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A Two-Grid Finite-Volume Method for the Schrödinger Equation

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Abstract. In this paper, some two-grid finite-volume methods are constructed for solving the steady-state Schrödinger equation. The method projects the original coupled problem onto a coarser grid, on which it is less expensive to solve, and then prolongates the approximated coarse solution back to the fine grid, on which it is not much more difficult to solve the decoupled problem. We have shown, both theoretically and numerically, that our schemes are more efficient and achieve asymptotically optimal accuracy as long as the mesh sizes satisfy $h=\mathcal{O}(H^2)$.

AMS subject classifications: 65N50, 65N30

Key words: Schrödinger equation, coupled equation, finite volume, two-grid.

1 Introduction

In this paper, we will study two-grid finite volume element discretization schemes for the following boundary value problem of the steady-state Schrödinger equation [1]:

$$-\Delta\psi(\mathbf{x})+V(\mathbf{x})\psi(\mathbf{x})=f(\mathbf{x}), \qquad \forall\mathbf{x}\in\Omega, \tag{1.1a}$$
$$\psi(\mathbf{x})=0, \qquad \forall\mathbf{x}\in\partial\Omega, \tag{1.1b}$$

where $\Omega\subset R^2$ is a convex polygonal domain, $f(\mathbf{x})$, $V(\mathbf{x})$ and unknown function $\psi(\mathbf{x})$ are complex-valued.

For any complex-valued function ψ, we denote its real part by ψ_1, the imaginary part by ψ_2. Then problem (1.1a)-(1.1b) is equivalent to the following coupled equations:

$$-\Delta\psi_1(\mathbf{x})+V_1(\mathbf{x})\psi_1(\mathbf{x})-V_2(\mathbf{x})\psi_2(\mathbf{x})=f_1(\mathbf{x}), \qquad \forall\mathbf{x}\in\Omega, \tag{1.2a}$$
$$-\Delta\psi_2(\mathbf{x})+V_1(\mathbf{x})\psi_2(\mathbf{x})+V_2(\mathbf{x})\psi_1(\mathbf{x})=f_2(\mathbf{x}), \qquad \forall\mathbf{x}\in\Omega, \tag{1.2b}$$
$$\psi_j(\mathbf{x})=0, \quad j=1,2, \qquad \forall\mathbf{x}\in\partial\Omega. \tag{1.2c}$$

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Finite volume method has the local conservation of certain physical quantities and the convenience in numerical implementation, so it has been efficiently used in lot of practical computations and extensively studied in theory [2–19, 35–43]. Zhou et al. constructed symmetric finite volume schemes for selfadjoint elliptic problems [2] in 2002 and for parabolic problems [6] in 2003 respectively. Also, there are different finite volume methods for elliptic problems [9, 11–13, 15]. Wang et al. [7] develop a second-order finite volume scheme to simulate three dimensional truncated pyramidal QDs in 2006, where the scheme has successfully computed all the confined energy states and visualized the corresponding wave functions. He et al. [8] proposed finite volume method based on stabilized finite elements for the nonstationary Navier-Stokes problem in 2007, where the resulting solution, verified by theoretical analysis and numerical experiments, achieves optimal accuracy, and so on.

On the other hand, the two-grid discretization method, proposed originally by Xu [20] in 1992, is an efficient numerical method. And it was further investigated and applied to solving many problems, such as nonlinear parabolic equations [21], nonlinear elasticity problems [22], nonlinear PDEs [23], Navier-Stokes equations [24, 25], evolution equations [26], two-phase mixed-domain PEMFC model [27], nonlinear natural convection system [28], Schrödinger equations [1, 29–34] and so on.

Later on, more authors connected finite volume method with two-grid method and obtained some important results, for instance, Bi et al. [35] constructed two-grid finite volume element method for linear and nonlinear elliptic problems in 2007; Chen et al. proposed semi-discrete two-grid finite volume element method for semilinear parabolic [36] and for second-order nonlinear hyperbolic equations [37] respectively in 2010; For nonlinear parabolic equations, Chen et al. [38] in 2009 and Zhang et al. [39] in 2011 constructed full-discrete two-grid finite volume element method respectively; Also Zhang [40] proposed two-grid characteristic finite volume element method for nonlinear parabolic equations in 2013; And Zhang [41] constructed semi-discrete two-grid finite volume element method for nonlinear convection-diffusion problems in 2011; Chen et al. [42] proposed two-grid characteristic finite volume element method for semilinear advection-dominated diffusion equations in 2013; Li et al. [43] show both wavelet preconditioners and multilevel preconditioners of linear systems which resulted from the finite volume method for elliptic boundary value problems in 2012. In the above results, some rigorous theoretical analyses are given, and some numerical experiments are presented to confirm the theoretical findings.

In this paper, we explore the two-grid finite volume method to decouple the systems of partial differential equations (1.2a)-(1.2c). Specifically, we extended the approach given in [2, 6] to solve the original problem directly on the coarse grid, and constructed a new finite volume method to solve the decoupled equations on the fine grid. The resulting solution, verified by theoretical analysis and numerical experiments, achieves optimal accuracy $(h+H^2)$ in H^1-norm.

The rest of the paper is organized as follows: Section 2 is a description and analysis of the finite volume method for Schrödinger equation. In Section 3, we construct the