Simulations of Atomic Gases on Frustrated Optical Lattices

Stefan Wessel *

Institute for Theoretical Physics III, University of Stuttgart, Germany

Abstract

We present results form quantum Monte Carlo simulations of ultra-cold bosonic atoms on frustrated optical lattices such as the triangular and the kagome lattice. For the triangular lattice case a supersolid state of matter emerges, resulting from a novel order-by-disorder effect in the quantum regime. On the kagome lattice no supersolid appears, instead the atoms form exotic valence-bond-solids with local bosonic resonances. The quantum melting of these solids into the superfluid takes place at weakly first-order quantum phase transitions. Relevant algorithmic improvements which allow for large-scale simulations of such systems are mentioned as well as possible experimental realizations of these scenarios based on current experimental advances in quantum optics.

Key words: ultra-cold atom-gases; optical lattices; lattice models; quantum Monte Carlo

Interest in the properties, phase transitions and various phases of strongly correlated systems has a very long history in condensed matter physics. The experimental realization of Bose-Einstein condensates (BEC) of ultra-cold bosonic atom gases [1] offered a novel possibility of studying such phenomena in precisely engineered systems. This goal was eventually achieved by placing the condensates on optical lattices [2,3] which allowed to access the strongly interacting regime. Strongly correlated systems on optical lattices have the advantage of being defect free and offer a high degree of control of the effective parameters describing these systems. Experimental studies so far focused on hyper-cubic lattice geometries in various dimensions, where the transition from a superfluid to a Mott-insulator was observed [2,3]. Here, we consider extensions of such studies for bosons on frustrated optical lattices, such as the triangular and the kagome lattice, where the interplay of classical frustration and quantum fluctuations provides an exciting means of stabilizing interesting quantum phases such as supersolid and valence-bond-solid (VBS) phases [4,5]. In particular, we consider strongly interacting bosons in the hard-core limit with an additional nearest-neighbor repulsion, described by the Hamiltonian

$$H = -t \sum_{\langle i,j \rangle} \left(a_i^\dagger a_j + a_j^\dagger a_i \right) + V \sum_{\langle i,j \rangle} n_i n_j - \mu \sum_i n_i,$$

where $a_i^\dagger$ (a_i) creates (destroys) a particle on site i, t denotes the nearest-neighbor hopping, V a nearest-neighbor repulsion, and μ the chemical potential that controls the filling of the lattice. Different proposals have been made, how bosonic systems with longer-ranged interactions can be realized in ultra-cold atom systems such as in dipolar gases [6], like BECs of Chromium atoms [7], or Bose-Fermi mixtures [8].

In our simulations, we employed the stochastic series expansion [9] quantum Monte Carlo (QMC) method with a directed loop update [10]. In order to reduce the effects of QMC freezing in the interaction dominated region, a decomposition of the Hamilto-

* Corresponding author.
Email address: wessel@theo3.physik.uni-stuttgart.de (Stefan Wessel).

nian based on triangular plaquettes instead of the conventional bond representation was used [11].

Considering first the case of a triangular lattice, we find that the interplay of classical frustration and quantum fluctuations stabilizes a supersolid state in a large parameter regime already in the hard-core limit, including the case of a half-filled lattice [4]. In such a supersolid state of matter, both the discrete lattice symmetry and the internal $U(1)$ symmetry are broken [12], in contrast to the case of a pure solid, where only the lattice symmetry is broken, and a BEC, where only the internal symmetry is broken. In the classical limit ($t = 0$), equivalent to the Ising model, two solid phases with densities $\rho = 1/3$ (and $\rho = 2/3$) exist, with one (two) out of the three sublattices being occupied [13], the other(s) being empty. Both solid phases extend into the phase diagram of the quantum model up to $t/V \approx 0.195$. At half-filling ($\rho = 1/2$), the classical model has an extensive ground state entropy [14]. This degeneracy is lifted by quantum fluctuations for $t > 0$, leading to a novel order-by-disorder effect with the emerging supersolid phase [4]. The supersolid extends beyond half-filling up to continuous quantum phase transition lines to the two solid phases. Doping these solids not towards, but away from half-filling leads to strong first-order quantum melting transitions into the large-t/V superfluid phase [4]. At these transitions a supersolid phase is rendered unstable by the proliferation of domain walls, that lower the kinetic energy of the system [15]. Our results are in good qualitative agreement with an earlier spin-wave calculation [16] and were confirmed by independed recent QMC simulations [17].

Spin-wave calculation [16] also predicted a supersolid phase of hard-core bosons on the kagome lattice. However, our QMC simulations did not confirm this prediction [5]. We obtained a phase diagram with a large-t/V superfluid phase and two low-t/V solid phases of densities $\rho = 1/3$ and $2/3$, respectively. These solids are however not fully rigid: E.g., for $\rho = 2/3$, one out of the three sublattices of the kagome lattice forms a solid backbone of occupied sites, whereas the remaining bosons locally resonate around every second hexagon in the kagome lattice, with three bosons per hexagon arranged in alternating patterns [5]. Such VBS phases were discussed recently in the context of quantum dimer models, valid for $t \ll V$ [18]. Here, we find such phases in a realistic, microscopic model, and also observed their quantum melting, which take place at very weakly first-order quantum phase transition. It will be exciting to observe such phases in future experiments with ultra-cold bosonic atoms on optical lattices.

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