Phase diagrams of Bose-Hubbard model

I.V. Stasyuk and T.S. Mysakovych

Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine, 1 Svientsitskii Str., 79011 Lviv, Ukraine, E–mail: ista@icmp.lviv.ua

The phase transitions in the many-state Bose-Hubbard model are investigated. The interest to this model greatly increased in last years due to the experimental realization of the optical lattices. This model can also be applied for the description of ionic conductivity and intercalation in crystals as well as kinetics of ionic adsorption on the crystal surfaces.

Single-particle Green's function is calculated in random phase approximation (which is an analog of Hubbard-I approximation for the case of fermionic Hubbard model) and the formalism of Hubbard operators is used. Single-particle excitations in the Mott insulator phase are studied (the existence of the energy gap at $\vec{k}=0$ which vanishes at ctitical point is a feature of this phase, reflecting the localized character of atoms) for the case when the interaction between three nearest bands is taken into account.

The regions of existence of superfluid and Mott insulator phases are established and phase diagrams in the plane (μ, t) (the chemical potential-transfer parameter) are built. The influence of temperature change on this transition is analysed and the phase diagram in the (T, μ) plane is calculated. The role of thermal activation of ion hopping is investigated by taking into account the temperature dependence of transfer parameter. The reconstruction of Mott-insulator lobes due to this effect is analysed.