**Modelling a two-level atom’s saturated absorption spectra using a Physics Informed Neural Network (PINN)**

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**Brief Introduction:**

The use of neural networks to help finding solutions in a data-driven manner is the beginning of a new paradigm. Current modelling approaches for spectroscopy prove inadequate for complex systems that are not analytically tractable, where traditional calculations are very computationally expensive. PINNs offer a generalizable approach that can be extended to a wide variety of materials. They also provide rapid inference, making them an approach worth studying.

Previous work in this field has focused on X-Ray absorption spectroscopy geared towards finding information about catalyst complexes. Most literature also only deals with traditional neural networks. We will be focusing on using *physics-informed* neural networks for quantum measurement, starting with a simple model and gradually extending applicability.

A PINN differs from a regular neural network by virtue of its loss function.The PINN uses the underlying physics (formulated as PDEs) as a regularizing loss term. This ensure that the neural network behaves accurately.

**Objectives:**

1. To predict a two-level atom’s absorption intensity, given relevant properties of the system such as photon frequency, using a PINN.

This can be extended into investigating field effects, splitting etc. as well.

1. In the second half of the project, we will explore the interaction of the atom with the quantum nature of the photon.

**Methods:**

1. We will be using Optical Bloch equations to model the underlying mechanics in a density matrix formulation.
2. For the neural network modelling, we will be using PyTorch and associated Python packages. The training will be done in a supervised learning approach. For this, we will require other traditional modelling tools such as QuTip as well, to serve as a source of data.
3. To compare with experimental results, we might also access the NIST spectra database.
4. We will be working on Github. Metrics that I want to log include training time, inference time, loss vs. amount of training data required, deviation from experimental results.
5. Physics informed neural networks require a GPU, due to their parallelisable nature.

**Plan:**

Week 1-3:

Understand the theoretical basis of the physics, previous literature in spectral analysis: identify potential further pitfalls and research landscape.

Week 4:

Prepare training data, via traditional simulation. Literature review of PINNs.

Week 5-6:

Start building the model, noting down metrics.

Week 7-8:

Tuning and testing of the model, also building extensions to the model (if feasible)

Week 9-11:

Live testing, performance validation, performance speed-ups

Week 12:

End-term preparation.

Expected outcomes:

1. To demonstrate an accurate and extendable physics informed neural network model of a two-state atom’s response to light.

Comments:

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