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Optimization of Explicit Symplectic Schemes for Time-Dependent Schrödinger Equations

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Abstract—In this paper, in order to conserve the discrete squared norm of the wave function, we propose a condition for optimizing the n-stage and n-order explicit symplectic schemes, which are applied to solving finite-dimensional canonical equations obtained by discretizing the time-dependent Schrodinger equations It is showed that the 'half unitary' (i e , symmetric) conditions proposed by Gray and Manolopoulos can automatically satisfy the optimal condition proposed in this paper for even n but not for odd n In particular, two-order or four-order optimized explicit symplectic schemes are obtained Calculations and comparisons with three kinds of explicit symplectic schemes are presented for a model in quantum systems © 2005 Elsevier Ltd. All rights reserved

Keywords—Symplectic scheme, Wave function, Schrodinger equation

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1. INTRODUCTION

The time evolution of quantum systems is described by the time-dependent Schrödinger equation (TDSE),

$$\imath \frac{\partial}{\partial t} \psi(t, \vec{r}) = H \psi(t, \vec{r}), \tag{1}$$

where H, the Hamiltonian operator, is a Hermite operator. Assume that H is real and does not depend on time apparently, e.g , $H = -(1/2)\nabla^2 + V(\vec{r})$. Let

$$\psi(t, \vec{r}) = \psi_r(t, \vec{r}) + \imath \psi_\imath(t, \vec{r}),$$

then equation (1) can be written as the following infinite-dimensional canonical equations,

$$\frac{\partial \psi_\imath}{\partial t} = -H\psi_r, \qquad \frac{\partial \psi_r}{\partial t} = H\psi_\imath. \tag{2}$$

The time-evolution of the wave function $\psi(t, \vec{r})$ is unitary, in other words, the time-evolution of vector $(\psi_r, \psi_\imath)^\top$ is symplectic and squared norm conserving [1]. TDSE can be discretized into the finite-dimensional canonical equations which conserve the discrete squared norm of the wave function. It is, therefore, natural and reasonable to search for a squared norm conserving symplectic scheme to solve it numerically. The symplectic schemes obtained by performing Cayley transformation or diagonal *Padê* approximation of $\exp(x)$ are both squared norm conserving, such as the Euler mid-point scheme [2,3]. These symplectic schemes, however, are implicit and their implementation contains iteration in every step. So, the computation cost is very expensive. When stability questions are not at issue, it often makes sense to use the explicit symplectic schemes (ESS) [4–8]. However, the conservation of the discrete squared norm, which is very important in quantum system, cannot be guaranteed by using ESS. By the expansion methods (under the zero boundary conditions) or discretization of second-order derivative in space by the central difference, the infinite-dimensional canonical equations (2) can be discretized into finite (m)-dimensional canonical equations in Hamiltonian system [1],

$$\frac{dD}{dt} = -SC, \qquad \frac{dC}{dt} = SD, \tag{3}$$

where S is a real symmetric matrix, $D = (d_1, d_2 \dots d_m)^\top$, $C = (c_1, c_2 \dots c_m)^\top$. This is a linear and separable Hamiltonian system with the Hamiltonian function $H(D, C) = (1/2)D^\top SD + (1/2)C^\top SC$. Zhu *et al.* [9] discussed the order conditions of n-stage and n-order ESS for the canonical equations (3) and optimized n-stage and n-order ESS replying on computational requirements. Gray *et al.* [10] discussed the order conditions and proposed a 'half unitary' condition to determine the coefficients of the ESS more conveniently. In this paper, we deduce the mathematical formulation of the condition which makes corresponding scheme conserve squared norm as accurately as possible. We call this condition the 'squared norm conserving' condition. Moreover, we show that the 'half unitary' condition [10] implies the 'squared norm conserving' condition' for even n.

The paper is organized as follows. In Section 2, we review some results presented by Zhu *et al.* and Gray *et al.* on the n-stage and n-order ESS for canonical equations (3). In Section 3, we present the idea of optimizing n-stage and n-order ESS and deduce the mathematical formulation of the 'squared norm conserving' condition. In Section 4, we give a numerical example in quantum system to compare the effect of three different kinds of four-stage and four-order ESS. The numerical results show that the optimized four-stage and four-order ESS can conserve the squared norm over long time evolution and is better than the other two kinds as far as the squared norm is concerned.

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