Two-state hard-core Bose-Hubbard model: beyond the random phase approximation

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The present study is a continuation of our previous works [1,2] considering the Bose-Einstein (BE) condensation in the Bose-Hubbard model with two local states and the particle hopping in the excited band only. The system is analyzed in the hard-core boson limit. Such a model is used for description of ultracold atoms in optical lattices as well as the dynamics of protons on the metal surface.

It was shown that the order of the phase transition into the phase with the BE condensate can change from the second order to the first one (related to BE condensation of "holes", while the second order transition leads mainly to the "particle" BE condensation). At the fixed concentration of bosons the system can separate on the normal phase and the phase with the BE condensate. The non-ergodic contribution due to the particle momentum distribution (fluctuations) increases significantly and becomes comparable with the ergodic one in the superfluid phase near the tricritical point.

Here a unified description of both thermodynamic (phase diagrams) and dynamic (single-particle excitation spectrum, density of states and momentum distribution) characteristics of the system by means of the temperature Green's function approach is presented. The correction up to the one sum over wave vector for the grand canonical potential of the system is calculated which provides improved expressions for occupations of states. Related changes of the system behaviour are analyzed and compared with the previous results.

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