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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.

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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 two-grid finite volume schemes and derive the error estimates. In Section 4, we provide numerical examples to verify the efficiency and effectiveness of the schemes.

2 The finite volume approximation

For any real-valued and complex-valued function, the inner product $(\cdot,\cdot)$ and standard Sobolev norms $(\|\cdot\|_{m,p},\|\cdot\|_{m,\infty})$ have been defined in the same way as in [44].

Then $\psi(\mathbf{x})$, the weak solution of problem (1.2a)-(1.2c), is defined as follows: Find $\psi(\mathbf{x})\in H_0^1\times H_0^1$ such that

$$A(\psi,\chi)=(f,\chi),\quad \forall\chi\in H_0^1\times H_0^1, \tag{2.1}$$

where

$$A(\psi,\chi)=(\nabla\psi_1,\nabla\chi_1)+(\nabla\psi_2,\nabla\chi_2)+(V_1\psi_1-V_2\psi_2,\chi_1)+(V_1\psi_2+V_2\psi_1,\chi_2), \tag{2.2a}$$

$$(f,\chi)=(f_1,\chi_1)+(f_2,\chi_2). \tag{2.2b}$$

Throughout this paper, we assume that

$$f_1(\mathbf{x}),f_2(\mathbf{x})\in L^2(\Omega);\quad V_1(\mathbf{x}),V_2(\mathbf{x})\in L^\infty(\Omega)\quad \text{and}\quad V_2(\mathbf{x})\geq 0. \tag{2.3}$$

Under the assumption (2.3), the variational problem (2.1) has a unique solution $\psi_h\in H^2(\Omega)\times H^2(\Omega)$, which satisfies (see, e.g., [1, Theorem 1]),

$$\|\psi\|_2\leq\|f\|, \tag{2.4}$$

and the bilinear form $A(\cdot,\cdot)$ satisfies

$$A(\chi,\chi)\gtrsim\|\chi\|_1^2,\quad \forall\chi\in H_0^1\times H_0^1. \tag{2.5}$$

Let T_h be a quasi-uniform triangulation of Ω with mesh size $h>0$, Z_h be the set of all nodes or vertices of T_h, $S_0^h\subset H_0^1$ be the corresponding piecewise linear finite element space.

For simplicity, let the notation "$\lesssim$" be equivalent to "$\leq C$" and "$\gtrsim$" be equivalent to "$\geq C$" for some positive constant C.

Then $\psi_h(\mathbf{x})$, the finite element approximation of problem (2.1), is defined as the following:

Find $\psi_h(\mathbf{x})\in S_0^h\times S_0^h$ such that

$$A(\psi_h,\chi_h)=(f,\chi_h),\quad \forall\chi_h\in S_0^h\times S_0^h. \tag{2.6}$$

It was shown in [1, Theorem 2] that

$$\|\psi-\psi_h\|_s\lesssim h^{2-s}\|\psi\|_2,\quad s=0,1, \tag{2.7}$$

where ψ_h satisfies (2.6).

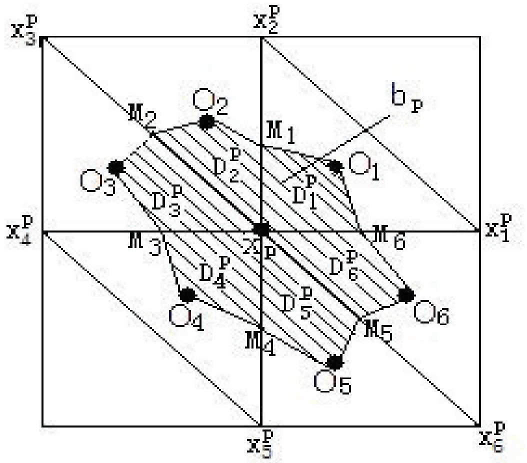

Figure 1: Barycenter Control Volume $b_p \in B^h$.

Now we construct a barycenter dual mesh B^h based upon T^h in the same way as in [2,11,12,35], as follows: for each $e \in T^h$, find the barycenter point O_i of e, then connect O_i by straight-line segments to the edge midpoints M_j of e. These segments decompose each e into three subregions. With each vertex $x_p \in Z_h$, we associate the barycenter control volume $b_p \in B^h$ (see Fig. 1), which consists of the union of the subregions sharing the vertex x_p.

Associated with b_p, we define a constant finite element spaces by

$$V_B = \{w \in L^\infty(\Omega) : w|_{b_p} = constant, \ \forall b_p \in B^h\}.$$

We then introduce $I_h : C(\bar{\Omega}) \to V_B$ satisfying

$$I_h w(x) = \begin{cases} w(x_p), & \forall x \in b_p \in B^h, \\ 0, & \text{others}. \end{cases} \tag{2.8}$$

The interpolation operator I_h has the following properties [11,35,39].

Lemma 2.1. *Let $e \in T^h$, For any $\chi \in S_0^h$, we have*

$$\int_e (\chi - I_h \chi) dx = 0, \tag{2.9a}$$

$$\|\chi - I_h \chi\|_{0,q,e} \lesssim h_e |\chi|_{1,q,e}, \quad 1 \le q \le \infty. \tag{2.9b}$$

Now we formulate the finite volume method for the problems (1.2a)-(1.2b) as follows. For any vertex x_p, integrating (1.2a)-(1.2b) over the barycenter control volume b_p and using Green's formula, we obtain

$$\begin{cases} -\int_{\partial b_p}\frac{\partial\psi_1}{\partial n}ds+\int_{b_p}(V_1\psi_1-V_2\psi_2)dx=\int_{b_p}f_1dx, & \forall b_p\in B^h,\\ -\int_{\partial b_p}\frac{\partial\psi_2}{\partial n}ds+v\int_{b_p}(V_2\psi_1+V_1\psi_2)dx=\int_{b_p}f_2dx, & \forall b_p\in B^h,\end{cases} \tag{2.10}$$

where n denotes the unit outer-normal of the domain.

In order to decouple the problems (1.2a)-(1.2b), approximating (2.10), we get the standard finite volume scheme (see, e.g., [2]):

Find $\psi^h\in S_0^h\times S_0^h$ such that

$$\begin{cases} -\int_{\partial b_p}\frac{\partial\psi_1^h}{\partial n}ds+\int_{b_p}V_1I_h\psi_1^hdx-\int_{b_p}V_2I_h\psi_2^hdx=\int_{b_p}f_1dx, & \forall b_p\in B^h,\\ -\int_{\partial b_p}\frac{\partial\psi_2^h}{\partial n}ds+\int_{b_p}V_2I_h\psi_1^hdx+\int_{b_p}V_1I_h\psi_2^hdx=\int_{b_p}f_2dx, & \forall b_p\in B^h.\end{cases} \tag{2.11}$$

Namely,

$$\begin{cases} -\sum_{x_p\in Z_h}\int_{\partial b_p}\frac{\partial\psi_1^h}{\partial n}I_h\chi_1ds+\sum_{x_p\in Z_h}\int_{b_p}V_1I_h\psi_1^hI_h\chi_1dx-\sum_{x_p\in Z_h}\int_{b_p}V_2I_h\psi_2^hI_h\chi_1dx\\ \quad=\sum_{x_p\in Z_h}\int_{b_p}f_1I_h\chi_1dx, \quad \forall\chi_1\in S_0^h,\\ -\sum_{x_p\in Z_h}\int_{\partial b_p}\frac{\partial\psi_2^h}{\partial n}I_h\chi_2ds+\sum_{x_p\in Z_h}\int_{b_p}V_2I_h\psi_1^hI_h\chi_2dx+\sum_{x_p\in Z_h}\int_{b_p}V_1I_h\psi_2^hI_h\chi_2dx\\ \quad=\sum_{x_p\in Z_h}\int_{b_p}f_2I_h\chi_2dx, \quad \forall\chi_2\in S_0^h.\end{cases} \tag{2.12}$$

By the following lemma (cf. [2, Lemma 2.1]),

Lemma 2.2. *If matrix $\mathcal{A}=(a_{ij})_{2\times2}$ satisfies $a_{ij}\in V_B$, $(1\le i,j\le 2)$, then*

$$-\sum_{b_p\in B^h}\int_{\partial b_p}(\nabla w)^T\mathcal{A}nI_hv=\int_\Omega(\nabla w)^T\mathcal{A}\nabla v, \quad \forall w,v\in S_0^h, \tag{2.13}$$

we have

$$-\sum_{x_p\in Z_h}\int_{\partial b_p}\frac{\partial\psi_i^h}{\partial n}I_h\chi_ids=(\nabla\psi_i^h,\nabla\chi_i), \quad i=1,2. \tag{2.14}$$

So we get a finite volume scheme as follows:

Find $\psi^h \in S_0^h \times S_0^h$ such that

$$A_h(\psi^h,\chi) = (f,\chi)_h, \quad \forall \chi \in S_0^h \times S_0^h, \tag{2.15}$$

where

$$\begin{aligned} A_h(\psi,\chi) =: &(\nabla\psi_1,\nabla\chi_1) + (V_1 I_h\psi_1, I_h\chi_1) - (V_2 I_h\psi_2, I_h\chi_1) \\ &+ (\nabla\psi_2,\nabla\chi_2) + (V_2 I_h\psi_1, I_h\chi_2) + (V_1 I_h\psi_2, I_h\chi_2), \end{aligned} \tag{2.16a}$$

$$(f,\chi)_h =: (f, I_h\chi) =: (f_1, I_h\chi_1) + (f_2, I_h\chi_2). \tag{2.16b}$$

Next we introduce the norm as follows:

$$\|w\|_h =: (I_h w, I_h w)^{\frac{1}{2}}, \quad \forall w \in S_0^h \times S_0^h. \tag{2.17}$$

So we can get

Lemma 2.3. *The norm $\|w\|_h$ is equivalent to the norm $\|w\|$, namely*

$$\|w\|_h \lesssim \|w\| \lesssim \|w\|_h, \quad \forall w \in S_0^h \times S_0^h. \tag{2.18}$$

Following from (2.16a) and (2.18), we have

Lemma 2.4. *Assume that* (2.3)*, then $A_h(\cdot,\cdot)$, the bilinear form in* (2.16a)*, satisfies*

$$|A_h(\psi,\chi)| \lesssim \|\psi\|_1 \|\chi\|_1, \qquad \forall \psi,\chi \in S_0^h \times S_0^h, \tag{2.19a}$$

$$A_h(\psi,\psi) \gtrsim \|\psi\|_1^2, \qquad \forall \psi \in S_0^h \times S_0^h. \tag{2.19b}$$

Therefore, by the Lax-Milgram theorem and Lemma 2.4, the problems (1.2a)-(1.2b) havs a unique solution $\psi^h \in S_0^h \times S_0^h$.

Next, to describe error estimates for the finite volume scheme (2.15), we will give some useful lemmas. By Friedrich inequality, we have

Lemma 2.5 ([45])**.** *Let*

$$g_e =: \frac{1}{measure(e)} \int_e g dx,$$

if $\forall g \in W^{1,p}(e)$, then

$$\|g - g_e\|_{0,p,e} \lesssim h\|g\|_{1,p,e}, \quad 1 \le p \le \infty.$$

So, we can get

Lemma 2.6. *For any $\psi \in S_0^h \times S_0^h$, we have*

$$|(f,\psi - I_h\psi)| \lesssim h^2 \|f\|_{1,p} \|\psi\|_{1,q}, \quad \forall f \in (W^{1,p}(\Omega))^2, \tag{2.20}$$

where $\frac{1}{p} + \frac{1}{q} = 1$, $1 \le p,q \le \infty$.

Proof. Let

$$f_{i,e} =: \frac{1}{measure(e)} \int_e f_i dx, \quad i=1,2, \quad \forall e \in T^h,$$

from (2.9a), (2.9b), Lemma 2.5 and Hölder inequality, we obtain

$$\begin{aligned}
|(f,\psi - I_h\psi)| =& \Big| \sum_{e\in T^h} \int_e [f_1(\psi_1 - I_h\psi_1) + f_2(\psi_2 - I_h\psi_2)]dx \Big| \\
=& \Big| \sum_{e\in T^h} \int_e [(f_1 - f_{1,e})(\psi_1 - I_h\psi_1) + (f_2 - f_{2,e})(\psi_2 - I_h\psi_2)]dx \Big| \\
\lesssim & \sum_{e\in T^h} (\|f_1 - f_{1,e}\|_{0,p,e} \|\psi_1 - I_h\psi_1\|_{0,q,e} + \|f_2 - f_{2,e}\|_{0,p,e} \|\psi_2 - I_h\psi_2\|_{0,q,e}) \\
\lesssim & h \sum_{e\in T^h} (\|f_1 - f_{1,e}\|_{0,p,e} |\psi_1|_{1,q,e} + \|f_2 - f_{2,e}\|_{0,p,e} |\psi_2|_{1,q,e}) \\
\lesssim & h^2 (\|f_1\|_{1,p} |\psi_1|_{1,q} + \|f_2\|_{1,p} |\psi_2|_{1,q}) \\
\lesssim & h^2 \|f\|_{1,p} \|\psi\|_{1,q}.
\end{aligned}$$

Thus, we complete the proof. □

By the following lemma (cf. (3.10) in [2]),

Lemma 2.7. *For any $\alpha \in W^{1,\infty}$, $w,v \in S_0^h$, then holds*

$$|(\alpha I_h w, I_h v) - (\alpha w, v)| \lesssim h^2 \|w\|_{1,p} \|v\|_{1,q}, \tag{2.21}$$

where $\frac{1}{p} + \frac{1}{q} = 1$, $1 \le p,q \le \infty$.

We have

Lemma 2.8. *If $V \in (W^{1,\infty})^2$, then*

$$|A(\psi,\chi) - A_h(\psi,\chi)| \lesssim h^2 \|\psi\|_{1,p} \|\chi\|_{1,q}, \quad \forall \psi,\chi \in S_0^h \times S_0^h, \tag{2.22}$$

where $\frac{1}{p} + \frac{1}{q} = 1$, $1 \le p,q \le \infty$.

Proof. From (2.2a) and (2.16a), noticing that $V \in (W^{1,\infty})^2$, we have

$$\begin{aligned}
|A(\psi,\chi) - A_h(\psi,\chi)| \lesssim & |(V_1\psi_1,\chi_1) - (V_1 I_h w_1, I_h\chi_1)| + |(V_2\psi_2,\chi_1) - (V_2 I_h\psi_2, I_h\chi_1)| \\
& + |(V_1\psi_2,\chi_2) - (V_1 I_h\psi_2, I_h\chi_2)| + |(V_2\psi_1,\chi_2) - (V_2 I_h\psi_1, I_h\chi_2)|.
\end{aligned} \tag{2.23}$$

Therefore, (2.22) follow from (2.21) and (2.23). □

Lemma 2.9. *ψ^h, the finite volume solution defined in* (2.15)*, has the estimate:*

$$\|\psi^h\|_1 \lesssim \|f\|. \tag{2.24}$$

Proof. From (2.19b), (2.15) and (2.18), we have

$$\begin{aligned}\|\psi^h\|_1^2 \lesssim & A_h(\psi^h,\psi^h) = (f,\psi^h)_h \\ \leq & \|f\|\|I_h\psi^h\| \lesssim \|f\|\|\psi^h\|.\end{aligned}$$

Therefore, (2.24) holds. □

Lemma 2.10. *If* $V \in (W^{1,\infty})^2$, $f \in (H^1)^2$, ψ_h, *the finite element solution defined in* (2.6), *and* ψ^h, *the finite volume solution defined in* (2.15), *have the estimates:*

$$|A(\psi^h - \psi_h,\chi)| \lesssim h^2 \|f\|_1 \|\chi\|_1, \quad \forall \chi \in S_0^h \times S_0^h, \tag{2.25a}$$

$$\|\psi_h - \psi^h\|_1 \lesssim h^2 \|f\|_1. \tag{2.25b}$$

Proof. From (2.6) and (2.15), we have

$$\begin{aligned}|A(\psi^h - \psi_h,\chi)| &= |A(\psi^h,\chi) - A(\psi_h,\chi)| = |A(\psi^h,\chi) - (f,\chi)| \\ &= |A(\psi^h,\chi) - A_h(\psi^h,\chi) + (f,\chi)_h - (f,\chi)| \\ &\lesssim |A(\psi^h,\chi) - A_h(\psi^h,\chi)| + |(f,\chi)_h - (f,\chi)|.\end{aligned} \tag{2.26}$$

Noticing (2.16b), (2.20), (2.22) and (2.24), where $p = q = 2$, from (2.26), we have

$$\begin{aligned}|A(\psi^h - \psi_h,\chi)| &\lesssim h^2 \|\psi^h\|_{1,p} \|\chi\|_{1,q} + h^2 \|f\|_{1,p} \|\chi\|_{1,q} \\ &\lesssim h^2 \|f\|_1 \|\chi\|_1.\end{aligned} \tag{2.27}$$

Therefore, (2.25a) holds. Furthermore, let $\chi = \psi^h - \psi_h$ in (2.25a), noticing (4.1), we obtain (2.25b). □

Theorem 2.1. *Assume that*

$$V \in (W^{1,\infty})^2, \quad f \in (H^1)^2 \quad \textit{and} \quad V_1 \geq 0 \quad \textit{in} \ \ \Omega.$$

Then ψ^h, *the finite volume approximation of* ψ, *has the error estimate:*

$$\|\psi - \psi^h\|_s \lesssim h^{2-s} \|f\|_1, \quad s = 0,1. \tag{2.28}$$

Proof. From (2.7), (2.25b) and (2.4), we obtain

$$\begin{aligned}\|\psi - \psi^h\|_s &\leq \|\psi - \psi_h\|_s + \|\psi_h - \psi^h\|_1 \lesssim h^{2-s} \|\psi\|_2 + h^2 \|f\|_1 \\ &\lesssim h^{2-s}(\|f\| + \|f\|_1) \lesssim h^{2-s} \|f\|_1, \quad s = 0,1.\end{aligned} \tag{2.29}$$

We complete the proof. □

3 The two-grid finite volume schemes

In this section, following the idea of decoupling in [1], we construct the two-grid finite volume algorithms for problem (1.1a)-(1.1b). The basic mechanisms in our approach is another finite element space $S_0^H\times S_0^H(\subset S_0^h\times S_0^h)$ defined on a coarser quasi-uniform triangulations of Ω with mesh size $H>h>0$.

Set the bilinear forms

$$\hat{A}_h(\psi,\chi)=:\int_\Omega \nabla\psi_1\cdot\nabla\chi_1 dx+(V_1 I_h\psi_1,I_h\chi_1)+\int_\Omega \nabla\psi_2\cdot\nabla\chi_2 dx+(V_1 I_h\psi_2,I_h\chi_2), \tag{3.1a}$$

$$N_h(\psi,\chi)=:(V_2\psi_1,I_h\chi_2)-(V_2\psi_2,I_h\chi_1). \tag{3.1b}$$

Algorithm 3.1.

Step 1. Find $\psi^H\in S_0^H\times S_0^H$ such that

$$A_H(\psi^H,\chi_H)=(f,\chi_H),\quad \forall\chi_H\in S_0^H\times S_0^H.$$

Step 2. Find $\psi_v^h\in S_0^h\times S_0^h$, such that

$$\hat{A}_h(\psi_v^h,\chi_h)+N_H(\psi^H,\chi_h)=(f,\chi_h)_h,\quad \forall\chi_h\in S_0^h\times S_0^h. \tag{3.2}$$

Theorem 3.1. *If $V\in(W^{1,\infty})^2$, $V_1\ge 0$, $f\in(H^1)^2$, then ψ_v^h, the two-grid finite volume solution defined in Algorithm* 3.1, *has the following error estimates:*

$$\|\psi^h-\psi_v^h\|_1\lesssim(h+H^2)\|f\|_1. \tag{3.3}$$

Consequently,

$$\|\psi-\psi_v^h\|_1\lesssim(h+H^2)\|f\|_1.$$

Proof. From (2.15) and (3.2), we have

$$A_h(\psi^h-\psi_v^h,\chi)=(V_2 I_h\psi_1^h-V_2\psi_1^H,I_h\chi_2)-(V_2 I_h\psi_2^h-V_2\psi_2^H,I_h\chi_1),\quad \forall\chi\in S_0^h\times S_0^h, \tag{3.4}$$

Noticing (2.3), (2.18), (2.9b), (2.24) and (2.28), We obtain

$$\begin{aligned}
&|(V_2 I_h\psi_2^h-V_2\psi_2^H,I_h\chi_1)|\\
\le&|(V_2 I_h\psi_2^h-V_2\psi_2^h,I_h\chi_1)|+|(V_2\psi_2^h-V_2\psi_2^H,I_h\chi_1)|\\
\le&(\|V_2(I_h\psi_2^h-\psi_2^h)\|+\|V_2(\psi_2^h-\psi_2^H)\|)\|I_h\chi\|\\
\le&(\|I_h\psi_2^h-\psi_2^h\|+\|\psi_2^h-\psi_2^H\|)\|\chi\|\|V_2\|_{0,\infty}\\
\lesssim&[h|\psi_2^h|_1+\|\psi_2-\psi_2^h\|+\|\psi_2-\psi_2^H\|]\|\chi\|\|V\|_{0,\infty}\\
\lesssim&[h\|f\|_0+\|\psi_2-\psi_2^h\|+\|\psi_2-\psi_2^H\|]\|\chi\|\\
\lesssim&(h+H^2)\|f\|_1\|\chi\|.
\end{aligned} \tag{3.5}$$

Following the idea of (3.5), it holds

$$|(V_2 I_h \psi_1^h - V_2 \psi_1^H, I_h \chi_2)| \lesssim (h+H^2)\|f\|_1 \|\chi\|. \tag{3.6}$$

We can easily check that

$$\hat{A}_h(w,w) \gtrsim \|w\|_1^2, \quad \forall w \in S_0^h \times S_0^h. \tag{3.7}$$

Taking $\chi = \psi^h - \psi_v^h$ in (3.4), from (3.5), (3.6) and (3.7), we obtain

$$\begin{aligned}\|\psi^h - \psi_v^h\|_1^2 \lesssim & |A_h(\psi^h - \psi_v^h, \psi^h - \psi_v^h)| \\ \lesssim & (h+H^2)\|f\|_1 \|\psi^h - \psi_v^h\|,\end{aligned}$$

Thus (3.3) holds.

From (2.28) and (3.3), it holds

$$\begin{aligned}\|\psi - \psi_v^h\|_1 \leq & \|\psi - \psi^h\|_1 + \|\psi^h - \psi_v^h\|_1 \\ \lesssim & h\|f\|_1 + (h+H^2)\|f\|_1 \\ \lesssim & (h+H^2)\|f\|_1.\end{aligned}$$

So, we complete the proof. □

Next, by slightly simplifying the coefficient matrix of the system in Step 2, we can get an alternative of Algorithm 3.2. Let the bilinear forms

$$\tilde{A}(\psi,\chi) =: \int_\Omega \nabla\psi_1 \cdot \nabla\chi_1 dx + \int_\Omega \nabla\psi_2 \cdot \nabla\chi_2 dx, \tag{3.8a}$$

$$\tilde{N}_h(\psi,\chi) =: (V_1\psi_1 - V_2\psi_2, I_h\chi_1) + (V_1\psi_2 + V_2\psi_1, I_h\chi_2). \tag{3.8b}$$

Algorithm 3.2.

Step 1. Find $\psi^H \in S_0^H \times S_0^H$ such that

$$A_H(\psi^H, \chi_H) = (f, \chi_H), \quad \forall \chi_H \in S_0^H \times S_0^H.$$

Step 2. Find $\psi_{v,*}^h \in S_0^h \times S_0^h$, such that

$$\tilde{A}_h(\psi_{v,*}^h, \chi_h) + \tilde{N}_H(\psi^H, \chi_h) = (f, \chi_h)_h, \quad \forall \chi_h \in S_0^h \times S_0^h. \tag{3.9}$$

Theorem 3.2. *If $V \in (W^{1,\infty})^2$, $V_1 \geq 0$, $f \in (H^1)^2$, then $\psi_{v,*}^h$, the two-grid finite volume solution defined in Algorithm 3.2, has the following error estimates:*

$$\|\psi^h - \psi_{v,*}^h\|_1 \lesssim (h+H^2)\|f\|_1. \tag{3.10}$$

Consequently,

$$\|\psi - \psi_{v,*}^h\|_1 \lesssim (h+H^2)\|f\|_1. \tag{3.11}$$

Proof. From (2.15) and (3.9), we can obtain

$$\begin{aligned}\tilde{A}(\psi^h-\psi^h_{v,*},\chi)=&-(V_2I_h\psi^h_2-V_2\psi^H_2,I_h\chi_1)+(V_1I_h\psi^h_1-V_1\psi^H_1,I_h\chi_1)\\&+(V_2I_h\psi^h_1-V_2\psi^H_1,I_h\chi_2)+(V_1I_h\psi^h_2-V_1\psi^H_2,I_h\chi_2),\quad \forall\chi\in S^h_0\times S^h_0, \end{aligned}\tag{3.12}$$

we can easily check that

$$\tilde{A}(w,w)\gtrsim\|w\|^2_1,\quad \forall w\in S^h_0\times S^h_0. \tag{3.13}$$

Taking $\chi=\psi^h-\psi^h_{v,*}$ in (3.12), and right-hand sides following the idea of (3.5), noticing (3.13), we can get

$$\begin{aligned}\|\psi^h-\psi^h_{v,*}\|^2_1\lesssim&|\tilde{A}(\psi^h-\psi^h_{v,*},\psi^h-\psi^h_{v,*})|\\ \lesssim&(h+H^2)\|f\|_1\|\psi^h-\psi^h_{v,*}\|,\end{aligned}\tag{3.14}$$

which implies that (3.10) holds. Furthermore, from (2.28) and (3.10), we get

$$\begin{aligned}\|\psi-\psi^h_{v,*}\|_1\le&\|\psi-\psi^h\|_1+\|\psi^h-\psi^h_{v,*}\|_1\\ \lesssim&h\|f\|_1+(h+H^2)\|f\|_1\\ \lesssim&(h+H^2)\|f\|_1.\end{aligned}$$

Thus, we complete the proof. □

4 Numerical example

In this section, we carry out the numerical examples to demonstrate the efficiency of our algorithms.

Example 4.1. For problem (1.1a)-(1.1b), let

$$V=1+i\quad\text{and}\quad V=\frac{1}{2}(x_1^2+x_2^2)+i\frac{1}{2}(x_1^2+x_2^2),$$

respectively, $\Omega=[0,1]\times[0,1]$, and f be so chosen that

$$\psi=(1-x_1)(1-x_2)\sin(x_1x_2)+i(1-x_1)x_2\sin[x_1(1-x_2)]$$

is the exact solution.

Here Ω is uniformly divided into families T_H and T_h of triangulations, and S^H_0, $S^h_0\subset H^1_0$ are linear finite element spaces defined on T_H,T_h respectively. We construct barycenter dual meshes B^h and B^H based upon T^h and T^H respectively. For $h=H^2$ and $H=1/4,1/8,1/16,1/32$, ψ^h_v and $\psi^h_{v,*}$ are computed by Algorithm 3.1 and Algorithm 3.2, respectively. Also ψ^h, the standard finite volume solution, and ψ^T_h, two-grid fine element

Table 1: Errors and CPU time of ψ_v^h and ψ^h, $V=1+i$.

mesh(h)	$\|\psi-\psi_v^h\|_1$	r	cpu(s)	$\|\psi-\psi^h\|_1$	r	cpu(s)
1/16	3.247E-2		0.22	3.244E-2		0.53
1/64	8.148E-3	3.989	3.05	8.141E-3	3.985	7.63
1/256	2.038E-3	3.998	54.37	2.036 E-3	3.998	123.72
1/1024	5.094E-4	4.000	1837.56	5.090 E-4	4.000	3331.99

Table 2: Errors and CPU time of ψ_v^h and ψ_h^T, $V=\frac{1}{2}(x_1^2+x_2^2)+i\frac{1}{2}(x_1^2+x_2^2)$.

mesh(h)	$\|\psi-\psi_v^h\|_1$	r	cpu(s)	$\|\psi-\psi_h^T\|_1$	r	cpu(s)
1/16	3.245E-2		0.26	3.244E-2		0.29
1/64	8.143E-3	3.985	4.20	8.142E-3	3.984	0.78
1/256	2.037E-3	3.998	59.64	2.036E-3	3.999	30.25
1/1024	5.114E-4	3.983	1463.55	5.090E-4	4.000	3845.05

Table 3: Errors and CPU time of $\psi_{v,*}^h$ and ψ_h^T, $V=1+i$.

mesh(h)	$\|\psi-\psi_{v,*}^h\|_1$	r	cpu(s)	$\|\psi-\psi_h^T\|_1$	r	cpu(s)
1/16	3.254E-2		0.21	3.253E-2		0.26
1/64	8.159E-3	3.988	3.84	8.162E-3	3.986	0.74
1/256	2.040E-3	4.000	55.35	2.041 E-3	3.999	30.28
1/1024	5.099E-4	4.001	1458.30	5.102 E-4	4.000	3910.43

Table 4: Errors and CPU time of $\psi_{v,*}^h$ and ψ^h, $V=\frac{1}{2}(x_1^2+x_2^2)+i\frac{1}{2}(x_1^2+x_2^2)$.

mesh(h)	$\|\psi-\psi_{v,*}^h\|_1$	r	cpu(s)	$\|\psi-\psi^h\|_1$	r	cpu(s)
1/16	3.246E-2		0.17	3.244E-2		0.19
1/64	8.144E-3	3.986	2.73	8.141E-3	3.985	2.84
1/256	2.036E-3	4.000	50.95	2.036E-3	4.999	64.292
1/1024	5.091E-4	3.999	1503.67	5.090E-4	4.000	3259.72

solution, are computed by (2.15) and Algorithm A1 in [1] respectively. From the numerical results from Table 1 to Table 4, we can see that

$$\|\psi-\psi_v^h\|_1 \approx \mathcal{O}(H^2)(\approx \mathcal{O}(h)) \quad \text{and} \quad \|\psi-\psi_{v,*}^h\|_1 \approx \mathcal{O}(H^2)(\approx \mathcal{O}(h)),$$

which coincide with the theoretical results obtained in Theorem 3.1 and Theorem 3.2, respectively. And, on running CPU time, we find that our two-grid finite volume methods are much more efficient than the standard finite volume method and the two-grid finite element method, when the calculation scale is too high.

5 Conclusions

In this paper, we constructed and analyzed two-grid finite volume schemes for the steady-state Schrödinger equation. The discretization schemes of the coupled equations on a fine grid are reduced to the finite volume schemes of the original equations on a much coarser grid together with the approximated discretization schemes of the decoupled equations on a finer grid. Both theoretical analysis and numerical examples show that our schemes work efficiently and can reach the optimal accuracy in H^1-norm.

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