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Solving the nonlinear Schrödinger equation using energy conserving Hamiltonian Boundary Value Methods

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Abstract. In this paper we study the use of energy-conserving methods, in the class of *Hamiltonian Boundary Value Methods*, for the numerical solution of the nonlinear Schrödinger equation.

Keywords: Hamiltonian Partial Differential Equations, Energy-conserving Runge-Kutta methods, Hamiltonian Boundary Value Methods, HBVMs, nonlinear Schrödinger equation.

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INTRODUCTION

Hamiltonian Partial Differential Equations (Hamiltonian PDEs) have been investigated since many years, especially in the context of multi-symplectic methods (see, e.g., [1, 13, 14]). In particular, after appropriate space discretization, one can still obtain a discrete Hamiltonian formulation of such equations, resulting into a corresponding discrete energy, which turns out to be conserved when appropriate boundary conditions (e.g., periodic) are prescribed. The discrete energy can be then conserved by using energy-conserving methods in the class of Hamiltonian Boundary Value Methods (HBVMs) [7, 6, 9], which are Runge-Kutta methods based on the concept of discrete line integral [12, 5]. We shall sketch the approach when a Fourier-Galerkin space semi-discretization is considered and periodic boundary conditions are prescribed for the nonlinear Schrödinger equation, thus extending to this equation recent results obtained for the nonlinear wave equation [4]. Let us consider the problem, which we write in a general form,¹

$$i\psi_t(x,t) + \psi_{xx}(x,t) + f'(|\psi(x,t)|^2)\psi(x,t) = 0, \quad (x,t) \in [a,b] \times [0,\infty) =: \Omega, \quad (1)$$

(with i denoting, as usual, the imaginary unit, the subscripts denoting the partial derivatives, and f' the derivative of f , a real valued function) and initial and boundary conditions given by

$$\psi(x,0) = \psi_0(x) \equiv u_0(x) + iv_0(x), \quad x \in [a,b], \quad \psi(a,t) = \psi(b,t), \quad \psi_x(a,t) = \psi_x(b,t), \quad t > 0. \quad (2)$$

We assume that the functions f and ψ_0 are sufficiently smooth, so that they define a regular solution $u(x,t)$. Equation (1) can be cast into the Hamiltonian form, by setting $\psi(x,y) \equiv u(x,t) + iv(x,t)$ and $y = (u, v)^\top$:

$$y_t = J\nabla\mathcal{H}[y], \quad \text{with} \quad J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad \text{and} \quad \nabla\mathcal{H} = \left(\frac{\delta}{\delta u}\mathcal{H}, \frac{\delta}{\delta v}\mathcal{H} \right)^\top$$

the vector of the functional derivatives of the *Hamiltonian functional* $\mathcal{H}[y] \equiv \mathcal{H}[u, v]$.² It can be easily checked that, because of the periodic boundary conditions,

$$\mathcal{H}[u, v] = \frac{1}{2} \int_a^b (v_x^2 + u_x^2 - f(u^2 + v^2)) dx = -\frac{1}{2} \int_a^b (v v_{xx} + u u_{xx} + f(u^2 + v^2)) dx. \quad (3)$$

We also consider the two quadratic functionals

$$\mathcal{M}_1[u, v] = \int_a^b (u^2 + v^2) dx \equiv \int_a^b |\psi|^2 dx, \quad \mathcal{M}_2[u, v] = \int_a^b (v_x u - u_x v) dx \equiv \text{Im} \int_a^b \bar{\psi} \psi_x dx. \quad (4)$$

¹ In the typical case, $f(r) = \pm r^2$.

² We shall use either one or the other notation, when convenient. Moreover, we shall sometimes omit the arguments, to simplify the notation.

The conservation laws for \mathcal{H} , \mathcal{M}_1 , and \mathcal{M}_2 are formulated in the following theorem [11].

Theorem 1 For problem (1)-(2), the following statements hold:

$$\mathcal{H}[u, v](t) = \mathcal{H}[u, v](0), \quad \mathcal{M}_1[u, v](t) = \mathcal{M}_1[u, v](0), \quad \mathcal{M}_2[u, v](t) = \mathcal{M}_2[u, v](0), \quad \forall t > 0.$$

In other words, (3) and (4) provide *conservation laws* for problem (1)-(2), whose numerical solution is considered in the next section. Later on, we sketch the main facts about HBVMs and, finally, we report on some numerical tests along with final conclusions.

NUMERICAL APPROXIMATION

In order to solve (1)-(2), we use a Fourier-Galerkin space semi-discretization, by expanding the solution in the following periodic orthonormal basis for $L^2([a, b])$,

$$c_0(x) \equiv \frac{1}{\sqrt{b-a}}, \quad c_j(x) = \sqrt{\frac{2}{b-a}} \cos\left(2j\pi \frac{x-a}{b-a}\right), \quad s_j(x) = \sqrt{\frac{2}{b-a}} \sin\left(2j\pi \frac{x-a}{b-a}\right), \quad j = 1, 2, \dots, \quad (5)$$

thus obtaining:

$$u(x, t) = \gamma_0(t)c_0(x) + \sum_{j \geq 1} \gamma_j(t)c_j(x) + \eta_j(t)s_j(x), \quad v(x, t) = \alpha_0(t)c_0(x) + \sum_{j \geq 1} \alpha_j(t)c_j(x) + \beta_j(t)s_j(x). \quad (6)$$

By introducing the infinite vectors

$$\mathbf{w}(x) = \begin{pmatrix} c_0(x) \\ c_1(x) \\ s_1(x) \\ c_2(x) \\ s_2(x) \\ \vdots \end{pmatrix}, \quad \mathbf{q}(t) = \begin{pmatrix} \gamma_0(t) \\ \gamma_1(t) \\ \eta_1(t) \\ \gamma_2(t) \\ \eta_2(t) \\ \vdots \end{pmatrix}, \quad \mathbf{p}(t) = \begin{pmatrix} \alpha_0(t) \\ \alpha_1(t) \\ \beta_1(t) \\ \alpha_2(t) \\ \beta_2(t) \\ \vdots \end{pmatrix}, \quad (7)$$

and the infinite matrix

$$D = \frac{2\pi}{b-a} \begin{pmatrix} 0 & & & & & & \\ & 1 \cdot \begin{pmatrix} 1 & \\ & 1 \end{pmatrix} & & & & & \\ & & & & & & \\ & & & 2 \cdot \begin{pmatrix} 1 & \\ & 1 \end{pmatrix} & & & \\ & & & & & & \\ & & & & & & \ddots \end{pmatrix}, \quad (8)$$

we see that (6) can be rewritten as $u(x, t) = \mathbf{w}(x)^\top \mathbf{q}(t)$, $v(x, t) = \mathbf{w}(x)^\top \mathbf{p}(t)$, and the problem can be formulated as the infinite-dimensional Hamiltonian ODE problem (where, as usual, the dot denotes the time derivative):

$$\begin{aligned} \dot{\mathbf{q}}(t) &= D^2 \mathbf{p}(t) - \int_a^b \mathbf{w}(x) f' \left((\mathbf{w}(x)^\top \mathbf{q}(t))^2 + (\mathbf{w}(x)^\top \mathbf{p}(t))^2 \right) \mathbf{w}(x)^\top \mathbf{p}(t) dx, \\ \dot{\mathbf{p}}(t) &= -D^2 \mathbf{q}(t) + \int_a^b \mathbf{w}(x) f' \left((\mathbf{w}(x)^\top \mathbf{q}(t))^2 + (\mathbf{w}(x)^\top \mathbf{p}(t))^2 \right) \mathbf{w}(x)^\top \mathbf{q}(t) dx, \end{aligned} \quad (9)$$

which is Hamiltonian with Hamiltonian function

$$H(\mathbf{q}, \mathbf{p}) = \frac{1}{2} \left[\mathbf{p}^\top D^2 \mathbf{p} + \mathbf{q}^\top D^2 \mathbf{q} - \int_a^b f \left((\mathbf{w}(x)^\top \mathbf{q})^2 + (\mathbf{w}(x)^\top \mathbf{p})^2 \right) dx \right]. \quad (10)$$

The following result can be easily shown, by taking into account that

$$\begin{aligned} u_x(x,t) &= \mathbf{w}'(x)^\top \mathbf{q}(t) \equiv [\tilde{D}\mathbf{w}(x)]^\top \mathbf{q}(t), \\ v_x(x,t) &= \mathbf{w}'(x)^\top \mathbf{p}(t) \equiv [\tilde{D}\mathbf{w}(x)]^\top \mathbf{p}(t), \end{aligned} \quad \tilde{D} = \frac{2\pi}{b-a} \begin{pmatrix} 0 & & & & \\ & 1 \cdot \begin{pmatrix} & -1 \\ 1 & \end{pmatrix} & & & \\ & & & & \\ & & & 2 \cdot \begin{pmatrix} & -1 \\ 1 & \end{pmatrix} & \\ & & & & \ddots \end{pmatrix}, \quad (11)$$

with $\tilde{D}^\top = -\tilde{D}$ and $\tilde{D}D = D\tilde{D}$.

Theorem 2 *The Hamiltonian (10) is equivalent to (3), via the expansions (6). Similarly, the quadratic functionals (4) are equivalent to*

$$M_1(\mathbf{q}, \mathbf{p}) = \int_a^b \left((\mathbf{w}(x)^\top \mathbf{q})^2 + (\mathbf{w}(x)^\top \mathbf{p})^2 \right) dx, \quad M_2(\mathbf{q}, \mathbf{p}) = 2\mathbf{q}^\top \tilde{D}\mathbf{p}, \quad (12)$$

respectively. Both (10) and (12) are constants of motion for the solution of (9).

In order to practically solve problem (9), the series in the expansions (6) are truncated after N terms (for a suitably large N). Consequently, the dimension of the vectors and matrices in (7)–(11) becomes $2N + 1$. By imposing that the residual be orthogonal to the functional subspace $\mathcal{V}_N = \text{span}\{c_0(x), c_1(x), s_1(x), \dots, c_N(x), s_N(x)\}$, which contains the approximation to the solution, the equation to be solved has dimension $4N + 2$, and formally is still given by (9). Moreover, also Theorem 2 continues to hold true, even though now the truncated invariants are only approximations to the corresponding original ones.³ Also, in order to obtain a practical computational procedure, the integrals (with periodic integrands) in (9) will be approximated, up to the round-off errors, using a composite trapezoidal rule defined at the discrete points

$$x_i = a + i(b-a)/m, \quad i = 0, \dots, m, \quad (14)$$

which is known to quickly converge to the corresponding integrals, provided that f is suitably regular. Consequently, in the sequel we shall assume m to be large enough to assure this requirement. In such a case, any symplectic Runge-Kutta method, applied to solve the truncated version of (9), will conserve the quadratic invariants (12) in the discrete solution (see, e.g., [15]) while, in general, it will fail to conserve the Hamiltonian (10).

For solving the Hamiltonian problem (9), one can consider the use of a HBVM(k, s) method, which is the k -stage Runge-Kutta method defined by the following Butcher tableau [6, 9]:

$$\begin{array}{c|c} c_1 & \\ \vdots & [b_j \sum_{\ell=0}^{s-1} P_\ell(c_j) \int_0^{c_i} P_j(\tau) d\tau]_{i,j=1,\dots,k} \\ c_k & \\ \hline & b_1 \dots b_k \end{array} \quad \text{where} \quad \int_0^1 P_i(x)P_j(x)dx = \delta_{ij}, \quad P_i \in \Pi_i, \quad i, j = 0, \dots, k,$$

P_i, P_j are the normalized and shifted Legendre polynomials, and $(b_i, c_i)_{i=1,\dots,k}$ the Legendre weights and abscissae, respectively. For such methods, the following result holds true [9, 5].

Theorem 3 *For all $k \geq s$, a HBVM(k, s) method applied to problem (9) with stepsize h :*

- is symmetric and of order $2s$;
- when $k = s$, it becomes the (symplectic) s -stage Gauss collocation method;
- is energy conserving (i.e., it conserves the Hamiltonian H) when f is a polynomial of degree $\nu \leq [2k/s]$;
- for general and suitably regular functions f , the energy error at each step is $O(h^{2k+1})$.

The last point, in turn, implies that a (at least *practical*) conservation of the energy is obtained, provided that f is suitably regular (which will be assumed hereafter), by choosing k large enough, also considering that the computational cost for implementing a HBVM(k, s) method depends essentially on s , rather than on k [8, 2, 3] (see also [5]).

³ Under regularity assumptions, they converge very fast to the continuous ones, as $N \rightarrow \infty$.

TABLE 1. Errors in the numerical invariants when solving problem (1)-(2) and (15).

method	maximum error in H	maximum error in M_1	maximum error in M_2
HBVM(2,2)	$2.3462 \cdot 10^{-06}$	$6.8834 \cdot 10^{-15}$	$2.5255 \cdot 10^{-17}$
HBVM(10,2)	$2.2204 \cdot 10^{-16}$	$2.4429 \cdot 10^{-04}$	$2.3111 \cdot 10^{-17}$

NUMERICAL TESTS

Let us now consider problem (1)-(2), with the following parameters:

$$a = -b = -20, \quad f(r) = 0.2526896 \cdot r^6, \quad u_0(x) = [\cosh(x)]^{-1}, \quad v_0(x) = 0, \quad (15)$$

which has a solution with a blow-up around $t^* \approx 2$. The corresponding Hamiltonian value is $H_0 \approx 0.24$, whereas the quadratic functionals have values $M_1 = 2$ and $M_2 = 0$, respectively. If we use the (practically) energy-conserving HBVM(10,2) method to perform 1000 steps with stepsize h , by using (see (14))

$$N = 100, \quad m = 1001, \quad h = 0.1, \quad (16)$$

then the numerical solution (correctly) blows-up after 20 integration steps, with an error in the invariants as listed in the last row of Table 1. On the other hand, by using the HBVM(2,2) method (i.e., the symplectic 2-stage Gauss method) with the same parameters as in (16), one obtains that while the quadratic invariants are preserved, the Hamiltonian function is not, as is shown in the second row of Table 1. However, in this latter case, the numerical solution *doesn't* blow-up, and *all* the 1000 integration steps are performed. Consequently, even though the mass and the momentum are numerically conserved, nevertheless, the Hamiltonian error is responsible for the wrong qualitative behavior of the numerical approximation.

In the future, we plan to investigate the numerical solution of (1)-(2) by means of EQUIP methods [10], which conserve *both* the Hamiltonian (10) and the quadratic invariants (12). This will hopefully further enhance the reliability of the numerical solution.

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