COMMUNICATIONS IN COMPUTATIONAL PHYSICS
Vol. **2**, No. 1, pp. 1-53

Commun. Comput. Phys.
February 2007

Recent Progress in Symplectic Algorithms for Use in Quantum Systems

Xue-Shen Liu[1,*], Yue-Ying Qi[1,2], Jian-Feng He[1,3] and Pei-Zhu Ding[1]

[1] *Institute of Atomic and Molecular Physics, Jilin University, Changchun 130012, P. R. China.*
[2] *School of Electrical Engineering, Jiaxing University, Jiaxing 314001, P. R. China.*
[3] *Department of Physics, School of Science, Beijing Institute of Technology, Beijing 100081, P. R. China.*

Received 20 December 2005; Accepted (in revised version) 5 April 2006

Available online 30 August 2006

Abstract. In this paper we survey recent progress in symplectic algorithms for use in quantum systems in the following topics: Symplectic schemes for solving Hamiltonian systems; Classical trajectories of diatomic systems, model molecule A_2B, Hydrogen ion H_2^+ and elementary atmospheric reaction $N(^4S)+O_2(X^3\Sigma_g^-)\rightarrow NO(X^2\Pi)+O(^3P)$ calculated by means of Runge-Kutta methods and symplectic methods; the classical dissociation of the HF molecule and classical dynamics of H_2^+ in an intense laser field; the symplectic form and symplectic-scheme shooting method for the time-independent Schrödinger equation; the computation of continuum eigenfunction of the Schrödinger equation; asymptotic boundary conditions for solving the time-dependent Schrödinger equation of an atom in an intense laser field; symplectic discretization based on asymptotic boundary condition and the numerical eigenfunction expansion; and applications in computing multi-photon ionization, above-threshold ionization, Rabbi oscillation and high-order harmonic generation of laser-atom interaction.

PACS: 47.10.Df, 02.70.-c, 34, 95.30.-k

Key words: Quantum system, symplectic algorithm, classical trajectory, Schrödinger equation, intense laser field.

Contents

1 Introduction 2

*Corresponding author. *Email addresses:* `liuxs@jlu.edu.cn` (X. S. Liu), `jess1234yao@yahoo.com.cn` (Y. Y. Qi), `hjf@bit.edu.cn` (J. F. He), `dpz@mail.jlu.edu.cn` (P. Z. Ding)

2 Hamiltonian systems and symplectic algorithms 3
3 Classical dynamics of molecular system in an intense laser field 12
4 Time-independent Schrödinger equation & symplectic-scheme shooting method 28
5 Interaction of atoms with intense laser field and the time-dependent Schrödinger equation 37
6 Conclusions 48

1 Introduction

The fundamental theorem of Hamiltonian mechanics says that the time-evolution of a Hamiltonian system is the evolution of symplectic transformation. In this sense, we say that the Hamiltonian system has a symplectic structure [1, 2]. Therefore, Ruth [3] and Feng [4] presented the symplectic algorithm for solving the Hamiltonian system, which leads to a new method for solving the Hamiltonian mechanics. It is now well known that the symplectic algorithm is a difference method that preserves the symplectic structure, and it is the method of choice in the long-time calculation and for preserving the structure of the system [5,7].

At present, the study and application of symplectic algorithms is well developed [4]-[27]. In particular, Feng [6] constructed symplectic difference schemes of Hamiltonian formalism via generating functions, and higher order symplectic schemes and multi-stage symplectic schemes were presented in [7, 8, 86]. Moreover, symplectic partitioned Runge-Kutta methods were deduced [12, 22], and multi-symplectic schemes were also established [24–27]. Up to now, symplectic methods have been applied to many fields, for example, to the nonlinear Schrödinger equation [28–32], celestial mechanics equation [33–35], time-evolution of quantum systems [36–39], molecular dynamics [40, 41], plasma physics [42], the KdV equation, the evolution of vortices in a rotating Bose–Einstein Condensate, and so on.

A quantum system is an infinite-dimensional Hamiltonian system. The time-evolution of the time-dependent Schrödinger equation preserves the normalization and symplectic product of the wave function. Thus, the time-dependent Schrödinger equation can be transformed into a Hamiltonian canonical equation. The square-preserving and symplectic scheme is the reasonable and natural way for solving the time-dependent Schrödinger equation. Therefore, the symplectic algorithm of the classical Hamiltonian system was extended to the time-evolution of quantum system [43, 44].

In this paper, we will review the applications of the symplectic algorithm of the classical Hamiltonian system to the quantum system. The topics of this review article include

a. Symplectic space, explicit symplectic schemes for linear separate Hamiltonian systems and tailored to the time-dependent Hamiltonian function;
b. The classical theory and classical trajectory methods and the classical dynamics of molecular system in an intense laser field;