Waves, Wires, and Weights: Numerical Adventures with the Schrödinger Equation

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1 Introduction

The time-dependent Schrödinger equation lies at the heart of quantum mechanics, dictating how the state of a quantum system evolves under the influence of potential energy landscapes. In contrast to classical mechanics, which predicts trajectories, the Schrödinger equation predicts wave functions, whose squared modulus yields probability densities. This shift from deterministic paths to probabilistic amplitudes marks a fundamental departure from classical intuition.

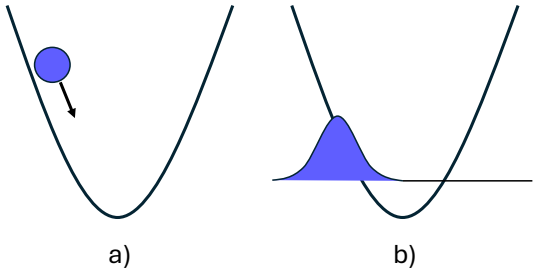

Figure 1:

From fundamental atomic models to emergent quantum technologies, the ability to solve the Schrödinger equation accurately and efficiently is essential for predicting quantum behavior. Yet, in most realistic settings, analytic solutions are unavailable. This necessitates the development of robust numerical approaches. In molecular systems, the Schrödinger equation governs the motion of nuclei on potential energy surfaces obtained from electronic structure calculations. Within the Born-Oppenheimer approximation, these nuclei behave as quantum particles subject to high-dimensional, often anharmonic potentials. For example, when modeling the movement of atoms within a molecule, it is common to reduce the full-dimensional problem to a few key internal coordinates, such as bond stretching or rotations. Even in such simplified spaces, the time evolution of a quantum state can reveal complex phenomena such as tunneling (where a particle passes through a potential barrier it classically could not cross), interference (where overlapping wave functions amplify or cancel each other), or wave packet spreading (the dispersion of a localized quantum state over time)—none of which are accessible through classical approximations.
This report investigates the numerical solution of the time-dependent Schrödinger equation in two spatial dimensions, a setting that permits the exploration of realistic molecular scenarios while maintaining computational tractability. Specifically, we consider model systems where the potential energy surface encodes features representative of atomic motions, reactive pathways, or coupled physi-

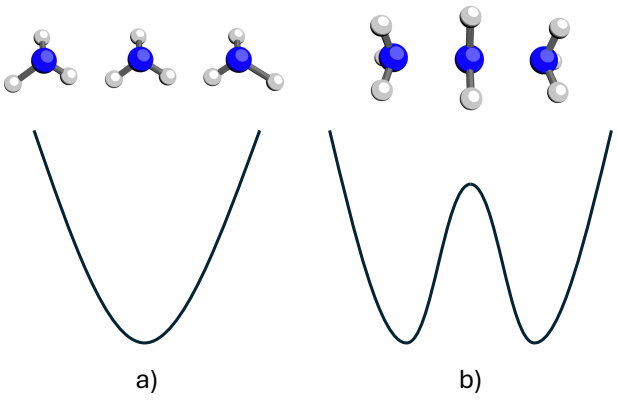

Figure 2:

cal effects.
To address this problem, we compare two distinct numerical strategies. The first is the finite element method (FEM), a classical and rigorously grounded approach based on variational formulations. The second leverages recent advances in machine learning: physics-informed neural networks (PINNs), which approximate the solution by minimizing the residual of the governing equations within a data-driven framework. While FEM offers precision and theoretical guarantees, PINNs provide flexibility and mesh-free generalization—particularly attractive for high-dimensional or inverse problems.
Through this dual lens, the report aims to highlight both the challenges and opportunities inherent in solving quantum dynamical equations numerically, and to evaluate the strengths of different computational paradigms in a physically meaningful context.

2 Finite Element Method

Model Problem: Schrödinger Equation

The Schrödinger equation is a second-order partial differential equation that describes the time evolution of a quantum system, represented by its wave function.
Let $\Omega \subset \mathbb{R}^n$ be a bounded Lipschitz domain and let $V : \Omega \times [0, T] \to \mathbb{R}$ be a given potential. We say that a function

$$u : \Omega \times [0, T] \to \mathbb{C}$$

is a **solution to the time-dependent Schrödinger equation, with homogeneous Dirichlet boundary conditions** if it satisfies the following system

of equations:

$$\begin{aligned} i\partial_t u(x,t) &= -\Delta u(x,t) + V(x,t)u(x,t), \quad x \in \Omega,\ t > 0, \\ \partial_t u(x,0) &= u_0(x), \quad x \in \Omega, \\ u(x,t) &= 0, \quad x \in \partial\Omega,\ t > 0, \end{aligned}$$

where Δ is the Laplacian operator, $V(x,t)$ is a potential, $\partial\Omega$ is the boundary of the domain Ω, and $u_0(x)$ is the initial condition at time $t = 0$.
Should we include this description?
The function $u(x,t)$ represents the wave function of the quantum system at position x and time t. The term $i\partial_t u(x,t)$ represents the time evolution of the wave function, while the term $-\Delta u(x,t)$ accounts for the kinetic energy of the system. The potential term $V(x,t)u(x,t)$ describes the interaction of the wave function with an external potential.

Weak Formulation of Schrödinger's Equation

To derive the weak formulation of the time dependent Schrödinger equation, we multiply the equation by $\bar{v}$ the complex conjugate of the test function $v(x,t) \in H_0^1(\Omega;\mathbb{C})$ and integrate over the domain Ω.

Sobolev Space with Complex Values Let $\Omega \subset \mathbb{R}^d$ be a bounded Lipschitz domain. We define the complex Sobolev space

$$H_0^1(\Omega;\mathbb{C}) := \left\{ u \in L^2(\Omega;\mathbb{C}) \;\middle|\; \nabla u \in L^2(\Omega;\mathbb{C}^d),\ u|_{\partial\Omega} = 0 \right\}.$$

This space is equipped with the inner product

$$\langle u, v \rangle_{H_0^1} := \int_\Omega \nabla u \cdot \nabla \bar{v}\, dx + \int_\Omega u\, \bar{v}\, dx,$$

and the associated norm

$$\|u\|_{H_0^1} := \sqrt{\langle u, u \rangle_{H_0^1}}.$$

By utilizing Greens' identity, we can transform the second order differential equation into a first order weak formulation:

$$\begin{aligned} \int_\Omega \Delta u \bar{v}\, dx &= \int_\Omega \nabla u \cdot \nabla \bar{v}\, dx - \int_{\partial\Omega} \nabla u \cdot n \bar{v}\, ds, \\ &= \int_\Omega \nabla u \cdot \nabla \bar{v}\, dx, \quad \text{(since } u \text{ vanishes on } \partial\Omega). \end{aligned}$$

This leads to the weak formulation of the Schrödinger equation:

$$i \int_\Omega (\partial_t u)\, \bar{v}\, dx = -\int_\Omega \nabla u \cdot \nabla \bar{v}\, dx + \int_\Omega V(x,t) u \bar{v}\, dx.$$

We take the complex conjugate of the test function v to ensure that the formulation aligns with the sesquilinear inner product in Hilbert spaces like $L^2(\Omega;\mathbb{C})$ and $H_0^1(\Omega;\mathbb{C})$.

Time Integration with the Euler Method

The Euler method is a simple and widely used numerical method for solving differential equations. It approximates the time derivative with a first order finite difference scheme. In the following we will use the backward Euler method, which gives an approximation of the time derivative as follows:

$$\partial_t u(x,t) \approx \frac{u^{t+\mathrm{dt}} - u^t}{\mathrm{dt}}, \tag{1}$$

The backward euler method allows us to solve the Schrödinger equation iteratively in each time step by finite elements method in space. The time resolution is controlled by the time step size dt, where t is the current time and $t + \mathrm{dt}$ is the next time step.
The backward Euler method has a remaining error of order $\mathcal{O}(\mathrm{dt})$, which means that the error decreases linearly with the time step size. This is sufficient for many applications, but for higher accuracy, higher order methods such as the Crank-Nicolson method or Runge-Kutta methods can be used.

Weak Formulation with Backward Euler Method

The time-discrete weak form of the Schrödinger equation becomes:

$$i \int_\Omega \left(\frac{u^{t+\mathrm{dt}} - u^t}{\mathrm{dt}} \right) \bar{v}\, dx = -\int_\Omega \nabla u^{t+\mathrm{dt}} \cdot \nabla \bar{v}\, dx + \int_\Omega V(x,t) u^{t+\mathrm{dt}} \bar{v}\, dx \tag{2}$$

By rearranging, the weak formulation takes the form, with implicit terms on the left and explicit (known) terms on the right:

$$i \int_\Omega u^{t+\mathrm{dt}} \bar{v} - \mathrm{dt} \int_\Omega u^{t+\mathrm{dt}} \bar{v} V(x,t)\, dx + \mathrm{dt} \int_\Omega \nabla u^{t+\mathrm{dt}} \cdot \nabla \bar{v} = i \int_\Omega u^t \bar{v}\, dx, \tag{3}$$

which can be solved iteratively for $u^{t+\mathrm{dt}}$ in each time step.

Existence and Uniqueness via the Lax-Milgram Theorem in Complex Hilbert Spaces

To establish the existence and uniqueness of solutions to the weak formulation of the Schrödinger equation, we can apply the Lax-Milgram theorem. This theorem provides conditions under which a sesquilinear form defines a unique solution to a linear functional equation in a Hilbert space.

Theorem 2.1 (Lax-Milgram Theorem)**.** *Let H be a complex Hilbert space with inner product $\langle \cdot, \cdot \rangle$ and norm $\| \cdot \|_H$. Let $a : H \times H \to \mathbb{C}$ be a sesquilinear form, i.e.,*

$$a(\cdot, v) \text{ is linear for all } v \in H, \quad a(u, \cdot) \text{ is conjugate-linear for all } u \in H.$$

Suppose that:

1. ***Boundedness of the sesquilinear form:*** *There exists $M > 0$ such that*

$$|a(u, v)| \leq M\|u\|_H\|v\|_H \quad \textit{for all } u, v \in H.$$

2. ***Boundedness of the linear form:*** *There exists $C > 0$ such that*

$$|L(v)| \leq C\|v\|_H \quad \textit{for all } v \in H.$$

3. ***Coercivity:*** *There exists $\alpha > 0$ such that*

$$\Re\, a(u, u) \geq \alpha\|u\|_H^2 \quad \textit{for all } u \in H.$$

Then for every bounded linear functional $L \in H^*$, there exists a unique $u \in H$ such that

$$a(u, v) = L(v) \quad \textit{for all } v \in H.$$

Application of the Lax-Milgram Theorem to the Discrete Schrödinger Equation

To properly ... Show that the left-hand side:

$$a(u, v) = \frac{i}{\mathrm{dt}} \int_\Omega u^{t+\mathrm{dt}} \overline{v}\, dx - \int_\Omega V(x, t) u^{t+\mathrm{dt}} \overline{v}\, dx + \int_\Omega \nabla u^{t+\mathrm{dt}} \cdot \nabla \overline{v}\, dx$$

is a sesquilinear form. And the right-hand side:

$$L(v) = \frac{i}{\mathrm{dt}} \int_\Omega u^t \overline{v}\, dx$$

is a bounded linear functional.

Scalar Product in $H_0^1(\Omega; \mathbb{C})$

We define the scalar product

$$\langle u, v \rangle_{H_0^1} := \int_\Omega \nabla u \cdot \nabla \overline{v}\, dx + \int_\Omega u\, \overline{v}\, dx.$$

This is a valid sesquilinear inner product because:

- It is **linear** in the first argument: $\langle \lambda u_1 + \mu u_2, v \rangle = \lambda \langle u_1, v \rangle + \mu \langle u_2, v \rangle$ for all $\lambda, \mu \in \mathbb{C}$.
- It is **conjugate-linear** in the second argument.
- It is **Hermitian**: $\langle u, v \rangle = \overline{\langle v, u \rangle}$.
- It is **positive-definite**: $\langle u, u \rangle = 0$ implies $u = 0$ in H_0^1.

Hence, $(H_0^1(\Omega; \mathbb{C}), \langle \cdot, \cdot \rangle_{H_0^1})$ is a Hilbert space.

Boundedness of the Sesquilinear and Linear Form.

Lemma 2.2 (Boundedness of $a(u,v)$)**.** *Let $u, v \in H_0^1(\Omega;\mathbb{C})$, $V \in L^\infty(\Omega)$ and $\tau > 0$. Then the sesquilinear form $a(u,v)$ is bounded, i.e., there exists $M > 0$ such that*

$$|a(u,v)| \leq M\|u\|_{H_0^1}\|v\|_{H_0^1}.$$

Proof. By triangle inequality, we can split the sesquilinear form into three terms:

$$|a(u,v)| \leq |\int_\Omega \nabla u \cdot \nabla \overline{v}\, dx| + \left|\frac{i}{\mathrm{dt}}\int_\Omega u\,\overline{v}\, dx\right| + \left|\int_\Omega V(x,t)u^{t+\mathrm{dt}}\overline{v}\, dx\right|.$$

We estimate each term separately.
(1) Stiffness term:

$$\begin{aligned}\left|\int_\Omega \nabla u \cdot \nabla \overline{v}\, dx\right| &\leq \int_\Omega |\nabla u||\nabla \overline{v}|\, dx = \int_\Omega |\nabla u||\nabla \overline{v}|\, dx = \int_\Omega |\nabla u||\nabla v|\, dx \\ &\leq \|\nabla u\|_{L^2(\Omega)}\|\nabla v\|_{L^2(\Omega)} \quad \text{(by Cauchy-Schwarz in } L^2(\Omega;\mathbb{C}^d)).\end{aligned}$$

(2) Mass term:

$$\begin{aligned}\left|\int_\Omega \frac{i}{\mathrm{dt}}u\,\overline{v}\, dx\right| &= \frac{1}{\mathrm{dt}}\left|\int_\Omega u\,\overline{v}\, dx\right| \leq \frac{1}{\mathrm{dt}}\int_\Omega |u||v|\, dx \\ &\leq \frac{1}{\mathrm{dt}}\|u\|_{L^2(\Omega)}\|v\|_{L^2(\Omega)} \quad \text{(again by Cauchy-Schwarz).}\end{aligned}$$

(3) Potential term:

$$\begin{aligned}\left|\int_\Omega V(x,t)u^{t+\mathrm{dt}}\overline{v}\, dx\right| &\leq \|V\|_{L^\infty(\Omega\times[0,T])}\int_\Omega |u^{t+\mathrm{dt}}||\overline{v}|\, dx \\ &\leq \|V\|_{L^\infty(\Omega\times[0,T])}\|u^{t+\mathrm{dt}}\|_{L^2(\Omega)}\|v\|_{L^2(\Omega)}.\end{aligned}$$

Combining all terms:

$$\begin{aligned}|a(u,v)| &\leq \|\nabla u\|_{L^2}\|\nabla v\|_{L^2} + \frac{1}{\mathrm{dt}}\|u\|_{L^2}\|v\|_{L^2} + \|V\|_{L^\infty}\|u^{t+\mathrm{dt}}\|_{L^2}\|v\|_{L^2} \\ &\leq M\left(\|\nabla u\|_{L^2}\|\nabla v\|_{L^2} + \|u\|_{L^2}\|v\|_{L^2}\right),\end{aligned}$$

where $M = \max\left(1, \frac{1}{\mathrm{dt}} + \|V\|_{L^\infty}\right)$.
Recalling the definition of the H_0^1 norm:

$$\|u\|_{H_0^1}^2 := \|\nabla u\|_{L^2}^2 + \|u\|_{L^2}^2.$$

We obtain the desired estimate:

$$|a(u,v)| \leq M\|u\|_{H_0^1}\|v\|_{H_0^1},$$

where $M = \max\left(1, \frac{1}{\mathrm{dt}} + \|V\|_{L^\infty}\right)$. ■

Lemma 2.3 (Boundedness of the linear form)**.** *Let $u^t \in L^2(\Omega;\mathbb{C})$ be given. Then the linear functional*

$$L(v) := \frac{i}{dt}\int_\Omega u^t\,\overline{v}\,dx$$

is bounded on $H_0^1(\Omega;\mathbb{C})$. That is, there exists a constant $C>0$ such that

$$|L(v)| \le C\|v\|_{H_0^1(\Omega)} \quad \forall v \in H_0^1(\Omega;\mathbb{C}).$$

Proof. We estimate each term separately using the Cauchy-Schwarz and Hölder inequalities.

$$\begin{aligned}
|L(v)| &\le \left|\frac{i}{\mathrm{dt}}\int_\Omega u^t(x)\,\overline{v(x)}\,dx\right| = \frac{1}{\mathrm{dt}}\left|\int_\Omega u^t(x)\,\overline{v(x)}\,dx\right| \\
&\le \frac{1}{\mathrm{dt}}\int_\Omega |u^t(x)|\,|v(x)|\,dx \quad \text{(by triangle inequality)} \\
&\le \frac{1}{\mathrm{dt}}\|u^t\|_{L^2(\Omega)}\|v\|_{L^2(\Omega)} \quad \text{(by Cauchy-Schwarz inequality).}
\end{aligned}$$

As in the last proof we can split $\|v\|_{L^2(\Omega)} = \frac{1}{2}\|v\|^2_{L^2(\Omega)} + \frac{1}{2}\|v\|^2_{L^2(\Omega)}$ and use the Poincaré inequality which gives us:

$$|L(v)| \le \frac{\tilde{C}}{2}\left(\|\nabla v\|^2_{L^2(\Omega)} + \|v\|^2_{L^2(\Omega)}\right) \le C\|v\|^2_{H_0^1(\Omega)},$$

where $C = \frac{1}{2\mathrm{dt}}\|u^t\|_{L^2(\Omega)}$.
Hence, L is bounded. ■

Coercivity of the Sesquilinear Form

Lemma 2.4 (Coercivity of the sesquilinear form)**.** *Let $a(u,v)$ be the sesquilinear form defined by*

$$a(u,v) = \int_\Omega \nabla u\cdot\nabla\overline{v}\,dx + \frac{i}{dt}\int_\Omega u\,\overline{v}\,dx - \int_\Omega V(x,t)u\,\overline{v}\,dx.$$

Then there exists a constant $\alpha>0$ such that

$$\Re a(u,u) \ge \alpha\|u\|^2_{H_0^1(\Omega)} \quad \forall u \in H_0^1(\Omega;\mathbb{C}).$$

Proof. We compute the real part of $a(u,u)$: Note: check again for minus signs looks weird

$$\begin{aligned}
\Re a(u,u) &= \Re\left(\int_\Omega |\nabla u|^2\,dx + \frac{i}{\mathrm{dt}}\int_\Omega |u|^2\,dx - \int_\Omega V(x,t)u\,\overline{u}\,dx\right) \\
&= \int_\Omega |\nabla u|^2\,dx - \int_\Omega V(x,t)|u|^2\,dx \\
&= ||\nabla u||^2_{L^2(\Omega)} - ||V||^2_{L^\infty(\Omega\times[0,T])}||u||^2_{L^2(\Omega)}.
\end{aligned}$$

By the boundedness of the potential term, we have:

$$\|V\|_{L^\infty(\Omega\times[0,T])} = C_V < \infty$$

By the Poincaré inequality, we have:

$$\|u\|^2_{L^2(\Omega)} \leq C_P||\nabla u||^2_{L^2(\Omega)} \quad \text{(for some constant } C_P > 0).$$

Thus, we can estimate for $\Re a(u,u)$:

$$\begin{aligned}\Re a(u,u) &= ||\nabla u||^2_{L^2(\Omega)} - C_V||u||^2_{L^2(\Omega)} \\ &\geq ||\nabla u||^2_{L^2(\Omega)} - C_V C_P||\nabla u||^2_{L^2(\Omega)} \\ &= (1 - C_V C_P)||\nabla u||^2_{L^2(\Omega)}.\end{aligned}$$

By definition of the H^1_0 norm and Poincaré inequality, we have:

$$\|u\|^2_{H^1_0(\Omega)} = ||\nabla u||^2_{L^2(\Omega)} + ||u||^2_{L^2(\Omega)} \leq (1 + C_P)||\nabla u||^2_{L^2(\Omega)}.$$

and therefore:

$$\|u\|^2_{L^2(\Omega)} \geq \frac{1}{1 + C_P}||\nabla u||^2_{H^1_0(\Omega)}.$$

Combining these estimates, we obtain:

$$\begin{aligned}\Re a(u,u) &\geq (1 - C_V C_P)||\nabla u||^2_{L^2(\Omega)} \\ &\geq \frac{1 - C_V C_P}{1 + C_P}||u||^2_{H^1_0(\Omega)}.\end{aligned}$$

Thus, we can choose $\alpha = \frac{(1-C_V C_P)}{(1+C_P)} > 0$ if $C_V < 1/C_P$ and the real part of the sesquilinear form is coercive.

■

We showed that every condition of the Lax-Milgram theorem is satisfied, thus a solution to the weak formulation of the Schrödinger equation exists and is unique.

3 Physics-Informed Neural Networks

Copilot: Physical Informed Neural Networks (PINNs) can be used to solve the Schrödinger equation by incorporating the physics of the problem into the training process. The neural network is trained to minimize a loss function that includes terms for the residual of the Schrödinger equation, initial conditions, and boundary conditions.

Classical PINN Loss for the Schrödinger Equation

Let $u_\theta : \Omega \times [0,T] \to \mathbb{C}$ be a neural network approximation to the solution of the time-dependent Schrödinger equation

$$i\,\partial_t u = -\Delta u + V(x,t)u.$$

We define the residual function

$$\mathcal{R}(x,t) := i\,\partial_t u_\theta(x,t) + \Delta u_\theta(x,t) - V(x,t)u_\theta(x,t).$$

The classical PINN loss functional is then given by

$$\mathcal{L}_{\text{PINN}}(\theta) = \lambda_{\text{PDE}} \cdot \frac{1}{N_f} \sum_{j=1}^{N_f} |\mathcal{R}(x_j,t_j)|^2 + \lambda_{\text{IC}} \cdot \frac{1}{N_0} \sum_{j=1}^{N_0} |u_\theta(x_j,0) - u_0(x_j)|^2 + \lambda_{\text{BC}} \cdot \frac{1}{N_b} \sum_{j=1}^{N_b} |u_\theta(x_j,t_j)|^2 ,$$

where:

- (x_j,t_j) are collocation points in $\Omega \times (0,T]$,
- $u_0(x)$ is the given initial condition,
- and $\lambda_{\text{PDE}}, \lambda_{\text{IC}}, \lambda_{\text{BC}}$ are weighting parameters for PDE residual, initial condition, and boundary condition losses, respectively.

Energy-Based PINN Loss via Weak Formulation

We consider a time discretization with step size Δt and define the semi-discrete Schrödinger equation via the backward Euler method:

$$i\frac{u^t - u^{t-1}}{\Delta t} = -\Delta u^t + V(x,t)u^t.$$

We define the bilinear form $a : H_0^1(\Omega;\mathbb{C}) \times H_0^1(\Omega;\mathbb{C}) \to \mathbb{C}$ and linear form $L^t : H_0^1(\Omega;\mathbb{C}) \to \mathbb{C}$ by

$$a(u,v) := \int_\Omega \left(\frac{i}{\Delta t} u\bar{v} + \nabla u \cdot \nabla \bar{v} + V(x,t)u\bar{v} \right) dx,$$
$$L^t(v) := \int_\Omega \frac{i}{\Delta t} u^{t-1}(x)\bar{v}(x)\,dx.$$

The energy-based loss at timestep t is defined by

$$\mathcal{L}^t_{\text{energy}}(\theta) := \left| a(u^t_\theta, v) - L^t(v) \right|^2 ,$$

where $v \in H_0^1(\Omega;\mathbb{C})$ is a test function (e.g., $v = u^t_\theta$), or the quantity can be integrated over a set of test functions or points.
The full loss over all timesteps is then

$$\mathcal{L}_{\text{energy}}(\theta) := \frac{1}{N_t} \sum_{t=1}^{N_t} \mathcal{L}^t_{\text{energy}}(\theta) + \lambda_{\text{IC}} \cdot \frac{1}{N_0} \sum_{j=1}^{N_0} |u_\theta(x_j,0) - u_0(x_j)|^2 + \lambda_{\text{BC}} \cdot \frac{1}{N_b} \sum_{j=1}^{N_b} |u_\theta(x_j,t_j)|^2 .$$

4 Experiments

Problem 1: Free Schrödinger Equation on the Unit Square

We consider the time-dependent Schrödinger equation on the unit square $\Omega = (0,1)^2$ with homogeneous Dirichlet boundary conditions and zero potential:

$$\begin{aligned} i\,\partial_t u(x,t) &= -\Delta u(x,t), && \text{in } \Omega \times (0,T), \\ u(x,t) &= 0, && \text{on } \partial\Omega \times (0,T), \\ u(x,0) &= u_0(x), && \text{in } \Omega. \end{aligned}$$

Analytical Solution

A known exact solution is given by the separable function

$$u(x,y,t) = \sin(\pi x)\sin(\pi y)e^{-i2\pi^2 t},$$

which satisfies:

- The homogeneous Dirichlet boundary conditions: $u(x,t) = 0$ on $\partial\Omega$ for all t,
- The initial condition: $u_0(x,y) = \sin(\pi x)\sin(\pi y)$,
- The PDE:

  $$\Delta u = -2\pi^2 \sin(\pi x)\sin(\pi y)e^{-i2\pi^2 t}, \quad \partial_t u = -i2\pi^2 \sin(\pi x)\sin(\pi y)e^{-i2\pi^2 t},$$

  hence

  $$i\,\partial_t u = -\Delta u.$$

Summary of Parameters

- Domain: $\Omega = (0,1)^2$
- Boundary conditions: $u = 0$ on $\partial\Omega$
- Initial condition: $u_0(x,y) = \sin(\pi x)\sin(\pi y)$
- Potential: $V(x,t) = 0$
- Exact solution: $u(x,y,t) = \sin(\pi x)\sin(\pi y)e^{-i2\pi^2 t}$

Problem 2: Schrödinger Equation with Time-Dependent Model Potential

Time-Discrete Weak Formulation (Backward Euler)

We discretize the time interval $[0,T]$ with step size $\Delta t > 0$ and denote $u^n \approx u(t_n)$ at time $t_n = n\Delta t$.

We use the backward Euler method for the time derivative:

$$\partial_t u(t_n) \approx \frac{u^n - u^{n-1}}{\mathrm{dt}}.$$

The time-discrete weak formulation reads: Given $u^{n-1} \in H_0^1(\Omega;\mathbb{C})$, find $u^n \in H_0^1(\Omega;\mathbb{C})$ such that for all test functions $v \in H_0^1(\Omega;\mathbb{C})$:

$$\left(\frac{i}{\Delta t}u^n, v\right)_{L^2(\Omega)} + (\nabla u^n, \nabla v)_{L^2(\Omega)} = \left(\frac{i}{\Delta t}u^{n-1}, v\right)_{L^2(\Omega)}.$$
$$i\int_\Omega u^n\,\overline{v}\,dx + \mathrm{dt}\int_\Omega \nabla u^n \cdot \nabla\overline{v}\,dx = i\int_\Omega u^{n-1}\,\overline{v}\,dx.$$

This is the variational equation to be solved at each time step t_n.

5 Discussion and Outlook

We can of course only evaluate the error of FEM and PINNs for the case where we have no potential, as we know the exact solution for this case.

Spacial Error Analysis

Here we show our numerical results for the error as a function of grid spacing with the FEM. We observe the expected convergence rate of $\mathcal{O}(h^2)$ for the FEM, except for very small grid spacings. For the PINNs, there is obviously no spacial error, as we dont use a grid.

Time Error Analysis and Energy Preservation

Here we show that for FEMs, the error in time is of order $\mathcal{O}(\Delta t)$ for the backward Euler method and that backward Euler does not preserve the energy of the system. This could also be connected to the boundary conditions, as with the Dirichlet boundary conditions, we have implicitly also assumed von Neumann boundary conditions. Possible improvements: Crank-Nicolson method and higher order time discretization schemes, as well as using periodic boundary conditions?
For PINNs, we observe that the error in time oscilates in time, which could be due to the fact that real and imaginary parts of the solution are not learned equally well. Under ideal conditions, the error should be constant in time.

Experiments on the time-dependent Model Potential

Here we show how the solutions of FEM and PINNs on the time-dependent model potential, for which there is no exact solution.