Hamiltonian learning nanoscale quantum magnets and multiorbital excitations with setpoint-dependent scanning tunneling spectroscopy

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Atomic-scale quantum many body systems provide a versatile platform to explore the emergence of quantum excitations in many-body systems. Here, we establish Hamiltonian learning strategies [1,2] to extract many-body Hamiltonians directly from scanning tunnel spectroscopy, applicable both to nanoscale quantum magnets and complex nanoscale multiorbital many-body excitations. First [1], we demonstrate this methodology experimentally with an artificial triplon quantum magnet based on cobalt phthalocyanine (CoPC) molecules on NbSe2. We show that this technique allows us to extract the Hamiltonian parameters of a quantum magnet from the differential conductance, including the substrate-induced spatial variation of the exchange couplings. Second [2], we introduce a molecular Hamiltonian learning strategy that infers the microscopic Hamiltonian parameters of a single adsorbed molecule directly from the setpoint-dependence of STM-IETS data. The method leverages the systematic evolution of spectral features as the STM tip tunes the local electrostatic environment for different tip-sample distances. We demonstrate this approach on iron phthalocyanine (FePC) on ferroelectric SnTe, training our algorithm on theory spectra from a realistic multiorbital model, including spin-orbit coupling, electrostatic interactions, local crystal field, and substrate effects. The algorithm, trained solely on theoretical many-body simulations, allows for reconstructing Hamiltonian parameters directly from experimental spectra. Our results establish setpoint-dependent spectroscopy as a flexible strategy for Hamiltonian learning in nanoscale quantum materials.[1] Rouven Koch, Robert Drost, Peter Liljeroth, and Jose L. Lado, Nano Letters, 25, 36, 13435–13440 (2025) [2] Greta Lupi, Adolfo O. Fumega, Mohammad Amini, Robert Drost, Peter Liljeroth, Jose L. Lado, arXiv:2601.19371 (2026)