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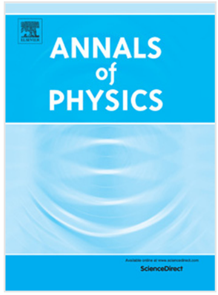

Checkerboard-supersolidity in a two-dimensional Bose-Holstein model

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Checkerboard-supersolidity in a two-dimensional Bose-Holstein model

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Abstract

Exploring supersolidity in naturally occurring and artificially designed systems has been and will continue to be an area of immense interest. Here we study the cooperation/competition of the superfluid and charge-density-wave (CDW) orders in a two-dimensional Bose-Holstein (BH) model where hard-core-bosons (HCBs) are coupled locally to optical phonons. In the parameter regimes of strong HCB-phonon coupling and nonadiabaticity, we find a novel mechanism for lattice-supersolidity (namely, sizeable same-sublattice tunneling in presence of large nearest-neighbor repulsion) in the system. The ground state phase diagram is obtained using Quantum Monte Carlo simulation involving stochastic-series-expansion technique. At densities not far from half filling and in the parameter regime where the double-hopping terms are non-negligible (negligible) compared to the nearest-neighbor hopping, we get checkerboard-supersolidity (phase separation) with CDW being characterized by ordering wavevector $\vec{Q} = (\pi, \pi)$.

Keywords: Supersolidity, Optical phonons, Hard-core bosons, Phase transition.

1. Introduction

Coexistence of diagonal long range orders [such as charge-density-wave (CDW) and spin-density-wave (SDW)] and off-diagonal long range orders [such as superconducting and superfluid (SF) states] in correlated electronic systems has long remained one of the central issues in condensed matter community. Lattice-supersolidity [1], which is the homogeneous coexistence of superconductivity/superfluidity and CDW realized in discrete lattices, has been observed in a number of three-dimensional [2, 3] (such as $BaBiO_3$ doped with K or Pb), quasi-two-dimensional [4, 5] (such as the dichalcogenide $2H - TaSe_2$ and $NbSe_2$; and layered molecular crystals) and quasi-one-dimensional systems [6, 7, 8] (such as the trichalcogenide $NbSe_3$ and doped spin ladder $Sr_{14}Cu_{24}O_{41}$). While phenomenological scenarios exist for understanding lattice-supersolidity [3, 9], a microscopic model that fully explains the coexistence-phenomena has been elusive.

Cold-atom systems in optical lattices provide opportunities for realizing supersolidity. Theoretically, lattice bosons with various types of interactions in diverse geometries have yielded supersolidity; a representative list of studies is given in Refs. [10, 11, 12, 13, 14, 15, 16, 17, 18, 19]. Recently, there has been an experimental creation of an optical lattice with effective long-range interactions that produced supersolidity [20]. In this experiment, the optical lattice is inside an optical cavity with infinite-range interaction beween atoms being mediated by a vacuum mode of the cavity.

There has been numerous studies of supersolidity involving hard-core-bosons (HCBs) [10, 11, 15, 16, 12, 13, 14]. Lattice models for quantum liquids as well as frustrated spin-half magnets involve HCBs [21, 22]. Local Cooper pairs can also be regarded as HCBs. Furthermore, in Bismuthates, such HCB-type Cooper pairs couple to the breathing mode of the oxygen cage surrounding the Bismuth ions [23, 24].

In this perspective, here we study the ground state properties of a two-dimensional (2D) Bose-Holstein (BH) model for HCBs on a square lattice. *The objective is to identify a mechanism of lattice-supersolidity that involves the ubiquitous particle-phonon interactions.* In contrast to a number of lattice models of the extended Bose-Hubbard type, the parameters (i.e., strength of HCB-phonon coupling, hopping term, and optical-phonon frequency) in our Bose-Holstein model either can be determined from experiments or can be obtained from band-structure calculations. In our model, the HCBs can hop to nearest-neighbor (NN) sites and experience the HCB-phonon interactions via a Holstein-type term.

Previously, exact diagonalization calculations were done on this model [25] for a small system (i.e., 4×4 lattice) to study the resulting phase diagram. Here we use stochastic-series-expansion (SSE) based quantum Monte Carlo (QMC) technique to simulate large-size lattices so that various phases in the thermodynamic limit can be identified more clearly. Unlike in the $t - V$ model, a checkerboard-SS is realized in our BH system due to the cooperative effect of non-negligible hopping within the same sublattice and large NN repulsion. At densities not far from half filling and at sufficiently large HCB-phonon couplings, phase coexistence occurs; furthermore, in the phase-coexistence region, the system tends to phase separate at stronger couplings.