CASUS
CENTER FOR ADVANCED SYSTEMS UNDERSTANDING

DSECOP Module: Learning the Schrödinger Equation

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Goals

CASUS CENTER FOR ADVANCED SYSTEMS UNDERSTANDING

- Relevant course: Quantum Mechanics 1 (Usually Junior year) (after students learn about Quantum Harmonic Oscillator)

- Physics goals:
  - Introduction to Time-Dependent Schrödinger Equation
  - Converting analytical solutions to code

- Machine learning goals:
  - Introduction to neural networks
  - Integrating physics domain knowledge into ML algorithms

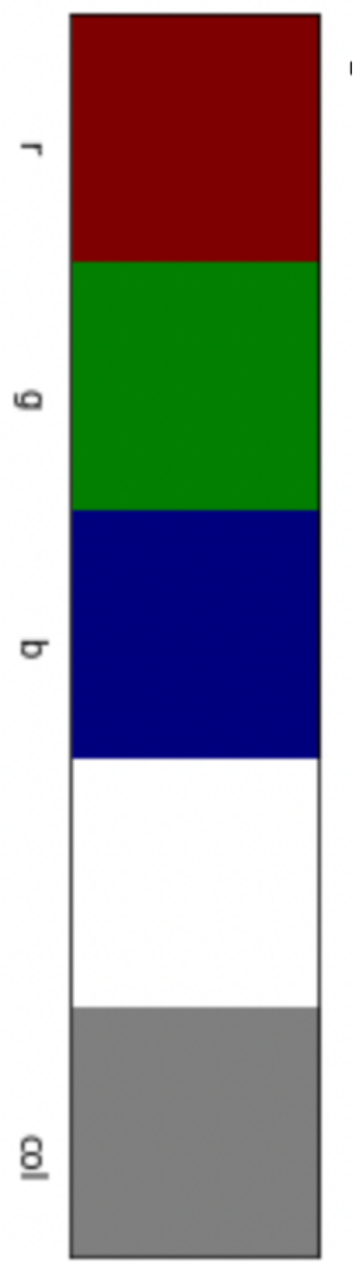
Structure

- Lesson 1: Introduction to Neural Networks
- Lesson 2: Brief background on machine learning and applications to physics
- Lesson 3: Solving the Time-Dependent Schrödinger Equation for a Quantum Harmonic Oscillator, using machine learning

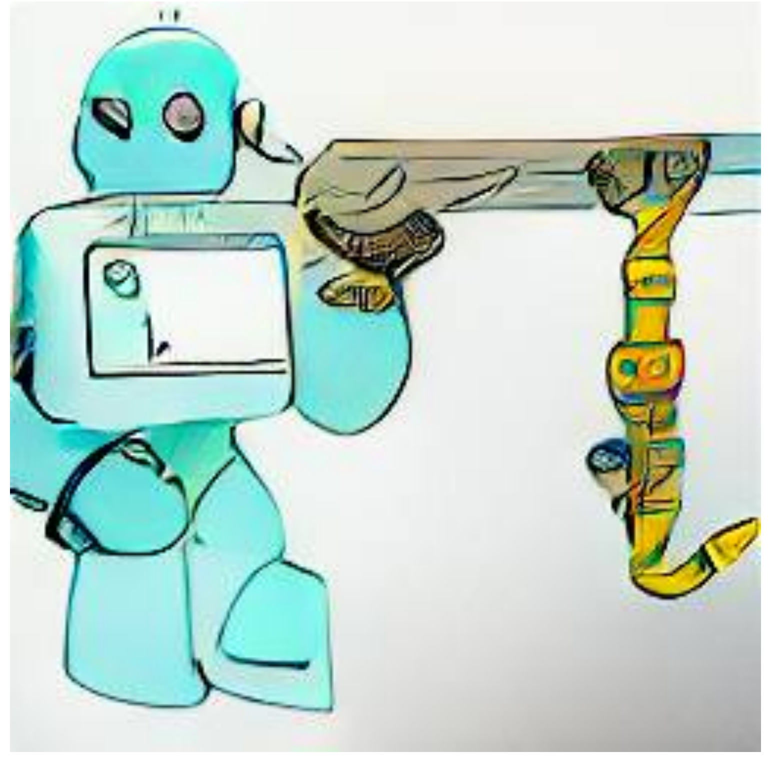
- Components:
  - In-built interactive demonstrations and exercises
  - Take-home reading and reference
  - Project ideas (trivial to ambitious)

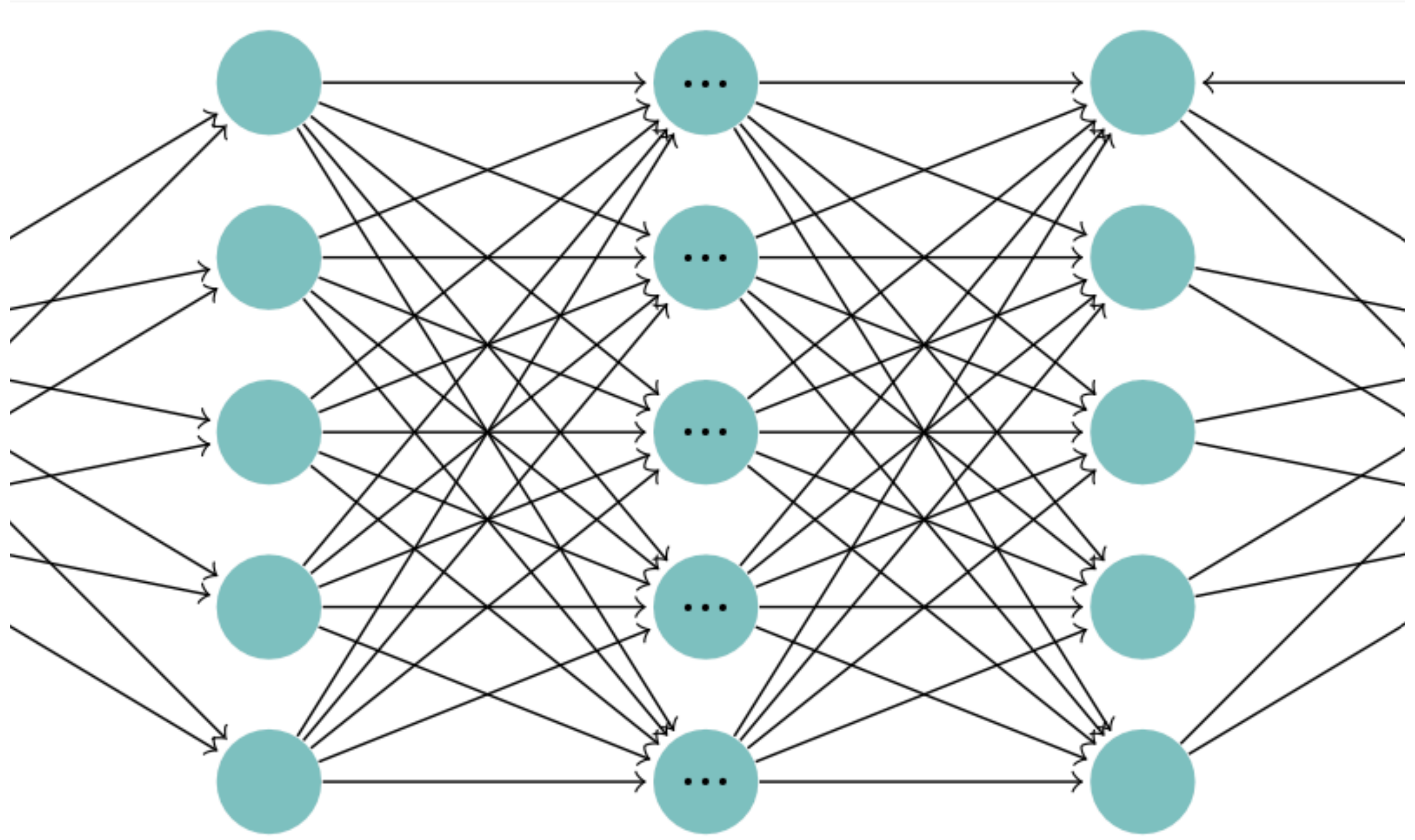
Lesson 1

Introduction to Neural Networks (with plumbing and colours)



RGB





Neural Network
(Trainable Parameters)

CMYK

Lesson 2

Broad introduction to machine learning

- Background for machine learning
- Brief explanation of:
  - Parts of ML workflow
  - Different ML models
  - Deep learning
- Applications to physics, and material to explore further (~70 references)

Lesson 3

Physics-Informed Neural Networks for a time evolving quantum QHO

A PINN is constructed for the solution of the Time-Dependent Schrödinger Equation

$$i\frac{\partial}{\partial t}\psi(x,t) - \hat{H}\psi(x,t) = 0$$

in the domain $x \in (-\pi, \pi), t \in (0,2\pi)$.

The Hamiltonian is given by

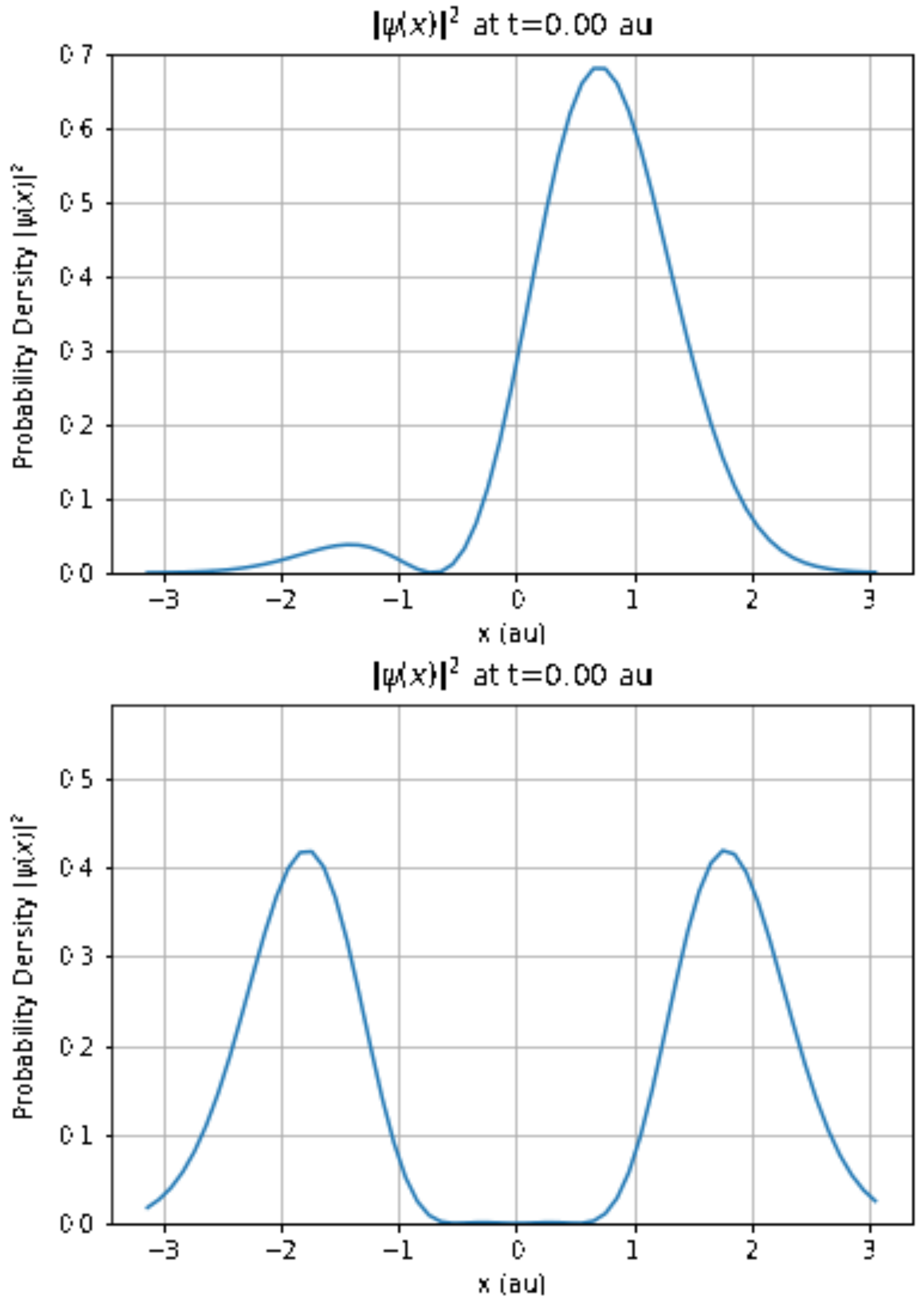
$$\hat{H}_x = -\frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{\omega^2}{2}x^2$$

The analytical solution $\psi_{m,n}(x,t) \in \mathbb{C}$ is

$$\psi_{m,n}(x,t) = \frac{1}{\sqrt{2}}\left(e^{(-iE_m t)}\phi_m(x) + e^{(-iE_n t)}\phi_n(x)\right)$$

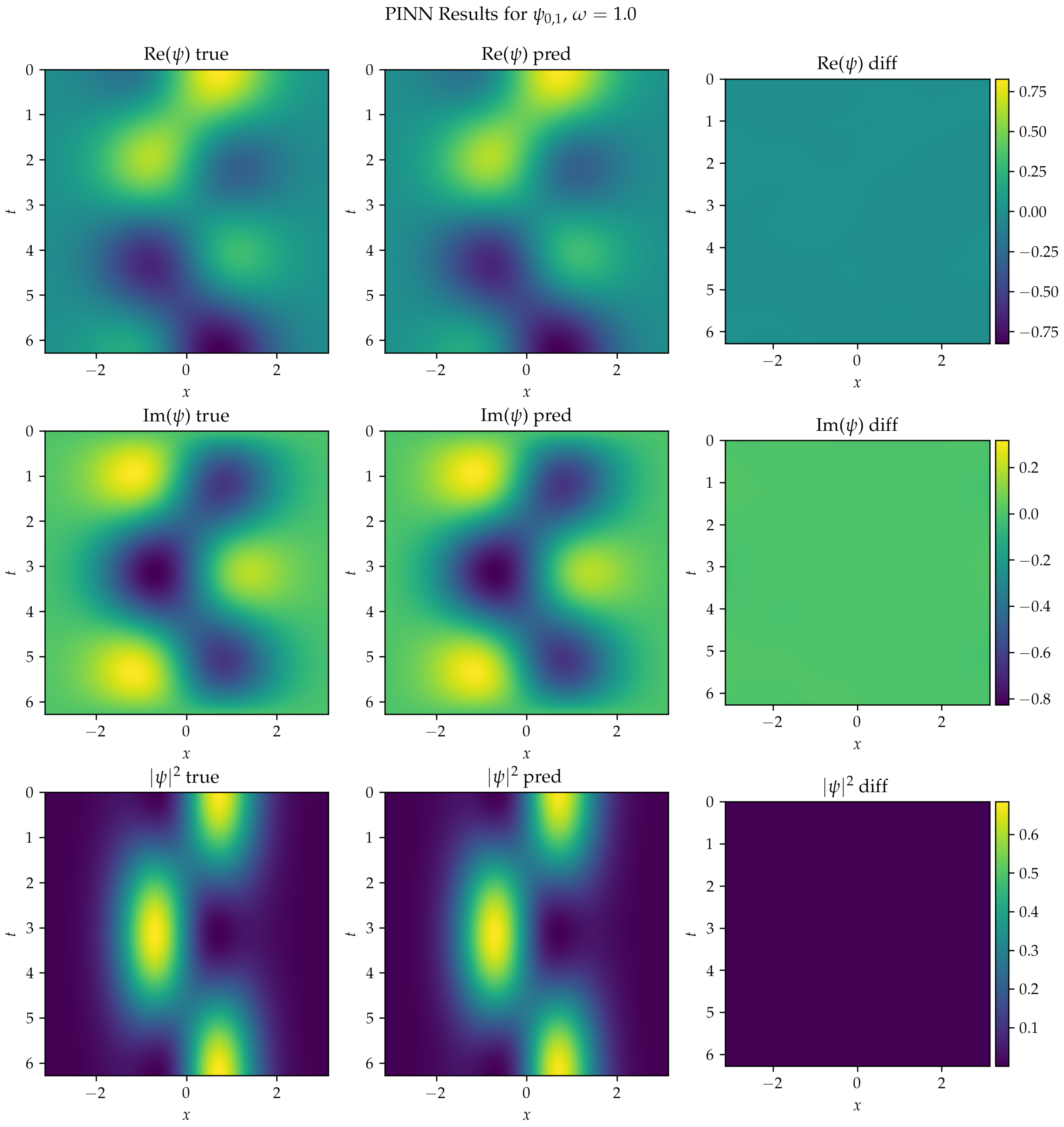
where $\psi_{m,n}$ is the wavefunction for a QHO consisting of the superposition of eigenstates ϕ_m and ϕ_n with E_i being the energy level of state ϕ_i.

The inputs of the PINN solver are x, t and ω, with the outputs being $u, v \in \mathbb{R}$, where $u = Re(\psi)$ and $v = Im(\psi)$ for a QHO with frequency ω.

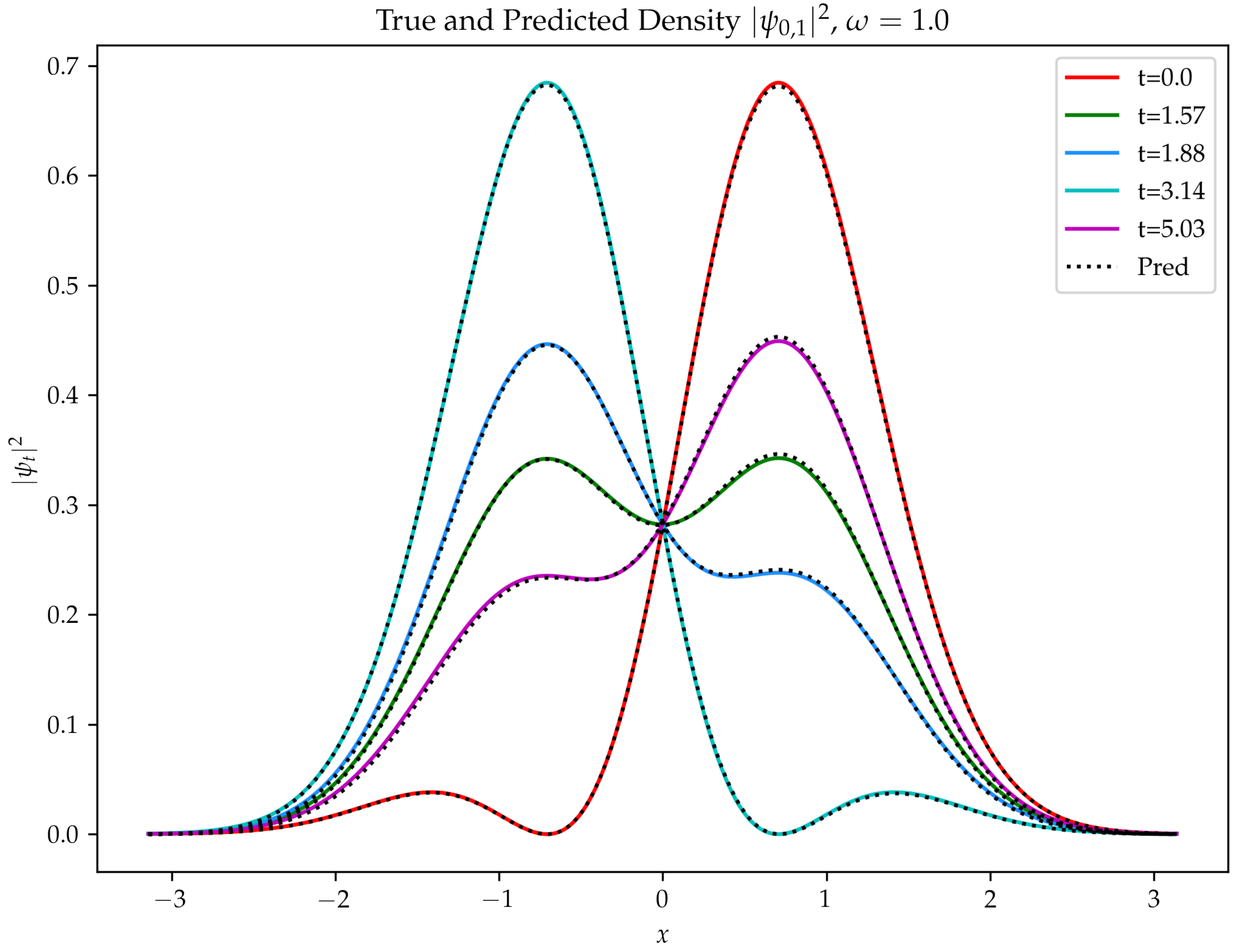


GIF of time evolving density

Lesson 3

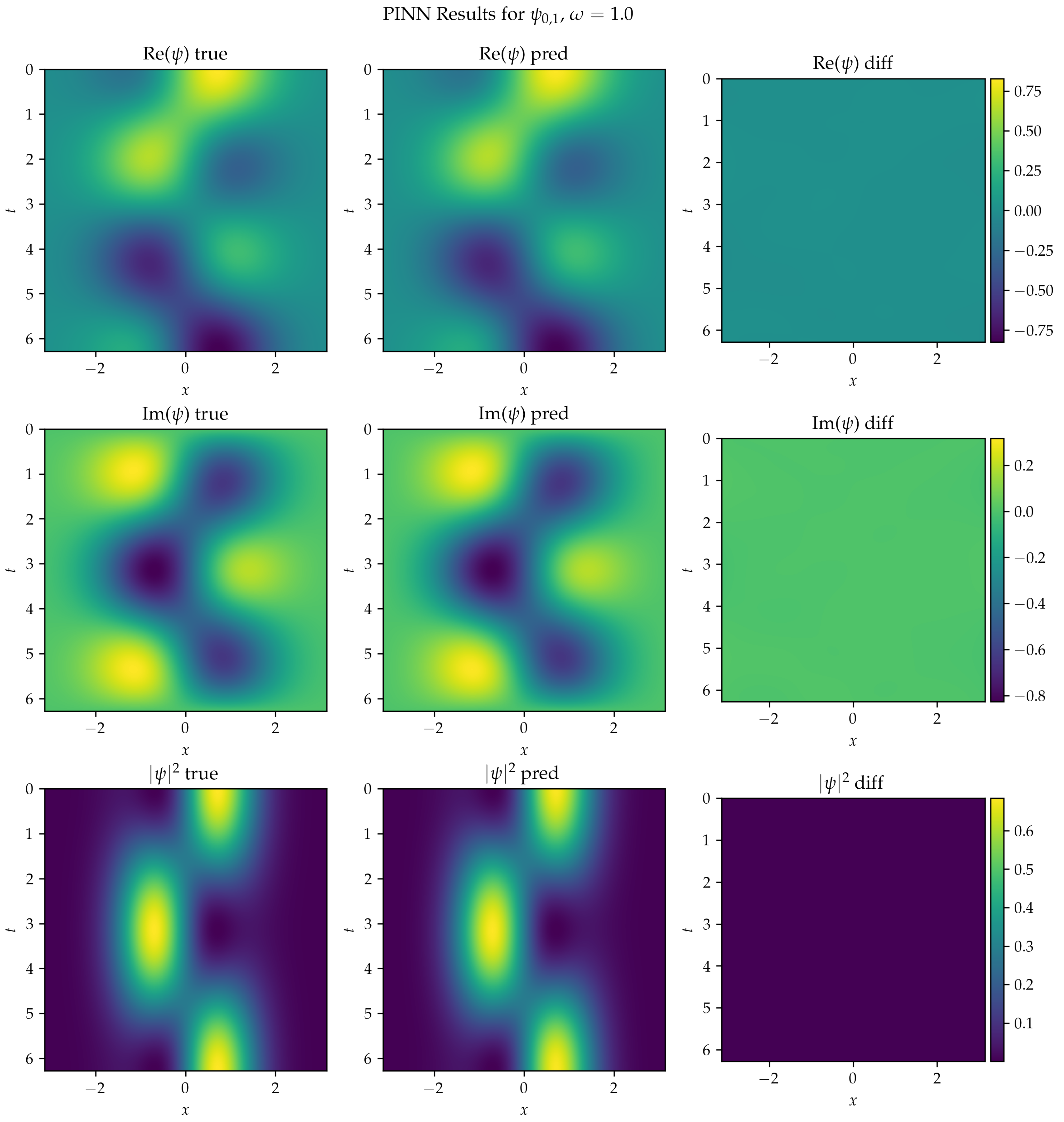


$x - t$ snapshot for true and predicted values for $\psi_{0,1}$ with ω = 1.0.
MSE_u = 1.60e-5, MSE_v = 1.37e-5

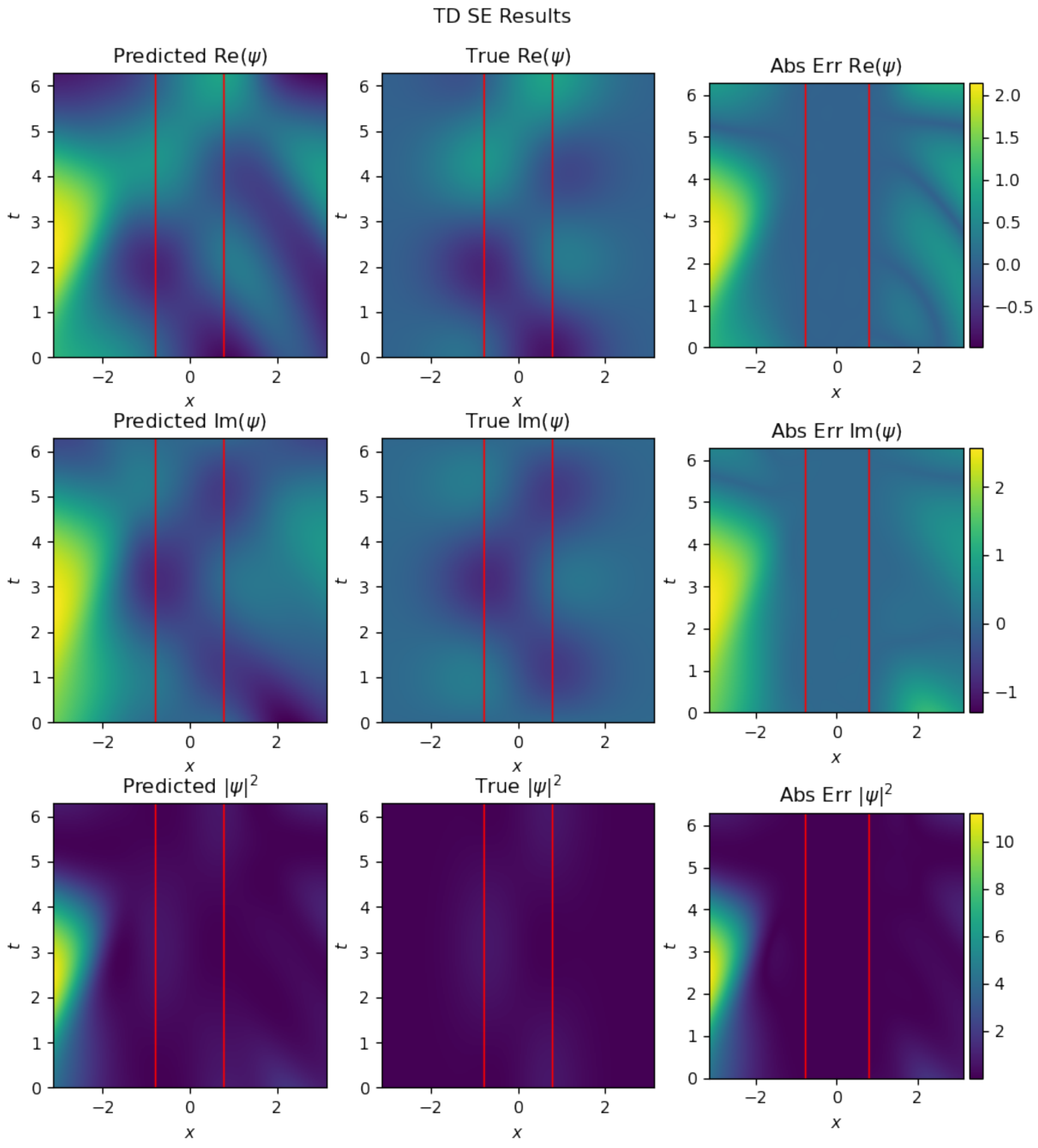


Probability Density $|\psi_t|^2$ at various time steps for $\psi_{0,1}$ with ω = 1.0.
Bold colours denote ground truth, dotted black line denotes corresponding predicted density.

Lesson 3



$x - t$ snapshot for true and predicted values for $\psi_{0,1}$with ω = 1.0.
MAE_u = 1.60e-3, MAE_v = 1.37e-3



$x - t$ snapshot for true and predicted values for $\psi_{0,1}$with ω = 1.0.
MAE_u = 0.27, MAE_v = 0.49

Lesson 3

For a system f, with solution $u(\mathbf{x}, t)$, governed by the following equation

$$f(u) := \frac{\partial u}{\partial t} + \mathcal{N}[u; \lambda], \mathbf{x} \in \Omega, t \in [T_0, T_\tau]$$

$$f(u) = 0$$

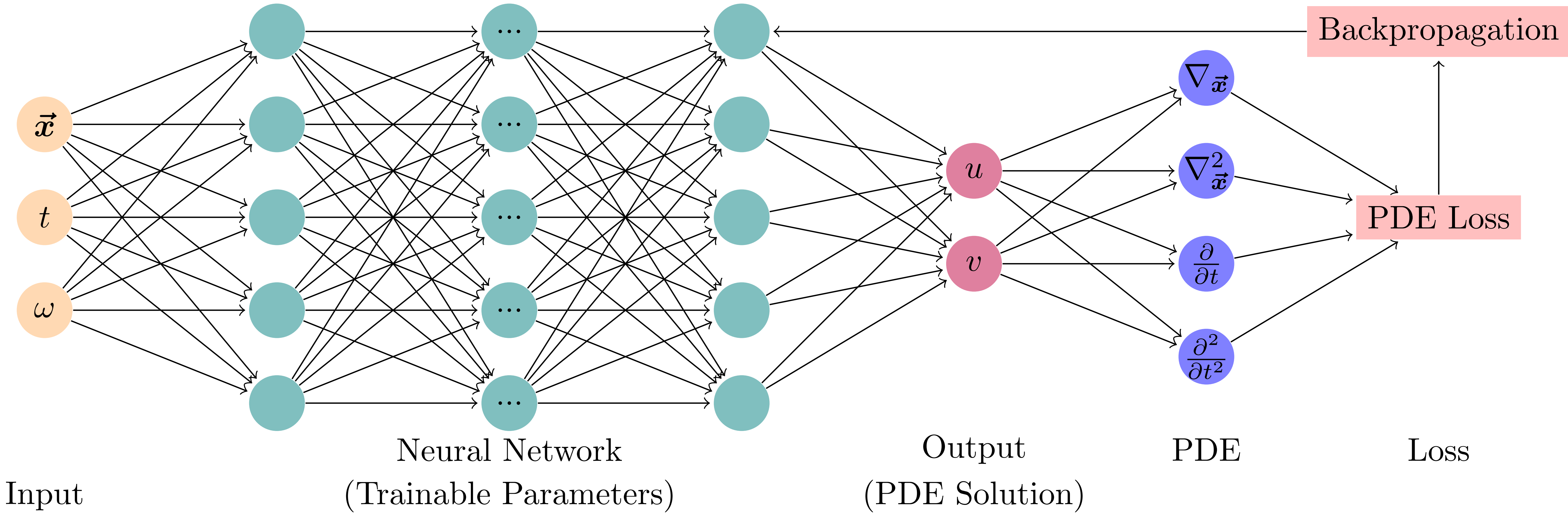
where $\mathcal{N}[u; \lambda]$ is a differential operator parameterised by λ, $\Omega \in \mathbb{R}^{\mathbb{D}}$, $\mathbf{x} = (x_1, x_2, \ldots, x_d)$

with boundary conditions

$\mathscr{B}(u, \mathbf{x}, t) = 0$ on $\partial\Omega$

and initial conditions

$\mathscr{T}(u, \mathbf{x}, t) = 0$ at T_0



PINN Architecture

Lesson 3

We construct u_{net}, a surrogate model for the true solution u.

$f_{net} = f(u_{net})$

The constraints imposed by the system are encoded in the loss term L for neural network optimisation.

$L = L_f + L_{BC} + L_{IC}$

where L_f denotes the error in the solution within the interior points of the system. This error is calculated for N_f collocation points.

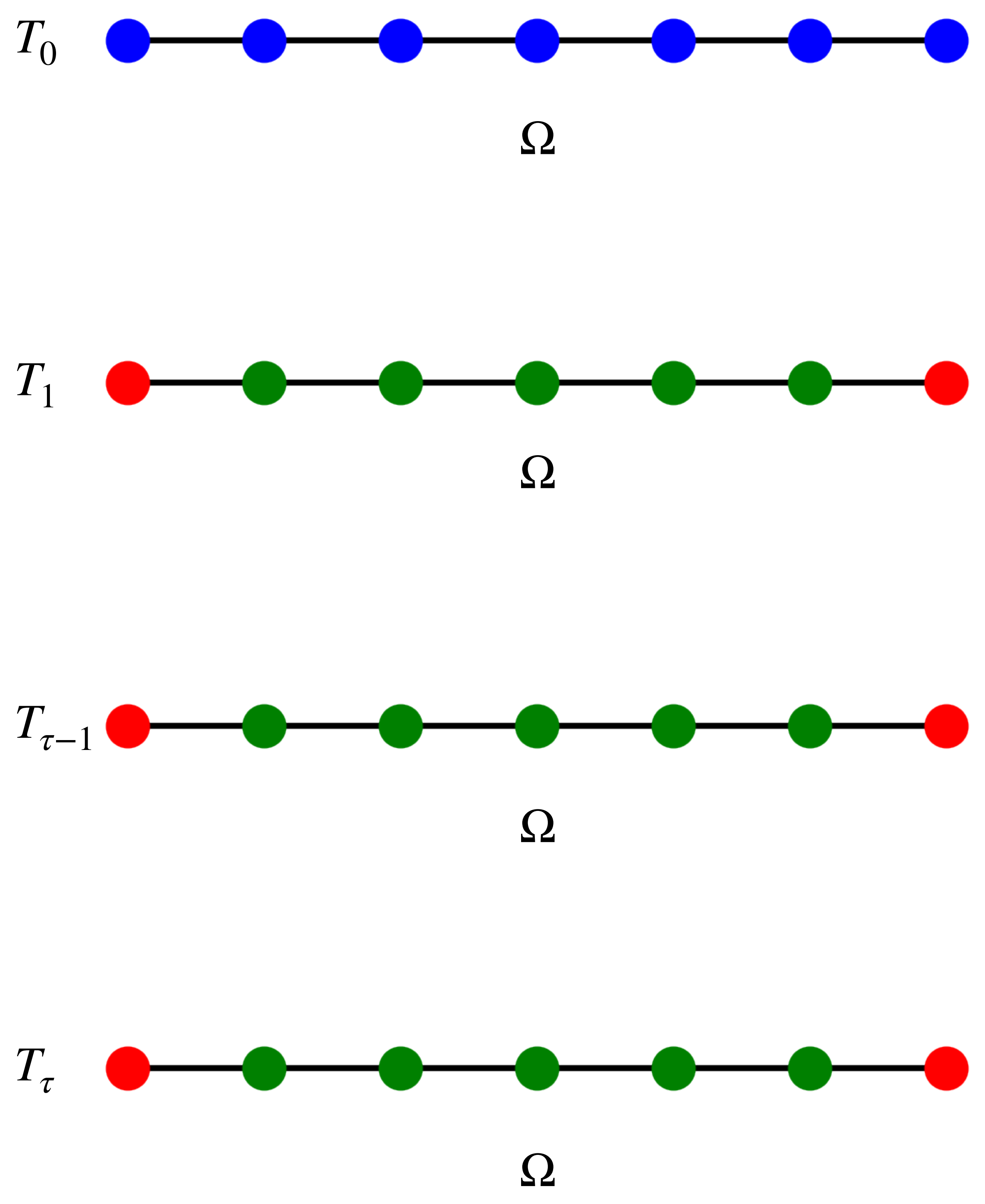
$$L_f = \frac{1}{N_f} \sum_{i=1}^{N_f} \left| f_{net}\left(\mathbf{x}_f^i, t_f^i\right) \right|^2$$

$$L_{BC} = \frac{1}{N_{BC}} \sum_{i=1}^{N_{BC}} \left| u\left(\mathbf{x}_{BC}^i, t_{BC}^i\right) - u^i \right|^2$$

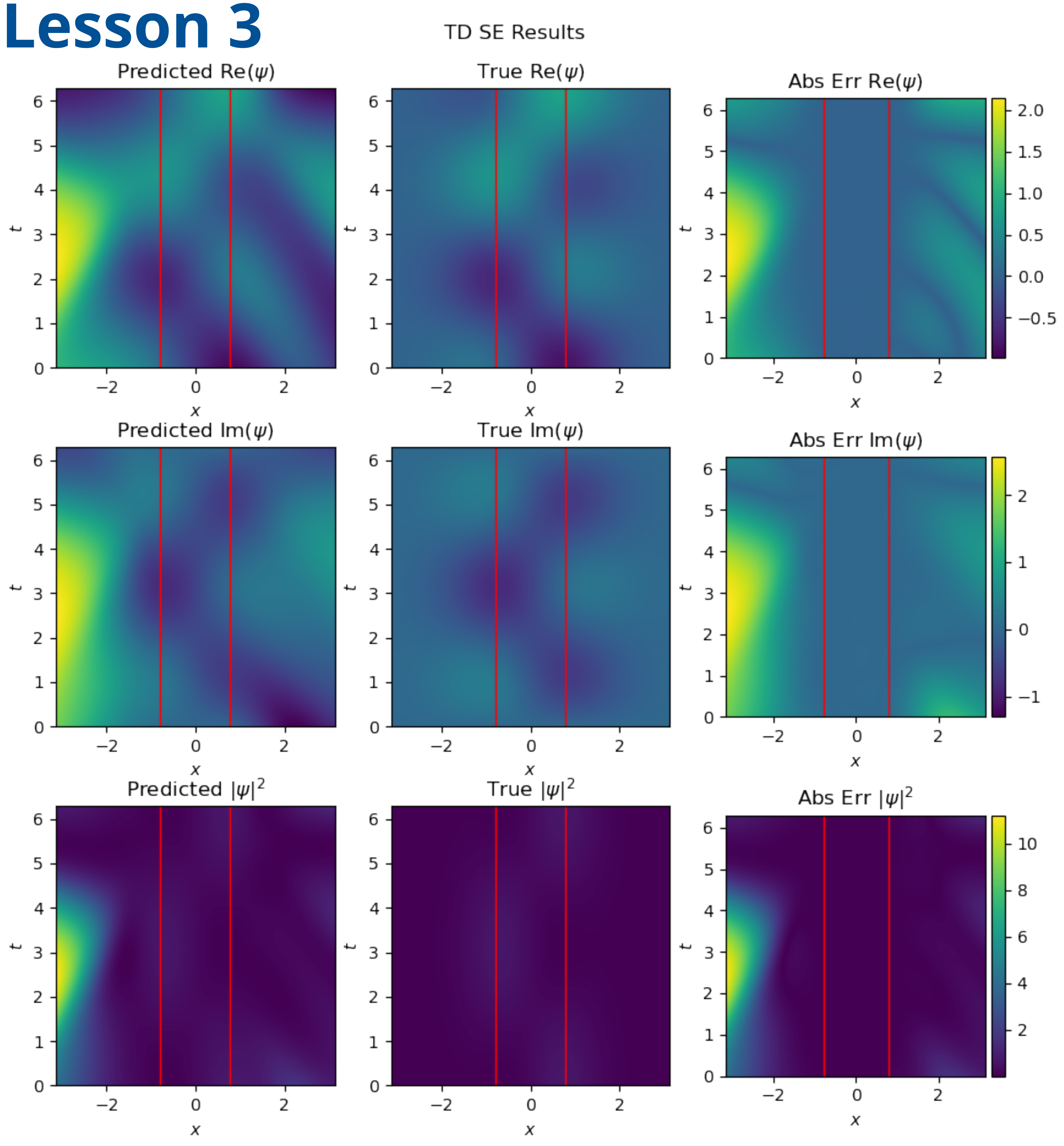
$$L_{IC} = \frac{1}{N_{IC}} \sum_{i=1}^{N_{IC}} \left| u\left(\mathbf{x}_{IC}^i, t_{IC}^i\right) - u^i \right|^2$$

L_{BC} and L_{IC} represent the constraints imposed by the boundary and initial conditions, calculated on a set of N_{BC} boundary points and N_{IC} initial points respectively, with u_i being the ground truth.

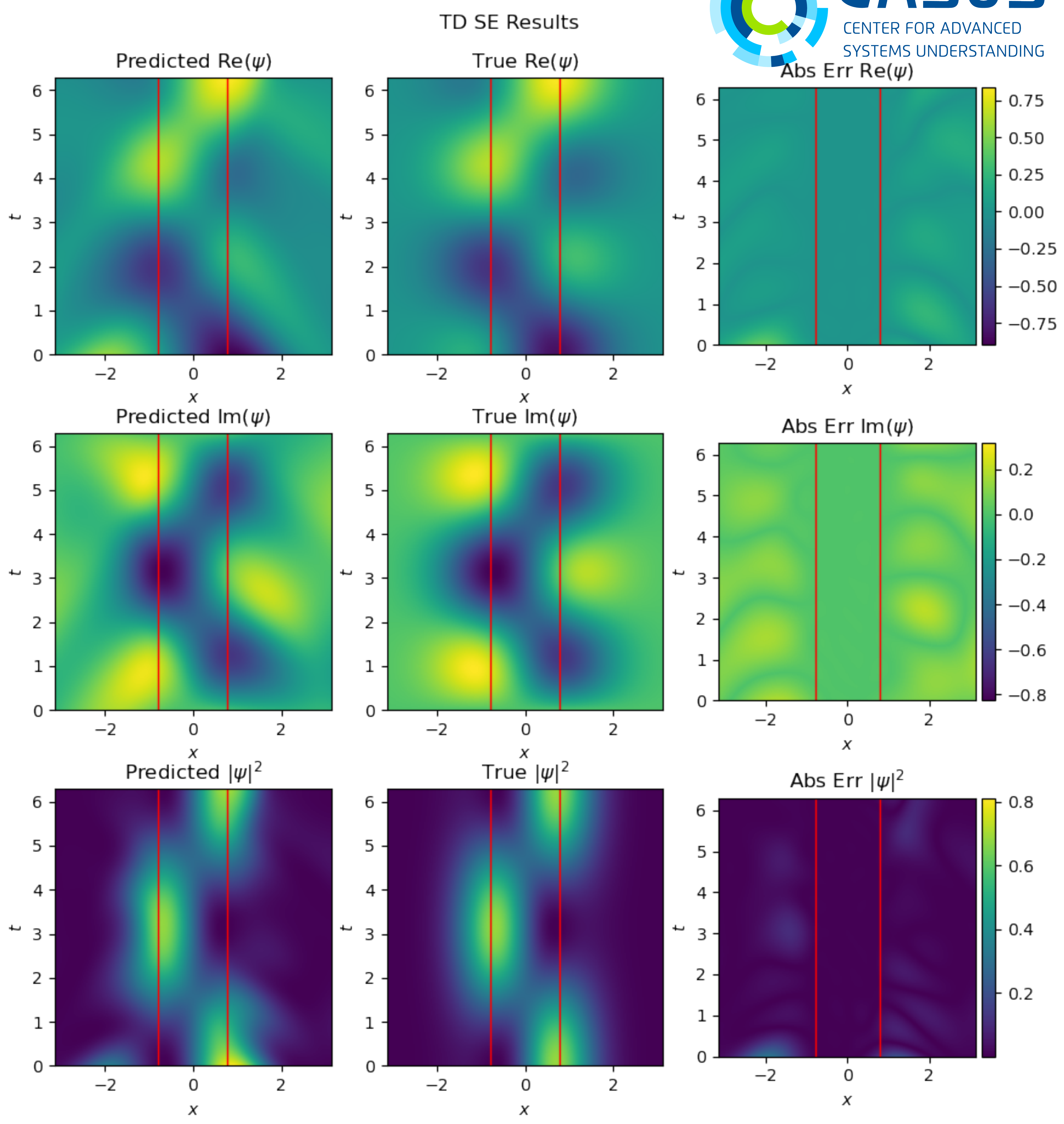
Distribution of Collocation Points



Lesson 3



FCN: MAE (density): 3.8673



PINN: MAE (density): 0.0010

Lesson 3

- Advantages of PINNs:
- Mesh free nature: Generate solutions for grids of arbitrary resolution
- Hybrid workflow: Generate extremely fast coarse solutions, further polished by iterative numerical schemes
- Automatic Differentiation: Well suited for integration into ML workflows
- Generalisable across PDE parameters. Train once, solve a large class of PDEs

Disadvantages of PINNs:

- For low dimensional problems, numerical approaches are faster with theoretical guarantees
- Lack of interpretability / Black box algorithm
- Learning high-resolution higher-dimensional system is resource intensive. However, once learnt, inference is very quick on that domain

Lesson Plan

- Take home - RobotPlumber exercise (2 hours)
- In class - General discussion of machine learning, applications in physics (1-2 hours)
- In class - TD Schrodinger Equation and PINN theoretical background (1-2 hours)
- Take home - Go through notebook (2 hours)
- Project (2 - 8 hours depending on the scope)

Conclusion

- Module can be used for a Quantum Mechanics course
- Based on feedback, easy to add other potentials like infinite square well
- First two lessons can be used for general ML information, third application module can be adapted to any course with a differential equation

The module is available under the DSECOP GitHub repository

Link:

https://github.com/GDS-Education-Community-of-Practice/DSECOP/tree/main/Learning_the_Schrodinger_Equation

Thank you
Questions Comments Concerns?

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Feedback form:
https://bit.ly/DSECOP-feedback

GitHub