional operators and in practice the above mentioned numerical methods can be applied only after a suitable space discretization of the operators L and B.

Semidiscretizations preserving symmetries or the Hamiltonian structure of PDEs have been considered recently in [17], [4], [9], [14].

In the KdV case one can consider semidiscretizations that describe an isospectral flow in a finite dimensional space. A famous example of such discretization was given by Kac and Van Moerbeke in [13], [12]. We refer to [18] for a study of the convergence of the solutions of the Kac-Van Moerbeke discretization to the solutions of (1.1).

The spectrum of the discrete Schroedinger operator is in any case just a discretization of the spectrum of L and what we are guaranteed to preserve with our time-stepping procedure it is just the discrete and obviously not the true spectrum of L.

In a more general way we are interested in finding discretizations of the operators L and B that are respectively self-adjoint and skew-adjoint with respect to an opportune discretization of the inner product of L_2. With straightforward computation it is possible to verify that, given $\phi \in L_2$, $[B, L]\phi = BL\phi - LB\phi = q_{xxx}\phi + 6qq_x\phi$ and the operator $[B, L]$ does not contain D or powers of D. This fact is a consequence of the rules of composition of the operator D. This feature plays an important role also in the discrete version of the problem and in the Kac-Van Moerbeke discretization it is represented by the fact that $[\tilde{B}, \tilde{L}]$ is a matrix with the same sparsity pattern as L.

We conjecture that considering restrictions of L and B on finite dimensional subspaces of functions in L_2, and imposing certain constraints of regularity on these functions it is possible to define other suitable discretizations $\tilde{L}$ and $\tilde{B}$ ensuring the desired properties of differentiation for $\tilde{D}$.

The main purpose of this note is to test the performance of Lie group integrators as applied to a semi discrete version of the KdV equation, and to discuss which features of the infinite dimensional problem should be maintained in the semi discrete system in order to apply these time integration strategies.

In the next section we will give a brief introduction to the methods of integration on manifolds based on the use of Lie group actions with particular consideration to the case of isospectral flows and sparse matrices.

In the third and last section we will consider the application of these methods to the discretization of the KdV equation.

2 Methods based on Lie group actions

Consider the differential equation

$$y^{'} = F(t, y), \qquad y \in \mathcal{M}$$

with $F(t,\cdot) \in X(\mathcal{M})$ a vector field on $\mathcal{M}$ assume that

$$F(t, y) = \lambda_*(f(t, y))(y). \tag{2.6}$$

Here $f : \mathbb{R} \times \mathcal{M} \to \mathfrak{g}$ and $\lambda_* : \mathfrak{g} \to X(\mathcal{M})$ and it is obtained as follows: assume

$$\Lambda : \mathrm{G} \times \mathcal{M} \to \mathcal{M}$$

is a Lie group action, choose

$$\phi : \mathfrak{g} \to \mathrm{G}$$

a coordinate map form $\mathfrak{g}$ on G, define

$$\lambda : \mathfrak{g} \times \mathcal{M} \to \mathcal{M}$$

a Lie algebra action by $\lambda(v, p) = \Lambda(\phi(v), p)$ and

$$\lambda_*(v)(p) = \left.\frac{d}{dt}\right|_{t=0} \lambda(tv, p)$$

and $f : \mathbb{R} \times \mathcal{M} \to \mathfrak{g}$. We will consider cases in which $\mathfrak{g} \subset \mathfrak{gl}(n)$.

Consider $d\phi_w : \mathfrak{g} \to \mathfrak{g}$,

$$d\phi_w(v) = \frac{d}{dt}|_{t=0}(\phi(v + tw)).$$

Then, given $p \in \mathcal{M}$, the vector field $\varphi(t, u) = \mathrm{d}\phi_u^{-1}(f(t, \lambda_p(u)))$, with $\lambda_p : \mathfrak{g} \to \mathcal{M}$ and $(\lambda_p(u) = \lambda(u, p))$ is such that

$$\lambda_p' \circ \varphi = F \circ \lambda_p.$$

As an immediate consequence if

$$u(t)' = \varphi(u(t)), \tag{2.7}$$

then

$$(\lambda_p \circ u)' = \lambda_p' \circ u' = \lambda_p' \circ \varphi \circ u = F \circ (\lambda_p \circ u).$$

It is possible to use a method of integration for ODEs on the Lie algebra equation (2.7) and transform back to the manifold $\mathcal{M}$ the obtained approximation at every time step. This leads to the following algorithm originally due to Munthe-Kaas:

Generalized RK-MK algorithm

$p := y_n$
for $i = 1$ to s do
  $u_i := h \sum a_{ij} \tilde{k}_j$
  $k_i = f(t_n + c_i h, \lambda(u_i, p)),$
  $\tilde{k}_i := \mathrm{d}\phi_{u_i}^{-1}(k_i)$
end do
$v := h \sum b_i \tilde{k}_i$
$y_{n+1} = \lambda(v, p)$

For a more extensive description of these methods we refer to the original article of Munthe-Kaas [15] and for its generalizations to [16] and [10]. Similar strategies have been explored by Zanna in [20] and [8] with particular focus on the application to isospectral flows.

Suppose now we want to apply the previous algorithm to an isospectral flow of the type

$$L_t = [B(L), L], \tag{2.8}$$

$L(0) = L_0$ with L $n \times n$ symmetric matrix, $L \in \mathrm{Sym}(n)$, and $B : \mathrm{Sym}(n) \to \mathfrak{so}(n)$, that here plays the role of f in (2.6). Given a coordinate map $\phi : \mathfrak{so}(n) \to \mathrm{SO}(n)$, the Lie algebra action

$$\lambda(P, S) := \phi(P)^* S \phi(P)$$

and consequently

$$\lambda_*(P)(S) = [P, S],$$

we recognize in (2.8) the framework required in (2.6).

Several possible choices are available for the coordinate map $\phi : \mathrm{SO}(n) \to \mathfrak{so}(n)$. Perhaps the most natural one consists in taking $\phi = \exp$ the matrix exponential, that leads to the following expression for $\mathrm{d}\phi_u^{-1}$,

$$\mathrm{d}\exp_u^{-1}(v) = \left.\frac{z}{e^z - z}\right|_{\mathrm{ad}_u}(v). \tag{2.9}$$

When $n \geq 4$, while some good techniques for the computation of the exponential of skew-symmetric matrices are available, [19] especially in the case of tridiagonal matrices, for computing (2.9) it is usual practice to consider truncations of the corresponding Taylor expansion of the same order in the step-size h of the considered Runge-Kutta method. An alternative way of approximating (2.9) is based on the use of Krylov techniques. Considering the subspace of $\mathfrak{so}(n)$

$$K_p(\mathrm{ad}_u, v) = \mathrm{span}\{v, \mathrm{ad}_u(v), \mathrm{ad}_u^2(v), \ldots, \mathrm{ad}_u^{p-1}(v)\},$$

and with $v_1, \ldots, v_p$ orthonormal basis with respect to the inner product $< w, v >= \mathrm{trace}(wv) = \sum_{i=1}^n \sum_{l=1}^n w_{i,l} v_{l,i}$, it is possible to consider the following approximation of (2.9)

$$V_p \mathrm{d}\phi_{H_p}^{-1}(\boldsymbol{e}_1)\|v\| \approx \mathrm{d}\phi_u^{-1}(v),$$

where $(H_p)_{i,j} =< v_i, \mathrm{ad}_u(v_j) >$, $j = 1, \ldots, p$ and $i = 1, \ldots, j+1$ and $V_p : \mathbb{R}^p \to K_p$ is such that $V_p(\boldsymbol{b}) = \sum_{k=1}^p v_i b_i$. Note that the order of the approximation coincides with the dimension of the Krylov subspace and then the cost of computing the above approximation is approximately the same of the truncated Taylor expansion, given that the cost for the inner products do not exceed $\mathcal{O}(n^2)$.

Among other choices for the coordinate map ϕ rational maps can be considered [5], and in particular all the diagonal Pade' approximants of the exponential map are suitable. For example if we consider $\phi(u) = (I - u/2)^{-1}(I + u/2)$, the Cayley map, we have $\mathrm{d}\phi_u^{-1}(v) = (I - u/2)v(I + u/2)$ in an explicit closed form.

A third and last option that we want to mention here is based on the composition of elementary exponentials, one can take for example $\phi(u) = e^{u_1 e_1} \cdots e^{u_d e_d}$, where $e_1, \ldots, e_d$ are a basis of the Lie algebra $\mathfrak{g}$ that in our case is $\mathfrak{so}(n)$.

The straightforward computation of $\mathrm{d}\phi_u^{-1}(v)$ implies high computational costs, but in the case of semi-simple Lie algebras over $\mathbb{C}$, it is possible to derive explicit expressions for $\mathrm{d}\phi_u^{-1}$ that can be computed at a competitive cost [16], these results do not apply in the $\mathfrak{so}(n, \mathbb{R})$ case.

In this last case one can instead opt for finding cheap approximations of the correct order for $\mathrm{d}\phi_u^{-1}(v)$ when $u, v \in \mathfrak{so}(n, \mathbb{R})$. In [5] and [6] the authors propose a strategy based on the use of compositions of elementary exponentials for constructing approximations of the exponential map of order p in the stepsize that are coordinates maps in their own right. Using such maps combined with the same order approximation of $\mathrm{d}\exp_u^{-1}$ gives a method of order p.

For $u \in \mathfrak{g}$, and $\mathfrak{g}$ of dimension d, let $e_1, \ldots, e_d$ be a basis for $\mathfrak{g}$, and $u = \sum_{l=1}^{d} u_l e_l$ consider

$$\phi(u) = \exp(\alpha_1(u)e_1) \cdots \exp(\alpha_d(u)e_d)$$

with $\alpha_j : \mathfrak{g} \to \mathbb{R}$ if the Jacobian of $[\alpha_1, \ldots \alpha_d]$ is invertible for u sufficiently close to the origin in $\mathfrak{g}$ $\phi(u)$ is a coordinate map. More generally consider

$$\phi(u) = \exp(U_1) \cdots \exp(U_k)$$

where the $\{U_i\}_{i=1}^{k}$ are defined as follows: let $\{S_i\}_{i=1}^{k}$ define a partition of the set of indices $\mathcal{I} = \{1, \ldots, d\}$, i.e.

$$\cup_{i=1}^{k} S_i = \mathcal{I}, \qquad S_i \cap S_j = O, \quad i \neq j;$$

we define now

$$U_i := \sum_{j \in S_i} \lambda_j(u) e_j,$$

with $\lambda_j : \mathfrak{g} \to \mathbb{R}$. Using the Baker-Campbell-Hausdorff (BCH) formula for $U_1, \ldots, U_k$ we find $Y(u) = \sum_{l=1}^{d} y_l(u) e_l$ such that $\phi(u) = \exp(Y(u))$ and also in this case if for u enough close to the origin the Jacobian of $[y_1, \ldots y_d]$ is invertible then ϕ is a coordinate map.

To illustrate this strategy we here give a special instance of these techniques that will prove itself useful in the special applications considered in the sequel.

We consider a symmetric composition for the coordinate map

$$\phi(u) = \exp(U_1) \cdots \exp(U_k) \cdots \exp(U_1),$$

where the U_i are defined as above and we consider $U_i^0 = \sum_{j\in S_i} u_j e_j$. Take now $\Lambda(u) = \sum_{l=1}^d \lambda_l(u) e_l$ with $\Lambda(u)$ representing an approximation of the symmetric Baker-Campbell-Hausdorff (BCH) formula for $U_1^0, \ldots, U_k^0$, for example a truncation at the $p/2+1$ term.

Suppose for example $p = 4$, we can express $\lambda_i(u) = u_i + q_i(u)$ and $Q(u) = \sum_{i=1}^d q_i(u) e_i$ is the second term in the symmetric BCH formula for $U_1^0, \ldots, U_k^0$ that can be expressed explicitly by

$$Q(u) = \tfrac{1}{12}\sum_{l=2}^{k-1} [U_1^0 + \cdots + U_{l-1}^0 + \tfrac{1}{2}U_l^0, [U_1^0 + \cdots + U_{l-1}^0, U_l^0]],$$

and for particular choices of the partition $\cup_{i=1}^k S_i = \mathcal{I}$ give explicit expressions for $q_i(u)$.

If $u \in \mathfrak{so}(n)$ is a skew-symmetric matrix, and we set for instance $U_i^0 = \boldsymbol{u}_i \boldsymbol{e}_i^{\mathrm{T}} - \boldsymbol{e}_i \boldsymbol{u}_i^{\mathrm{T}}$ with $\boldsymbol{u}_i = -[0, \ldots, 0, u_{i,i+1}, \ldots, u_{i,n}]^{\mathrm{T}}$ and $\boldsymbol{e}_i$ the i-th vector of the canonical basis of $\mathbb{R}^n$, then after some elementary algebra one can express $Q(u)$ with the following sum of skew-symmetric matrices

$$\begin{aligned} Q \; &= \tfrac{1}{12}\sum_{l=2}^{n-1} 2(\bar{\boldsymbol{u}}_l \hat{\boldsymbol{u}}_l^{\mathrm{T}} - \hat{\boldsymbol{u}}_l \bar{\boldsymbol{u}}_l^{\mathrm{T}}) + \tfrac{1}{2}(\bar{\boldsymbol{u}}_l \boldsymbol{u}_l^{\mathrm{T}} - \boldsymbol{u}_l \bar{\boldsymbol{u}}_l^{\mathrm{T}}) + \\ &\tfrac{1}{12}\sum_{l=2}^{n-1} \boldsymbol{u}_l \left(\sum_{k=1}^{l-1} u_{k,l}\boldsymbol{u}_k - \check{\boldsymbol{u}}_l\right)^{\mathrm{T}} - \left(\sum_{k=1}^{l-1} u_{k,l}\boldsymbol{u}_k - \check{\boldsymbol{u}}_l\right)\boldsymbol{u}_l^{\mathrm{T}} + \\ &\tfrac{1}{12}\sum_{l=2}^{n-1} \tfrac{1}{2}\boldsymbol{u}_l^{\mathrm{T}}\boldsymbol{u}_l \left(\hat{\boldsymbol{u}}_l \boldsymbol{e}_l^{\mathrm{T}} - \boldsymbol{e}_l \hat{\boldsymbol{u}}_l^{\mathrm{T}}\right) + \check{\boldsymbol{u}}_l \boldsymbol{e}_l^{\mathrm{T}} - \boldsymbol{e}_l \check{\boldsymbol{u}}_l^{\mathrm{T}}, \end{aligned}$$

with

$$\boldsymbol{e}_k^{\mathrm{T}} \bar{\boldsymbol{u}}_l = \begin{cases} -\boldsymbol{u}_k^{\mathrm{T}}\boldsymbol{u}_l & k = 1, \ldots, l-1 \\ 0 & \text{otherwise,} \end{cases}$$

and

$$\boldsymbol{e}_k^{\mathrm{T}} \hat{\boldsymbol{u}}_l = \begin{cases} u_{k,l} & k = 1, \ldots, l-1 \\ 0 & \text{otherwise,} \end{cases}$$

and

$$\boldsymbol{e}_k^{\mathrm{T}} \check{\boldsymbol{u}}_l = \begin{cases} \boldsymbol{u}_k^{\mathrm{T}}\hat{\boldsymbol{u}}_l & k = 1, \ldots, l-1 \\ 0 & \text{otherwise.} \end{cases}$$

The cost of computing Q is in this case $\approx 5n^3$, but if the rows of the matrix u are such that just one elemant per row is nonzero then the complexity reduces to $\approx 5n^2$. This is in fact the case of the application we will present in next section.

Parametrising the element $u \in \mathfrak{g}$ with the step-size h it is easy to realize that $\phi(hu) = \exp(hu) + \mathcal{O}(h^5)$ in the previous example, for this reason it is possible to take the series of $\mathrm{d}\exp_{hu}^{-1}$ truncated at order 4 as an order four approximation of $\mathrm{d}\phi_{hu}^{-1}$.

In the case of sparse matrices, the main drawback in the application of these methods is due to the fact that the application of $w = \mathrm{d}\phi_u^{-1}(v)$ with u and v sparse gives a result w of sparsity that is reduced with the order of the method. This implies that at each time step, in the computation of the Lie algebra action in the method, the coordinate map is applied to matrices of decreasing sparsity. To avoid this problem it is possible to use methods that are simply based on the composition of elementary flows for which however the number of exponentials to be computed is much higher than in this case [7].

3 Discrete KdV and Lie group integrators

In this section we consider the use of the methods described in the previous section in the numerical integration of the following system of differential equations:

$$\frac{dR_n}{dt} = e^{-R_{n-1}(t)} - e^{-R_{n+1}(t)} \tag{3.10}$$

for $n = 2, \ldots, N-1$ with $\frac{dR_1}{dt} = -e^{-R_2(t)}$ and $\frac{dR_N}{dt} = e^{-R_{N-1}(t)}$, and setting $a_i = \frac{1}{2}e^{-\frac{1}{2}R_i(t)}$ for $i = 1, \ldots, N$ and $b_i = a_i a_{i+1}$ for $i = 1, \ldots, N-1$ we define the following $(N+1) \times (N+1)$ matrices

$$L = \begin{bmatrix} 0 & a_1 & 0 & \dots & 0 \\ a_1 & \ddots & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & a_N \\ 0 & \dots & 0 & a_N & 0 \end{bmatrix} \qquad B = \begin{bmatrix} 0 & 0 & b_1 & \dots & 0 \\ 0 & \ddots & \ddots & \ddots & \vdots \\ -b_1 & \ddots & \ddots & \ddots & b_{N-1} \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \dots & -b_{N-1} & 0 & 0 \end{bmatrix}.$$

We will apply the techniques described in the previous section to the isospectral flow

$$L_t = [B, L],$$

in order to obtain a numerical approximation of $R_i(t)$ $i = 1, \ldots, N$ that preserves the spectrum of the operator L. We will then use the obtained approximations to derive a numerical solution of the KdV equation.

Consider the solutions of the scaled version of (3.10) obtained by replacing $R_k(t)$ with $r_k(t) = h_x^{-2}R_k(t/h_x^3)$. Consider then an interpolating function $r_{h_x}(x,t)$ whose values in the nodes $x_k = kh_x$ coincide with $r_k(t)$ and define $U_{h_x}(x + h_x^{-2}tc, t) := r_{h_x}(x,t)$ in [18] it is shown how U_{h_x} converge to the general solution of

$$U_t = 1/3U_{xxx} - UU_x.$$

We notice that in the case of matrices of the sparsity of B the coordinate map described at the end of previous section will be computed in a number of $\mathcal{O}(n^2)$ operations, this appears to be competitive compared with the algorithms that efficiently compute exponentials of skew-symmetric sparse matrices and that in any case require $\mathcal{O}(n^3)$ operations.

In the numerical experiments we will actually consider the periodic version of the above L and B obtained allowing for an extra coefficient $a_{N+1} = \frac{1}{2}e^{-\frac{1}{2}R_{N+1}(t)}$ and

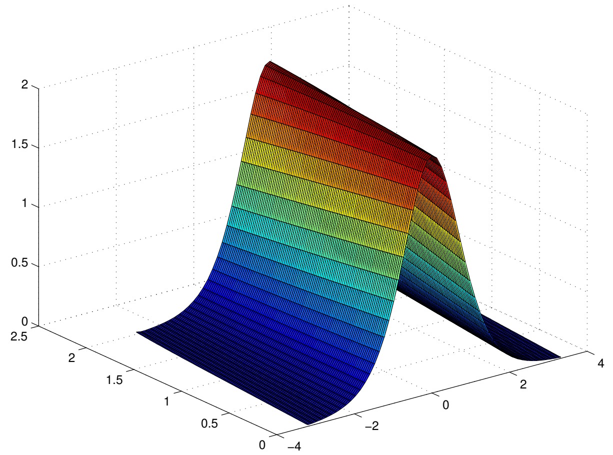

Figure 1: Evolution of one soliton solution.

$b_{N+1} = a_N * a_{N+1}$ placed in the right up corner and left low corner of the matrices L and B respectively.

In figure (1) we report the evolution of one soliton computed using the RKMK algorithm of the previous section combined with the coordinate map described at the end of that section.

In our example on the space interval $[-2, 2]$ we took $N = 65$ and $h_x = 4/65$ we integrated for $t \in [0, 2]$ with 100 steps and initial value $2\text{sech}^2(x)^2$. The final error at $t = 2$ measured in the L_2 norm $(\|\cdot\|_2/N)$ is 0.0898.

In figure (2) we have plotted the initial value of the solution and the computed value at $t = 2$, shape and hight of the soliton are preserved.

The simulation of two interacting solitons has not been properly tested yet and in any case it appears more difficult, numerical instability occurs for big enough t.

In [11] Goodman and Lax observed that the semi discrete scheme of [12] coincides with the use of a special finite difference discretization for the conservation law

$$u_t + (\frac{1}{2}u^2)_x = 0, \tag{3.11}$$

namely

$$\frac{d}{dt}u_n + u_n \frac{u_{n+1} - u_{n-1}}{2\Delta} = 0. \tag{3.12}$$

Using the explicit classical Runge-Kutta of order 4 (RK-4) for integrating the system (3.11) Goodman and Lax observed an oscillatory behaviour in the numerical solution for times t grater than a certain critical time. This unstable behaviour appears as a disadvantage also in our context and sets limits to the possibility of using the Kac-Van Moerbeke discretization for numerical purposes. Our attempts to find alternative more stable semidiscretizations for the Lax formulation of the KdV that maintain the geometrical properties of the ininite dimensional problem have for the moment not been successful.

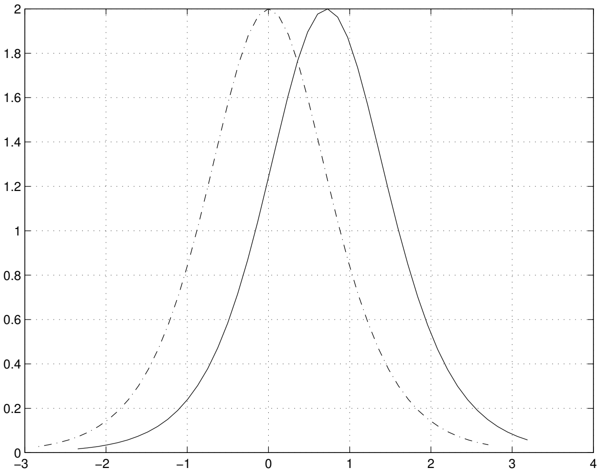

Figure 2: Evolution of one soliton solution.

Given the good features of pseudo-spectral methods in handling problems of the same type of the KdV equation, [1], we will try in the future to combine these semidiscretization strategies with the ideas of this note.

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