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From Short-Sighted to Far-Sighted: A Comparative Study of Recursive Machine Learning Approaches for Open Quantum Systems

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Abstract: Accurately modeling the dynamics of open quantum systems is critical for advancing quantum technologies, yet traditional methods often struggle with balancing accuracy and efficiency. Machine learning (ML) offers a promising alternative, particularly through recursive models that predict system evolution based on the past history. While these models have shown success in predicting single observables, their effectiveness in more complex tasks, such as forecasting the full reduced density matrix (RDM), remains unclear. In this work, we extend history-based recursive ML approaches to complex quantum systems, comparing four physics-informed neural network (PINN) architectures: (i) single-RDM-predicting PINN (SR-PINN), (ii) SR-PINN with simulation parameters (PSR-PINN), (iii) multi-RDMs-predicting PINN (MR-PINN), and (iv) MR-PINN with simulation parameters (PMR-PINN). We apply these models to two representative open quantum systems: the spin-boson (SB) model and the Fenna-Matthews-Olson (FMO) complex. Our results demonstrate that single-RDM-predicting models (SR-PINN and PSR-PINN) are limited by a narrow history window, failing to capture the full complexity of quantum evolution and resulting in unstable long-term predictions, especially in nonlinear and highly correlated dynamics. In contrast, multi-RDMs-predicting models (MR-PINN and PMR-PINN) provide more accurate predictions by extending the forecast horizon, incorporating long-range temporal correlations, and mitigating error propagation. Surprisingly, including simulation parameters explicitly, such as temperature and reorganization energy, in PSR-PINN and PMR-PINN does not consistently improve accuracy and, in some cases, even reduces performance. This suggests that these parameters are already implicitly encoded in the RDM evolution, making their inclusion redundant and adding unnecessary complexity. These findings highlight the limitations of short-sighted recursive forecasting in complex quantum systems and demonstrate the superior stability and accuracy of far-sighted approaches for long-term predictions.

Key words: machine learning, quantum dissipative dynamics, open quantum system.

Open quantum systems describe quantum systems interacting with their environment, playing a fundamental role in quantum computing, quantum memory, quantum transport, proton tunneling in DNA and energy transfer in photosynthesis [1-5]. Their dynamics are captured by the reduced density matrix (RDM), which evolves under both the system internal dynamics and the influence of its environment.

Modeling the influence of environment is challenging due to its high-dimensional nature. Mixed quantumclassical methods [6-17] simplify the problem by treating the system quantum mechanically while approximating the environment classically, significantly reducing computational cost. However, these methods often struggle to capture detailed balance [18-20] or subtle quantum correlations [21]. Fully quantum approaches, including path-

integral [22-30] and quantum master equation-based methods [31-38], provide more accurate descriptions but are computationally expensive, particularly in regimes with strong system-environment coupling or where fine discretization is needed for numerical stability.

Recently, machine learning (ML) has emerged as a promising tool for learning complex spatiotemporal dynamics in high-dimensional systems [39-61]. One widely used ML strategy is the recursive approach, where the future evolution of a quantum state is predicted iteratively based on a short history of past evolution. This method has been successfully applied to the relaxation dynamics of the two-state spin-boson (SB) model [40,43,44,60], even enabling extrapolation beyond the trained time window [40]. However, previous applications have been limited to predicting a single observable—such as the population difference in the SB model—and have relied solely on singlestep prediction models.

In this work, we extend recursive ML approaches to more complex quantum systems, focusing on predicting the full RDM rather than just a single observable. We examine four physics-informed neural network (PINN)-based architectures: (i) the single-RDM-predicting PINN (SR-PINN), (ii) the SR-PINN with simulation parameters (PSR-PINN), (iii) the multi-RDMs-predicting PINN (MR-PINN), and (iv) the MR-PINN with simulation parameters (PMR-PINN). These architectures are tested on the relaxation dynamics of the SB model and the exciton energy transfer (EET) process in the Fenna-Matthews-Olson (FMO) complex.

From our results, we underscore the limitations of short-sighted, single-RDM-predicting models (SR-PINN and PSR-PINN) in capturing long-term system dynamics, especially in systems with intricate behavior. These models, constrained by a narrow history window, fail to predict long-term quantum evolution accurately, as they cannot fully capture the complexity of system evolution. In contrast, far-sighted models—such as MR-PINN and PMR-PINN—overcome these limitations by extending the forecast horizon, allowing them to incorporate long-range temporal correlations and achieve more stable predictions.

Although we initially anticipated that incorporating simulation parameters such as reorganization energy (λ), characteristic frequency (γ), and temperature (T) would improve accuracy, our findings show that these parameters do not consistently enhance performance and, in some instances, actually degrade it. This suggests that the relevant effects of these parameters are already implicitly encoded in the RDM evolution, making their explicit inclusion unnecessary in certain cases.

To build our case, let's consider an open quantum system (S), consisting of n states interacting with an external environment (E). As stated before, the dynamics of the system is governed by the RDM, which evolves non-unitarily due to environmental effects. While the full system follows unitary evolution described by the Liouville–von Neumann equation, tracing out the environmental degrees of freedom introduces a superoperator $\mathbf{R}$ that encodes dissipation and decoherence. Under the assumption that the initial state is separable between the system and environment ($\rho(0) = \rho_S(0) \otimes \rho_E(0)$), mathematically it can be described as

$$\begin{aligned}\rho_S(t) &= \mathbf{Tr}_E\left(\mathbf{U}(t,0)\,\rho(0)\,\mathbf{U}^{\dagger}(t,0)\right)\\ &= -i\,[\mathbf{H}_S, \rho_S(t)] + \mathbf{R}[\rho_S(t)],\end{aligned} \tag{1}$$

where $\rho_S(t)$ is the RDM of the system at time t, $\mathbf{Tr}_E$ denotes the partial trace over the environment, $\mathbf{R}$ is a superoperator that encodes the effects of the environment and $\mathbf{U}(t, 0)$ and $\mathbf{U}^{\dagger}(t, 0)$ are the forward and backward time-evolution operators, respectively.

In the recursive ML framework, modeling the time evolution of Eq. (1) is formulated as learning a mapping function $\mathcal{M}$ that maps the input descriptors into predicted RDMs. In general, we have

$$\mathcal{M}: \{\mathbb{R}^{n\times n}\}^{k'} \rightarrow \{\mathbb{R}^{n\times n}\}^{l}, \tag{2}$$

where $\{\mathbb{R}^{n\times n}\}^{k'}$ is a collection of k' input matrices (of size $n \times n$) that encode physical information such as historical RDM data, initial conditions, and simulation parameters, and $\{\mathbb{R}^{n\times n}\}^{l}$ is a sequence of l predicted RDMs corresponding to different time steps. In our study, we consider four distinct approaches for predicting the time evolution of RDM:

The *SR-PINN approach*: This method predicts the RDM at the next time step based solely on a fixed-length history of past RDMs. The recursive mapping function is defined as

$$\mathcal{M}_{\text{rec}}: \{\mathbb{R}^{n\times n}\}^{k'} \rightarrow \mathbb{R}^{n\times n}, \tag{3}$$

with

$$\mathcal{M}_{\text{rec}}[\rho_S(t_{k-k'+1}), \rho_S(t_{k-k'+2}), \ldots, \rho_S(t_k) = \rho_S(t_{k+1}). \tag{4}$$

The procedure is applied iteratively: after predicting $\rho_S(t_{k+1})$, this new RDM is appended to the history while the oldest entry is removed, keeping the memory size constant at k'.

The *PSR-PINN approach*: To improve prediction accuracy, additional simulation parameters $\mathbf{p}$ (e.g., system–environment coupling, characteristic frequency, temperature) are incorporated into the input. The mapping function becomes

$$\mathcal{M}_{\text{rec}}: \mathbb{R}^{p} \times \{\mathbb{R}^{n\times n}\}^{k'} \rightarrow \mathbb{R}^{n\times n}, \tag{5}$$

such that

$$\mathcal{M}_{\text{rec}}\left[\mathbf{p}, [\rho_S(t_{k-k'+1}), \ldots, \rho_S(t_k)]\right] = \rho_S(t_{k+1}). \tag{6}$$

As with the standard SR-PINN, the process is applied recursively with a fixed history length.

The MR-PINN approach: Rather than predicting a single RDM at a time, the MR-PINN approach forecasts a block of future RDMs in one step. Its mapping function is defined by

$$\mathcal{M}_{\text{rec}}: \{\mathbb{R}^{n\times n}\}^{k'} \rightarrow \{\mathbb{R}^{n\times n}\}^{N_f}, \tag{7}$$

with

$$\begin{aligned}&\mathcal{M}_{\text{rec}}[\rho_S(t_{k-k'+1}), \ldots, \rho_S(t_k)]\\ &= [\rho_S(t_{k+1}), \rho_S(t_{k+2}), \ldots, \rho_S(t_{k+N_f})].\end{aligned} \tag{8}$$

In this case, the model outputs N_f future RDMs simultaneously, thus providing a multi-step prediction without requiring iterative updating.

The PMR-PINN approach: This variant extends the MRPINN method by including simulation parameters in the prediction. The mapping is defined as

$$\mathcal{M}_{\text{rec}}: \mathbb{R}^{p} \times \{\mathbb{R}^{n\times n}\}^{k'} \rightarrow \{\mathbb{R}^{n\times n}\}^{N_f}, \tag{9}$$

so that