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Phase Transitions in Insulating 1D Electron Systems

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Abstract. We study the ground state phase diagram of different extensions of the one-dimensional Hubbard model at half filling by numerically diagonalizing finite systems with the Lanczos and DMRG method. We discuss the different kinds of insulator-insulator phase transitions that may occur in these models and the remaining open questions regarding their phase diagrams. First numerical results obtained on the IBM RS/6000 SP at the Scientific Supercomputing Center (SSC) Karlsruhe are presented.

1 Introduction

In recent years various new materials have been synthesized and studied, whose electronic and magnetic properties are marked by quasi one-dimensional (1D) chain and ladder structures [1–3]. These systems have received considerable interest due to the discovery of quasi-1D conductors and high- T_C superconductivity in cuprate materials.

To understand the physics of such materials governed by strong electronic interactions and reduced dimensionality, model studies on 1D correlated electron systems are necessary.

In addition to the motivation by experiments on novel materials, model studies of 1D correlated electron systems are of theoretical interest as well, since in 1D some model systems like e. g. the Hubbard model can either be solved exactly [4] or treated approximately by powerful field theoretical methods. The availability of analytic results in some limiting cases allows to efficiently test the accuracy of numerical calculations.

Such correlated electron systems are characterized by two phenomena unique for 1D systems: the separation of the energy scales for spin- and charge excitations (“spin-charge separation”) [4–6] — in contrast to the situation in conventional metals — and their instability towards the formation of a Peierls-distortion of the lattice.

For real, quasi-1D metallic materials both phenomena should play an important role for their electronic properties. However, their interplay has not been fully understood even in simple models. Before addressing these issues in the metallic phase of such 1D systems it is important to have a good understanding of their behaviour in the insulating case. This motivates the numerical study of the interplay between these phenomena in 1D correlated insulators.

In 1D insulators the ground state phase diagram may consist of insulating phases of different types, distinguished either by the mechanism that creates the energy gap in the insulator (like e.g. *band* or *correlated insulator*) or the ordering type of the ground state (like e.g. *charge density wave* (CDW) or *spin density wave* (SDW)-like ordering).

The availability of increasingly powerful high-performance supercomputers as well as the development of new numerical techniques like the so called Density-Matrix Renormalization Group (DMRG) method [7] allow a very accurate numerical diagonalization of 1D model Hamiltonians for large systems (system lengths $L > 100$) providing accurate and detailed information about the phase diagram.

Since numerical diagonalization techniques like the Lanczos method or DMRG are especially well suited to obtain ground state properties like the ground state energy, its corresponding eigenvector or static correlation functions, we will focus on the study of such properties. The most natural physical quantities to calculate are therefore the ground state energy and the spin (Δ_S) and charge (Δ_C) excitation gaps which are obtained for a half-filled system by the relations

$$\Delta_S = E_0(N = L, S_z = 1) - E_0(N = L, S_z = 0) \quad (1)$$

$$\Delta_C = E_0(N = L + 1, S_z = 0) + E_0(N = L - 1, S_z = 0) - E_0(N = L, S_z = 0) \quad (2)$$

where $E_0(N, S_z)$ is the ground state energy, L the system length, N the number of electrons in the system, and S_z the z -component of the total spin.

2 Models

As a microscopic model of a 1D correlated electron system we study the Hubbard model with various extensions. Two kinds of insulator-insulator transitions may occur: the transition from a band to a correlated (or Mott) insulator, and the transition between a CDW and a SDW-like phase. Both of them will be explained in more detail below.

2.1 Transition from a band to a correlated insulator

We distinguish the band insulator from the correlated insulator in a 1D electron system by the behaviour of the spin and charge gaps. We consider a system to be a band insulator when these two gaps are equal ($\Delta_S = \Delta_C$) and a correlated insulator when the charge gap is larger than the spin gap ($\Delta_C > \Delta_S$). In the absence of SU(2) symmetry breaking terms the correlated insulator is called a Mott insulator, if $\Delta_S = 0$ in this insulating phase.

2.2 Ionic Hubbard model

The so-called “ionic” Hubbard model was discussed e.g. in the context of the physics of ferroelectric perovskites [8–10]. Its Hamiltonian is given by

$$H = -t \sum_{i,\sigma} \left(c_{i\sigma}^\dagger c_{i+1\sigma} + h.c. \right) + U \sum_i n_{i\uparrow} n_{i\downarrow} + \frac{\Delta}{2} \sum_i (-1)^i n_i \quad (3)$$

where $c_{i\sigma}^\dagger$ creates an electron on site i with spin σ , $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$, t is the nearest-neighbour hopping amplitude, U the on-site Hubbard interaction, and Δ the modulation of the on-site energies. For $U = 0$ the ground state of this model is a band insulator at half-filling, its elementary excitation spectrum consists of particle-hole excitations over a band gap induced by the modulation Δ of the on-site energies. On the other hand, for $U \gg 0$, the gap is controlled entirely by the Coulomb interaction U , thus the system is a correlated insulator in this regime with $\Delta_S = 0$. The nature of the intermediate region was the subject of different numerical and analytical studies in recent years [11,12].

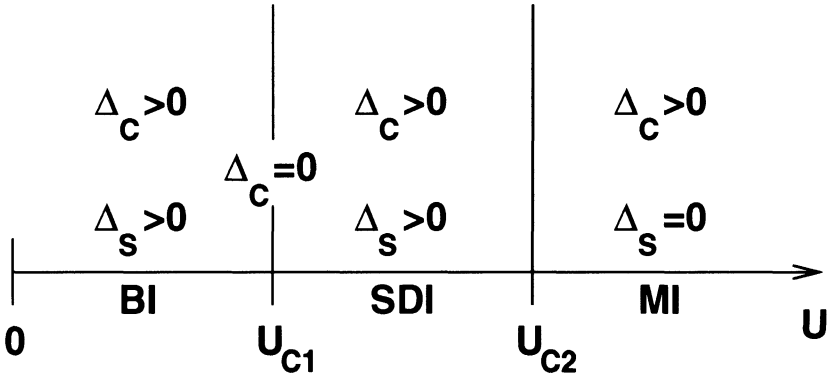


Fig. 1. Schematic ground state phase diagram of the ionic Hubbard model at half-filling obtained from bosonization (taken from Ref. [12]).

Fabrizio *et al.* [12] derived a schematic phase diagram within the framework of bosonization techniques as reproduced in Fig. 1. The authors of Ref. [12] find that for small but finite U the band insulator (BI) should persist up to a critical value U_{C1} at which Δ_C should vanish and the system should be conducting even at half filling. With further increasing U they predict a “spontaneously dimerized” (SDI) phase, which should undergo a continuous

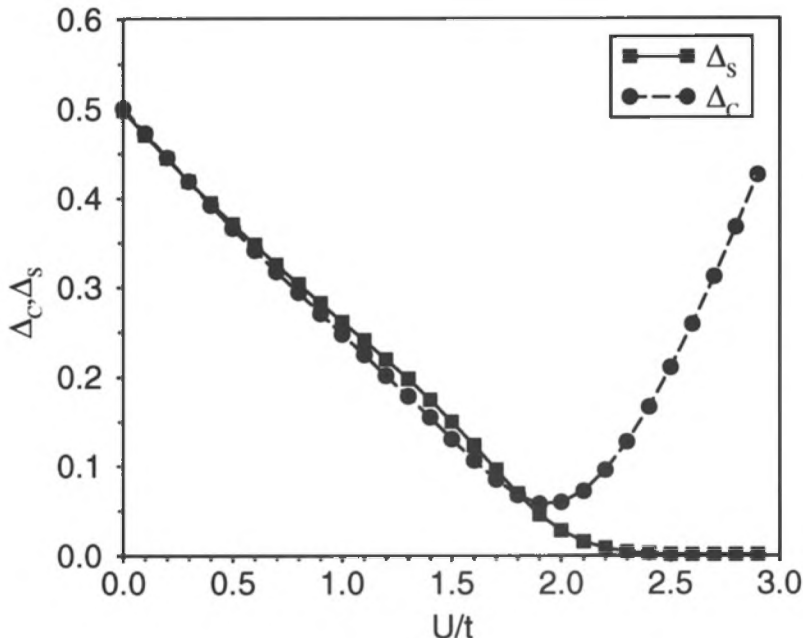


Fig. 2. First results for the spin (Δ_S) and charge (Δ_C) gap of the 1D ionic Hubbard model in the thermodynamic limit at half-filling with on-site energy modulation $\Delta = 0.5t$ as a function of the on-site Coulomb repulsion U . The ground state energies were obtained by DMRG calculations ($L = \{30, 40, 50, 60\}$) and extrapolated to the infinite chain.

transition into the correlated (or Mott) insulating (MI) phase at a second critical value U_{C2} .

We have started to explore the behaviour of the spin and charge gaps numerically and to compare our results with the remarkably rich scenario for the phase diagram in Fig. 1. We use the DMRG method which allows us to study long chains (up to $L = 60$) with open boundary conditions and to extrapolate to the thermodynamic limit with much higher accuracy than it is possible with exact diagonalization (Lanczos method) as was done in Ref. [11] with inconclusive results.

In Fig. 2 first results for the U dependence of Δ_C and Δ_S are shown. The scaling behaviour of the spin and charge gaps with chain length L is

approximated by [13]

$$\Delta_i(L) = \Delta_i^\infty + \frac{A_i}{L} + \frac{B_i}{L^2} \quad (4)$$

where $i \in \{S, C\}$. Extrapolation to the infinite chain limit is then done by fitting this second order polynomial in $1/L$ to the calculated finite chain results. Though the data presented in Fig. 2 are still preliminary, it can be seen already that up to approximately $U \sim 0.4t$ the band insulator with $\Delta_C = \Delta_S$ persists, and that for $U > 2.3t$ the system is a Mott insulator with $\Delta_C > 0$ and $\Delta_S = 0$. The nature of the intermediate transition region remains yet to be understood and the possible occurrence of the spontaneously dimerized phase in this region still has to be verified. More DMRG calculations are needed to explore the Δ dependence and the behaviour of static correlation functions in the ground state.

2.3 Peierls–Hubbard model

Extended Hubbard models that include a Peierls distortion of the lattice are discussed as possible models e. g. for dimerized chain materials like polyacetylen [14,15]. The Peierls-Hubbard model is given by the Hamiltonian

$$H = -t \sum_{i,\sigma} (1 + \Delta(-1)^i) \left(c_{i\sigma}^\dagger c_{i+1\sigma} + h.c. \right) + U \sum_i n_{i\uparrow} n_{i\downarrow} \quad (5)$$

where the modulation Δ of the hopping amplitude is assumed to result from a static alternating distortion of the lattice. Similar to the ionic Hubbard model, the Peierls-Hubbard model at half-filling is a band insulator at $U = 0$ and a correlated insulator for large U . From bosonization studies evidence exists [16] that like in the ionic model the band insulating phase might persist also for small but finite $U > 0$, such that a transition from band to correlated insulator occurs at a finite critical value U_C .

In order to establish the existence of this transition we have started DMRG studies of the spin and charge gaps for this model as well. This is ongoing work and will lead to first results soon. The goal is a better understanding of the nature of the possible insulator-insulator transition in this model as well as its connection to the physics of the ionic Hubbard model. The existence of a band insulator to Mott insulator transition in the half-filled Peierls-Hubbard model will naturally imply important consequences for the doped metallic phase.

2.4 Transition from a CDW to a Mott insulator: U - V Hubbard model

The transition from a CDW to a Mott insulator phase with dominating SDW correlations is realized in the phase diagram of the Hubbard model with

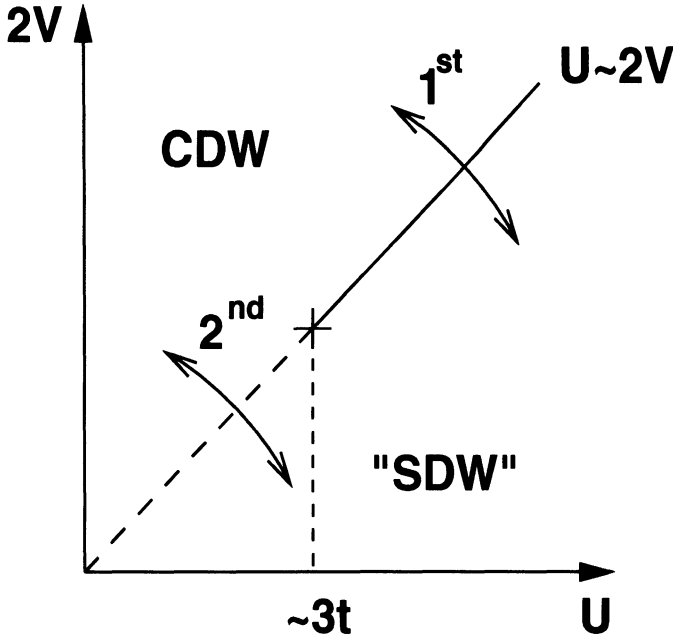


Fig. 3. Schematic ground state phase diagram of the 1D U - V Hubbard model at half-filling. For $U > 0$ and $V > 0$ a transition between a CDW and a Mott phase with SDW correlations is observed and evidence exists for a tricritical point around $(U, V) \sim (3t, 1.5t)$.

additional nearest-neighbour Coulomb repulsion V . In the CDW state one has $\Delta_C > \Delta_S > 0$, whereas in the Mott phase with SDW correlations the spin gap is $\Delta_S = 0$ and only $\Delta_C > 0$. The Hamiltonian of this model is given by

$$H = -t \sum_{i,\sigma} (c_{i\sigma}^\dagger c_{i+1\sigma} + h.c.) + U \sum_i n_{i\uparrow} n_{i\downarrow} + V \sum_i n_i n_{i+1} \quad (6)$$

where $n_i = \sum_\sigma n_{i\sigma}$. The extended U - V Hubbard model has been studied using different techniques [17]. In the weak-coupling limit, the phase diagram is analytically obtained by field theoretical calculations [18]. On the other hand, in the strong coupling limit perturbation theory gives the phase boundary of the CDW-Mott insulator transition [19]. The intermediate region has been studied by numerical techniques like exact diagonalization, quantum Monte Carlo [20,21], and short chain DMRG calculations [22].

In Fig. 3 the schematic phase diagram is shown summarizing the results of previous studies of the extended Hubbard model Eq. (6). The phase boundary between the CDW phase and the Mott insulator phase with SDW correlations

lies slightly above the line where $U = 2V$. In the weak coupling limit up to $U \sim 3t$ the transition across this line is believed to be second order, for larger values of U it may become a first order transition. A change in the order of a phase transition along the corresponding phase boundary requires the existence of a tricritical point at the location where this change of order takes place. However, the existence and exact location of the tricritical point remains still unclear.

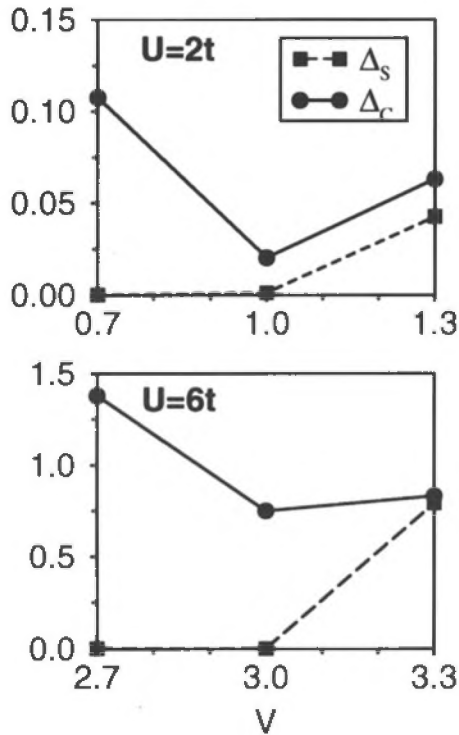


Fig. 4. First results for the half-filled 1D U - V Hubbard model. Δ_C and Δ_S as extrapolated to the infinite chain limit are shown as a for three values of V with $U = 2t$ (top) and $U = 6t$ (bottom). The energy gaps were obtained by numerical DMRG calculations for finite size chains of lengths $L = \{40, 60, 80, 100\}$.

For a so far limited parameter set we have calculated Δ_S and Δ_C for the U - V Hubbard model at half-filling using the DMRG method. For each set of parameters (U, V) we calculated the energy gaps for different chain lengths

$L = \{40, 60, 80, 100\}$ using open boundary conditions and with extrapolation to the infinite chain length limit using the finite size scaling ansatz Eq. (4).

First preliminary results obtained this way are shown in Fig. 4. For two values of U , one below ($U = 2t$) and one above ($U = 6t$) the presumed tricritical point, Δ_S and Δ_C are plotted for different values of V . For each value of U we have chosen three values for the nearest-neighbour repulsion V : $V < U/2$, $V = U/2$, and $V > U/2$. The energy gaps for $V < U/2$ clearly show the signature of the Mott insulator phase, namely $\Delta_S = 0$ and $\Delta_C > 0$, whereas for the chosen value $V > U/2$ the system is clearly in the CDW phase, where $\Delta_C > \Delta_S > 0$. The precise behaviour at the phase boundary has yet to be studied. For U below the tricritical point it might be possible that at the transition line between the Mott insulator with SDW correlations and the CDW phase (dashed line in Fig. 3) the charge gap vanishes completely ($\Delta_C = 0$), implying the system would be metallic on that line. However, for U above the critical value a first order transition is expected with $\Delta_C > 0$ for all V . Though the preliminary results of Fig. 4 do not yet allow any final conclusion about the transition region around $U \sim 2V$, it can be seen that for $U = 2t$ at $U = 2V$ the charge gap is quite small already, whereas for $U = 6t$ it remains comparable for $U = 2t$ to its values for $V < U/2$ and $V > U/2$. By calculating the gaps for more (U, V) parameter sets we hope to answer this question in the future.

3 Calculations on the IBM RS/6000 SP at the SSC

All calculations are performed on the IBM RS/6000 SP supercomputer at the SSC Karlsruhe using a parallelized Lanczos exact diagonalization program (PARLAN) and DMRG programs. All programs are written in the C++ programming language and make use of additional library routines written in FORTRAN 77 (BLAS, LAPACK, ESSL, and parts of the Lanczos routine).

The programs are parallelized using the MPI communication protocol to simultaneously diagonalize systems with different parameter sets and to allow the treatment of bigger matrices in the exact diagonalization procedure by storing them on different processing nodes.

Due to the nature of the required operations as well as to the lower efficiency of C++ compilers in vectorizing the code (e.g. on the Fujitsu VPP600 at the Leibniz-Rechenzentrum, Munich) our programs do not benefit very strongly from vector CPUs; the general purpose POWER architecture of the IBM RS/6000 computers is much better suited to our needs. In addition, the availability of both AIX based IBM RS/6000 workstations and the development RS/6000 SP system at the University of Augsburg, all integrated by a DCE/DFS installation, provide us with an optimal basis for development and testing of programs to be used on the RS/6000 SP at the SSC Karlsruhe.

We developed and tested the programs on the IBM RS/6000 SP at the University of Augsburg where we used up to 8 processing nodes, each equipped

with 256 MB RAM. However, to study the necessary chain lengths this is not sufficient. In contrast, the IBM RS/6000 SP at the SSC Karlsruhe with a big number of processing nodes with 500 MB or even 2 GB RAM each has shown to be a very well suited machine for our needs.

During development and testing, we made intensive use of the debugging and profiling tools included with the IBM compilers.

Typically, we run our programs on the RS/6000 SP at the SSC in in the production class using 10-30 processors for each job, making use of the maximum available 500 MB per node. Depending on the length of the chains (especially in the DMRG calculations) the necessary CPU time is close to the maximum available 240 min. in this class. In addition, when necessary we have done special serial program runs in the application class using the full available 2GB RAM.

4 Conclusion

In conclusion, we have started to study numerically the ground state phase diagram of three different extended Hubbard models at half-filling — the ionic Hubbard model, the Peierls-Hubbard model, and the U - V Hubbard model — by means of exact diagonalization and DMRG calculations. Selected preliminary results already obtained on the IBM RS/6000 SP at the SSC Karlsruhe were shown.

Despite the fact that these models have been studied already for quite some time, many questions regarding their ground state phase diagram still remain open, as we tried to briefly illustrate above. In the continuation of our numerical analysis we hope to be able to answer some of them, in particular in connection to the band insulator – Mott insulator transition. State-of-the-art numerical techniques like DMRG in combination with the computational power and flexibility of modern parallel supercomputers like the RS/6000 SP provide an efficient tool to address those questions.

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