Multisymplectic Spectral Methods for the Gross-Pitaevskii Equation

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Abstract. Recently, Bridges and Reich introduced the concept of multisymplectic spectral discretizations for Hamiltonian wave equations with periodic boundary conditions [5]. In this paper, we show that the 1D nonlinear Schrodinger equation and the 2D Gross-Pitaevskii equation are multi-symplectic and derive multi-symplectic spectral discretizations of these systems. The effectiveness of the discretizations is numerically tested using initial data for multi-phase solutions.

1 The Multisymplectic Approach

A Hamiltonian PDE with N space dimensions is said to be *multisymplectic* if it can be written as

$$\boldsymbol{M}\boldsymbol{z}_t + \sum_{i=1}^N \boldsymbol{K}_i \, \boldsymbol{z}_{x_i} = \boldsymbol{\nabla}_z \boldsymbol{S}(\boldsymbol{z}), \qquad \boldsymbol{z} \in \mathbb{R}^d, \tag{1}$$

where $M, K_i \in \mathbb{R}^{d \times d}$ are skew-symmetric matrices and $S : \mathbb{R}^d \to \mathbb{R}$ is a smooth function [1]. Associated with (1) are the N+1 two-forms

$$\omega(U,V) = V^T \boldsymbol{M} U, \quad \kappa_i(U,V) = V^T \boldsymbol{K}_i U, \quad U, V \in \mathbb{R}^d$$
(2)

which define a symplectic structure associated with time and the space directions x_i , respectively. System (1) implies the existence of a multi-symplectic conservation law

$$\partial_t \omega + \sum_{i=1}^N \partial_{x_i} \kappa_i = 0, \tag{3}$$

when U, V are any two solutions of the variational equation associated with (1)

$$\boldsymbol{M}dz_t + \sum_{i=1}^N \boldsymbol{K}_i dz_{x_i} = D_{zz}S(z)dz.$$

One consequence of multi-symplecticity is that when the Hamiltonian S(z) is independent of x_i and t, the PDE has an energy conservation law (ECL) [4]

$$\frac{\partial E}{\partial t} + \sum_{i=1}^{N} \frac{\partial F_i}{\partial x_i} = 0, \quad E = S(z) - \frac{1}{2} z^T \sum_{i=1}^{N} \mathbf{K}_i z_{x_i}, \quad F_i = \frac{1}{2} z^T \mathbf{K}_i z_t \qquad (4)$$

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$$\sum_{i=1}^{N} \frac{\partial I_i}{\partial t} + \sum_{i=1}^{N} \frac{\partial G}{\partial x_i} = 0, \quad G = S(z) - \frac{1}{2} z^T \boldsymbol{M} z_t, \quad I_i = \frac{1}{2} z^T \boldsymbol{M} z_{x_i}.$$
 (5)

When the local conservation laws are integrated over the domain in \mathbb{R}^N , using periodic boundary conditions, we obtain the global conservation of the total energy and total momentum.

Multi-symplectic integrators are approximations to (1) which conserve a discretization of the multi-symplectic conservation law (3). This newly emerging class of integrators has proven very promising as it includes simple and fast schemes with remarkable conservation properties for local as well as global invariants (cf. [1] - [5]).

The nonlinear Schrödinger (NLS) equation in two space dimensions with an external potential models the mean-field dynamics of a dilute-gas Bose Einstein condenstate (BEC) [7]. In this case the equation is referred to as the Gross-Pitaevskii (GP) equation. Numerical experiments with the GP equation are used to provide insight into BEC stability properties. The NLS equation and the GP equation can be formulated as multi-symplectic systems. In order that the numerical discretization reflects the geometric properties of the PDE, we investigate the use of multi-symplectic spectral integrators for the NLS and GP equations.

1.1 The multi-symplectic form of the 1D nonlinear Schrödinger equation

The focusing one dimensional nonlinear Schrödinger (NLS) equation,

$$iu_t + u_{xx} + 2|u|^2 u = 0, (6)$$

can be written in multisymplectic form by letting u = p + iq and introducing the new variables $v = p_x$, $w = q_x$ [2]. Separating (6) into real and imaginary parts, the multi-symplectic form (eq. (1) with N=1) for the NLS equation is obtained with

and Hamiltonian $S(z) = \frac{1}{2} \left[\left(p^2 + q^2 \right)^2 + \left(v^2 + w^2 \right) \right]$. The multi-symplectic conservation law for the NLS equation is given by

$$\partial_t [\boldsymbol{d}p \wedge \boldsymbol{d}q] + \partial_x [\boldsymbol{d}p \wedge \boldsymbol{d}v + \boldsymbol{d}q \wedge \boldsymbol{d}w] = 0.$$
⁽⁷⁾

Implementing relations (4)-(5) for the NLS equation we obtain the energy conservation law (ECL)

$$\frac{1}{2}\left[\left(p^2+q^2\right)^2-\left(v^2+w^2\right)\right]_t+\left[p_tv+q_tw\right]_x=0.$$
(8)

1.2 The multi-symplectic form of the 2D Gross-Pitaevskii equation

After rescaling the physical variables, the Gross-Pitaevskii (GP) equation is given by

$$iu_t = -\frac{1}{2} \left(u_{xx} + u_{yy} \right) + \alpha |u|^2 u + V(x, y)u \tag{9}$$

where u(x, y, t) is the macroscopic wave function of the condensate and $V(\mathbf{x})$ is an experimentally generated macroscopic potential. The parameter α determines whether (9) is repulsive ($\alpha = 1$, defocusing nonlinearity), or attractive ($\alpha = -1$, focusing nonlinearity). Although in BEC applications both signs of α are relevant, here we will concentrate on (9) with repulsive nonlinearity. As in [7], we consider the family of periodic lattice potentials given by

$$V(x,y) = -\left(A_1 \operatorname{sn}_1^2 + B_1\right) \left(A_2 \operatorname{sn}_2^2 + B_2\right) + \left(m_1 k_1 \operatorname{sn}_1\right)^2 + \left(m_2 k_2 \operatorname{sn}_2\right)^2 \quad (10)$$

where $\operatorname{sn}_i = \operatorname{sn}(m_i x, k_i)$ denote the Jacobian elliptic sine functions, with elliptic moduli k_i . A nice feature of this potential is that it has some closed form solutions which can be used for comparative purposes.

The GP equation can be reformulated as a multisymplectic PDE by letting u = p + iq and $v_1 = p_x$, $v_2 = p_y$, $w_1 = q_x$, $w_2 = q_y$. Then, with the state vector $z = (p, q, v_1, w_1, v_2, w_2)$, the skew-symmetric matrices

and Hamiltonian $S(z) = -\frac{1}{4} \left[\left(p^2 + q^2 \right)^2 + 2V \left(p^2 + q^2 \right) - \left(v_1^2 + w_1^2 + v_2^2 + w_2^2 \right) \right],$ the system can be written in the canonical form (1).

The multi–symplectic conservation law

$$\partial_t \omega + \partial_x \kappa_1 + \partial_y \kappa_2 = 0 \tag{11}$$

where ω and κ_i are given by (2).

The energy conservation law is

$$\frac{\partial e}{\partial t} + \frac{\partial f_1}{\partial x} + \frac{\partial f}{\partial y} = 0 \tag{12}$$

with energy density

$$e = -\frac{1}{4} \left[\left(p^2 + q^2 \right)^2 + 2V \left(p^2 + q^2 \right) - \left(pv_{1x} + qw_{1x} + pv_{2y} + qw_{2y} \right) \right]$$
(13)

and the two energy fluxes

$$f_{1} = -\frac{1}{4} \left(p v_{1t} + q w_{1t} - p_{t} v_{1} - q_{t} w_{1} \right), \ f_{2} = -\frac{1}{4} \left(p v_{2t} + q w_{2t} - p_{t} v_{2} - q_{t} w_{2} \right).$$

In this case the ECL for the GP equation becomes

$$\left[\left(p^2 + q^2 \right)^2 + 2V \left(p^2 + q^2 \right) + \left(v_1^2 + w_1^2 + v_2^2 + w_2^2 \right) \right]_t \\ -2 \left[\left(p_t v_1 + q_t w_1 \right)_x + \left(p_t v_2 + q_t w_2 \right)_y \right] = 0.(14)$$

2 The Spectral Discretization

Bridges and Reich [5] have shown that using the Fourier transforms leaves the multi–symplectic nature of a PDE unchanged and that the discrete Fourier system recovers the standard spectral discretizations leading to a system of Hamiltonian ODEs which can be integrated by standard symplectic integrators. We briefly summarize these results.

Consider the space $L_2(I)$ of *L*-periodic, square integrable functions in I = [-L/2, L/2] and let $U = \mathcal{F}u$ denote the discrete Fourier transform of $u \in L_2(I)$. Here $\mathcal{F} : L_2 \to l_2$ denotes the Fourier operator which gives the complex-valued Fourier coefficients $U_k \in \mathbb{C}$, $k = -\infty, \ldots, -1, 0, 1, \ldots, \infty$, which we collect in the infinite-dimensional vector $U = (\ldots, U_{-1}, U_0, U_1, \ldots) \in l_2$. Note that $U_{-k} = U_k^*$. We also introduce the L_2 inner product, which we denote by (u, v) and the l_2 inner product, which we donote by $\langle U, V \rangle$. The inverse Fourier operator \mathcal{F}^{-1} : $l^2 \to L^2$ is defined by $\langle V, \mathcal{F}u \rangle = (\mathcal{F}^{-1}V, u)$. Furthermore, partial differentiation with respect to $x \in I$ simply reduces to $\partial_x u = \mathcal{F}^{-1}\Theta U$ where $\Theta : l_2 \to l_2$ is the diagonal spectral operator with entries $\theta_k = i2\pi k/L$.

These definitions can be generalized to vector-valued functions $z \in L_2^d(I)$. Let $\hat{\mathcal{F}} : L_2^d(I) \to l_2^d$ be defined such that $Z = (Z^1, \ldots, Z^d) = \hat{\mathcal{F}}z = (\mathcal{F}z^1, \ldots, \mathcal{F}z^d)$. Thus with a slight abuse of notations and after dropping the hats, we have $Z = \mathcal{F}z, z = \mathcal{F}^{-1}Z$, and $\partial_x z = (\partial_x z^1, \ldots, \partial_x z^d) = (\mathcal{F}^{-1}\Theta Z^1, \ldots, \mathcal{F}^{-1}\Theta Z^d) = \mathcal{F}^{-1}\Theta Z$

Applying these operators to the multi–symplectic PDE (1), one obtains an infinite dimensional system of ODEs

$$\boldsymbol{M}\partial_t \boldsymbol{Z} + \boldsymbol{K}\boldsymbol{\Theta}\boldsymbol{Z} = \boldsymbol{\nabla}_{\boldsymbol{Z}}\bar{\boldsymbol{S}}(\boldsymbol{Z}), \quad \bar{\boldsymbol{S}}(\boldsymbol{Z}) = \int_{-L}^{L} \boldsymbol{S}(\mathcal{F}^{-1}\boldsymbol{Z})\,d\boldsymbol{x}.$$
 (15)

This equation can appropriately be called a multi–symplectic spectral PDE with associated multi–symplectic and energy conservation laws

$$\partial_t \Omega_k + \theta_k \mathcal{K}_k = 0, \quad \Omega = \mathcal{F}\omega, \quad \mathcal{K} = \mathcal{F}\kappa,$$
 (16)

$$\partial_t E_k + \theta_k F_k = 0, \quad E = \mathcal{F}e, \quad F = \mathcal{F}f.$$
 (17)

Bridges and Reich show that the truncated Fourier series,

$$U_k = \frac{1}{\sqrt{N}} \sum_{l=1}^N u_l e^{-\theta_k (l-1)\Delta x}, \ u_l = u(x_l), \ x_l = -\frac{L}{2} + (l-1)\Delta x, \ \Delta x = \frac{L}{N},$$

with

$$\theta_k = \begin{cases} i \frac{2\pi}{L} (k-1) \text{ for } k = 1, \dots, N/2, \\ 0 & \text{ for } k = N/2 + 1 \\ -\theta_{N-k+2} & \text{ for } k = N/2 + 2, \dots, N \end{cases}$$

gives a multi–symplectic spatial discretization [5]. Therefore to mantain the multi–symplecticity a discrete integrator that is symplectic in time should be used, such as the implicit midpoint method.

The 1D NLS equation The beauty of the spectral multi–symplectic scheme (15) is that in many cases, such as those considered in this paper, one can recover the standard spectral discretization of the original equation in complex form. That is, using a spectral discretization of the spatial derivatives one obtains a multi–symplectic Hamiltonian system of ODEs which can be integrated using standard symplectic methods such as the implicit midpoint rule.

Let $\mathcal{D}^{n}(u)$ be the spectral discretization of $\frac{\partial^{n} u}{\partial x^{n}}$, $\mathcal{D}^{n}(u) = \mathcal{F}^{-1}\{\Theta^{n}\mathcal{F}u\}$, and $\mathcal{C}(u) = 2|u|^{2}u$. Then the multi-symplectic spectral method for the 1D NLS, using the implicit midpoint rule in time, is given by

$$i\frac{u^1 - u^0}{\Delta t} + \mathcal{D}^2(u^{1/2}) + \mathcal{C}(u^{1/2}) = 0,$$
(18)

where $u^{1/2} = (u^1 + u^0)/2$ and $u^j = u(x, j\Delta t)$. Scheme (18) is denoted as MS-S in the numerical experiments.

The numerically induced residual R_i of the ECL is given by

$$R_i = \frac{E_i^1 - E_i^0}{\Delta t} + D^1(F_i^{1/2}), \tag{19}$$

where $E^n = \frac{1}{2} \left(|u^n|^4 - |D^1(u^n)|^2 \right)$ and $F^{1/2} = Re \left\{ \left(\frac{u^1 - u^0}{\Delta t} \right)^* D^1(u^{1/2}) \right\}$. This residual of the ECL is due to *local* non–conservation of energy under numerical discretization, and it can be compared with the global energy error

$$\Delta E^j = |E^j - E^0|.$$

Note the relation

$$\frac{E^j - E^{j-1}}{\Delta t} = \sum_i R_i^j$$

The 2D GP equation As before, we let $\mathcal{D}_i^n(x)$ be the spectral discretization of $\frac{\partial^n u}{\partial x_i^n}$, $\mathcal{D}_i^n(u) = \mathcal{F}^{-1}{\{\Theta_i^n \mathcal{F}u\}}$ and $\mathcal{C}(u) = |u|^2 u - V(x, y)u$. Then the multi–symplectic spectral method for the 2D GP equation, using the second order implicit midpoint rule in time, is given by

$$i\frac{u^1 - u^0}{\Delta t} + \mathcal{D}_1^2(u^{1/2}) + \mathcal{D}_2^2(u^{1/2}) + \mathcal{C}(u^{1/2}) = 0,$$
(20)

where $u^{1/2} = (u^1 + u^0)/2$ and $u^j = u(x, y, j\Delta t)$. Scheme (20) is denoted as GP-MS in the numerical experiments.

The numerically induced residual R_i of the ECL is given by

$$R = \frac{E^{1} - E^{0}}{\Delta t} - 2\left(D_{1}^{1}\left(F_{1}^{1/2}\right) + D_{2}^{1}\left(F_{2}^{1/2}\right)\right)$$

with

$$E^{j} = \left(|u^{j}|^{4} + 2V|u|^{2} + |D_{1}^{1}(u^{j})|^{2} + |D_{2}^{1}(u^{j})|^{2} \right),$$
(21)

and

$$F_i^{1/2} = Re\left\{ \left(\frac{u^1 - u^0}{\Delta t}\right)^* D_i^1(u^{1/2}) \right\}.$$
 (22)

We are interested in simulating multi-phase quasi-periodic (in time) solutions to the NLS and GP equations under periodic boundary conditions.

3 Numerical Experiments

The 1D NLS equation: We consider initial conditions of the form

$$u_0(x) = a(1 + \epsilon \cos \mu x) \tag{23}$$

where a = 0.5, $\epsilon = 0.1$, $\mu = 2\pi/L$ and L is either (a) $L = 2\sqrt{2\pi}$ or (b) $L = 4\sqrt{2\pi}$ [2]. Initial data (a) and (b) correspond to multi-phase solutions, near the plane wave, which are characterized by either one or two excited modes, respectively. We refer to these cases as the one mode and two mode case.

In [2], a multi-symplectic centered cell discretization (obtained by concatenating two implicit midpoint schemes) as well as an integrable-symplectic discretization (an integrable spatial discretization with symplectic integrator in time) were developed for the NLS equation. The multi-symplectic centered cell discretization is denoted as MS-CC in the subsequent discussion. The geometric integrators were shown to be more efficient than standard integrators in preservation of geometric features of the system such as local and global conserved quantities, quasiperiodic character of the motion and qualitative features of the waveform. However, among the geometric integrators, performance varied. The integrable-symplectic scheme reproduced more faithfully the qualitative features of the wave profile than the MS-CC scheme.

In this paper, we show that the MS spectral discretization captures the qualitative features of the waveform better than the MS centered cell discretization. We begin with initial data (a) for the one mode case. Figures 1 show the conservation of the residual energy R(x,t) using the MS-S and the MS-CC discretizations, respectively, with N = 64, $\Delta t = 2.5 \times 10^{-3}$, T = 450 - 500. The error in the ECL obtained using the spectral scheme is several orders of magnitude smaller than the ECL obtained with the centered cell scheme (similarly for the corresponding error in the global energy, not shown). The surfaces of the one-mode case obtained with MS-S and MS-CC are essentially identical and the global momentum and norm are conserved exactly by both schemes, up to the error criterion of 10^{-14} in the iteration procedure in these implicit schemes (not shown).

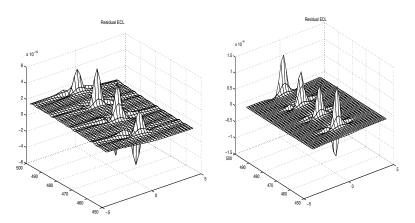


Fig. 1. The residual ECL, R(x,t), of the NLS one mode case obtained using a) the MS-S scheme and b) the MS-CC sceme with N = 64, $\Delta t = 2.5 \times 10^{-3}$, T = 450 - 500.

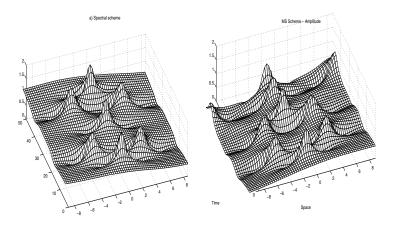


Fig. 2. The surface |u(x,t)| of the NLS two mode case obtained using a) the MS-S scheme and b) the MS-CC sceme with N = 64, $\Delta t = 5 \times 10^{-3}$, T = 0 - 50.

Figures 2 show the surfaces |u(x,t)| of the waveform obtained using MS-S and MS-CC, respectively for initial data (b) with discretization parameters N = 64, $\Delta t = 5 \times 10^{-3}$, T = 0 - 50. The MS-S scheme correctly captures the quasiperiodic motion and produces results which are comparable to those obtained using the integrable-symplectic scheme (see [2]). On the other hand, using the MS-CC integrator, the onset of numerically induced temporal chaos is observed at approximately t = 25. The temporal chaos is characterized by a random switching in time of the location of the spatial excitations in the waveform, see Figure 2(b). However, for the duration of the simulation 0 < t <500, switching in the spatial excitations does not occur using the MS-S scheme. As in the one mode case, the ECL is preserved better by the MS-S scheme. Since a significant improvement in the qualitative features of the solution is obtained with the MS-S scheme in 1D, MS spectral schemes should prove to be a valuable tool in integrating multi-dimensional PDEs.

The 2D GP equation: In the following experiments periodic boundary conditions in x and y are imposed and we use a fixed $N \times N$ spatial lattice with N = 32. The time step used throughout is $\Delta t = 2 \times 10^{-3}$. We begin by considering solutions of (9) with an elliptic function potential (10) that has the following choice of constants: $k_1 = k_2 = 1/2$, $m_1 = m_2 = 1$, $A_1 = A_2 = -1$, $B_1 = B_2 = -A_1/k_1^2$ and the initial condition

$$u_0(x,y) = \sqrt{B_1}\sqrt{B_2} \mathrm{dn}(m_1 x, k_1) \mathrm{dn}(m_2 x, k_2).$$
(24)

This is initial data for a linearly stable stationary solution of the GP equation.

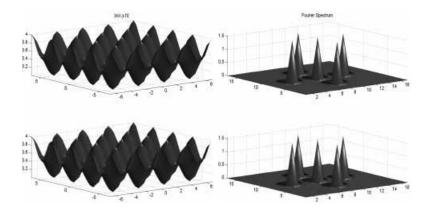


Fig. 3. Stable periodic potential with constants $k_1 = k_2 = 1/2$, $m_1 = m_2 = 1$, $A_1 = A_2 = -1$, $B_1 = B_2 = -A_1/k_1^2$ and initial condition (24): a) Surface; b) Fourier spectrum.

The evolution of the solution obtained using the GP-MS scheme (20) is shown in Figure 3. The surface |u(x, y, t)| is given in the first column and the fourier spectrum is given in the second column. The plots are at t = 0 and t = 60, top and bottom figures respectively. As analytically determined in [7], this solution is clearly stable. In further numerical simulations (not shown) for 0 < t < 1000, the solution obtained with GP-MS (20) remains stable with no growth in the Fourier modes. The ECL is preserved on the order of 10^{-3} and the error in the global energy oscillates in a bounded fashion as is typical of the behavior of a symplectic integrator.

Next, we examine the solution obtained using the elliptic function potential (10) with the values of the constants now specified to be $k_1 = k_2 = 1/2$, $m_1 = m_2 = 1$, $A_1 = A_2 = 1$, $B_1 = B_2 = -A_1$ and the initial condition

$$u_0(x,y) = \sqrt{B_1}\sqrt{B_2} \operatorname{cn}(m_1 x, k_1) \operatorname{cn}(m_2 x, k_2).$$
(25)

Figure 3 shows the surface of the waveform |u(x, y, t)| and the fourier spectrum obtained using the GP-MS scheme (20) at t = 0 and t = 60, in the same order as before.

Obviously, this solution is unstable, as reported in [7]. The onset of the instability occurs between t = 15 and t = 20 and by t = 60 a significant number of additional Fourier modes have become excited. The ECL, as well as the global invaariants are well preserved by the GP-MS discretization. Even working with this coarse lattice, we are able to recover the main qualitative features of the solution. As for the 1D NLS equation, for two dimensional systems we already see the power of multi-symplectic spectral integrators. A more detailed study of the performance of the GP-MS scheme, relative to standard integrators, with respect to the local conservation of energy and momentum as well as the global invariants, will be presented elsewhere.

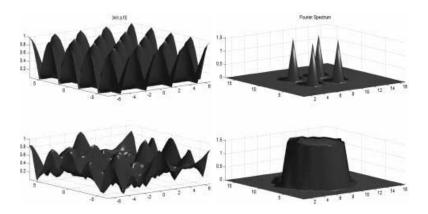


Fig. 4. Unstable periodic potential with constants $k_1 = k_2 = 1/2$, $m_1 = m_2 = 1$, $A_1 = A_2 = 1$, $B_1 = B_2 = -A1$ and initial condition (25): a) Surface; b) Fourier spectrum.

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