Investigation of the Bose-Hubbard model using dynamical mean-field theory

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Understanding the effects of strong-correlations in many-body systems is one of the major goals of the modern condensed matter physics. To achieve this goal physicists develop simplified models that capture the essence of strong-correlations. An example is the Bose-Hubbard model. While it does capture strong-interaction effects and has a simple form, it is still difficult to solve. This model also describes the experiments with cold atoms in optical lattices. Parallelly more accurate approximation schemes are searched for. A very successful one is the dynamical mean-field theory (DMFT) and its bosonic counterpart, the bosonic dynamical mean-field theory (B-DMFT). Owing to its unusual expansion scheme in renormalized perturbation theory it provides better and more accurate results, in particular, where other methods are no longer reliable.

In this Thesis we present our investigation of the Bose-Hubbard model within the B-DMFT. Firstly we focus on both the derivation of the model and the method to solve it. We provide the basic theories standing behind each. We also present technical details of the continuous-time quantum Monte Carlo algorithm - a very successful method for solving the impurity problem associated with the B-DMFT. The self-written and tested Fortran 90/95 program based on that algorithm has been used to obtain the physical results in this Thesis. Next we focus on results obtained within the B-DMFT for the Bose-Hubbard model on a cubic lattice. We present results for both the static properties and the spectral functions. These are obtained for all ranges of interaction strength, from weak through intermediate to strong regimes. We compare the performance of the B-DMFT with other methods, mainly the static mean-field theory. While in the limiting cases the agreement is good, as expected, for intermediate interaction strength the B-DMFT provides some quantitative and qualitative corrections. We also study the Bose-Hubbard model on a square lattice with an additional infinite-range interaction. We present results for the static properties of the model. We compare the performance of the B-DMFT method with that of the static mean-field theory. Both similarities and differences are found and discussed. We also provide a first thorough study of the spectral functions of the model.