Mott transition and dimerization in the one-dimensional SU($n$) Hubbard model

K. Buchta, Ö. Legeza, E. Szirmai, and J. Sólyom

Research Institute for Solid State Physics and Optics, H-1525 Budapest, P. O. Box 49, Hungary

(Dated: September 18, 2018)

The one-dimensional SU($n$) Hubbard model is investigated numerically for $n = 2, 3, 4$, and 5 at half filling and $1/n$ filling using the density-matrix renormalization-group (DMRG) method. The energy gaps and various quantum information entropies are calculated. In the half-filled case, finite spin and charge gaps are found for arbitrary positive $U$ if $n > 2$. Furthermore, it is shown that the transition to the gapped phase at $U_c = 0$ is of Kosterlitz-Thouless type and is accompanied by a bond dimerization both for even and odd $n$. In the $1/n$-filled case, the transition has similar features as the metal-insulator transition in the half-filled SU($2$) Hubbard model. The charge gap opens exponentially slowly for $U > U_c = 0$, the spin sector remains gapless, and the ground state is non-dimerized.

PACS numbers: 71.10.Fd

I. INTRODUCTION

Recently, the SU($n$)-symmetric generalization of the standard SU($2$) Hubbard model has been intensively studied theoretically, since this model may mimic strongly correlated electron systems where the orbital degrees of freedom of $d$ and $f$ electrons play important role.

Although the standard SU($2$) Hubbard model is exactly solvable in one dimension by Bethe’s ansatz and is well known to exhibit—at half filling—a Mott transition at $U_c = 0$, no such rigorous statement could be formulated for higher $n$ values. It is expected, however, that at generic fillings the one-dimensional SU($n$) Hubbard model behaves like an $n$-component Luttinger liquid while gaps may be generated at special fillings of the band, namely at half filling or $1/n$ filling.

The one-dimensional half-filled SU($n$) Hubbard model has been studied in the large $n$ limit and it has been shown that the charge and spin modes— that are decoupled for $n = 2$—become coupled and gap is generated in all of them. Moreover, it has been found that the system is spontaneously dimerized if $n$ is even. The role of umklapp processes in the half-filled model has been studied by the analytic multiplicative renormalization-group method in fermionic representation, too. It has been shown that in fact the umklapp processes couple the spin and charge modes if $n > 2$ and the spectrum is fully gapped for arbitrary values of the Coulomb repulsion. The question of dimerization has not been addressed in that work.

The $1/n$-filled case has been investigated analytically using the bosonized version of the model and numerically with quantum Monte Carlo simulation. It has been shown that at this special filling, i.e., when the number of particles is equal to the number of sites, the spin and charge degrees of freedom are decoupled and gap opens in the charge mode only. The spin modes remain gapless. Furthermore, it was inferred from the numerical calculations that for $n > 2$, unlike in the $n = 2$ case, the charge gap opens at a finite positive $U_c$. For smaller positive $U$ values the system shows metallic behavior. Since the contributions of the leading umklapp processes for commensurate fillings— except for half filling—are not logarithmically divergent, the special case of $1/n$ filling for $n > 2$ could not be analyzed in the framework of the usual analytic renormalization-group procedure.

In this paper, we present a careful numerical analysis of the one-dimensional SU($n$)-symmetric Hubbard model for $n = 2, 3, 4$, and 5 using the density-matrix renormalization-group (DMRG) method. Besides the question where the Mott transition takes place in the $1/n$-filled model we will consider the problem of dimerization in the half-filled case, since Marston and Affleck predicted dimerization for even $n$ only. This is done by calculating the one-site and two-site entropies whose behavior may be a better indicator of where and how a quantum phase transition occurs than the study of opening of gaps, which is notoriously difficult for a Kosterlitz-Thouless transition.

The setup of the paper is as follows. The Hamiltonian is presented and the role of umklapp processes at commensurate fillings is discussed in Sec. II. A few questions concerning the numerical procedure used in the paper are presented in Sec. III. In Sec. IV, the accuracy is tested on the SU($2$) Hubbard model. The results obtained for half-filled and $1/n$-filled systems for $n > 2$ are given in Sec. V and VI, respectively. The conclusions are summarized in Sec. VII.

II. THE HAMILTONIAN AND THE ROLE OF UMKLAPP PROCESSES

The Hamiltonian of the SU($n$) Hubbard model is written in the form

$$ \mathcal{H} = -t \sum_{i=1}^{N} \sum_{\sigma=1}^{n} (c_{i,\sigma}^\dagger c_{i+1,\sigma} + c_{i+1,\sigma}^\dagger c_{i,\sigma}) + \frac{U}{2} \sum_{i=1}^{N} \sum_{\sigma,\sigma'=1}^{n} n_{i,\sigma} n_{i,\sigma'}. $$

(1)
where \( N \) is the number of sites in the chain, \( c_{i,\sigma}^\dagger \) (\( c_{i,\sigma} \)) creates (annihilates) an electron at site \( i \) with spin \( \sigma \), the spin index is allowed to take \( n \) different values, \( n_{i,\sigma} \) is the particle-number operator, \( t \) is the hopping integral between nearest neighbor sites, and \( U \) is the strength of the on-site Coulomb repulsion. In what follows \( t \) will be taken as the unit of energy. The dimensionless \( U \) and the dimensionless gaps used in the paper are obtained by dividing their physical values by \( t \).

The term \( \sigma = \sigma' \) could have been kept in the last summation, as it is usually done in the literature, in order to display clearly the SU(\( n \)) symmetry. We prefer this form where the Coulomb repulsion acts between particles of different spin index only. Since it is forbidden to have two particles of the same spin on the same site, the two expressions differ in a shift in the energy only.

At generic fillings, this model is equivalent to an \( n \)-component Luttinger liquid. It has one symmetric (charge) and \( n - 1 \) antisymmetric (spin) gapless bosonic modes. At special fillings, where umklapp processes may become relevant, we will be interested especially in the modes. At special fillings, where umklapp processes may become relevant, we will be interested especially in the charge and spin modes. At such fillings, the leading umklapp term corresponds to scattering of \( n \) particles from one of the Fermi points to the opposite one. In this case, the effective term in the Hamiltonian is proportional to

\[
\int \! dx \cos [2\sqrt{n}\phi_c(x)].
\]

As can be seen, this term involves the charge sector only. On the other hand, for a \( p/q \)-filled band with \( q < n \), several terms may appear in (3) as leading \( (l = q) \) umklapp processes. When written in terms of the bosonic fields, both charge and spin modes appear in them. For example in the SU(3) model, where in addition to the charge mode there are two spin modes, in the half-filled case, the contribution of the two-particle umklapp processes is proportional to

\[
\int \! dx \left( \cos \left[ \frac{\sqrt{2}}{3} \left( 2\sqrt{2}\phi_c(x) + 2\phi_{2s}(x) \right) \right] + \cos \left[ \frac{\sqrt{2}}{3} \left( 2\sqrt{2}\phi_c(x) + \sqrt{3}\phi_{1s}(x) - \phi_{2s}(x) \right) \right] + \cos \left[ \frac{\sqrt{2}}{3} \left( 2\sqrt{2}\phi_c(x) - \sqrt{3}\phi_{1s}(x) - \phi_{2s}(x) \right) \right] \right).
\]

These terms are relevant and the corresponding soliton excitations couple the charge and spin modes. Therefore, gap is generated not only in the charge sector but in the spin sector as well, if \( q < n \), in agreement with Refs. 2 and 7.

### III. NUMERICAL PROCEDURE

#### A. Numerical accuracy

The numerical calculations presented in this paper have been performed on finite chains with open or periodic boundary condition (OBC or PBC, respectively) using the DMRG technique and the dynamic block-state selection (DBSS) approach. All data shown in
the figures were obtained with OBC unless stated otherwise. We have set the threshold value of the quantum information loss \( \chi \) to \( 10^{-5} \) and the minimum number of block states \( M_{\text{min}} \) to 256. All eigenstates have been targets independently using four DMRG sweeps until the entropy sum rule has been satisfied. The accuracy of the Davidson diagonalization routine has been set to \( 10^{-7} \) and the largest dimension of the superblock Hamiltonian was around three millions.

In the DBSS procedure the DMRG parameters are set dynamically. The maximum number of block states \( (M_{\text{max}}) \) that our program could handle was 2500, 1500, 800, and 256 for \( n = 2, 3, 4, \) and 5, respectively. This determines the maximal chain length that can be treated reliably with the accuracy prescribed in terms of \( \chi \). For small \( U (U < 1) \), where the coherence length is large, the block entropy grows very rapidly with increasing block size and the upper cutoff on the number of block states is reached at \( N \approx 90 \) for the SU(3) model and at \( N \approx 30 \) for the SU(4) model. For these \( U \) values and for such chain lengths the truncation error was of the order of \( 10^{-6} \) for a few DMRG iteration steps and the absolute error of our calculation is in the range of \( 10^{-4} \). Calculations on longer systems would give less reliable results and this imposes a serious limitation on the accuracy of the results obtained by finite-size extrapolation.

B. Detecting and locating phase transitions

The most common procedure to locate quantum phase transitions numerically is to calculate energy gaps. If the SU\((n)\) symmetry is not broken in the ground state and the band is \( p/q \) filled, in a system with \( N \) lattice sites, the number of particles with spin index \( \sigma \) is \( N_{\sigma} = N p/q \). The ground-state energy is denoted by \( E_0(N) \). The spin and charge gaps corresponding to the increase of energy when changing the spin of a particle or changing the number of particles were calculated according to the formulae

\[
\begin{align*}
\Delta_{\sigma}(N) &= E_{\sigma+1,-1}(N) - E_0(N), \\
\Delta_{c}(N) &= E_{\sigma+1}(N) + E_{\sigma-1}(N) - 2E_0(N),
\end{align*}
\]

where \( E_{\sigma+1}(N) \) is the lowest energy eigenvalue of the Hamiltonian when \( N_{\sigma} \) is increased by one for a given spin, \( E_{\sigma-1}(N) \) is the lowest energy when \( N_{\sigma} \) is decreased by one for a given spin, and \( E_{\sigma+1,-1}(N) \) is the lowest energy when the number of particles with spin \( \sigma \) is increased by one while the number of particles with a different \( \sigma' \) is decreased by one.

Since—as will be seen—it is difficult to study numerically the closing of energy gaps for small \( U \) values, an alternative approach to study quantum phase transitions has been suggested by several groups\cite{21, 22, 23, 24}. It uses the anomalies appearing in the generalized \( l \)-site entropy functions. These functions are easily accessible in DMRG and require to target the ground-state wavefunction only. Moreover, they are expected to have better finite-size scaling properties than the energy gaps.

The von Neumann entropy of a single site can be determined from \( s_i = -\text{Tr} \rho_i \ln \rho_i \), where the reduced density matrix \( \rho_i \) of site \( i \) is obtained from the wavefunction of the total system by tracing out all configurations of all other sites. In a similar manner generalized \( l \)-site entropies can be calculated which are often better indicators of quantum phase transitions than the one-site entropy. In our DMRG approach, the one- \( (s_i) \) and two-site \( (s_{i,i+1}) \) entropies at the center of the chain, for \( i = N/2 \) or \( i = N/2 + 1 \) and the block entropy of the left half of the system (corresponding to \( l = N/2 \)) are calculated at the end of each DMRG sweeps.

It turned out that for the SU\((n)\) Hubbard model the same single-site entropy is obtained when it is calculated on neighboring sites in the center of the chain. The sites are equivalent. The two-site entropy \( s_{i,i+1} \) is, however, different when it is considered at \( i = N/2 \) or \( i = N/2 + 1 \). An indication of the existence of bond dimer order, the breaking of translational symmetry can be obtained—as an alternative to the usual dimer order parameter—from the difference of two-site entropies,

\[
D_s(N) = s_{N/2,N/2+1} - s_{N/2+1,N/2+2}.
\]

As it has been shown in Ref. \cite{15} and will be discussed below, usually the dimer entropy difference converges faster than the energy gap, and it may be more convenient to analyze this quantity. In the next sections, we will use \( D_s \) to study the phase diagram as a function of \( U \).

As has been pointed out recently by two of the authors\cite{20} further information about possible nonuniform phases can be obtained from the study of the length dependence of the von Neumann entropy of a block of \( l \) sites in a finite chain, \( s(l), l = 0, \ldots, N \), and its Fourier spectrum,

\[
\tilde{s}(q) = \frac{1}{N} \sum_{l=0}^{N} e^{-iql} s(l).
\]

A finite peak at a nonzero wave vector indicates a corresponding modulation of the state. E. G., in a dimerized (trimerized) state the \( q = \pi \) \((q = 2\pi/3)\) Fourier component is nonvanishing. Furthermore, in a gapless model the central charge can be derived\cite{21, 22, 23, 24} from the initial slope of the length dependence of \( s(l) \). This can help to distinguish better gapped and gapless regimes.

C. Finite-size scaling

The large-\( N \) limit of the energy gaps and entropies can be obtained if appropriate scaling functions are used. In a critical, gapless model, in leading order, the gap \( \Delta(N) \) is expected to scale to zero as \( 1/N \). In a non-critical model the scaling depends on the boundary condition. The leading correction is exponential, if PBC is used:

\[
\Delta(N) = \Delta + c \frac{1}{N^{1/2}} \exp(-N/\xi),
\]
while for OBC the corrections are algebraic, and $\Delta(N)$ is expected to vary as

$$\Delta(N) = \Delta + a/N^2 + O(N^{-4}).$$

(11)

Therefore, the following fitting ansatz was used to evaluate the results obtained with OBC,

$$\Delta(N) = \Delta + a/N + b/N^2,$$

(12)

with $\Delta$, $a$, and $b$ as free parameters.

Local quantities, however, are expected to have a better scaling property even for OBC. For non-critical models the end effects decay exponentially with a finite correlation length, and the leading correction to the local quantities $s_{N/2}(N)$, $s_{N/2N+1}(N)$, and $D_s(N)$ is expected to have the form

$$A(N) = A + dN^{-\beta} \exp(-N/2\xi),$$

(13)

where $A$ is any of the local quantities listed above. This form is qualitatively similar to (10), except that $N/2$—the distance of the middle of the chain from the boundary—appears in the exponential and the exponent of the algebraic prefactor is a priori unknown.

IV. THE SU(2) MODEL AS A REFERENCE SYSTEM

Since numerical accuracy and proper finite-size scaling are crucial in the present work, we have tested our approach first on the half-filled SU(2) Hubbard model, where exact results are available.

The energy of all eigenstates that have been determined using DMRG with PBC agreed up to 5 digits with the numerical solution of the Bethe-ansatz equations. The $U$ dependence of the spin and charge gaps and the finite-size extrapolation are shown in Figs. 1 and 2 respectively.

Although the spin gap has a maximum as a function of $U$, this is a finite-size effect. Using (10) for the extrapolation to the thermodynamic limit, the spin gap scales to $\Delta_s = 6(1) \times 10^{-4}$ for small and large $U$ while it is of the order of $10^{-3}$ in the intermediate region. Here and in what follows the digits in parentheses are the one-standard-deviation uncertainty in the last digits of the given value. The root-mean-square error (the norm of residuals) of the fit denoted by $\kappa$ was $10^{-6}$.

The charge gap decreases monotonically with decreasing $U$, and the extrapolated values obtained using (10) are finite, opening exponentially slowly,

$$\Delta(U) = a \exp[-c(U - U_c)^{-\sigma}],$$

(14)

which is characteristic to a Kosterlitz-Thouless transition. The non-universal constants $a$ and $c$ and the exponent $\sigma$ were estimated together with $U_c$ by a least square fit. The best fit with error $\kappa = 5 \times 10^{-4}$ could be achieved with $a = 100.513$, $c = 8.931$, $\sigma = 0.517$, and $U_c = 0.024$.

If $\sigma$ is fixed to $\sigma = 0.5$ the parameters $a$ and $c$ change only slightly, and the best fit with error $\kappa = 8 \times 10^{-4}$ gives $U_c = 0.075$. This can be taken as an indicator of the accuracy since the exact result is $U_c = 0$.

The one-site and two-site entropies measured in the middle of the chain as well as the dimerization in the two-site entropy obtained for chains with up to $N = 128$ sites as a function of $U$ are plotted in Fig. 3. It is worth mentioning that the block entropy measured for the symmetric superblock configuration shows similar behavior as the two-site entropy.

The one-site, two-site and block entropies take their maximal value at $U = 0$, corresponding to the equipartition of local states, and no anomaly can be seen for $U > 0$ in agreement with the known analytic result.
The one-site entropy could be fitted well with a parabola

$$s_{N/2} = s_0 - AU^2,$$  \hspace{1cm} (15)

yielding $s_0 = 1.3863$, $A = 0.009293$, with error $\kappa = 5 \times 10^{-9}$. This parabolic fit is also shown in Fig. 3. The constant $s_0$ and the coefficient $A$ are in very good agreement with the exact result, $s_0 = \ln 4$ and $A = [7\zeta(3)/2\pi^2]/2 = 0.0092057$.

Although the two-site-entropy is markedly different on neighboring bonds in finite systems, the dimerization of the two-site entropy defined by 5 scales to $D_s = 5(1) \times 10^{-4}$ for all $U$, which should be considered as zero, in agreement with the known result that the SU(2) Hubbard model is not dimerized.

From these calculations we conclude that a value less than about $5 \times 10^{-4}$ either for the gap or the dimerization of the two-site entropy should be taken as zero.

\section{V. HALF-FILLED SU(n) MODELS}

The renormalization-group calculations\textsuperscript{27} have shown that at half filling the charge mode is always gapped. When $n > 2$, this mode is coupled to the spin sector and this generates gaps in the spin modes, as well. Moreover, Marston and Affleck\textsuperscript{2} have pointed out that for even $n$ the ground state is a charge-density wave state where the charge density is centered on the bonds, i.e., the system is spontaneously dimerized.

Since the arguments leading to this result cannot be straightforwardly extended to odd $n$ we have done calculations both for even and odd $n$ to compare the behavior of the SU(4) Hubbard model to that of the SU(3) and SU(5) models.

\subsection{A. Models with even $n$}

As has been shown, in the SU(2) model already, where relatively long chains could be studied, the energy gaps could not be determined for small $U$ values with better accuracy than $5 \times 10^{-4}$. Since the upper cutoff on the number of DMRG block states is reached for relatively small system sizes, $N = 32$ already in the SU(4) model, determination of the $N \rightarrow \infty$ limit of the energy spectrum with the same accuracy is not possible with our computational facilities. We have calculated the energy gaps for a few large $U$ values, where longer chains up to $N = 64$ could be treated. Although the extrapolated gaps are somewhat larger than those reported in Ref. 4 e.g., for $U = 4$ we have found $\Delta_c = 0.69(4)$ and $\Delta_s = 0.26(2)$, the results demonstrate clearly that in fact both gaps are finite.

Since our primary aim for the half-filled case was to study dimerization, we have analyzed the ground state entropy functions. The one-, and two-site entropies and the dimerization of the two-site entropy are shown in Fig. 3 for different chain lengths. While the one-site entropy shows no sign of dimerization, bond dimerization is apparent in the two-site entropy. Unfortunately the limitation for small $U$ values discussed above applies also in the case when the extrapolated values of $D_s$ are calculated. Although there is no doubt that $D_s$ is finite for not too small $U$, and in the large-$N$ limit, the dimerization of the two-site entropy seems to grow exponentially as a function of $U$, resembling a Kosterlitz-Thouless transition, no reliable finite-size scaling analysis could be done to determine $U_c$ where $D_s$ and the energy gaps become finite. The reason is that if a smaller $\chi$ is required in the calculation for the longest chain with $N = 64$ sites, smaller $D_s$ is obtained, thus our results shown for $N = 64$ overestimate $D_s$.

We try to infer $U_c$ from the behavior of the one-site entropy. As seen, it is a continuous function of $U$ with a maximum at $U = 0$ and without any anomaly for $U > 0$. For small $U$ values it can be fitted well (with error $\kappa = 1 \times 10^{-7}$) by a parabola with $s_0 = 2.7723$ (the exact value is $s_0 = \ln 16$) and $A = 0.0404$.

This analytic behavior and the results obtained for the dimerization are in complete agreement with the prediction by Marston and Affleck\textsuperscript{2}. 

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig3}
\caption{One-site and two-site entropy and dimerization of the two-site entropy in the middle of the chain as a function of $U$ for the half-filled SU(2) Hubbard model. The two sets of curves for the two-site entropy correspond to $i = N/2$ and $i = N/2 + 1$. The dashed lines are guide to the eye and the solid line is our parabolic fit.}
\end{figure}
B. Models with odd $n$

We will now compare the results described above with the behavior of the SU($n$) model for odd $n$. The $U$ dependence of the spin gap obtained by DMRG for the SU(3) half-filled Hubbard model and the finite-size extrapolation are shown in Fig. 5. The corresponding plots for the charge gaps are shown in Fig. 6.

The extrapolated values obtained using Eq. (12) are summarized in Table I. They were fitted with a four-parameter curve (14). The least-square fit (also shown in Fig. 5) for the spin gap with error $\kappa = 8 \times 10^{-7}$ gives $a = 1.089$, $c = 4.9256$, $\sigma = 0.607$, and $U_c = 0.054$. When $\sigma$ is fixed to $\sigma = 0.5$ we obtain $U_c = 0.098$ with error $\kappa = 2 \times 10^{-6}$.

For the charge gap the same procedure gives $a = 1.0855$, $c = 5.0492$, $\sigma = 0.9060$ and $U_c = 0.0913$ with error $\kappa = 5 \times 10^{-7}$ (this curve is also shown in Fig. 6) or $U_c = 0.099$ with error $\kappa = 2 \times 10^{-5}$ if $\sigma = 0.5$.

| $U$  | $\Delta_s$ | $\Delta_c$ |
|------|------------|------------|
| 0.1  | 0.0010(5)  | 0.0017(4)  |
| 0.25 | 0.0016(4)  | 0.0021(4)  |
| 0.5  | 0.0040(4)  | 0.0035(4)  |
| 1    | 0.0129(3)  | 0.0086(3)  |
| 2    | 0.0618(2)  | 0.0339(3)  |
| 2.5  | 0.0497(1)  | 0.0559(2)  |
| 3    | 0.1537(2)  | 0.0794(2)  |
| 3.5  | 0.2047(2)  | 0.1057(1)  |
| 4    | 0.2586(1)  | 0.1318(1)  |

TABLE I: Extrapolated values of the spin and charge gaps in the thermodynamic limit for the half-filled SU(3) Hubbard model.

The one- and two-site entropies and the dimerization appearing in the latter one are shown in Fig. 7 for system sizes up to $N = 90$. The one-site entropy possesses a maximum at $U = 0$, and none of the entropy functions show any sign of anomaly for $U > 0$. The one-site entropy can be fitted with a parabola giving $s_0 = 2.0791$ (the exact value is $s_0 = \ln 8$) and $A = 0.0197$ with $\kappa = 5 \times 10^{-7}$. Bond dimerization is signaled again by the two-site entropy, since $D_s$ remain finite in the large-$N$ limit for all finite $U$ values. Eq. (11) with fixed $\sigma = 0.5$ gives $a = 18.324$, $c = 5.827$, and $U_c = 0.013$ with error $\kappa =$.
5 × 10⁻⁷.

![Site entropy comparison](image1)

![Two-site entropy comparison](image2)

![Spin entropy comparison](image3)

**FIG. 7:** Entropy functions plotted as in Fig. 3 but for the half-filled SU(3) Hubbard model.

This finding, the dimerization of the half-filled SU(3) model has been corroborated by the study of the length dependence of the block entropy. We have determined the von Neumann entropy of blocks of length \( l \) for various chain lengths and calculated the Fourier components. It was found that an oscillatory component is superimposed on the smoothly increasing dependence of the block entropy. We have determined the Fourier components of the von Neumann entropy of blocks of length \( l \) for various chain lengths and calculated the Fourier components.

![Entropy functions comparison](image4)

**FIG. 8:** Finite-size scaling of the \( q = \pi \) Fourier component of the half-filled SU(\( n \)) Hubbard model for \( n = 2, 3, 4 \) at \( U = 4 \).

**VI. 1/\( n \)-FILLED SU(\( n \)) MODELS**

The other interesting situation which in a certain sense is the analogon of the half-filled SU(2) model is the 1/\( n \)-filled band, where the number of electrons is equal to the number of lattice sites. In this case umklapp processes in which \( n \) particles with different spin indices are scattered across from \( k_F \) to \(-k_F \) (or vice versa) may become relevant. An earlier study of the model using both analytic and numerical quantum Monte Carlo approach suggested that the spin gap vanishes for all \( U \), while the charge gap opens exponentially slowly for \( U > U_c \) but with finite \( U_c \). Since these numerical calculations have been performed for relatively short chains up to \( N = 30 \) sites, in this section we investigate in detail the same problem for the SU(3) model on longer chains using a different and hopefully more accurate procedure, and check the results for SU(4) and SU(5) models, too.

**A. SU(3) model at one-third filling**

The \( U \) dependence of the spin gap obtained by DMRG for the SU(3) one-third-filled Hubbard model and the finite-size extrapolation are shown in Fig. 9. The corresponding plots for the charge gaps are shown in Fig. 10.

As it is seen, for the chain lengths available the spin gap is a decreasing function of \( U \) and it scales to zero slower than 1/\( N \). An upper bound \( \Delta_s = 0.003(2) \) is obtained for all \( U \) if (12) is used for the extrapolation. A better fit can be achieved by the ansatz

\[
\Delta(N) = \Delta + a/N^b,
\]

with the exponent \( b \) as a free parameter. This fit gives \( \Delta_s = 0.0006(3) \) with \( b \) varying between 0.9 and 0.98. This difference is an indicator of the limits of our calculations. As mentioned earlier a gap 5 × 10⁻⁴ should be taken to
for small values, as well. Our finite-size scaling analysis had also predicted small but finite charge gap. The extrapolated values were fitted with the four-parameter function (14). The best estimates for the parameters are: $a = 8.68$, $c = 28.12$, $\sigma = 1.62(3)$, and $U_c = 0.03(3)$ (this curve is also shown in Fig. 11). The error of the fit is $\kappa = 2 \times 10^{-4}$. The fit with fixed $\sigma = 0.5$ gives $U_c = 0.36$ with error $\kappa = 2 \times 10^{-3}$. These $U_c$ values are much smaller than the one found Ref. 3. Even though it has been emphasized in that work that the extrapolated charge gap can be fitted with $U_c$ varying between 0 and 2.2, their best estimate was $U_c = 2.2$. The curve using their parameter values, $a = 45.050$, $c = 6.567$, and $\sigma = 0.5$ is also plotted in Fig. 11. It is clearly seen that this curve is well below our extrapolated data even for large $U$. The authors of Ref. 3 supported their finding by a theoretical estimate for the critical coupling $U_c$ which they have found to be the order of unity. Our best estimate at least an order of magnitude smaller.

| $U$   | $\Delta_c$ | $U$   | $\Delta_c$ |
|-------|------------|-------|------------|
| 0.1   | 0.0037(4)  | 2     | 0.0065(3)  |
| 0.25  | 0.0039(5)  | 2.25  | 0.0101(3)  |
| 0.5   | 0.0043(4)  | 2.5   | 0.0183(2)  |
| 1     | 0.0048(4)  | 2.75  | 0.0360(2)  |
| 1.25  | 0.0049(4)  | 3     | 0.0702(2)  |
| 1.5   | 0.0051(4)  | 3.5   | 0.2090(1)  |
| 1.75  | 0.0053(3)  | 4     | 0.4421(1)  |

TABLE II: Extrapolated values of the charge gap in the thermodynamic limit for the one-third-filled SU(3) Hubbard model.

Since the numerical results on the gap do not give a definite answer whether $U_c$ is finite or not, while Ref. 3 gives analytic arguments in favor of a finite critical value, we looked for further numerical evidence by studying the entropy functions. Our results are shown in Fig. 7. The one-site entropy possesses a maximum at $U = 0$. It shows no anomaly for $U > 0$. For small $U$, it can be fitted with the a quadratic $U$ dependence with $s_0 = 1.9076$ (the exact value is $s_0 = 3 \ln 3 - 2 \ln 2$) and $A = 0.0138$ with $\kappa = 2 \times 10^{-7}$.

A somewhat different behavior is obtained when the entropy of bigger blocks are considered. This effect is most pronounced when the entropy for a block of length $l = N/2$ is considered. The block entropy as a function of the block length oscillates now with a period of three, the Fourier spectrum has a peak at $q = 2\pi/3$, however, this component vanishes in the large $N$ limit, indicating that the system remains uniform. When the $U$ dependence of the blocks of length $l = N/2$ is taken, this quantity, in contrast to what has been seen for the single-site entropy, does not have its maximum at $U = 0$, but at a somewhat larger value. This is seen in Fig. 12.

The accuracy, the allowed quantum information loss was $\chi = 10^{-4}$ in this calculation, which allowed us to consider chains with $N = 120$ sites, but this does not influence the shape of the curves. The location of the maximum is shifted by less then one percent. The inset in the figure shows the finite-size scaling of $U_c$, the location of the maximum of the curves. Similar calculation have been performed for the excited state with $N + 1$ or $N - 1$ particles. The $U_c$ values obtained from the maximum are also shown in the inset. Extrapolation to the $N \to \infty$ limit gives a critical $U_c$ that is smaller than 0.1. Similar result is observed for the two-site entropy. The location

be zero. Thus we conclude that the spin gap vanishes in the large-$N$ limit for all positive $U$. In contrast to this, the charge gap is a monotonically increasing function of $U$ for all finite system sizes. It scales to finite values not only if $U$ is large enough but for small $U$ values, as well. Our finite-size scaling analysis predicts small but finite charge gap. The extrapolated values are given in Table I. These values are larger than those given in Ref. 3 where the longest chain used in the finite size scaling analysis had $N = 30$ sites. The reason for the discrepancy is that the $1/N^2$ corrections in Eq. 11 can be seen for longer systems only. The extrapolated values were fitted with the four-parameter function (14). The best estimates for the parameters are: $a = 8.68$, $c = 28.12$, $\sigma = 1.62(3)$, and $U_c = 0.03(3)$ (this curve is also shown in Fig. 11). The error of the fit is $\kappa = 2 \times 10^{-4}$. The fit with fixed $\sigma = 0.5$ gives $U_c = 0.36$ with error $\kappa = 2 \times 10^{-3}$. These $U_c$ values are much smaller than the one found Ref. 3. Even though it has been emphasized in that work that the extrapolated charge gap can be fitted with $U_c$ varying between 0 and 2.2, their best estimate was $U_c = 2.2$. The curve using their parameter values, $a = 45.050$, $c = 6.567$, and $\sigma = 0.5$ is also plotted in Fig. 11. It is clearly seen that this curve is well below our extrapolated data even for large $U$. The authors of Ref. 3 supported their finding by a theoretical estimate for the critical coupling $U_c$ which they have found to be the order of unity. Our best estimate at least an order of magnitude smaller.

![FIG. 9: Spin gap plotted as in Fig. 1 but for the one-third-filled SU(3) Hubbard model.](image1)

![FIG. 10: Charge gap plotted as in Fig. 2 but for the one-third-filled SU(3) Hubbard model.](image2)
which is related to the number of soft modes, using the

\[ U > 3 \]

is found, our calculation indicates that it is only 2 for all positive

\[ N \]

with

\[ s = 0 \]

vanishes for any anomaly for \( U > 0 \). The dimerization of the two-site entropy seems to scale to zero, since for any \( U \) it scales to a value less than \( D_s = 0.02(3) \). Although for finite systems the Fourier spectrum of the block entropy \( \tilde{s}(q) \) has a peak at \( q = \pi / 2 \), it scales to zero in the thermodynamic limit. The ground state is in fact uniform.

Due to the similarity in the behavior of the half-filled SU(2), one-third-filled SU(3), and quarter-filled SU(4) models, we suggest that—in disagreement with the result obtained by Assaraf et al. who predicted vanishing charge gap for \( U < 2.8 \)—the charge gap opens exponentially slowly at \( U_c = 0 \).

The entropy functions of the \( 1/5 \)-filled SU(5) model have been calculated for chains up to \( N = 30 \) lattice sites only. Although no reliable finite-size scaling could be performed, our results indicate similar features as seen in the other \( 1/n \)-filled models. The one-site entropy possesses a maximum at \( U = 0 \) and it is a smooth function of \( U \). We expect, therefore, that in this case as well the Mott transition occurs at \( U_c = 0 \).

**VII. CONCLUSION**

In summary, we have studied the one-dimensional SU(\( n \)) (\( n = 2, 3, 4 \), and 5) Hubbard model using the density-matrix renormalization-group method. Excitation gaps, \( l \)-site entropies, and Fourier spectrum of the block entropy have been calculated numerically. The numerical accuracy has been controlled by the quantum in-
formation loss $\chi$ which also sets a limit on the largest chain lengths whose properties could be determined with an a priori defined accuracy. Our method has been tested on the SU(2) Hubbard model in order to see similarities and differences when the $n > 2$ cases are studied.

First, the model at half filling has been studied. The prediction based on a large-$n$ analytical calculation, that the SU($n$) chain is bond dimerized for even $n > 2$ has been verified numerically, and it has been shown that exactly the same behavior is found for odd $n$. For the half-filled models both the spin and charge excitation gaps are finite for all finite Coulomb repulsion $U$, and they open exponentially slowly, indicating a Kosterlitz-Thouless transition at $U_c = 0$. Since finite-size scaling is notoriously difficult in the neighborhood of a Kosterlitz-Thouless transition, we have studied the behavior of several entropy functions. They show no anomalies for $U > 0$ which also supports that $U_c = 0$. This is, however, not a usual metal-insulator transition. The dimerization for $n > 2$ has been corroborated by the peak at $q = \pi$ in the Fourier spectrum of the length dependence of the block entropy.

Next, $1/n$-filled systems have been studied. It has been shown that the one-third-filled SU(3) model and the quarter-filled SU(4) model behave exactly in the same way as the half-filled SU(2) model. Although the length dependence of the block entropy shows a characteristic oscillation with a period of $1/n$, the corresponding Fourier components vanish in the thermodynamic limit, confirming that the ground state is spatially uniform. The spin gap vanishes while the charge gap opens exponentially slow for $U > 0$. Moreover, the best fit gives a value for $U_c$ that is very close to zero. The location of the transition has been checked by studying the $U$ dependence of various entropy functions. While the one-site entropy has its maximum at $U = 0$, this is not the case for larger blocks. Nevertheless, their maximum shifts to $U = 0$ in the large $N$ limit. Within our numerical accuracy the opening of the charge gap happens with a Kosterlitz-Thouless type transition at $U_c = 0$. The fifth-filled SU(5) Hubbard model shows similar behavior. Of course, a finite but very small $U_c < 0.1$ cannot be excluded, but even such a small value indicates that the role of higher order umklapp processes needs to be reexamined.

In a recent work it has been shown that the entropy profile of the SU(2) Hubbard model for different $U$ values as a function of the band filling indicates clearly the Mott transition at half filling for any positive $U$. Extension of this work to SU($n$) models might provide further evidence or discredit our result that in all cases studied $U_c = 0$.

Acknowledgments

This research was supported in part by the Hungarian Research Fund (OTKA) Grants No. T 043330, F 046356 and NF 61726 and the János Bolyai Research Fund. The authors acknowledge computational support from Dynaflex Ltd under Grant No. IgB-32.

---

1. J. Hubbard, Proc. Roy. Soc. A 276, 238 (1963); ibid. 277, 237 (1964); ibid. 281, 401 (1964); ibid. 285, 542 (1965).
2. J. B. Marston and I. Affleck, Phys. Rev. B 39, 11538 (1989).
3. R. Assaraf, P. Azaria, M. Caffarel, and P. Lecheminant, Phys. Rev. B 60, 2299 (1999).
4. R. Assaraf, P. Azaria, E. Boulat, M. Caffarel, and P. Lecheminant, Phys. Rev. Lett. 93, 016407 (2004).
5. C. Honerkamp and W. Hofstetter, Phys. Rev. Lett. 92, 170403 (2004).
6. F. F. Assaad, Phys. Rev. B 71, 075103 (2005).
7. E. Szirmai and J. Sólyom, Phys. Rev. B 71, 205108 (2005).
8. E. Szirmai and J. Sólyom, Phys. Rev. B 74, 155110 (2006).
9. E. H. Lieb and F. Y. Wu, Phys. Rev. Lett. 20, 1445 (1968).
10. S. R. White, Phys. Rev. Lett. 69, 2863 (1992); Phys. Rev. B 48, 10345 (1993).
11. P. Zanardi, Phys. Rev. A 65, 042101 (2002).
12. L.-A. Wu, M. S. Sarandy, and D. A. Lidar, Phys. Rev. Lett. 93, 250404 (2004).
13. S.-J. Gu, S.-S. Deng, Y.-Q. Li, and H.-Q. Lin, Phys. Rev. Lett. 93, 086402 (2004).
14. Ö. Legeza and J. Sólyom, Phys. Rev. Lett. 96, 116401 (2006).
15. T. Giamarchi and A. J. Millis, Phys. Rev. B 46, 9325 (1992).
16. For a review, see, e.g., J. Sólyom, Adv. Phys. 28, 201 (1979); and A. O. Gogolin, A. A. Nersesyan, A. M. Tsvelik, Bosonization and Strongly Correlated Systems (Cambridge University Press, Cambridge, 1998).
17. Ö. Legeza, J. Röder, and B. A. Hess, Phys. Rev. B 67, 125114 (2003).
18. Ö. Legeza and J. Sólyom, Phys. Rev. B 70, 205118 (2004).
19. K. Buchta, G. Fáth, Ö. Legeza and J. Sólyom, Phys. Rev. B 72, 054433 (2005).
20. Ö. Legeza, J. Sólyom, L. Tincani and R. M. Noack, cond-mat/0610499 (2006).
21. C. Holzhey, F. Larsen, and F. Wilczek, Nucl. Phys. B424, 443 (1994).
22. P. Calabrese and J. Cardy, J. Stat. Mech.: Theor. Exp. P06002 (2004).
23. I. Affleck and A. W. W. Ludwig, Phys. Rev. Lett. 67, 161 (1991).
24. N. Laflorencie, E. S. Sorensen, M-S Chang and I. Affleck, Phys. Rev. Lett. 96, 100603 (2006).
25. D. Larsson and H. Johansson, Phys. Rev. Lett. 95, 196406 (2005).
26. V. V. Franca and K. Capelle, (unpublished, cond-mat/0605207).