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Machine-learning-corrected quantum dynamics calculations JUN DAI, University of British Columbia, A. JASINSKI, J. MONTANER, R. C. FORREY, Penn State University, B. H. YANG, P. C. STANCIL, University of Georgia, N. BALAKRISHNAN, University of Nevada, R. A. VARGAS-HERNNDEZ, R .V. KREMS, University of British Columbia — Quantum scattering calculations must generally rely on approximations. All approximations introduce errors. The impact of these errors is often difficult to assess because they depend on the Hamiltonian parameters and the particular observable under study. In this work, we illustrate a general, system and approximation-independent, approach to improve the accuracy of quantum dynamics approximations. The method is based on a Bayesian machine learning (BML) algorithm that is trained by a small number of rigorous results and a large number of approximate calculations, resulting in ML models that accurately capture the dependence of the dynamics results on the quantum dynamics parameters. Most importantly, the present work demonstrates that the BML models can generalize quantum results to different dynamical processes. Thus, a ML model trained by a combination of approximate and rigorous results for a certain inelastic transition can make accurate predictions for different transitions without rigorous calculations. This opens the possibility of improving the accuracy of approximate calculations for quantum transitions that are out of reach of rigorous scattering calculations.

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