Quantum Monte Carlo for Molecular Dipole Moments

Dr. Peter Reynolds
Physics Directorate, Army Research Office

Date: Friday, Oct 12, 2018
Time: 1100
Location: Spanagel Hall, Room 117

Abstract

I will describe how the advent of laser cooling and trapping of atoms and ions progressed to the achievement of quantum degeneracy in ultra-dilute atomic gases, and then to their trapping in optical lattices. These incredibly dilute gasses can be used in a variety of unexpected ways, from altering chemical reaction dynamics, to serving as concept atomtronic devices (generalizing electronics with the many additional degrees of freedom afforded by atoms), to the creation of physical embodiments of model Hamiltonians. The latter is an intriguing way to "solve" numerically intractable models such as the Fermi Hubbard model, believed to be at the heart of high-temperature superconductivity. Trapping molecules in optical lattices opens even more opportunities. Competing phases are expected to be realized with the introduction of long-ranged dipolar interactions. As the strength of the dipole moment is a key parameter in this competition, it is necessary to know it for the molecules that might be cooled and trapped in future optical lattice experiments. To that end, we have computed the dipole moment for some specific molecules of interest to the community because they are candidates in such experiments. One in particular, LiSr, is extremely weakly bound and has never been made, yet has desirable properties of coupling by both electric and magnetic interactions. Traditional methods of computing the binding energy and the dipole moment converge very poorly for this molecule. We therefore employ a Quantum Monte Carlo approach, which is considered the gold standard for accuracy. This approach will be described, and our results will be presented.

Biography

Dr. Peter Reynolds is the Senior Research Scientist and Chief Scientist for the Physical Sciences at the Army Research Office (ARO). Dr. Reynolds received his PhD in Physics from MIT where he did research in statistical mechanics, particularly critical phenomena and phase transitions in disordered lattice models. After receiving his PhD at MIT, he accepted a position as an assistant research professor at Boston University, and subsequently served as a staff scientist at Lawrence Berkeley Laboratory. After almost 8 years at Berkeley, he accepted a position at the Office of Naval Research (ONR) as a Program Manager in Atomic and Molecular Physics, and continued his own research in continuum quantum Monte Carlo methods. He joined ARO in 2003, and has served as the Associate Director for Physical Sciences and Division Chief of Physics prior to being appointed to the Senior Research Scientist position. His career at DoD spans 30 years during which he has been involved in selecting and managing a large portfolio of research. Currently he also coordinates the Discovery Essential Research Area (ERA) within the Army Research Lab, which includes identifying, creating, developing and exploiting innovative new scientific discoveries for the Army, including exploiting the "2nd Quantum revolution" for new and leap-ahead capabilities across a variety of domains.