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Nicholas Metropolis Award for Outstanding Doctoral Thesis Work in Computational Physics: Quantum many-body physics of ultracold molecules in optical lattices: models and simulation methods

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Experimental progress in generating and manipulating synthetic quantum systems, such as ultracold atoms and molecules in optical lattices, has revolutionized our understanding of quantum many-body phenomena and posed new challenges for modern numerical techniques. Ultracold molecules, in particular, feature long-range dipole-dipole interactions and a complex and selectively accessible internal structure of rotational and hyperfine states, leading to many-body models with long range interactions and many internal degrees of freedom. Additionally, the many-body physics of ultracold molecules is often probed far from equilibrium, and so algorithms which simulate quantum many-body dynamics are essential. Numerical methods which are to have significant impact in the design and understanding of such synthetic quantum materials must be able to adapt to a variety of different interactions, physical degrees of freedom, and out-of-equilibrium dynamical protocols. Matrix product state (MPS)-based methods, such as the density-matrix renormalization group (DMRG), have become the de facto standard for strongly interacting low-dimensional systems. Moreover, the flexibility of MPS-based methods makes them ideally suited both to generic, open source implementation as well as to studies of the quantum many-body dynamics of ultracold molecules. After introducing MPSs and variational algorithms using MPSs generally, I will discuss my own research using MPSs for many-body dynamics of long-range interacting systems. In addition, I will describe two open source implementations of MPS-based algorithms in which I was involved, as well as educational materials designed to help undergraduates and graduates perform research in computational quantum many-body physics using a variety of numerical methods including exact diagonalization and static and dynamic variational MPS methods. Finally, I will mention present research on ultracold molecules in optical lattices, such as the exploration of many-body physics with polyatomic molecules, and the next generation of open source matrix product state codes. This work was performed in the research group of Prof. Lincoln D. Carr.