Numerical simulation of interaction between Schrödinger field and Klein–Gordon field by multisymplectic method

Linghua Kong *, Ruxun Liu, Zhenli Xu

Department of Mathematics, University of Science and Technology of China, Hefei, Anhui 230026, PR China

Abstract

We propose a multisymplectic scheme to solve the coupled Klein–Gordon–Schrödinger system. The scheme preserves the multisymplectic geometry structure exactly by satisfying the discrete multisymplectic conservation law, and can simulate the original waves well in a long time. This scheme also has discrete quasi-norm conservation law. Numerical experiments demonstrate the consistency between the theoretical analysis and the numerical results.

Keywords: Klein–Gordon–Schrödinger system; Multisymplectic scheme; Conservation law; Long time behavior; Solitons

1. Introduction

The coupled Klein–Gordon–Schrödinger (KGS) system [1–3]

\[
\begin{align*}
    i \psi_t + \frac{1}{2} \psi_{xx} + \psi \varphi &= 0, \quad i^* = \sqrt{-1}, \\
    \varphi_{tt} - \varphi_{xx} + \varphi - |\psi|^2 &= 0,
\end{align*}
\]

(1)
is a classical model which describes the interaction between conservative complex neutron field and neutral meson Yukawa in quantum field theory. Here \(\psi(x, t)\) and \(\varphi(x, t)\) are complex and real functions, respectively. Its mathematical properties, such as the global strong stability and solitary wave solution, have been studied by many authors [1–4]. Zhang and Chang [5,6] exhibited energy conservative schemes and analyzed their convergence.

Multisymplecticity is an intrinsical geometric property for many PDEs. So it is natural to require a numerical method preserving this property. Based on this idea, Bridges and Reich [7,8] introduced the concept of multisymplectic scheme (MS), which possesses a completely local multisymplectic conservation law. They showed that the Gauss–Legendre collocation method both in space and time directions led to a MS which preserves the discrete multisymplectic conservation law. MS has attracted much attention and been applied...
serves the discrete quasi-norm conservation law. In Section 3, some numerical experiments are performed by
multisymplectic scheme of KGS system reported in Section 4.

The problem (1)–(3) has conservative quantity

$$E = \int_{x_L}^{x_R} \psi(x)^2 dx = E_0,$$

where \(E_0\) is a constant depending only on initial values. This property will be studied theoretically and numerically in the following sections.

The paper is organized as follows. In Section 2, we simply review the multisymplectic integrator firstly. The multisymplectic formation in one-dimensional space variable is

$$M\partial_t z + K\partial_x z = \nabla_x S(z),$$

where \(M\) and \(K\) are \(n \times n\) skew-symmetry matrices, and \(z \in \mathbb{R}^n\) is a state variable, and \(S: \mathbb{R}^n \rightarrow \mathbb{R}\) is a smooth Hamiltonian function.

The multisymplectic conservation law

$$\partial_t \omega + \partial_x \kappa = 0, \quad \text{where} \quad \omega = dz \wedge M dz, \kappa = dz \wedge K dz,$$

holds for the multisymplectic formation (5). This can be obtained by taking wedge with the variational formation of (5) and making use of \(dz \wedge dz = 0\).

Taking inner product with (5) by \(z_i\) and \(z_{ix}\), respectively, we obtain the local energy conservation law (LECL) and the local momentum conservation law (LMCL), respectively,

$$\partial_t E + \partial_x F = 0, \quad \text{where} \quad E = S(z) - \frac{1}{2} z^T K z, F = \frac{1}{2} z^T K z_t,$$

$$\partial_t G + \partial_x I = 0, \quad \text{where} \quad I = S(z) - \frac{1}{2} z^T M z, G = \frac{1}{2} z^T M z_x.$$

Definition. A scheme is called multisymplectic scheme (MS) if it satisfies the discrete formation of the multisymplectic conservation law (6).

If Euler mid-point schemes are adopted in both time and spatial directions, we get the following Preissmann scheme

$$M\partial_t z_{i+1/2} + K\partial_x z_{i+1/2} = \nabla_x S \left( z_{i+1/2} \right),$$

where \(h, \tau\) are spatial and time step sizes, respectively; \(z_{i+1/2} = \frac{1}{2} \left( z_{i+1} + z_i \right)\).

The Preissmann scheme (9) is a MS since it satisfies discrete multisymplectic conservation law (see [7]).

Setting \(\psi = p + i q, \varphi = p_x + i q_x = f + i g, \varphi_t = v, \varphi_x = w, z = (p, q, f, g, \varphi, v, w)^T\), the multisymplectic formation of the KGS system (1) is
\[
\begin{aligned}
-q_t + \frac{1}{2}f_x &= -\varphi p_x, \\
p_t + \frac{1}{2}g_x &= -\varphi q_x, \\
-\frac{1}{2}p_x &= -\frac{1}{2}f, \\
-\frac{1}{2}q_x &= -\frac{1}{2}g, \\
-v_t + \frac{1}{2}w_x &= \frac{1}{2}\varphi - \frac{1}{2}(p^2 + q^2), \\
\frac{1}{2}\varphi_x &= \frac{1}{2}v, \\
-\frac{1}{2}\varphi_x &= -\frac{1}{2}w.
\end{aligned}
\] (10)

Therefore the matrices \(M\) and \(K\) in (5) are

\[
M = \frac{1}{2} \begin{bmatrix}
0 & -2 & 0 & 0 & 0 & 0 & 0 \\
2 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\end{bmatrix}, \quad K = \frac{1}{2} \begin{bmatrix}
0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 \\
-1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 \\
\end{bmatrix},
\]

respectively, and the Hamiltonian function is

\[
S(z) = -\frac{1}{2}\varphi(p^2 + q^2) + \frac{1}{4}(\varphi^2 + v^2 - w^2 - f^2 - g^2).
\]

For the three local conservation laws corresponding to (6)–(8), we have

\[
\begin{aligned}
\omega(z) &= -2dp \wedge dq - d\varphi \wedge dv, \\
\kappa(z) &= dp \wedge df + dq \wedge dg + d\varphi \wedge dw; \\
E(z) &= -\frac{1}{2}\varphi(p^2 + q^2) + \frac{1}{4}(\varphi^2 + v^2 - pf_x - qg_x - \varphi w_x), \\
F(z) &= \frac{1}{4}(pf_x + qg_x + \varphi w_x - fp_t - gq_t - vw); \\
I(z) &= -\frac{1}{2}\varphi(p^2 + q^2) + \frac{1}{4}(\varphi^2 - w^2 - f^2 - g^2 + \varphi v_t) + \frac{1}{2}(pq_t - qp_t), \\
G(z) &= \frac{1}{4}(-2pg + 2fq - \varphi v_t + vw).
\end{aligned}
\]

Applying scheme (9) to (10) yields a MS for the KGS system (1)

\[
\begin{aligned}
-\delta_t q_{j+1/2}^{i+1/2} + \frac{1}{2} \delta_x f_{i+1/2}^{j+1/2} &= -\varphi_{j+1/2}^{i+1/2} f_{i+1/2}^{j+1/2}, \\
\delta_t p_{j+1/2}^{i+1/2} + \frac{1}{2} \delta_x g_{i+1/2}^{j+1/2} &= -\varphi_{j+1/2}^{i+1/2} g_{i+1/2}^{j+1/2}, \\
\delta_t p_{j+1/2}^{i+1/2} = f_{i+1/2}^{j+1/2}, \quad \delta_t q_{j+1/2}^{i+1/2} = g_{i+1/2}^{j+1/2}, \\
-\delta_t v_{j+1/2}^{i+1/2} + \delta_x w_{i+1/2}^{j+1/2} &= \varphi_{j+1/2}^{i+1/2} - \left[ \left( p_{j+1/2}^{i+1/2} \right)^2 + \left( q_{j+1/2}^{i+1/2} \right)^2 \right], \\
\delta_t v_{j+1/2}^{i+1/2} = v_{i+1/2}^{j+1/2}, \quad \delta_t w_{j+1/2}^{i+1/2} = w_{i+1/2}^{j+1/2}.
\end{aligned}
\] (11)

The multisymplecticity of the scheme (11) can be easily verified with

\[
\delta_t \omega_{j+1/2}^{i+1/2} + \delta_x \eta_{j+1/2}^{i+1/2} = 0.
\] (12)

Variables \(f, g, v, w\) in (11) can be eliminated by a standard algebraic procedure. We thus derive the following more practical scheme:
Theorem. Scheme (13) has discrete quasi-norm conservation quantity

\[ \text{Norm} = h \sum_i |\psi_i^{j+1} + \psi_{i+1}^{j+1}|^2 = \cdots = h \sum_i |\psi_0(x_i) + \psi_0(x_{i+1})|^2. \] (14)

Proof. Multiply the first equation of (13) by \( \psi_i^{j+1} + \psi_{i+1}^{j+1} \), sum over \( i \), and take the imaginary part, where \( \overline{\psi} \) is the complex conjugate of \( \psi \), we have

\[
\begin{aligned}
&h \sum_i \left( \psi_{i+1}^{j+1} \overline{\psi}_{i+1}^{j+1} + \psi_{i+1}^{j+1} \overline{\psi}_i^{j+1} + \psi_i^{j+1} \overline{\psi}_i^{j+1} + \psi_{i+1}^{j+1} \overline{\psi}_{i+1}^{j+1} \right) - h \sum_i \left( \psi_{i+1}^{j+1} \overline{\psi}_{i+1}^{j+1} + \psi_i^{j+1} \overline{\psi}_i^{j+1} + \psi_{i+1}^{j+1} \overline{\psi}_i^{j+1} + \psi_i^{j+1} \overline{\psi}_{i+1}^{j+1} \right) \\
&= h \sum_i (\psi_i^{j+1} + \psi_{i+1}^{j+1}) (\overline{\psi}_i^{j+1} + \overline{\psi}_{i+1}^{j+1}) - h \sum_i (\psi_i^{j+1} + \psi_{i+1}^{j+1}) (\overline{\psi}_i^{j+1} + \overline{\psi}_{i+1}^{j+1}) \\
&= h \sum_i |\psi_i^{j+1} + \psi_{i+1}^{j+1}|^2 - h \sum_i |\psi_i^{j+1} + \psi_{i+1}^{j+1}|^2 = 0.
\end{aligned}
\]

In other words, (14) is true. This finishes the proof. \( \square \)

Remark 1. The discrete form of LECL (7) and LMCL (8) are not preserved exactly by scheme (11). The residual of LECL (7) is denoted

\[ \text{Res}^i = \sum_i \left( \frac{E_{i+1/2}^{j+1} - E_{i+1/2}^j}{\tau} + \frac{E_{i+1/2}^{j+1} - E_{i+1/2}^{j+1/2}}{h} \right). \] (15)

3. Numerical experiments

In this section, we will carry some numerical experiments to test the performance of the MS (13). In all of the following experiments, the initial conditions (2) are always chosen such that \( |\psi_0(x)|, \varphi_0(x), \varphi_1(x) \) decay to zero rapidly as \( |x| \to \infty \). The computational domain is large enough such that the boundary conditions (3) are satisfied.

The KGS system (1) has analytic solitary wave solutions (see [4])

\[
\begin{aligned}
\psi(x, t, v) &= \frac{3}{4 \sqrt{1 - v^2}} \sech^2 \left( \frac{1}{2 \sqrt{1 - v^2}} (x - vt - x_0) \right) \exp \left( i (v x + \frac{1-c^2+v^2}{2(1-v^2)} t) \right), \\
\varphi(x, t, v) &= \frac{3}{4 (1-v^2)} \sech^2 \left( \frac{1}{2 \sqrt{1-v^2}} (x - vt - x_0) \right),
\end{aligned}
\] (16)

where \( v \) is the propagating velocity of the wave and \( x_0 \) is the initial phase.

3.1. Solitary wave solution

The purpose of the present numerical experiments is to verify numerically that the proposed scheme (13) (i) exhibits a second-order convergence rate, and (ii) preserves the soliton shape well, and (iii) has conservative quantity Norm.
We take \( v = 0.8, x_0 = 0 \) in (16) and calculate the problem in \([-10, 10]\) up to \( t = 1\) to test the discrete error in space. We choose a relatively small time step \( \tau = 0.005\) such that the error from the time discretization is negligible comparing to those from the space, and solve the KGS system (1) with different mesh size \( h\). The \( \|\text{error}\|_\infty \) and convergence rate are presented in Table 1. The convergence rate is calculated using the formula

\[
\text{Order} \approx \frac{\ln(\|\text{error}(h_2)\|_\infty/\|\text{error}(h_1)\|_\infty)}{\ln(h_2/h_1)},
\]

where error\( (h_k) = \psi_{h_k}^i - \psi(x_i, t_j) \) is the error with \( h_k \) spatial step size.

Chosen \( v = 0.8, x_0 = -10, \tau = 0.01, h = 0.05 \) and \(-20 \leq x \leq 20\), we study solitary wave simulated by the MS (13). Fig. 1 shows the wave shape of \( |\psi| \) both numerical and exact solutions at various time stages, and Table 2 shows the conservative quantity Norm (14) and energy residual Res (15).

Since the table about time convergence rate is very similar to Table 1, we do not reproduce it here. From Tables 1 and 2 and Fig. 1, we can draw the following: (i) scheme (13) exhibits the expected convergence rate 2; (ii) it can simulate the solitary wave well; (iii) it conserves the Norm (14) exactly within the roundoff error; (iv) the residual Res (15) of discrete LECL (7) is small.

In the following two subsections, we will study head-on and overtaking collisions of two solitary waves, respectively. The initial data are chosen as

| Table 1 |
| The convergence rate in space for the scheme (13) |
| \( h \) | 0.2 | 0.1 | 0.05 | 0.025 | 0.0125 |
| \( \|\text{error}\|_\infty \) | 3.0700E–2 | 7.9153E–3 | 1.9986E–3 | 5.0090E–4 | 1.2554E–4 |
| Order | 1.956 | 1.986 | 1.997 | 1.996 |

| Table 2 |
| Conserved quantity and energy residual at various time stages |
| \( t \) | 0 | 10 | 20 | 30 |
| Norm | 19.98506504431 | 19.98506504431 | 19.98506504431 | 19.98506504431 |

Fig. 1. Numerical and exact solutions comparison at various time stages.
\[
\left\{
\begin{array}{l}
\psi_0(x) = \psi(x - p_1, 0, v_1) + \psi(x - p_2, 0, v_2), \\
\varphi_0(x) = \varphi(x - p_1, 0, v_1) + \varphi(x - p_2, 0, v_2), \\
\varphi_1(x) = \frac{2}{\pi} \varphi(x - p_1, t, v_1)|_{t=0} + \frac{2}{\pi} \varphi(x - p_2, t, v_2)|_{t=0},
\end{array}
\right.
\]

where \( p_1, v_1 \) and \( p_2, v_2 \) are the initial phases and propagating velocities of the first soliton and the second one, respectively. The exact solutions are difficult to be found, but some interesting phenomena can be numerically observed.

3.2. Head-on collisions

We study the collisions of two solitary waves at two distinct cases:

Case I. \( v_1 = 0.8, \quad p_1 = -10, \quad v_2 = -0.6, \quad p_2 = 5 \).

This case is two colliding solitary waves with different amplitudes, velocities and initial phases. We solve the problem in \([-30, 30]\) up to \( t = 20 \). Fig. 2 shows the waves shape of \( \varphi \) at various time stages with mesh sizes \( h = 0.075, \tau = 0.00625 \) (dashed ‘—’ —’) and \( h = 0.025, \tau = 0.005 \) (solid line ‘—’). Fig. 3 plots the \( x - t \) pictures of

Fig. 2. Numerical solution with mesh sizes, ‘—’; \( h = 0.025, \tau = 0.005; \) ‘—–’; \( h = 0.075, \tau = 0.00625 \).

Fig. 3. Head-on collision solitary waves for case I of \( |\psi| \) (left) and \( \varphi \) (right).
$|\psi|$, $\varphi$ with mesh size $h = 0.075$, $\tau = 0.00625$. Fig. 4 shows the conservative quantity $\text{Norm}$ and residual $\text{Res}$ with the evolution of time. From these pictures we find that some ripples both appear after the collisions despite of the refinement of mesh size; moreover, quasi-norm $\text{Norm}$ is preserved well; the small residual takes on quasi-periodic changes.

**Case II.** $v_1 = 0.6$, $p_1 = 10$ and $v_2 = -0.6$, $p_2 = -10$.

This case is symmetric collisions, i.e., the collisions of solitary waves with equal amplitudes and opposite velocities. Moreover, their initial phases are symmetric about origin. The problem is solved in $[-50, 50]$ up to $t = 30$ with mesh size $h = 0.1$, $\tau = 0.03$. Fig. 5 shows the evolution of the waves. As is seen from the picture, the solitary waves propagate in their original directions, however, with slightly smaller speeds. The collisions also result in a pair of symmetric new soliton-like waves. These are very interesting phenomena.

### 3.3. Overtaking solitons

We choose parameters in (18) as $v_1 = 0.9$, $p_1 = -25$ and $v_2 = 0.4$, $p_2 = -10$.

This is two overtaking solitary waves both propagating to the right with distinct initial phases. We solve this problem in $[-60, 60]$ with mesh size $h = 0.1$, $\tau = 0.02$, and calculate up to $t = 50$. Fig. 6 exhibits the evolution of the dispersive wave $|\psi|, \varphi$. Judging from Fig. 6, we observe the wave with larger amplitude absorbs
some of the smaller one after interaction, while the smaller one splits into new soliton-like waves successively. These very interesting phenomena are similar to those in [17,18].

4. Conclusions

The MS is presented for the KGS system. It preserves the intrinsic multisymplectic geometry structure character and quasi-norm. Numerical experiments illustrate the superiorities of MS: it can simulate various waves and has long term behaviors, etc.

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