Critical properties of the Bose-Hubbard model

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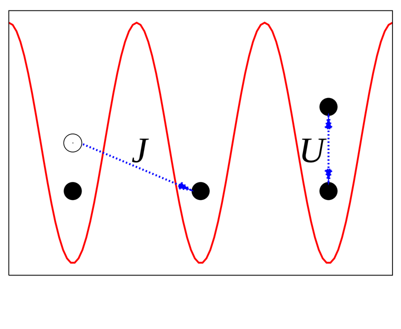
We study certain critical properties of the superfluid-to-Mott insulator quantum phase transition of the Bose-Hubbard model at zero temperature. By converting Kato's perturbation series into an efficient numerical algorithm and by applying the method of effective action, we gain access to the phase boundary as well as the superfluid and the condensate density. These calculations allow us to determine the critical exponents in two ways. One of these is based on variational perturbation theory, while the other requires more numerical effort.

The Bose-Hubbard model

The Bose-Hubbard model (BHM) describes ultracold bosons in optical lattices [1]. The grand canonical BH Hamiltonian reads

$$\hat{H}_{\rm BH} = \frac{U}{2}\sum_{i=1}^{M}\hat{n}_i(\hat{n}_i-1) - J\sum_{\langle i,j\rangle}\hat{b}_i^\dagger\hat{b}_j - \mu\sum_{i=1}^{M}\hat{n}_i \; .$$

- Particles tunnel from site i to a neighboring site j, as denoted by the index $\langle i,j\rangle$. The tunneling strength J quantifies the corresponding decrease of the kinetic energy.
- A pair of particles sitting on the same site leads to an interaction energy U increasing the system energy.



The BHM exhibits a quantum phase transition from the Mott insulator to a superfluid because of the competition between the tunneling dynamics and the repulsive on-site interaction of the bosons [2, 3].

Method of effective action

The following calculations base on the method of the effective potential [4, 5], which can be deduced by introducing sources and drains into the dimensionless BH Hamiltonian with strength η and η^* at the first step,

$$\hat{H}_{SD} = \underbrace{\frac{1}{2}\sum_{i=1}^{M}\hat{n}_i(\hat{n}_i-1) - \mu/U\sum_{i=1}^{M}\hat{n}_i}_{:=\hat{H}_0}\underbrace{-J/U\sum_{\langle i,j\rangle}\hat{b}_i^\dagger\hat{b}_j + \sum_{i=1}^{M}(\eta^*\hat{b}_i + \eta\hat{b}_i^\dagger)}_{:=\hat{V}} \; .$$

After expanding the free energy into a series in $|\eta|^2$ and carrying out a Legendre transformation $\Gamma = \mathcal{F}/M - \eta^*\psi - \eta\,\psi^*$, one arrives at the effective potential

$$\Gamma(J/U, |\psi|^2) = f_0 - \frac{1}{c_2}|\psi|^2 + \frac{c_4}{c_2^4}|\psi|^4 + \left(\frac{c_6}{c_2^6} - \frac{4c_4^2}{c_2^7}\right)|\psi|^6 + \mathcal{O}(|\psi|^8)$$

$$:= f_0 + \alpha_2|\psi|^2 + \alpha_4|\psi|^4 + \alpha_6|\psi|^6 = f_0 + \sum_{i=1}^{\ell}\alpha_{2i}|\psi|^{2i}$$

with the order parameter $\psi = \langle\hat{a}_i\rangle$. Since $\partial\Gamma/\partial\psi = -\eta^*$, and since the original BH system is recovered by setting $\eta = \eta^* = 0$, the system adopts that order parameter $\psi_{0,\ell}$ which minimizes Γ. The condensate density is connected to the order parameter by $\rho_{c,\ell} = |\psi_{0,\ell}|^2$ and depends on the maximum order ℓ of the expansion. Therefore we get

$$\rho_{c,2} = -\frac{\alpha_2}{2\alpha_4} \quad \text{and} \quad \rho_{c,3} = \frac{-\alpha_4 + \sqrt{\alpha_4^2 - 3\alpha_2\alpha_6}}{3\alpha_6} \; .$$

By adding a "twist" θ/L to the creation and annihilation operators via $\hat{b}_i \to e^{ix\theta/L}\hat{b}_i$, we are also able to calculate the superfluid density [6]:

$$\rho_{{\rm sf},\ell} = \lim_{\theta/L\to 0}\frac{1}{M(J/U)}\left(\frac{L}{\theta}\right)^2\left[\Gamma(\theta/L) - \Gamma(0)\right] \; .$$

The process-chain approach

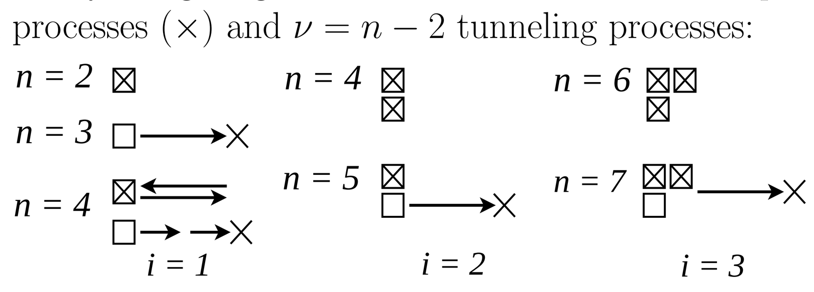
To calculate the free energy of $\hat{H}_{SD}$ we use Kato's formulation of the perturbation series [7]

$$\mathcal{F} = M\left(f_0 + \sum_{i=1}^{\infty}c_{2i}|\eta|^{2i}\right) = E_m + \sum_{n=1}^{\infty}{\rm tr}\left[\sum_{\{\alpha_\ell\}}{\rm S}^{\alpha_1}\hat{\rm V}{\rm S}^{\alpha_2}\ldots{\rm S}^{\alpha_{\rm n}}\hat{\rm V}{\rm S}^{\alpha_{\rm n+1}}\right]$$

with

$$S^\alpha = \begin{cases} -|m\rangle\langle m| & \text{for } \alpha = 0 \\ \sum_{i\neq m}\frac{|i\rangle\langle i|}{(E_m-E_i)^\alpha} & \text{for } \alpha > 0 \end{cases} \quad \text{and} \quad \sum_{i=1}^{n+1}\alpha_i = n-1 \; .$$

The states $|i\rangle$ with eigenvalues E_i are eigenvectors of the Hamiltonian $\hat{H}_0$ and $|m\rangle$ is the ground state of the Mott insulator. The perturbation $\hat{V}$ is given by the tunneling term and by the source and drain term. This formulation delivers process chains with various intermediate states [8]. As every coefficient c_{2i} is connected to i creations and i annihilations of a particle, we can express the nth-order series by using diagrams which consist of i creation processes (□), i annihilation processes (×) and $\nu = n - 2$ tunneling processes:



Condensate and superfluid density

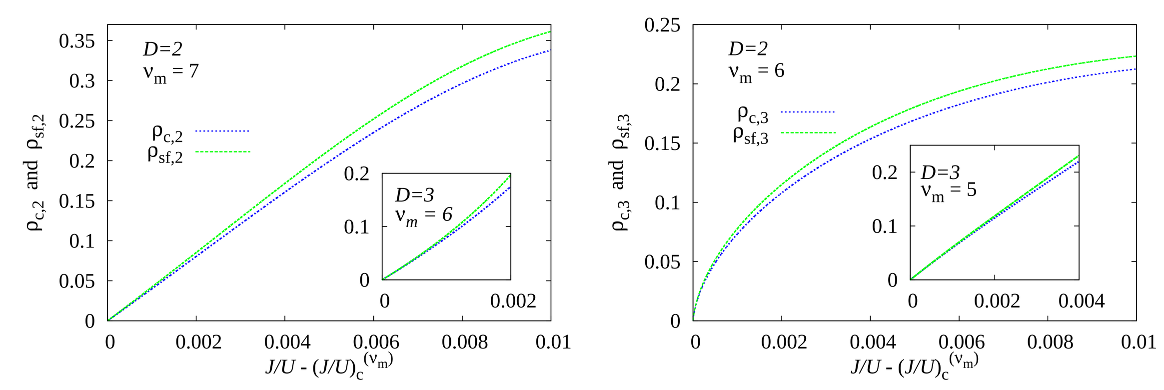


FIGURE 1: Superfluid density $\rho_{sf,\ell}$ and condensate density $\rho_{c,\ell}$ for $D = 2$ and $D = 3$. The respective maximal hopping order ν_m is stated in the figure. For the superfluid density the twist is set to $\theta/L = 0.001$. Whereas both densities shown in the upper figure increase linearly, the densities in the lower figure differ from each other, since only the densities for $D = 3$ show a linear behavior.

Critical exponents

The BHM lies in the universality class of the $(D+1)$-dimensional XY-model [1]. That means $D = 3$ is the upper critical dimension of the BHM and the mean-field critical exponents $\beta_c = 1$ for the condensate density and $\upsilon = 1$ for the superfluid density are valid. The expected results for $D = 2$ are listed in the left part of Tab. 1.
In principle the critical exponents should be given by the logarithmic derivative

$${\rm d}\log\rho := \lim_{J/U-(J/U)_c\to 0}\frac{{\rm d}\log\rho}{{\rm d}\log\left(J/U - (J/U)_c\right)}$$

of the densities ρ. We found two methods for obtaining the critical exponents of the two-dimensional BHM. The $|\psi|^4$-approach relies on the odd-order results of the coefficients c_{2i} and the $|\psi|^6$-approach uses the even-order results.

$|\psi|^4$-approach This method uses the densities for $\ell = 2$. As one can recognize in Fig. 1 both densities increase linearly which means the method of effective action delivers the critical exponents $\beta_c = \upsilon = 1$ of mean-field theory.
The variational perturbation theory (VPT) [9, 10] transforms a weak-coupling series with $x \ll 1$ to a strong-coupling series of the form

$$g_n(x) = x^{p/q}\sum_{i=0}^{n}b_m\left(x^{-2/q}\right)^i \quad \text{with} \quad x \gg 1 \; .$$

The ratio p/q, which is equal to the critical exponent, is called the *leading-power behavior in* x and $2/q$ is the *approach to the leading-power behavior*. By applying the logarithmic derivative to the densities we get an expansion of the critical exponents in $J/U \ll 1$. These series are transformed to the strong-coupling regime with the help of the VPT. Since it holds $p = 0$ for the strong-coupling series of the critical exponents, we only have to determine the variational parameter q self-consistently. The obtained results for $\nu_m = 3, 5, 7$ are linearly fitted so that we finally get the critical exponents.

$|\psi|^6$-approach Here we use the densities with $\ell = 3$. As one can see in Fig. 2 the logarithmic derivative of the condensate density for $D = 3$ converges always to one but for $D = 2$ the derivative shows a linear part which delivers values for the critical exponents unequal to one after a linear extrapolation. The results of this procedure for $\nu_m = 4, 6$ are also extrapolated linearly leading to nontrivial critical exponents.

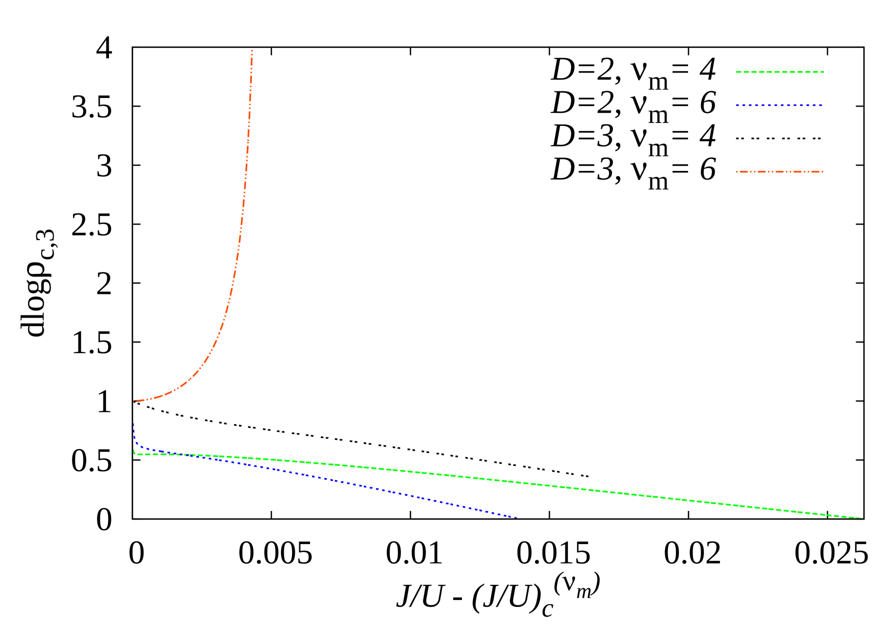


FIGURE 2: Logarithmic derivative of the condensate density $\rho_{c,3}$ for various orders ν_m and dimensionalities $D = 2, 3$. While for $D = 3$ the derivative converges to one, the extrapolated linear part of the derivative of $D = 2$ converges to approximately 2/3.

Ref.	[11]	[12]	[13]	$\|\psi\|^4$	$\|\psi\|^6$
β_c	0.6930	0.6962	0.6970	0.7028	0.7029
υ	0.6676	0.6697	0.6716	0.6784	0.6681

TABLE 1: Critical exponents of the BHM for $D = 2$. Listed are various reference values as well as our results obtained for the densities with $\ell = 2$ and $\ell = 3$.

Determination of the phase boundary

Due to the Ginzburg-Landau theory the point of phase transition is defined by the condition $\alpha_2(J/U) = 0$, thus, it is determinable by the coefficient c_2 alone. In the following the determination of the phase boundary of the square lattice is presented. Two methods lead to estimates for the phase boundary:

- The point of phase transition is given by that J/U which marks the radius of convergence so that

$$c_2 = \sum_{\nu=1}^{\nu_m}\gamma^{(\nu)}\left(\frac{J}{U}\right)^\nu$$

diverges. The coefficients $\gamma^{(\nu)}$ form an almost perfect geometric series so that a linear extrapolation of $\gamma^{(\nu-1)}/\gamma^{(\nu)}$ over $1/\nu$ leads to the phase boundary at $\nu = \infty$ [14, 15, 16].

- The zeros $(J/U)_0^{(\nu_m)}$ of the Taylor expansion

$$\alpha_2^{(\nu_m)} = \sum_{\nu=1}^{\nu_m}a^{(\nu)}\left(\frac{J}{U}\right)^\nu$$

of $1/c_2$ mark the phase boundary. These zeros are then linearly extrapolated to $\nu\to\infty$ by plotting them over $1/\nu$. Here one gets two phase boundaries since even and odd orders require a separate extrapolation.

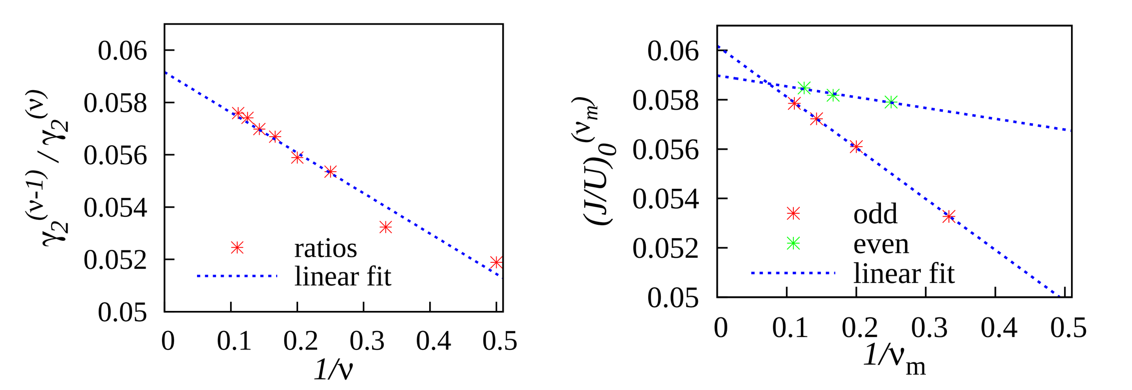


FIGURE 3: The extrapolation schemes for the determination of the phase boundary for $D = 2$. The left figure shows the ratios $\gamma_2^{(\nu-1)}/\gamma_2^{(\nu)}$ and the right figure shows the zeros $(J/U)_0^{(\nu_m)}$, which are both fitted linearly.

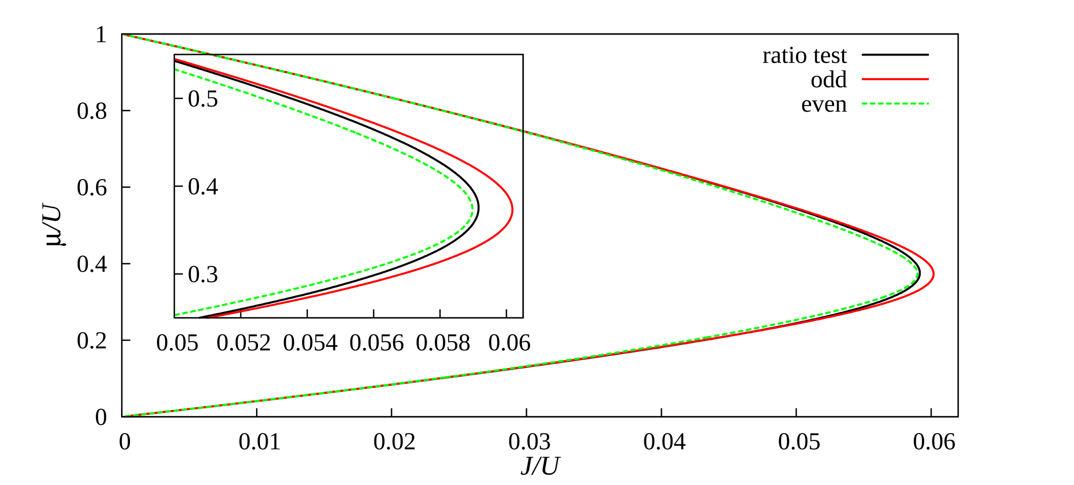


FIGURE 4: Phase boundary of the square lattice. The extrapolated results of the ratio test applied to c_2 and of the zeros of $\alpha_2^{(\nu_m)}$ are both plotted. The inset shows the tip of the Mott lobe. The phase boundaries determined by the zeros act as upper and lower bounds on the results of the ratio test.

Outlook

- Extension of these methods such that they yield the critical properties of the BHM with even higher accuracy.
- These methods are not restricted to the BHM and should be adaptable in a straightforward manner to modified BHM (e.g., other lattice geometries, nnn interaction) or even to other models like the JaynesCummings model which has been already studied with the process-chain approach [17].

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