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# An Implicit Solver for the Time-Dependent Kohn-Sham Equation

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**Abstract.** The implicit numerical methods have the advantages on preserving the physical properties of the quantum system when solving the time-dependent Kohn-Sham equation. However, the efficiency issue prevents the practical applications of those implicit methods. In this paper, an implicit solver based on a class of Runge-Kutta methods and the finite element method is proposed for the time-dependent Kohn-Sham equation. The efficiency issue is partially resolved by three approaches, i.e., an $h$-adaptive mesh method is proposed to effectively restrain the size of the discretized problem, a complex-valued algebraic multigrid solver is developed for efficiently solving the derived linear system from the implicit discretization, as well as the OpenMP based parallelization of the algorithm. The numerical convergence, the ability on preserving the physical properties, and the efficiency of the proposed numerical method are demonstrated by a number of numerical experiments.

**AMS subject classifications**: 35Q41, 81Q05, 65M60, 65M55, 65M50

**Key words**: Time-dependent Kohn-Sham equation, implicit midpoint scheme, finite element methods, h-adaptive mesh methods, complex-valued algebraic multigrid methods.

## 1. Introduction

Suppose that there is an electronic structure system consisting of $M$ nuclei and $N$ electrons. The evolution of this many-body system in the nonrelativistic sense is fundamentally controlled by the time-dependent Schrödinger equation (TDSE)

$$i\frac{\partial}{\partial t}\Psi = H\Psi \quad \text{in } \mathbb{R}^3, \tag{1.1}$$

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where $i$ denotes the imaginary unit, $H$ consists of the kinetic energy operator for each particle as well as the classical Coulomb interactions between each pair of particles, and $\Psi := \Psi(\vec{X}_1, \ldots, \vec{X}_M, \vec{x}_1, \ldots, \vec{x}_N, t)$ is the high dimensional wavefunction depending on the position of each particle and a time variable. It is this high dimensionality of the wavefunction $\Psi$ which makes the analysis and computation on the TDSE very challenging. The time-dependent Kohn-Sham (TDKS) density functional theory is one of the most successful approximation models towards partially overcoming this challenge, which can be written as

$$\begin{aligned} i\frac{\partial}{\partial t}\psi_j &= \left(-\frac{1}{2}\nabla^2 - \sum_l \frac{z_l}{|\vec{x} - \vec{R}_l|} + \int \frac{\rho(\vec{x}', t)}{|\vec{x} - \vec{x}'|} d\vec{x}' + v_{ALDA}(\rho)\right)\psi_j \\ &=: \left(-\frac{1}{2}\nabla^2 + V_{KS}\right)\psi_j, \quad j = 1, \ldots, N, \end{aligned} \tag{1.2}$$

where $\rho(\vec{x}, t) = \sum_j |\psi_j(\vec{x}, t)|^2$ is the time-dependent electron density, $z_l$ and $\vec{R}_l$ for $l = 1, \ldots, M$ denote the nuclear charge and position of the $l$-th nucleus, and $V_{KS}$ denotes the Kohn-Sham potential consisting of the external potential, the Hartree potential, as well as the exchange-correlation potential, respectively. Here, an adiabatic approximation for the exchange-correlation potential, denoted by $v_{ALDA}$, is considered. Guaranteed by the Runge-Gross theorem [22], the time-dependent electron density $\rho(\vec{x}, t)$ is used as a fundamental variable to represent an evolved many-body system. It is noted that the electron density $\rho$ is a four dimensional variable in a three dimensional space. This huge reduction of the dimension brings the possibility on quality analysis and simulation for the many-body system. So far, the TDKS equation has been widely used in a variety of applications such as material science, nano-optics, and attosecond science, etc. Please refer to [21] and references therein for more details on the application of the TDKS equation.

There have been lots of numerical methods in the market to solve the TDKS equation in the time domain, people may refer to [3,7,14] and references therein for detail. People may also refer to [11, 16, 28] for numerical methods of Schrödinger equation. Among those grid-based numerical methods, the finite difference methods [1], the finite element methods [3,8,9,17,18,27], the discontinuous Galerkin methods [20], the wavelet methods [12] etc. are popular for the spatial discretization, while there are Runge-Kutta methods, commutator-free Magnus expansion methods, etc. for the temporal discretization. It is worth mentioning that the comparison of the performance of those time propagators, including the linear multistep methods, can be found from a recent paper [14]. However, it should be pointed out that the memory issue of the solver is missed there, and that many factors would affect the performance of those solvers, for example, the performance of the linear solver for the implicit methods. Due to their advantage on the memory requirement, the single step methods such as the Runge-Kutta methods have attracted much attention in solving the time-dependent problems. Furthermore, some implicit one-step solvers have the property on well preserving the physical structure of the TDKS equation. These advantages make the solvers such as