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An SAV Method for Imaginary Time Gradient Flow Model in Density Functional Theory

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Abstract. In this paper, based on the imaginary time gradient flow model in the density functional theory, a scalar auxiliary variable (SAV) method is developed for the ground state calculation of a given electronic structure system. To handle the orthonormality constraint on those wave functions, two kinds of penalty terms are introduced in designing the modified energy functional in SAV, i.e., one for the norm preserving of each wave function, another for the orthogonality between each pair of different wave functions. A numerical method consisting of a designed scheme and a linear finite element method is used for the discretization. Theoretically, the desired unconditional decay of modified energy can be obtained from our method, while computationally, both the original energy and modified energy decay behaviors can be observed successfully from a number of numerical experiments. More importantly, numerical results show that the orthonormality among those wave functions can be automatically preserved, without explicitly preserving orthogonalization operations. This implies the potential of our method in large-scale simulations in density functional theory.

AMS subject classifications: 65N30, 37M05
Key words: Density functional theory, gradient flow, scalar auxiliary variable, unconditional energy stability, orthonormalization free.

1 Introduction

The Kohn-Sham density functional theory (KSDFT) [13] is one of the most successful approximation models of the many-body Schrödinger equation. Thanks to the Hohenberg-

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Kohn theorem, the ground state electron density is used as a fundamental variable to describe the many-body problem. This is a huge reduction on the dimensionality since the ground state electron density is a three dimensional variable while the wave function in the original many-body system is a $3N$ dimensional one. However, it is still very challenging to develop efficient numerical methods for the KSDFT, due to the singularity from the external potential, the orthonormality constraint for those wave functions, etc. Besides the popular self-consistent field iteration [22,23], minimizing total energy [10,26] is an alternative approach for the ground state calculation. In this direction, the gradient flow method is a competitive method due to its feature on energy dissipation, in which there have been many pioneer works on developing numerical methods [19,27,30]. Among all these methods, the emerging scalar auxiliary variable (SAV) method has been attracting more and more attention since its excellent performance in the simulation.

The SAV method has been proposed in [32,33] for solving the Allen-Cahn and Cahn-Hilliard equations. The main idea of SAV [25] is to introduce a scalar auxiliary variable which is a square root function to reformulate a gradient flow model into an equivalent form. For the reformulated system, it is easy to construct a linear scheme with unconditional energy stability, which in turn solves the original model. The original SAV method has the following remarkable features [17]: i) At each time step, only decoupled, linear systems with constant coefficients need to be solved (efficiency); ii) The first- and second-order SAV schemes are unconditionally energy stable (stability); iii) The form of nonlinear part of total energy is not restricted, so it applies to a large class of gradient flows (flexibility). Due to the above advantages, several works have been completed based on this method. The convergence and error analysis of the SAV method for gradient flow have been developed in [31]. The high-order scalar auxiliary variable (HSAV) method was presented in [16], and it has been shown that the newly proposed schemes could be reached in arbitrarily high order in time. In [7], the generalized scalar auxiliary variable method (G-SAV) was proposed where the definition form of the auxiliary variable was extended. More variants of the SAV method for solving Allen-Cahn type equations can be found in [20,21].

By using the method mentioned above, the SAV method has already been widely used in variable problems. In [29], a second order SAV Crank-Nicolson (SAV-CN) scheme was adopted to solve the Peng-Robinson EOS problem. In [1], a second order SAV pseudo-spectral scheme was proposed to handle the dynamics of general nonlinear Schrödinger/Gross-Pitaevskii equations. In [12], an SAV-Gauss collocation finite element method was used to study nonlinear Schrödinger equation. In [8], a second order SAV modified Crank-Nicolson scheme was proposed and analyzed for the epitaxial thin film growth model. Recently, in [35], a modified SAV scheme was constructed to solve the ground state solutions of one- and multi-component Bose-Einstein Condensates (BECs). It is mentioned that there is a norm preserving constraint in the problem, which is removed by the authors by introducing a penalty term in the expression of total energy. With this strategy, the unconditional decay of the modified total energy can be obtained both theoretically and numerically, while the norm constraint can be satisfied automatically.