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.

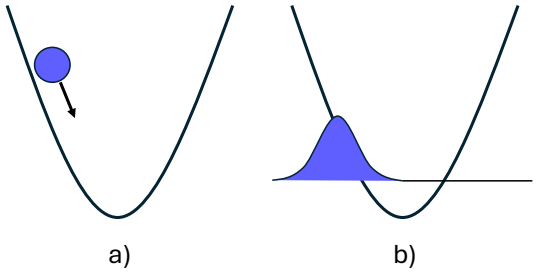

Figure 1:

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-

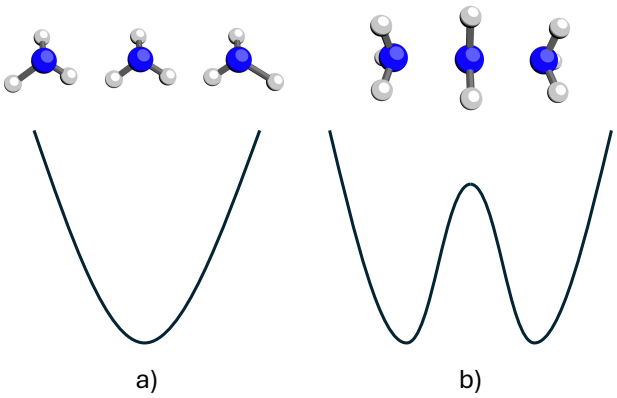

Figure 2:

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

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** if it satisfies the following system of equations:

$$i\partial_t u(x,t) = -\Delta u(x,t) + V(x,t)u(x,t), \quad x \in \Omega,\ t > 0, \tag{1}$$

$$\partial_t u(x,0) = u_0(x), \quad x \in \Omega, \tag{2}$$

$$u(x,t) = g(x,t), \quad x \in \Gamma_D, t > 0, \tag{3}$$

$$\partial_n u(x,t) = h(x,t), \quad x \in \Gamma_N, t > 0. \tag{4}$$

where Δ is the Laplacian operator, $V(x,t)$ is the potential, and $u(x,t)$ is the wave function and the boundary of the domain is split into Dirichlet boundary Γ_D and Neumann boundary Γ_N (homogeneous Dirichlet?). The initial condition is given by $u_0(x)$.

Weak Formulation of Schrödinger's Equation

v is not needed to be in Sobolev space can also do other spaces but when is it elegant to do the transition to Sobolev spaces?
Multiplying the Schrödinger equation by a test function $v(x,t) \in H_0^1(\Omega;\mathbb{C})$ and integrating over the domain Ω, we obtain:

$$i\int_\Omega (\partial_t u)\,\bar{v}\,dx = -\int_\Omega \nabla u \cdot \nabla \bar{v}\,dx + \int_\Omega V(x,t)u\bar{v}\,dx, \tag{5}$$

where $v := v(x,t)$ is a test function in $H_0^1(\Omega;\mathbb{C})$.

Time discretisation of Schrödinger's Equation

Using an implicit time discretisation scheme, we can rewrite the time derivative as:

$$\partial_t u(x,t) \approx \frac{u^{t+\mathrm{dt}} - u^t}{\mathrm{dt}}, \tag{6}$$

We need to choose what to handle implicit and explicit on the right hand side of the weak formulation. In the following, we will treat the term with the potential $V(x,t)$ explicitly and the term with the Laplacian implicitly. This simplifies the numerical treatment of the mass term, because the potential can introduce stiffness in the system, if it is large and has rapid variations.
The weak form of the Schrödinger equation becomes:

$$i\int_\Omega \left(\frac{u^{t+\mathrm{dt}} - u^t}{\mathrm{dt}}\right)\bar{v}\,dx = -\int_\Omega \nabla u^{t+\mathrm{dt}} \cdot \nabla \bar{v}\,dx + \int_\Omega V(x,t)u^{t+\mathrm{dt}}\bar{v}\,dx \tag{7}$$

Rearranging, we get:

$$i\int_\Omega u^{t+\mathrm{dt}}\bar{v} - \mathrm{dt}\int_\Omega u^{t+\mathrm{dt}}\bar{v}V(x,t)\,dx + \mathrm{dt}\int_\Omega \nabla u^{t+\mathrm{dt}} \cdot \nabla \bar{v} = i\int_\Omega u^t\bar{v}\,dx, \tag{8}$$

which can be solved iteratively using a time-stepping method.
Note: In the following, we will denote the dependence of u and v on x and t explicitly, while $t + \mathrm{dt}$ refers to the next time step.

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

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

and the associated norm

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

Lax-Milgram Theorem for complex Problems

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*
$$|a(u, v)| \le M \|u\|_H \|v\|_H \quad \text{for all } u, v \in H.$$
2. ***Boundedness of the linear form:*** *There exists $C > 0$ such that*
$$|L(v)| \le C \|v\|_H \quad \text{for all } v \in H.$$
3. ***Coercivity:*** *There exists $\alpha > 0$ such that*
$$\Re\, a(u, u) \ge \alpha \|u\|_H^2 \quad \text{for all } u \in H.$$

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

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

Apply Lax Milgram

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*

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

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

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

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

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

(2) Mass term:

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

(3) Potential term:

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

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

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

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

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

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

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

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

$$\Re a(u,u) \geq \alpha \|u\|^2_{H^1_0(\Omega)} \quad \forall u \in H^1_0(\Omega;\mathbb{C}).$$

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

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

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.

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.