SFB/TRR 21 - Seminar
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Ultracold Molecules in Crystals of Light: A Highly Tunable System for Exploring Novel Materials and Quantum Physics

Ultracold molecules at sub-microKelvin temperatures and trapped in crystals of light (optical lattices) present a new regime of physical chemistry and a new state of matter: complex dipolar matter. We present models for the quantum many-body statics and dynamics of present experiments on polar bi-alkali dimer molecules. We are developing and will discuss Hamiltonians and simulations for upcoming experiments on dimers beyond the alkali metals, including biologically and chemically important naturally occurring free radicals like the hydroxyl free radical (OH), as well as symmetric top polyatomic molecules like methyl fluoride (CH_3F). These systems offer surprising opportunities in modeling and design of new materials, in addition to well-known exciting possibilities in quantum computing applications. For example, symmetric top polyatomics can be used to study quantum molecular magnets and quantum liquid crystals. Our numerical method of choice is massively parallel high performance computing via variational matrix-product-state (MPS) algorithms, a highly successful form of data compression used to treat lowly entangled dynamics and statics of many-body systems with large Hilbert spaces; we supplement our calculations with exact diagonalization and simpler variational, perturbative, and other approaches. We use MPS algorithms not only to produce experimentally measurable quantum phase diagrams but also to explore the dynamical interplay between internal and external degrees of freedom inherent in complex dipolar matter. Our group maintains open source code (openTEBD and openMPS) available freely and used widely. We have worked and will continue to work closely with experimentalists throughout our projects, and make detailed use of ultracold molecular properties and constants to provide concrete and accurate explanations, guidance, and inspiration.

[1] Kenji Maeda, M. L. Wall, and L. D. Carr, ``Hyperfine structure of OH molecule in electric and magnetic fields,'' New J. Phys., to be submitted (2014)
[2] M. L. Wall, Kenji Maeda, and L. D. Carr, ``Realizing topological states with polyatomic symmetric top molecules,'' Phys. Rev. Lett., under review, arXiv:1402.0465 (2014)
[3] M. L. Wall, Kenji Maeda, and L. D. Carr, ``Simulating quantum magnets with symmetric top molecules,'' Ann. Phys. (Berlin) 525, 845 (2013)
[4] M. L. Wall, E. Bekaroglu and L. D. Carr, ``The Molecular Hubbard Hamiltonian: Field Regimes and Molecular Species,'' Phys. Rev. A, 88, 023605 (2013)
[5] M. L. Wall and Lincoln D. Carr, ``Out of equilibrium dynamics with Matrix Product States,'' New J. Phys. 14, 125015 (2012)
[6] L. D. Carr, David DeMille, Roman V. Krems, and Jun Ye, ``Cold and Ultracold Molecules: Science, Technology, and Applications,'' New J. Phys. 11, 055049 (2009)

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