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Charge density plateaux and insulating phases in the t-J model with ladder geometry

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Abstract. We discuss the occurrence and the stability of charge density plateaux in ladder-like t-J systems (at zero magnetization M=0) for the cases of 2- and 3-leg ladders. Starting from isolated rungs at zero leg coupling, we study the behaviour of plateaux-related phase transitions by means of first order perturbation theory and compare our results with Lanczos diagonalizations for t-J ladders $(N=2\times8)$ with increasing leg couplings. Furthermore we discuss the regimes of rung and leg couplings that should be favoured for the appearance of the charge density plateaux.

PACS. 71.10.Fd Lattice fermion models (Hubbard model, etc.) – 71.27.+a Strongly correlated electron systems; heavy fermions – 75.10.-b General theory and models of magnetic ordering – 75.10.Jm Quantized spin models

1 Introduction

The t-J model has been introduced as the first order correction of the extreme atomic limit of the Hubbard model [1,2] and is considered the simplest model including the low energy physics of doped ladder systems [3,4]. The phase diagram of the two leg Hubbard model has been investigated in [5] by means of a renormalization group approach valid for small values of the on-site Coulomb interaction U but for arbitrary charge density and arbitrary hopping along the rungs. The phase diagram is classified as different C_xS_y phases which denotes x gapless charge modes and y gapless spin modes. They have shown under which condition a phase of C_1S_0 appears which is analog of either a superconductor or chargedensity wave. The extension of this approach to the Nleg Hubbard model can be found in [6] where the dimensional crossover as $N \to \infty$ is discussed. The charge and spin gap for the two leg Hubbard model and its dependence on the on-site Coulomb interaction and the rung hopping parameter t have been calculated by means of the density matrix renormalization group (DMRG) and compared with the previous weak-coupling RG [7]. The effect of an additional nearest neighbour Coulomb repulsion V has been studied in [8]. A charge order (metalinsulator) transition was found at charge density $\rho = 1/2$

The values of the charge density (and magnetization) at the plateaux are fixed by the geometry of the system (e.g. the number of legs in a ladder system).

In this paper we will study the ground states of the t-J Hamiltonian on a ladder with n legs (n=2,3)

$$H^{[n]} = tH_r^{[n]} + t'H_l^{[n]}. (1.1)$$

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from a homogeneous state to a charge density wave. The influence of an anisotropy between leg and rung couplings in Hubbard and t-J models on specific correlations, which signal the metal-insulator transition, has been investigated in [9]. The metal-insulator transition is accompanied by the opening of a gap, which appears as a plateau in the charge density $\rho(\mu)$ as a function of the chemical potential μ . The charge density plateau in $\rho(\mu)$ looks similar to the plateaux in the magnetization curve M(B) found in the spin ladder systems and one might ask whether the mathematical foundations for both plateaux are the same. This is indeed the case and becomes evident if one maps the t-J Hamiltonian on a spin-1 Hamiltonian with broken SU(3) symmetry [10]. The Lieb-Schultz-Mattis theorem [11] has been extended to quasi onedimensional fermionic systems [12] and the momenta of low-lying excitations could be classified thereby. The quantization rule of Oshikawa, Yamanaka and Affleck [13] predicts as well possible plateaux in the charge density $\rho(\mu)$.

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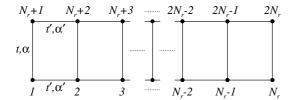


Fig. 1. Structure of a two leg ladder with open boundary conditions and $2N_r$ sites.

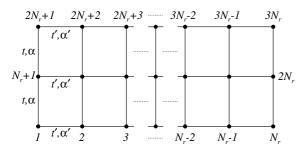


Fig. 2. Structure of a three leg ladder with open boundary conditions and $3N_r$ sites.

 t,t^{\prime} are the hopping parameters, and

$$H_r^{[n]} = \sum_{x=1}^{N_r} h_r^{[n]}(x, \alpha), \quad \alpha = J/t,$$

$$H_l^{[n]} = \sum_{x=1}^{N_r - 1} h_l^{[n]}(x, \alpha') \quad \alpha' = J'/t'$$
(1.2)

define the contributions of the couplings along the rungs and legs, respectively. The spin exchange is included in the ratios $\alpha = J/t$, $\alpha' = J'/t'$. The latter are depicted in Figures 1 and 2 for the cases of a two and a three leg ladder.

A charge density plateau in $\rho(\mu)$ – where μ is the chemical potential – is signaled by discontinuous changes in the slope of the ground state energy per site as function of ρ (cf. Eq. (2.12)). They emerge immediately in the "local rung approximation" [9] (or "bond operator theory" [14]), where the ground states are direct products of rung cluster states. The corresponding energies turn out to be piecewise linear in ρ .

It is the purpose of this paper to go beyond the local rung approximation by means of a systematic perturbation theory in the leg coupling t'. To first order, this leads to an effective interaction between the rung cluster states. The corresponding effective Hamiltonians are defined on a chain with N_r sites – where N_r is the number of rungs – and can be diagonalized numerically.

The outline of the paper is as follows: In Section 2 we first treat the two leg ladder. Here, the effective Hamiltonians for $\rho < 1/2$ and $\rho > 1/2$ look like modified t-J models on a chain with N_T sites.

In Section 3 we extend all considerations to the three leg ladder, where plateaux appear at $\rho=1/3$ and $\rho=2/3$. First order perturbation theory in t' leads to three different effective Hamiltonians in the regimes $0 \le \rho \le 1/3, \, 1/3 \le \rho \le 2/3, \, 2/3 \le \rho \le 1$. In Section 4 we compare the perturbative results with Lanczos diagonalizations on ladder systems and discuss consequences for the phase diagram.

2 T - J model on a two leg ladder

According to the notation given in Figure 1 the couplings along the rungs and legs which enter into the t-J-Hamiltonian on a two leg ladder are given by:

$$h_r^{[2]}(x,\alpha) = h(x, x + N_r, \alpha),$$

$$h_l^{[2]}(x,\alpha') = h(x, x + 1, \alpha')$$

$$+h(x + N_r, x + 1 + N_r, \alpha').$$
(2.1)

For our purposes it is convenient to represent these couplings in terms of "constrained" permutation operators

$$h(x, y, \tilde{\alpha}) = -P_{01}(x, y) + \frac{\tilde{\alpha}}{2}Q_{11}(x, y).$$
 (2.3)

Here, $P_{01}(x, y)$ is a permutation operator, which permutes the states at x and y, if they are occupied by one hole (0) and one electron (1). This operator allows the hopping of electrons and holes and forbids the double occupancy of each site x with two electrons.

If both sites x and y are occupied with electrons, the operator

$$Q_{11}(x,y) = P(x,y) - 1, (2.4)$$

$$Q_{11}(x,y)|x,y\rangle = |y,x\rangle - |x,y\rangle \tag{2.5}$$

first interchanges the electrons at x and y; afterwards the original state is subtracted.

2.1 0th order perturbation theory in t'

The lowest energy eigenstates of the rungs $(x, x+N_r)$ with Hamiltonian $h(x, x+N_r, \alpha)$ can be easily calculated.

$$|Q(x) = 0\rangle = |0,0\rangle$$

$$|Q(x) = 1\rangle = \frac{1}{\sqrt{2}}(|\sigma,0\rangle + |0,\sigma\rangle)$$

$$|Q(x) = 2\rangle = \frac{1}{\sqrt{2}}(|+,-\rangle - |-,+\rangle).$$
(2.6)

The right-hand side defines the states on the sites x and $x+N_r$ of the rung; 0 means hole with charge zero. Q(x)=1 means one electron with spin $\sigma=\pm 1$. Q(x)=2 represents an electron pair coupled antiferromagnetically to a total spin 0. Therefore, we have charges 0,1 and 2 for $|Q(x)=0\rangle$, $|Q(x)=1\rangle$ and $|Q(x)=2\rangle$ respectively. The eigenvalues are given by the following equations.

$$h(x, x + N_r, \alpha)|Q(x)\rangle = \varepsilon_n|Q(x)\rangle$$
 (2.7)

$$\varepsilon_0 = 0; \varepsilon_1 = -1; \varepsilon_2 = -\alpha.$$
 (2.8)

In the limit of vanishing leg couplings t' = 0, the system of decoupled rungs has the following ground state.

(1) For $\rho = \frac{Q}{2N_r} = \frac{1}{2} - \frac{q}{N_r} \le \frac{1}{2}$; $q = 0, 1, 2, \ldots$ and $\alpha < 2$ the ground state is a direct product of $(N_r - 2q)$ rung states $|Q(x) = 1(\sigma)\rangle$ and 2q states with $|Q(x) = 0\rangle$.

Note that for $\alpha < 2$, the creation of a pair state $|Q(x) = 2\rangle$ and a charge zero state $|Q(x) = 0\rangle$ from two charge 1 states $|Q(x) = 1(\sigma = +1)\rangle$ and $|Q(x) = 1(\sigma = -1)\rangle$ is not energetically favorable, since

$$\varepsilon_0 + \varepsilon_2 > 2\varepsilon_1.$$
 (2.9)

Therefore, the ground state energy turns out to be

$$E_1^{(0)}(\rho,\alpha) = (N_r - 2q)\varepsilon_1 + 2q\varepsilon_0$$

= -2N_r\rho. (2.10)

(2) For $\rho=\frac{Q}{2N_r}=\frac{1}{2}+\frac{q}{N_r}\geq\frac{1}{2};\ q=0,1,2,\ldots$ and $\alpha<2$ the ground state is a direct product of (N_r-2q) rung state $|Q(x)=1\rangle$ and 2q states $|Q(x)=2\rangle$ with electron pairs. In this case the ground state energy is

$$E_2^{(0)}(\rho, \alpha) = (N_r - 2q)\varepsilon_1 + 2q\varepsilon_2$$

= $2N_r\rho(1 - \alpha) - (2 - \alpha)N_r$. (2.11)

Note, in both regimes $\rho \leq 1/2$ and $\rho \geq 1/2$ the ground state energy is linear in ρ . The first derivative of the ground state energy

$$\mu = \frac{d}{d\rho} \frac{E}{2N_r} \tag{2.12}$$

is related to the chemical potential which has a discontinuity at $\rho = \frac{1}{2}$.

$$\mu = \begin{cases} -1 & \text{for } \rho \le \frac{1}{2} \\ 1 - \alpha & \text{for } \rho \ge \frac{1}{2}, \end{cases}$$
 (2.13)

This is the first indication of a charge density plateau at $\rho = 1/2$ in the t-J model on a two leg ladder.

To zeroth order in the leg coupling (t'), the eigenstates of the t-J Hamiltonian (1.1) are product states of N_r rung states:

$$|Q(1), Q(2), \dots, Q(N_r)\rangle = \prod_{x} |Q(x)\rangle.$$
 (2.14)

The rung quantum numbers $Q(x) = 0, 1(\sigma = \pm 1), 2$ are subjected to the conservation of total charge Q,

$$\sum_{x} Q(x) = Q. \tag{2.15}$$

Moreover, the total spin, which originates from the spin of charge 1 states $|Q(x) = 1\rangle$, is assumed to be zero here:

$$\sum_{x} \sigma(x)\delta_{Q(x),1} = 0. \tag{2.16}$$

Therefore the ground states with energies (2.10), (2.11) are highly degenerate for $\rho \neq 0, 1/2, 1$.

2.2 1st order perturbation theory in t'

A first order perturbation theory demands a computation of the transition matrix elements:

$$\langle Q'(1), Q'(2), \dots, Q'(N) | H_l^{[2]} | Q(1), Q(2), \dots, Q(N) \rangle = \sum_{x=1}^{N_r - 1} \mathcal{A} \langle Q'(x), Q'(x+1) | h_l^{[2]}(x, \alpha') | Q(x), Q(x+1) \rangle$$
(2.17)

where

$$\mathcal{A} = \prod_{y \neq x, x+1} \delta_{Q'(y), Q(y)},$$

and the diagonalization of the resulting effective Hamiltonian on a chain with N_r -sites. The matrix elements of the leg operators between the rung states equation (2.6)

$$\langle Q'(1), Q'(2)|h_l^{[2]}(1, \alpha')|Q(1), Q(2)\rangle \equiv$$

$$(Q'(1), Q'(2); Q(1), Q(2)), \qquad (2.18)$$

– the explicit spin dependence of the electrons has been omitted here – are listed in the following equations:

$$(0,0;0,0) = 0,$$
 $(\sigma,0;\sigma,0) = 0,$ (2.19)

$$(\sigma'_1, \sigma'_2; \sigma_1, \sigma_2) = \frac{\alpha'}{4} \langle \sigma'_1, \sigma'_2 | P(1, 2) - 1 | \sigma_1, \sigma_2 \rangle, (2.20)$$

$$(\sigma, 0; 0, \sigma) = -1,$$
 $(\sigma, 2; 2, \sigma) = -\frac{1}{2},$ (2.21)

$$(2, \sigma; 2, \sigma) = -\frac{\alpha'}{4}, \qquad (2, 2; 2, 2) = -\frac{\alpha'}{2}. \quad (2.22)$$

From these equations we can read off the effective Hamiltonian on a chain with N_r sites. Since the ground state structure differs for $\rho \leq \frac{1}{2}$ and $\rho \geq \frac{1}{2}$ as described in Section 2, we have to consider these two cases separately.

(1) For $\rho \leq 1/2$ only rung states with Q(x)=0 and Q(x)=1 are involved. From equations (2.19) and (2.20) we see that the effective Hamiltonian

$$\hat{H}_1(\alpha') = \sum_{r=1}^{N_r - 1} \hat{h}_1(x, x + 1, \alpha')$$
 (2.23)

with couplings:

$$\hat{h}_1(x, x+1, \alpha') = -P_{01}(x, x+1) + \frac{\alpha'}{4}Q_{11}(x, x+1)$$
 (2.24)

can be identified with a t-J model (2.3) on a chain with coupling $\alpha'/2$, which is just half of the leg coupling. Note also that the charge density on the chain with N_r sites

$$\rho_1 = \frac{Q}{N_r} = 2\rho \tag{2.25}$$

is just twice the charge density of the two leg ladder. In first order perturbation theory we get for the ground state energy on the two leg ladder:

$$E(\rho, t = 1, \alpha; t', \alpha') = -2N_r \rho + t' \hat{E}_1(\rho_1 = 2\rho, \alpha_1 = \alpha'/2) + O(t'^2). \quad (2.26)$$

Here $\hat{E}_1(\rho_1, \alpha_1)$ is the ground state energy of the "effective" t-J Hamiltonian (2.23) on a chain with N_r sites. According to equation (2.12) we can calculate the chemical potential from the first derivative with respect to the charge density:

$$\mu_1(\rho, \alpha; t', \alpha') = -1 + t'\hat{\mu}_1(\rho_1, \alpha_1)$$
 (2.27)

where

$$\hat{\mu}_1(\rho_1, \alpha_1) = \frac{1}{N_r} \frac{d\hat{E}_1}{d\rho_1}$$
 (2.28)

is the chemical potential of the t-J model on a chain with N_r sites and $\alpha_1 = \alpha'/2$ at $\rho_1 = 2\rho$.

(2) For $\rho \geq 1/2$ only rung states with $Q(x) = 1(\sigma = \pm 1)$ and Q(x) = 2 are involved. From equations (2.20–2.22) we see that the first part of the effective Hamiltonian:

$$\hat{H}_2(\alpha') = \sum_{r=1}^{N_r - 1} \hat{h}_2(x, x + 1, \alpha')$$
 (2.29)

with couplings:

$$\hat{h}_2(x, x+1, \alpha') = \left\{ -P_{21}(x, x+1) + \frac{\alpha'}{2} Q_{11}(x, x+1) + D_2(x, x+1) \right\}$$
(2.30)

is indeed a t-J model, if we treat electron pair states $|Q(x) = 2\rangle$ as quasi-holes. The third term (D_2) on the right-hand side of (2.30):

$$\langle Q(x), Q(x+1) | \hat{h}_2(x, x+1) | Q(x), Q(x+1) \rangle = \begin{cases} 0 & Q(x) = 1, \quad Q(x+1) = 1 \\ -\frac{\alpha'}{2} & Q(x) = 2, \quad Q(x+1) = 1 \\ -\alpha' & Q(x) = 2, \quad Q(x+1) = 2 \end{cases}$$
(2.31)

takes into account the non-vanishing diagonal terms (2.22). The ground state energy $\hat{E}_2(\rho_2, \alpha_2)$ of the effective Hamiltonian

$$\hat{H}_2 = \sum_x \hat{h}_2(x, x+1, \alpha') \tag{2.32}$$

on a chain of N_r sites fixes the first order perturbation correction to the ground state energy of the two leg ladder system:

$$E(\rho, t = 1, \alpha; t', \alpha') = -2N_r[1 - \alpha/2 - \rho(1 - \alpha)] + \frac{t'}{2}\hat{E}_2(\rho_2, \alpha_2) + O(t'^2) \quad (2.33)$$

where

$$\rho_2 = 2(1 - \rho), \quad \alpha_2 = \alpha'.$$
(2.34)

Finally, we get the following relation between the chemical potential $\mu(\rho, \alpha; t', \alpha')$ of the two leg ladder

$$\hat{\mu}_2(\rho_2, \alpha_2) = \frac{1}{N_r} \frac{d\hat{E}_2}{d\rho_2},$$
(2.35)

and for the effective Hamiltonian (2.32) on a chain of N_r sites:

$$\mu_2(\rho, \alpha; t', \alpha') = 1 - \alpha - \frac{t'}{2}\hat{\mu}_2(\rho_2, \alpha_2).$$
 (2.36)

Combining (2.27) and (2.36), we get for the width of the charge density plateau at $\rho = \frac{1}{2}$ in the first order perturbation theory:

$$W(\alpha, t', \alpha') \equiv \mu_2 - \mu_1$$

= 2 - \alpha - t' [\hat{\text{\$\theta}}_2(\rho_2 = 1, \alpha')/2
+ \hat{\text{\$\theta}}_1(\rho_1 = 1, \alpha'/2)]. (2.37)

3 Charge density plateaux on a three leg ladder

The perturbation treatment of the leg couplings will be applied now on the three leg ladders. The geometry and the notion of states can be seen in Figure 2.

The Hamiltonian (1.1) for the 3-leg (n = 3) case is again constructed from t - J couplings (2.3) on the rungs and the legs, respectively, and is given by the components

$$h_r^{[3]}(x,\alpha) = h(x, x + N_r, \alpha) + h(x + N_r, x + 2N_r, \alpha),$$

$$h_l^{[3]}(x,\alpha') = \sum_{l=1}^{3} h(x + (l-1)N_r, x + 1 + (l-1)N_r, \alpha').$$
(3.1)

3.1 0th order perturbation theory in t'

The lowest energy eigenstates on the rung Hamiltonian $h_r^{[3]}(x,\alpha)$ have been calculated in [15]

$$\begin{split} |Q(x)=0\rangle &= |0,0,0\rangle \\ |Q(x)=1\rangle &= \frac{1}{2} \left\{ |\sigma,0,0\rangle + \sqrt{2}|0,\sigma,0\rangle + |0,0,\sigma\rangle \right\} \\ |Q(x)=2\rangle &= \frac{1}{\sqrt{4+2b^2}} \{ |0,+,-\rangle - |0,-,+\rangle \\ &+ b|+,0,-\rangle - b|-,0,+\rangle \\ &+ |+,-,0\rangle - |-,+,0\rangle \} \\ |Q(x)=3\rangle &= \frac{1}{\sqrt{6}} \{ |\sigma,\sigma,-\sigma\rangle - 2|\sigma,-\sigma,\sigma\rangle \\ &+ |-\sigma,\sigma,\sigma\rangle \} \end{split} \tag{3.2}$$

with

$$b = \frac{-2}{\varepsilon_2} = \left(\sqrt{\alpha^2 + 8} - \alpha\right)/2, \qquad (3.3)$$

$$\sigma = \pm 1.$$

We have four types of states with charges Q(x) = 0, 1, 2, 3 respectively. Even charge states with Q(x) = 0, 2 carry total spin 0 and look like "composite bosons". Odd charge

states with Q(x) = 1,3 have total spin 1/2 and look like "composite fermions". The energies of the four states are:

$$\varepsilon_0 = 0, \quad \varepsilon_1 = -\sqrt{2}$$

$$\varepsilon_2 = -\frac{1}{2} \left(\sqrt{\alpha^2 + 8} + \alpha \right), \quad \varepsilon_3 = -\frac{3}{2} \alpha. \quad (3.4)$$

If we compute the ground state energy of the three leg ladder in the limit of vanishing leg coupling t'=0, we have to discriminate the following three cases:

(1) regime:
$$0 \le \rho \le 1/3$$
 $(\rho = 1/3 - 2q/3N_r)$

The ground state is a direct product of $N_r - 2q$ rung states $|Q(x) = 1(\sigma)\rangle$ with charge 1 and 2q rung states $|Q(x) = 0\rangle$ with charge 0.

$$E_1^{(0)}(\rho,\alpha) = (N_r - 2q)\varepsilon_1 + 2q\varepsilon_0 = 3N_r\rho\varepsilon_1. \tag{3.5}$$

The creation of a charge 2 state (|Q(x)| = 2) and a charge 0 state (|Q(x)| = 0) from two charge 1 states costs energy, since

$$\varepsilon_0 + \varepsilon_2 > 2\varepsilon_1 \quad \text{for} \quad \alpha < \frac{3}{\sqrt{2}}$$
 (3.6)

(2) regime:
$$1/3 \le \rho \le 2/3$$
 $(\rho = 1/3 + 2q/3N_r)$

The ground state is a direct product of $N_r - 2q$ rung states with charge 1 and 2q rung states with charge 2.

$$E_2^{(0)}(\rho, \alpha) = (N_r - 2q)\varepsilon_1 + 2q\varepsilon_2$$

= $N_r\{(2 - 3\rho)\varepsilon_1 + (3\rho - 1)\varepsilon_2\}.$ (3.7)

The creation of a charge 3 state and a charge 1 state from two charge 2 states costs energy since

$$\varepsilon_1 + \varepsilon_3 \ge 2\varepsilon_2 \quad \text{for} \quad \alpha > 0$$
 (3.8)

(3) regime:
$$2/3 \le \rho \le 1$$
 $(\rho = 1 - 2q/3N_r)$

The ground state is a product of $N_r - 2q$ rung states with charge 3 and 2q with charge 2.

$$E_3^{(0)}(\rho,\alpha) = (N_r - 2q)\varepsilon_3 + 2q\varepsilon_2(\alpha)$$

= $N_r\{(3\rho - 2)\varepsilon_3 + 3(1-\rho)\varepsilon_2\}.$ (3.9)

Note that the ground state energies are linear again in the charge density. Therefore, we get for the chemical potentials:

$$\mu(\rho) = \frac{1}{3N_r} \frac{dE}{d\rho} \tag{3.10}$$

$$\mu_1^{(0)}(\rho, \alpha) = \varepsilon_1 \qquad \text{for} \qquad 0 \le \rho \le 1/3 ,$$

$$\mu_2^{(0)}(\rho, \alpha) = \varepsilon_2 - \varepsilon_1 \qquad \text{for} \qquad 1/3 \le \rho \le 2/3 ,$$

$$\mu_3^{(0)}(\rho, \alpha) = \varepsilon_3 - \varepsilon_2 \qquad \text{for} \qquad 2/3 \le \rho \le 1 . \tag{3.11}$$

These are the results for the zeroth order (t'=0) in the leg couplings $[h_l \text{ in } (3.1)].$

Table 1. Effective couplings for a three leg ladder.

ρ	$0 \le \rho \le \frac{1}{3}$	$\frac{1}{3} \le \rho \le \frac{2}{3}$	$\frac{2}{3} \le \rho \le 1$
$Q_{\rm rung}$	Q = 0, 1	Q = 1, 2	Q = 2, 3
μ_{0th}	$arepsilon_1$	$\varepsilon_2 - \varepsilon_1$	$\varepsilon_3 - \varepsilon_2$
$ ho_{ ext{eff.}}$	$\rho_1 = 3\rho$	$\rho_2 = 2 - 3\rho$	$\rho_3 = 3\rho - 2$
H_{eff} .	$t_1\hat{H}_1(lpha_1)$	$t_2\hat{H}_2(lpha_2)$	$t_3\hat{H}_3(lpha_3)$
$t_{ m eff.}$	$t_1 = t'$	$t_2 = \frac{b^2 + 2\sqrt{2}b + 2}{4(b^2 + 2)}t'$	$t_3 = \frac{3}{2(b^2 + 2)}t'$
$\alpha_{\mathrm{eff.}}$	$\alpha_1 = \frac{3}{8}\alpha'$	$\alpha_2 = \frac{3(b^2 + 2)}{2(b^2 + 2\sqrt{2}b + 2)}\alpha'$	$\alpha_3 = \frac{2(b^2+2)}{3}\alpha'$
μ_{1st}	$t_1\hat{\mu}_1(\rho_1,\alpha_1)$	$-t_2\hat{\mu}_2(ho_2,lpha_2)$	$t_3\hat{\mu}_3(\rho_3,\alpha_3)$

3.2 1st order perturbation theory in t'

The first order calculation starts from the matrix elements of the leg couplings (3.1) between the zeroth order states (3.2). The results of this tedious calculation are summarized in Table 1.

The first row defines the 3 regimes of charge density ρ . In each regime, the zeroth order ground state is built up from direct products of rung cluster states with charge Q listed in the second row. The chemical potentials (3.10–3.11) in zeroth order are listed in the third row.

First order perturbation theory in the leg couplings leads to the effective Hamiltonians with nearest neighbour interactions on a chain of N_r sites in each sector of ρ (5th row of Tab. 1). These Hamiltonians contain two parts:

$$t_{j}\hat{H}_{j}(\alpha_{j}) = t_{j} \sum_{x=1}^{N_{r}-1} \hat{h}_{j}(x, x+1, \alpha_{j}), \quad (j=1, 2, 3),$$

$$= t_{j}[H_{t-J}(t=1, \alpha=\alpha_{j}) + D_{j}]. \quad (3.12)$$

The first one is of the t-J type (2.3) with effective hopping parameter t_j (6th row of Tab. 1) and spin coupling α_j (7th row of Tab. 1).

The second part D_j , j=1,2,3 with $D_1\equiv 0$ takes into account diagonal terms, which are not present in the t-J Hamiltonian:

$$\langle 1, 2|\hat{h}_2(x, x+1, \alpha')|1, 2\rangle = \frac{-(b^2+3)}{8(b^2+2)}\alpha'$$
 (3.13)

$$\langle 2, 2|\hat{h}_2(x, x+1, \alpha')|2, 2\rangle = \frac{-(b^4 + 2b^2 + 3)}{2(b^2 + 2)^2}\alpha'$$
 (3.14)

$$\langle 2, 3|\hat{h}_3(x, x+1, \alpha')|2, 3\rangle = \frac{-\alpha'}{2}$$
 (3.15)

$$\langle 3, 3|\hat{h}_3(x, x+1, \alpha')|3, 3\rangle = \frac{-\alpha'}{2}.$$
 (3.16)

Note that in the three leg ladder case the effective hopping terms t_2 and t_3 as well as the effective couplings α_2

and α_3 depend on the rung coupling α via (3.3). This does not occur in the two leg ladder case.

If we denote the ground state energies of the effective Hamiltonian H_j on a chain with N_r sites by $E_j(\rho_j, \alpha_j)$ and the corresponding chemical potential by

$$\hat{\mu}_j(\rho_j, \alpha_j) = \frac{1}{N_r} \frac{d\hat{E}_j}{d\rho_j} \tag{3.17}$$

we can express the first order correction to the chemical potential of the three leg ladder in terms of (3.17) (last row of Tab. 1). The relation between the charge density ρ on the ladder system and the charge density ρ_j in the effective one dimensional system can be found in the 4th row of Table 1.

4 Numerical results

In this section we are going to present numerical results for the ground state energies and the chemical potentials of the two and three leg ladder. Our results were obtained with open boundary conditions to facilitate the comparison with future DMRG calculations which can be done on larger systems. Other boundary conditions – e.g. periodic ones – can be incorporated as well.

4.1 Two leg ladders

The ground state energies $\hat{E}_j(\rho_j, \alpha_j)$ of the effective Hamiltonians \hat{H}_j j=1,2 (cf. (2.23) and (2.29)) on a chain with N_r sites have been computed for $N_r=8,10,12,14,16,(18)^1$ and

$$\alpha' = 2.7, \ \alpha_1 = \frac{\alpha'}{2} = 1.35, \ \alpha_2 = \alpha' = 2.7.$$
 (4.1)

For $\rho_1 = 0$ and $\rho_2 = 0$ these energies are known:

$$\hat{E}_1(\rho_1 = 0, \alpha_1) = 0, \qquad (4.2)$$

$$\hat{E}_2(\rho_2 = 0, \alpha_2) = -\alpha_2(N_r - 1). \tag{4.3}$$

For $\rho_1 = 1$ and $\rho_2 = 1$ the ground state energies are given by the nearest neighbour Heisenberg chain (with open boundary conditions)

$$\hat{E}_1(\rho_1 = 1, \alpha_1 = \alpha'/2) = \frac{1}{2}\hat{E}_2(\rho_2 = 1, \alpha_2 = \alpha')$$
. (4.4)

The finite-size dependence has been analyzed with an ansatz:

$$\hat{e}_j(\rho_j, \alpha_j) = \frac{\hat{E}_j(\rho_j, \alpha_j)}{N_r + N_j(\rho_j)}, \qquad j = 1, 2,$$
 (4.5)

for the ground state energies per site.

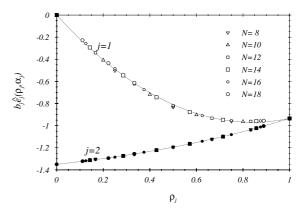


Fig. 3. Ground state energies per site $b_j \hat{e}_j(\rho_j, \alpha_j)$ (Eqs. (4.5) and (4.9)) for the effective Hamiltonians \hat{H}_j (j=1,2) of the two leg ladder with $\alpha_2=\alpha'=2.7$ – results for $N_r=8,10,\ldots,(18)$ and optimized polynomial fits.

Table 2. Parameters $a_j^{(0,1,2)}$, j=1,2 in the fit (4.9) for the energies $b_j \hat{e}_j(\rho_j,\alpha_j)$ shown in Figure 3.

j	$a_j^{(0)}$	$a_j^{(1)}$	$a_j^{(2)}$
1	-0.9346	-1.3769	0.0167
2	0.4154	-0.2384	0.0580

From (4.3) we get

$$N_2(\rho_i = 0) = -1. (4.6)$$

A finite-size analysis of the Heisenberg chain (t-J) chain at $\rho=1$ yields

$$N_i(\rho_i = 1) = -0.6, \qquad j = 1, 2,$$
 (4.7)

which means that finite-size effects change with ρ_j . We assume here a linear interpolation:

$$N_i(\rho_i) = -1 + 0.4\rho_i, \qquad j = 1, 2,$$
 (4.8)

between the boundary values (4.6) and (4.7).

Indeed, this procedure has the effect, that the data points for N=12,14,16,(18) follow unique curves $\hat{e}_1(\rho_1,\alpha_1)$ and $\hat{e}_2(\rho_2,\alpha_2)/2$ as is demonstrated in Figure 3.

The smooth dependence on the charge densities can be parametrized in such a way

$$b_j \hat{e}_j(\rho_j, \alpha_j) = b_j \hat{e}_j(\rho_j = 0, \alpha_j)$$

+ $\rho_j \left(a_j^{(0)} + a_j^{(1)} (1 - \rho_j) + a_j^{(2)} (1 - \rho_j)^2 \right)$ (4.9)

that the constraints (4.2-4.4) are built in explicitly:

$$b_1 = 1.0, \ \hat{e}_1(\rho_1 = 0, \alpha_1) = 0,$$

 $b_2 = 1/2, \ \hat{e}_2(\rho_2 = 0, \alpha_2) = -\alpha'.$ (4.10)

In Table 2 we list the coefficients of the fit (4.9).

In Figure 4 we compare the first order predictions (2.26), (2.33) for the ground state energies per

 $^{^{1}}$ The 18-site systems have been evaluated for Q=0,2,4,6,16,18. For the Q values inbetween, the dimension of the Hilbert spaces exceeded our computer capacities.

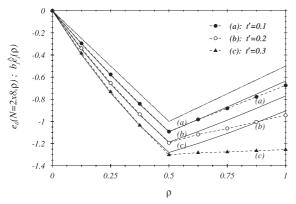


Fig. 4. Zero (dotted line) and first order (solid lines) predictions for two leg ladders with $\alpha=0.5, \alpha'=2.7$ and leg couplings t'=0.1(a), 0.2(b), 0.3(c) as well as the corresponding Lanczos energies for a 2×8 -site ladder (dashed lines).

rung with a Lanczos diagonalization on a two leg ladder with 8 rungs and couplings $\alpha=0.5,~\alpha'=2.7,~t'=0.1(a),0.2(b),0.3(c)$. The charge density plateau at $\rho=1/2$ is clearly visible in the discontinuous change of the slope in the energy per rung as function of ρ .

A remarkable agreement between Lanczos diagonalization (dashed curve) and the perturbative result including first order corrections (solid curve) is achieved for $\rho < 1/2$. A comparison with the zeroth order result (dotted curve) demonstrates that first order corrections are significant.

The situation for $\rho > 1/2$ is different. Here, we observe deviations between the Lanczos diagonalization (dashed curve) and the perturbative results (solid curve) which increase monotonically with t' and ρ . Note, that the spin coupling J' along the legs $(J' = t'\alpha')$ is already close to J'=1 for t'=0.3 and $\alpha'=2.7$. This means in particular for $\rho = 1$, where the t - J model reduces to a Heisenberg model with spin couplings J = 0.5 and J' = 0.81 (for t'=0.3 and $\alpha'=2.7$), that the product ansatz (2.14) with rung cluster states (2.6) is an inadequate starting point for a perturbative expansion. We expect improvements, if we start with a direct product of more complex clusters – e.g. plaquettes on the two leg ladder. Moreover, bound states (hole-pairs) may change the properties of ground state at large charge density $(\rho \to 1)$. This is indeed the case for $\alpha > 2$ [16].

Let us next turn to the phase diagram of the two leg ladder, which is defined by a vanishing plateau width $W(\alpha,t',\alpha')$ [(2.37)]. In general one has to discuss the phase boundary in the three dimensional parameter space (α,t',α') . In first order perturbation theory in t' (cf. Eq. (2.37)), however, it is sufficient to discuss the boundary in the plane $(2-\alpha)/t'$ versus α' :

$$\frac{2-\alpha}{t'} = \Delta(\alpha')$$

$$= \frac{1}{2}\hat{\mu}_2(\rho_2 = 1, \alpha') + \hat{\mu}_1(\rho_1 = 1, \alpha'/2). \quad (4.11)$$

We have determined the chemical potentials $\mu_1(\rho_1 = 1, \alpha'/2)$, $\mu_2(\rho_2 = 1, \alpha')$ from a numerical calculation of

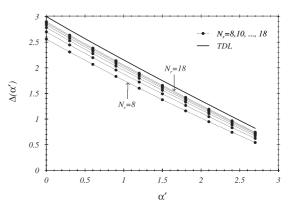


Fig. 5. α' -dependence (first order result) of the plateau width of the chemical potential of a two leg ladder at $\rho=1/2$ – finite system results and BST-evaluation of the thermodynamical limit (TDL).

the ground state energies per site (4.5) on systems with $N_r = 8, 10, 12, 14, 16, (18)$ and

$$\alpha' = 0.0, 0.3, \dots, 2.7$$
.

The α' -dependence of $\Delta(\alpha')$ (right-hand side of (4.11)) is shown in Figure 5. There is a monotonic finite-size dependence and the thermodynamical limit (solid curve) is estimated with the Bulirsch-Stoer (BST) algorithm [17]. The gapped phase with a nonvanishing plateau at $\rho=1/2$ is characterized by

$$\frac{2-\alpha}{t'} > \Delta(\alpha') \tag{4.12}$$

i.e. the formation of a plateau at $\rho = 1/2$ is favoured for

- small rung couplings $\alpha = J/t < 2$
- large leg couplings $\alpha' = J'/t'$.

4.2 Three leg ladders

The ground state energies $\hat{E}_j(\rho_j, \alpha_j)$ of the effective Hamiltonians (5th row of Tab. 1, Eqs. (3.12–3.16)) on a chain with N_r sites have been computed for $N_r = 8, 10, \ldots, 16, (18)$ and

$$\alpha = 0.5, \ \alpha' = 2.7$$
 (4.13)
 $\alpha_1 = 1.0125, \ \alpha_2 = 2.041, \ \alpha_3 = 6.132.$

The finite-size dependence has been analyzed with an ansatz of the type (4.5) for the ground state energies per site $\hat{e}_j(\rho_j, \alpha_j)$.

The constraints at $\rho_j = 0$ and at $\rho_j = 1$ are taken into account in the linear interpolations

 $N_3(\rho_3) = -1 + 0.232\rho_3$.

$$N_j(\rho_j) = -1 + 0.4\rho_j, \qquad j = 1, 2,$$

(4.14)

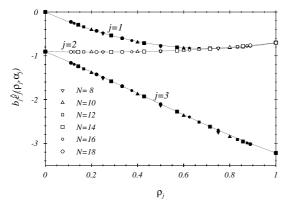


Fig. 6. Ground state energies per site $b_j \hat{e}_j(\rho_j, \alpha_j)$ (4.5, 4.9) for the effective Hamiltonians \hat{H}_j (j = 1, 2, 3) of the three leg ladder with $\alpha = 0.5, \alpha' = 2.7$ – results for $N_r = 8, 10, \ldots, (18)$ and optimized polynomial fits.

Table 3. Parameters $a_j^{(0,1,2)}$, j=1,2,3 in the fits for the energies $b_j \hat{e}_j(\rho_j,\alpha_j)$ shown in Figure 6.

j	$a_j^{(0)}$	$a_j^{(1)}$	$a_j^{(2)}$
1	-0.7010	-1.6209	-0.0260
2	0.2054	-0.4364	0.1630
3	-2.3129	-0.4460	0.5739

The factors b_i in Figure 6, (4.16)

$$b_j = \frac{t_j}{t'} \tag{4.15}$$

reflect the "renormalization" of the hopping term (6th row in Tab. 1). A plot of $b_j e_j(\rho_j, \alpha_j)$, j = 1, 2, 3, $\alpha = 0.5$, $\alpha' = 2.7$ on the finite systems is shown in Figure 6.

The data points do not scatter with the system size but follow unique curves, which can be considered as a reliable estimate of the thermodynamical limit. Their dependence on the effective charge densities $\rho_{\rm eff}$ (fourth row in Tab. 1) is parametrized by an ansatz of type (4.9). The resulting coefficients with

$$\begin{split} b_1 &= 1.0, & \hat{e}_1(\rho_1 = 0, \alpha_1) = 0, \\ b_2 &= 0.49618, & \hat{e}_2(\rho_2 = 0, \alpha_2) = -\frac{8}{3}\alpha_2\frac{b^4 + 2b^2 + 3}{2(b+2)^2}, \\ b_3 &= 0.44028, & \hat{e}_3(\rho_3 = 0, \alpha_3) = -\alpha_3\frac{b^4 + 2b^2 + 3}{2(b+2)^2}, (4.16) \end{split}$$

are listed in Table 3.

Looking at the phase diagram of the three leg ladder we have to distinguish four regimes in the three dimensional parameter space of α, t', α' :

I plateaux at
$$\rho = 1/3, 2/3$$

II plateau at
$$\rho = 1/3$$
, no plateau at $\rho = 2/3$

III plateau at
$$\rho = 2/3$$
, no plateau at $\rho = 1/3$

IV no plateau.

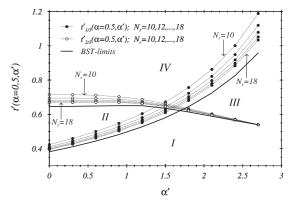


Fig. 7. First order results for the (t', α') -dependence of the boundaries of the plateau regimes (I-IV) of a three leg ladder – finite system results and BST-evaluation of the TDL.

The phase boundaries are defined by the vanishing of the plateau width (cf. rows 3 and 8 in Tab. 1):

$$\begin{split} \rho &= 1/3: \\ W_{1/3} &= \varepsilon_2 - 2\varepsilon_1 \\ &-t' \left(b_2 \hat{\mu}_2(\rho_2 = 1, \alpha_2) + b_1 \hat{\mu}_1(\rho_1 = 1, \alpha_1) \right) \\ \rho &= 2/3: \\ W_{2/3} &= \varepsilon_3 + \varepsilon_1 - 2\varepsilon_2 \\ &+t' \left(b_3 \hat{\mu}_3(\rho_3 = 0, \alpha_3) + b_2 \hat{\mu}_2(\rho_2 = 0, \alpha_2) \right). \end{split} \tag{4.18}$$

In first order perturbation theory the widths are linear in t^\prime and it is therefore convenient to represent the phase boundaries in the form

$$t'_{1/3} = t'_{1/3}(\alpha, \alpha')$$

$$= \frac{\varepsilon_2 - 2\varepsilon_1}{(b_1\hat{\mu}_1(\rho_1 = 1, \alpha_1) + b_2\hat{\mu}_2(\rho_2 = 1, \alpha_2))}$$

$$t'_{2/3} = t'_{2/3}(\alpha, \alpha')$$

$$= -\frac{\varepsilon_3 + \varepsilon_1 - 2\varepsilon_2}{(b_3\hat{\mu}_3(\rho_3 = 0, \alpha_3) + b_2\hat{\mu}_2(\rho_2 = 0, \alpha_2))}.$$
(4.19)

The four phases defined above are characterized by

$$\begin{array}{ll} \mathrm{I} & t'_{1/3}(\alpha,\alpha') \geq t' \geq 0 \,, & t'_{2/3}(\alpha,\alpha') \geq t' \geq 0 \,, \\ \mathrm{II} & t'_{1/3}(\alpha,\alpha') \geq t' \geq 0 \,, & t' \geq t'_{2/3}(\alpha,\alpha') \,, \\ \mathrm{III} & t' \geq t'_{1/3}(\alpha,\alpha') \,, & t'_{2/3}(\alpha,\alpha') \geq t' \geq 0 \,, \\ \mathrm{IV} & t' \geq t'_{1/3}(\alpha,\alpha') \,, & t' \geq t'_{2/3}(\alpha,\alpha') \,. \end{array}$$

We have computed the phase boundaries $t'_{1/3}(\alpha, \alpha')$ and $t'_{2/3}(\alpha, \alpha')$ from the ground state energies of the effective Hamiltonians \hat{H}_j (3.12) on systems with $10, 12, \ldots, (18)$ sites for

$$\alpha = 1/2$$
, $\alpha' = 0.0, 0.3, \dots, 2.7$.

This projection of the phase diagram is shown in Figure 7. The thermodynamical limits (TDLs; solid curves) are estimated with the BST algorithm [17].

5 Discussion and perspectives

Quasi onedimensional quantum systems – like the Heisenberg model or the t-J model – defined on ladders with l legs show a characteristic sequence of gaps in their spectrum. They appear as plateaux in the magnetization curve M(B) and the charge density $\rho(\mu)$ (as functions of the magnetic field B and chemical potential μ , respectively) for the spin and charge degrees of freedom. The quantization rule of Oshikawa, Yamanaka and Affleck [13] defines the values of M and ρ where these might occur. The mechanism which creates the plateaux can be studied in a perturbation expansion in the leg couplings t'; $\alpha' = J'/t'$ fixed. To zeroth order the ground states – at fixed magnetization M and/or charge density ρ – are products of rung cluster states. The latter can be classified by a cluster spin S_3 and charge Q. First order perturbation theory leads to an effective interaction between the rung cluster states.

We have studied in this paper the 0th and 1st order perturbation expansion in the leg coupling t' (for α' fixed) on two and three leg ladders. The magnetization – given by the total spin – has been assumed to be zero. Our results on the two leg ladder can be summarized as follows:

i) The ground state in the two regimes

$$0 \le \rho \le 1/2$$
 $(Q = 0, 1)$
 $1/2 \le \rho \le 1$ $(Q = 1, 2)$

is built up from a direct product of rung cluster states with Q = 0, 1 and Q = 1, 2, respectively.

Even charge states (Q=0,2) have total spin 0 and are bosonic, odd charge states (Q=1,(3 for the 3-leg ladder)) have total spin 1/2 and are fermionic. For $\rho=0,1/2,1$ all rung cluster states have the same charge Q=0,1,2, respectively.

- ii) The effective Hamiltonian, which describes the interaction between the rung cluster states in first order perturbation theory, looks like a generalized t-J model on a chain, if we treat fermionic states (Q=1) as electrons, bosonic ones (Q=0,2) as holes. A comparison of the perturbative results with exact diagonalizations yields good agreement for the ground state energies in the first regime $(\rho < 1/2, \, t' \le 0.3)$, but increasing deviations with ρ and t' in the second one.
- iii) Increasing the size of the cluster we started with, will improve these results and might reveal further gaps in the spectrum. In a next step we will consider a direct product of plaquette cluster states on the two leg ladder (Fig. 1). Here, cluster ground states with charges Q(x) = 0, 1, 2, 3, 4 occur, which might induce additional plateaux at $\rho = 1/4$ and $\rho = 3/4$. Indeed, evidence for the existence of a long range charge density wave state in the t-J two leg ladder at $\rho = 3/4$ has been found in a DMRG calculation [18].
- iv) We have studied the stability of the charge density plateau and the phase diagram in the regime where first order perturbation theory is applicable. We found that the formation of a charge density plateau is favoured for

- small values of the couplings $\alpha = J/t$ on the rungs
- large values of the couplings $\alpha' = J'/t'$ on the legs.

In the three leg ladder case, the ground states in 0th order are built up again from rung cluster states with two charges:

$$0 \le \rho \le 1/3 \qquad (Q = 0, 1)$$

$$1/3 \le \rho \le 2/3 \qquad (Q = 1, 2)$$

$$2/3 \le \rho \le 1 \qquad (Q = 2, 3).$$

For $\rho=0,1/3,2/3,1$ all the rung clusters have the same charges: $Q=0,\,Q=1,\,Q=2,\,Q=3,$ respectively.

The method developed here for ladder systems should be applicable whenever finite clusters containing the "large" couplings can be defined in a natural way. If we for instance consider the t-J model on a Shastry-Sutherland lattice [19], the "large" couplings on the diagonals define two site clusters. The same arguments we developed here for the two leg ladder (with two site clusters) can be repeated and we expect again a charge density plateau at $\rho=1/2$. Of course the effective interaction between the cluster states depend on the geometry of the lattice and are therefore different for the Shastry-Sutherland lattice and the two leg ladder.

The method developed here for charge density plateaux is also applicable to magnetization plateaux provided that finite clusters containing the "large" couplings can be defined in a natural way. Again, the Heisenberg model on a Shastry-Sutherland lattice [19] is a good example.

However, for a realistic description of the experimentally found magnetization plateaux M=S/N=1/6,1/8,1/16 (S total spin, N total number of sites) one should start from clusters which at least – requiring integer total spin for the clusters – contain 6,8,16 sites! Of course the computation of the cluster ground states and in particular of their interaction becomes more involved for decreasing magnetization values.

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