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UNIFORM IN TIME ERROR ANALYSIS OF HDG APPROXIMATION FOR SCHRÖDINGER EQUATION BASED ON HDG PROJECTION

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Abstract. This paper presents error analysis of hybridizable discontinuous Galerkin (HDG) time-domain method for solving time dependent Schrödinger equations. The numerical trace and numerical flux are constructed to preserve the conservative property for the density of the particle described. We prove that there exist the superconvergence properties of the HDG method, which do hold for second-order elliptic problems, uniformly in time for the semidiscretization by the same method of Schrödinger equations provided that enough regularity is satisfied. Thus, if the approximations are piecewise polynomials of degree r, the approximations to the wave function and the flux converge with order $r+1$. The suitably chosen projection of the wave function into a space of lower polynomial degree superconverges with order $r+2$ for $r \geq 1$ uniformly in time. The application of element-by-element postprocessing of the approximate solution which provides an approximation of the potential convergence with order $r+2$ for $r \geq 1$ in L^2 is also uniformly in time.

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1. Introduction

In this paper, we propose a new semidiscretization by hybridizable discontinuous Galerkin (HDG) method for the following time dependent Schrödinger equation

$$\begin{cases} \frac{\partial u}{\partial t} - i\Delta u = f & t > 0, x \in \Omega \subset R^d, \\ u|_{\partial\Omega} = g & t > 0, \\ u|_{t=0} = u_0(x) & x \in \Omega \subset R^d. \end{cases} \tag{1.1}$$

Keywords and phrases: HDG, error estimate, superconvergence, Schrödinger equations.

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In order to define a HDG method for the time dependent Schrödinger equation (1.1), we introduce an auxiliary flux variable and rewrite it in terms of a system of first order partial differential equations

$$\begin{cases} -\nabla u = \boldsymbol{q} & x \in \Omega \subset R^d, \\ \frac{\partial u}{\partial t} + i\nabla \cdot \boldsymbol{q} = f & t > 0, x \in \Omega \subset R^d, \\ u|_{\partial\Omega} = g & t > 0, \\ u|_{t=0} = u_0(x) & x \in \Omega \subset R^d, \end{cases} \tag{1.2}$$

where $i = \sqrt{-1}$, $u(x,t)$ is a complex unknown density function defined in $\Omega \times [0,T]$ and Ω is bounded and convex (or smooth). The Schrödinger equation above may describe many physical phenomena in optics and mechanics.

In [20, 33], the authors propose the traditional analytical methods of Schrödinger equations by using plane wave analysis and perturbation technique, but only handle simple planner structures or weak perturbations. However, recently numerical methods of the time dependent Schrödinger equation provide an efficient and flexible alternative choice to study quantum structures from the simple model to the complicated geometric configurations such as quantum wells. Up to date a lot of numerical approximations have been investigated extensively to the development of efficient methods for the Schrödinger equation, including the finite difference methods [3, 19, 23], the finite element methods [1, 2, 22, 29], the DG methods [13] and for others [7, 21]. In the light of a fully discrete scheme presented by Jin and Wu [22] and Wang [34], Crank–Nicolson methods are employed for time discretization and the different finite element methods are employed for the spatial discretization for the Schrödinger equation. It turns out that the schemes are unconditionally stable and their convergence have the optimal orders, but they are implicit. In [2], Antoine *et al.* introduced some proper non-reflecting boundary conditions or absorbing boundary conditions for the linear Schrödinger equations, constructed the fully discrete schemes by applying the Crank–Nicolson scheme in time and Galerkin finite element approximations in space for the resulting initial-boundary value problems. In [13], Dong *et al.* developed and analyzed a discontinuous Galerkin (DG) method for one-dimensional stationary Schrödinger equations with open boundary conditions which had highly oscillating solutions and proved that the DG approximation converges optimally with respect to the mesh size h in L^2 norm.

In this paper, we introduce and analyze a hybridizable DG methods proposed in [8, 10] for the linear non-stationary Schrödinger equation. An important property of the resulting numerical method is the conservation for the probability density of the particles. Our method follows closely with the discontinuous Galerkin methods proposed in [5] for the heat equation [25], for the time-harmonic Maxwell equations [16, 27], for the convection diffusion equation and [28] for the incompressible Navier–Stokes equations, but is different from the DG/LDG method in [13, 15, 24]. We propose a local discontinuous Galerkin-hybridizable method. When applied to the second order elliptic equation, this method uses polynomials of degree $r \geq 0$ to approximate u and each component of the flux $\boldsymbol{q} = -\nabla u$. Some analysis of the HDG methods were proposed [8, 12] which is based on the use of suitably chosen projections. In these papers, it showed that the HDG methods have the same convergence properties as the Raviart–Thomas (RT) methods [30]. It showed that the postprocessing could be computed and converged to u with order $r+2$ for $r \geq 1$ and that the approximation to $\boldsymbol{q}$ converges with order $r+1$ for $r \geq 1$ in all of the above mentioned papers. In this paper, we will prove that these results also hold in our setting uniformly in time provided that the exact solution is smooth enough.

There are some similarities between our method and those in [5, 6, 14]. The convergence or superconvergence results for HDG methods for elliptic problems obtained in [8] and heat equations obtained in [5] were extended them to the semidiscrete HDG methods. Here we extend to our Schrödinger problems the convergence or superconvergence results for the discretization by HDG methods of second-order elliptic problems [2, 7, 29]. Moreover, we also use energy techniques and parabolic duality arguments. The energy techniques are very well known and can be found in many literatures. The duality technique of evolution equations was also used in [5]. Here, we use a variation of the duality arguments used in many literature. It is based on an estimate of the

$L^1(0,T;L^2(\Omega))$-norm of the solution of the dual problem and incorporates the fact that the projection of the error we are trying to estimate lies in a finite dimensional space.

The organization of this paper is the following. In Section 2, we state and discuss our main results for the HDG method under consideration. Their proofs are displayed in detail in Section 3. In Section 4, some conclusions are summarized.

2. Main results

2.1. HDG method

In order to represent our results, we need to introduce the HDG methods which are constructed by Cockburn *et al.* [8–11, 26]. To do that, let us introduce some notation. We denote by $\Omega_h = \{K\}$ a triangulation of the domain Ω, which are shape-regular simplexes K, and define the following three boundary sets associated to this triangulation: firstly, the set of faces of all the elements $\Gamma_h = \{\partial K : K \in \Omega_h\}$, secondly, the set of interior faces Γ_h^i, and lastly, the set of boundary faces Γ_h^∂. We say that $F \in \Gamma_h^i$ if there are two simplexes K_1 and K_2 in Ω_h such that $F = \partial K_1 \bigcap \partial K_2$, and we say that $F \in \Gamma_h^\partial$ if there are the simplex K in Ω_h such that $F = \partial K \bigcap \partial\Omega$. It is obvious that $\Gamma_h = \Gamma_h^\partial \bigcup \Gamma_h^i$.

For each time t on the interval $[0,T]$, the method yields a scalar approximation $u_h(t)$ to the wave function $u(t)$, a vector approximation $\boldsymbol{q}_h(t)$ to the flux $\boldsymbol{q}(t)$, and a scalar approximation $\hat{u}_h(t)$ to the trace of $u(t)$ on element boundaries. The hybridized Galerkin methods seek an approximation $(\boldsymbol{q}_h, u_h, \lambda_h)$ to the exact solution $(\boldsymbol{q}(t)|_\Omega, u(t)|_\Omega, u(t)|_{\Gamma_h\setminus\partial\Omega})$ in a finite-dimensional space $\boldsymbol{V}_h \times W_h \times M_h$ of the form

$$\begin{aligned}
\boldsymbol{V}_h &= \{\boldsymbol{v} \in L^2(\Omega) : \boldsymbol{v}|_K \in \boldsymbol{V}(K), \forall K \in \Omega_h\},\\
W_h &= \{w \in L^2(\Omega) : w|_K \in W(K), \forall K \in \Omega_h\},\\
M_h &= \{m \in L^2(\partial\Gamma_h) : m|_F \in M(e), \forall F \in \Gamma_h\},
\end{aligned}$$

respectively, where

$$W(K) = \mathscr{P}_r(K), \quad \boldsymbol{V}(K) = \boldsymbol{P}_r(K), \quad M(F) = \mathscr{P}_r(F).$$

Here $\mathscr{P}_r(K)$ is the space of polynomials of total degree at most r and $\boldsymbol{P}_r(K) = [\mathscr{P}_r(K)]^d$.

The weak formulation of a HDG method for equations (1.2) is to find an approximation $(\boldsymbol{q}_h, u_h, \lambda_h)$ in the finite element space $\boldsymbol{V}_h \times W_h \times M_h$ such that

$$(\boldsymbol{v}, \boldsymbol{q}_h)_{\Omega_h} - (\nabla\cdot\boldsymbol{v}, u_h)_{\Omega_h} + \langle \boldsymbol{v}\cdot\boldsymbol{n}, \hat{u}_h\rangle_{\Gamma_h} = 0, \tag{2.1a}$$

$$\left(\frac{\partial u_h}{\partial t}, w\right)_{\Omega_h} - i(\boldsymbol{q}_h, \nabla w)_{\Omega_h} + i\langle \hat{\boldsymbol{q}}_h\cdot\boldsymbol{n}, w\rangle_{\Gamma_h} = (f, w)_{\Omega_h}, \tag{2.1b}$$

$$\langle \hat{u}_h, \nu\rangle_{\Gamma_h^\partial} = \langle g, \nu\rangle_{\Gamma_h^\partial}, \tag{2.1c}$$

$$\langle \hat{\boldsymbol{q}}_h\cdot\boldsymbol{n}, \nu\rangle_{\Gamma_h\setminus\Gamma_h^\partial} = 0, \tag{2.1d}$$

$$u_h|_{t=0} = \Pi_W^H u_0, \tag{2.1e}$$

hold for all test functions $\boldsymbol{v} \in \boldsymbol{V}_h, w \in W_h$, and $\nu \in M_h$, with a numerical trace for the flux defined by

$$\hat{u}_h = \begin{cases} P_\partial g & \text{on } \Gamma_h^\partial,\\ \lambda_h & \text{on } \Gamma_h\setminus\Gamma_h^\partial, \end{cases} \tag{2.2}$$

where P_∂ denotes an L^2-projection defined as follows: $P_\partial : L^2(\Gamma_h) \to M_h$ and Π_W^H is the HDG projection which is defined in Section 2.3. Given a function $\xi \in L^2(\Gamma_h)$, and an arbitrary simplex $F \in \Gamma_h$, the restriction of $P_\partial\xi$

to a face F of K is defined as the element of $\mathscr{P}_r(F)$ that satisfies

$$\langle P_\partial\ \xi - \xi, \mu\rangle_F = 0, \quad \forall \mu \in \mathscr{P}_r(F). \tag{2.3}$$

However, the numerical traces $\hat{\boldsymbol{q}}_h$ is assumed to be the following simple form:

$$\hat{\boldsymbol{q}}_h = \boldsymbol{q}_h + \tau(u_h - \hat{u}_h)\cdot \boldsymbol{n} \quad \text{on } \Gamma_h, \tag{2.4}$$

where τ is the stable parameter which is related with the projections.

Above and through, we use the notation

$$(u,w)_{\Omega_h} = \sum_{K\in\Omega_h}(u,w)_K, \quad \langle u,w\rangle_{\Gamma_h} = \sum_{K\in\Omega_h}\langle u,w\rangle_{\partial K},$$

where

$$(u,w)_K = \int_K u\bar{w}\mathrm{d}x, \qquad \forall K \in R^d,$$
$$\langle u,w\rangle_{\partial K} = \int_{\partial K} u\bar{w}\mathrm{d}s, \quad \forall \partial K \in R^{d-1}.$$

Here $\bar{w}$ is the complex conjugate of w and $\boldsymbol{n}$ is the unit outward normal vector. Besides, for vector functions $\boldsymbol{q}$ and $\boldsymbol{v}$, the notations are similarly defined with the integrand being the vector inner-product $\boldsymbol{q}\cdot\boldsymbol{v}$. This completes the definition of the method.

2.2. The conservation of semi-discrete HDG

In this subsection, we provide the conservative result of HDG. We define the probability density and the current density for the continuous problem (1.1) or (1.2). We introduce them in case of one dimension. Consider a single electron whose probability density is given by

$$p(x,t) = u\cdot\bar{u},$$

and whose probability current density is given by

$$I(x,t) = -i\left(u\cdot\frac{\partial\bar{u}}{\partial x} - \bar{u}\cdot\frac{\partial u}{\partial x}\right).$$

If u is the solution of the problem (1.1), then probability density p and current density I satisfy the following continuity equation:

$$\frac{\partial p}{\partial t} - \frac{\partial I}{\partial x} = 0.$$

Similarly, we define the probability density and the current density for HDG (2.1) by the following form:

$$p_h(x,t) = u_h\cdot\bar{u}_h,$$

and

$$I_h(x,t) = -i\left(u_h\cdot\frac{\partial\bar{u}_h}{\partial x} - \bar{u}_h\cdot\frac{\partial u_h}{\partial x}\right).$$

Theorem 2.1. *Let u_h be the solution of the problem (2.1) and p_h is the probability density. Then HDG is conservative,* i.e.,

$$\frac{\partial}{\partial t}\int_{\Omega_h} p_h \mathrm{d}x = 0.$$

2.3. Projections

In this subsection we introduce the HDG projection, which plays an important role in our error analysis. **The HDG projection**: The projection $(\boldsymbol{\Pi}_V^H, \Pi_W^H) : \boldsymbol{H}^1(\Omega_h)\times H^1(\Omega_h) \to \boldsymbol{V}_h \times W_h$. Given a vector value function $(\boldsymbol{\phi}, \zeta) \in \boldsymbol{H}^1(\Omega_h)\times H^1(\Omega_h)$ and an arbitrary simplex $K \in \Omega_h$, the restrict of projection value $(\boldsymbol{\Pi}_V^H\boldsymbol{\phi}, \Pi_W^H\ \zeta)$ to K is defined on the element of $(\mathscr{P}^r(K))^d \times \mathscr{P}^r(K)$ that satisfies

$$(\boldsymbol{\Pi}_V^H\boldsymbol{\phi} - \boldsymbol{\phi}, \boldsymbol{v})_K = 0, \qquad \forall \boldsymbol{v} \in (\mathscr{P}^{r-1}(K))^d,\ r \geq 1, \tag{2.5a}$$

$$(\Pi_W^H\ \zeta - \zeta, w)_K = 0, \qquad \forall w \in \mathscr{P}^{r-1}(K),\ r \geq 1, \tag{2.5b}$$

$$\langle \boldsymbol{\Pi}_V^H\boldsymbol{\phi}\cdot\boldsymbol{n} + \tau\Pi_W^H\ \zeta, \mu\rangle_F = \langle \boldsymbol{\phi}\cdot\boldsymbol{n} + \tau\zeta, \mu\rangle_F, \qquad \forall \mu \in \mathscr{P}^r(F), F \in \partial K. \tag{2.5c}$$

$(\boldsymbol{\Pi}_V^H, \Pi_W^H)$ is called the HDG projection which has the following approximation results, see [18].

Proposition 2.2. *Suppose $r \geq 0$, $\tau|_{\partial K}$ is nonnegative and $\tau_K^{\max} := \max\ \tau|_{\partial K} \geq 0$. Then the system (2.5) is uniquely solvable for $(\boldsymbol{\Pi}_V^H\boldsymbol{q}, \Pi_W^H u)$. Furthermore, there is a constant C independent of K and τ such that*

$$\|\boldsymbol{\Pi}_V^H\boldsymbol{q} - \boldsymbol{q}\|_K \leq Ch_K^{l_q+1}|\boldsymbol{q}|_{\boldsymbol{H}^{l_q+1}(K)} + Ch_K^{l_u+1}\tau_K^*|u|_{H^{l_u+1}(K)}, \tag{2.6a}$$

$$\|\Pi_W^H u - u\|_K \leq C\frac{h_K^{l_q+1}}{\tau_K^{\max}}|\nabla\cdot\boldsymbol{q}|_{\boldsymbol{H}^{l_q}(K)} + Ch_K^{l_u+1}|u|_{H^{l_u+1}(K)}, \tag{2.6b}$$

for l_u, l_q in $[0, r]$. Here $\tau_K^* = \max\{\tau|_{\partial K\setminus F^*}\}$, where F^* is a face of K at which $\tau|_{\partial K}$ is maximum.

To discuss the error analysis and present error estimates, we use some norms. We denote the norm and seminorm on any Sobolev space by $\|\cdot\|_D$ and $|\cdot|_D$, respectively. We set

$$\|(\boldsymbol{q}, u)\|_{a,T,\Omega} = \|\boldsymbol{q}\|_{L^2(L^2)} + \|u_t\|_{L^1(L^2)}, \quad \|(\boldsymbol{q}, u)\|_{b,T,\Omega} := \|\boldsymbol{q}(0)\|_{L^2} + \|\boldsymbol{q}_t\|_{L^1(L^2)} + \|u_t\|_{L^2(L^2)}.$$

We are now ready to state our main results.

Theorem 2.3. *Assume that the exact solution $(u, \boldsymbol{q})$ of (1.2) is in the space $H^{r+1}(\Omega_h)\times\boldsymbol{H}^{r+1}(\Omega_h)$. For any $T > 0$ and any $r \geq 0$, we have*

$$\|u - u_h\|_{L^\infty(L^2(\Omega_h))} \leq C(\|u - \Pi_W^H u\|_{L^\infty(L^2(\Omega_h))} + \|(\boldsymbol{q} - \boldsymbol{\Pi}_V^H\boldsymbol{q}, u - \Pi_W^H u)\|_{a,T,\Omega}),$$

$$\|\boldsymbol{q} - \boldsymbol{q}_h\|_{L^\infty(L^2(\Omega_h))} \leq C(\|u - \Pi_W^H u\|_{L^\infty(L^2(\Omega_h))} + \|(\boldsymbol{q} - \boldsymbol{\Pi}_V^H\boldsymbol{q}, u - \Pi_W^H u)\|_{b,T,\Omega}),$$

$$\|\hat{u}_h - u_h + \Pi_W^H u - P_\partial u\|_{L^\infty(L^2(\Gamma_h))} \leq C(\|u - \Pi_W^H u\|_{L^\infty(L^2(\Omega_h))} + \|(\boldsymbol{q} - \boldsymbol{\Pi}_V^H\boldsymbol{q}, u - \Pi_W^H u)\|_{b,T,\Omega}).$$

Theorem 2.4. *Assume that the exact solution $(u, \boldsymbol{q})$ of (1.2) is in the space $H^{r+1}(\Omega_h)\times\boldsymbol{H}^{r+1}(\Omega_h)$, and the domain Ω is a convex polyhedral domain of R^d such that $\forall\psi \in H_0^1(\Omega)\cap H^2(\Omega)$, the elliptic regularity inequality*

$$\|\psi\|_{H^2(\Omega)} \leq C\|\Delta\psi\|_{L^2(\Omega)}.$$

For any $T > 0$ and any $r \geq 1$, we have

$$\|P_{r-1}(\Pi_W^H u - u_h)\|_{L^\infty(L^2(\Omega_h))} \leq Ch\Big(\|u - \Pi_W^H u\|_{L^\infty(L^2(\Omega_h))} + \|(\boldsymbol{q} - \boldsymbol{\Pi}_V^H \boldsymbol{q}, u - \Pi_W^H u)\|_{a,T,\Omega} + \|(\boldsymbol{q} - \boldsymbol{\Pi}_V^H \boldsymbol{q}, u - \Pi_W^H u)\|_{b,T,\Omega}\Big).$$

2.4. Postprocessing

Finally, as done in [8], we finish this section by showing how to discover the superconvergence results to postprocess u_h to get a better approximation to u defined as follows. Here, we present the postprocessing method.

The method: way of getting a good gradient: Since $\boldsymbol{q} = -\nabla u$, we can use the approximation $\boldsymbol{q}_h$ as a way of getting an improved gradient. We follow [17, 31, 33], using the L^2 projection of u_h to determine the L^2 projection of the postprocessed in the space $\mathscr{P}_{r-1}(K)$, we find

$$u_h^* \in \Pi_{K\in\mathcal{T}_h}\mathscr{P}_{r+1}(K),$$

satisfying for all $K \in \mathcal{T}_h$

$$\begin{aligned} (u_h^*, w)_K &= (u_h, w)_K \qquad &&\forall w \in \mathscr{P}_{r-1}(K), \\ (\nabla u_h^*, \nabla w)_K &= (\boldsymbol{q}_h, w)_K \qquad &&\forall w \in \mathscr{P}_{r-1}^{\perp}(K), \end{aligned} \tag{2.7}$$

where $\mathscr{P}_{r-1}^{\perp}(K)$ denote the L^2 orthogonal complement of $\mathscr{P}_{r-1}(K)$ in $\mathscr{P}_{r+1}(K)$.

Theorem 2.5. *Assume that all conditions in Theorem 2.4 hold. Then for any $r \geq 0$, we have*

$$\|u - u_h^*\|_{L^\infty(L^2(\Omega_h))} \leq Ch^{r+2}(\|f\|_{L^\infty(H^r(\Omega_h))} + \|\boldsymbol{q}\|_{L^1(H^{r+1}(\Omega_h))} + \|u\|_{L^2(H^{r+1}(\Omega_h))} + \|u_t\|_{L^1(H^{r+1}(\Omega_h))}).$$

The results of Theorem 2.3 with convergence order $r+1$ are optimal. Under the assumption of the elliptic regularity, the following theorem provides the superconvergence with order $r+2$ if the approximations are piecewise polynomial with degree r.

Theorem 2.6. *Assume that all conditions in Theorem 2.4 hold. Then for any $r \geq 1$, we have*

$$\|\Pi_W^H u - u_h\|_{L^\infty(L^2(\Omega_h))} \leq Ch\Big(\|(\boldsymbol{q} - \boldsymbol{\Pi}_V^H \boldsymbol{q}, u - \Pi_W^H u)\|_{a,T,\Omega} + \|(\boldsymbol{q} - \boldsymbol{\Pi}_V^H \boldsymbol{q}, u - \Pi_W^H u)\|_{b,T,\Omega})\Big).$$

3. Proofs

In this section, we present detailed proofs of all our results.

3.1. Conservation of HDG scheme for Schrödinger equation

Theorem 2.1 which describes the conversation of scheme (2.1) is proved in this subsection.

Proof. Taking $\boldsymbol{v} = \boldsymbol{q}_h$ in (2.1a) and $w = u_h$ in (2.1b), respectively, we have that

$$\int_{\Omega_h} \frac{\partial u_h}{\partial t}\bar{u}_h \mathrm{d}x = i\int_{\Omega_h} \boldsymbol{q}_h \nabla \bar{u}_h \mathrm{d}x - i\int_{\Gamma_h} \hat{\boldsymbol{q}}_h \cdot \boldsymbol{n}\bar{u}_h \mathrm{d}s, \tag{3.1a}$$

$$\|\boldsymbol{q}_h\|^2_{L^2(\Omega_h)} - \int_{\Omega_h} \nabla\cdot\boldsymbol{q}_h \bar{u}_h \mathrm{d}x + \int_{\Gamma_h} \boldsymbol{q}_h\cdot\boldsymbol{n}\bar{\hat{u}}_h \mathrm{d}s = 0. \tag{3.1b}$$

Integrating by parts on the second term of (3.1b), we conclude that

$$\|\boldsymbol{q}_h\|^2_{L^2(\Omega_h)} + \int_{\Omega_h} \boldsymbol{q}_h \nabla\bar{u}_h \mathrm{d}x + \int_{\Gamma_h} \boldsymbol{q}_h\cdot\boldsymbol{n}(\bar{\hat{u}}_h - \bar{u}_h)\mathrm{d}s = 0. \tag{3.2}$$

Inserting (3.2) into (3.1a) implies that

$$\frac{\partial u_h}{\partial t}\bar{u}_h = -i\Big(\|\boldsymbol{q}_h\|^2_{L^2(\Omega_h)} + \int_{\Gamma_h} \boldsymbol{q}_h\cdot\boldsymbol{n}(\bar{\hat{u}}_h - \bar{u}_h)\mathrm{d}s\Big) - i\int_{\Gamma_h} \hat{\boldsymbol{q}}_h\cdot\boldsymbol{n}\bar{u}_h\mathrm{d}s. \tag{3.3}$$

By the definition of the probability density,

$$\frac{\partial p_h}{\partial t} = \frac{\partial u_h}{\partial t}\bar{u}_h + u_h\frac{\partial \bar{u}_h}{\partial t} = \frac{\partial u_h}{\partial t}\bar{u}_h + \overline{\frac{\partial u_h}{\partial t}\bar{u}_h}. \tag{3.4}$$

Substituting (3.3) into (3.4), we have that

$$\begin{aligned}\int_{\Omega_h} \frac{\partial p_h}{\partial t}\mathrm{d}x &= i\int_{\Gamma_h} (-\boldsymbol{q}_h\cdot\boldsymbol{n}(\bar{\hat{u}}_h - \bar{u}_h) - \hat{\boldsymbol{q}}_h\cdot\boldsymbol{n}\bar{u}_h + \bar{\boldsymbol{q}}_h\cdot\boldsymbol{n}(\hat{u}_h - u_h)\mathrm{d}s + \bar{\hat{q}}_h\cdot\boldsymbol{n}u_h)\mathrm{d}s \\ &= i\int_{\Gamma_h} ((\hat{\boldsymbol{q}}_h - \boldsymbol{q}_h)\cdot\boldsymbol{n}(\bar{\hat{u}}_h - \bar{u}_h) - (\hat{u}_h - u_h)(\bar{\hat{q}}_h - \bar{\boldsymbol{q}}_h)\cdot\boldsymbol{n})\mathrm{d}s,\end{aligned}$$

by the single value of $\hat{u}_h$ and $\hat{\boldsymbol{q}}_h$. Using the definition of the numerical flux $\hat{\boldsymbol{q}}_h$ (2.4), we have that

$$\frac{\partial}{\partial t}\int_{\Omega_h} p_h\mathrm{d}x = i\int_{\Gamma_h} (\tau(\hat{u}_h - u_h)(\bar{\hat{u}}_h - \bar{u}_h) - \tau(\bar{\hat{u}}_h - \bar{u}_h)(\hat{u}_h - u_h))\mathrm{d}s = 0.$$

So HDG method for the linear Schrödinger equation is conversative. This completes the proof. □

3.2. Error analysis

In this subsection, we describe the error analysis of HDG approximation: Theorems 2.3–2.6.

The proof of the error estimates is based on the so-called error equations and the properties of the projection. The error equations are that

$$\Big(\frac{\partial(u-u_h)}{\partial t}, w\Big)_{\Omega_h} + i(\nabla\cdot(\boldsymbol{q}-\boldsymbol{q}_h), w)_{\Omega_h} + i\langle(\boldsymbol{q}_h - \hat{\boldsymbol{q}}_h)\cdot\boldsymbol{n}, w\rangle_{\Gamma_h} = 0, \tag{3.5a}$$

$$(\boldsymbol{v}, \boldsymbol{q}-\boldsymbol{q}_h)_{\Omega_h} - (\nabla\cdot\boldsymbol{v}, u-u_h)_{\Omega_h} + \langle\boldsymbol{v}\cdot\boldsymbol{n}, u-\hat{u}_h\rangle_{\Gamma_h} = 0, \tag{3.5b}$$

$$\langle u-\hat{u}_h, \nu\rangle_{\partial\Omega} = 0, \quad u(0)-u_h(0) = 0, \tag{3.5c}$$

$$\langle(\boldsymbol{q}-\hat{\boldsymbol{q}}_h)\cdot\boldsymbol{n}, \nu\rangle_{\Gamma_h\backslash\partial\Omega} = 0, \tag{3.5d}$$

for all the test functions $(\boldsymbol{v}, w, \nu) \in \boldsymbol{V}_h \times W_h \times M_h$.

Lemma 3.1. *Let* $(u, \boldsymbol{q})$ *and* $(u_h, \boldsymbol{q}_h)$ *be the solutions of the problem* (1.1) *and the problem* (2.1) *respectively,* $(\boldsymbol{\Pi}_V^H, \Pi_W^H)$ *be the projection defined by* (2.5). *Then we have that*

$$\begin{aligned}&\left(\frac{\partial(\Pi_W^H u - u_h)}{\partial t}, \Pi_W^H u - u_h\right)_{\Omega_h} + i\|\boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h\|_{L^2(\Omega_h)}^2 + i\langle \tau(P_\partial u - \hat{u}_h - \Pi_W^H u + u_h)^2, 1\rangle_{\Gamma_h}\\ &\quad= -i(\boldsymbol{q} - \boldsymbol{\Pi}_V^H \boldsymbol{q}, \boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h)_{\Omega_h} - \left(\frac{\partial(u - \Pi_W^H u)}{\partial t}, \Pi_W^H u - u_h\right)_{\Omega_h}.\end{aligned}$$

Proof. Taking $w = \Pi_W^H u - u_h$ in (3.5a) and $\boldsymbol{v} = \boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h$ in (3.5b), we have that

$$\begin{aligned}&\left(\frac{\partial(\Pi_W^H u - u_h)}{\partial t}, \Pi_W^H u - u_h\right)_{\Omega_h} + i(\nabla\cdot(\boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h), \Pi_W^H u - u_h)_{\Omega_h}\\ &\quad + i\langle(\boldsymbol{q}_h - \hat{\boldsymbol{q}}_h)\cdot\boldsymbol{n}, \Pi_W^H u - u_h\rangle_{\Gamma_h}\\ &\quad = -i(\nabla\cdot(\boldsymbol{q} - \boldsymbol{\Pi}_V^H \boldsymbol{q}), \Pi_W^H u - u_h)_{\Omega_h} - \left(\frac{\partial(u - \Pi_W^H u)}{\partial t}, \Pi_W^H u - u_h\right)_{\Omega_h},\end{aligned}$$

and

$$\begin{aligned}&i\|\boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h\|_{L^2(\Omega_h)}^2 - i(\nabla\cdot(\boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h), \Pi_W^H u - u_h)_{\Omega_h} + i\langle u - \hat{u}_h, \boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h\cdot\boldsymbol{n}\rangle_{\Gamma_h}\\ &\quad = -i(\boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h, \boldsymbol{q} - \boldsymbol{\Pi}_V^H \boldsymbol{q})_{\Omega_h}.\end{aligned}$$

By the integration by parts and the orthogonality of the $\boldsymbol{\Pi}_V^H$, we have that

$$(\nabla\cdot(\boldsymbol{q} - \boldsymbol{\Pi}_V^H \boldsymbol{q}), \Pi_W^H u - u_h)_{\Omega_h} = \langle(\boldsymbol{q} - \boldsymbol{\Pi}_V^H \boldsymbol{q})\cdot\boldsymbol{n}, \Pi_W^H u - u_h\rangle_{\Gamma_h}.$$

Summing the above three equations, we have that

$$\begin{aligned}&\left(\frac{\partial(\Pi_W^H u - u_h)}{\partial t}, \Pi_W^H u - u_h\right)_{\Omega_h} + i\|\boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h\|_{L^2(\Omega_h)}^2 + i\langle(\boldsymbol{q}_h - \hat{\boldsymbol{q}}_h)\cdot\boldsymbol{n}, \Pi_W^H u - u_h\rangle_{\Gamma_h}\\ &\quad + i\langle\boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h\cdot\boldsymbol{n}, u - \hat{u}_h\rangle_{\Gamma_h} + i\langle(\boldsymbol{q} - \boldsymbol{\Pi}_V^H \boldsymbol{q})\cdot\boldsymbol{n}, \Pi_W^H u - u_h\rangle_{\Gamma_h}\\ &\quad = -\left(\frac{\partial(u - \Pi_W^H u)}{\partial t}, \Pi_W^H u - u_h\right)_{\Omega_h} - i(\boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h, \boldsymbol{q} - \boldsymbol{\Pi}_V^H \boldsymbol{q})_{\Omega_h}.\end{aligned}$$

In order to obtain the result, we must simplify the sum of the three boundary integration terms. We noticed that

$$i\langle P_\partial \boldsymbol{q} + \hat{\boldsymbol{q}}_h)\cdot\boldsymbol{n}, u - \hat{u}_h\rangle_{\Gamma_h} = 0,$$

by the single value of $\hat{\boldsymbol{q}}_h, P_\partial u, P_\partial \boldsymbol{q}$ and $\hat{u}_h$ on the interior boundary and the definition of $\hat{u}_h$ (2.2). Recombining the above four boundary integration terms, we have that

$$\begin{aligned}&\langle(\boldsymbol{q}_h - \hat{\boldsymbol{q}}_h)\cdot\boldsymbol{n}, \Pi_W^H u - u_h\rangle_{\Gamma_h} + \langle\boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h\cdot\boldsymbol{n}, u - \hat{u}_h\rangle_{\Gamma_h}\\ &\quad + \langle(\boldsymbol{q} - \boldsymbol{\Pi}_V^H \boldsymbol{q})\cdot\boldsymbol{n}, \Pi_W^H u - u_h\rangle_{\Gamma_h} - \langle P_\partial \boldsymbol{q} + \hat{\boldsymbol{q}}_h)\cdot\boldsymbol{n}, u - \hat{u}_h\rangle_{\Gamma_h}\\ &\quad = \langle(\Pi_V^H \boldsymbol{q} - \boldsymbol{q}_h - P_\partial \boldsymbol{q} + \hat{\boldsymbol{q}}_h)\cdot\boldsymbol{n}, P_\partial u - \hat{u}_h - \Pi_W^H u + u_h\rangle_{\Gamma_h},\end{aligned}$$

by the orthogonality of the L^2 projection P_∂. On the other hand, we have

$$\begin{aligned}\langle(\Pi_V^H \boldsymbol{q} - \boldsymbol{q}_h - P_\partial \boldsymbol{q} + \hat{\boldsymbol{q}}_h)\cdot \boldsymbol{n}, \mu\rangle_{\Gamma_h} =& \langle(\Pi_V^H \boldsymbol{q} - P_\partial \boldsymbol{q} - \boldsymbol{q}_h + \hat{\boldsymbol{q}}_h)\cdot \boldsymbol{n}, \mu\rangle_{\Gamma_h}\\ =& \langle \tau(P_\partial u - \Pi_V^H u - \hat{u}_h + u_h), \mu\rangle_{\Gamma_h},\end{aligned}$$

by the definition of HDG projection (2.5c) and the definition of the numerical flux (2.4). Combining the above all equations can obtain shortly the result of the lemma. This completes the proof. □

In order to prove the first result of Theorem 2.3, we need the following propositions.

Proposition 3.2. *Assume that the complex function $z(t) = a(t) + ib(t)$ is continuous differential. For all $t \in R^+$, $0 < |z|^2 = a^2(t) + b^2(t) \le R < +\infty$. $\min\{\frac{a}{b}, \frac{b}{a}\}$ is bounded,* i.e., $\min\{|\frac{a}{b}|, |\frac{b}{a}|\} \le \frac{Q_z}{2}$. *Then for all $T \ge 0$*

$$\left|\int_0^T \left(\left(\frac{\partial a}{\partial t}, b\right)_{\Omega_h} - \left(\frac{\partial b}{\partial t}, a\right)_{\Omega_h}\right)\mathrm{d}t\right| \le Q_z R.$$

Proposition 3.3 (seen in [23])**.** *Assume that the functions $A(t)$ and $B(t)$ are nonnegative in $L^\infty(R^+)$. $S(t)$ satisfies that*

$$S^2(t) + \int_0^t y(s)\mathrm{d}s \le A(t) + \int_0^t B(s)S(s)\mathrm{d}s.$$

Then for any $T > 0$

$$S^2(T) + \int_0^T y(s)\mathrm{d}s \le \left(\left[\max_{0\le t\le T} A(t)\right]^{\frac{1}{2}} + \frac{1}{2}\int_0^T B(s)\mathrm{d}s\right)^2. \tag{3.6}$$

3.2.1. The proof of the first estimates in Theorem 2.3

Proof. By decomposing all terms of the expression of Lemma 3.1 into the real parts and imaginary parts and the simple algebraic computation, we have that

$$\begin{aligned}\frac{1}{2}\frac{\partial}{\partial t}\|\Pi_W^H u - u_h\|_{\Omega_h}^2 &= Re\left(\frac{\partial(\Pi_W^H u - u_h)}{\partial t}, \Pi_W^H u - u_h\right)_{L^2(\Omega_h)}\\ &= -Im(\boldsymbol{q} - \boldsymbol{\Pi}_V^H \boldsymbol{q}, \boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h)_{\Omega_h} - Re\left(\frac{\partial(u - \Pi_W^H u)}{\partial t}, \Pi_W^H u - u_h\right),\end{aligned} \tag{3.7a}$$

$$\begin{aligned}&\|\boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h\|_{L^2(\Omega_h)}^2 + \langle \tau|P_\partial u - \hat{u}_h - \Pi_W^H u + u_h|^2, 1\rangle_{\Gamma_h}\\ &\quad= -Im\left(\frac{\partial(\Pi_W^H u - u_h)}{\partial t}, \Pi_W^H u - u_h\right)_{\Omega_h} + Re(\boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h, \boldsymbol{q} - \boldsymbol{\Pi}_V^H \boldsymbol{q})_{\Omega_h}\\ &\qquad+ \left(\frac{\partial(u - \Pi_W^H u)}{\partial t}, \Pi_W^H u - u_h\right).\end{aligned} \tag{3.7b}$$

Integrating (3.7a) on the interval $[0, T]$ with respective to the time and using the initial condition $(u_h - \Pi_W^H u)(0) = 0$, we deduce that

$$\frac{1}{2}\|(\Pi_W^H u - u_h)(T)\|_{\Omega_h}^2 \le \int_0^T \left|\left(\frac{\partial(u - \Pi_W^H u)}{\partial t}, \Pi_W^H u - u_h\right)_{\Omega_h}\right| + |(\boldsymbol{q} - \boldsymbol{\Pi}_V^H \boldsymbol{q}, \boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h)_{\Omega_h}|\mathrm{d}t. \tag{3.8}$$

Applying Proposition 3.2 with $a(t) = Re(\Pi_W^H u - u_h)$, $b(t) = Im(\Pi_W^H u - u_h)$ and $R = \left|\int_0^T \left(\frac{\partial(u-\Pi_W^H u)}{\partial t}, \Pi_W^H \bar{u} - \bar{u}_h\right)_{\Omega_h} \mathrm{d}t\right| + \left|\int_0^T (\boldsymbol{q} - \boldsymbol{\Pi}_V^H \boldsymbol{q}, \boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h)_{\Omega_h} \mathrm{d}t\right|$ in the above equation, we imply that there exists a constant Q_u^H such that

$$\left|\int_0^T Im\left(\frac{\partial \Pi_W^H u - u_h}{\partial t}, \Pi_W^H u - u_h\right)_{L^2(\Omega_h)} \mathrm{d}t\right|$$
$$\leq Q_u^H \left|\int_0^T \left(\frac{\partial(u-\Pi_W^H u)}{\partial t}, \Pi_W^H u - u_h\right)_{\Omega_h} \mathrm{d}t\right| + Q_u^H \left|\int_0^T (\boldsymbol{q} - \boldsymbol{\Pi}_V^H \boldsymbol{q}, \boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h)_{\Omega_h} \mathrm{d}t\right|.$$

Inserting the above inequality into the second equation of (3.7b) and combining (3.8), we derive that

$$\frac{1}{2}\|(\Pi_W^H u - u_h)(T)\|_{L^2(\Omega_h)}^2 + \int_0^T (\|\boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h\|_{L^2(\Omega_h)}^2 + \langle \tau |P_\partial u - \hat{u}_h - \Pi_W^H u + u_h|^2, 1\rangle_{\Gamma_h})\mathrm{d}t$$
$$\leq (Q_u^H + 2)\left|\int_0^T \left(\frac{\partial(u-\Pi_W^H u)}{\partial t}, \Pi_W^H u - u_h\right)\mathrm{d}t\right| + (Q_u^H + 2)\left|\int_0^T (\boldsymbol{q} - \Pi_V^H \boldsymbol{q}, \boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h)_{\Omega_h} \mathrm{d}t\right|.$$

By the module of complex number, Cauchy–Schwartz inequality and Yong's inequality, we have that

$$\frac{1}{2}\|(\Pi_W^H u - u_h)(T)\|_{L^2(\Omega_h)}^2 + \int_0^T (\|\boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h\|_{L^2(\Omega_h)}^2 + \langle \tau |P_\partial u - \hat{u}_h - \Pi_W^H u + u_h|^2, 1\rangle_{\Gamma_h})\mathrm{d}t$$
$$\leq (Q_u + 2)\int_0^T \left\|\frac{\partial(u-\Pi_W^H u)}{\partial t}\right\|_{L^2(\Omega_h)} \|\Pi_W^H u - u_h\|_{L^2(\Omega_h)}\mathrm{d}t + C\int_0^T \|\boldsymbol{q} - \boldsymbol{\Pi}_V^H \boldsymbol{q}\|_{L^2(\Omega_h)}^2 \mathrm{d}t.$$

By using directly Proposition 3.3 with $S(t) = \|(\Pi_W^H u - u_h)(t)\|_{L^2(\Omega_h)}$, $y(s) = \|\boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h\|_{L^2(\partial\Omega_h)}^2 + \langle \tau |P_\partial u - \hat{u}_h - \Pi_W^H u + u_h|^2, 1\rangle_{\Gamma_h}$, $A(t) = \int_0^T \|\boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}\|_{L^2(\Omega_h)}^2$ and $B(s) = \|\frac{\partial(u-\Pi_W^H u)}{\partial t}\|_{L^2(\Omega_h)}$, we conclude the following corollary.

Corollary 3.4. *For any $T > 0$,we have that*

$$\frac{1}{2}\|(\Pi_W^H u - u_h)(T)\|_{L^2(\Omega_h)}^2 + \int_0^T \|\boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h\|_{L^2(\Omega_h)}^2 + \langle \tau |P_\partial u - \hat{u}_h - \Pi_W^H u + u_h|^2, 1\rangle_{\Gamma_h}$$
$$\leq C\|\boldsymbol{q} - \boldsymbol{\Pi}_V^H \boldsymbol{q}\|_{L^2(L^2)}^2 + C\|(\Pi_W^H u - u)_t\|_{L^1(L^2)}^2.$$

In this manner, the first estimate of Theorem 2.3 is obtained. □

Next, we prove the second and the third estimates of Theorem 2.3. We need following result before we present their proof.

Lemma 3.5. *For any $T > 0$, we have that*

$$\frac{1}{2}\|(\boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h)(T)\|_{L^2(\Omega_h)}^2 + \frac{1}{2}\|\tau^{\frac{1}{2}}(P_\partial u - \hat{u}_h - \Pi_W^H u + u_h)(T)\|_{L^2(\Gamma_h)}^2$$
$$+ \int_0^T \left\|\frac{\partial}{\partial t}(\Pi_W^H u - u_h)\right\|_{L^2(\Omega_h)}^2 \mathrm{d}t$$

$$\leq C\|(\boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h)(0)\|^2_{L^2(\Omega_h)} + C\int_0^T \left[\left\| \frac{\partial(u - \Pi_W^H u)}{\partial t} \right\|^2_{L^2(\Omega_h)} \right.$$
$$\left. + \|\boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h\|_{L^2(\Omega_h)} \left\| \frac{\partial(\boldsymbol{q} - \boldsymbol{\Pi}_V^H \boldsymbol{q})}{\partial t} \right\|_{L^2(\Omega_h)} \right] \mathrm{d}t.$$

Proof. In order to prove the result of lemma, we need to make slight changes to the aforementioned error equations (3.1). As the conclusion is an error estimate on the flux function and time-derivative of the wave function, we only need to differentiate the (b) and (c) equations with respect to time, at the same time keep the (a) and (d) equations in (3.1). Since the test function is only a function of the space variable and it is independent of time, we will get the following system of error equations

$$\left(\frac{\partial(u-u_h)}{\partial t}, w\right)_{\Omega_h} + i(\nabla\cdot(\boldsymbol{q}-\boldsymbol{q}_h), w)_{\Omega_h} + i\langle(\boldsymbol{q}_h - \hat{\boldsymbol{q}}_h)\cdot\boldsymbol{n}, w\rangle_{\Gamma_h} = 0, \tag{3.9a}$$

$$\left(\boldsymbol{v}, \frac{\partial}{\partial t}(\boldsymbol{q}-\boldsymbol{q}_h)\right)_{\Omega_h} - \left(\nabla\cdot\boldsymbol{v}, \frac{\partial}{\partial t}(u-u_h)\right)_{\Omega_h} + \left\langle \boldsymbol{v}\cdot\boldsymbol{n}, \frac{\partial}{\partial t}(u-\hat{u}_h)\right\rangle_{\Gamma_h} = 0, \tag{3.9b}$$

$$\langle \partial_t(\Pi_W^H u - \hat{u}_h), \mu\rangle_{\partial\Omega} = 0, \tag{3.9c}$$

$$\langle(\boldsymbol{\Pi}_V^H \boldsymbol{q} - \hat{\boldsymbol{q}}_h)\cdot\boldsymbol{n}, w\rangle_{\Gamma_h\backslash\partial\Omega} = 0, \qquad (\Pi_W^H u - u_h)|_{t=0} = 0, \tag{3.9d}$$

for all $(\boldsymbol{v}, w, \mu) \in \boldsymbol{V}_h \times W_h \times M_h$.

Following the error equations (3.9a) and (3.9b) and using the definition of the projection $(\boldsymbol{\Pi}_V^H, \Pi_W^H)$ (2.5), we have that

$$\left(\frac{\partial(\Pi_W^H u - u_h)}{\partial t}, w\right)_{\Omega_h} + i(\nabla\cdot(\boldsymbol{\Pi}_V^H\boldsymbol{q} - \boldsymbol{q}_h), w)_{\Omega_h} + i\langle(\boldsymbol{q}_h - \hat{\boldsymbol{q}}_h)\cdot\boldsymbol{n}, w\rangle_{\Gamma_h}$$
$$+ i\langle \boldsymbol{q} - \boldsymbol{\Pi}_V^H\boldsymbol{q})\cdot\boldsymbol{n}, w\rangle_{\Gamma_h}, = -\left(\frac{\partial(u - \Pi_W^H u)}{\partial t}, w\right)_{\Omega_h}, \tag{3.10a}$$

$$\left(\boldsymbol{v}, \frac{\partial}{\partial t}(\boldsymbol{\Pi}_V^H\boldsymbol{q} - \boldsymbol{q}_h)\right)_{\Omega_h} - \left(\nabla\cdot\boldsymbol{v}, \frac{\partial(\Pi_W^H u - u_h)}{\partial t}\right)_{\Omega_h} + \left\langle \boldsymbol{v}\cdot\boldsymbol{n}, \frac{\partial(u-\hat{u}_h)}{\partial t}\right\rangle_{\Gamma_h}$$
$$= -\left(\boldsymbol{v}, \frac{\partial(\boldsymbol{q} - \boldsymbol{\Pi}_V^H\boldsymbol{q})}{\partial t}\right)_{\Omega_h}. \tag{3.10b}$$

Taking $w = \partial_t(\Pi_W^H u - u_h)$ and $\boldsymbol{v} = i(\boldsymbol{\Pi}_V^H\boldsymbol{q}_h - \boldsymbol{q}_h)$ in (3.10a) and (3.10b), respectively, and summing the two resulting equations, we have that

$$\left\|\frac{\partial}{\partial t}(\Pi_W^H u - u_h)\right\|^2_{L^2(\Omega_h)} + i\left(\boldsymbol{\Pi}_V^H\boldsymbol{q} - \boldsymbol{q}_h, \frac{\partial}{\partial t}(\boldsymbol{\Pi}_V^H\boldsymbol{q} - \boldsymbol{q}_h)\right)_{\Omega_h}$$
$$+ i\left\langle(\boldsymbol{q}_h - \hat{\boldsymbol{q}}_h)\cdot\boldsymbol{n}, \frac{\partial(\Pi_W^H u - u_h)}{\partial t}\right\rangle_{\Gamma_h} + i\left\langle(\boldsymbol{\Pi}_V^H\boldsymbol{q} - \boldsymbol{q}_h)\cdot\boldsymbol{n}, \frac{\partial(u-\hat{u}_h)}{\partial t}\right\rangle_{\Gamma_h}$$
$$+ i\langle(\boldsymbol{q} - \boldsymbol{\Pi}_V^H\boldsymbol{q})\cdot\boldsymbol{n}, w\rangle_{\Gamma_h}$$
$$= -\left(\frac{\partial(u - \Pi_W^H u)}{\partial t}, \frac{\partial(\Pi_W^H u - u_h)}{\partial t}\right)_{\Omega_h} - i\left(\boldsymbol{\Pi}_V^H\boldsymbol{q} - \boldsymbol{q}_h, \frac{\partial(\boldsymbol{q} - \boldsymbol{\Pi}_V^H\boldsymbol{q})}{\partial t}\right)_{\Omega_h}. \tag{3.11}$$

For the sake of convenience, we denote the numerical trace approximation error by $\hat{\varepsilon}_h^u = P_\partial u - \hat{u}_h - \Pi_W^H u + u_h$. It follows from the boundary condition (2.1c) and the definition of numerical trace (2.1d) and (2.4) and the definition of HDG projection (2.5c) that

$$\left\langle (\hat{\boldsymbol{q}} - \boldsymbol{q}_h) \cdot \boldsymbol{n}, \frac{\partial(\Pi_W^H u - u_h)}{\partial t} \right\rangle_{\Gamma_h} + \left\langle (\boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h) \cdot \boldsymbol{n}, \frac{\partial(u - \hat{u}_h)}{\partial t} \right\rangle_{\Gamma_h} - \left\langle (\boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h) \cdot \boldsymbol{n}, \frac{\partial(u - \Pi_W^H u)}{\partial t} \right\rangle_{\Gamma_h} = \left\langle \tau \hat{\varepsilon}_h^u, \frac{\partial \hat{\varepsilon}_h^u}{\partial t} \right\rangle_{\Gamma_h}.$$

Inserting the above equation into (3.11) presents that

$$\left\| \frac{\partial}{\partial t}(\Pi_W^H u - u_h) \right\|_{L^2(\Omega_h)}^2 + i \left(\boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h, \frac{\partial}{\partial t}(\boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h) \right)_{\Omega_h} + i \left\langle \tau \hat{\varepsilon}_h^u, \frac{\partial \hat{\varepsilon}_h^u}{\partial t} \right\rangle_{\Gamma_h}$$
$$= - \left(\frac{\partial(u - \Pi_W^H u)}{\partial t}, \frac{\partial(\Pi_W^H u - u_h)}{\partial t} \right)_{\Omega_h} - i \left(\boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h, \frac{\partial(\boldsymbol{q} - \boldsymbol{\Pi}_V^H \boldsymbol{q})}{\partial t} \right)_{\Omega_h}.$$

After integrating over the interval $[0, T]$ with respective to the time for the above equation and using the initial condition (3.5d) and numerical trace, we consider the imaginary part of the resulting equation,

$$\begin{aligned}
&\frac{1}{2}\|(\boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h)(T)\|_{L^2(\Omega_h)}^2 + \frac{1}{2}\|\tau^{\frac{1}{2}} \hat{\varepsilon}_h^u(T)\|_{L^2(\Gamma_h)}^2 \\
&\quad = -Im \int_0^T \left[\left(\frac{\partial(u - \Pi_W^H u)}{\partial t}, \frac{\partial(\Pi_W^H u - u_h)}{\partial t} \right)_{\Omega_h} - i \left(\boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h, \frac{\partial(\boldsymbol{q} - \boldsymbol{\Pi}_V^H \boldsymbol{q})}{\partial t} \right)_{\Omega_h} \right] \mathrm{d}t \\
&\qquad + \|(\boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h)(0)\|_{L^2(\Omega_h)}^2 \\
&\quad \leq \int_0^T \Big[\left\| \frac{\partial(u - \Pi_W^H u)}{\partial t} \right\|_{L^2(\Omega_h)}^2 + \delta \left\| \frac{\partial(\Pi_W^H u - u_h)}{\partial t} \right\|_{L^2(\Omega_h)}^2 \\
&\qquad + \|\boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h\|_{L^2(\Omega_h)} \left\| \frac{\partial(\boldsymbol{q} - \boldsymbol{\Pi}_V^H \boldsymbol{q})}{\partial t} \right\|_{L^2(\Omega_h)} \Big] \mathrm{d}t + \|(\boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h)(0)\|_{L^2(\Omega_h)}^2,
\end{aligned} \tag{3.12}$$

where δ is a small enough constant.

Applying Proposition 3.2, there exists the constant Q_q^H such that

$$\begin{aligned}
&Im \int_0^T \left(\boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h, \frac{\partial}{\partial t}(\boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h) \right)_{\Omega_h} \mathrm{d}t + Im \int_0^T \left\langle \tau(u_h - \hat{u}_h), \frac{\partial(u_h - \hat{u}_h)}{\partial t} \right\rangle_{\Gamma_h} \mathrm{d}t \\
&\quad \leq Q_q^H \int_0^T \Big[\left\| \frac{\partial(u - \Pi_W^H u)}{\partial t} \right\|_{L^2(\Omega_h)}^2 + \delta \left\| \frac{\partial(\Pi_W^H u - u_h)}{\partial t} \right\|_{L^2(\Omega_h)}^2 \\
&\qquad + \|\boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h\|_{L^2(\Omega_h)} \left\| \frac{\partial(\boldsymbol{q} - \boldsymbol{\Pi}_V^H \boldsymbol{q})}{\partial t} \right\|_{L^2(\Omega_h)} \Big] \mathrm{d}t + Q_q^H \|(\boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h)(0)\|_{L^2(\Omega_h)}^2.
\end{aligned}$$

Following that, similarly, we consider the integration of the real part,

$$\begin{aligned}
&\int_0^T \left\|\frac{\partial}{\partial t}(\Pi_W^H u - u_h)\right\|_{L^2(\Omega_h)}^2 \mathrm{d}t \\
&= Im \int_0^T \left(\mathbf{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h, \frac{\partial}{\partial t}(\mathbf{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h)\right)_{\Omega_h} \mathrm{d}t + Im \int_0^T \left\langle \tau\hat{\varepsilon}_h^u, \frac{\partial \hat{\varepsilon}_h^u}{\partial t}\right\rangle_{\Gamma_h} \mathrm{d}t \\
&\quad - Re \int_0^T \left(\frac{\partial(u - \Pi_W^H u)}{\partial t}, \frac{\partial(\Pi_W^H u - u_h)}{\partial t}\right)_{\Omega_h} \mathrm{d}t + Im \int_0^T \left(\mathbf{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h, \frac{\partial(\boldsymbol{q} - \mathbf{\Pi}_V^H \boldsymbol{q})}{\partial t}\right)_{\Omega_h} \mathrm{d}t \\
&\le Q_q^H \|(\mathbf{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h)(0)\|_{L^2(\Omega_h)}^2 + (Q_q^H + 1)\int_0^T \Bigg[\left\|\frac{\partial(u - \Pi_W^H u)}{\partial t}\right\|_{L^2(\Omega_h)}^2 \\
&\quad + \|\mathbf{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h\|_{L^2(\Omega_h)} \left\|\frac{\partial(\boldsymbol{q} - \mathbf{\Pi}_V^H \boldsymbol{q})}{\partial t}\right\|_{L^2(\Omega_h)}\Bigg]\mathrm{d}t + \delta \int_0^T \left\|\frac{\partial(\Pi_W^H u - u_h)}{\partial t}\right\|_{L^2(\Omega_h)}^2.
\end{aligned}$$

So we have that

$$\begin{aligned}
\int_0^T \left\|\frac{\partial}{\partial t}(\Pi_W^H u - u_h)\right\|_{L^2(\Omega_h)}^2 \mathrm{d}t \le & C Q_q^H \|(\mathbf{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h)(0)\|_{L^2(\Omega_h)}^2 + C Q_q^H \int_0^T \Bigg[\left\|\frac{\partial(u - \Pi_W^H u)}{\partial t}\right\|_{L^2(\Omega_h)}^2 \\
& + \|\mathbf{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h\|_{L^2(\Omega_h)} \left\|\frac{\partial(\boldsymbol{q} - \mathbf{\Pi}_V^H \boldsymbol{q})}{\partial t}\right\|_{L^2(\Omega_h)}\Bigg]\mathrm{d}t.
\end{aligned}$$

Summing the above inequalities and (3.12) induces the result. This completes the proof. □

3.2.2. The proof of the second and the third estimates in Theorem 2.3

Proof. The result follows by using the Proposition 3.3 with $S^2(t) = \frac{1}{2}\|\mathbf{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h)(t)\|_{L^2(\Omega_h)}^2 + \frac{1}{2}\|\sqrt{\tau}\hat{\varepsilon}_h^u(s)\|_{L^2(\Omega_h)}^2$, $y(s) = \|\frac{\partial}{\partial s}(\Pi_W^H u - u_h)\|_{L^2(\Omega_h)}^2$, $A = \|(\mathbf{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h)(0)\|^2 + \int_0^t \|\frac{\partial}{\partial t}(u - \Pi_W^H u)\|_{L^2(\Omega_h)}^2 \mathrm{d}s$ and $B(s) = \|\mathbf{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}\|_{L^2(\Omega_h)}$. □

Next, we discuss the estimate of $P_{r-1}(\Pi_W^H u - u_h)$ in Theorem 2.4 by the dual techniques. To state it, we introduce the dual problem

$$\psi_t - i\Delta\psi = 0 \quad \text{on } \Omega \times (0, T), \tag{3.13a}$$
$$\psi = 0 \quad \text{on } \partial\Omega \times (0, T), \tag{3.13b}$$
$$\psi(T) = \theta \quad \text{on } \Omega, \tag{3.13c}$$

or the first order equations form

$$\boldsymbol{\varphi} + \nabla\psi = 0 \quad \text{on } \Omega \times (0, T), \tag{3.14a}$$
$$\psi_t + i\nabla \cdot \boldsymbol{\varphi} = 0 \quad \text{on } \Omega \times (0, T), \tag{3.14b}$$
$$\psi = 0 \quad \text{on } \partial\Omega \times (0, T), \tag{3.14c}$$
$$\psi(T) = \theta \quad \text{on } \Omega, \tag{3.14d}$$

According to the dual argument, we consider the following quantity

$$\|P_{r-1}(\Pi_W^H u - u_h)(T)\|_{L^2(\Omega_h)} = \sup_{\theta\in W_h} \frac{(P_{r-1}(\Pi_W^H u - u_h)(T),\theta)}{\|\theta\|_{L^2(\Omega_h)}}.$$

Then we will present the upper bound of quantity $(P_{r-1}(\Pi_W^H u - u_h)(T),\theta)$ by the error equation and solution of the dual problem (3.14). To continue the our estimates, we need the regularity estimates represented in the following proposition.

Together with the estimates obtained in the previous sections, we need the parabolic regularity estimates or stable properties described in the following result. Its proof is given in the appendix.

Proposition 3.6. *Assume that ψ be the solution of dual problem (3.2.2). Then we have that*

$$\|\nabla\psi\|^2_{L^2(L^2)} \le \|\theta\|^2_{L^2(\Omega_h)}, \quad \forall\theta\in L^2(\Omega_h),$$

and

$$\|\Delta\psi\|^2_{L^2(L^2)} \le C\|\theta\|^2_{L^2(\Omega_h)}, \quad \forall\theta\in L^2(\Omega_h).$$

Lemma 3.7. *Let u and u_h be the solutions of the problem (1.2) and the problem (2.1), respectively, and ψ be the solution of dual problem (3.14). Then for any $T>0$, we have that*

$$\begin{aligned}
&(P_{r-1}(\Pi_W^H u - u_h)(T),\theta)_{\Omega_h}\\
&\quad = \int_0^T i(\mathbf{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h, \nabla I_h\psi - \mathbf{\Pi}^{BDM}\nabla\psi)_{\Omega_h} + i(\Pi_W^H u_t - u_t, I_h\psi - P_{r-1}\psi)_{\Omega_h}\\
&\qquad + (\partial_t(\Pi_W^H u - u_h), P_{r-1}\psi - I_h\psi)_{\Omega_h} + i(\mathbf{\Pi}_V^H\boldsymbol{q} - \boldsymbol{q}, \mathbf{\Pi}^{BDM}\nabla\psi - \nabla P_L\psi)_{\Omega_h},
\end{aligned} \tag{3.15}$$

where P_L is the L^2 projection into W_h and I_h is any interpolation operator from $L^2(\Omega)$ into $W_h\cap H_0^1(\Omega)$.

Proof. It follows from the dual problem (3.14d), Newton–Leibniz formula and the initial condition $(\Pi_W^H u - u_h)(0) = 0$ that

$$\begin{aligned}
&(P_{r-1}(\Pi_W^H u - u_h)(T),\theta)_{\Omega_h} = (P_{r-1}(\Pi_W^H u - u_h)(T),\psi(T))_{\Omega_h}\\
&\quad = \int_0^T \left[\left(\frac{\partial}{\partial t}P_{r-1}(\Pi_W^H u - u_h),\psi\right)_{\Omega_h} + \left(P_{r-1}(\Pi_W^H u - u_h),\frac{\partial\psi}{\partial t}\right)_{\Omega_h}\right]\mathrm{d}t = J.
\end{aligned} \tag{3.16}$$

By the orthogonality of L^2 projection P_{r-1} and the dual equation (3.14b), we have that

$$\begin{aligned}
J &= \int_0^T \left[\left(\frac{\partial}{\partial t}P_{r-1}(\Pi_W^H u - u_h), P_{r-1}\psi\right)_{\Omega_h} - i(P_{r-1}(\Pi_W^H u - u_h), P_{r-1}\nabla\cdot\boldsymbol{\varphi})_{\Omega_h}\right]\mathrm{d}t\\
&= \int_0^T \left[\left(\frac{\partial}{\partial t}(\Pi_W^H u - u_h), P_{r-1}\psi\right)_{\Omega_h} - i((\Pi_W^H u - u_h), P_{r-1}\nabla\cdot\boldsymbol{\varphi})_{\Omega_h}\right]\mathrm{d}t.
\end{aligned}$$

Using the error equation (3.5b) and the well-known property of the projections $\boldsymbol{\Pi}^{BDM}$ and P_{r-1}, *i.e.*, the so-called weak commutativity property, we imply that

$$J=\int_0^T\left[\left(\frac{\partial}{\partial t}(\Pi_W^H u-u_h),P_{r-1}\psi\right)_{\Omega_h}+i(\boldsymbol{\Pi}_V^H\boldsymbol{q}-\boldsymbol{q}_h,\boldsymbol{\Pi}^{BDM}\boldsymbol{\varphi})_{\Omega_h}\right.$$
$$\left.+(\boldsymbol{q}-\boldsymbol{\Pi}_V^H\boldsymbol{q},\boldsymbol{\Pi}^{BDM}\nabla\psi)_{\Omega_h}+i\langle u-\hat{u}_h,\boldsymbol{\Pi}^{BDM}\boldsymbol{\varphi}\cdot\boldsymbol{n}\rangle_{\Gamma_h}\right]\mathrm{d}t.$$

By the dual equation (3.14a) and the error equation (3.5a), we conclude that

$$\begin{aligned}i(\boldsymbol{\Pi}_V^H\boldsymbol{q}-\boldsymbol{q}_h,\boldsymbol{\Pi}^{BDM}\boldsymbol{\varphi})_{\Omega_h}&=i(\boldsymbol{\Pi}_V^H\boldsymbol{q}-\boldsymbol{q}_h,-\boldsymbol{\Pi}^{BDM}\nabla\psi)_{\Omega_h}\\&=i(\boldsymbol{\Pi}_V^H\boldsymbol{q}-\boldsymbol{q}_h,-\boldsymbol{\Pi}^{BDM}\nabla\psi+\nabla I_h\psi)_{\Omega_h}-i(\boldsymbol{\Pi}_V^H\boldsymbol{q}-\boldsymbol{q}_h,\nabla I_h\psi)_{\Omega_h}\\&=i(\boldsymbol{\Pi}_V^H\boldsymbol{q}-\boldsymbol{q}_h,-\boldsymbol{\Pi}^{BDM}\nabla\psi+\nabla I_h\psi)_{\Omega_h}+i\langle\boldsymbol{q}-\hat{\boldsymbol{q}}_h,I_h\psi\rangle_{\Gamma_h}\\&\quad+\left(\frac{\partial(u-\Pi_W^H u)}{\partial t},I_h\psi\right)_{\Omega_h}+\left(\frac{\partial(\Pi_W^H u-u_h)}{\partial t},I_h\psi\right)_{\Omega_h}.\end{aligned}$$

By the definitions of the projection $(\boldsymbol{\Pi}_V^H,\Pi_W^H)$ (2.5a) and (2.5b), we have that

$$\begin{aligned}(\boldsymbol{q}-\boldsymbol{\Pi}_V^H\boldsymbol{q},\boldsymbol{\Pi}^{BDM}\nabla\psi)_{\Omega_h}&=(\boldsymbol{q}-\boldsymbol{\Pi}_V^H\boldsymbol{q},\boldsymbol{\Pi}^{BDM}\nabla\psi-\nabla P_L\psi)_{\Omega_h},\\\left(\frac{\partial(u-\Pi_W^H u)}{\partial t},I_h\psi\right)_{\Omega_h}&=\left(\frac{\partial(u-\Pi_W^H u)}{\partial t},I_h\psi-P_{r-1}\psi\right)_{\Omega_h}.\end{aligned}$$

Next, we compute two boundary terms $\langle u-\hat{u}_h,\boldsymbol{\Pi}^{BDM}\boldsymbol{\varphi}\cdot\boldsymbol{n}\rangle_{\Gamma_h}$ and $\langle(\boldsymbol{q}-\hat{\boldsymbol{q}}_h)\cdot\boldsymbol{n},I_h\psi\rangle_{\Gamma_h}$. By the single-value of $\hat{u}_h$ and $\Pi^{BDM}\boldsymbol{\varphi}$ in the interior faces, we have that

$$\langle u-\hat{u}_h,\boldsymbol{\Pi}^{BDM}\boldsymbol{\varphi}\cdot\boldsymbol{n}\rangle_{\Gamma_h\backslash\partial\Omega}=0.$$

Using $\hat{u}_h|_{\partial\Omega}=P_\partial u|_{\partial\Omega}$ and the definition of the projection P_∂ implies that

$$\langle u-\hat{u}_h,\boldsymbol{\Pi}^{BDM}\boldsymbol{\varphi}\rangle_{\partial\Omega}=\langle u-P_\partial u,\boldsymbol{\Pi}^{BDM}\boldsymbol{\varphi}\cdot\boldsymbol{n}\rangle_{\partial\Omega}=0.$$

Adding the above two equations, we get that

$$\langle u-\hat{u}_h,\boldsymbol{\Pi}^{BDM}\boldsymbol{\varphi}\cdot\boldsymbol{n}\rangle_{\Gamma_h}=0.$$

It follows from the single-value of $\boldsymbol{q}$, $\hat{\boldsymbol{q}}_h$ and $I_h\psi$ in the interior faces that

$$\langle(\boldsymbol{q}-\hat{\boldsymbol{q}}_h)\cdot\boldsymbol{n},I_h\psi\rangle_{\Gamma_h\backslash\partial\Omega}=0.$$

We notice $I_h\psi=0$ by the boundary condition of the dual problem (3.14c). So we have

$$\langle(\boldsymbol{q}-\hat{\boldsymbol{q}}_h)\cdot\boldsymbol{n},I_h\psi\rangle_{\partial\Omega}=0.$$

Adding the above two equations, we get that

$$\langle(\boldsymbol{q}-\hat{\boldsymbol{q}}_h)\cdot\boldsymbol{n},I_h\psi\rangle_{\Gamma_h}=0.$$

Substituting the above these equations into (3.16) and rearranging all the terms, we obtain that

$$\begin{aligned}(P_{r-1}(\Pi_W^H u - u_h)(T), \theta)_{\Omega_h} = \int_0^T \Bigg[& \left(\frac{\partial(\Pi_W^H u - u_h)}{\partial t}, P_{r-1}\psi - I_h\psi \right)_{\Omega_h} \\ & + i(\boldsymbol{q} - \boldsymbol{\Pi}_V^H \boldsymbol{q}, \boldsymbol{\Pi}^{BDM}\nabla\psi - \nabla P_L\psi)_{\Omega_h} \\ & + i(\boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h, \nabla I_h\psi - \boldsymbol{\Pi}^{BDM}\nabla\psi)_{\Omega_h} \\ & + i\left(\frac{\partial(u - \Pi_W^H u)}{\partial t}, I_h\psi - P_{r-1}\psi \right)_{\Omega_h} \Bigg] \mathrm{d}t.\end{aligned}$$

This completes the proof. □

To obtain the result of Theorem 2.4, we need have these estimates of $P_{r-1}\psi - I_h\psi$, $\boldsymbol{\Pi}^{BDM}\nabla\psi - \nabla P_L\psi$ and $\boldsymbol{\Pi}^{BDM}\nabla\psi - \nabla I_h\psi$, which are seen in Proposition 3.6 of [4].

Proposition 3.8. *The projection $\boldsymbol{\Pi}^{BDM}$ is defined in [4]. I_h is any interpolation operator from $L^2(\Omega)$ into $W_h \cap H_0^1(\Omega)$. Then there exist the approximation results,*

$$\begin{aligned}&\|P_{r-1}\psi - I_h\psi\| \le Ch^2\|\psi\|_{H^2}, \\ &\|\boldsymbol{\Pi}^{BDM}\nabla\psi - \nabla P_L\psi\| \le Ch\|\psi\|_{H^2}, \\ &\|\boldsymbol{\Pi}^{BDM}\nabla\psi - \nabla I_h\psi\| \le Ch\|\psi\|_{H^2}.\end{aligned}$$

Proof of Theorem 2.4. The superconvergence estimate of $P_{r-1}(\Pi_W^H u - u_h)(T)$.

Proof. Following the identity (3.15) of Lemma 3.6 and using Cauchy–Schwartz inequality, we have that

$$\begin{aligned}\|P_{r-1}(\Pi_W^H u - u_h)(T)\|_{L^2(\Omega_h)} &= \sup_{\theta\in W_h} \frac{(P_{r-1}(\Pi_W^H u - u_h)(T), \theta)}{\|\theta\|_{L^2(\Omega_h)}} \\ \le \sup_{\theta\in W_h} \frac{1}{\|\theta\|_{L^2(\Omega_h)}} \int_0^T \Bigg[& \left\| \frac{\partial(\Pi_W^H u - u_h)}{\partial t} \right\|_{L^2(\Omega_h)} \|P_{r-1}\psi - I_h\psi\|_{L^2(\Omega_h)} \\ & + \|\boldsymbol{q} - \boldsymbol{\Pi}_V^H \boldsymbol{q}\|_{L^2(\Omega_h)} \|\boldsymbol{\Pi}^{BDM}\nabla\psi - \nabla P_L\psi\|_{L^2(\Omega_h)} \\ & + \|\boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h\|_{L^2(\Omega_h)} \| - \boldsymbol{\Pi}^{BDM}\nabla\psi + \nabla I_h\psi\|_{L^2(\Omega_h)} \\ & + \left\| \frac{\partial(u - \Pi_W^H u)}{\partial t} \right\|_{L^2(\Omega_h)} \|I_h\psi - P_{r-1}\psi\|_{L^2(\Omega_h)} \Bigg] \mathrm{d}t.\end{aligned}$$

Substituting the bounds of Proposition 3.8 into the above inequality and using Theorem 2.1 and the elliptic regularity, we have that

$$\begin{aligned}\|P_{r-1}(\Pi_W^H u - u_h)(T)\|_{L^2(\Omega_h)} \le & Ch \left\| \frac{\partial(\Pi_W^H u - u_h)}{\partial t} \right\|_{L^2(L^2(\Omega_h))} + Ch\|\boldsymbol{q} - \boldsymbol{\Pi}_V^H \boldsymbol{q}\|_{L^2(L^2(\Omega_h))} \\ & + Ch\|\boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h\|_{L^2(L^2(\Omega_h))} + Ch \left\| \frac{\partial(u - \Pi_W^H u)}{\partial t} \right\|_{L^2(L^2(\Omega_h))}.\end{aligned}$$

This completes the proof. □

Proof of Theorem 2.5. The superconvergence of the postprocessing method.

Proof. By the equations (2.7) defining the postprocessed approximation u_h^* and the orthogonalities of the HDG projection (2.5a) and the L^2 projection P_L, we have that

$$\begin{aligned}(u-u_h^*,w)_K&=(P_{r-1}(\Pi_W^H u-u_h),w)_K \qquad \forall w\in\mathscr{P}_{r-1}(K),\\ (\nabla(u-u_h^*),\nabla w)_K&=(\Pi_V^H\boldsymbol{q}-\boldsymbol{q}_h,\nabla w)_K \qquad \forall w\in\mathscr{P}_{r-1}^{\perp}(K).\end{aligned}$$

By Poincare inequality and the well-known argument give that

$$\|u-u^*\|_K\le Ch_K^{r+2}\|u\|_{H^{r+2}(K)}+C\|P_{r-1}(\Pi_W^H u-u_h)\|_K+Ch_K\|\Pi_V^H\boldsymbol{q}-\boldsymbol{q}_h\|_K.$$

Applying the results of Theorems 2.3 and 2.4 can prove Theorem 2.5. □

The conclusion of Theorem 2.3 with convergence order $r+1$ is an optimal convergence result. Note that we do not assume the regularity condition here. In many relevant literatures, people derive higher order convergence for the finite element scheme of similar equations under sufficient regularity conditions. Thus a natural question is whether our finite element method has superconvergence result. Theorem 2.6 answers this question. Let us discuss this point in detail.

Proof of Theorem 2.6. Superconvergence.

Lemma 3.9. *$(u,\boldsymbol{q})$ and $(u_h,\boldsymbol{q}_h)$ are the exact solution and the approximation solution of the problems (1.2) and (2.1). Then for any $T>0$, we have that*

$$\begin{aligned}((\Pi_W^H u-u_h)(T),\theta)=&\int_0^T\left(\frac{\partial(\Pi_W^H u-u_h)}{\partial t},\psi-\Pi_W^H\psi\right)_{\Omega_h}+(\boldsymbol{q}-\boldsymbol{\Pi}_V^H\boldsymbol{q},\boldsymbol{\Pi}_V^H\nabla\psi-\nabla P_L\psi)_{\Omega_h}\\ &+(\boldsymbol{q}_h-\boldsymbol{\Pi}_V^H\boldsymbol{q},\boldsymbol{\Pi}_V^H\boldsymbol{\varphi}-\boldsymbol{\varphi})_{\Omega_h}+\left(\frac{\partial(u-\Pi_W^H u)}{\partial t},\Pi_W^H\psi-P_{r-1}\psi\right)_{\Omega_h}.\end{aligned}$$

Proof. It follows from the dual problem (3.14d), Newton–Leibniz formula and the initial condition $(\Pi_W^H u-u_h)(0)=0$ that

$$\begin{aligned}((\Pi_W^H u-u_h)(T),\theta)&=\int_0^T\left[\left(\frac{\partial(\Pi_W^H u-u_h)}{\partial t},\psi\right)_{\Omega_h}+\left(\Pi_W^H u-u_h,\frac{\partial\psi}{\partial t}\right)_{\Omega_h}\right]\mathrm{d}t\\ &=\int_0^T\left[\left(\frac{\partial(\Pi_W^H u-u_h)}{\partial t},\psi\right)_{\Omega_h}+i(\Pi_W^H u-u_h,\nabla\cdot\boldsymbol{\varphi})_{\Omega_h}\right]\mathrm{d}t. \qquad (3.17)\end{aligned}$$

We discuss the second term of the equation (3.17):

$$\begin{aligned}(\Pi_W^H u-u_h,\nabla\cdot\boldsymbol{\varphi})_{\Omega_h}&=(\Pi_W^H u-u_h,\nabla\cdot\boldsymbol{\Pi}_V^H\boldsymbol{\varphi})_{\Omega_h}+(\Pi_W^H u-u_h,\nabla\cdot(\boldsymbol{\varphi}-\boldsymbol{\Pi}_V^H\boldsymbol{\varphi}))_{\Omega_h}\\ &=(\Pi_W^H u-u_h,\nabla\cdot\boldsymbol{\Pi}_V^H\boldsymbol{\varphi})_{\Omega_h}+\langle\Pi_W^H u-u_h,(\boldsymbol{\varphi}-\boldsymbol{\Pi}_V^H\boldsymbol{\varphi})\cdot\boldsymbol{n}\rangle_{\Gamma_h}, \qquad (3.18)\end{aligned}$$

by the integration by parts and the property of the projection $\mathbf{\Pi}_V^H$ (2.5a). Using the error equation (3.5b) with $\boldsymbol{v} = \mathbf{\Pi}_V^H \boldsymbol{\varphi}$ and the dual equation (3.14a) for the first term of right hand of the equation (3.18), we have that

$$\begin{aligned}
&(\Pi_W^H u - u_h, \nabla \cdot \mathbf{\Pi}_V^H \boldsymbol{\varphi})_{\Omega_h} \\
&\quad = (\mathbf{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h, \mathbf{\Pi}_V^H \boldsymbol{\varphi})_{\Omega_h} + \langle u - \hat{u}_h, \mathbf{\Pi}_V^H \boldsymbol{\varphi} \cdot \boldsymbol{n} \rangle_{\Gamma_h} + (\boldsymbol{q} - \mathbf{\Pi}_V^H \boldsymbol{q}, \mathbf{\Pi}_V^H \boldsymbol{\varphi})_{\Omega_h} \\
&\quad = (\mathbf{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h, \mathbf{\Pi}_V^H \boldsymbol{\varphi} - \boldsymbol{\varphi})_{\Omega_h} + (\boldsymbol{q}_h - \mathbf{\Pi}_V^H \boldsymbol{q}, \nabla \psi)_{\Omega_h} \\
&\qquad + \langle u - \hat{u}_h, \mathbf{\Pi}_V^H \boldsymbol{\varphi} \cdot \boldsymbol{n} \rangle_{\Gamma_h} + (\boldsymbol{q} - \mathbf{\Pi}_V^H \boldsymbol{q}, \mathbf{\Pi}_V^H \boldsymbol{\varphi})_{\Omega_h}.
\end{aligned}$$

Inserting the above equation into (3.18) gives that

$$\begin{aligned}
(\Pi_W^H u - u_h, \nabla \cdot \boldsymbol{\varphi})_{\Omega_h} =& (\mathbf{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h, \mathbf{\Pi}_V^H \boldsymbol{\varphi} - \boldsymbol{\varphi})_{\Omega_h} + (\boldsymbol{q}_h - \mathbf{\Pi}_V^H \boldsymbol{q}, \nabla \psi)_{\Omega_h} + (\boldsymbol{q} - \mathbf{\Pi}_V^H \boldsymbol{q}, \mathbf{\Pi}_V^H \boldsymbol{\varphi})_{\Omega_h} \\
&+ \langle u - \hat{u}_h, \mathbf{\Pi}_V^H \boldsymbol{\varphi} \cdot \boldsymbol{n} \rangle_{\Gamma_h} + \langle \Pi_W^H u - u_h, (\boldsymbol{\varphi} - \mathbf{\Pi}_V^H \boldsymbol{\varphi}) \cdot \boldsymbol{n} \rangle_{\Gamma_h}.
\end{aligned}$$

We discuss the second term of the above equation:

$$\begin{aligned}
(\boldsymbol{q}_h - \mathbf{\Pi}_V^H \boldsymbol{q}, \nabla \psi)_{\Omega_h} =& (\boldsymbol{q}_h - \mathbf{\Pi}_V^H \boldsymbol{q}, \nabla \Pi_W^H \psi)_{\Omega_h} + (\boldsymbol{q}_h - \mathbf{\Pi}_V^H \boldsymbol{q}, \nabla(\psi - \Pi_W^H \psi))_{\Omega_h} \\
=& - i \left(\frac{\partial (u_h - \Pi_W^H u)}{\partial t}, \Pi_W^H \psi \right)_{\Omega_h} - i \left(\frac{\partial (u - \Pi_W^H u)}{\partial t}, \Pi_W^H \psi \right)_{\Omega_h} \\
&+ \langle (\hat{\boldsymbol{q}}_h - \boldsymbol{q}) \cdot \boldsymbol{n}, \Pi_W^H \psi \rangle_{\Gamma_h} + \langle (\boldsymbol{q}_h - \mathbf{\Pi}_V^H \boldsymbol{q}) \cdot \boldsymbol{n}, \psi - \Pi_W^H \psi \rangle_{\Gamma_h},
\end{aligned} \tag{3.19}$$

by using the error equation (3.5a) for the first term of the first equal, integration by parts for the second term in the first equal, and the definition of the projection Π_W^H. Combining the equations from (3.17) to (3.19), we have that

$$\begin{aligned}
((\Pi_W^H u - u_h)(T), \theta) = \int_0^T & \left(\frac{\partial (\Pi_W^H u - u_h)}{\partial t}, \psi - \Pi_W^H \psi \right)_{\Omega_h} + (\boldsymbol{q} - \mathbf{\Pi}_V^H \boldsymbol{q}, \mathbf{\Pi}_V^H \nabla \psi - \nabla P_L \psi)_{\Omega_h} \\
&+ (\boldsymbol{q}_h - \mathbf{\Pi}_V^H \boldsymbol{q}, \mathbf{\Pi}_V^H \boldsymbol{\varphi} - \boldsymbol{\varphi})_{\Omega_h} + \left(\frac{\partial (u - \Pi_W^H u)}{\partial t}, \Pi_W^H \psi - P_{r-1} \psi \right)_{\Omega_h} \\
&+ \langle u - \hat{u}_h, \mathbf{\Pi}_V^H \boldsymbol{\varphi} \cdot \boldsymbol{n} \rangle_{\Gamma_h} + \langle \Pi_W^H u - u_h, (\boldsymbol{\varphi} - \mathbf{\Pi}_V^H \boldsymbol{\varphi}) \cdot \boldsymbol{n} \rangle_{\Gamma_h} \\
&+ \langle (\hat{\boldsymbol{q}}_h - \boldsymbol{q}) \cdot \boldsymbol{n}, \Pi_W^H \psi \rangle_{\Gamma_h} + \langle (\boldsymbol{q}_h - \mathbf{\Pi}_V^H \boldsymbol{q}) \cdot \boldsymbol{n}, \psi - \Pi_W^H \psi \rangle_{\Gamma_h}.
\end{aligned}$$

We only prove that the sum of the last four terms is vanished in the above equation. Indeed, by the single value of $P_\partial u, P_\partial \boldsymbol{q}, \hat{u}_h$ and $\hat{\boldsymbol{q}}_h$, definition of numerical trace (2.2), equation (2.3) and boundary condition (3.14c)

$$\begin{aligned}
&\langle u - \hat{u}_h, \mathbf{\Pi}_V^H \boldsymbol{\varphi} \cdot \boldsymbol{n} \rangle_{\Gamma_h} + \langle \Pi_W^H u - u_h, (\boldsymbol{\varphi} - \mathbf{\Pi}_V^H \boldsymbol{\varphi}) \cdot \boldsymbol{n} \rangle_{\Gamma_h} \\
&\qquad + \langle (\hat{\boldsymbol{q}}_h - \boldsymbol{q}) \cdot \boldsymbol{n}, \Pi_W^H \psi \rangle_{\Gamma_h} + \langle (\boldsymbol{q}_h - \mathbf{\Pi}_V^H \boldsymbol{q}) \cdot \boldsymbol{n}, \psi - \Pi_W^H \psi \rangle_{\Gamma_h} \\
&\quad = \langle P_\partial u - \hat{u}_h, (\mathbf{\Pi}_V^H \boldsymbol{\varphi} - \boldsymbol{\varphi}) \cdot \boldsymbol{n} \rangle_{\Gamma_h} + \langle \Pi_W^H u - u_h, (\boldsymbol{\varphi} - \mathbf{\Pi}_V^H \boldsymbol{\varphi}) \cdot \boldsymbol{n} \rangle_{\Gamma_h} \\
&\qquad + \langle (\hat{\boldsymbol{q}}_h - P_\partial \boldsymbol{q}) \cdot \boldsymbol{n}, \Pi_W^H \psi - \psi \rangle_{\Gamma_h} + \langle (\boldsymbol{q}_h - \mathbf{\Pi}_V^H \boldsymbol{q}) \cdot \boldsymbol{n}, \psi - \Pi_W^H \psi \rangle_{\Gamma_h} \\
&\quad = \langle u_h - \Pi_W^H u + P_\partial u - \hat{u}_h, (\mathbf{\Pi}_V^H \boldsymbol{\varphi} - \boldsymbol{\varphi}) \cdot \boldsymbol{n} \rangle_{\Gamma_h} \\
&\qquad + \langle (\hat{\boldsymbol{q}}_h - P_\partial \boldsymbol{q}) \cdot \boldsymbol{n} - (\boldsymbol{q}_h - \mathbf{\Pi}_V^H \boldsymbol{q}) \cdot \boldsymbol{n}, \Pi_W^H \psi - \psi \rangle_{\Gamma_h} \\
&\quad = \langle u_h - \Pi_W^H u + P_\partial u - \hat{u}_h, (\mathbf{\Pi}_V^H \boldsymbol{\varphi} - \boldsymbol{\varphi}) \cdot \boldsymbol{n} + \tau (\Pi_W^H \psi - \psi) \rangle_{\Gamma_h} = 0,
\end{aligned}$$

by the definition of HDG projection (2.5c) and numerical flux (2.4). Combining the above two equations implies the result. This completes the proof. □

We immediately obtain the following consequence of the result of Lemma 3.9 by Cauchy–Schwartz inequality.

Corollary 3.10. *For all $T > 0$, we have that*

$$
\begin{aligned}
\|(\Pi_W^H u - u_h)(T)\| \le & \|\boldsymbol{\Pi}_V^H \boldsymbol{q} - \boldsymbol{q}_h\|_{L^\infty(L^2)} \sup_{\theta \in W_h} \frac{\|\boldsymbol{\Pi}_V^H \boldsymbol{\varphi} - \boldsymbol{\varphi}\|_{\Omega_h}}{\|\theta\|_{L^2(\Omega_h)}} \\
& + \left\| \frac{\partial(u_h - \Pi_W^H u)}{\partial t} \right\|_{L^2(L^2)} \sup_{\theta \in W_h} \frac{\|\psi - \Pi_W^H \psi\|_{L^1(L^2)}}{\|\theta\|_{L^2(\Omega_h)}} \\
& + \left\| \frac{\partial(u - \Pi_W^H u)}{\partial t} \right\|_{L^2(L^2)} \sup_{\theta \in W_h} \frac{\|P_{r-1}\psi - \Pi_W^H \psi\|_{L^1(L^2)}}{\|\theta\|_{L^2(\Omega_h)}} \\
& + \|\boldsymbol{q} - \boldsymbol{\Pi}_V^H \boldsymbol{q}\|_{L^\infty(L^2)} \sup_{\theta \in W_h} \frac{\|\boldsymbol{\Pi}_V^H \nabla \psi - \nabla P_L \psi\|_{L^1(L^2)}}{\|\theta\|_{L^2(\Omega_h)}},
\end{aligned}
$$

where $(\psi, \boldsymbol{\varphi})$ is the solution of the dual problem (3.13) or (3.14).

To obtain Theorem 2.6, we have the estimates of all projection approximations. The following proposition presents the estimates we need.

Proposition 3.11. *Assume that the following elliptic regularity holds, i.e., for any function $\psi \in H_0^1(\Omega)$, we have the elliptic regularity inequality*

$$\|\psi\|_{H_0^1(\Omega)} \le C_{reg} \|\Delta \psi\|.$$

Then we have that

$$
\begin{aligned}
\|\nabla \psi - \nabla P_L \psi\|_{L^2(\Omega)} &\le Ch \|\Delta \psi\|_{L^2(\Omega)}, \\
\|\psi - P_{r-1}\psi\|_{L^2(\Omega)} &\le Ch \|\nabla \psi\|_{L^2(\Omega)}.
\end{aligned}
$$

These estimates can be seen in [5]. Combining the approximation estimates with the similar parabolic regularity estimates

$$\|\Delta \psi\|_{L^2(L^2)}^2 \le C\|\theta\|, \quad \forall \theta \in H^1(\Omega),$$

by Proposition 3.3. Using the Cauchy–Schwartz inequality directly get the following result:

$$
\begin{aligned}
\|(\Pi_W^H u - u_h)(T)\|_{L^2} = \sup_{\theta \in W_h} \frac{((\Pi_W^H u - u_h)(T), \theta)}{\|\theta\|_{L^2(\Omega_h)}} \le Ch \Big(\| \frac{\partial(\Pi_W^H u - u_h)}{\partial t} \|_{L^2(L^2)} \\
+ \left\| \frac{\partial(u - \Pi_W^H u)}{\partial t} \right\|_{L^2(L^2)} + \|\boldsymbol{q} - \boldsymbol{\Pi}_V^H \boldsymbol{q}\|_{L^2(L^2)} + \|\boldsymbol{q}_h - \boldsymbol{\Pi}_V^H \boldsymbol{q}\|_{L^2(L^2)} \Big).
\end{aligned}
$$

Using Theorem 2.3 completes the proof of Theorem 2.6.

4. Conclusion

In this paper the numerical trace and numerical flux are constructed to preserve the conservative property for the density of the particle described. We prove that there exist the superconvergence properties of HDG method, which do hold for second-order elliptic problems, uniformly in time for the semidiscretization by the same method of Schrödinger equations provided that enough regularity is satisfied.

Based on current research, we are going to work on the error analysis to the fully discrete HDG scheme for Schrödinger equation with non-zero potential. Besides, some numerical experiments will be carry out to validate the theoretical results.

Appendix A. Proofs of some auxiliary results

Proof of Proposition 3.2 on boundness.

Proof. Without the loss of the general, we assume that $\frac{b}{a}$ is bounded, *i.e.*, $|\frac{b}{a}| \leq \frac{Q_z}{2}$.

$$\int_0^T (b\frac{\partial a}{\partial t} - a\frac{\partial b}{\partial t})\mathrm{d}t = \int_0^T \frac{a_t b - b_t a}{a^2} \cdot a^2 \mathrm{d}t = \int_0^T -\left(\frac{b}{a}\right)_t \cdot a^2 \mathrm{d}t,$$

by the rule of the division derivation.

$$\int_0^T -\left(\frac{b}{a}\right)_t \cdot a^2 \mathrm{d}t = a^2(\xi) \int_0^T -\left(\frac{b}{a}\right)_t \cdot \mathrm{d}t = a^2(\xi)\left(\frac{b}{a}(0) - \frac{b}{a}(T)\right),$$

by the integral mean value theorem.

$$\left| a^2(\xi)\left(\frac{b}{a}(0) - \frac{b}{a}(T)\right)\right| \leq Q_z R,$$

by the bound of $\frac{b}{a}$ and $|z| \leq R$. This completes the proof. □

Proof of Proposition 3.6 on parabolic regularity.

Proof. We decomposing the complex function ψ into its real part and imaginary part $\psi = \psi_R + i\psi_I$ with ψ_R and ψ_I being real functions. Multiply the dual equation (3.13a) by $\bar{\psi}$ and integrate the resulting equation over Ω, we have that

$$\int_\Omega \left(\frac{\partial \psi}{\partial t}\psi - i\Delta\psi\psi\right)\mathrm{d}x = \int_\Omega \left(\frac{\partial \psi}{\partial t}\psi - i|\nabla\psi|^2\right)\mathrm{d}x = 0,$$

by the integration by parts and the boundary condition (3.13c). Substituting $\psi = \psi_R + i\psi_I$ into the first term of the above equation and with the simple algebraic computation, we have that

$$\frac{\partial}{\partial t}(\|\psi_R\|^2_{L^2(\Omega)} + \|\psi_I\|^2_{L^2(\Omega)}) + i\int_\Omega \left(\frac{\partial \psi_I}{\partial t}\psi_R - \frac{\partial \psi_R}{\partial t}\psi_I\right)\mathrm{d}x + i|\|\nabla\psi\|^2_{L^2(\Omega)} = 0.$$

Taking the real part and imaginary part, respectively, we have that

$$\frac{\partial}{\partial t}(\|\psi_R\|^2_{L^2(\Omega)} + \|\psi_I\|^2_{L^2(\Omega)}) = 0, \tag{A.1}$$

and

$$\|\nabla\psi\|^2_{L^2(\Omega)} = -\int_\Omega \left(\frac{\partial \psi_I}{\partial t}\psi_R - \frac{\partial \psi_R}{\partial t}\psi_I\right)\mathrm{d}x. \tag{A.2}$$

It follows (A.1) and initial condition (3.14d) from that

$$\psi_R = \theta(x) \sin t \quad \text{and} \quad \psi_R = \theta(x) \cos t.$$

Substituting the above equations into (A.2) implies the first estimate. Using the same techniques can prove the second inequality. This finish the proof. □

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References

[1] I. Alonso-Mallo and N. Reguera, A high order finite element discretization with local absorbing boundary conditions of the linear Schrödinger equation. *J. Comput. Phys.* **220** (2006) 409–421.
[2] X. Antoine, C. Besse and V. Mouysset, Numerical schemes for simulation of the two-dimensional Schrödinger equation using non-reflecting boundary conditions. *Math. Comput.* **73** (2004) 1779–1799.
[3] A. Borzi and E. Decker, Analysis of a leap-frog pseudospectral scheme for the Schrödinger equation. *J. Comput. Appl. Math.* **193** (2006) 65–88.
[4] F. Brezzi and M. Fortin, Mixed and Hybrid Finite Element Methods. Springer-Verlag, New York (1991) 90–132.
[5] B. Chabaud and B. Cockburn, Uniform-in-time superconvergence of HDG methods for the heat equation. *Math. Comput.* **81** (2012) 107–129.
[6] H. Chen, R. Ewing and R. Lazarov, Superconvergence of mixed finite element methods for parabolic problems with nonsmooth initial data. *Numer. Math.* **78** (1998) 495–521.
[7] E.T. Chung, Q. Du and J. Zou, Convergence analysis of a finite volume method for Maxwell's equations in nonhomogeneous media. *SIAM J. Numer. Anal.* **41** (2003) 37–63.
[8] B. Cockburn, B. Dong and J. Guzmán, A superconvergent LDG-hybridizable Galerkin method for second-order elliptic problems. *Math. Comput.* **77** (2008) 1887–1916.
[9] B. Cockburn, B. Dong and J. Guzman, A hybridizable and superconvergent discontinuous Galerkin method for biharmonic problems. *J. Scient. Comput.* **40** (2009) 141–187.
[10] B. Cockburn, J. Guzman and H. Wang, Superconvergent discontinuous Galerkin methods for second-order elliptic problems. *Math. Comput.* **78** (2009) 1–24.
[11] B. Cockburn, J. Gopalakrishnan and R. Lazarov, Unified hybridization of discontinuous Galerkin, mixed, and continuous Galerkin methods for second order elliptic problems. *SIAM J. Numer. Anal.* **47** (2009) 1319–1365.
[12] B. Cockburn, W. Qiu and M. Solano, A priori error analysis for HDG methods using extensions from subdomains to achieve boundary conformity. *Math. Comput.* **83** (2014) 665–699.
[13] B. Dong, C. Shu and W. Wang, A new multiscale discontinuous Galerkin method for the one-dimensional stationary Schrödinger equation. *J. Sci Comput.* **66** (2016) 321–345.
[14] R. Ewing and R. Lazarov, Superconvergence of the mixed finite element approximations of parabolic problems using rectangular finite elements. *East-West J. Numer. Math.* **1** (1993) 199–212.
[15] K. Fan, W. Cai and X. Ji, A generalized discontinuous Galerkin (GDG) method for Schrödinger equations with nonsmooth solutions, *J. Comput. Phys.* **227** (2008) 2387–2410.
[16] G. Fu, W. Qiu and W. Zhang, An analysis of HDG methods for convection-dominated diffusion problems. *ESAIM: M2AN* **49** (2015) 225–256.
[17] L. Gastaldi and R.H. Nochetto, Sharp maximum norm error estimates for general mixed finite element approximations to second order elliptic equations. *RAIRO Model. Math. Anal. Numer.* **23** (1989) 103–128.
[18] J. Gopalakrishnan, B. Cockburn and F.J. Sayas, A projection-based error analysis of HDG methods. *Math. Comput.* **79** (2010) 1351–1367.
[19] H. Han, J. Jin and X. Wu, A finite difference method for the one-dimensional time-dependent Schrödinger equation on unbounded domain. *Comput. Math. Appl.*, **50** (2005) 1345–1362.
[20] P. Harrison, Quantum Wells, Wires and Dots. John Wiley & Sons, New York (2000).
[21] M. Javidi and A. Golbabai, Numerical studies on nonlinear Schrödinger equations by spectral collocation method with preconditioning. *J. Math. Anal. Appl.* **333** (2007) 1119–1127.
[22] J. Jin and X. Wu, Analysis of finite element method for one-dimensional time-dependent Schrödinger equation on unbounded domain. *J. Comput. Appl. Math.* **220** (2008) 240–256.
[23] H. Liao, Z. Sun and H. Shi, Error estimate of fourth-order compact scheme for linear Schrödinger equations. *SIAM J. Numer. Anal.* **47** (2010) 4381–4401.
[24] T. Lu, W. Cai and P. Zhang, Conservative local discontinuous Galerkin methods for time dependent Schrödinger equation. *Int. J. Numer. Anal. Model.* **2** (2014) 72–80.
[25] P. Lu, H. Chen and W. Qiu, An absolutely stable hp-HDG method for the time-harmonic Maxwell equations with high wave number. *Math. Comput.* **86** (2017) 1553–1577.

[26] N.C. Nguyen, J. Peraire and B. Cockburn, Hybridizable discontinuous Galerkin methods, in Spectral and High Order Methods for Partial Differential Equations. Springer (2011) 63–84.

[27] W. Qiu and K. Shi, An HDG method for convection diffusion equation. *J. Scient. Comput.* **66** (2016) 346–357.

[28] W. Qiu and K. Shi, A superconvergent HDG methods for the incompressible Navier–Stokes equations on general polyhedral meshes. *IMA J. Numer. Anal.* **36** (2016) 1–18.

[29] L. Ramdas Ram-Mohan, Finite Element and Boundary Element Applications in Quantum Mechanics. Oxford University Press, Oxford (2002).

[30] P.A. Raviart and J.M. Thomas, A mixed finite element method for second order elliptic problems, in Mathematical Aspects of Finite Element Method. Vol. 606 of *Lecture Notes in Math.*, edited by I. Galligani and E. Magenes. Springer-Verlag, New York (1977) 292–315.

[31] F.J. Says, From Raviart–Thomas to HDG: a personal voyage. Preprint arXiV: 1307.2491 (2013)

[32] L. Schiff, Quantum Mechanics. McGraw-Hill, New York (1968).

[33] R. Stenberg, Postprocessing schemes for some mixed finite elements. *RAIRO Model. Math. Anal. Numer.* **25** (1991) 151–167.

[34] J. Wang, A new error analysis of Crank–Nicolson Galerkin FEMs for a generalized nonlinear Schrödinger equation. *J. Sci. Comput.* **60** (2014) 390–407.