On Error Estimates of the Crank-Nicolson-Polylinear Finite Element Method with the Discrete TBC for the Generalized Schrödinger Equation in an Unbounded Parallelepiped

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Abstract. We deal with an initial-boundary value problem for the generalized time-dependent Schrödinger equation with variable coefficients in an unbounded \( n \)-dimensional parallelepiped \( (n \geq 1) \). To solve it, the Crank-Nicolson in time and the polylinear finite element in space method with the discrete transparent boundary conditions is considered. We present its stability properties and derive new error estimates \( O(\tau^2 + |h|^2) \) uniformly in time in \( L^2 \) space norm, for \( n \geq 1 \), and mesh \( H^1 \) space norm, for \( 1 \leq n \leq 3 \) (a superconvergence result), under the Sobolev-type assumptions on the initial function. Such estimates are proved for methods with the discrete TBCs for the first time.

Keywords: time-dependent Schrödinger equation, unbounded domain, Crank-Nicolson scheme, finite element method, discrete transparent boundary conditions, stability, error estimates, superconvergence.

1 Introduction

The linear time-dependent Schrödinger equation is the key one in many physical fields. It should be often solved in unbounded space domains. A number of approaches were developed to deal with such problems using approximate transparent boundary conditions (TBCs) at the artificial boundaries.

Among the best methods of such kind are those using the so-called discrete TBCs remarkable by the clear mathematical background and the corresponding rigorous stability results in theory as well as the complete absence of spurious reflections in practice. They first were constructed and studied for the standard Crank-Nicolson in time finite-difference schemes, see [15] and also [23], in the cases of the infinite or semi-infinite axis and strip. Later families of finite-difference schemes with general space averages were treated in [11,21,15]. In particular, they include the linear and bilinear FEMs in space.

In this paper, we consider the Crank-Nicolson-polylinear FEM in an unbounded \( n \)-dimensional parallelepiped \( (n \geq 1) \), present results on its stability
with respect to the initial data and a free term as well as on exploiting the
discrete TBCs and mainly derive the corresponding new error estimates $O(\tau^2 + |h|^2)$
uniform in time and in $L^2$ norm (for $n \geq 1$) and mesh $H^1$ norm (for $1 \leq n \leq 3$
in space under the Sobolev-type assumptions on the initial function. The latter estimate is a superconvergence result. Such estimates are proved for the methods with the discrete TBCs for the first time. Importantly, the error estimates contain no mesh steps in negative powers like for other approximate TBCs, see [67], that is one more advantage of using the discrete TBCs.

2 The IBVP and numerical methods to solve it

We deal with the initial-boundary value problem (IBVP) for the time-dependent
generalized Schrödinger equation with $n \geq 1$ space variables

$$
ih\rho D_t \psi = \mathcal{H}\psi := -\tfrac{k^2}{\hbar^2} \text{div}(B \nabla \psi) + V\psi \quad \text{on} \quad \Pi \times (0,T),$$

$$
\psi|_{\partial\Pi} = 0, \quad \psi|_{t=0} = \psi^0(x) \quad \text{on} \quad \Pi. \quad (2)
$$

Hereafter $\psi = \psi(x,t)$ is the complex-valued unknown wave function, $i$ is the
imaginary unit and $\hbar > 0$ is a physical constant. The $x = (x_1, \ldots, x_n)$-depending
coefficients $\rho, V \in L^\infty(\Pi)$ and the $n \times n$ matrix $B \in L^\infty(\Pi)$ are real-valued
and satisfy $\rho(x) \geq \rho_0 > 0$ and $B(x) \geq B_0 I > 0$ on $\Pi$, where $I$ is the unit matrix
(wheras $V$ can have any sign in general). Here $\Pi := \mathbb{R}$ for $n = 1$ or, for $n \geq 2,$
$\Pi := \mathbb{R} \times \Pi_1$ is the infinite parallelepiped, with $\Pi_1 := (0, X_2) \times \cdots \times (0, X_n).$

Also $D_t = \frac{\partial}{\partial t}$ and $D_i = \frac{\partial}{\partial x_i}$ are the partial derivatives, and the operators $\text{div}$
and $\nabla$ are taken with respect to space variables.

We also assume that, for some (sufficiently large) $X_0 > 0,$

$$\rho(x) = \rho_\infty, \quad B(x) = \text{diag}(B_{1\infty}, \ldots, B_{n\infty}), \quad V(x) = V_\infty \quad \text{for} \quad |x_1| \geq X_0, \quad (3)$$

where $\text{diag}(B_{1\infty}, \ldots, B_{n\infty})$ is the diagonal matrix with the listed positive diagonal entries. More generally, it could be easily assumed that $\rho, B$ and $V$ have different constant values for $x_1 \leq -X_0$ and for $x_1 \geq X_0.$ Let $X_1 > X_0,$ and

$\Omega = \Omega_X = (-X_1, X_1)$ for $n = 1$ or $\Omega = \Omega_X = (-X_1, X_1) \times \Pi_1$ for $n \geq 2.$

We consider the weak solution $\psi \in C([0,T]; H^1_0(\Pi))$ having $D_t \psi \in C([0,T];
L^2(\Pi))$ and satisfying the integral identity

$$
ih (D_t \psi(\cdot,t), \varphi)_{L^2(\Pi)} = \mathcal{H} \mathcal{I} (\psi(\cdot,t), \varphi) \quad \text{for any} \quad \varphi \in H^1_0(\Pi), \quad \text{on} \quad [0,T], \quad (4)
$$

and the initial condition $\psi|_{t=0} = \psi^0 \in H^1_0(\Pi).$ Hereafter we use the standard complex Lebesgue and Sobolev spaces (and subspaces), the weighted complex Lebesgue space $L^2(\rho; \mathcal{L}(\Omega))$ endowed by the inner product $(w, \varphi)_{L^2(\rho; \mathcal{L}(\Omega))} := (\rho w, \varphi)_{L^2(\Omega)},$ and the $\mathcal{H}$-related Hermitian-symmetric sesquilinear form

$$
\mathcal{L}_G (w, \varphi) := \tfrac{h^2}{2} (B \nabla w, \nabla \varphi)_{L^2(\Omega)} + (V w, \varphi)_{L^2(\Omega)}, \quad \text{with} \quad G = \Pi, \Omega, \text{etc.}
$$

We define a non-uniform mesh in $x_1$ on $\mathbb{R}$ containing the points $\pm X_1$ and being
uniform with a step $0 < h_1 < X_1$ outside $[-X_1 + h_1, X_1 - h_1] \supset [-X_0, X_0].$ We
also define non-uniform meshes in \( x_2, \ldots, x_n \) respectively on \([0, X_2], \ldots, [0, X_n]\) (containing the ends of the segments). They induce the partition of \( \Pi \) into finite elements that are rectangular parallelepipeds without common internal points. Let \(|h|\) be their maximal diagonal length. Let \( S_h(\Pi) \) be the (infinite-dimensional) subspace of functions in \( H^1_0(\Pi) \) that are polylinear over each element. Clearly \( S_h(\Pi) \subset C(\Pi) \cap L^2(\Pi) \). Let \( S_h \) be the restriction of \( S_h(\Pi) \) to \( \Omega \).

Let \( \mathcal{W}_h(\Pi) \) be the non-uniform mesh \( 0 = t_0 < \ldots < t_M = T \) with steps \( \tau_m := t_m - t_{m-1} \). We put \( \tau_{\text{max}} := \max_{1 \leq m \leq M} \tau_m \) and \( \hat{\tau}_m := \frac{\tau_m + \tau_{m+1}}{2} \) for \( 1 \leq m \leq M-1 \) and \( \hat{\tau}_0 := \frac{\tau_1}{2} \). We define the time mesh operators

\[
\partial_t Y^m := \frac{Y^m - Y^{m-1}}{\tau_m}, \quad \hat{\partial}_t Y^m := \frac{Y^{m+1} - Y^m}{\hat{\tau}_m}, \quad \bar{\Pi} Y^m := \frac{Y^{m-1} + Y^m}{2}.
\]

We introduce the Crank-Nicolson-polylinear FEM approximate solution \( \Psi: \mathcal{W}_h(\Pi) \to S_h(\Pi) \) satisfying the integral identity

\[
(\partial_t \Psi^m, \varphi)_{L^2(\Pi)} = (\hat{\partial}_t \varphi)_{L^2(\Pi)} = \mathcal{H}(\bar{\Pi} \varphi, \varphi) \quad \forall \varphi \in S_h(\Pi),
\]

(compare with (4)), and the initial condition \( \Psi|_{t=0} = \Psi^0 \in S_h(\Pi) \), where \( \Psi^0 \) is an approximation for \( \varphi^0 \).

Let \( \ell^m(\varphi) \) be a conjugate linear functional on \( S_h(\Pi) \) that we add to the right-hand side of (5) to study stability in more detail and to derive error estimates.

**Proposition 1.** Let \( \ell^m(\varphi) = (F^m, \varphi)_{L^2(\Pi)} \) with \( F^m \in L^2(\Pi) \) for \( 1 \leq m \leq M \). Then there exists a unique approximate solution \( \Psi \) and the following first stability bound holds

\[
\max_{0 \leq m \leq M} \| \Psi^m \|_{L^2(\Pi)} \leq \| \Psi^0 \|_{L^2(\Pi)} + \frac{2}{h} \sum_{m=1}^{M} \| F^m \|_{L^2(\Pi)} \tau_m.
\]

We introduce also the “energy” norm such that

\[
\| w \|_{H^1(\Pi)}^2 := \mathcal{H}(w, w) + \hat{\nu} \| w \|_{L^2(\Pi)}^2 \geq \delta \| w \|_{L^2(\Pi)}^2
\]

for any \( w \in H^1_0(\Pi) \), (7) with some real numbers \( \hat{\nu} \) and \( \delta > 0 \). Inequality (7) is knowingly valid for \( \hat{\nu} \) so large that \( \frac{\delta}{\hat{\nu} \lambda_0} V(x) + (\hat{\nu} - \delta) \rho(x) \geq 0 \) on \( \Omega \) with \( \lambda_0 := \sum_{k=2}^{n} (\bar{\pi}_k)^2 \) (here \( \lambda_0 = 0 \) for \( n = 1 \)). We define also the corresponding dual mesh depending norm

\[
\| w \|_{H^{-1}(\Pi)}^2 := \max_{\varphi \in S_h(\Pi)} | \langle w, \varphi \rangle_{\Pi} | \leq c \| w \|_{H^{-1}(\Pi)},
\]

where \( \langle w, \varphi \rangle_{\Pi} \) is the conjugate duality relation on \( H^{-1}(\Pi) \times H^1_0(\Pi) \) and \( H^{-1}(\Pi) = [H^1_0(\Pi)]^* \). Hereafter \( c \) and \( c_1 \) are generic constants independent of the meshes, any functions and \( T \) whereas \( c_0 \) denotes absolute constants (fixed numbers).
Proposition 2. Let $f_m^\infty(\varphi) = (F^m, \varphi)_\Omega$ with $F^m \in H^{-1}(\Omega)$ for $1 \leq m \leq M$ and $F^0 \in H^{-1}(\Omega)$ be arbitrary. Then there exists a unique approximate solution $\Psi$ and the following second stability bound holds
\[
\max_{0 \leq m \leq M} \|\Psi^m\|_{\mathcal{H}^0(\Omega)} \leq \|\Psi^0\|_{\mathcal{H}^0(\Omega)} + 4 \sum_{m=1}^{M} \left( \frac{\ell_m}{L} \|F^m\|_{H^{-1}(\Omega)} + \|\partial_1 F^m\|_{H^{-1}(\Omega)} \right) \tau_m + \|F^0\|^{(-1)}_h. \tag{8}
\]

Method 5 cannot be directly used in practice because of the infinite number of unknowns at each time level. Nevertheless it is possible to restrict the method to $\Omega$ provided that $\Psi^0 \in S_{0h} := \{ \varphi \in S_h; \varphi(x) = 0 \text{ on } \Omega \setminus \Omega_0 \}$, where $\Omega_0 := \Omega_{x_1-h_1,x_2-\ldots,x_n}$, and $\mathcal{W}_M$ is uniform with the step $\tau = \frac{\ell_s}{M}$. Let both assumptions be valid up to the end of the section.

By definition, the discrete TBCs are conditions at the artificial boundaries $x_1 = \pm X_1$ allowing to accomplish the restriction (they are non-local in $x_2, \ldots, x_n$ and $t$). To write down them explicitly, for clarity, we confine ourselves by the case of the uniform mesh in $x_k$ with the step $h_k = \frac{X_k}{J_k}$, for $2 \leq k \leq n$, and define the related well-known direct and inverse discrete sine Fourier transforms
\[
P^{(q)} = (F_k P)^{(q)} := \frac{2}{J_k} \sum_{j=1}^{J_k-1} P_j \sin \frac{\pi q j}{J_k}, \quad 1 \leq q \leq J_k - 1,
\]
\[
P_j = (F_k^{-1} P^{(q)}) := \sum_{q=1}^{J_k-1} P^{(q)} \sin \frac{\pi q j}{J_k}, \quad 1 \leq j \leq J_k - 1.
\]
The related eigenvalues of the 1D linear in $x_k$ FEM counterparts of the operators $-D^2_k$ and the unit one (for zero Dirichlet boundary values at $x_k = 0, X_k$) are
\[
\lambda_q^{(k)} = \left( \frac{2}{h_k} \sin \frac{\pi q h_k}{2X_k} \right)^2, \quad \sigma_q^{(k)} = 1 - \frac{2}{3} \sin^2 \frac{\pi q h_k}{2X_k} \in \left( \frac{1}{3}, 1 \right).
\]

Denote by $\omega_{h_1}$ the internal part of the introduced uniform mesh in $\bar{\Omega}$ and define the related mesh inner product
\[
(U, W)_{\omega_{h_1}} := \sum_{j_2=1}^{J_2-1} \cdots \sum_{j_n=1}^{J_n-1} U_{j_2, \ldots, j_n} W_{j_2, \ldots, j_n} h_2 \cdots h_n \quad \text{for } n \geq 2
\]
or set $(U, W)_{\omega_{h_1}} := UW^*$ for $n = 1$, where $W^*$ is the complex conjugate for $W$.

Recall that the discrete convolution of mesh functions $R, Q: \mathcal{W}_M \to \mathbb{C}$ is given by $(R * Q)^m := \sum_{p=0}^{m} R^p Q^{m-p}$ for $0 \leq m \leq M$.

Proposition 3. The restriction $\Psi|_{\Omega}$ of the above approximate solution obeys the integral identity on $\Omega$
\[
h_i \langle \mathcal{L}_\psi \Psi^m, \varphi \rangle_{L^2(\Omega)} = \mathcal{L}_\psi (\mathcal{S}_c \Psi^m, \varphi)
\]
\[
- \frac{h^2}{2} B_1 \infty (\mathcal{S}_c \Psi^m_{X_1}, \varphi|_{x_1 = X_1})_{\omega_{h_1}} + \frac{h^2}{2} B_1 \infty (\mathcal{S}_c \Psi^m_{-X_1}, \varphi|_{x_1 = -X_1})_{\omega_{h_1}} \tag{9}
\]
Then the solution to Proposition 4.

Hand side of (9) to study stability in more detail.

Here \( \Phi_{\pm X_1} = \{ \Phi^0 |_{x_1 = \pm X_1}, \ldots, \Phi^m |_{x_1 = \pm X_1} \} \) is a vector-function.

The operator \( \Phi^m \) in the discrete TBC has the form

\[
\Phi^m := F_2^{-1} \ldots F_n^{-1} \left[ \sigma_{q_2}^{(2)} \ldots \sigma_{q_n}^{(n)} R_q \Phi^m \right] \quad \text{on } \mathbb{T}_M
\]

for any \( \Phi: \omega_{\pm} \times \mathbb{T}_M \to \mathbb{C} \) such that \( \Phi^0 = 0 \), where \( \Phi^m := \{ \Phi^0, \ldots, \Phi^m \} \), \( \Phi^m : (F_{q_1} \ldots (F_{q_2})^{(q_2)} \ldots)^{(q_n)} \) and \( q = (q_2, \ldots, q_n) \). Here the kernel \( R_q \) can be computed by the recurrent formulas

\[
R_q^0 = c_1q, \quad R_q^1 = -c_1q \kappa q \mu q, \quad R_q^m = \frac{2m - 3}{m} \kappa q \mu q R_q^{m-1} - \frac{m - 3}{m} \kappa q^2 R_q^{m-2}, \quad m \geq 2,
\]

with the coefficients defined by

\[
c_1q = -\frac{|\alpha q|^{1/2}}{2} e^{-\sqrt{2} \alpha q}, \quad \kappa q = -e^{\sqrt{2} \alpha q}, \quad \mu q = \frac{\beta q}{|\alpha q|} \in (-1, 1),
\]

\[
\alpha q = 2a q + \frac{1}{3} \hbar^2 q^2 \neq 0, \quad \arg \alpha q \in (0, 2\pi), \quad \beta q = 2 \text{Re} a q + \frac{1}{3} \hbar^2 q^2 |\alpha q|^2,
\]

\[
a q = -\frac{V}{\hbar^2 \rho_{\infty}} + \frac{1}{2 \hbar^2 \rho_{\infty}} \left( B_2 \frac{\lambda_{q_2}^{(2)}}{\sigma_{q_2}^{(2)}} + \cdots + B_n \frac{\lambda_{q_n}^{(n)}}{\sigma_{q_n}^{(n)}} \right) + i \frac{2 \rho_{\infty}}{\hbar^2 \rho_{\infty}}.
\]

The next lemma is important to prove stability results for method [9], [10].

**Lemma 1.** The operator \( \Phi^m \) satisfies the inequalities [2,3]

\[
\text{Im} \sum_{l=1}^{m} (S_{\Phi^l} \Phi^i, \Phi^j)_{\omega_{\pm} \tau} \geq 0, \quad \text{Im} \sum_{l=1}^{m} (S_{\Phi^l} \Phi^i, (i \hbar \omega_{\pm} + \sqrt{\rho q}) \Phi^j)_{\omega_{\pm} \tau} \geq 0
\]

on \( \mathbb{T}_M \), for any \( \Phi: \omega_{\pm} \times \mathbb{T}_M \to \mathbb{C} \) such that \( \Phi^0 = 0 \) and \( \rho \geq -\frac{\sqrt{\rho_{\infty}}} {\rho_{\infty}} \) (see [3]).

Let \( \ell^m(\varphi) \) be a conjugate linear functional on \( S_h \) that we add to the right-hand side of \( (11) \) to study stability in more detail.

**Proposition 4.** Let \( \ell^m(\varphi) = (F^m, \varphi)_{L^2(\Omega)} \) with \( F^m \in L^2(\Omega) \) for \( 1 \leq m \leq M \). Then the solution to (9), (10) is unique and satisfies the first stability bound

\[
\max_{0 \leq m \leq M} \| \Phi^m \|_{L^2(\Omega)} \leq \| \Phi^0 \|_{L^2(\Omega)} + \frac{2}{\hbar} \sum_{m=1}^{M} \| F^m \|_{L^2(\Omega), 1} \frac{\tau}{\rho_{\infty}}.
\]

We introduce the “energy” norm on \( \Omega \) such that

\[
\| w \|_{L^2(\Omega) + \delta_{\rho}:\Omega}^2 := \mathcal{L}_{\Omega}(w, w) + \sqrt{\rho} \| w \|_{L^2(\Omega)}^2 > 0,
\]

for any \( \varphi \in S_h \) and \( 1 \leq m \leq M \), and the initial condition

\[
\psi_{t=0} = \psi^0 \in S_h.
\]

(10)
Proposition 5. satisfies the second stability bound $F$.

The following first error estimate holds

Proposition 6. $H$.

$\theta$ space averages depending on a parameter $\langle \rangle$ where

Here $\sigma \psi$ on $\Omega$.

formulas (12), see also [14]. For the linear and bilinear FEMs (for $\theta$ of those from [13] (given specifically for general FEM). The case $n$ let condition (7) be valid and

$3$ Error estimates

Let condition (17) be valid and $\sigma w$ be the elliptic projection of $w \in H^1_0(\Pi)$ onto $S_h(\Pi)$ such that

$L_\Pi(\sigma w, \varphi) + \hat{v}(\sigma w, \varphi)_{L^2(\Pi)} = L_\Pi(w, \varphi) + \hat{v}(w, \varphi)_{L^2(\Pi)}$.

for any $\varphi \in S_h(\Pi)$. Note that $\sigma w$ exists and is unique. We also assume below that $B \in W^{1,\infty}(\Pi)$ and then the following error estimate holds

$\|w - \sigma w\|_{L^2(\Pi)} \leq c|\nabla|^2(\mathcal{H}_\rho + \hat{v})w|_{L^2(\Pi)}$ for any $w \in H^2(\Pi) \cap H^1_0(\Pi)$.

We consider $\mathcal{H}_\rho := \frac{1}{\rho} \mathcal{H}$ as an unbounded operator in $L^2(\Pi)$ with $\mathcal{D}(\mathcal{H}_\rho) = H^2(\Pi) \cap H^1_0(\Pi)$. Assume below that $\psi^0 \in \mathcal{D}(\mathcal{H}_\rho^3)$.

Proposition 6. The following first error estimate holds

$\max_{0 \leq m \leq M} \|\psi - \Psi\|^m_{L^2(\Pi)} \leq \|\psi^0 - \sigma \psi^0\|_{L^2(\Pi)}$

$+ c(1 + T) \left\{ T_{\max} |\mathcal{H}_\rho^3\psi^0|_{L^2(\Pi)} + |\nabla|^2(\mathcal{H}_\rho^2\psi^0)_{L^2(\Pi)} + \|\psi^0\|_{L^2(\Pi)} \right\}$. (18)

Here $\sigma \psi^0$ can be replaced by $\psi^0$. 

The numerical results for the method can be found in [4,15,16].
Proof. 1. For \( y \in L^1(0, T) \), define the average (the projection on the time mesh) \([y]^m := \frac{1}{T_m} \int_{t_m}^{t_{m+1}} y(t) dt\), \(1 \leq m \leq M\), and notice that

\[
\sum_{m=1}^{M} \|u(m)\|_B \tau_m \leq \int_0^T \|u(\cdot, t)\|_B \, dt,
\]

where \(\| \cdot \|_B = \| \cdot \|_{L^2(\Omega)}\) or \(\| \cdot \|_{H^{\psi, \nu}}\), and \(u \in L^1(0, T; B)\), and

\[
[y]^m - \bar{\sigma} y^m \leq c_0 \tau_m^2 \|D_t^2 y\|^m, \quad 1 \leq m \leq M, \quad \text{for} \quad y \in W^{2,1}(0, T).
\]

2. Applying \(|\cdot|\) to identity (1), we get

\[
\langle i\hbar [D_t \psi]^m, \varphi \rangle_{L^2(\Omega)} = \mathcal{L}_H ([\psi]^m, \varphi) \quad \text{for any} \quad \varphi \in H^0_0(\Omega) \quad \text{and} \quad 1 \leq m \leq M.
\]

Then for any \( \eta : \mathbb{R}^D \rightarrow S_h(\Omega) \) from identities (5) and (21) it follows that

\[
\langle i\hbar \bar{\sigma} \psi, \varphi \rangle_{L^2(\Omega)} = i\hbar \bar{\sigma} \psi, \varphi \rangle_{L^2(\Omega)} - \mathcal{L}_H ([\psi] - \bar{\sigma} \eta)^m, \varphi)
\]

Let \( \eta^m := \sigma \psi^m, 0 \leq m \leq M \). By identity (16) and \( [D_t y] = \bar{\sigma} y \) we get

\[
\langle i\hbar \bar{\sigma} \psi, \varphi \rangle_{L^2(\Omega)} - \mathcal{L}_H ([\psi] - \bar{\sigma} \psi)^m, \varphi)
\]

where (after rearranging the summands)

\[
F = -([\mathcal{H} \psi] - \bar{\sigma} \mathcal{H} \psi) + i\hbar \rho [D_t (\psi - \sigma \psi)] + \bar{\sigma} \mathcal{H}_\rho (\psi - \sigma \psi).
\]

Let now \( h = 1 \). Proposition (1) together with (19) lead to the bound

\[
\max_{0 \leq m \leq M} \| (\psi - \sigma \psi)^m \|_{L^2(\Omega)} \leq \| \psi^0 - \sigma \psi^0 \|_{L^2(\Omega)} + 2 \sum_{m=1}^{M} \| F^m \|_{L^2(\Omega)} \tau_m
\]

\[
\leq \| \psi^0 - \sigma \psi^0 \|_{L^2(\Omega)} + 2 \sum_{m=1}^{M} \| [\mathcal{H}_\rho \psi] - \bar{\sigma} \mathcal{H}_\rho \psi \|_{L^2(\Omega)} \tau_m
\]

\[
+ 2 \int_0^T \| D_t (\psi - \sigma \psi) \|_{L^2(\Omega)} \, dt + 2|\bar{\sigma}| T \max_{0 \leq m \leq M} \| (\psi - \sigma \psi)^m \|_{L^2(\Omega)}.
\]

The formula \( \psi - \psi = \psi - \sigma \psi - \mathbf{H} - \sigma \psi \) and estimates (17) and (20) imply

\[
\max_{0 \leq m \leq M} \| (\psi - \psi)^m \|_{L^2(\Omega)} \leq \| \psi^0 - \sigma \psi^0 \|_{L^2(\Omega)}
\]

\[
+ \frac{c \tau_m^2}{\max_{0 \leq m \leq M} \| (\mathcal{H}_\rho + \bar{\sigma}) \psi^m \|_{L^2(\Omega)}} \int_0^T \| D_t \mathcal{H}_\rho \psi \|_{L^2(\Omega)} \, dt + |\bar{\sigma}| T \max_{0 \leq m \leq M} \| (\mathcal{H}_\rho + \bar{\sigma}) \psi^m \|_{L^2(\Omega)}.
\]
Under the above assumptions, the solution to problem \(1\), \(2\) satisfies the bound
\[
\max_{0 \leq t \leq T} \|D_t^k \psi\|_{L^2(\Omega)} \leq \|(D_t^k \psi)\|_{t=0} \|L^2(\Omega)\) = \|H^k_\rho \psi^0\|_{L^2(\Omega)}), \quad 0 \leq k \leq 3, \tag{25}
\]
and the property \(D_t^k \psi = D_t^{k-1}(-iH_\rho)^l \psi\) for \(1 \leq l \leq k\). Therefore
\[
\max_{0 \leq m \leq M} \|(\psi - \Psi)^m\|_{L^2(\Omega)} \leq \|\Psi^0 - \sigma \psi^0\|_{L^2(\Omega)} + c \left\{ T \tau^2 \|H^3_\rho \psi^0\|_{L^2(\Omega)} + T|h|^2 \|H^2_\rho \psi^0\|_{L^2(\Omega)} + \|\psi^0\|_{L^2(\Omega)} \right\}.
\]
Note that for \(\hat{\psi} = 0\) the estimate is simplified.

The following multiplicative inequality holds
\[
\|H^l_\rho \psi^0\|_{L^2(\Omega)}^{\leq 3} \leq \|H^{l+1}_\rho \psi^0\|_{L^2(\Omega)} \|H^{l-1}_\rho \psi^0\|_{L^2(\Omega)} \quad \text{for } l = 1, 2. \tag{26}
\]
Using \(17\) for \(w = \psi^0\) together with \(26\) for \(l = 1\), we complete the proof. \(\square\)

**Corollary 1.** Let \(\psi^0(x) = 0\) for \(|x_1| \geq X_0\), \(\Psi^0 \in S_{0h}\) and \(\overline{\mathbb{M}}\) be uniform. Then for the solution to \(9\), \(10\) the following first error estimate holds
\[
\max_{0 \leq m \leq M} \|(\psi - \Psi)^m\|_{L^2(\Omega)} \leq \|\Psi^0 - \psi^0\|_{L^2(\Omega)} + 2 \left\{ C_1 \|\Psi^0\|_{L^2(\Omega)} + \|\psi^0\|_{L^2(\Omega)} \right\}.
\]

The result immediately follows from Proposition 6. Notice also that, for \(1 \leq n \leq 3\), for the interpolant \(s\psi^0\) in \(S_{0h}\) for \(\psi^0\), the following error estimate holds
\[
\|s\psi^0 - \psi^0\|_{L^2(\Omega)} \leq c|h|^2 \left\{ C_1 \|\Psi^0\|_{L^2(\Omega)} + \|\psi^0\|_{L^2(\Omega)} \right\},
\]
thus one can set simply \(\Psi^0 := s\psi^0\). Other possible choices of \(\Psi^0\) with the same error estimate, for any \(n \geq 1\), are the \(L^2(\Omega_0)\) (possibly with a weight like \(\rho\)) projection of \(\psi^0\) onto \(S_{0h}\) or its elliptic projection onto \(S_{0h}\) like \(16\) (with \(\Pi\) replaced by \(\Omega_0\) and any \(\varphi \in S_{0h}\)).

**Remark 1.** Importantly, all the above results can be essentially generalized rather easily. For example, in the 2D case, the problem in an unbounded domain \(\Pi\) of general shape with smooth boundary and several half-strip-like outlets to infinity can be treated by using combined linear triangle elements inside \(\Pi\) except outlets and bilinear rectangular elements inside outlets.

Let \(B \in W^{2,\infty}(\Pi)\) and \(\rho, V \in W^{1,\infty}(\Pi)\).

**Proposition 7.** Let \(H^3_\rho \psi^0 \in H^1_0(\Pi)\), \(1 \leq n \leq 3\) and \(\Psi^0 := s\psi^0\). Then the following second error estimate holds
\[
\max_{0 \leq m \leq M} \|s\psi^m - \Psi^m\|_{H^{l+\bar{\rho}; \Pi}} \leq c(1 + T) \left\{ \tau^2 \left\{ \|H^3_\rho \psi^0\|_{H^{l+\bar{\rho}; \Pi}} + \|H^2_\rho \psi^0\|_{H^{l+\bar{\rho}; \Pi}} \right\} + |h|^2 \left\{ \|H^2_\rho \psi^0\|_{L^2(\Omega)} + \|\psi^0\|_{L^2(\Omega)} \right\} \right\}.
\]
Here \(s\psi^m\) is the interpolant in \(S_{h(\Pi)}\) for \(\psi^m\), \(0 \leq m \leq M\).
Applying Proposition 2, now we get

\[ \|w\|_{H^{-1}(\Omega)} \leq \hat{\delta}^{-1/2} \|w\|_{L^2(\Omega)}, \quad \|w\|_{L^2(\Omega)} \leq \hat{\delta}^{-1/2} \|w\|_{H^{1/2}(\Omega)}. \]  

(28)

Then setting \( \hat{c} := 1 + \frac{|\hat{\nu}|}{\hat{\delta}} \), we also get

\[ \|Hw\|_{H^{-1}(\Omega)} \leq \|H + \hat{\nu}w\|_{H^{-1}(\Omega)} + |\hat{\nu}| \|\rho w\|_{H^{-1}(\Omega)} \leq \hat{c} \|w\|_{H^{1/2}(\Omega)}. \]  

(29)

For \( y \in L^1(0, T) \), define two more averages (projections on the time mesh)

\[ [y]_2^m := \frac{1}{2\tau_m} \int_{t_{m-1}}^{t_m} y(t) dt, \quad \langle y \rangle_0^m := \frac{1}{\tau_m} \int_{t_{m-1}}^{t_m} y(t) dt, \quad 1 \leq m \leq M - 1, \]

\[ \hat{\nu}_0^m := |\hat{\nu}|, \quad \hat{\nu}_m^m := \frac{2}{\tau_m} \int_{t_0}^{t_m} y(t) dt, \]

where \( e_m(t) \) is the “hat” function linear on all segments \( [t_{l-1}, t_l] \) and such that \( e_m(t_{l-1}) = 1 \) and \( e_m(t_l) = 0 \) for all \( t \neq m \).

Notice that the following relations hold

\[ \hat{\nu}_m^m = \langle D_t y \rangle_0^m, \quad \hat{\nu}_m^m = \langle D_t \sigma \rangle_0^m, \quad 1 \leq m \leq M - 1, \]

\[ \langle y \rangle_0^m = \frac{\tau_m}{2} \langle D_t y \rangle_0^m, \quad \langle y \rangle_0^m = \frac{\tau_m}{2} \langle D_t \sigma \rangle_0^m, \quad \text{for } y \in W^{1,1}(0, T), \]  

(30)

\[ \sum_{m=0}^{M-1} \|\langle u \rangle_0^m\|_{L^2} \leq \int_0^T \|u(\cdot, t)\| dt, \quad \sum_{m=0}^{M-1} \|\langle u \rangle_0^m\|_{L^2} \leq \int_0^T \|u(\cdot, t)\| dt, \]  

(31)

\[ \|\langle y \rangle_0^m - \langle y \rangle_0^m\|_{L^2} \leq c_0 \tau_m^2 \|\langle D_t y \rangle_0^m\|_{L^2}, \quad 1 \leq m \leq M - 1, \quad \text{for } y \in W^{2,1}(0, T). \]  

(32)

(33)

2. Let first \( \Psi^0 \in S_h(\Omega) \) be arbitrary. We go back to the error identity (22). Applying Proposition 2 now we get

\[ \max_{0 \leq m \leq M} \|\langle \Psi - \sigma \psi \rangle_0^m\|_{H^{1/2}(\Omega)} \leq \|\Psi^0 - \sigma \psi^0\|_{H^{1/2}(\Omega)} \]

\[ + 4 \sum_{m=0}^{M-1} \|\hat{\nu} F_m^m \|_{H^{-1}(\Omega)} \hat{\tau}_m + 4 |\hat{\nu}| \sum_{m=1}^{M} \|F_m^m \|_{H^{-1}(\Omega)} \hat{\tau}_m + 4 \|F_0^m \|_{H^{-1}(\Omega)} \]  

(34)

where the right-hand side is slightly transformed and \( F \) is given by (23). We introduce the decomposition

\[ F = F_\tau + \rho F_h, \quad F_\tau := -\langle [\hat{\psi} - \sigma \psi] \rangle_0, \quad F_h := i[D_t (\psi - \sigma \psi)] + i\hat{\nu}_t (\psi - \sigma \psi) \]

as well as set \( F_\tau^0 := 0 \) and \( F_h^0 = i[D_t (\psi - \sigma \psi)]_{t=0} + i(\psi^0 - \sigma \psi^0) \).
Applying sequentially relations (30), (31), (17) and (32), we obtain

\[
S_T := |\tilde{v}| \sum_{m=1}^{M} \|F_m^m\|_{H_{H}^{-1}(H)} \tau_m + \sum_{m=0}^{M-1} \|\hat{\partial}_t F_m^m\|_{H_{H}^{-1}(H)} \tau_m
\]

\[
\leq \hat{c} \left[ |\tilde{v}| \sum_{m=1}^{M} \left( \|([\psi] - \tilde{\tau}_v \psi)^m\|_{H + \hat{\psi}; H} \tau_m + \sum_{m=1}^{M-1} \left( \|\langle D_2 \psi \rangle - [D_t \psi]^2 \|_{H + \hat{\psi}; H} \tau_m \right. \right.
\]

\[
+ \left. \left( \|\tilde{\tau}_v \psi \|_{H + \hat{\psi}; H} \right) \right) \sum_{m=1}^{M} \|D^2 \psi \|_{H + \hat{\psi}; H} \tau_m
\]

\[
\leq \hat{c} c_0 \tau_{\max}^2 \left\{ |\tilde{v}| \sum_{m=1}^{M} \left( \|D^2 \psi \|_{L^2(H)} \tau_m \right. \right.
\]

\[
+ \left. \left( \|D^2 \psi \|_{H_{H}^{-1}(H)} \tau_m \right) \right) \sum_{m=1}^{M} \|\hat{\partial}_t F_m^m\|_{H_{H}^{-1}(H)} \tau_m
\]

\[
\leq \hat{c} c_0 \tau_{\max}^2 \left\{ |\tilde{v}| \sum_{m=1}^{M} \left( \|D^2 \psi \|_{L^2(H)} \tau_m \right. \right.
\]

\[
+ \left. \left( \|D^2 \psi \|_{H_{H}^{-1}(H)} \tau_m \right) \right) \sum_{m=1}^{M} \|\hat{\partial}_t F_m^m\|_{L^2(H)} \tau_m \right\} dt, \quad (35)
\]

The left inequality (28) implies

\[
S_h := |\tilde{v}| \sum_{m=1}^{M} \|\rho F_h^m\|_{H_{H}^{-1}(H)} \tau_m + \|\rho F_h^0\|_{H_{H}^{-1}(H)} + \sum_{m=0}^{M-1} \|\hat{\rho} \hat{\partial}_t F_h^m\|_{H_{H}^{-1}(H)} \tau_m
\]

\[
\leq \delta^{-1/2} \left[ |\tilde{v}| \sum_{m=1}^{M} \|F_h^m\|_{L^2(H)} \tau_m + \|F_h^0\|_{L^2(H)} + \sum_{m=0}^{M-1} \|\hat{\partial}_t F_h^m\|_{L^2(H)} \tau_m \right], \quad (36)
\]

and further the error estimate (17) leads to

\[
\|F_h^m\|_{L^2(H)} \leq \|D_t (\psi - \sigma \psi)\|_{L^2(H)} + |\tilde{v}| \|\psi^0 - \sigma \psi^0\|_{L^2(H)}
\]

\[
\leq c h^2 \|D_t (\mathcal{H}_\rho + \hat{\psi})\|_{L^2(H)} + |\tilde{v}| \|\mathcal{H}_\rho + \hat{\psi}\|_{L^2(H)}. \quad (37)
\]

Applying sequentially relations (30), (31), (17) and (32), we also obtain

\[
\sum_{m=0}^{M-1} \|\hat{\rho} \hat{\partial}_t F_h^m\|_{L^2(H)} \tau_m
\]

\[
\leq \sum_{m=0}^{M-1} \left( \|D^2 (\psi - \sigma \psi)\|_{L^2(H)} + |\tilde{v}| \|D_t (\psi - \sigma \psi)\|_{L^2(H)} \right) \tau_m
\]

\[
\leq c h^2 \sum_{m=0}^{M-1} \|D^2 (\mathcal{H}_\rho + \hat{\psi})\|_{L^2(H)} + |\tilde{v}| \|D_t (\mathcal{H}_\rho + \hat{\psi})\|_{L^2(H)} \tau_m
\]

\[
\leq c h^2 \int_0^T \|D^2 (\mathcal{H}_\rho + \hat{\psi})\|_{L^2(H)} + |\tilde{v}| \|D_t (\mathcal{H}_\rho + \hat{\psi})\|_{L^2(H)} dt. \quad (38)
\]
Inserting into (34) all the estimates (35)-(38) together with the estimate for $\sum_{m=1}^{M} \| F_{\mathcal{H}}^{m} \|_{L^{2,p}(\Omega)} \tau_{m}$ used in the preceding proof in (24), we derive

$$\max_{0 \leq m \leq M} \| (\psi - \sigma \psi)^{m} \|_{\mathcal{H}^{1/2}; \Omega} \leq \| \psi^{0} - \sigma \psi^{0} \|_{\mathcal{H}^{1/2}; \Omega} + 4 \mathcal{S}_{\tau} + 4 \mathcal{S}_{h}$$

$$\leq c \max_{0 \leq m \leq M} \left\{ \| \mathcal{D}_{t}^{2} \psi \|_{t=0} + \int_{0}^{T} \left( \| \mathcal{D}_{t} \psi \|_{H^{1/2}; \Omega} + \sum_{l=0}^{3} \| \mathcal{D}_{t}^{l} \psi \|_{H^{1/2}; \Omega} \right) dt \right\}$$

$$+ c |h|^{2} \left( \| \mathcal{D}_{t} \psi \|_{H^{1/2}; \Omega} + \int_{0}^{T} \| \mathcal{D}_{t} \mathcal{D}_{t} \psi \|_{H^{1/2}; \Omega} dt \right)$$

$$+ c |h|^{2} \left( \| \mathcal{D}_{t} \psi \|_{H^{1/2}; \Omega} + \int_{0}^{T} \| \mathcal{D}_{t} \mathcal{D}_{t} \psi \|_{H^{1/2}; \Omega} dt \right)$$

Once again for $\tilde{v} = 0$ the estimate is essentially simplified.

Under all the above assumptions, the solution to problem (1), (2) satisfies the following second error estimate:

$$\| w - \sigma w \|_{H^{1/2}; \Omega} \leq c h^{2} \left( \sum_{p \neq q} \| \mathcal{D}_{p}^{2} \mathcal{D}_{q} w \|_{L^{2}(\Omega)} + \sum_{p=1}^{n} \| \mathcal{D}_{p}^{2} w \|_{L^{2}(\Omega)} \right)$$

$$\leq c_{1} h^{2} \left( \| \mathcal{H}_{p} w \|_{H^{1/2}; \Omega} + \| w \|_{H^{1/2}; \Omega} \right)$$

for any $w \in \mathcal{D}(\mathcal{H}_{p})$ such that $\mathcal{H}_{p} w \in H_{0}^{1}(\Omega)$, taking into account the above regularity assumptions on $B, \rho$ and $V$, where the first sum is taken over all $p$ and $q$ from 1 to $n$ excepting $p = q$ and disappearing for $n = 1$. This estimate allows to pass from (39) to the final estimate (27) by the triangle inequality together with inequalities (26) and

$$\| \mathcal{H}_{p}^{l} \psi^{0} \|_{H^{1/2}; \Omega} \leq \| (\mathcal{H}_{p} + \tilde{v}) \mathcal{H}_{p}^{l} \psi^{0} \|_{L^{2,p}(\Omega)} \| \mathcal{H}_{p}^{l} \psi^{0} \|_{L^{2,p}(\Omega)}, \quad l = 0, 1, \quad \square$$

**Corollary 2.** Let $\psi^{0}(x) = 0$ for $|x| \geq X_{0}, 1 \leq n \leq 3$ and $\psi^{0} = s \psi^{0}$ on $\Omega$ and $\overline{\mathcal{A}_{T}}$ be uniform. Then for the solution to (9), (10) the following second error
estimate holds

$$\max_{0 \leq m \leq M} \|s\psi^m - \Psi^m\|_{H+\bar{\nu}; \Omega} \leq c(1 + T) \left\{ h^2 \left( \|\mathcal{H}_\rho^3 \psi^0\|_{H+\bar{\nu}; \Omega} + \|\mathcal{H}_\rho^2 \psi^0\|_{H+\bar{\nu}; \Omega} \right) \right. $$

$$+ \left. |h| \left( \|\mathcal{H}_\rho^3 \psi^0\|_{L^2; \omega(\Omega)} + \|\psi^0\|_{L^2; \omega(\Omega)} \right) \right\}. $$

The result immediately follows from Proposition 7.

Note that the norm $\| \cdot \|_{H+\bar{\nu}; \Omega}$ is equivalent to $\| \cdot \|_{H^1(\Omega)}$ and $\|s \cdot \|_{H^1(\Omega)}$ is actually the mesh counterpart of the latter norm.

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