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Novel Conservative Methods for Schrödinger Equations with Variable Coefficients over Long Time

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Abstract. In this paper, we propose a wavelet collocation splitting (WCS) method, and a Fourier pseudospectral splitting (FPSS) method as comparison, for solving one-dimensional and two-dimensional Schrödinger equations with variable coefficients in quantum mechanics. The two methods can preserve the intrinsic properties of original problems as much as possible. The splitting technique increases the computational efficiency. Meanwhile, the error estimation and some conservative properties are investigated. It is proved to preserve the charge conservation exactly. The global energy and momentum conservation laws can be preserved under several conditions. Numerical experiments are conducted during long time computations to show the performances of the proposed methods and verify the theoretical analysis.

AMS subject classifications: 37M05, 65M70, 65T60

Key words: Schrödinger equation, wavelet collocation method, splitting technique, conservative property.

1 Introduction

The Schrödinger equations are very important in many branches of physics and applied mathematics, such as nonlinear quantum field theory, condensed matter, nonlinear optics, hydrodynamics, self-focusing in laser pulse, thermodynamic process in meso

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scale systems, plasma and so on [1–7]. Meanwhile, most of real physical equations possess variable coefficient. For example, the dispersion-managed optical fibers and soliton lasers, certain inhomogeneous optical fibers, arterial mechanics, Laser-atom interaction and so on [8–13].

In this paper, firstly we consider the one-dimensional nonlinear Schrödinger (1D-NLS) equation with variable coefficients:

$$i\psi_t+\alpha(t)\psi_{xx}+v(x)\psi+\beta(t)|\psi|^2\psi=0, \tag{1.1a}$$
$$\psi(x,0)=\varphi(x), \tag{1.1b}$$

where $\alpha(t)$, $v(x)$ and $\beta(t)$ are bounded real functions, $\psi(x,t)$ is the complex-valued wave function, and $\alpha(t)$ is related to the second order dispersion coefficient. As usual, $i=\sqrt{-1}$, and $\varphi(x)$ is a smooth function such that

$$E_1(\varphi)=\int_{\mathbb{R}}|\varphi(x)|^2dx<+\infty, \tag{1.2}$$

(the so-called L_2-function). The 1D-NLS system admits following conservation laws

Proposition 1.1. The solution ψ of Eq. (1.1) satisfies:

(1) Global charge conservation:

$$\mathcal{Q}(\psi)=\int_{\mathbb{R}}|\varphi|^2dx=\mathcal{Q}(\varphi); \tag{1.3}$$

(2) Global momentum conservation:

$$\mathcal{M}(\psi)=\int_{\mathbb{R}}(\Re(\psi)\Im(\psi_x)-\Re(\psi_x)\Im(\psi))dx=\mathcal{M}(\varphi), \tag{1.4}$$

where $\Re$ and $\Im$ stand for the real part and the imaginary part, respectively;

(3) Global energy conservation: if $\alpha(t)$ and $\beta(t)$ are independent of t (i.e. $\alpha(t)=\alpha$, $\beta(t)=\beta$), then

$$\begin{aligned}\mathcal{E}(\psi)&=\int_{\mathbb{R}}\Big(\alpha|\psi_x|^2-v(x)|\psi|^2-\frac{\beta}{2}|\psi|^4\Big)dx\\&=\int_{\mathbb{R}}\Big(\alpha|\varphi_x|^2-v(x)|\varphi|^2-\frac{\beta}{2}|\varphi|^4\Big)dx=\mathcal{E}(\varphi).\end{aligned} \tag{1.5}$$

We will consider the following equations from the general form of Eq. (1.1):

(1) Cubic 1D-NLS equation

$$i\psi_t+\alpha(t)\psi_{xx}+\beta(t)|\psi|^2\psi=0. \tag{1.6}$$

The theoretical investigation of Eq. (1.6) can be found in [4] and references therein. We assume the solution ψ exists globally and satisfies $\lim_{|x|\to+\infty}(|\psi|+|\psi_x|)=0$.