Supporting Information for "Physics-Informed Neural Networks and Beyond: Enforcing Physical Constraints in Quantum Dissipative Dynamics"

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Table S1. Mean Absolute Error (MAE) averaged over time steps from 0.8 to 1 ps for the diagonal elements $\tilde{\boldsymbol{\rho}}_{\mathrm{S_{nn}}}$ in the FMO complex, considering different memory times, denoted as t_m. In the table, n represents the state site number, and Avg(n) denotes the average MAE across all sites. Additionally, the MAE for trace is calculated and averaged over all time steps within the same time interval (0.8 to 1 ps). We used unconstrained NNs where all the models had nearly identical validation mean square error (loss), approximately 1.0×10^{-7}.

	Average MAE for each site n								MAE for Trace
n	1	2	3	4	5	6	7	Avg(n)	
$t_m = 0.2$ ps	1.50e-3	1.0e-1	1.30e-1	1.05e-1	9.42e-2	3.10e-2	1.22e-2	6.80e-2	7.31e-4
$t_m = 0.4$ ps	9.77e-3	2.15e-3	1.12e-2	1.96e-3	1.23e-3	1.92e-3	9.44e-4	4.18e-3	2.79e-3
$t_m = 0.6$ ps	8.10e-4	5.01e-3	1.19e-3	5.46e-4	1.35e-3	1.48e-3	1.46e-3	1.16e-3	1.17e-3
$t_m = 0.8$ ps	3.27e-3	2.92e-3	2.49e-3	1.34e-3	2.59e-4	6.04e-4	5.75e-4	1.63e-3	9.10e-4

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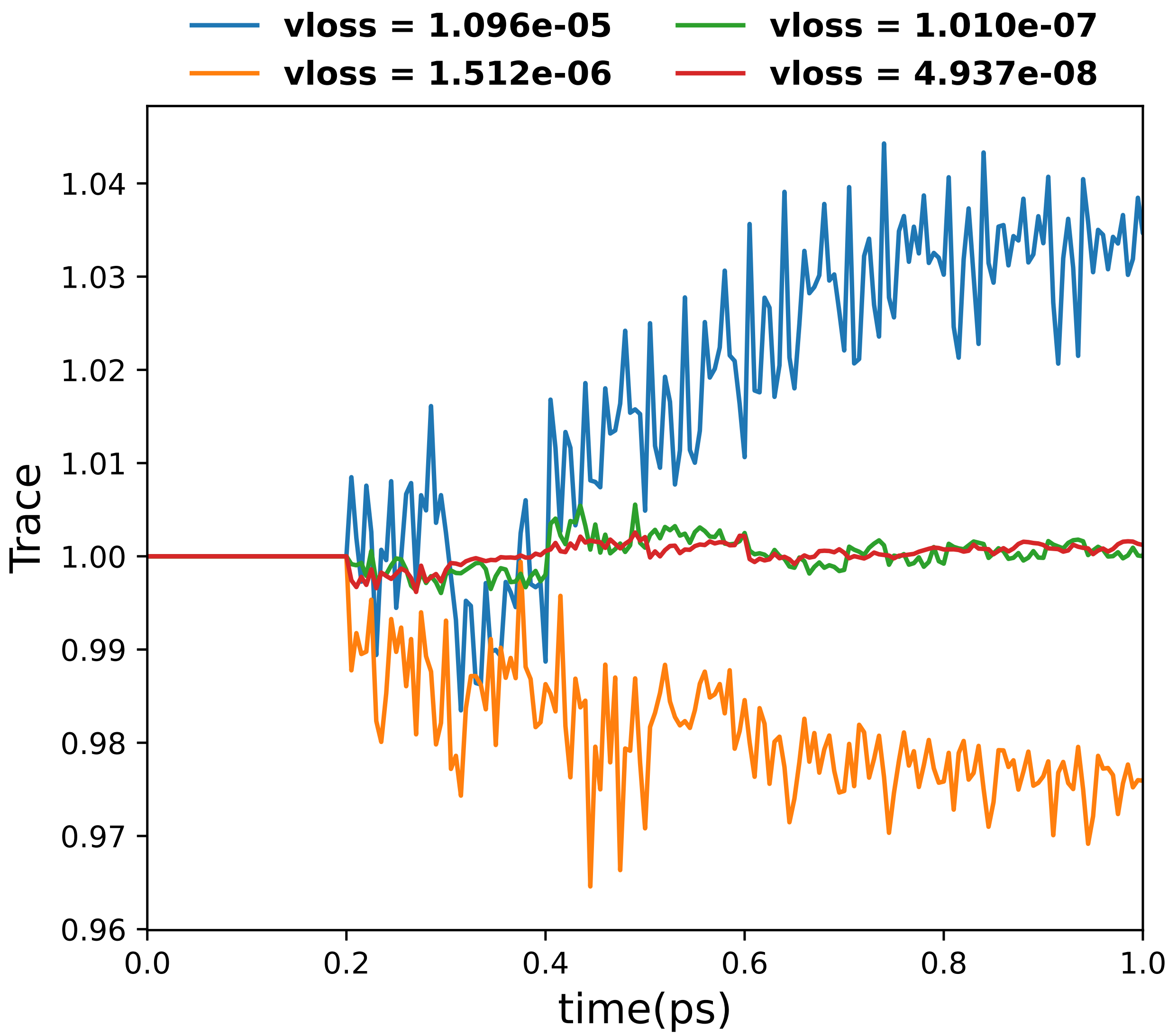

Figure S1. Comparison of trace conservation for unconstrained NN with varying validation loss (vloss). The considered system is the 7-site FMO complex, where an initial dynamics of 0.2 ps, exhibiting ideal trace conservation, is used as the seed for model predictions based on reference calculations. The initial excitation is located on site-1, with parameters $\gamma = 400$ cm^{-1}, $\lambda = 40$ cm^{-1}, and temperature $T = 90$ K. Further details on training and prediction are provided in the Results and Discussion section of the main text.

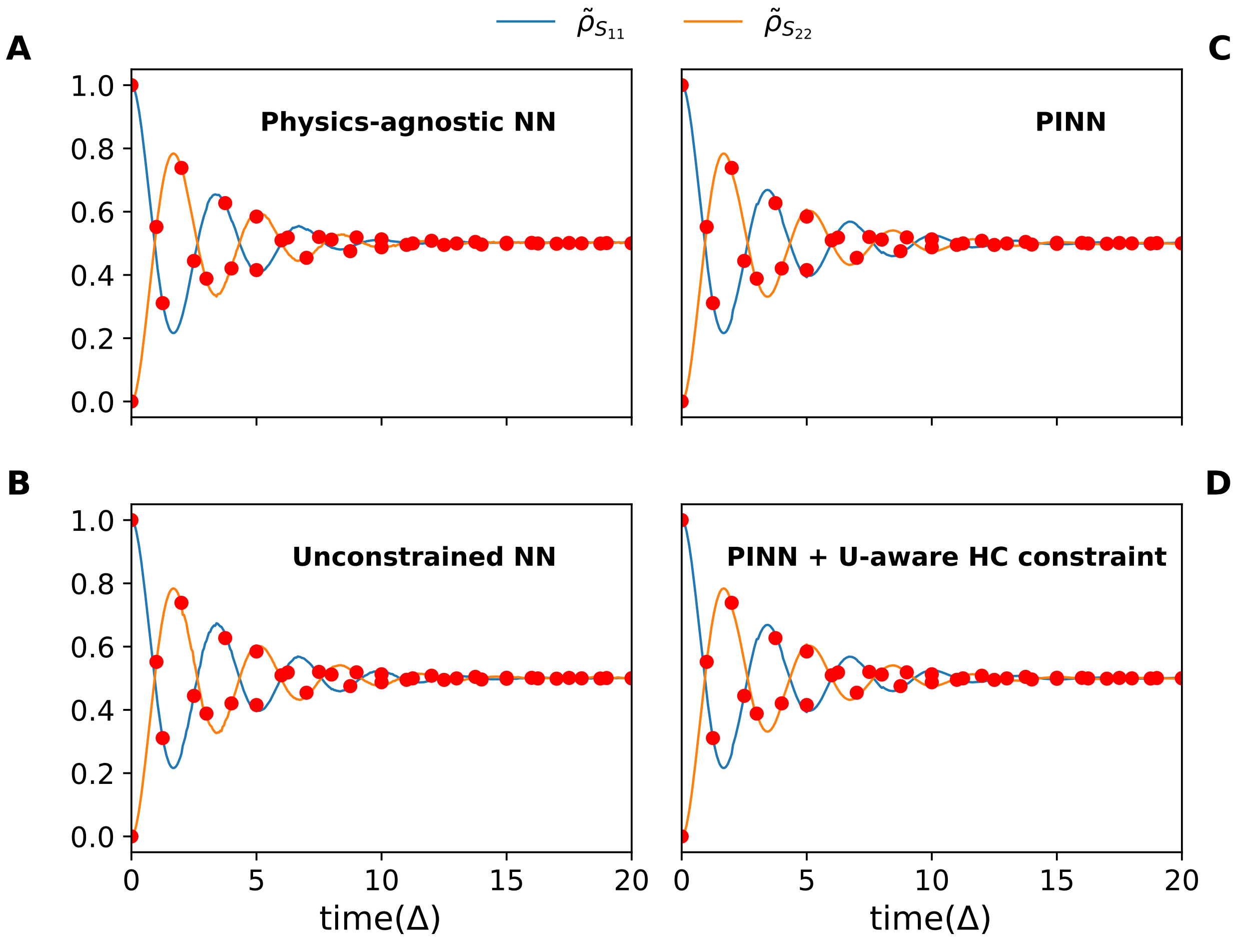

Figure S2. Population dynamics of the two states in the symmetric SB model as a function of time. Results are presented for an unseen trajectory with $\gamma/\Delta = 9.0$, $\lambda/\Delta = 0.6$, and $\beta\Delta = 1.0$. A short HEOM dynamics with a time length of $t_m\Delta = 2.0$ was used as a seed and recursive dynamics was propagated with 20 time steps in one shot. The results are compared with HEOM results (dots).

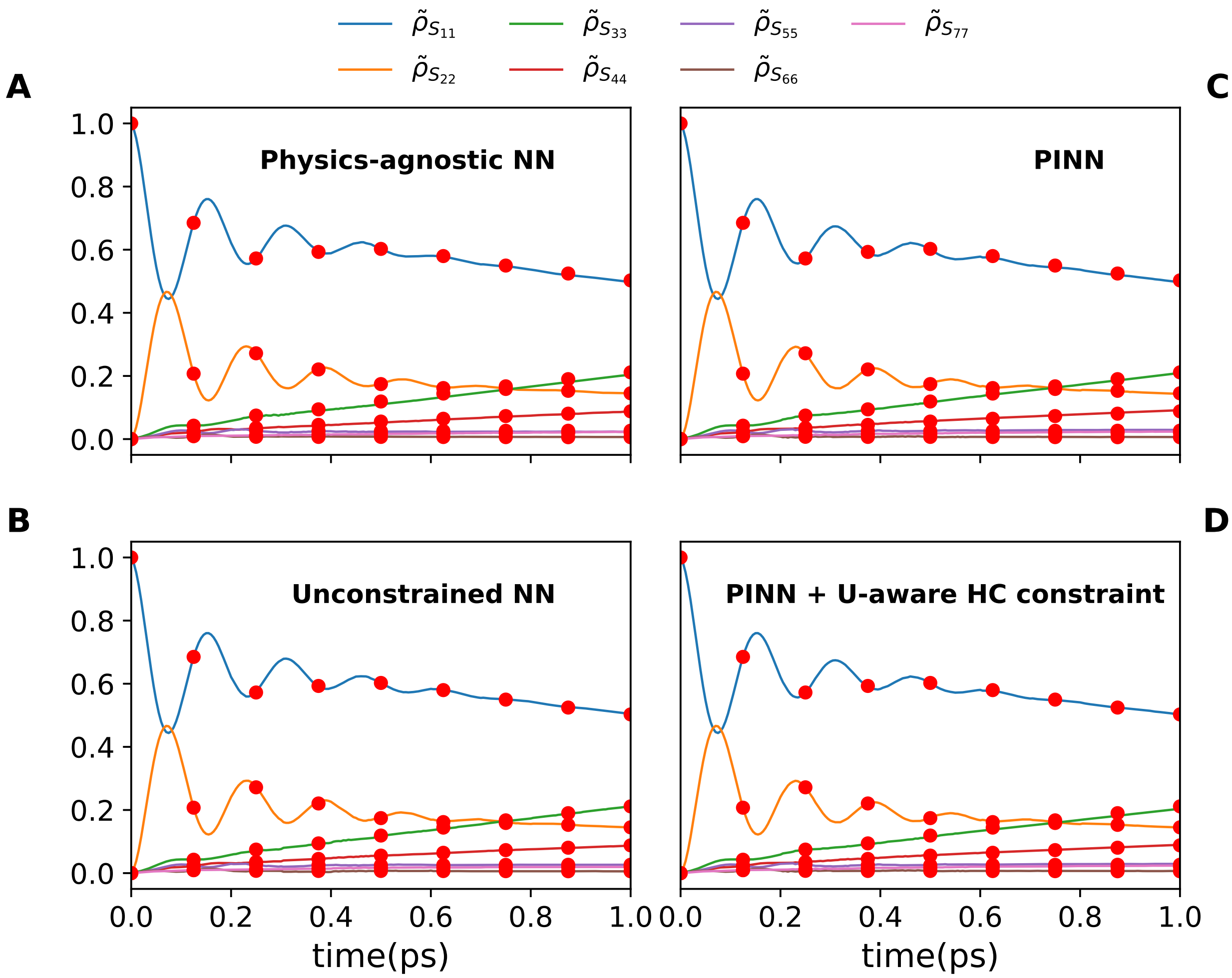

Figure S3. Excitation energy transfer in the 7-site FMO complex as a function of time. Results are presented for an unseen trajectory with $\gamma = 400.0\ \mathrm{cm}^{-1}$, $\lambda = 40.0\ \mathrm{cm}^{-1}$, and $T = 90.0$ K. A short LTLME dynamics with a time length of $t_m\Delta = 0.2$ ps was used as a seed and recursive dynamics was propagated with 20 time steps in one shot. The results are compared with LTLME results (dots).