

A SPACETIME DPG METHOD FOR THE SCHRÖDINGER EQUATION

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ABSTRACT. A spacetime Discontinuous Petrov Galerkin (DPG) method for the linear time-dependent Schrödinger equation is proposed. The spacetime approach is particularly attractive for capturing irregular solutions. Motivated by the fact that some irregular Schrödinger solutions cannot be solutions of certain first order reformulations, the proposed spacetime method uses the second order Schrödinger operator. Two variational formulations are proved to be well posed: a strong formulation (with no relaxation of the original equation) and a weak formulation (also called the “ultraweak formulation”, that transfers all derivatives onto test functions). The convergence of the DPG method based on the ultraweak formulation is investigated using an interpolation operator. A standalone appendix analyzes the ultraweak formulation for general differential operators. Reports of numerical experiments motivated by pulse propagation in dispersive optical fibers are also included.

1. INTRODUCTION

This paper is devoted to exploring a weak formulation and an accompanying numerical technique for the Schrödinger equation with Dirichlet boundary conditions. Let $\Omega_0 \subset \mathbb{R}^n$ ($n \geq 1$) be an open bounded domain with Lipschitz boundary. The space variable x lies in Ω_0 while the time variable t lies in the open interval $(0, T)$ with $T < \infty$. The classical form of Schrödinger initial boundary value problem reads as follows:

$$i\partial_t u - \Delta_x u = f, \quad x \in \Omega_0, \quad 0 < t < T, \quad (1.1a)$$

$$u(x, t) = 0, \quad x \in \partial\Omega_0, \quad 0 < t < T, \quad (1.1b)$$

$$u(x, 0) = 0, \quad x \in \Omega_0, \quad (1.1c)$$

where ∂_t denotes the time derivative $\partial/\partial t$ and Δ_x denotes the Laplacian with respect to the spatial variable x . Here f is any given function in $L^2(\Omega)$ and $\Omega = \Omega_0 \times (0, T)$ throughout.

The numerical technique we want to apply to (1.1) is the Discontinuous Petrov-Galerkin (DPG) method [14]. Among its desirable properties are mesh independent stability, inheritance of discrete stability from the wellposedness of the undiscretized problem, and the availability of a canonical error indicator computed as part of the solution. The DPG method has been successfully applied to a wide variety of problems such as second order elliptic problems [11], convective phenomena [9, 10, 13], elasticity [2, 7, 21, 22], Stokes flow [7, 25], and spacetime problems [15, 16, 28]. It seems natural therefore that the DPG method should work for (1.1) as well. In this paper, we will show that the DPG method does indeed faithfully approximate the solutions of (1.1) *provided* we do not recast (1.1) into a first order system.

Many applications of interest come as a first order system even if they are often displayed as second order partial differential equations. For example, the second order heat equation is really a combination of two first order equations, namely the Fourier law of heat conduction

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and the conservation of energy. Similarly, the linear elasticity equation while often displayed as a second order equation for displacement, is really a combination of the two first order equations, the constitutive (Hooke's) law and the equation of static equilibrium. Thus its no surprise that it makes physical sense to bring back the heat equation or the elasticity equation to first order form before discretizing. However, it makes no physical sense to do this for the Schrödinger equation as its not derived from first order physical laws.

It makes no mathematical sense either. One might be tempted to introduce a “flux” τ , formulate the first order system $i\partial_t u - \operatorname{div}_x \tau = f$ and $\nabla_x u - \tau = g$, and claim its equivalence to (1.1) when $g = 0$. This claim is false because while the Schrödinger problem (1.1) is wellposed for $f \in L^2(\Omega)$, *the first order system cannot be wellposed in $L^2(\Omega)$* . Indeed, denoting the norm of $L^2(\Omega)$ by $\|\cdot\|_\Omega$, if the first order system were wellposed, then there are constants $C_1, C_2 > 0$ such that $\|u\|_\Omega + \|\tau\|_\Omega \leq C_1\|f\|_\Omega + C_2\|g\|_\Omega$. But then the second equation of the system implies that $\|\nabla_x u\|_\Omega = \|g + \tau\|_\Omega \leq C_1\|f\|_\Omega + 2C_2\|g\|_\Omega$ for any solution u , which is false: In the next two paragraphs we will exhibit a Schrödinger solution for which $\|\nabla_x u\|_\Omega = \infty$ even when $g = 0$ and $f \in L^2(\Omega)$.

First observe that given any $f(x, t)$ in $L^2(\Omega)$, it is possible to solve (1.1) by the “method of Galerkin approximations” [18] (distinct from the Galerkin finite element method). Let $e_k(x)$ in $H_0^1(\Omega_0)$ and $\omega_k^2 > 0$ be an eigenpair of Δ_x satisfying

$$-\Delta_x e_k = \omega_k^2 e_k \quad \text{a.e. in } \Omega_0, \quad (1.2)$$

normalized so that $\|e_k\|_{\Omega_0} = 1$ for all natural numbers $k \geq 1$. Since Fubini's theorem for product measures implies that $f(\cdot, t)$ is in $L^2(\Omega_0)$, the following definitions make sense:

$$f_k(t) = \int_{\Omega_0} f(x, t) \bar{e}_k(x) dx, \quad u_k(t) = -i \int_0^t e^{i\omega_k^2(t-s)} f_k(s) ds, \quad (1.3a)$$

$$F_M(x, t) = \sum_{k=1}^M f_k(t) e_k(x), \quad U_M(x, t) = \sum_{k=1}^M u_k(t) e_k(x). \quad (1.3b)$$

It is not difficult to show (see the proof of Theorem 2.4 below) that $u = \lim_{M \rightarrow \infty} U_M$ exists in $L^2(\Omega)$ and solves (1.1).

Now consider the one-dimensional case $\Omega_0 = (0, 1)$ where $\omega_k = k\pi$ and choose

$$f(x, t) = \sum_{k=1}^{\infty} \frac{1}{k} e^{i\omega_k^2 t} e_k(x) \quad \text{in } L^2(\Omega).$$

Then by the orthonormality of e_k , we have that $f_k(s) = e^{i\omega_k^2 s}/k$, $u_k(t) = -ite^{i\omega_k^2 t}/k$,

$$\begin{aligned} \|U_M\|_\Omega^2 &= \sum_{k=1}^M \int_0^T |u_k(t)|^2 dt = \sum_{k=1}^M \int_0^T \left| \frac{-it}{k} e^{i\omega_k^2 t} \right|^2 dt = \frac{T^3}{3} \sum_{k=1}^M \frac{1}{k^2} \\ \|\nabla_x U_M\|_\Omega^2 &= \sum_{k=1}^M \omega_k^2 \int_0^T |u_k(t)|^2 dt = T^3 \sum_{k=1}^M \frac{\omega_k^2}{3k^2} = \frac{\pi^2}{3} T^3 M. \end{aligned}$$

The solution u is the limit of U_M . The above calculations clearly show that as $M \rightarrow \infty$, while $\|u\|_\Omega = \lim_{M \rightarrow \infty} \|U_M\|_\Omega = (T^3 \pi^2 / 18)^{\frac{1}{2}}$, the limit of $\|\nabla_x U_M\|_\Omega$ diverges. *Thus it is possible to obtain a Schrödinger solution u whose H^1 -norm is infinite even when $f \in L^2(\Omega)$* . Note that finer arguments are needed to understand the regularity of Schrödinger solutions in unbounded domains, which although a topic of wide mathematical interest [27], is not our concern here.

To our knowledge, this paper is the first work to analyze the feasibility of the DPG methodology for a system without ready access to an equivalent first order formulation. The second order form necessitates formulations in the non-standard graph spaces of the second order Schrödinger operator. One of the contributions of this paper is the proof of wellposedness of a strong and a weak formulation of (1.1) in these graph spaces. The general spaces and arguments required for this analysis are collected in a standalone Appendix A anticipating uses outside of the Schrödinger example. The analysis in Appendix A is motivated by the modern theory of Friedrichs systems [17] but applies beyond Friedrichs systems. Borrowing the approach of [17], we are able to prove wellposedness without developing a trace theory for the graph spaces. The other contributions involve the numerical implications of this wellposedness. Numerical methods using the strong formulation must use conforming finite element subspaces of the graph spaces. On the other hand, numerical methods using the weak formulation need only use existing standard finite element spaces. In either case, an interpolation theory in the Schrödinger graph norm is needed to estimate convergence rates. We address this issue in one space dimension.

In the next section, we investigate wellposedness (in the sense of Hadamard) for a strong and weak variational formulation for the Schrödinger problem. This will require an abstract definition of a boundary operator and duality pairings in a graph space. Such abstract definitions that apply beyond the Schrödinger setting are in Appendix A. Their particular realizations for the Schrödinger case are used in section 2. To avoid repetitions of the general definitions in the specific case, we will often refer to Appendix A in section 2. Section 3 provides a verification of a density assumption made in section 2. Section 4 details our construction of a conforming finite element space and interpolation error estimates. Section 5 points to an application in dispersive optical fibers and contains some numerical results.

2. FUNCTIONAL SETTING AND WELLPOSEDNESS

We now provide a functional setting within which a strong and a weak formulation of the spacetime Schrödinger problem can be proved to be well posed (i.e., *inf-sup* stable). The analysis is an application of the general theory detailed in Appendix A.

The classical form of the problem is already presented in (1.1). Recalling that $\Omega = \Omega_0 \times (0, T)$, define these parts of $\partial\Omega$:

$$\Gamma = \partial\Omega_0 \times [0, T] \cup \Omega_0 \times \{0\}, \quad \Gamma^* = \partial\Omega_0 \times [0, T] \cup \Omega_0 \times \{T\}$$

(see Fig. 1). Then the initial and boundary conditions together can be written as $u|_{\Gamma} = 0$. We want to write (1.1) as an operator equation (see (A.8)) to apply the general results of Appendix A. To this end, consider the setting of Appendix A with

$$A = A^* = i\partial_t - \Delta_x, \quad k = l = m = 1, \quad d = n + 1,$$

The space $W = W^*$ is then defined by (A.2)–(A.3), namely $W = W^* = \{u \in L^2(\Omega) : i\partial_t u - \Delta_x u \in L^2(\Omega)\}$. The operator $D = D^* : W \rightarrow W'$ is defined by (A.5)–(A.6), namely $\langle Dw, \tilde{w} \rangle_W = (Aw, \tilde{w})_{\Omega} - (w, A\tilde{w})_{\Omega}$ for all $w, \tilde{w} \in W$. As usual, let $\mathcal{D}(\bar{\Omega})$ denote the restrictions of functions from $\mathcal{D}(\mathbb{R}^{n+1})$ to Ω . The operator D (often called the “boundary operator” in the theory of Friedrichs systems [17]), satisfies

$$\langle D\phi, \psi \rangle_W = \int_{\partial\Omega} in_t \phi \bar{\psi} + \int_{\partial\Omega} \phi (n_x \cdot \nabla_x \bar{\psi}) - \int_{\partial\Omega} (n_x \cdot \nabla_x \phi) \bar{\psi} \quad (2.1)$$

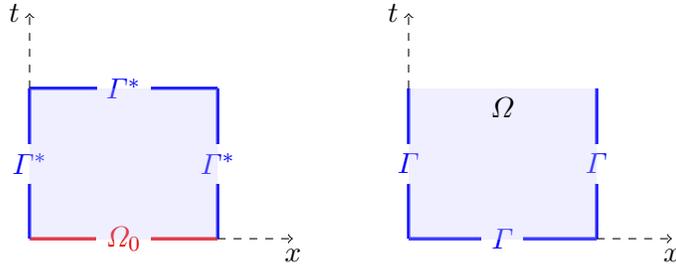


FIGURE 1. Schematic of the spacetime domain

for all $\phi, \psi \in \mathcal{D}(\bar{\Omega})$. Note that although the integrals on the right hand side need not exist for all functions in W , D is defined on all W through (A.5).

Although we set the differential operators A and A^* to be equal above, note that we consider each as an unbounded operator with its own domain. We set the domain of A to

$$\text{dom}(A) = \{u \in W : \langle Dv, u \rangle_W = 0, \forall v \in \mathcal{V}^*\}, \quad (2.2)$$

where $\mathcal{V}^* = \{\varphi \in \mathcal{D}(\bar{\Omega}) : \varphi|_{\Gamma^*} = 0\}$. The domain of the adjoint is given by the usual [3, 24] general prescription: $\text{dom}(A^*) = \{s \in L^2(\Omega)^l : \text{there is an } \ell \in L^2(\Omega)^m \text{ such that } (Av, s)_\Omega = (v, \ell)_\Omega \text{ for all } v \in \text{dom}(A)\}$. Here $(\cdot, \cdot)_\Omega$ denotes the (complex) inner product in $L^2(\Omega)$. Finally, as in the appendix, set $V = \text{dom}(A)$ and $V^* = \text{dom}(A^*)$ with the understanding that both V and V^* are endowed with the W -topology, while $\text{dom}(A)$ and $\text{dom}(A^*)$ have the topology of $L^2(\Omega)$.

For the above set A, A^* and $\text{dom}(A)$, the conditions (A-a) and (A-b) in Appendix A are immediate, while condition (A-c) is easily verified using (2.1). Hence Lemma A.2 shows that $\text{dom}(A^*)$ equals

$$V^* = {}^\perp D(V). \quad (2.3)$$

Rewriting (2.2) in the same style,

$$V = {}^\perp D(\mathcal{V}^*). \quad (2.4)$$

Thus V and V^* are closed subspaces of W . Let $\mathcal{V} = \{\varphi \in \mathcal{D}(\bar{\Omega}) : \varphi|_\Gamma = 0\}$.

Lemma 2.1. $\mathcal{V} \subset V$ and $\mathcal{V}^* \subset V^*$.

Proof. Equation (2.1) implies $\langle D\phi, \phi^* \rangle_W = 0$ for all $\phi \in V$ and $\phi^* \in \mathcal{V}^*$. Hence, any $\phi \in \mathcal{V}$ is also in ${}^\perp D(\mathcal{V}^*)$, which by (2.4) implies that $\phi \in V$. Thus $\mathcal{V} \subset V$.

If $\phi^* \in \mathcal{V}^*$, then (2.2) shows that $\langle D\phi^*, u \rangle_W = 0$ for all $u \in V$, i.e., $\phi^* \in {}^\perp D(V)$, which by (2.3) implies ϕ^* is in V^* . \square

In (2.4), \mathcal{V}^* may be replaced by V^* provided a density result is available, as we show next.

Assumption 1. Suppose \mathcal{V}^* is dense in V^* and \mathcal{V} is dense in V .

Lemma 2.2. *If Assumption 1 holds, then ${}^\perp D(\mathcal{V}^*) = {}^\perp D(V^*)$ and ${}^\perp D(\mathcal{V}) = {}^\perp D(V)$.*

Proof. Clearly $\mathcal{V}^* \subseteq V^*$ implies ${}^\perp D(\mathcal{V}^*) \supseteq {}^\perp D(V^*)$. To prove the reverse containment, suppose $w \in {}^\perp D(\mathcal{V}^*)$ and $v^* \in V^*$. By density, there is a sequence \tilde{v}_n in \mathcal{V}^* satisfying $\lim_{n \rightarrow \infty} \|\tilde{v}_n - v^*\|_W = 0$. Since $\langle D\tilde{v}_n, w \rangle_W = 0$, by continuity of D , we have $\langle Dv^*, w \rangle_W = 0$. Hence $w \in {}^\perp D(V^*)$. The second identity is proved similarly. \square

2.1. Strong formulation. The strong formulation of the Schrödinger problem (1.1) is based on these sesquilinear and conjugate linear forms:

$$a(u, v) = (Au, v)_\Omega, \quad l(v) = (f, v)_\Omega.$$

Problem 2.3 (Strong formulation). *Given any $f \in L^2(\Omega)$, find $u \in V$ satisfying*

$$a(u, v) = l(v), \quad \forall v \in L^2(\Omega).$$

Theorem 2.4. *Suppose Assumption 1 holds. Then the linear Schrödinger operator $A : V \rightarrow L^2(\Omega)$ is a continuous bijection. Hence Problem 2.3 is well posed.*

Proof. To prove the surjectivity of A , suppose $f \in L^2(\Omega)$. Recall the definitions of e_k , u_k and f_k from (1.2) and (1.3). Clearly, $AU_M = F_M$. Since U_M and any $\varphi \in \mathcal{V}^*$ are smooth enough for integration by parts using $\varphi|_{\Gamma^*} = 0$ and $U_M|_\Gamma = 0$, we have

$$\begin{aligned} (i\partial_t U_M, \varphi)_\Omega &= (U_M, i\partial_t \varphi)_\Omega \\ (\Delta U_M, \varphi)_\Omega &= (U_M, \Delta \varphi)_\Omega. \end{aligned}$$

Hence $\langle D\varphi, U_M \rangle_W = (A\varphi, U_M)_\Omega - (\varphi, AU_M)_\Omega = 0$ for all $\varphi \in \mathcal{V}^*$. By (2.4), this implies that U_M is in V .

Next, we show that U_M is a Cauchy sequence in V . For any $N > M$,

$$\begin{aligned} \|U_M - U_N\|_\Omega^2 &= \sum_{k=M+1}^N \int_0^T |u_k(t)|^2 dt \leq \frac{1}{2} T^2 \sum_{k=M+1}^\infty \int_0^T |f_k(t)|^2 dt, \\ \|A(U_M - U_N)\|_\Omega^2 &= \|F_M - F_N\|_\Omega^2 \leq \sum_{k=M+1}^\infty \int_0^T |f_k(t)|^2 dt, \end{aligned}$$

both of which converge to 0 as $M \rightarrow \infty$, because $f \in L^2(\Omega)$. Thus U_M is Cauchy. It must therefore have an accumulation point u in V . Moreover, since Au and f are $L^2(\Omega)$ -limits of the same sequence $F_M = AU_M$, we have $Au = f$. Thus $A : V \rightarrow L^2(\Omega)$ is surjective.

We use a similar argument (with u_k defined by integrals from T to t) to show that $A = A^* : V^* \rightarrow L^2(\Omega)$ is also surjective. We omit the details, but note that the only difference is that instead of (2.4), we must now use

$$V^* = {}^\perp D(\mathcal{V}),$$

which follows from (2.3), Assumption 1 and Lemma 2.2. Finally, since $\ker(A) = {}^\perp \text{ran}(A^*)$, the surjectivity of $A^* : V^* \rightarrow L^2(\Omega)$ shows that $A : V \rightarrow L^2(\Omega)$ is injective, thus completing the proof of the stated bijectivity. \square

Remark 2.5. An example of a standard wellposedness result for the Schrödinger equation obtained using semigroup theory is [23, Theorem 4.8.1], which proves that there is one and only one solution to (1.1) whenever $f \equiv 0$ and $u(x, 0)$ is in $H^2(\Omega) \cap H_0^1(\Omega)$. In Theorem 2.4, we have shown (by a different method) that the existence of a unique solution holds for any $f \in L^2(\Omega)$. Note that in the above proof, we used Assumption 1 only to obtain injectivity. If one opts to use the results of [23] (with $u(x, 0) \equiv 0$ and $f \equiv 0$) to conclude injectivity, then there is no need to place Assumption 1 in Theorem 2.4.

2.2. A weak formulation. Now we consider a mesh-dependent weak formulation that is the basis of the DPG method. This formulation, sometimes called the “ultraweak” formulation, is given in a general setting in Problem A.4 of Appendix A. We apply this to our example of the Schrödinger equation.

The spacetime domain Ω is partitioned into a mesh Ω_h of finitely many open elements K such that $\bar{\Omega} = \cup_{K \in \Omega_h} \bar{K}$ where $h = \max_{K \in \Omega_h} \text{diam}(K)$. Particularizing the general definitions in Appendix A (see (A.9) through (A.11)) to the Schrödinger example, we let $A_h = A_h^*$ be the Schrödinger operator applied element by element and let $W_h = W_h^* = \{w \in L^2(\Omega) : A(w|_K) \in L^2(K) \text{ for all } K \in \Omega_h\}$. The operator $D_h : W_h \rightarrow W_h'$ is defined by $\langle D_h w, v \rangle_{W_h} = (A_h w, v)_\Omega - (w, A_h v)_\Omega$ for all $w, v \in W_h$ and let $D_{h,V} : V \rightarrow W_h'$ denote $D_h|_V$. The range of $D_{h,V}$, denoted by Q , is made into a complete space by the norm $\|q\|_Q = \inf_{v \in D_{h,V}^{-1}(\{q\})} \|v\|_W$. Abbreviating the duality pairing $\langle \cdot, \cdot \rangle_{W_h}$ by $\langle \cdot, \cdot \rangle_h$, define the sesquilinear form $b((u, q), v) = (u, A_h v)_\Omega + \langle q, v \rangle_h$ on $(L^2(\Omega) \times Q) \times W_h$.

Problem 2.6 (Ultraweak formulation). Given $F \in W_h'$, find $u \in L^2(\Omega)$ and $q \in Q$ such that

$$b((u, q), v) = F(v), \quad \forall v \in W_h.$$

Theorem 2.7. *Suppose Assumption 1 holds. Then Problem 2.6 is well posed, i.e., there is a $C > 0$ such that given any $F \in W_h'$, there is a unique solution $(u, q) \in L^2(\Omega) \times Q$ to Problem 2.6 and it satisfies*

$$\|u\|_\Omega^2 + \|q\|_Q^2 \leq C \|F\|_{W_h'}^2.$$

Moreover, if $F(v) = (f, v)_\Omega$ for some $f \in L^2(\Omega)$, then u is in V and $q = D_h u$.

Proof. The result follows from Theorem A.5. Since Lemma 2.2 together with (2.4) implies (A.12) and Theorem 2.4 implies (A.13), the assumptions of Theorem A.5 are verified. \square

3. VERIFICATION OF THE DENSITY ASSUMPTION

In the next three sections, Ω_0 is set to be the interval $(0, L)$ and $\Omega = (0, L) \times (0, T)$ where $L, T > 0$. The purpose of this section is to verify the density assumption (Assumption 1) in this case of one space dimension.

Theorem 3.1. *Let $\Omega = (0, L) \times (0, T)$. Then $\mathcal{V}^* = \{\varphi \in \mathcal{D}(\bar{\Omega}) : \varphi|_{\Gamma^*} = 0\}$ is dense in V^* and $\mathcal{V} = \{\varphi \in \mathcal{D}(\bar{\Omega}) : \varphi|_\Gamma = 0\}$ is dense in V .*

Proof. Since the proofs of both the stated density results are similar, we will only show the proof of density of \mathcal{V}^* in V^* .

Step 1. Extend: Let $\Omega_l = (-L, 0] \times (0, T)$ and $\Omega_r = [L, 2L) \times (0, T)$. Define an operator G that extends functions on Ω to $\hat{\Omega} \equiv \Omega_l \cup \Omega \cup \Omega_r$ by

$$Gw(x, t) = \begin{cases} -w(-x, t), & (x, t) \in \Omega_l, \\ -w(2L - x, t), & (x, t) \in \Omega_r, \end{cases}$$

(and $Gw(x, t) = w(x, t)$ for all $(x, t) \in \Omega$). Let G' be the reverse operator that maps functions on $\hat{\Omega}$ to Ω by $G'\bar{w}(x, t) = \bar{w}(x, t) - \bar{w}(-x, t) - \bar{w}(2L - x, t)$, for all $(x, t) \in \Omega$ (see Figure 2). Such definitions are to be interpreted a.e., so that for example, Gw is well defined for any w in $L^2(\Omega)$. It is easy to see by a change of variable that

$$(Gf, g)_{\hat{\Omega}} = (f, G'g)_\Omega, \quad \forall f \in L^2(\Omega), g \in L^2(\hat{\Omega}). \quad (3.1)$$

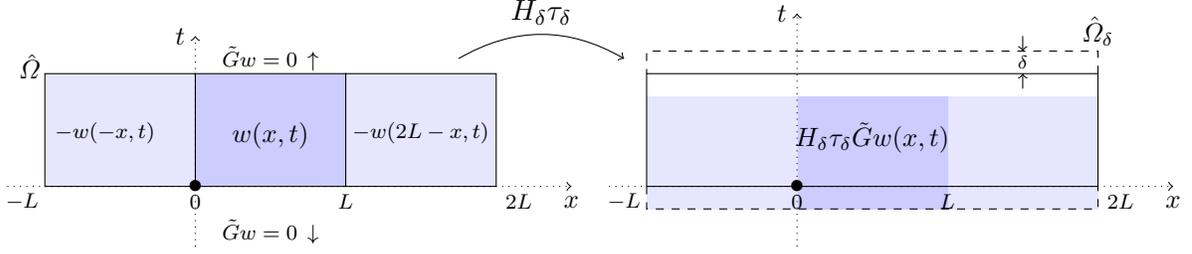


FIGURE 2. Extension and translation in the proof of Theorem 3.1.

Next, we claim that

$$AGv = GA v, \quad \forall v \in V^*. \quad (3.2)$$

Clearly, Gv is in $L^2(\hat{\Omega})$. Let $\varphi \in \mathcal{D}(\hat{\Omega})$. Let $\langle AGv, \varphi \rangle_{\mathcal{D}(\hat{\Omega})}$ denote the action of the distribution AGv on φ . Then $\langle AGv, \varphi \rangle_{\mathcal{D}(\hat{\Omega})} = (Gv, A\varphi)_{\hat{\Omega}} = (v, G'A\varphi)_{\Omega}$ because of (3.1). By the chain rule applied to the smooth function φ , we find that

$$G'A\varphi = AG'\varphi. \quad (3.3)$$

Hence,

$$\langle AGv, \varphi \rangle_{\mathcal{D}(\hat{\Omega})} = (v, AG'\varphi)_{\Omega} = (Av, G'\varphi)_{\Omega} - \langle Dv, G'\varphi \rangle_W. \quad (3.4)$$

Now observe that $G'\varphi|_{\Gamma} = 0$. Hence by Lemma 2.1, $G'\varphi$ is in V . Since $v \in V^*$ and $G'\varphi \in V$, the last term of (3.4) must vanish by (2.3). Thus $\langle AGv, \varphi \rangle_{\mathcal{D}(\hat{\Omega})} = (Av, G'\varphi)_{\Omega} = (GA v, \varphi)_{\hat{\Omega}}$, completing the proof of the claim (3.2). In view of (3.2), we conclude that Gv is in $W(\hat{\Omega})$ whenever $v \in V^*$.

Step 2. Translate: Let $\tilde{G}v$ denote the extension of Gv by zero to \mathbb{R}^2 , i.e., $\tilde{G}v$ equals Gv on $\hat{\Omega}$ and equals zero elsewhere. Let τ_δ be the translation operator in the $-t$ direction by δ , i.e., $(\tau_\delta w)(x, t) = w(x, t + \delta)$. It is well known ([3]) that

$$\lim_{\delta \rightarrow 0} \|\tau_\delta g - g\|_{\mathbb{R}^2} = 0, \quad \forall g \in L^2(\mathbb{R}^2). \quad (3.5)$$

Let $\hat{\Omega}_\delta = (-L, 2L) \times (-\delta, T + \delta)$ and let H_δ denote the restriction of functions on \mathbb{R}^2 to $\hat{\Omega}_\delta$. By a change of variable,

$$(\tau_\delta \tilde{G}f, g)_{\hat{\Omega}_\delta} = (Gf, \tau_{-\delta}g)_{\hat{\Omega}}, \quad \forall f \in L^2(\Omega), g \in L^2(\hat{\Omega}_\delta). \quad (3.6)$$

We now claim that

$$AH_\delta \tau_\delta \tilde{G}v = H_\delta \tau_\delta \tilde{G}Av, \quad \forall v \in V^*. \quad (3.7)$$

Indeed, for any $\varphi \in \mathcal{D}(\hat{\Omega}_\delta)$, the action of the distribution $AH_\delta \tau_\delta \tilde{G}v$ on φ equals

$$\begin{aligned} \langle AH_\delta \tau_\delta \tilde{G}v, \varphi \rangle_{\mathcal{D}(\hat{\Omega}_\delta)} &= (\tau_\delta \tilde{G}v, A\varphi)_{\hat{\Omega}_\delta} = (Gv, A\tau_{-\delta}\varphi)_{\hat{\Omega}} = (v, G'A\tau_{-\delta}\varphi)_{\Omega} = (v, AG'\tau_{-\delta}\varphi)_{\Omega} \\ &= (Av, G'\tau_{-\delta}\varphi)_{\Omega} - \langle Dv, G'\tau_{-\delta}\varphi \rangle_W, \end{aligned}$$

where we have used (3.6), (3.1), and (3.3) consecutively. Since $(G'\tau_{-\delta}\varphi)|_{\Gamma} = 0$, Lemma 2.1 shows that $G'\tau_{-\delta}\varphi$ is in V , and consequently the last term above vanishes for all $v \in V^*$. Continuing and using (3.1) and (3.6) once more, $\langle AH_\delta \tau_\delta \tilde{G}v, \varphi \rangle_{\mathcal{D}(\hat{\Omega}_\delta)} = (GA v, \tau_{-\delta}\varphi)_{\hat{\Omega}} = (\tau_\delta \tilde{G}Av, \varphi)_{\hat{\Omega}_\delta}$. This proves (3.7).

Step 3. Mollify: Consider the mollifier $\rho_\varepsilon \in \mathcal{D}(\mathbb{R}^2)$, for each $\varepsilon > 0$, defined by $\rho_\varepsilon(x, t) = \varepsilon^{-2} \rho_1(\varepsilon^{-1}x, \varepsilon^{-1}t)$, where

$$\rho_1(x, t) = \begin{cases} k e^{-\frac{1}{1-x^2-t^2}} & \text{if } x^2 + t^2 < 1, \\ 0 & \text{if } x^2 + t^2 \geq 1, \end{cases}$$

and k is a constant chosen so that $\int_{\mathbb{R}^2} \rho_1 = 1$. It is well known ([3]) that when any function w in $L^2(\mathbb{R}^2)$ is convolved with ρ_ε , the result $\rho_\varepsilon * w$ is infinitely smooth and satisfies

$$\lim_{\varepsilon \rightarrow 0} \|w - \rho_\varepsilon * w\|_{\mathbb{R}^2} = 0, \quad \forall w \in L^2(\mathbb{R}^2). \quad (3.8)$$

Consider any small enough $\delta > 0$, say $\delta < \min(L/2, T/2)$, and define two functions $v_\varepsilon = \rho_\varepsilon * \tau_\delta \tilde{G}v$ and $a_\varepsilon = \rho_\varepsilon * \tau_\delta \tilde{G}Av$. Note that the two smooth functions Av_ε and a_ε need not coincide everywhere. However, because of (3.7), they coincide on Ω whenever $\varepsilon < \delta/2$:

$$Av_\varepsilon = a_\varepsilon \quad \text{on } \Omega.$$

Let us therefore set δ to, say, $\delta = 3\varepsilon$ and let $\varepsilon < \min(L/2, T/2)/3$ go to zero. Note that

$$\begin{aligned} \|Av_\varepsilon - Av\|_\Omega &= \|a_\varepsilon - Av\|_\Omega = \|\rho_\varepsilon * \tau_\delta \tilde{G}Av - Av\|_\Omega \\ &\leq \|\rho_\varepsilon * \tau_\delta \tilde{G}Av - \tau_\delta \tilde{G}Av\|_{\mathbb{R}^2} + \|\tau_\delta \tilde{G}Av - \tilde{G}Av\|_{\mathbb{R}^2}, \\ \|v_\varepsilon - v\|_\Omega &\leq \|\rho_\varepsilon * \tau_\delta \tilde{G}v - \tau_\delta \tilde{G}v\|_\Omega + \|\tau_\delta \tilde{G}v - v\|_\Omega \\ &\leq \|\rho_\varepsilon * \tau_\delta \tilde{G}v - \tau_\delta \tilde{G}v\|_{\mathbb{R}^2} + \|\tau_\delta \tilde{G}v - \tilde{G}v\|_{\mathbb{R}^2}. \end{aligned}$$

Using (3.8) and (3.5) it now immediately follows that

$$\lim_{\varepsilon \rightarrow 0} \|v_\varepsilon - v\|_W = 0.$$

To conclude, examine the value of v_ε at points $z = (0, t)$ for any $0 < t < T$, namely

$$v_\varepsilon(0, t) = \int_{\mathbb{R}} \int_{\mathbb{R}} \rho_\varepsilon(-x', t - t') (\tau_\delta \tilde{G}v)(x', t') dx' dt'.$$

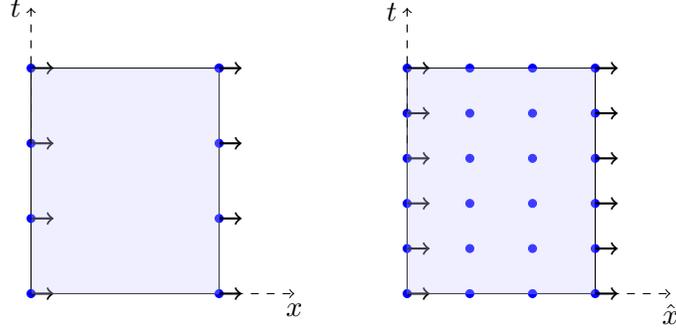
The integrand of the inner integral is the product of an even function (ρ_ε) of x' and an odd function $\tau_\delta \tilde{G}v$ of x' . Hence $v_\varepsilon(0, t) = 0$. The same holds for points $z = (L, t)$. Moreover, since $\tau_\delta \tilde{G}v(y)$ is identically zero in a neighborhood of $z = (T, x)$ for all $0 < x < L$, we conclude that $v_\varepsilon|_{\Gamma^*} = 0$. \square

4. ERROR ESTIMATES FOR THE IDEAL DPG METHOD

Continuing to consider the set Ω as defined in Section 3, we now proceed to analyze the convergence of the ideal DPG method for Problem 2.6. The ideal DPG method finds u_h and q_h in finite dimensional subspaces $U_h \subset L^2(\Omega)$ and $Q_h \subset Q$ respectively, satisfying

$$b((u_h, q_h), v) = F(v), \quad \text{for all } v \in T(U_h \times Q_h). \quad (4.1)$$

Here $T : L^2(\Omega) \times Q \rightarrow W_h$ is defined by $(T(z, r), v) = b((z, r), v)$ for all $v \in W_h$ and any $(z, r) \in L^2(\Omega) \times Q$. The main feature of the ideal DPG method is that the wellposedness of Problem 2.6 implies quasioptimality of the method's error [14]. The wellposedness of Problem 2.6 follows from Theorem 2.7, now that we have verified Assumption 1 in Theorem 3.1. Hence to obtain convergence rates for specific subspaces, we need only develop interpolation error estimates. Since the interpolation properties of the L^2 -conforming U_h are standard, we need only discuss those of Q_h . To study this, we will create a spacetime finite element space $V_h \subset V$, then identify


 FIGURE 3. Degrees of freedom in the $p = 3$ (left) and $p = 5$ (right) cases.

Q_h as $D_h(V_h)$, and finally establish interpolation estimates for Q_h using those for V_h . Note that V_h will be used only in the proof (and not in the computations).

To transparently present the ideas, we shall limit ourselves to the very simple case of a uniform mesh Ω_h of spacetime square elements of side length h . Let \mathcal{E}_h denote the set of edges of Ω_h . On any $E \in \mathcal{E}_h$, let $P_p(E)$ denote the space of polynomials on the edge of degree at most p . On any $K \in \Omega_h$, let $Q_p(K)$ denote the space of polynomials of degree at most p in x and at most p in t . To begin the finite element construction, we consider the reference element $\hat{K} = (0, 1) \times (0, 1)$ and the element space $Q_p(\hat{K})$, endowed with the following degrees of freedom: For any $w \in H^3(K)$, and for each $i \in \{0, 1, \dots, p-2\}$ and $j \in \{0, 1, 2, \dots, p\}$, write $x_i = i/(p-2)$ and $t_j = j/p$ and set

$$\sigma_{ij}(w) = w(x_i, t_j), \quad \sigma_j^0(w) = \partial_x w(0, t_j), \quad \sigma_j^1(w) = \partial_x w(1, t_j).$$

Together, these form a set Σ with $(p-1)(p+1) + 2(p+1)$ linear functionals. The triple $(\hat{K}, Q_p(\hat{K}), \Sigma)$ is a unisolvent finite element, in the sense of [8], as we show next.

Lemma 4.1. *Suppose $p \geq 3$. Then any polynomial $w \in Q_p(\hat{K})$ is uniquely defined by the values of its degrees of freedom σ in Σ .*

Proof. Suppose $w \in Q_p(\hat{K})$ and $\sigma(w) = 0$ for all $\sigma \in \Sigma$. Then $w_j(x) = w(x, t_j)$ is a polynomial of degree p in one variable (x). The Hermite and Lagrange degrees of freedom on $t = t_j$ imply $w_j = 0$. Now, fixing x , observe that the polynomial $w(x, t)$ is of degree at most p in the variable t and has $p+1$ zeros. Hence $w \equiv 0$ and the proof is complete since $\dim Q_p(\hat{K})$ equals the number of degrees of freedom. \square

Next, consider the global finite element space $W_h^p(\Omega) = \{w \in L^2(\Omega) : \partial_t w \text{ and } \partial_{xx} w \text{ are in } L^2(\Omega) \text{ and } w|_K \in Q_p(K) \text{ for all } K \in \Omega_h\}$. Each element $K \in \Omega_h$ is obtained by mapping the reference element \hat{K} by $T_K : \hat{K} \rightarrow K$, $T_K(\hat{x}, \hat{t}) = (h\hat{x} + x_K, h\hat{t} + t_K)$, where (x_K, t_K) is the lower left corner vertex of K , and the element space $Q_p(K)$ is the pull back of the reference element space $Q_p(\hat{K})$ under this map. The space $W_h^p(\Omega)$ can be controlled by a global set of degrees of freedom obtained by mapping the reference element degrees of freedom and, as usual, coalescing those that coincide at the mesh element interfaces.

On the reference element \hat{K} , the degrees of freedom define an interpolation operator

$$\hat{\Pi}w = \sum_{\sigma \in \Sigma} \sigma(w) \varphi_\sigma$$

where, as usual, $\{\varphi_\eta \in Q_p(\hat{K}) : \eta \in \Sigma\}$ is the set of shape functions obtained as the dual basis of Σ . By the Sobolev inequality in two dimensions, $\hat{\Pi} : H^3(\hat{K}) \rightarrow Q_p(\hat{K})$ is continuous. Similarly, the global degrees of freedom define an interpolation operator $\Pi : H^3(\Omega) \rightarrow W_h^p(\Omega)$ satisfying

$$(\Pi w) \circ T_K = \hat{\Pi}(w \circ T_K). \quad (4.2)$$

Lemma 4.2. *If $w \in H^{p+1}(\Omega)$, then for all $p \geq 3$,*

$$\begin{aligned} \|w - \Pi w\|_\Omega &\leq Ch^{p+1}|w|_{H^{p+1}(\Omega)} \\ \|\partial_t(w - \Pi w)\|_\Omega &\leq Ch^p|w|_{H^{p+1}(\Omega)} \\ \|\partial_{xx}(w - \Pi w)\|_\Omega &\leq Ch^{p-1}|w|_{H^{p+1}(\Omega)}. \end{aligned}$$

Proof. Changing variables $(x, t) = T_K(\hat{x}, \hat{t})$ as (\hat{x}, \hat{t}) runs over \hat{K} , integrating, and using (4.2),

$$\|w - \Pi w\|_K = h\|\hat{w} - \hat{\Pi}\hat{w}\|_{\hat{K}} \quad (4.3a)$$

$$\|\partial_t(w - \Pi w)\|_K = \|\partial_{\hat{t}}(\hat{w} - \hat{\Pi}\hat{w})\|_{\hat{K}} \quad (4.3b)$$

$$\|\partial_{xx}(w - \Pi w)\|_K = h^{-1}\|\partial_{\hat{x}\hat{x}}(\hat{w} - \hat{\Pi}\hat{w})\|_{\hat{K}}. \quad (4.3c)$$

On the reference element, since $H^{p+1}(\hat{K}) \hookrightarrow H^3(\hat{K})$, the interpolation operator $\hat{\Pi} : H^{p+1}(\hat{K}) \rightarrow Q_p(\hat{K})$ is continuous. Moreover $\hat{\Pi}\hat{w} = \hat{w}$ for all $\hat{w} \in Q_p(\hat{K})$. Hence, the Bramble-Hilbert Lemma yields a $\hat{C} > 0$ such that $\|\hat{w} - \hat{\Pi}\hat{w}\|_{H^3(\hat{K})} \leq \hat{C}|\hat{w}|_{H^{p+1}(\hat{K})}$ for all $\hat{w} \in H^{p+1}(\hat{K})$. Since $|\hat{w}|_{H^{p+1}(\hat{K})} \leq Ch^p|w|_{H^{p+1}(K)}$, combining with (4.3) and summing over all the elements in Ω_h , we obtain the result. \square

Now we are ready to present the main result of this section. Set $V_h = W_h^p(\Omega) \cap V$ and

$$Q_h = D_h(V_h), \quad U_h = \{u \in L^2(\Omega) : u|_K \in Q_{p-1}(K) \text{ for all } K \in \Omega_h\}. \quad (4.4)$$

Theorem 4.3. *Let $p \geq 3$. Suppose $u \in V \cap H^{p+1}(\Omega)$ and $q = D_h u$ solve Problem 2.6 and suppose $U_h \times Q_h$ is set by (4.4). Then, there exists a constant C independent of h such that the discrete solution $u_h \in U_h$ and $q_h \in Q_h$ solving (4.1) satisfies*

$$\|u - u_h\|_\Omega + \|q - q_h\|_Q \leq Ch^r|u|_{H^{r+2}(\Omega)} \quad (4.5)$$

for $2 \leq r \leq p - 1$.

Proof. By [14, Theorem 2.2] the ideal DPG method is quasioptimal:

$$\begin{aligned} \|(u, q) - (u_h, q_h)\|_{U \times Q}^2 &\leq C \inf_{(z_h, r_h) \in U_h \times Q_h} \|(u, q) - (z_h, r_h)\|_{U \times Q}^2 \\ &= C \inf_{(z_h, r_h) \in U_h \times Q_h} (\|u - z_h\|_\Omega^2 + \|q - r_h\|_Q^2). \end{aligned}$$

Because of the standard approximation estimate $\inf_{z_h \in U_h} \|u - z_h\|_\Omega \leq Ch^r|u|_{H^r(\Omega)}$ for $0 \leq r \leq p - 1$, it suffices to focus on $\|q - r_h\|_Q$. Since $q = D_h u$, by the definition of Q -norm (A.14), and the fact that any r_h in Q_h equals $D_h v_h$ for some $v_h \in V_h$, we have

$$\inf_{r_h \in Q_h} \|q - r_h\|_Q \leq \inf_{v_h \in V_h} \|u - v_h\|_W \leq \|u - \Pi u\|_W.$$

Applying Lemma 4.2, the result follows. \square

We conclude this section by examining a property of Q_h that is useful for computations. Let \mathcal{E}_h^i and \mathcal{E}_h^- denote the set of vertical and horizontal (closed) mesh edges, respectively, and $\mathcal{E}_h^+ = \mathcal{E}_h^i \cup \mathcal{E}_h^-$. Let E_h^i and E_h^+ denote the closed set formed by the union of all edges in \mathcal{E}_h^i and \mathcal{E}_h^+ , respectively. Let $Q_h^i = \{r \in L^2(E_h^i) : r|_F \in P_p(F) \text{ for all } F \in \mathcal{E}_h^i\}$ and $Q_h^+ = \{r \in L^2(E_h^+) : r \text{ is continuous on } E_h^+ \text{ and } r|_F \in P_p(F) \text{ for all } F \in \mathcal{E}_h^+ \text{ and } r|_\Gamma = 0\}$. For any $v_h \in V_h$, since v_h is a polynomial on each element, we may integrate by parts element by element to get

$$\begin{aligned} \langle D_h v_h, \psi \rangle_h &= (A_h v_h, \psi)_h - (v_h, A_h \psi)_h \\ &= \sum_{K \in \Omega_h} \int_{\partial K} in_t v_h \bar{\psi} + \int_{\partial K} v_h n_x (\partial_x \bar{\psi}) - \int_{\partial K} n_x (\partial_x v_h) \bar{\psi}, \end{aligned}$$

for all $\psi \in \mathcal{D}(\bar{\Omega})$. Thus $q = D_h v_h$ satisfies

$$\langle q, \psi \rangle_h = \sum_{K \in \Omega_h} \int_{\partial K} q^+ (in_t \bar{\psi}) + \int_{\partial K} q^+ n_x (\partial_x \bar{\psi}) - \int_{\partial K} q^i (n_x \bar{\psi}),$$

where $q^+ = v_h|_{E_h^+}$ and $q^i = \partial_x v_h|_{E_h^i}$. In computations, one may therefore identify Q_h with the interfacial polynomial space $Q_h^+ \times Q_h^i$ whose components are of degree at most p .

5. NUMERICAL RESULTS

This section is motivated by our interest in simulating electromagnetic pulse propagation in dispersive optical fibers. Nonlinear, dispersive Maxwell equations in the context of optical fibers have been studied extensively [1]. The common approach to model dispersive, intensity-dependent nonlinearities is based on several simplifying approximations. These approximations include a slowly varying pulse envelope, a quasi-monochromatic optical field, a specific polarization maintained along the fiber length, and approximation of nonlinear terms as perturbations of the purely linear case. With these assumptions, the full Maxwell equations are reduced [1, 26] to the “nonlinear Schrödinger equation”

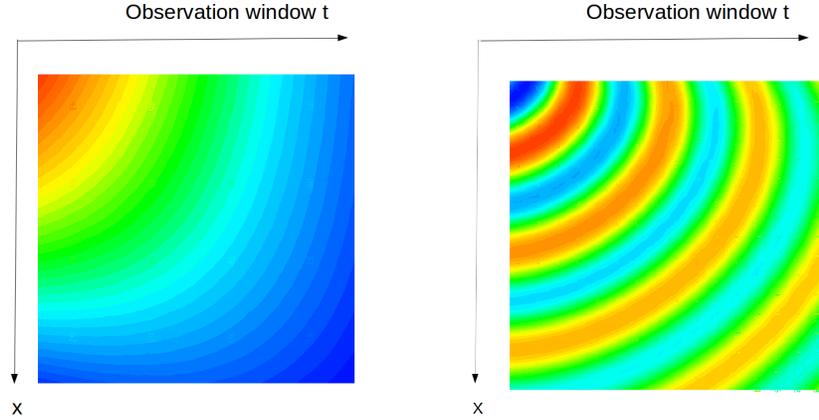
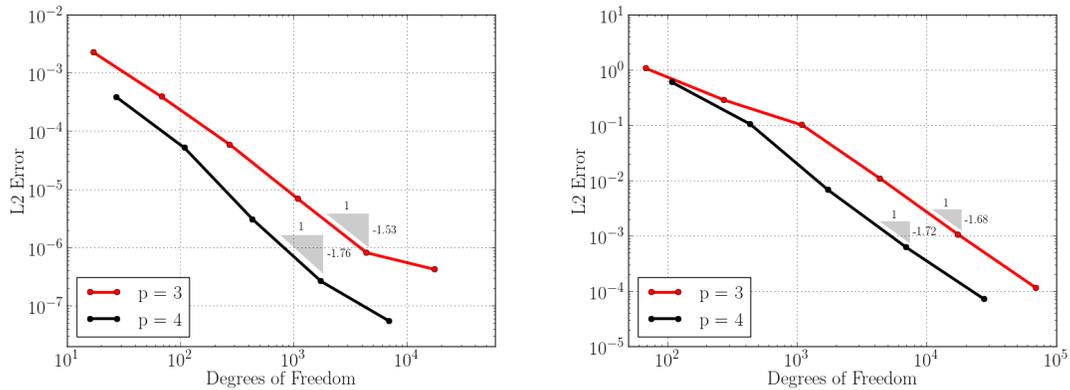
$$i \frac{\partial a}{\partial x} - \frac{\beta}{2} \frac{\partial^2 a}{\partial t^2} + \gamma |a|^2 a = 0,$$

where x is the distance along the fiber, t is an observation window (in time), β is some given fiber-dependent constant, and a is a complexified amplitude of the pulse.

Since the roles of x and t in this application may be confusing, we switch them to agree with the previous sections and consider the simple case of $\gamma = 0$. In other words, we present numerical results obtained using a practical DPG method applied to the one dimensional Schrödinger problem

$$\begin{aligned} i \partial_t u - \frac{\beta}{2} \partial_{xx} u &= f, & 0 < x < 1, 0 < t < 1, \\ u(x, 0) &= u_0(x), & 0 < x < 1, \\ u(0, t) &= u_l(t), & 0 < t < 1, \\ u(1, t) &= u_r(t), & 0 < t < 1. \end{aligned}$$

To describe the method we used in practice, first set $b((u, q), v)$ using the Schrödinger operator $A = i \partial_t - (\beta/2) \partial_{xx}$ and recall (4.1). As mentioned in the previous section, the action of any $q = D_h u$ on the boundary of each element, can be viewed as a combination of two *independent* boundary actions of variables q^+ and q^i that are of the same polynomial order.

FIGURE 4. Plots of solutions. *Left:* Case (a). *Right:* Case (b).FIGURE 5. Rates of convergence. *Left:* Results from case (a) with the complex Gaussian solution. *Right:* Results from the case (b) with the wave packet of frequency $\omega = 20$.

However, we are led to implement a slightly different space because our computational tool is a standard Petrov-Galerkin code supporting the exact sequence elements of the first type [20]. Accordingly, q^+ is discretized with (continuous) traces of H^1 conforming elements of order p but q^l is discretized with (discontinuous) traces of the compatible $H(\text{div})$ conforming elements of order $p - 1$, i.e., one order less than required by the presented interpolation theory. Let \tilde{Q}_h represent this reduced space. The next modification needed in our implementation is an approximation of T . Let $T_h(z, r) \in W_h^{\Delta p}$ be defined by $(T_h(z, r), v) = b((z, r), v)$ for all $v \in W_h^{\Delta p}$ and any $(z, r) \in U_h \times \tilde{Q}_h$, where $W_h^{\Delta p} = \{w \in W_h : w|_K \in Q_{p+\Delta p}(K) \text{ for all } K \in \Omega_h\}$. Thus the practically implemented method, in contrast to (4.1), finds $u_h \in U_h$ and $q_h \in \tilde{Q}_h$ satisfying

$$b((u_h, q_h), v) = F(v)$$

for all $v \in T_h(U_h \times \tilde{Q}_h)$. In all the results presented below, no significant differences were seen between $\Delta p = 1$ and $\Delta p = 2$, so we only report the results obtained with $\Delta p = 1$.

We report the observed rates of convergence for two problems: (a) The first case is when the exact solution is a complex Gaussian

$$u(x, t) = \frac{MT_0}{\sqrt{T_0^2 - i\beta t}} e^{-\frac{x^2}{T_0^2 - i\beta t}}, \quad (5.1)$$

where M, T_0 , and β are fiber-dependent constants (see [26]). Our simulations used non-dimensionalized units of $M = T_0 = 1.5$ and $\beta = 2.5$. (b) The second example uses an exact solution which is a wave packet traveling along the fiber whose in-packet oscillations are of moderately high wavenumber ω , namely

$$u(x, t) = a_0 e^{-\frac{x^2 + t^2}{\omega^2}}, \quad (5.2)$$

where the amplitude $a_0 = (2/\omega^2)^{1/4}$ and the wavenumber is $\omega = 20$. Plots of solutions in either case are displayed in Figure 4.

The observed convergence rates are displayed in Figure 5 (the left plot shows results from case (a) and the right plot shows results from case (b)). We experiment with $p = 3$ and $p = 4$ cases. For the ideal DPG method using the $U_h \times Q_h$ in (4.4), Theorem 4.3 implies that the convergence rate in terms of the number of degrees of freedom $n = O(h^{-2})$ is $O(n^{-s})$ where $s = (p - 1)/2$. We observe from Figure 5 that in spite of reducing Q_h to \tilde{Q}_h and in spite of approximating T by T_h , we continue to observe a rate higher than s . Namely, in the $p = 3$ case, while we expected a rate of $s \leq 1$, the observed rate is $s \approx 1.5$. In the $p = 4$ case, while the expected rate is $s \leq 1.5$, the observed rate is between 1.5 and 2. An improved error analysis explaining these observations is yet to be found.

Note the flattening out of the curves in left plot of Figure 5. This is due to conditioning issues. As with any method using second order derivatives, we should be wary of conditioning. Indeed, the DPG system with $p = 3$ or $p = 4$, after 4 or 5 uniform refinements, has a condition number in the vicinity of $O(10^{10})$. Therefore, the roundoff effect becomes apparent after we achieve an error threshold around 10^{-6} or 10^{-7} . This is the cause of convergence curves flattening out in case (a). In case (b), due to $\omega = 20$, we start with a higher error so the loss of digits due to conditioning issues is postponed.

APPENDIX A. ABSTRACT WEAK FORMULATION

In this section, we consider a boundary value problem involving a general partial differential operator. We derive a mesh-dependent weak formulation of the boundary value problem and show that it is possible to identify sufficient conditions for its wellposedness. This section can be read independently of the remainder of the paper.

Let $\Omega \subseteq \mathbb{R}^d$ be a bounded open set in $d \geq 1$ dimensions and let $k, l, m \geq 1$ be integers. Let A be a differential operator such that i th component of Au is

$$[Au]_i = \sum_{j=1}^m \sum_{|\alpha| \leq k} \partial^\alpha (a_{ij\alpha} u_j), \quad (\text{A-a})$$

where $a_{ij\alpha} : \Omega \rightarrow \mathbb{C}$ are functions for all $i = 1, \dots, l$, $j = 1, \dots, m$, and all multi-indices $\alpha = (\alpha_1, \dots, \alpha_d)$ whose length is $|\alpha| = \alpha_1 + \dots + \alpha_d \leq k$. As usual, $\partial^\alpha = \partial_1^{\alpha_1} \dots \partial_d^{\alpha_d}$. The formal adjoint of A is given by

$$[A^*v]_j = \sum_{i=1}^l \sum_{|\alpha| \leq k} (-1)^{|\alpha|} \overline{a_{ji\alpha}} \partial^\alpha v_j. \quad (\text{A.1})$$

We assume that the coefficients $a_{ij\alpha}$ are such that

$$A^*u \in \mathcal{D}'(\Omega)^m \quad \text{for all } u \in L^2(\Omega)^l. \quad (\text{A-b})$$

E.g., (A-b) is satisfied if $a_{ij\alpha}$ are smooth.

For any nonempty open subset $S \subseteq \Omega$, define the space

$$W(S) = \{u \in L^2(S)^m : Au \in L^2(S)^l\}, \quad (\text{A.2})$$

normed by $\|u\|_{W(S)} = (\|u\|_S^2 + \|Au\|_S^2)^{1/2}$, and the space

$$W^*(S) = \{u \in L^2(S)^l : A^*u \in L^2(S)^m\} \quad (\text{A.3})$$

normed by $\|u\|_{W^*(S)} = (\|u\|_S^2 + \|A^*u\|_S^2)^{1/2}$. Here and throughout, $(\cdot, \cdot)_\Omega$ and $\|\cdot\|_\Omega$ denotes the inner product and the norm, respectively, in $L^2(\Omega)$ or its Cartesian products. To simplify notation, we abbreviate $W = W(\Omega)$, $W^* = W^*(\Omega)$. Clearly these are inner product spaces.

Lemma A.1. *The spaces $W(S)$ and $W^*(S)$ are Hilbert spaces.*

Proof. Since the proofs for $W(S)$ and $W^*(S)$ are similar, we only show the first. Suppose u_n is a Cauchy sequence in $W(S)$. Then u_n is Cauchy in $L^2(S)^m$ and Au_n is Cauchy in $L^2(S)^l$. Hence there is a $u \in L^2(S)^m$ and $f \in L^2(S)^l$ such that $\|u - u_n\|_S \rightarrow 0$ and $\|f - Au_n\|_S \rightarrow 0$. We will show that u is in $W(S)$.

Let $\phi \in \mathcal{D}(S)^l$. For each $w \in L^2(S)^m$, the distributional action of Aw on $\bar{\phi}$, denoted by $\langle Aw, \phi \rangle_{\mathcal{D}(S)^l}$, equals $(w, A^*\phi)_S$. If w is also in $W(S)$, then

$$(Aw, \phi)_S = \langle Aw, \phi \rangle_{\mathcal{D}(S)^l} = (w, A^*\phi)_S, \quad (\text{A.4})$$

for all ϕ in $\mathcal{D}(S)^l$. To complete the proof, we apply (A.4) with $w = u_n$ to get

$$\langle Au, \phi \rangle_{\mathcal{D}(S)^l} = (u, A^*\phi)_S = \lim_{n \rightarrow \infty} (u_n, A^*\phi)_S = \lim_{n \rightarrow \infty} (Au_n, \phi)_S = (f, \phi)_S$$

for all ϕ in $\mathcal{D}(S)^l$. Hence $Au = f$ and u is in $W(S)$. \square

Next, define bounded linear operators $D_S : W(S) \rightarrow W^*(S)'$ and $D_S^* : W^*(S) \rightarrow W(S)'$ by

$$\langle D_S w, \tilde{w} \rangle_{W^*(S)} = (Aw, \tilde{w})_S - (w, A^*\tilde{w})_S, \quad (\text{A.5})$$

$$\langle D_S^* \tilde{w}, w \rangle_{W(S)} = (A^*\tilde{w}, w)_S - (\tilde{w}, Aw)_S, \quad (\text{A.6})$$

for all $w \in W(S)$ and $\tilde{w} \in W^*(S)$. When $S = \Omega$, we abbreviate D_S and D_S^* to D and D^* , respectively. Here, like in (A.4), and in the remainder, we use $\langle \cdot, \cdot \rangle_X$ to denote the action of a linear functional in X' on an element of X .

Next we will view $A : \text{dom}(A) \subset L^2(\Omega)^m \rightarrow L^2(\Omega)^l$ as an unbounded linear operator, whose domain (denoted by $\text{dom}(A)$) is chosen so that

$$\mathcal{D}(\Omega)^m \subseteq \text{dom}(A). \quad (\text{A-c})$$

This implies that A is a densely defined operator. Then, identifying the dual of (Cartesian products of) $L^2(\Omega)$ with itself, recall that the adjoint $A^* : \text{dom}(A^*) \subset L^2(\Omega)^l \rightarrow L^2(\Omega)^m$ is a uniquely defined (unbounded) closed linear operator [3, 24] on $\text{dom}(A^*) = \{s \in L^2(\Omega)^l : \text{there is an } \ell \in L^2(\Omega)^m \text{ such that } (Av, s)_\Omega = (v, \ell)_\Omega \text{ for all } v \in \text{dom}(A)\}$, satisfying $(Av, \tilde{v})_\Omega = (v, A^*\tilde{v})_\Omega$ for all $v \in \text{dom}(A)$ and $\tilde{v} \in \text{dom}(A^*)$. Note that $\mathcal{D}(\Omega)^l \subseteq \text{dom}(A^*)$. Note also that by an abuse of notation, we have used A^* to denote both the differential operator in (A.1) and the adjoint operator of the unbounded A .

When $\text{dom}(A)$ is endowed with the topology of $W(\Omega)$, we call it V , i.e., although V and $\text{dom}(A)$ coincide as sets, V has the topology of $W(\Omega)$ and $\text{dom}(A)$ has the topology of $L^2(\Omega)^m$. Similarly, $\text{dom}(A^*)$ is called V^* when it is endowed with the topology of $W^*(\Omega)$. For the next result, recall that the left annihilator of any subspace R of the dual space X' of any Banach space X is defined by ${}^\perp R = \{w \in X : \langle s', w \rangle_X = 0 \text{ for all } s' \in R\}$.

Lemma A.2. *In the setting of (A-a), (A-b) and (A-c), we have $V^* = {}^\perp D(V)$.*

Proof. According to the (above-mentioned) definition of $\text{dom}(A^*)$, for any $\tilde{v} \in \text{dom}(A^*) = V^*$, there is an $\ell \in L^2(\Omega)^l$ such that

$$(Av, \tilde{v})_\Omega = (v, \ell)_\Omega, \quad \forall v \in V. \quad (\text{A.7})$$

Due to (A-c), we may choose v in $\mathcal{D}(\Omega)^m$. By (A-b), $A^*\tilde{v}$ is a distribution and by (A.7) this distribution is in $L^2(\Omega)^m$ and equals ℓ . In particular, \tilde{v} is in $W^*(\Omega)$. Hence (A.5) is applicable, and in combination with (A.7) yields $\langle Dv, \tilde{v} \rangle_{W^*(\Omega)} = (Av, \tilde{v})_\Omega - (v, \ell)_\Omega = 0$ for all $v \in V$. Hence $\tilde{v} \in {}^\perp D(V)$ and we have proved that $V^* \subseteq {}^\perp D(V)$. The reverse containment is also easy to prove. \square

We are interested in the boundary value problem of finding u satisfying

$$Au = f, \quad u \in V, \quad (\text{A.8})$$

given $f \in L^2(\Omega)^l$. Homogeneous boundary conditions are incorporated in V . Consider the scenario where Ω is partitioned into a mesh Ω_h of finitely many open elements K such that $\bar{\Omega} = \cup_{K \in \Omega_h} \bar{K}$. Here the index h denotes $\max_{K \in \Omega_h} \text{diam}(K)$. Recall D_K and D_K^* by replacing S by K in (A.5) and (A.6). Additionally, set

$$W_h = \prod_{K \in \Omega_h} W(K), \quad (W_h^*)' = \prod_{K \in \Omega_h} W^*(K)'. \quad (\text{A.9})$$

The spaces W_h^* and W_h' are defined similarly. The component on an element K of functions in such product spaces are indicated by placing K as subscript, e.g., for any w in W_h , the component of w on element K is denoted by w_K . Let $D_h : W_h \rightarrow (W_h^*)'$ be the continuous linear operator defined by

$$\langle D_h w, v \rangle_{W_h^*} = \sum_{K \in \Omega_h} \langle D_K w_K, v_K \rangle_{W^*(K)}$$

for all $w \in W_h$ and $v \in W_h^*$. To simplify notation, we abbreviate $\langle D_h w, v \rangle_{W_h^*}$ to $\langle D_h w, v \rangle_h$, i.e., duality pairing in W_h^* is simply denoted by $\langle \cdot, \cdot \rangle_h$. For any $w \in W_h$, we denote by $A_h w$ the function obtained by applying A to w_K , element by element, for all $K \in \Omega_h$. The resulting function $A_h w$ is an element of $\prod_{K \in \Omega_h} L^2(K)^l$, which is identified to be the same as $L^2(\Omega)^l$. The operator $A_h^* : W_h^* \rightarrow L^2(\Omega)^m$ is defined similarly. Thus

$$\langle D_h w, v \rangle_h = (A_h w, v)_\Omega - (w, A_h^* v)_\Omega \quad (\text{A.10})$$

for all $w \in W_h$ and $v \in W_h^*$.

Lemma A.3. *For all $w \in W$ and $v \in W^*$, we have $\langle D_h w, v \rangle_h = \langle Dw, v \rangle_W$.*

Proof. If $w \in W$ and $v \in W^*$, then $A_h w = Aw$ and $A_h^* v = A^* v$. Using this in (A.10), $\langle D_h w, v \rangle_h = (Aw, v)_\Omega - (w, A^* v)_\Omega = \langle Dw, v \rangle_{W^*}$ whenever w is in W and v is in W^* . \square

To derive the mesh-dependent weak formulation, multiply (A.8) by a test function $v \in W_h$ and apply the definition of D_K . Summing over all $K \in \Omega_h$, we obtain $(u, A_h^* v)_\Omega + \langle D_h u, v \rangle_h = (f, v)_\Omega$ for all v in W_h^* . Let

$$Q = \{r \in (W_h^*)' : \text{there is a } v \in V \text{ such that } r = D_h v\}. \quad (\text{A.11})$$

Setting $D_h u$ to be a new unknown q in Q , we have thus derived the following weak formulation with $F(v) = (f, v)_\Omega$.

Problem A.4. Given any $F \in (W_h^*)'$, find $u \in L^2(\Omega)^m$ and $q \in Q$ such that

$$(u, A_h^* v)_\Omega + \langle q, v \rangle_h = F(v), \quad \forall v \in W_h^*.$$

Theorem A.5. In the setting of (A-a), (A-b) and (A-c), suppose

$$V = {}^\perp D^*(V^*), \text{ and} \quad (\text{A.12})$$

$$A : V \rightarrow L^2(\Omega)^l \text{ is a bijection.} \quad (\text{A.13})$$

Then, Problem A.4 is well posed. Moreover, if $F(v) = (f, v)_\Omega$ for some $f \in L^2(\Omega)^l$, then the unique solution u of Problem A.4 is in V , solves (A.8), and satisfies $q = D_h u$.

Before we prove this theorem, we must note how our assumptions allow a natural topology on Q . Specifically, (A.12) implies that V is a closed subspace of W . It is also a closed subspace of W_h since W is continuously embedded in W_h . The same embedding also shows that the restriction of D_h to V , denoted by $D_{h,V} : V \rightarrow (W_h^*)'$, is continuous. Note that Q is the range of $D_{h,V}$. For any r in Q , we use $D_{h,V}^{-1}(\{r\})$ to denote the pre-image of r , i.e., set of all $v \in V$ such that $r = D_h v$. The continuity of $D_{h,V}$ implies that $D_{h,V}^{-1}(\{0\})$ is a closed subspace of V . Hence

$$\|q\|_Q = \inf_{v \in D_{h,V}^{-1}(\{q\})} \|v\|_W \quad (\text{A.14})$$

is a norm on Q . This quotient norm makes Q complete. The wellposedness result of Theorem A.5 is to be understood with Q endowed with this norm.

A.1. A proof of wellposedness. We now give a proof of Theorem A.5. Recall that the right annihilator of any subspace $S \subseteq X$ is defined by $S^\perp = \{w' \in W' : \langle w', s \rangle_W = 0 \text{ for all } s \in S\}$. The next lemma is used below to prove uniqueness.

Lemma A.6. If (A.12) holds, then $D_h V \subseteq (V^*)^\perp$.

Proof. Let $w \in V \subseteq W_h$. Then for any $\tilde{v} \in V^*$, the functional $D_h w \in (W_h^*)'$ satisfies $\langle D_h w, \tilde{v} \rangle_h = \langle Dw, \tilde{v} \rangle_{W^*}$ by Lemma A.3. But $\langle Dw, \tilde{v} \rangle_{W^*} = -\langle D^* \tilde{v}, w \rangle_W = 0$ since (A.12) shows that $w \in {}^\perp D^*(V^*)$. Hence $D_h w \in (V^*)^\perp$. \square

Proof of Theorem A.5. We verify the uniqueness and inf-sup conditions of the Babuška theory to obtain wellposedness. To verify the uniqueness condition, we must prove that if

$$(u, A_h^* v)_\Omega + \langle q, v \rangle_h = 0, \quad \forall v \in W_h^*, \quad (\text{A.15})$$

then u and q vanishes. Since $q = D_h z$ for some $z \in V$, by virtue of Lemma A.6, $\langle q, v \rangle_h = 0$ for any v in V^* . Hence (A.15) implies

$$(u, A_h^* v)_\Omega = 0, \quad \forall v \in V^*. \quad (\text{A.16})$$

In particular, since $\mathcal{D}(\Omega)^l \subseteq V^*$, this implies that $Au = 0$ and therefore $u \in W$. Hence (A.5) and (A.16) imply $\langle Du, v \rangle_{W^*} = 0$, or equivalently $\langle D^* v, u \rangle_W = 0$ for all $v \in V^*$. Thus $u \in$

${}^\perp D^*(V^*) = V$. The bijectivity of $A : V \rightarrow L^2(\Omega)^l$ then implies that $u = 0$. Returning to (A.15) and setting $u = 0$, we see that $\langle q, v \rangle_h = 0$ for all $v \in W_h^*$, so $q = 0$ as well.

It only remains to prove the inf-sup condition

$$\|w\|_{W_h^*} \leq C_1 \sup_{0 \neq x \in X} \frac{|b(x, w)|}{\|x\|_X}, \quad (\text{A.17})$$

where $X = L^2(\Omega)^m \times Q$ and $b((u, q), w) = (u, A_h^* w)_\Omega + \langle q, w \rangle_h$. Given any $w \in W_h^* \subseteq L^2(\Omega)^l$, we use the bijectivity of $A : V \rightarrow L^2(\Omega)^l$ and the Banach Open Mapping theorem to obtain a v in V satisfying $Av = w$, and $\|v\|_W \leq C\|w\|_{W_h^*}$. Then, setting $z = v + A_h^* w$ and $r = D_h v$, we have $\|r\|_Q \leq \|v\|_W \leq C\|w\|_{W_h^*}$ and $\|z\|_\Omega \leq (C + 1)\|w\|_{W_h^*}$. Hence

$$\begin{aligned} \|w\|_{W_h^*}^2 &= (A_h v, w)_\Omega + (A_h^* w, A_h^* w)_\Omega = (v + A_h^* w, A_h^* w)_\Omega + \langle D_h v, w \rangle_h \\ &= \|(z, r)\|_X \frac{b((z, r), w)}{\|(z, r)\|_X} \leq C_1 \|w\|_{W_h^*} \sup_{0 \neq x \in X} \frac{|b(x, w)|}{\|x\|_X}, \end{aligned}$$

where C_1 depends only on C . Hence (A.17) follows. \square

Remark A.7. Various elements of the arguments used in this proof are well-known in the DPG literature – see e.g., [12, § 6.2]. A generalization of these ideas to make a unified theory for DPG approximations of all Friedrichs systems was attempted in [4]. However, [4, equation (2.17)] is not correct (a counterexample is easily furnished by the Laplace example) and unfortunately that equation is used in [4, Lemma 2.4 and Corollary 2.5] to prove the existence of a solution for Problem A.4. The above proof provides a corrigendum to [4] and shows that the results claimed there for symmetric Friedrichs systems are indeed correct for operators of the form (A-a) with $k = 1$ and with V and V^* set respectively to the null spaces of the operators $B - M$ and $B + M^*$ defined there.

Remark A.8. The above analysis is applicable beyond Friedrichs systems as the example of Schrödinger equation shows. “Instead of working with one equation of higher than first order,” writes Friedrichs in his early work [19], “we prefer to work with a system of equations of first order.” We have already noted the difficulties in reformulating the Schrödinger equation as a first order system. The modern theory of Friedrichs systems (for operators of the form (A-a) with $l = m$) starts with the assumption that $\|(A + A^*)\phi\|_\Omega \leq C\|\phi\|_\Omega$ for all $\phi \in \mathcal{D}(\Omega)^l$ – see [17, equation (T2)]. This assumption does not hold for the Schrödinger operator.

A.2. An alternate proof of wellposedness. Another proof of Theorem A.5 can be given using the following two lemmas.

Lemma A.9. $V^* = \{y \in W_h^* : \langle q, y \rangle_h = 0 \text{ for all } q \in Q\}$.

Proof. If $y \in V^*$, then for any $z \in V$, using Lemmas A.3 and A.2, we have $\langle D_h z, y \rangle_h = \langle Dz, y \rangle_{W^*} = 0$, i.e., $\langle q, y \rangle_h = 0$ for all $q \in Q$.

To prove the reverse containment, let $y \in W_h^*$ satisfy $\langle D_h z, y \rangle_h = 0$ for all $z \in V$. For any $\phi \in \mathcal{D}(\Omega)^m$, the distribution $A^* y$ satisfies $\langle A^* y, \phi \rangle_{\mathcal{D}(\Omega)^m} = (y, A\phi)_\Omega = (A_h^* y, \phi)_\Omega + \overline{\langle D_h \phi, y \rangle_h}$. The last term is zero, because by (A-c), $\mathcal{D}(\Omega)^m \subseteq \text{dom}(A) = V$. Hence $A^* y = A_h^* y$ and y is in W^* . Thus by Lemma A.3, $\langle D_h z, y \rangle_h = \langle Dz, y \rangle_W = 0$, so $y \in {}^\perp D(V)$. Hence y is in V^* by Lemma A.2. \square

Lemma A.10. *Suppose (A.12) holds. Then, for all $q \in Q$,*

$$\inf_{v \in D_{h,V}^{-1}(\{q\})} \|v\|_W = \sup_{0 \neq y \in W_h^*} \frac{|\langle q, y \rangle_h|}{\|y\|_{W_h^*}}.$$

Proof. The supremum, denoted by s , is attained by the function \tilde{u}_q in W_h^* satisfying

$$(A_h^* \tilde{u}_q, A_h^* y)_\Omega + (\tilde{u}_q, y)_\Omega = -\langle q, y \rangle_h, \quad \forall y \in W_h^*, \text{ and} \quad (\text{A.18})$$

$$s = \|\tilde{u}_q\|_{W_h^*}. \quad (\text{A.19})$$

Choosing $y \in \mathcal{D}(\Omega)^l$ in (A.18), we conclude that the distribution $A(A_h^* \tilde{u}_q)$ is in $L^2(\Omega)^l$. Hence (A.10) is applicable with $w = A_h^* \tilde{u}_q$ and we obtain

$$A_h A_h^* \tilde{u}_q + \tilde{u}_q = 0 \quad (\text{A.20a})$$

$$D_h A_h^* \tilde{u}_q = q. \quad (\text{A.20b})$$

Now let $u_q = A_h^* \tilde{u}_q$. Then (A.20a) implies $A_h u_q = -\tilde{u}_q$, which implies $A_h^* A_h u_q = -A_h^* \tilde{u}_q = -u_q$. Combining with (A.20b), we have

$$A_h^* A_h u_q + u_q = 0 \quad (\text{A.21a})$$

$$D_h u_q = q. \quad (\text{A.21b})$$

Next, we show that u_q is in V . By (A.12), it suffices to prove that $u_q \in {}^\perp D^*(V^*)$. For any \tilde{v} in V^* , we have, using Lemma A.3, $\langle D^* \tilde{v}, u_q \rangle_W = -\overline{\langle D u_q, \tilde{v} \rangle_{W^*}} = -\overline{\langle D_h u_q, \tilde{v} \rangle_h} = -\langle q, \tilde{v} \rangle_h$. The last term is zero because $q = D_h z$ for some $z \in V$ and $\langle q, \tilde{v} \rangle = \langle D z, \tilde{v} \rangle_{W^*} = 0$ by Lemma A.2. Hence $u_q \in {}^\perp D^*(V^*) = V$.

The infimum of the lemma is $\|q\|_Q$. By virtue of (A.19), to complete the proof, it suffices to show that $\|q\|_Q = \|u_q\|_W = \|\tilde{u}_q\|_{W_h^*}$. The last equality is obvious from $u_q = A_h^* \tilde{u}_q$ and $A_h u_q = -\tilde{u}_q$, hence we need only show that $\|q\|_Q = \|u_q\|_W$. Standard variational arguments show that the infimum defining $\|q\|_Q$ is attained by a unique minimizer $v_q \in V$ satisfying $\|q\|_Q = \|v_q\|_W$, $D_h v_q = q$ and $(A_h v_q, A_h v)_\Omega + (v_q, v)_\Omega = 0$ for all $v \in D_{h,V}^{-1}(\{0\})$. Choosing a v in $\mathcal{D}(K)$ (whose extension by zero is in $D_{h,V}^{-1}(\{0\})$), we conclude that distribution $A^*(A_h v_q)|_K$ is in $L^2(K)^m$ for any $K \in \Omega_h$. Therefore $A_h^* A_h v_q$ is in $L^2(\Omega)^m$. In view of (A.21), this means that $v_q = u_q$. \square

Second proof of Theorem A.5. According to [5, Theorem 3.3], it suffices to prove that there are positive constants c_0, \hat{c} such that

$$c_0 \|u\|_\Omega \leq \sup_{0 \neq y \in Y_0} \frac{|(u, A_h^* y)_\Omega|}{\|y\|_{W_h^*}} \quad \forall u \in L^2(\Omega)^m, \quad (\text{A.22})$$

$$\hat{c} \|q\|_Q \leq \sup_{0 \neq y \in W_h^*} \frac{|\langle q, y \rangle_h|}{\|y\|_{W_h^*}} \quad \forall q \in Q. \quad (\text{A.23})$$

where $Y_0 = \{y \in W_h^* : \langle q, y \rangle_h = 0 \text{ for all } q \in Q\}$.

Since (A.23) follows with $\hat{c} = 1$ from Lemma A.10, we only need to prove (A.22). First note that since V is closed (by (A.12)), A is a closed operator. By (A.13), the range of A is closed. By the Closed Range Theorem for closed operators, range of A^* is closed. Also, the well-known identity $\ker(A^*) = \text{ran}(A)^\perp$, in combination with (A.13), implies that A^* is injective. Hence there exists a $C > 0$ such that

$$C \|y\|_\Omega \leq \|A^* y\|_\Omega \quad \forall y \in \text{dom}(A^*) = V^*. \quad (\text{A.24})$$

This implies the following inf-sup condition:

$$C\|y\|_{W^*} \leq \sup_{u \in L^2(\Omega)^m} \frac{|(u, A^*y)_\Omega|}{\|u\|_\Omega} \quad \forall y \in V^*.$$

To complete the proof, we note that by standard arguments the order of arguments in the inf and sup may be reversed to get

$$\inf_{u \in L^2(\Omega)^m} \sup_{y \in V^*} \frac{|(u, A^*y)_\Omega|}{\|u\|_\Omega \|y\|_{W^*}} = \inf_{y \in V^*} \sup_{u \in L^2(\Omega)^m} \frac{|(u, A^*y)_\Omega|}{\|u\|_\Omega \|y\|_{W^*}} \geq C.$$

By Lemma A.9, $Y_0 = V^*$, thus completing the proof of (A.22). \square

Remark A.11. The idea behind Lemma A.10 (to consider the two related problems (A.20) and (A.21), one with essential boundary conditions and the other with natural boundary conditions) was first presented in [5, 6], tailored to the specific needs of a Maxwell problem. A generalization for first order operators was presented later in [28]. The argument to prove (A.22) using the Closed Range Theorem, was first presented for the case of first order Sobolev spaces in [5, Theorem 6.6].

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