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Layer-Splitting Methods for Time-Dependent Schrödinger Equations of Incommensurate Systems

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Abstract. This work considers numerical methods for the time-dependent Schrödinger equation of incommensurate systems. By using a plane wave method for spatial discretization, the incommensurate problem is lifted to a higher dimension that results in semidiscrete differential equations with extremely demanding computational cost. We propose several fully discrete time stepping schemes based on the idea of "layer-splitting", which decompose the semidiscrete problem into sub-problems that each corresponds to one of the periodic layers. Then these schemes handle only some periodic systems in the original lower dimension at each time step, which reduces the computational cost significantly and is natural to involve stochastic methods and parallel computing. Both theoretical analysis and numerical experiments are provided to support the reliability and efficiency of the algorithms.

AMS subject classifications: 35Q40, 35Q41, 65L05, 65L20

Key words: Incommensurate system, time-dependent Schrödinger equation, time stepping scheme.

1 Introduction

Recently there have been extensive research efforts on low dimensional materials with multilayer structures [7, 12, 26, 27, 31]. The mechanical and electronic properties of such

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systems depend heavily on the stacking arrangement, which allows various manipulation to create heterostructure devices [6, 29]. The lattice periods of the individual layers are generally incommensurate due to the difference in the crystal structure and also due to misorientation between the adjacent layers [10, 28, 32]. Meanwhile, in the experiments of ultracold atoms [11, 30] and photonic crystals [33, 37] the incommensurate potentials are created by the interference of laser or the modulation of the refractive indeces and people have observed the localized-extended transition in the time evolution of the quantum waves.

The absence of periodicity in the incommensurate systems presents an essential challenge to atomic/electronic structure calculations since the Bloch theorem can not be applied directly. The conventional numerical method to study such systems is to strain them to some commensurate supercells such that the periodicity can be retained [19, 20, 23, 36]. However, this type of approaches are usually very expensive and there is no verification of the approximation error. Recently, a plane wave method has been proposed to study the quasicrystals [17] and eigenvalue problems of the incommensurate systems [8, 38], which in principle gets rid of the modeling error and is efficient in numerical simulations. Despite many advantages of the plane wave method for incommensurate systems, it has been shown in [8, 38] that this method essentially lifts the problem into a higher dimensional space and therefore results in a discrete problem with huge degrees of freedom, especially when the system consists of many periodic layers and when a large energy cutoff is used for the plane wave discretization. This difficulty needs to be resolved so that one can achieve "affordable" simulations with high accuracy for incommensurate systems, in particular, for the time-dependent problems.

The goal of this paper is to apply the plane wave method to the time-dependent Schrödinger equations of incommensurate systems for spacial discretization, and then design efficient time-stepping schemes to cure the problem of dimension lifting. Our idea is to split the total Hamiltonian operator such that each part is related to one of the periodic layers in the incommensurate system. Based on this "layer-splitting" idea, semidiscrete problem is split into low dimensional sub-problems, and the wavefunctions are evolving by several periodic operators at each time step rather than an incommensurate one, which can reduce the computational cost significantly (see more discussions in Section 4). The layer-splitting methods are natural to involve parallel computing and stochastic algorithms, thus very beneficial for simulating large-scale systems.

The algorithms developed in this paper are analogous to the so-called operator splitting methods [13, 25, 35] that have been widely used in the numerical solutions of partial differential equations, especially for the time-dependent Schrödinger equations (see e.g. [3–5, 24]). In particular, we mention two recent works that are more related to this paper. In [22], the quantum dynamics of some quasiperiodic systems were studied, by using plane wave methods for spatial discretization and an operator splitting method for time stepping to handle the kinetic and potential parts separately. In [9], an operator splitting technique was adopted to decompose a four dimensional Wigner equation into two sub-equations with lower dimension, which are then discretized by a charac-