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Journal of Computational and Applied Mathematics 193 (2006) 65–88
JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS
www.elsevier.com/locate/cam

Analysis of a leap-frog pseudospectral scheme for the Schrödinger equation☆

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Received 24 December 2004

Abstract

The numerical properties of a leap-frog pseudospectral scheme for the Schrödinger equation are analyzed. Stability, second-order accuracy in time, and spectral accuracy in space are discussed considering the linear Schrödinger equation with potential in a periodic setting. Further issues regarding phase error, gauge invariance, conservation properties, and commutation relations are addressed. Results of numerical experiments are reported to demonstrate the validity and limitations of the theoretical findings and for comparison with the well known Crank–Nicholson finite difference scheme.

MSC: 65M06; 65M70; 65M12; 65T50; 65Z05

Keywords: Schrödinger equation; Pseudospectral method; Leap-frog scheme; Stability and accuracy analysis

1. Introduction

Two decades ago Kosloff and Kosloff [20] proposed a leap-frog pseudospectral (LFPS) method for solving the Schrödinger equation in a periodic setting and, since then, the LFPS scheme has been successfully applied to various quantum computation problems; see [16,20,19,18,21,25] and references therein.

☆ Supported in part by the Austrian Science Fund FWF project P18136-N13 "Quantum optimal control of semiconductor nanostructures".
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doi:10.1016/j.cam.2005.04.066

As emphasized in the early paper [20], spectral methods [7,14] provide accurate numerical representations of evolving quantum systems. In fact they allow—in contrast to, e.g., finite difference or finite element methods [2,9,11,12,17,22,24]—the 'spectrally accurate' representation of specific properties of quantum mechanical time evolution.

Nowadays, the study of quantum dynamics is experiencing a renewed intensive effort motivated by nanoscience research [15], where investigation of quantum phenomena at atomic and molecular level beyond macroscopic averaging is required. This research work requires accurate simulation of quantum systems motivating the study of highly accurate discretization schemes like the one considered in this paper. Besides accuracy, the spectral approach allows for exact representation of commutation relations and preserves conservation laws. Its use is further motivated by recent regularity results concerning solutions to the Schrödinger equation given in [6]. Also notice that typically quantum wave packets [26] decay exponentially in classically forbidden regions of phase space and thus Fourier grids are most appropriate to represent these wave functions.

Quantum systems are genuinely time-dependent requiring the implementation of efficient quantum evolution operators. These operators should reflect time-reversal invariance and guarantee stable and accurate solutions as is the case of LFPS methods. An additional feature of LFPS schemes regarding time evolution is their immediate applicability to cases where time-dependent potentials are considered, in contrast to exact in time propagation schemes [4] or propagation schemes based on Tchebychev polynomials expansion of the evolution operator [21,25]. Time-dependent Hamiltonians arise in, e.g., quantum optimal control problems [5,15,23]. Furthermore, the LFPS approach allows a viable and simple generalization to higher-order time propagators; see the class of extended LFPS schemes considered in [16].

Our present contribution to the development and application of LFPS methods is to provide stability and accuracy estimates for the LFPS scheme applied to linear Schrödinger equations in a periodic multi-dimensional setting.

For the purpose of our analysis we report, in the next section, results concerning existence and regularity properties of solutions. While most of these results are well known, some of them are recent and provide the appropriate analytical setting for analyzing the pseudospectral scheme considered in this paper. In Section 3, the Fourier pseudospectral discretization method is illustrated and some related approximation properties are reported, which will be used in the forthcoming Section 4 dedicated to the numerical analysis of LFPS discretization of the Schrödinger equation. In this section stability of the LFPS scheme under restriction of the time step size is discussed. Then, in the second part of this section, second-order accuracy in time and spectral accuracy in space is proved. These results are stated in terms of discrete L^2-norms and therefore they do not provide immediate insight on the error in the phase occurring during time evolution. Because the phase plays an important role in the physical interpretation of quantum phenomena, we discuss in Section 5 phase error and the related problem of gauge invariance. The theoretical discussion on the numerical properties of the LFPS scheme is completed in Section 6 where conservation laws and commutation relations are considered.

In Section 7, results of numerical experiments are reported for the purpose of validating the theoretical findings and for comparison of the LFPS scheme with the largely used Crank–Nicholson finite difference scheme. The latter provides solutions which are second-order accurate in space and in time. However, we show that second-order accuracy in space is not sufficient to provide correct wave-packet evolution. Further results show that the LFPS scheme compares favorably in the presence of moderate discontinuous potentials. Concerning the LFPS scheme, all results of experiments with free wave packets confirm second-order accuracy in time and spectral accuracy in space. In particular, it is shown that errors due to time