Dimensional Crossover of the Phase Diagram within a Layered Bose-Hubbard System

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Abstract

We study the Bose-Hubbard model with a varying number of coupled two dimensional layers, and present the corresponding crossover from two to three dimensions exhibited by its phase diagram. In addition, we shortly introduce the method utilized, called process-chain approach.

Model

The pure Bose-Hubbard model describing Bose particles on a lattice which are allowed to tunnel between neighboring lattice sites with **tunneling strength** J, while repelling each other when occupying the same site with **interaction energy** U has the grand-canonical Hamiltonian

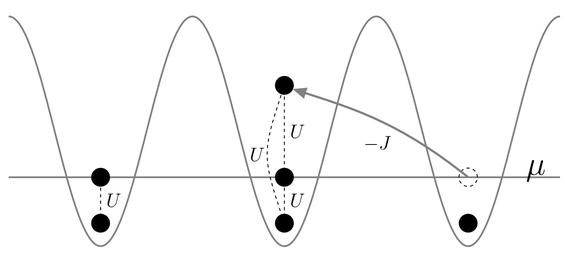

Fig. 1: Schematic display of the Bose-Hubbard model

$$\widehat{H}_{\mathrm{BH}} = \frac{1}{2}\sum_i \left(\hat{n}_i\left(\hat{n}_i - 1\right) - \mu/U\,\hat{n}_i\right) - J/U \sum_{\langle i,j\rangle} \hat{b}_i^\dagger\,\hat{b}_j. \tag{1}$$

The Hamiltonian cannot be solved analytically, but for the limits of vanishing and diverging tunneling strength one can obtain the following results:

- for $J/U \to 0$: the Bose particles are localized at lattice sites and the first excited state is separated from the ground state by a finite energy gap (**Mott insulator**)
- for $J/U \to \infty$: every Bose particle is homogeneously distributed over the lattice occupying the same state (**BEC, superfluid**)

Varying the ratio J/U leads to a critical value $(J/U)_c$ at which the energy gap between ground state and first excited state closes and the system exhibits a **quantum phase transition** from Mott insulator to superfluid.
In this work the **phase diagram**, i.e. the dependency of $(J/U)_c$ on the chemical potential μ/U, is studied in general, and in particular the differences between two and three dimensions. To this intent, systems with multiple two dimensional Bose-Hubbard layers allowing tunneling between neighboring layers as described by (1) are examined.

Methods

In order to calculate the critical value $(J/U)_c$ the system's response to the attempt of coupling particles into or out of the lattice through spatially homogeneous sources and drains, as expressed by the extended Hamiltonian

$$\widehat{H} = \frac{1}{2}\sum_i \left(\hat{n}_i\left(\hat{n}_i - 1\right) - \mu/U\,\hat{n}_i\right) - J/U \sum_{\langle i,j\rangle} \hat{b}_i^\dagger\,\hat{b}_j + \sum_i \left(\eta\,\hat{b}_i^\dagger + \eta^*\,\hat{b}_i\right) \tag{2}$$

is studied, as suggested in [3].
The intuitive idea behind this is that in the Mott insulator state the system should resist sufficiently small source strength η while in the superfluid state some response for arbitrarily small values of η is expected.
At zero temperature, the free energy $\mathcal{F}$ is given by the ground state expectation value of the Hamiltonian, $\mathcal{F}(J/U, \mu/U, \eta, \eta^*) = \langle\widehat{H}\rangle$ and can be expanded in the form

$$\mathcal{F}(J/U, \mu/U, \eta, \eta^*) = M\left(f_0(J/U, \mu/U) + \sum_{k=1}^{\infty} c_{2k}(J/U, \mu/U)\,|\eta|^{2k}\right). \tag{3}$$

It can be shown that the critical value $(J/U)_c$ is given by the radius of convergence of $c_2(J/U, \mu/U)$. The calculation of the coefficient $c_2(J/U, \mu/U)$ is accomplished by means of the **process-chain approach** devised by Eckardt [2], that utilizes Kato's explicit formulation of perturbation theory. The occurring terms can be visualized by diagrams as done up to second order in J/U in Fig. 2.

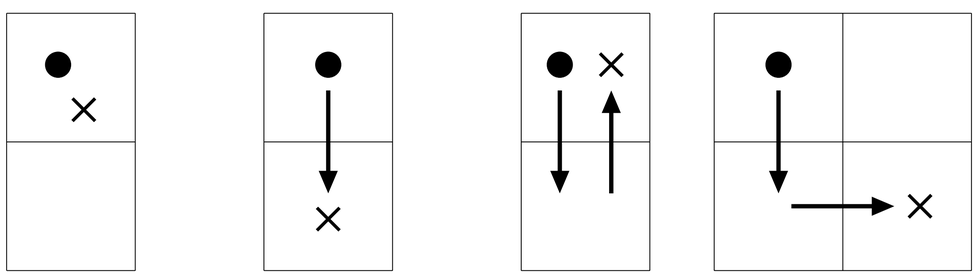

Fig. 2: Diagrams for determining c_2 up to second order in J/U

Results

As a measure of quality the phase diagram obtained with the process-chain approach is compared with **Quantum Monte Carlo (QMC)** data, here displayed for a 3d lattice and compared with data taken from [1].
In Fig. 4 one can see the excellent agreement between both methods.

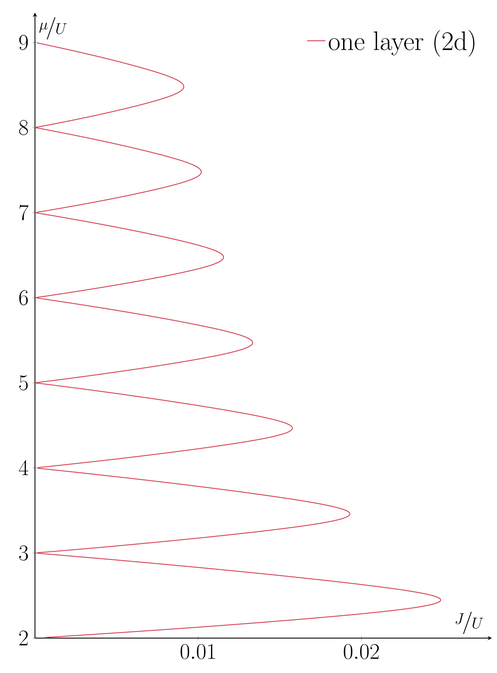

Fig. 3: The phase diagram for a 2d lattice

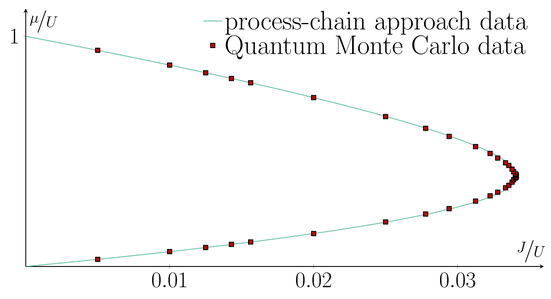

Fig. 4: Comparison between the phase diagram obtained with the process-chain approach and QMC data for a 3d lattice

The process-chain approach makes use of the indistinguishability of the Bose particles resulting in a vanishing influence of the filling factor on the computational load, so that the process-chain allows one to reach arbitrarily high filling factors. This is in contrast to and a major advantage over QMC-simulations, that scale very poorly with the number of bosons, restricting the analysis in [1] to a filling factor of one.
In Fig. 3 the phase diagram for a 2d lattice is displayed with a filling factor ranging from three up to nine.

Last the phase diagrams in two and three dimensions as well as the diagrams for multiple layers are presented; in Fig. 5 displayed are two, three, five, ten and twenty layers. As is to be expected, the diagrams vary from the two dimensional diagram monotonously with increasing number of layers to the three dimensional diagram.

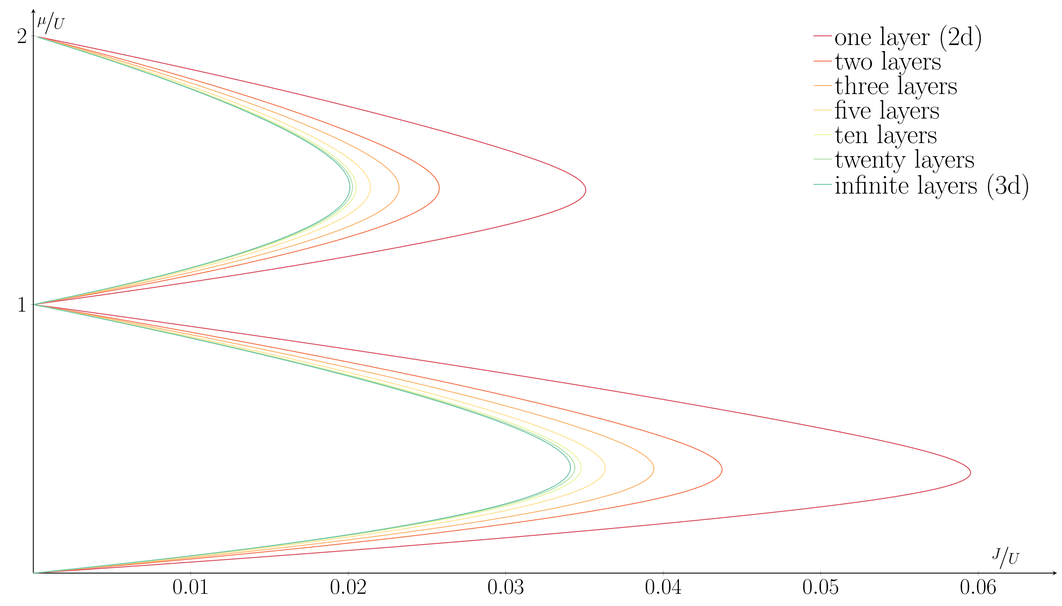

Fig. 5: Comparison of phase diagrams for various numbers of layers

Outlook

The interest in the transition from the two dimensional to the three dimensional Bose-Hubbard model originates from the fundamental change in the model expressed by the change from the non-trivial **critical exponent** in two dimensions to the trivial critical exponent in three dimensions (upper critical dimension). The presented method might lead to a better understanding of the underlying physics.

Literature

[1] B. Capogrosso-Sansone, N. V. Prokof'ev, and B. V. Svistunov. Phase diagram and thermodynamics of the three-dimensional Bose-Hubbard model. *Phys. Rev. B*, **75**(134302), 2007.

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[3] D. Hinrichs, A. Pelster, and M. Holthaus. Perturbative calculation of critical exponents for the Bose-Hubbard model. *Applied Physics B*, **113**(1), 2013.