

Bose-Fermi-Hubbard model in the truncated Hilbert space limit

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We investigate the phase transitions in the Bose-Fermi-Hubbard model proposed for description of thermodynamics and energy spectrum of the ultracold mixtures of Bose- and Fermi-atoms in optical lattices. The study of the fermion subsystem influence on the phase transition (PT) from the normal (Mott insulator, MI) phase to the superfluid (SF) one with the Bose-Einstein condensate is our main task. Consideration is performed for the case of infinitely small fermion transfer in the limit of truncated basis of the single-site states of bosons ($n_i \leq 1$ for hard-core bosons, and $n_i \leq 2$). The boson-fermion interaction U' is taken into account exactly while the hopping t_0 of bosons is considered within the mean-field approximation.

The regime of fixed values of chemical potentials (μ and μ' , respectively) of Bose- and Fermi-particles is the basic one in our study. Analyzing the behavior of the BE condensate order parameter and the grand canonical potential, we have built the (μ, μ') , (μ, t_0) and (μ, T) phase diagrams at $T = 0$ and at the nonzero temperatures. It is shown: i) in the cases when transition to the SF phase is accompanied by the change of mean number of fermions, the PT order changes from the 2nd to the 1st one; this result corresponds to the literature data (DMRG calculations for harmonic trap); ii) at non-zero temperatures, the re-entrant transitions (when the SF phase is an intermediate one) can exist; iii) there are two types of SF phase that differ by fermion concentration; iiiii) the shape of the MI phase regions (so-called lobes) in the (μ, t_0) diagrams and the localization of the 1st order PT segments on them depend on the μ' level position.

Using the fermion-hole transformation, a correspondence between cases of the B-F on-site repulsion and attraction is established. Based on the phase diagrams, built within the framework of the grand canonical ensemble, the conditions of the SF phase existence at $U' > 0$ and $U' < 0$ are analyzed. The diagrams (U', t_0) , that illustrate the difference of behaviour of the BF mixture in these cases, are obtained. A relation to available experiments data is discussed.