A space–time Trefftz discontinuous Galerkin method for the linear Schrödinger equation

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Linear Schrödinger equation

We consider the following **homogeneous**, time-dependent Schrödinger equation on a space–time cylinder $Q = \Omega \times I$, where $\Omega \subset \mathbb{R}^d$, $d \in \mathbb{N}$, with Lipschitz boundary $\partial\Omega$ and $I = (0, T)$, for some $T > 0$:

$$i\frac{\partial \psi}{\partial t} + \Delta\psi - V\psi = 0, \qquad \text{in } Q, \tag{1.1a}$$

$$\psi = g_{\mathrm{D}}, \qquad \text{on } \partial\Omega \times I, \tag{1.1b}$$

$$\psi(\mathbf{x}, 0) = \psi_0(\mathbf{x}), \quad \text{on } \Omega. \tag{1.1c}$$

- $V : \Omega \to \mathbb{R}$ is a piecewise-constant potential.

Model problem

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Some applications of the model (1.1):

- ✓ It is the fundamental equation of quantum mechanics [Lifshitz and Landau, 1965].
- ✓ Optics (called “paraxial wave equation”) [Grella, 1982].
- ✓ Underwater acoustics (called “parabolic equation”) [Keller and Papadakis, 1977].

Why space-time Trefftz-DG?

Space–time methods:

- ✓ High-order accuracy in both space and time variables at once.
- ✓ Approximate solution is available in the whole space–time cylinder Q.
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Trefftz discontinuous Galerkin:

- ✓ Test and trial spaces are spanned by local solutions to the PDE.
- ✓ Less DoFs compared to polynomial approximations.
- ✓ Efective for highly oscillatory solutions.
- ✓ DG methods are specially suitable to be combined with Trefftz bases.
- ✓ No volume integrals involved.
- × For non-homogeneous PDEs (terms with derivatives of different order) the method requires non-polynomial basis functions.

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⋆There is a very small number of works on space–time methods for the Schrödinger equation compared to the heat equation:

- [Karakashian and Makridakis, 1998] (CG in space + DG in time).
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- [Demkowicz et al., 2017] (Space–time Discontinuous Petrov Galerkin).
- [Gómez and Moiola, 2022] (accepted for publication on SIAM Numerical Analysis).

Description of the Trefftz DG method

Let the time interval $(0,T)$ be partitioned as $0 = t_0 < t_1 < \ldots < t_N = T, \quad I_n := (t_{n-1}, t_n)$.
For each $n = 1, \ldots, N$, we assume to have a polytopic partition $\mathscr{T}^{\mathbf{x}}_{h_{\mathbf{x}},n} = \{K_{\mathbf{x}}\}$ of Ω.

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The space–time finite element mesh is given by

$$\mathscr{T}_h(Q) := \left\{ K = K_{\mathbf{x}} \times I_n \; : \; K_{\mathbf{x}} \in \mathscr{T}^{\mathbf{x}}_{h_{\mathbf{x}},n}, \; n = 1, \ldots, N \right\}.$$

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We define the local and global Trefftz spaces:

$$\mathbf{T}(K) := \left\{w \in H^1\left(I_n; L^2(K_{\mathbf{x}})\right) \cap L^2\left(I_n; H^2(K_{\mathbf{x}})\right) \text{ s.t. } i\frac{\partial w}{\partial t} + \Delta w - V|_K w = 0 \text{ on } K = K_{\mathbf{x}} \times I_n\right\},$$

$$\mathbf{T}(\mathcal{T}_h) := \left\{w \in L^2(Q)^{d+1} \ \middle|\ w|_K \in \mathbf{T}(K),\ \forall K \in \mathcal{T}_h(Q)\right\}.$$

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For any finite-dimensional subspace $\mathbb{T}_p(\mathscr{T}_h)\subset\mathbf{T}(\mathscr{T}_h)$ the proposed Trefftz-DG method applied to (1.1) seeks an approximation $\psi_{hp}(\mathbf{x},t)\in\mathbb{T}_p(\mathscr{T}_h)$ of the exact solution $\psi(\mathbf{x},t)\in\mathbf{T}(\mathscr{T}_h)$ such that for any test function $s_{hp}\in\mathbb{T}_p(\mathscr{T}_h)$ the following equation is satisfied for all $K\in\mathscr{T}_h(Q)$

$$\int_K \psi_{hp}\overline{\left(i\frac{\partial s_{hp}}{\partial t}+\Delta s_{hp}-Vs_{hp}\right)}\,\mathrm{d}V$$
$$+\oint_{\partial K}\left[i\widehat{\psi}_{hp}\overline{s_{hp}}n^t_K+\left(\widehat{\nabla\psi}_{hp}\overline{s_{hp}}-\widehat{\psi}_{hp}\nabla\overline{s_{hp}}\right)\cdot\vec{\mathbf{n}}^x_K\right]\mathrm{d}S=0,$$

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$$+ \oint_{\partial K} \left[i\widehat{\psi}_{hp}\overline{s_{hp}} n^t_K + \left(\widehat{\nabla\psi_{hp}}\overline{s_{hp}} - \widehat{\psi}_{hp}\nabla\overline{s_{hp}}\right)\cdot \vec{\mathbf{n}}^x_K \right] \mathrm{d}S = 0,$$

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$$+ \oint_{\partial K} \left[i\widehat{\psi}_{hp} \overline{s_{hp}} n^t_K + \left(\widehat{\nabla \psi_{hp}} \overline{s_{hp}} - \widehat{\psi}_{hp} \nabla \overline{s_{hp}} \right) \cdot \vec{\mathbf{n}}^x_K \right] \mathrm{d}S = 0,$$

The so-called *numerical fluxes* $\widehat{\psi}_{hp}$ and $\widehat{\nabla\psi}_{hp}$ are approximations of the traces of ψ_{hp} and $\nabla\psi_{hp}$ on $\mathscr{F}_h$. We choose them as:

$$\widehat{\psi}_{hp} := \begin{cases} \psi_{hp}^-, & \text{on } \mathscr{F}_h^{\mathrm{space}}, \\ \psi_{hp}, & \text{on } \mathscr{F}_h^{T}, \\ \psi_0, & \text{on } \mathscr{F}_h^{0}, \\ \{\{\psi_{hp}\}\} - i\beta\, [[\nabla\psi_{hp}]]_{\mathbf{N}}, & \text{on } \mathscr{F}_h^{\mathrm{time}}, \\ g_{\mathrm{D}}, & \text{on } \mathscr{F}_h^{\mathrm{D}}, \end{cases}$$

$$\widehat{\nabla\psi}_{hp} := \begin{cases} \{\{\nabla\psi_{hp}\}\} + i\alpha\, [[\psi_{hp}]]_{\mathbf{N}}, & \text{on } \mathscr{F}_h^{\mathrm{time}}, \\ \nabla\psi_{hp} + i\alpha\,(\psi_{hp} - g_{\mathrm{D}})\, \vec{\mathbf{n}}_\Omega^x, & \text{on } \mathscr{F}_h^{\mathrm{D}}, \end{cases}$$

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The stabilization parameters α and β are set as $\alpha^{-1} = \beta \sim h$.

After summing over all the elements $K \in \mathscr{T}_h(Q)$ and substituting the definition of the numerical fluxes, the following Trefftz-DG variational formulation is obtained:

$$\text{Seek } \psi_{hp} \in \mathbb{T}_p(\mathscr{T}_h) \text{ such that: } \mathscr{A}\left(\psi_{hp};\, s_{hp}\right) = \ell(s_{hp}), \quad \forall s_{hp} \in \mathbb{T}_p(\mathscr{T}_h), \tag{1.2}$$

where

$$\begin{aligned}
\mathscr{A}\left(\psi_{hp};\, s_{hp}\right) := & \int_{\mathscr{F}_h^{\text{space}}} i\psi_{hp}^{-}\left[\!\left[\overline{s_{hp}}\right]\!\right]_t \mathrm{d}\mathbf{x} + \int_{\mathscr{F}_h^T} i\psi_{hp}\overline{s_{hp}}\,\mathrm{d}\mathbf{x} \\
& + \int_{\mathscr{F}_h^{\text{time}}} \Big(\{\!\{\nabla\psi_{hp}\}\!\} \cdot \left[\!\left[\overline{s_{hp}}\right]\!\right]_{\mathbf{N}} + i\alpha \left[\!\left[\psi_{hp}\right]\!\right]_{\mathbf{N}} \cdot \left[\!\left[\overline{s_{hp}}\right]\!\right]_{\mathbf{N}} - \{\!\{\psi_{hp}\}\!\} \left[\!\left[\nabla\overline{s_{hp}}\right]\!\right]_{\mathbf{N}} \\
& \qquad + i\beta \left[\!\left[\nabla\psi_{hp}\right]\!\right]_{\mathbf{N}} \left[\!\left[\nabla\overline{s_{hp}}\right]\!\right]_{\mathbf{N}} \Big) \mathrm{d}S + \int_{\mathscr{F}_h^{\mathrm{D}}} \left(\nabla\psi_{hp} \cdot \vec{\mathbf{n}}_\Omega^x + i\alpha\psi_{hp}\right) \overline{s_{hp}}\,\mathrm{d}S, \\
\ell(s_{hp}) := & \int_{\mathscr{F}_h^0} i\psi_0 \overline{s_{hp}}\,\mathrm{d}\mathbf{x} + \int_{\mathscr{F}_h^{\mathrm{D}}} g_{\mathrm{D}} \left(\nabla\overline{s_{hp}} \cdot \vec{\mathbf{n}}_\Omega^x + i\alpha\overline{s_{hp}}\right) \mathrm{d}S.
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After summing over all the elements $K \in \mathcal{T}_h(Q)$ and substituting the definition of the numerical fluxes, the following Trefftz-DG variational formulation is obtained:

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$$+ \int_{\mathcal{F}_h^{\text{time}}} \Big(\{\{\nabla\psi_{hp}\}\} \cdot \left[\left[\overline{s_{hp}}\right]\right]_{\mathbf{N}} + i\alpha \left[\left[\psi_{hp}\right]\right]_{\mathbf{N}} \cdot \left[\left[\overline{s_{hp}}\right]\right]_{\mathbf{N}} - \{\{\psi_{hp}\}\} \left[\left[\nabla\overline{s_{hp}}\right]\right]_{\mathbf{N}}$$
$$+ i\beta \left[\left[\nabla\psi_{hp}\right]\right]_{\mathbf{N}} \left[\left[\nabla\overline{s_{hp}}\right]\right]_{\mathbf{N}} \Big)\,\mathrm{d}S + \int_{\mathcal{F}_h^{\mathrm{D}}} \left(\nabla\psi_{hp}\cdot\vec{\mathbf{n}}_\Omega^x + i\alpha\psi_{hp}\right)\overline{s_{hp}}\,\mathrm{d}S,$$

$$\ell(s_{hp}) := \int_{\mathcal{F}_h^0} i\psi_0\overline{s_{hp}}\,\mathrm{d}\mathbf{x} + \int_{\mathcal{F}_h^{\mathrm{D}}} g_{\mathrm{D}} \left(\nabla\overline{s_{hp}}\cdot\vec{\mathbf{n}}_\Omega^x + i\alpha\overline{s_{hp}}\right)\mathrm{d}S.$$

⋆ The definitions of $\mathscr{A}(\cdot;\,\cdot)$ and $\ell(\cdot)$ in the variational formulation (1.2) are independent of the potential V, which has an effect only on the discrete space.

Theoretical results

We define the following mesh-dependent semi-norms:

$$
\begin{aligned}
|||w|||_{\mathrm{DG}}^2 := & \|[\![w]\!]_t\|_{L^2(\mathscr{F}_h^{\mathrm{space}})}^2 + \frac{1}{2}\|w\|_{L^2(\mathscr{F}_h^T \cup \mathscr{F}_h^0)}^2 + \left\|\alpha^{1/2} w\right\|_{L^2(\mathscr{F}_h^{\mathrm{D}})}^2 \\
& + \left\|\alpha^{1/2} [\![w]\!]_{\mathbf{N}}\right\|_{L^2(\mathscr{F}_h^{\mathrm{time}})^d}^2 + \left\|\beta^{1/2} [\![\nabla w]\!]_{\mathbf{N}}\right\|_{L^2(\mathscr{F}_h^{\mathrm{time}})}^2, \\
|||w|||_{\mathrm{DG+}}^2 := & |||w|||_{\mathrm{DG}}^2 + \|w^-\|_{L^2(\mathscr{F}_h^{\mathrm{space}})}^2 + \left\|\alpha^{-1/2} \{\{\nabla w\}\}\right\|_{L^2(\mathscr{F}_h^{\mathrm{time}})^d}^2 \\
& + \left\|\alpha^{-1/2} \nabla w \cdot \vec{\mathbf{n}}_\Omega^x\right\|_{L^2(\mathscr{F}_h^{\mathrm{D}})} + \left\|\beta^{-1/2} \{\{w\}\}\right\|_{L^2(\mathscr{F}_h^{\mathrm{time}})}^2.
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$$|||w|||_{\mathrm{DG+}}^2 := |||w|||_{\mathrm{DG}}^2 + \|w^-\|_{L^2(\mathscr{F}_h^{\mathrm{space}})}^2 + \left\|\alpha^{-1/2}\{\{\nabla w\}\}\right\|_{L^2(\mathscr{F}_h^{\mathrm{time}})^d}^2 + \left\|\alpha^{-1/2}\nabla w \cdot \vec{\mathbf{n}}_\Omega^x\right\|_{L^2(\mathscr{F}_h^{\mathrm{D}})} + \left\|\beta^{-1/2}\{\{w\}\}\right\|_{L^2(\mathscr{F}_h^{\mathrm{time}})}^2.$$

⋆ Even though $|||\cdot|||_{\mathrm{DG}}$ and $|||\cdot|||_{\mathrm{DG+}}$ are just seminorms on $H^1(\mathscr{T}_h)$, they are indeed norms on $\mathbf{T}(\mathscr{T}_h)$.

Well-posedness

Proposition 1 (Coercivity)

For all $w \in \mathbf{T}(\mathscr{T}_h)$ the following identity holds: $\mathfrak{Im}\left(\mathscr{A}\left(w;\ w\right)\right) = |||w|||_{\mathrm{DG}}^2.$

Proposition 1 (Coercivity)

For all $w \in \mathbf{T}(\mathscr{T}_h)$ the following identity holds: $\mathfrak{Im}\left(\mathscr{A}(w;\ w)\right) = |||w|||^2_{\mathrm{DG}}$.

Proposition 2 (Continuity)

The sesquilinear form $\mathscr{A}(\cdot;\ \cdot)$ and the linear functional $\ell(\cdot)$ are continuous in the following sense:

$$|\mathscr{A}(v;\ w)| \leq 2|||v|||_{\mathrm{DG}+}\ |||w|||_{\mathrm{DG}}, \qquad \forall v, w \in \mathbf{T}(\mathscr{T}_h),$$

$$|\ell(v)| \leq \left(2\left\|\psi_0\right\|^2_{L^2(\mathscr{F}_h^0)} + 2\left\|\alpha^{1/2} g_{\mathrm{D}}\right\|^2_{L^2(\mathscr{F}_h^{\mathrm{D}})}\right)^{1/2} |||w|||_{\mathrm{DG}+}, \qquad \forall v \in \mathbf{T}(\mathscr{T}_h).$$

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Theorem 1 (Quasi-optimality)

For any finite-dimensional subspace $\mathbb{T}_p(\mathscr{T}_h)$ of $\mathbf{T}(\mathscr{T}_h)$ there exists a unique solution $\psi_{hp} \in \mathbb{T}_p(\mathscr{T}_h)$ satisfying (1.2). Furthermore, the following quasi-optimality condition holds:

$$|||\psi - \psi_{hp}|||_{\mathrm{DG}} \leq 3 \inf_{s_{hp} \in \mathbb{T}_p(\mathscr{T}_h)} |||\psi - s_{hp}|||_{\mathrm{DG}+}. \tag{1.5}$$

Condition 1

For any Schrödinger solution $\psi \in \mathscr{C}^{p+1}(K)$, for each element $K \in \mathscr{T}_h$, we require that the discrete space $\mathbb{T}_p(K)$ contains an element whose Taylor polynomial centered at some $(\mathbf{z}, s)$ matches that of ψ; i.e., there exists $\mathbf{a}(\mathbf{z}, s) \in \mathbb{C}^{n_{d,p}}$ that satisfies

$$T^{p+1}_{(\mathbf{z},s)}\left[\sum_{\ell=1}^{n_{d,p}} a_\ell(\mathbf{z}, s)\phi_\ell\right](\mathbf{x}, t) = T^{p+1}_{(\mathbf{z},s)}[\psi](\mathbf{x}, t), \tag{1.6}$$

where $\{\phi_\ell\}_{\ell=1}^{n_{d,p}}$ is a basis of $\mathbb{T}_p(K)$.

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Theorem 2

Let $p \in \mathbb{N}$. Let $\psi \in \mathbf{T}(\mathscr{T}_h) \cap \mathscr{C}^{p+1}(Q)$ be the exact solution of (1.1) and $\psi_{hp} \in \mathbb{T}_p(\mathscr{T}_h)$ be the Trefftz-DG approximation solving (1.2) with $\mathbb{T}_p(\mathscr{T}_h)$ satisfying Condition 1 for all $K \in \mathscr{T}_h(Q)$.
Then there exists a constant C independent on the mesh size such that

$$|||\psi - \psi_{hp}|||_{\mathrm{DG}} \leq C \sum_{K = K_{\mathbf{x}} \times (t_{n-1}, t_n) \in \mathscr{T}_h(Q)} \max\{h_{K_{\mathbf{x}}}, h_n\}^p \|\psi\|_{H^{p+1}(K)}.$$

Condition 1

For any Schrödinger solution $\psi \in \mathscr{C}^{p+1}(K)$, for each element $K \in \mathscr{T}_h$, we require that the discrete space $\mathbb{T}_p(K)$ contains an element whose Taylor polynomial centered at some $(\mathbf{z}, s)$ matches that of ψ; i.e., there exists $\mathbf{a}(\mathbf{z}, s) \in \mathbb{C}^{n_{d,p}}$ that satisfies

$$T^{p+1}_{(\mathbf{z},s)}\left[\sum_{\ell=1}^{n_{d,p}} a_\ell(\mathbf{z}, s)\phi_\ell\right](\mathbf{x}, t) = T^{p+1}_{(\mathbf{z},s)}[\psi](\mathbf{x}, t), \tag{1.6}$$

where $\{\phi_\ell\}_{\ell=1}^{n_{d,p}}$ is a basis of $\mathbb{T}_p(K)$.

Theorem 2

Let $p \in \mathbb{N}$. Let $\psi \in \mathbf{T}(\mathscr{T}_h) \cap \mathscr{C}^{p+1}(Q)$ be the exact solution of (1.1) and $\psi_{hp} \in \mathbb{T}_p(\mathscr{T}_h)$ be the Trefftz-DG approximation solving (1.2) with $\mathbb{T}_p(\mathscr{T}_h)$ satisfying Condition 1 for all $K \in \mathscr{T}_h(Q)$.
Then there exists a constant C independent on the mesh size such that

$$|||\psi - \psi_{hp}|||_{\mathrm{DG}} \leq C \sum_{K = K_{\mathbf{x}} \times (t_{n-1}, t_n) \in \mathscr{T}_h(Q)} \max\{h_{K_{\mathbf{x}}}, h_n\}^p \, \|\psi\|_{H^{p+1}(K)}.$$

⋆ In the paper the theory is developed to allow for general $\psi \in H^{p+1}(\mathscr{T}_h)$.

Sketch of the proof of Condition 1

We aim to prove that for each $K \in \mathscr{T}_h$, there exists $\mathbf{a}(\mathbf{z}, s) \in \mathbb{C}^{n_{d,p}}$ that satisfies

$$\sum_{\ell=1}^{n_{d,p}} a_\ell(\mathbf{z}, s)\, T^{p+1}_{(\mathbf{z},s)}[\phi_\ell](\mathbf{x}, t) = T^{p+1}_{(\mathbf{z},s)}[\psi](\mathbf{x}, t). \tag{1.7}$$

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- The above problem translates into a rectangular linear system $\mathbf{Ma}(\mathbf{z}, s) = \mathbf{b}$, where $\mathbf{M} \in \mathbb{C}^{r_p \times n_{d,p}}$ and $\mathbf{b} \in \mathbb{C}^{r_p}$, with $r_p := \dim\left(\mathbb{P}_p(K)\right) \geq n_{d,p}$.

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- The choice of the basis functions ϕ_ℓ must guarantee that $\mathbf{M}$ is full-rank.

The local space $\mathbb{T}_p(K)$ is defined for each $K = K_{\mathbf{x}} \times I_n \in \mathscr{T}_h(Q)$ and for $p \in \mathbb{N}$ as the following set of complex exponentials:

$$\mathbb{T}_p(K) := \mathrm{span}\left\{\phi_\ell(\mathbf{x},t),\ \ell = 1,\dots,n_{d,p}\right\},\ \text{ where} \tag{1.8}$$
$$\phi_\ell(\mathbf{x},t) := \mathrm{e}^{i\left(k_\ell \mathbf{d}_\ell{}^\top \mathbf{x} - (k_\ell{}^2 + V|_K)t\right)}\ \text{ for } \ell = 1,\dots,n_{d,p},$$

for some parameters $\{k_\ell\} \subset \mathbb{R}$ and directions $\{\mathbf{d}_\ell\} \subset \mathscr{S}_1^d := \{\mathbf{v} \in \mathbb{R}^d, |\mathbf{d}| = 1\}$, which can be chosen differently in each cell K.

Best approximation

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Proposition 3

Let $d = 1$, $p \in \mathbb{N}$, $n_{1,p} = 2p + 1$ and the parameters $\{k_\ell\}_{\ell=1}^{2p+1} \subset \mathbb{R}$ be all different from one another. Let

$$\phi_\ell(x, t) = e^{\left(k_\ell x - (k_\ell^2 + V|_K)t\right)}, \qquad \ell = 1, \dots, 2p + 1, \tag{1.9}$$

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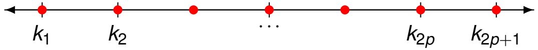

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Let $d = 2$ and $n_{2,p} = (p+1)^2$. Let the parameters k_m and $\theta_{m,\lambda}$ satisfy the following conditions:

$$k_m \in \mathbb{R} \text{ for } m = 0,\dots,p, \text{ with } k_{m_1}^2 \neq k_{m_2}^2 \text{ for } m_1 \neq m_2 \text{ and } k_m \neq 0,$$

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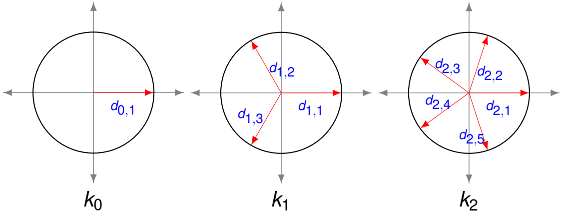

Numerical experiments

Square-well potential in $(1+1)$ dimensions

Let us consider the (1+1)-dimensional Schrödinger equation (1.1) on $Q = (-2,2) \times (0,1)$ with homogeneous Dirichlet boundary conditions and the following square-well potential:

$$V(x) = \begin{cases} 0, & x \in (-1,1), \\ V_*, & x \in (-2,2) \setminus (-1,1), \end{cases} \tag{1.10}$$

for some $V_* > 0$. The initial condition is taken as an eigenfunction (bound state) of $-\partial_x^2 + V$ on $(-2,2)$

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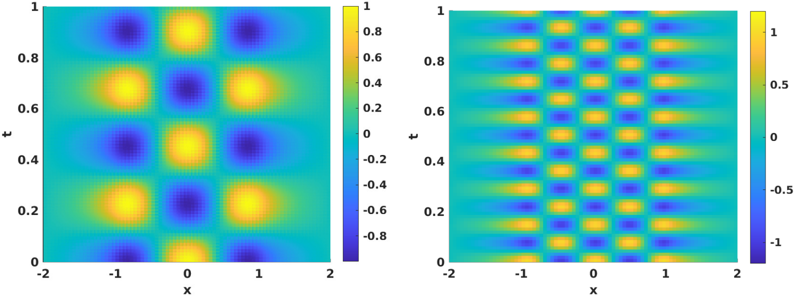
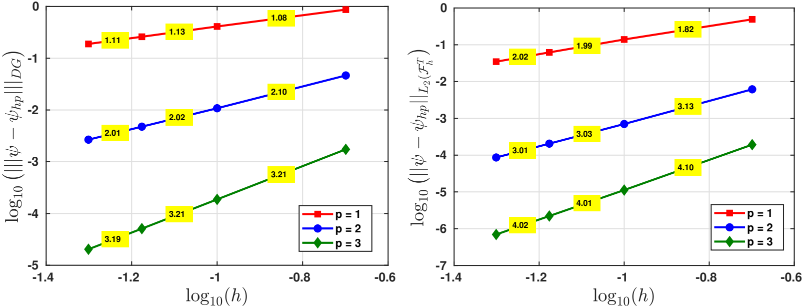


(a) $\mathfrak{Re}\left(\psi_{hp}\right)$ for $V_*=20$

(b) $\mathfrak{Re}\left(\psi_{hp}\right)$ for $V_*=50$

Figure 1: Trefftz-DG approximation ψ_{hp} in the space–time cylinder Q for the $(1+1)$-dimensional square-well potential problem (1.10) computed with $p=3$.



(a) Error in DG norm

(b) Error in L_2 norm at $T = 1$

Figure 2: Trefftz-DG error for the $(1+1)$-dimensional problem with square well potential (1.10) with $V_* = 20$. The numbers in the yellow rectangles are the empirical algebraic convergence rates in h.

Choice of the k_m parameters

We first note that in this experiment we know the time frequency of the exact solution, which is $\omega = k_*^2$. Therefore it is natural to expect the approximation to be better if our basis functions oscillate at the same time frequency.

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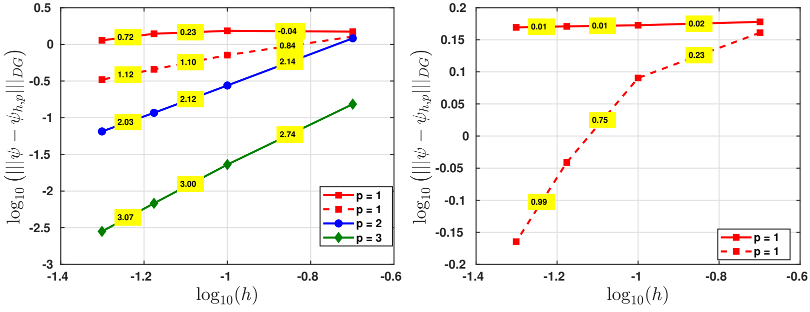

(a) $V_* = 50$ (b) $V_* = 100$

Figure 3: Trefftz-DG error measured in DG norm for the (1 + 1) dimensional problem with square-well potential 1.10 with $V_* = 50$ ($k_* \approx 6.6394$) and $V_* = 100$ ($k_* \approx 9.6812$), and for $k_\ell \in \{-p, \ldots, p\}$ (continuous line), which is the same choice of the previous plots, and $k_\ell \in \{0, \pm k_*\}$ (dashed line).

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