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THESIS DEFENSE: Quantum many-body physics with ultracold atoms and molecules: exact dynamics and machine learning

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Quantum many-body physics poses a substantial computational challenge resulting from the exponential growth of the wave function complexity and many non-trivial correlations encoded in it. Studying many-body systems is thus a demanding quest that is being tackled via various methods. The research described within this thesis concerns
two parallel approaches that are gaining the attention of the scientific community: quantum simulations with ultracold molecules and interpretable machine learning.
The first research path is a detailed analysis of the ultracold system of two interacting molecules in a one-dimensional trap. By comparing with the two-atom system in a harmonic

trap, we identify differences in spectra and reactions to the external fields introduced by the molecular character of the system, i.e., rotational levels, anisotropic shortrange interactions, and stronger dipolar interactions. Exactly these richer properties of molecules could allow for discovering new exotic phases of matter and simulating phenomena that are inaccessible for the physics of ultracold atoms. Inspired by materials with both electric and magnetic orders, in the next step, we focus on the interplay of the electric and magnetic properties of the two-body molecular system, analyze magnetization diagrams, and study the quench dynamics.

Alternatively, quantum many-body problems can be solved via numerical methods. Among them, machine learning algorithms are gaining significant momentum. However, so far, they have mostly enabled only the recovery of known results (but at much lower computational cost). Moreover, we usually lack the understanding of how the machine solves the problem at hand. Therefore, we propose a way to combine the efficiency of neural networks with Hessian-based interpretability and reliability methods like influence functions. In principle, these universal and model-independent tools allow to unravel the logic hidden in the machine and thus increase the chance to understand the physics of the problem. We show their power on the fundamental one-dimensional Fermi-Hubbard model and on the experimental data obtained from the Floquet realization of the topological two-dimensional Haldane model.

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