

# 三耦合薛定谔方程组的离散线积分方法

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**摘要:**三耦合薛定谔方程组具有能量守恒特性,用保能量算法数值模拟三耦合薛定谔方程组孤立波的演化行为具有重要意义.将三耦合薛定谔方程组转化成典则哈密顿系统,利用 Boole 离散线积分方法进行数值求解,得到三耦合薛定谔方程的一个新的保能量格式.利用新格式数值模拟方程组在不同参数下孤立波的行为.数值结果表明离散线积分方法可以很好模拟方程组孤立波的行为和保方程的能量守恒.

**关键词:**三耦合薛定谔方程组;哈密顿系统;离散线积分方法;谱方法

**中图分类号:**O241.5

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在长时间数值模拟微分方程时,与经典数值方法(如 Runge-Kutta 方法和多步方法)相比较,保结构方法(如辛几何算法和多辛算法等)具有保持微分方程守恒特性的优越性.近年来保能量方法成为保结构算法研究热点<sup>[1-5]</sup>.1996 年,文献[6]首次提出了保能量的离散梯度方法.后来,文献[7]提出了保能量离散变分导数方法求解非线性波动方程.文献[8-9]提出了平均向量场方法.这些方法在数值模拟哈密顿系统时能保持系统的能量守恒.最近,文献[10-11]提出了新的保能量守恒的离散线积分方法,可以构造哈密顿系统任意阶精度的高阶保能量格式.本文利用离散线积分方法求解具有能量守恒特性的三耦合薛定谔方程组.

## 1 三耦合薛定谔方程组

三耦合薛定谔方程组是科学与工程中的一个重要数学模型,广泛应用于光纤通信、生物物理、流体力学和量子力学等学科中.分析和求解三耦合薛定谔方程组成了数学家和物理学家们常研究的课题之一.在本文中,研究如下三耦合薛定谔方程组<sup>[12]</sup>

$$\begin{cases} i \frac{\partial \psi_1}{\partial t} + \alpha_1 \frac{\partial^2 \psi_1}{\partial x^2} + (\sigma |\psi_1|^2 + e |\psi_2|^2 + \sigma |\psi_3|^2) \psi_1 = 0, \\ i \frac{\partial \psi_2}{\partial t} + \alpha_2 \frac{\partial^2 \psi_2}{\partial x^2} + (e |\psi_1|^2 + \sigma |\psi_2|^2 + e |\psi_3|^2) \psi_2 = 0, \\ i \frac{\partial \psi_3}{\partial t} + \alpha_3 \frac{\partial^2 \psi_3}{\partial x^2} + (\sigma |\psi_1|^2 + e |\psi_2|^2 + \sigma |\psi_3|^2) \psi_3 = 0. \end{cases} \quad (1)$$

设初始条件  $\psi_1(x, 0) = (\psi_1)_0(x)$ ,  $\psi_2(x, 0) = (\psi_2)_0(x)$ ,  $\psi_3(x, 0) = (\psi_3)_0(x)$ ,  $x \in R, t > 0$ ,  $\alpha_1, \alpha_2, \alpha_3$  是弥散系数,  $\sigma$  是描述波包自调制的 Landau 常数,  $e$  是描述波包交叉调制的波相互作用的系数.方程组(1)具有如下能量守恒特性

$$\begin{aligned} E(t) = \int & -\frac{\alpha_1}{2} |\psi_1|^2 - \frac{\alpha_2}{2} |\psi_2|^2 - \frac{\alpha_3}{2} |\psi_3|^2 + \frac{\sigma}{4} (|\psi_1|^2)^2 + (|\psi_2|^2)^2 + (|\psi_3|^2)^2 + \\ & \frac{\sigma}{2} |\psi_1|^2 |\psi_3|^2 + \frac{e}{2} |\psi_2|^2 (|\psi_1|^2 + |\psi_3|^2) dx = E(0). \end{aligned} \quad (2)$$

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## 2 三耦合薛定谔方程的哈密顿形式

令  $\psi_1 = q_1(x, t) + iq_2(x, t)$ ,  $\psi_2 = q_3(x, t) + iq_4(x, t)$ ,  $\psi_3 = q_5(x, t) + iq_6(x, t)$ , 方程组(1)等价于

$$\begin{cases} q_{1t} = -\alpha_1 q_{2xx} - (\sigma(q_1^2 + q_2^2) + e(q_3^2 + q_4^2) + \sigma(q_5^2 + q_6^2))q_2, \\ q_{2t} = \alpha_1 q_{1xx} + (\sigma(q_1^2 + q_2^2) + e(q_3^2 + q_4^2) + \sigma(q_5^2 + q_6^2))q_1, \\ q_{3t} = -\alpha_2 q_{4xx} - (e(q_1^2 + q_2^2) + \sigma(q_3^2 + q_4^2) + e(q_5^2 + q_6^2))q_4, \\ q_{4t} = \alpha_2 q_{3xx} + (e(q_1^2 + q_2^2) + \sigma(q_3^2 + q_4^2) + e(q_5^2 + q_6^2))q_3, \\ q_{5t} = -\alpha_3 q_{6xx} - (\sigma(q_1^2 + q_2^2) + e(q_3^2 + q_4^2) + \sigma(q_5^2 + q_6^2))q_6, \\ q_{6t} = \alpha_3 q_{5xx} + (\sigma(q_1^2 + q_2^2) + e(q_3^2 + q_4^2) + \sigma(q_5^2 + q_6^2))q_5. \end{cases} \quad (3)$$

方程组(3)可表示成如下典则哈密顿系统

$$\frac{dz}{dt} = J \frac{\delta H(z)}{\delta z}, J = \begin{pmatrix} 0 & -1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}, \quad (4)$$

其中  $z = (q_1, q_2, q_3, q_4, q_5, q_6)^T$ , 相应的哈密顿函数为

$$H(z) = \int_{\Omega} \frac{\sigma}{4} ((q_1^2 + q_2^2)^2 + (q_3^2 + q_4^2)^2 + (q_5^2 + q_6^2)^2) + \frac{\sigma}{2} (q_1^2 + q_2^2)(q_5^2 + q_6^2) + \frac{e}{2} (q_3^2 + q_4^2)((q_1^2 + q_2^2) + (q_5^2 + q_6^2)) - \frac{\alpha_1}{2} (q_{1x}^2 + q_{2x}^2) - \frac{\alpha_2}{2} (q_{3x}^2 + q_{4x}^2) - \frac{\alpha_3}{2} (q_{5x}^2 + q_{6x}^2) dx. \quad (5)$$

为了离散哈密顿偏微分方程(4), 在空间的方向, 选择用傅里叶拟谱方法离散<sup>[13-14]</sup>. 设傅里叶拟谱微分矩阵  $D_k$  离散  $k$  阶偏微分算子, 则  $D_1$  和  $D_2$  分别是一阶  $\partial_x$  和二阶  $\partial_{xx}$  谱微分矩阵可表示如下:

$$(D_1)_{i,j} = \begin{cases} \frac{1}{2} \mu (-1)^{i+j} \cot(\mu \frac{x_i + x_j}{2}), & i \neq j, \\ 0, & i = j, \end{cases} \quad (D_2)_{i,j} = \begin{cases} \frac{1}{2} \mu^2 (-1)^{i+j+1} \frac{1}{\sin^2(\mu \frac{x_i - x_j}{2})}, & i \neq j, \\ -\mu^2 \frac{N^2 + 2}{12}, & i = j, \end{cases}$$

其中  $i, j = 0, 1, \dots, N-1$ ,  $\mu = \frac{2\pi}{L}$ ,  $L$  是空间积分区间的长度,  $N$  是一个正偶数. 方程组(1)的半谱离散格式如下:

$$\frac{dq_{1i}}{dt} = -\alpha_1 (D_2 Q_2)_i - \sum_{j=0}^{N-1} (\sigma(q_{1j}^2 + q_{2j}^2) + e(q_{3j}^2 + q_{4j}^2) + \sigma(q_{5j}^2 + q_{6j}^2)) q_{2j}, \quad (6)$$

$$\frac{dq_{2i}}{dt} = \alpha_1 (D_2 Q_1)_i + \sum_{j=0}^{N-1} (\sigma(q_{1j}^2 + q_{2j}^2) + e(q_{3j}^2 + q_{4j}^2) + \sigma(q_{5j}^2 + q_{6j}^2)) q_{1j}, \quad (7)$$

$$\frac{dq_{3i}}{dt} = -\alpha_2 (D_2 Q_4)_i - \sum_{j=0}^{N-1} (e(q_{1j}^2 + q_{2j}^2) + \sigma(q_{3j}^2 + q_{4j}^2) + e(q_{5j}^2 + q_{6j}^2)) q_{4j}, \quad (8)$$

$$\frac{dq_{4i}}{dt} = \alpha_2 (D_2 Q_3)_i + \sum_{j=0}^{N-1} (e(q_{1j}^2 + q_{2j}^2) + \sigma(q_{3j}^2 + q_{4j}^2) + e(q_{5j}^2 + q_{6j}^2)) q_{3j}, \quad (9)$$

$$\frac{dq_{5i}}{dt} = -\alpha_3 (D_2 Q_6)_i - \sum_{j=0}^{N-1} (\sigma(q_{1j}^2 + q_{2j}^2) + e(q_{3j}^2 + q_{4j}^2) + \sigma(q_{5j}^2 + q_{6j}^2)) q_{6j}, \quad (10)$$

$$\frac{dq_{6i}}{dt} = \alpha_3 (D_2 Q_5)_i + \sum_{j=0}^{N-1} (\sigma(q_{1j}^2 + q_{2j}^2) + e(q_{3j}^2 + q_{4j}^2) + \sigma(q_{5j}^2 + q_{6j}^2)) q_{5j}. \quad (11)$$

格式(6)~(11)式可写成如下有限维典则的哈密顿系统:

$$\frac{dZ}{dt} = f(Z) = \bar{N}H(Z), \bar{J} = \begin{pmatrix} 0 & -I & 0 & 0 & 0 & 0 \\ I & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -I & 0 & 0 \\ 0 & 0 & I & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -I \\ 0 & 0 & 0 & 0 & I & 0 \end{pmatrix}, \quad (12)$$

其中  $Z = [Q_1^T, Q_2^T, Q_3^T, Q_4^T, Q_5^T, Q_6^T]^T$ ,  $Q_1 = (q_{1,0}, q_{1,1}, \dots, q_{1,n-1})^T$ , 其他类推.  $I$  是  $N \times N$  单位矩阵, 相应的哈密顿函数为

$$H(Z) = \sum_{i=0}^{N-1} \frac{\sigma}{4} ((q_{1i}^2 + q_{2i}^2)^2 + (q_{3i}^2 + q_{4i}^2)^2 + (q_{5i}^2 + q_{6i}^2)^2) + \frac{\sigma}{2} (q_{1i}^2 + q_{2i}^2)(q_{5i}^2 + q_{6i}^2) + \frac{e}{2} (q_{3i}^2 + q_{4i}^2)((q_{1i}^2 + q_{2i}^2) + (q_{5i}^2 + q_{6i}^2)) + \frac{\alpha_1}{2} (Q_1^T D_2 Q_1 + Q_2^T D_2 Q_2) + \frac{\alpha_2}{2} (Q_3^T D_2 Q_3 + Q_4^T D_2 Q_4) + \frac{\alpha_3}{2} (Q_5^T D_2 Q_5 + Q_6^T D_2 Q_6). \quad (13)$$

### 3 三耦合薛定谔方程的 Boole 离散线积分方法

哈密顿系统(12)的能量  $H(Z)$  是一个守恒常量. 利用离散线积分方法对该系统(12)进行求解. 设由初值  $Z_0$  得到的  $t = h$  处的数值解  $Z_1$ . 在这里, 考虑最简单的连接  $Z_0$  和  $Z_1$  的路径为

$$\sigma(ch) = cZ_1 + (1-c)Z_0, c \in [0, 1]. \quad (14)$$

如果在  $t = 0$  和  $t = h$  的能量相等, 也就是

$$H(Z_1) - H(Z_0) = H(\sigma(h)) - H(\sigma(0)) = \int_0^h \nabla H(\sigma(t))^T \sigma'(t) dt = h \int_0^1 \nabla H(\sigma(ch))^T \sigma'(ch) dc = h \int_0^1 \nabla H((cZ_1 + (1-c)Z_0))^T (Z_1 - Z_0) dc = h \left[ \int_0^1 \nabla H(cZ_1 + (1-c)Z_0) dc \right]^T (Z_1 - Z_0) = 0. \quad (15)$$

设

$$Z_1 = Z_0 + h \bar{J} \int_0^1 \nabla H(cZ_1 + (1-c)Z_0) dc. \quad (16)$$

事实上,  $\bar{J}$  是反对称的, 则可以得到

$$\left[ \int_0^1 \nabla H(cZ_1 - (1-c)Z_0) dc \right]^T \frac{Z_1 - Z_0}{h} = \left[ \int_0^1 \nabla H(cZ_1 + (1-c)Z_0) dc \right]^T \bar{J} \left[ \int_0^1 \nabla H(cZ_1 + (1-c)Z_0) dc \right] = 0. \quad (17)$$

如果  $H \in \Pi_v$ , 在(16)式右侧的被积函数就有  $v-1$  度, (16)式能够精确的数值积分, 也就相当于一个基于  $v$  的等距横坐标在  $[0, 1]$  区间上的牛顿-科茨公式. 由于  $f(\cdot) = \bar{J} \nabla H(\cdot)$ , 对格式(16)数值离散后, 可得到  $Z_1 = Z_0 + h \sum_{i=1}^v \beta_i f(c_i Z_1 + (1-c_i)Z_0) \equiv Z_0 + h \sum_{i=1}^v b_i f(Y_i)$ , 其中  $c_i = \frac{i-1}{v-1}$ ,  $Y_i = \sigma(c_i) \equiv c_i y_1 + (1-c_i)y_0$ ,  $i = 1, \dots, v$ ,  $\{b_i\}$  是正交权重

$$b_i = \int_0^1 \prod_{j=1, j \neq i}^v \frac{t - c_j}{c_i - c_j} dt, i = 1, \dots, v. \quad (18)$$

在这里, 考虑到计算效率的问题, 选用 Boole 公式, 当  $v=5$  时, 可以得到系统(12)的离散线积分格式

$$Z_1 = Z_0 + \frac{h}{90} \bar{J} (7 \nabla H(Z_0) + 32 \nabla H(\frac{3Z_0 + Z_1}{4}) + 12 \nabla H(\frac{Z_0 + Z_1}{2}) + 32 \nabla H(\frac{Z_0 + 3Z_1}{4}) + 7 \nabla H(Z_0)), \quad (19)$$

显然该格式是对称的, 并且具有四阶精度. 若  $H$  是阶小于等于 4 的多项式哈密顿函数, 格式(19)一定是精

确保能量的.

### 4 数值模拟

为了有效地验证构造的离散线积分格式(19)的保能量守恒特性,定义相对能量误差为  $RE(t) = \left| \frac{H(Z^n) - H(Z^0)}{H(Z^0)} \right|$ , 其中  $H(Z^0)$  为初始能量.

#### 4.1 数值模拟 1

首先考虑  $e=1$  时孤立波的碰撞情况. 设三耦合薛定谔方程组初始条件为

$$\begin{cases} \psi_1(x) = a_0(1 - \epsilon \cos(lx)), \\ \psi_2(x) = b_0(1 - \epsilon \cos(l(x + \theta))), \\ \psi_3(x) = c_0(1 - \epsilon \cos(lx)), \end{cases} \quad (20)$$

其中  $\alpha_1 = \alpha_2 = \alpha_3 = e = 1, l = 0.5$ . 取周期边界条件为  $[-4\pi, 4\pi]$ , 时间步长  $\Delta t = 0.005$ , 空间置配点  $N = 128$ . 图 1 表示当  $a_0 = b_0 = c_0 = 0.3, \epsilon = 0.1, \theta = 0$  时利用离散线积分格式模拟三耦合薛定谔方程组在  $t = [0, 100]$  的数值解. 图 2 表示当  $a_0 = 0.2, b_0 = 0.3, c_0 = 0.2, \epsilon = 0.1, \theta = 0$  时利用离散线积分格式模拟三耦合薛定谔方程组在  $t = [0, 100]$  的数值解. 图 3 表示方程在  $t = [0, 100]$  内的相对能量误差. 显然, 离散线积分格式(19)有很好的计算精度, 并且可以精确地保持方程(12)的能量守恒特性.

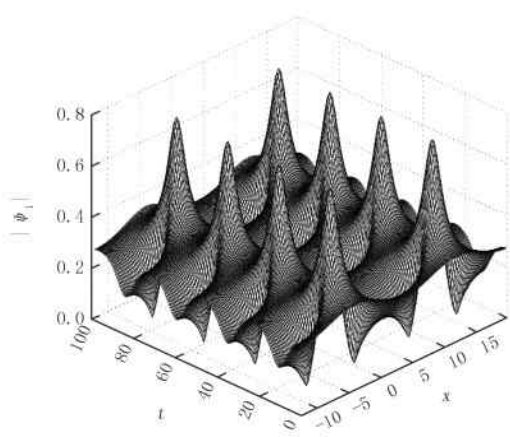


图 1 当  $a_0=b_0=c_0=0.3$  时  $|\psi_1|$  的数值解

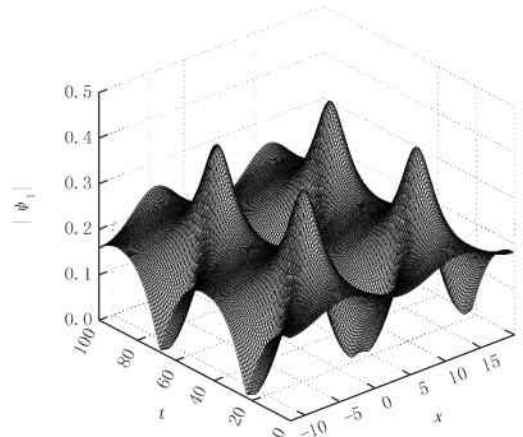


图 2 当  $a_0=0.2, b_0=0.3, c_0=0.2$  时  $|\psi_1|$  的数值解

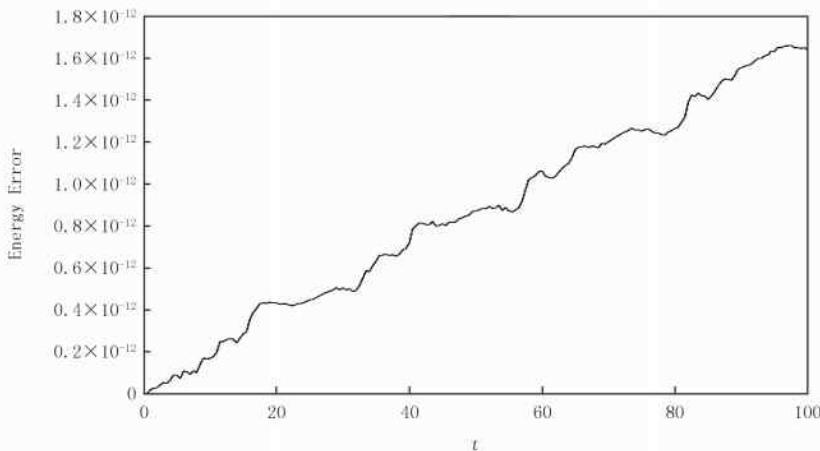


图 3 孤立波在  $t \in [0, 100]$  内的相对能量误差变化

## 4.2 数值模拟 2

下面考虑在  $\varepsilon = \frac{2}{3}$  时孤立波的演化情况. 初始条件(20)不变, 图4表示当  $a_0 = b_0 = c_0 = 0.3, \varepsilon = 0.1, \theta = \frac{9\pi}{4}$  时孤立波的演化情况. 图5表示当  $a_0 = 0.3, b_0 = 0.4, c_0 = 0.3, \varepsilon = 0.1, \theta = 0$  时孤立波的演化情况. 图6表示方程在  $t = [0, 100]$  内的相对能量误差. 根据图4~6可以看出, 离散线积分格式同样具有好的计算精度和保系统的能量守恒特性.

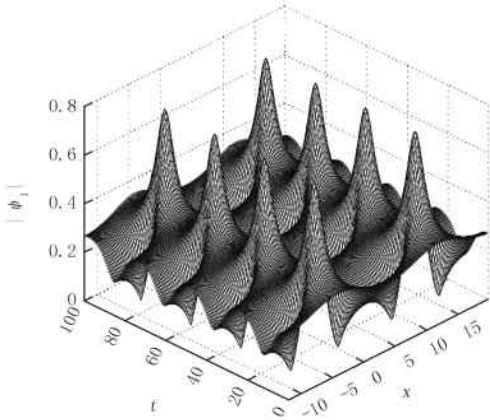


图4 当  $a_0 = b_0 = c_0 = 0.3, \varepsilon = 0.1, \theta = \frac{9\pi}{4}$  时  $|\psi_1|$  的数值解

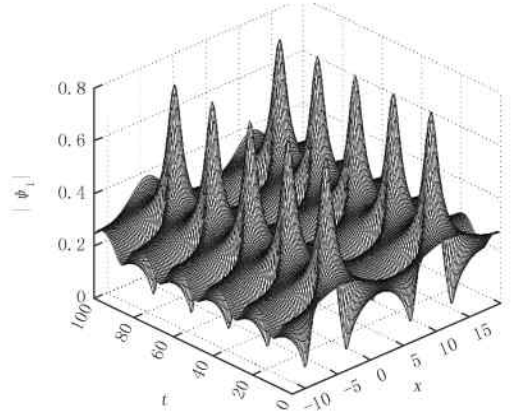


图5 当  $a_0 = 0.3, b_0 = 0.4, c_0 = 0.3, \varepsilon = 0.1, \theta = 0$  时  $|\psi_1|$  的数值解

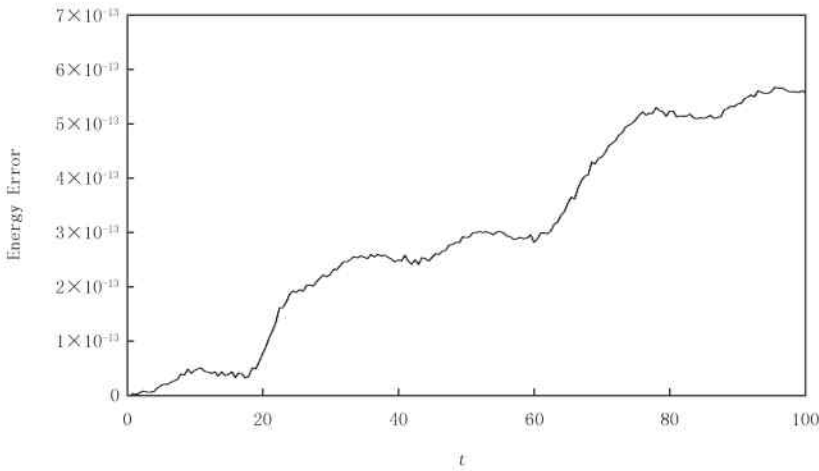


图6 孤立波在  $t \in [0, 100]$  内的相对能量误差变化

## 5 结论

基于 Boole 离散线积分方法, 构造了三耦合薛定谔方程组的离散线积分格式. 利用构造的离散线积分格式数值模拟孤立波的演化行为并分析格式的相对能量误差. 数值结果表明, 该方法可以很好地模拟孤立波的演化行为, 且精确地保持方程组的能量守恒. 在数值模拟三耦合薛定谔方程组中, 本文基于 Boole 离散线积分方法的数值格式在保能量方面具有明显的优越性.

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## Discrete line integral method for 3-coupled Schrödinger equations

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**Abstract:** Three coupled Schrodinger equations have the energy conservation property. Energy conservation numerical method of three coupled Schrodinger equations has important meaning in simulating the solitary wave behaviors of the equations. In this paper, three coupled Schrodinger equations were transformed into the classical Hamilton system, the Boole discrete line integral method was applied to the classical Hamilton system. The new energy conserving schemes of three coupled Schrodinger equations is obtained. The new scheme is applied to simulate the solitary wave behaviors with different parameters. The numerical results show that the discrete line integral method can well simulate the solitary wave behaviors of the equations and preserve the energy conservation.

**Keywords:** 3-coupled Schrödinger equations; Hamilton system; discrete line integral method; spectral method

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