Dynamics and thermodynamics of the Bose-Hubbard model

N. Elstner and H. Monien
Physikalisches Institut, Universität Bonn, Nußallee 12, D-53115 Bonn, Germany
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We report results from a systematic analytic strong-coupling expansion of the Bose-Hubbard model in one- and two-spatial dimensions. We obtain numerically exact results for the dispersion of single-particle and single-hole excitations in the Mott insulator. The boundary of the Mott phase can be determined with previously unattainable accuracy in one and two dimensions. In one dimension, we observe the occurrence of reentrant behavior from the compressible to the insulating phase in a region close to the critical point, which was conjectured in earlier work. Our calculation can be used as a benchmark for the development of numerical techniques for strongly correlated systems. [S0163-1829(99)04319-2]

Quantum phase transitions in strongly correlated systems have attracted a lot of interest in recent years. In fermionic systems the Mott transition is complicated by the fact that in unfrustrated systems the antiferromagnetic transition and localization transition occur at the same point (see, e.g., Ref. 1). For interacting Bose systems with spin zero, the situation is much simpler and one can focus on the physics of the Mott transition. Strongly interacting bosonic systems are not only of academic interest. Physical realizations include Josephson junction arrays, granular and short-correlation-length superconductors, flux lattices in type-II superconductors, and possibly in the future ultracold atoms in a periodic potential.[2–4]

To be specific, we investigate the generic model for the Mott transition, the Hubbard model, for bosons (BH model),

$$H=-t\sum_{\langle i,j\rangle}(b_i^\dagger b_j+b_j^\dagger b_i)+\frac{1}{2}U\sum_i \hat{n}_i(\hat{n}_i-1)-\mu\sum_i \hat{n}_i, \tag{1}$$

where the $b_i^\dagger$ and b_i are bosonic creation and annihilation operators, $\hat{n}_i=b_i^\dagger b_i$ is the number of particles on site i, t the hopping-matrix element, $U>0$ the on-site repulsion, and μ the chemical potential. With short-range interactions, only the model has two phases at zero temperature: a superfluid phase and a Mott phase. Much of the physics of the model was already understood qualitatively in an early paper by Fisher *et al.*[5] and subsequent papers (see, e.g., Refs. 6–8).

It is, however, interesting to obtain a quantitative understanding of the model—for example to compare with experiments. To this end, the BH model has been studied numerically by quantum Monte Carlo simulations[9–15] in one- and two-spatial dimensions. Recently, the one-dimensional case was also investigated using the density-matrix renormalization group (DMRG).[16] This study found indications for an unexpected reentrant behavior from the superfluid to the Mott insulator as a function of the hopping amplitude t for certain values of the chemical potential.

In this paper we report a systematic analytic strong-coupling series to high order for the Bose-Hubbard model. Previous attempts that were restricted to rather low order[17] showed promising results but were not sufficient to investigate the asymptotic behavior of the series. Recently Gelfand[18] proposed a method for a linked cluster expansion with degenerate states. We have implemented the series expansion of the ground state and the first excited state as a linked cluster expansion on a computer. The results show a spectacular convergence of the Pade approximants for the phase diagram in one and two dimensions. The critical points can be determined to a previously unattainable accuracy (relative errors of $\approx 10^{-3}$). In particular, we are able to confirm convincingly that in one dimension there is reentrant behavior of the Mott phase. The series calculation can be used as a benchmark for development of numerical techniques for strongly correlated systems (e.g., DMRG).

We start by writing down the ground state in the atomic limit (the hopping-matrix element $t\to 0$). In the atomic limit the number of bosons per site is fixed to an integer number, for example, n_0. Then the ground state of the Mott insulator with a fixed number n_0 of particles per site is given by

$$|n_0\rangle_{\rm Mott}^{(0)}=\prod_{i=1}^{N}\frac{1}{\sqrt{n_0!}}(b_i^\dagger)^{n_0}|0\rangle \tag{2}$$

with energy

$$E_{\rm Mott}^{(0)}/N=\tfrac{1}{2}n_0(n_0-1)U-\mu n_0. \tag{3}$$

Perturbation theory for the ground-state energy $E_{\rm Mott}$ can be formulated as a linked cluster expansion, see, e.g., Ref. 19 and the ground-state energy can be obtained in the thermodynamic limit ''relatively easily.''

The Mott transition is obtained by studying charge excitations on top of the Mott phase. The charge excitations are gapped in the incompressible Mott phase and become gapless at the Mott transition. In the atomic limit charge excitations are created by adding or removing a particle onto or from a particular site i

$$|n_0;i\rangle_{\rm part}^{(0)}=\frac{1}{\sqrt{n_0+1}}b_i^\dagger|n_0\rangle_{\rm Mott}^{(0)}, \tag{4}$$

$$|n_0;i\rangle_{\rm hole}^{(0)}=\frac{1}{\sqrt{n_0}}b_i|n_0\rangle_{\rm Mott}^{(0)}. \tag{5}$$

Their energy relative to the ground state is given by

$$E^{(0)}_{\text{part}} = Un_0 - \mu, \tag{6}$$

$$E^{(0)}_{\text{hole}} = -U(n_0 - 1) + \mu \tag{7}$$

for particles and holes, respectively showing that the charge excitations are degenerate. This degeneracy is lifted as soon as the hopping amplitude t is finite. In the atomic limit the energy of the excited states vanishes for a chemical potential $\mu_c^{(0)} = Un_0$ and the system becomes compressible.

A systematic strong-coupling expansion of the energy of the charge excitations complicated due to the high degeneracy. The problem how to write down a linked cluster expansion for degenerate states was solved only recently by Gelfand.[18] The idea is to construct perturbatively an effective Hamiltonian $H^{\text{eff}}_{i,j}$ in the subspace of the degenerate states $|n_0;i\rangle^{(0)}_{\text{part/hole}}$ by a similarity transformation

$$H^{\text{eff}}_{i,j}(t) = S_{i,\nu}(t) H_{\nu,\lambda} S_{\lambda,j}(t)$$

with

$$S_{i,\nu}(t) = S^{-1}_{\nu,i}(t), \tag{8}$$

where Greek indices run over states in the full Hilbert space while Latin indices are restricted to the degenerate manifold of single-particle and single-hole states (4) and (5), respectively. Then the linked cluster theorem applies to $H^{\text{eff}}_{i,j}(t) - E_{\text{Mott}}(t)$. In the case of a homogeneous system $H^{\text{eff}}_{i,j}$ depends only on the difference of indices $i-j$ and is easily diagonalized by a Fourier transform. This way one can determine the full dispersion $E(\mathbf{k};t,\mu)$ of the charge excitations. In many ways the linked cluster expansion is similar to a exact diagonalization study of small systems—however in the linked cluster expansion it is possible to remove all finite-size effects in each order and one obtains the full dispersion in the thermodynamic limit.

The spectrum $E(\mathbf{k};t,\mu)$ takes on the form

$$E_{\text{part}}(\mathbf{k};t,\mu) = \epsilon_{\text{part}}(\mathbf{k};t) - \mu, \tag{9}$$

$$E_{\text{hole}}(\mathbf{k};t,\mu) = -\epsilon_{\text{hole}}(\mathbf{k};t) + \mu \tag{10}$$

in complete analogy to Eqs. (6) and (7). For positive values of the hopping-matrix element t the smallest (largest) eigenvalue in the particle (hole) sector is always located at a wave vector $\mathbf{k}=0$. The upper and lower phase boundary of the Mott phase are thus given by $\mu_{\text{upper}}(t) = \epsilon_{\text{part}}(\mathbf{k}=\mathbf{0};t)$ and $\mu_{\text{lower}}(t) = \epsilon_{\text{hole}}(\mathbf{k}=\mathbf{0};t)$, respectively. As a consequence the single charge gap $\Delta(t) = \epsilon_{\text{part}}(\mathbf{k};t) - \epsilon_{\text{hole}}(\mathbf{k};t)$, determines also the width $\mu_{\text{upper}}(t) - \mu_{\text{lower}}(t)$ of the insulating region. With increasing hopping t the distance between the upper and lower boundary decreases until finally at some critical value t_c the energy to remove a particle and the energy to add a particle become degenerate and the Mott insulator vanishes altogether.

We will first discuss the BH model, Eq. (1) on a two-dimensional lattice. We investigated both the square and triangular lattice and calculated the series for occupation numbers $n_0=1$ and $n_0=2$ up to 13th and 10th order, respectively. The dispersion, $\epsilon(\mathbf{k})$ of the particle and hole excitations for $n_0=1$ on the square lattice is shown in Fig. 1. The different shape of the two curves reflects the particle-hole asymmetry of the model Hamiltonian (1). The series were found to converge very rapidly. Figure 1 was obtained by summation of the 13th order series. It turned out to be almost indistinguishable from the result of the 10-term series even for $t/U=0.055$, which is not far from the critical endpoint t_c of the Mott lobe. The particle and hole excitations both have a pronounced extremum at wave vector $\mathbf{k}=\mathbf{0}$ and are separated by a gap Δ. For values of the chemical potential μ in this range all single charge excitations are gapped and the system is insulating.

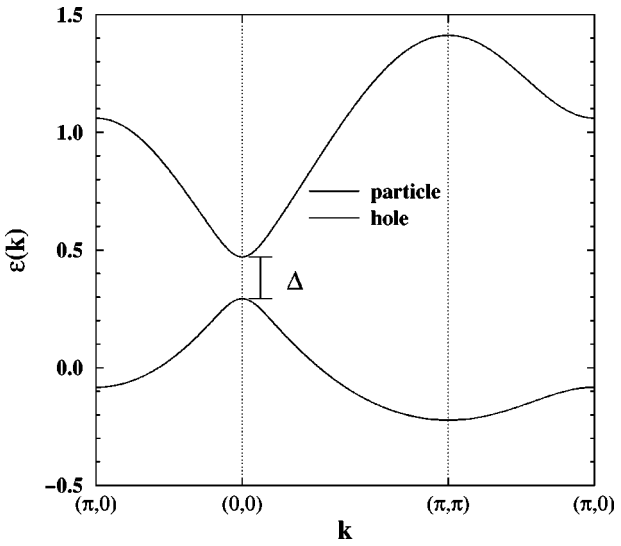

FIG. 1. Dispersion of the single-particle and single-hole states of the square lattice Bose-Hubbard model at $t/U=0.055$.

The phase diagram shown in Fig. 2 is obtained by a Pade analysis of the series for the single particle gap, Δ. Scaling theory[5] predicts that in the neighborhood of the critical point $(t_c,\ \mu_c)$ the single particle gap $\Delta(t)$ as a function of the hopping-matrix element t has the general form: $\Delta(t) = A(t)(t_c - t)^{z\nu}$, where $A(t)$ is a regular function of t and $z\nu$ is the dynamical critical exponent. We use the following pro-

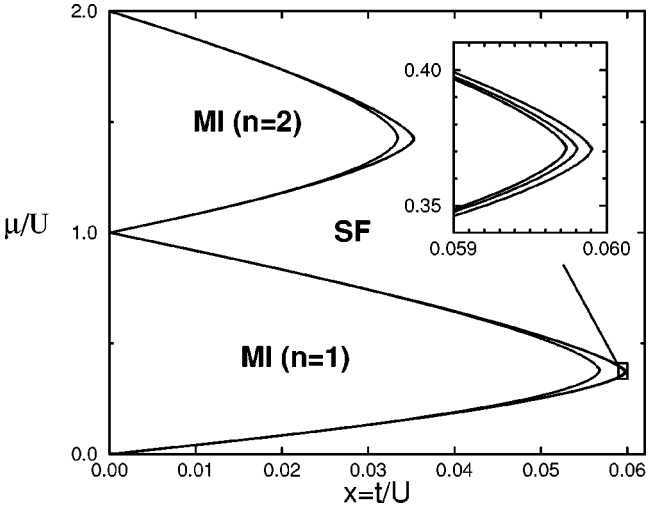

FIG. 2. Phase diagram of the square lattice constructed using a Pade analysis of the series. The Mott phases are denoted by **MI** and the superfluid region by **SF**. The left curve is the lowest order Pade approximant (4th-order series) the right curve represents all the higher approximants. The inset shows a resolution of the region around the critical point. Note the scale!

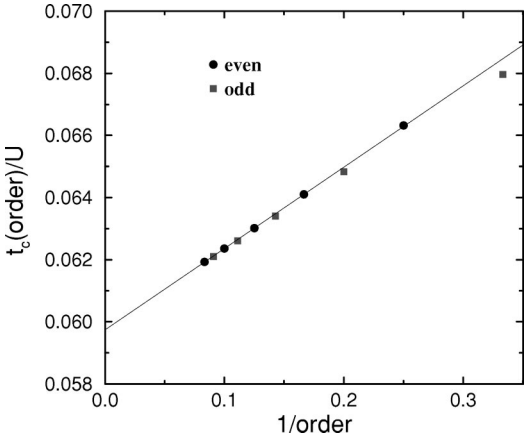

FIG. 3. 1/order extrapolation of the critical point (t_c).

cedure to extrapolate the series.[20] We calculate the logarithmic derivative of the series of the gap with respect to t, which results in

$$\frac{\partial \ln[\Delta(t)]}{\partial t} = \frac{z\nu}{t - t_c} + \frac{A'(t)}{A(t)}. \tag{11}$$

The right-hand side of Eq. (11) is well approximated by a Pade approximant. The pole of the Pade approximants for $\partial \ln[\Delta(t)]/\partial t$ then determines the critical point t_c and the residuum determines the dynamical critical exponent $z\nu$. We then integrate the Pade approximants numerically to obtain the single-particle gap $\Delta(t)$. With the exception of the lowest approximant all others approximant turn out to be almost indistinguishable from each other indicating a rapid convergence. The results are shown in Fig. 2. To observe any change at all in the higher approximants we have magnified the region around the critical point in the inset. The chemical potential is a regular function of the hopping-matrix element t. We used Pade analysis to check the scaling prediction and found for the critical point $t_c \approx 0.0599$ and the critical exponent $\nu \approx 0.69$. This has to be compared with the known value for the three-dimensional xy model,[21] $\nu = 0.6693 \pm 0.0010$, obtained by Borel summation of field theoretical results. The difference between the two results is of the order of a few per cent. Obviously, the Pade analysis has a tendency to slightly overestimate the value of the critical point, which in turn induces an error in the value of the critical exponent.

It is also possible to extract the critical hopping-matrix element t and the chemical potential at the critical point μ_c directly from the series. In each order k of the expansion the single-particle gap $\Delta(t)$ vanishes at some effective critical value $t_c^{(k)}$ with a corresponding effective $\mu_c^{(k)}$. Plotting $t_c^{(k)}$ and $\mu_c^{(k)}$ vs $1/k$ one finds again a rapid convergence as shown in Fig. 3. Extrapolation to $k \to \infty$ allows to determine accurately the critical point: $t_c = 0.05974 \pm 0.00004$ and $\mu_c = 0.371 \pm 0.001$.

We now turn to the one-dimensional case. From scaling theory[5] the critical behavior of the system is expected to be that of a Kosterlitz-Thouless transition[22] for which the gap closes according to $\Delta(t) \propto A(t) \exp(-W/\sqrt{t_{\mathrm{KT}} - t})$ for $|t_{\mathrm{KT}} - t| \ll 1$, where $A(t)$ is a regular function of t. The asymptotic form of the gap makes it difficult to approximate $\Delta(t)$ directly. Therefore, we analyze the series for $\ln[\Delta(t)]^2$.

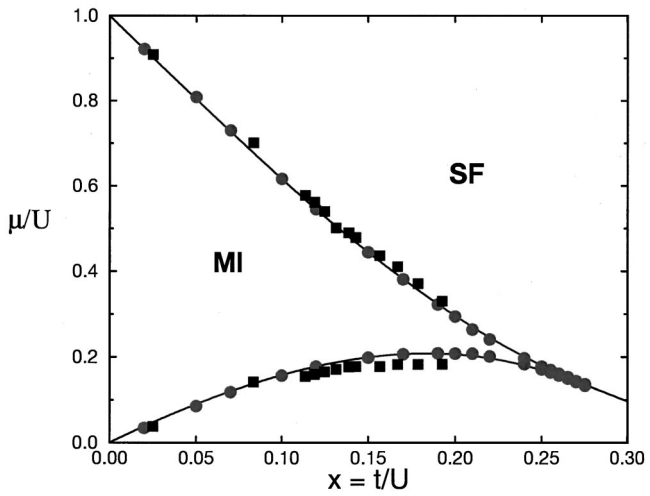

FIG. 4. Comparison of the phase diagram obtained from series expansion (solid line), DMRG (solid circles) and QMC (solid squares). The Mott phase is denoted by **MI** and the superfluid phase by **SF**.

The Pade analysis of the series yields spectacular agreement with the recent DMRG study of the phase diagram[16] as is shown in Fig. 4 where we compare results from the series analysis with numerical data of quantum Monte Carlo (QMC) simulations by Batrouni and Scalettar[10] and DMRG data.[16] The agreement between the series and the DMRG data is excellent. Both calculations show that for a fixed chemical potential as a function of the hopping matrix element t the Mott phase is reentrant meaning that by increasing the kinetic energy one returns to a *localized* state! The series analysis confirms the surprising behavior observed in the DMRG[16] calculation.

A simple intuitive way of understanding this phenomenon is the fact that Mott lobe is particle-hole asymmetric for the lattice problem. Starting from strong coupling ($U \gg t$) it is clear that the effect of the kinetic energy is to delocalize the particles. The delocalization decreases the average number of particles per site if the chemical potential is held fixed. On the other hand, in the weak coupling limit ($U \ll t$) the bosons condense at the lower band edge so that for increasing bandwidth (t) and fixed chemical potential the average number of particles per site is decreasing. The nonmonotonic behavior of the density can be understood simply as a result of two limiting cases. Thus starting from the Mott phase the number of particles per site first decreases and then increases leading to a second Mott transition for a well-defined range of the chemical potential.

The uncertainties in the precise location of the Kosterlitz-Thouless transition are still comparatively large. We use a Pade analysis of $\ln^2\Delta(t) \propto (t_{\mathrm{KT}} - t)^{-1}$. This quantity has a simple pole at the critical point that can be captured by rational function. This method turned out to give excellent results. We estimate the point for Kosterlitz-Thouless transition to be located at $t_{\mathrm{KT}}/U = 0.26 \pm 0.01$ and $\mu_{\mathrm{KT}}/U = 0.16 \pm 0.01$.

In conclusion, series expansion techniques were applied to investigate the zero-temperature properties of the Bose-Hubbard model in one and two dimensions. We determine the complete spectrum of single-particle and single-hole ex-

citations in the Mott phase. The phase diagram in one and two dimensions is obtained *quantitatively* and the critical-end points of the Mott insulator regions are determined. In two dimensions, this is so far the only quantitative investigation of the complete phase diagram of this problem. In one dimensions, the series shows almost perfect agreement with a recent DMRG study and provides a conclusive confirmation for counterintuitive reentrance behavior from the compressible to the insulating phase near the Kosterlitz-Thouless point.

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