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Mott-insulator shells in the three-dimensional Bose-Hubbard model with harmonic confinement MAKOTO YAMASHITA, NTT Basic Research Laboratories — Ultracold atomic gases in optical lattices provide the ideal stages for investigating the fundamental many-body problems in condensed-matter physics. Recently, the superfluid-Mott insulator (MI) transition of a Bose-Einstein condensate in a three-dimensional optical lattice was precisely measured by using a two-photon spectroscopy. It has been found that, in the strong interaction regime, the number of atoms at the lattice sites takes the integer values raging from one to five and its spatial distribution forms the shell structure, namely MI shells. To quantitatively understand these experimental results, we numerically study the ground-state properties of the three-dimensional (3D) Bose-Hubbard model with harmonic confinement. We have developed the highly efficient numerical method based on the Gutzwiller approximation, which can be applied to a large system consisting of more than one million of lattice sites. The MI shells observed in the experiments are successfully reproduced by the calculations using the appropriate parameters. We show the systematic analyses of the 3D Bose-Hubbard model and compare them with the recent experimental results.

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