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Quantum Monte Carlo simulations of bosons with complex interactions[1]

VALERY ROUSSEAU, Louisiana State University

Many of the most exciting materials and phenomena being studied today, from oxide heterostructures to topological insulators or iron-based superconductors, are the ones in which an understanding of how quantum particles interact with each other is essential. In the last decade, the development and the improvement of quantum Monte Carlo algorithms combined with the increased power of computers has opened the way to the exact simulation of Hamiltonians that include various types of interactions, such as inter-species conversion terms or ring-exchange terms. Simultaneously, developments made in the field of optical lattices, laser cooling and magneto/optical trapping techniques have led to ideal realizations of such Hamiltonians. A wide variety of phases can be present, including Mott insulators and superfluids, as well as more exotic phases such as Haldane insulators, supersolids, counter-superfluids, or the recently proposed Feshbach insulator. These experimental realizations of the various forms of the Hubbard model can have interesting applications, in particular they provide a possible way of performing quantum computing, and have also given rise to a new field known as Atomtronics, the equivalent of Electronics where the carriers are replaced by atoms. I will illustrate these ideas with examples of Hamiltonians that have been studied and some results. In order to study these systems, it is crucial to identify the various phases that are present, which can be characterized by a set of order parameters. Of particular importance in this task is the superfluid density. It is well known that the superfluid density can be related to the response of the free energy to a boundary phase twist, or to the fluctuations of the winding number. However, these relationships break down when complex interactions are involved. To address this problem, I will propose a general expression of the superfluid density, derived from real and thought experiments. I will discuss two interesting applications of my method to the SF transition of softcore bosons with 2nd neighbor hopping and to atom-molecule mixtures.

Reference: "Superfluid density in continuous and discrete spaces: Avoiding misconceptions," Phys. Rev. B 90, 134503 (2014)

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