Thermodynamics and dynamics of the two-state Bose-Hubbard model in the effective pseudospin representation

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Phase transition into the phase with the Bose-Einstein (BE) condensate in the Bose-Hubbard model with two local states and the particle hopping in the excited band only is investigated. Instability connected with such a transition (appearing at excitation energies δ less than the particle hopping parameter $|t'_0|$) is considered. The re-entrant behaviour of spinodales is revealed in the region of positive values of chemical potential in the hard-core boson (HCB) limit (no more than one particle per site regardless of state – excited or ground – which it occupies). Contrary to the two-level ordinary HCB case, where particles are described by the Pauli statistics, our single-site problem is a three-level one. The effective pseudospin representation is used, where operators σ_i^α are quite similar to spin operators for $S = 1/2$ but the anticommutator of σ_i^+ and σ_i^- is equal to the total occupation of respective states instead of unity.

It is found that the order of the phase transition can change in the case $\mu > 0$ becoming the first one. First order phase transitions also exist at negative values of δ (under the condition $\delta > \delta_{\text{crit}} \approx -0.12|t'_0|$). At $\mu < 0$ the phase transition mostly remains to be of the second order. The behaviour of the BE condensate order parameter is analyzed, the (Θ, μ) and $(|t'_0|, \mu)$ phase diagrams are built and localization of tricritical points is established. A possibility of separation on the normal phase and the phase with the BE condensate at the fixed average concentration of bosons is demonstrated.

The boson Green function and the single-particle spectral density are calculated in the random phase approximation. The excitation spectrum of the "hole" type at concentrations $n \leqslant 1$ or the "particle" type at $n \geqslant 0$ has a band structure. Its reconstruction (gap disappearance and the change from the quadratic dispersion law to the linear one at $\vec{q} \sim 0$) at the first order phase transition is jump-like with a simultaneous appearance of the negative component in the spectral density.