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Spectrum of boundary states in the open Hubbard chain

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Abstract. We use the Bethe ansatz solution for the one-dimensional Hubbard model with open boundary conditions and applied boundary fields to study the spectrum of bound states at the boundary. Depending on the strength of the boundary potentials, one finds that the true ground state contains a single charge or, for boundary potentials comparable with the Hubbard interaction, a pair of electrons in a bound state. If these are left unoccupied one finds holon and spinon bound states. We compute the finite size corrections to the low-lying energies in this system and use the predictions of boundary conformal field theory to study the exponents related to the orthogonality catastrophe.

1. Introduction

The recent advances in the understanding of boundary effects in low-dimensional quantum systems due to the predictions of boundary conformal field theory [1–3] and the formulation of Bethe ansatz soluble models on open lattices with potentials applied on the boundary sites [4–7] have opened new possibilities to study the effects of correlations and quantum fluctuations on long-standing problems such as the orthogonality catastrophe [8, 9] and edge singularities in optical absorption experiments [10–12].

The effect of electronic correlations on the bulk critical behaviour of $(1+1)$-dimensional quantum systems has been studied successfully in the Tomonaga–Luttinger model which then can be handled using field theoretical methods [13–15]. Studies of integrable lattice models have added insights to this problem since, for example the dependence of critical exponents on microscopic parameters and their behaviour due to lattice effects (back scattering, Mott transition) can be computed exactly [16–18]. Similarly, one expects additional information from studies of lattice models for interacting electrons with open boundaries [4, 19, 20]. Besides giving a deeper understanding of previous predictions, these lattice models have features not easily included into the continuum description: local chemical potentials in the former lead to a sequence of bound states (see, e.g. [21]) which are expected to influence the critical properties of the boundary.

In this paper we consider the Hubbard model on a chain of L sites subject to an additional chemical potential p at the first site. The Hamiltonian is given by

$$\mathcal{H} = -\sum_{\sigma,\, j=1}^{L-1} (c^{\dagger}_{j,\sigma} c_{j+1,\sigma} + \mathrm{hc}) + 4u \sum_{j=1}^{L} n_{j\uparrow} n_{j\downarrow} + \mu \hat{N} - \frac{h}{2}(\hat{N} - 2\hat{N}_{\downarrow}) - p(\hat{N}_{1,\uparrow} + \hat{N}_{1,\downarrow}). \tag{1.1}$$

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For $p = 0$ this model has been solved by Schulz using the coordinate Bethe ansatz [4]. Recently, this solution has been extended to non-vanishing p [19] and the integrability of the model has been established in the framework of the quantum inverse scattering method [22]. The Bethe ansatz equations (BAE) determining the spectrum of (1.1) in the N_e-particle sector with magnetization $M = \frac{1}{2}N_e - N_\downarrow$ read [19]

$$\begin{aligned} &\mathrm{e}^{\mathrm{i}k_j 2(L+1)} s_p(k_j) = \prod_{\beta=1}^{N_\downarrow} e_{2u}(\eta_j - \lambda_\beta) e_{2u}(\eta_j + \lambda_\beta) \qquad j = 1, \ldots, N_e \\ &\prod_{j=1}^{N_e} e_{2u}(\lambda_\alpha - \eta_j) e_{2u}(\lambda_\alpha + \eta_j) = \prod_{\substack{\beta=1 \\ \beta\neq\alpha}}^{N_\downarrow} e_{4u}(\lambda_\alpha - \lambda_\beta) e_{4u}(\lambda_\alpha + \lambda_\beta) \qquad \alpha = 1, \ldots, N_\downarrow \end{aligned} \tag{1.2}$$

with $e_n(x) = \frac{x+\mathrm{i}\frac{n}{2}}{x-\mathrm{i}\frac{n}{2}}$, $s_p(k_j) = \left(\frac{1-p\mathrm{e}^{-\mathrm{i}k_j}}{1-p\mathrm{e}^{\mathrm{i}k_j}}\right)$ and $\eta_j = \sin k_j$. The energy of the corresponding eigenstate of (1.1) is

$$E = \sum_{j=1}^{N_e} \left(\mu - \frac{h}{2} - 2\cos k_j\right) + hN_\downarrow. \tag{1.3}$$

Using the global spin- and η-pairing SU(2) symmetry of the Hubbard model the Bethe states extended by those obtained by application of the corresponding raising operators have been shown to form a complete basis of the Hilbert space of the system [23]. A non-zero boundary potential destroys the η-symmetry of the model and the question of completeness should be considered again. Numerical solutions of (1.2) for small p show that there exist complex combinations of two k and one λ which coincide with one η-pair in the limit of $p \to 0$. In the following we only consider the ground state and the low-lying excitations of the system, so we can neglect these kinds of complex solutions as they belong to the highly excited states of the system [24]. However, for sufficiently strong attractive boundary potentials $p > 1$ we find that there exist other complex solutions which turn out to correspond to bound states in these potentials (note that these states do not appear in the case $p < 1$ studied in [19]). These solutions need to be considered to obtain the true ground state of the system. We find that despite the presence of several complex parameters in the ground-state configuration the low-energy spectrum of the many-particle system can still be described in the Tomonaga–Luttinger picture equivalent to two $c = 1$ conformal field theories. The case $p > 1$ will be studied in detail in the next section.

2. Boundary bound states

From a physical point of view it is clear that the ground state of the model contains a bound state at the first site for sufficiently large p. Numerical solutions of the BAE show that this is indeed the fact for $p > 1$ where a complex quasimomentum k is present in the ground-state configuration. A similar situation has been found in the XXZ Heisenberg chain with a boundary magnetic field [21, 25] and in a continuum model related to the Kondo problem [26].

Increasing the boundary potential further we find that additional complex parameters are added to the gound-state solution of (1.2). In the thermodynamic limit ($L \to \infty$) we have to distinguish three different regions where the BAE describing the ground state are modified due to the presence of these complex roots†:

† In principle one is free to leave the bound states empty. This gives rise to another continuum of states. These states become important if one considers, for example, multiple Fermi edge singularities in the presence of bound states [12, 27].

I. $1 < p < p_1 = u + \sqrt{1+u^2}$

$$\mathrm{e}^{\mathrm{i}k_j 2(L+1)} s_p(k_j) = \prod_{\beta=1}^{N_\downarrow} e_{2u}(\eta_j - \lambda_\beta) e_{2u}(\eta_j + \lambda_\beta) \qquad j = 1, \ldots, N_e - 1$$

$$e_{2u-2t}(\lambda_\alpha) e_{2u+2t}(\lambda_\alpha) \prod_{j=1}^{N_e-1} e_{2u}(\lambda_\alpha - \eta_j) e_{2u}(\lambda_\alpha + \eta_j) = \prod_{\substack{\beta=1 \\ \beta\neq\alpha}}^{N_\downarrow} e_{4u}(\lambda_\alpha - \lambda_\beta) e_{4u}(\lambda_\alpha + \lambda_\beta) \qquad (2.1)$$

$$\alpha = 1, \ldots, N_\downarrow$$

with the complex solution $k_{N_e} = \mathrm{i}\ln(p)$ (with exponential accuracy in the limit $L \to \infty$) and $t = -\mathrm{i}\sin k_{N_e} = \frac{1}{2}(p - \frac{1}{p}) < u$. The contribution of this bound state to the energy (1.3) is given by $E_1 = -p - \frac{1}{p} + \mu - \frac{h}{2}$. This complex solution corresponds to a charge bound to the first site, as the quasimomenta k parametrize the charge part of the states.

II. $p_1 < p < p_2 = 2u + \sqrt{1+4u^2}$

Larger values of the boundary potential lead to an additional complex solution in the spin part: $\lambda_{N_\downarrow} = \mathrm{i}(t-u)$ ($t > u$ in this region) and the following modified BAE:

$$\mathrm{e}^{\mathrm{i}k_j 2(L+1)} s_p(k_j) = e_{4u-2t}(\eta_j) e_{2t}(\eta_j) \prod_{\beta=1}^{N_\downarrow - 1} e_{2u}(\eta_j - \lambda_\beta) e_{2u}(\eta_j + \lambda_\beta)$$

$$j = 1, \ldots, N_e - 1$$

$$\prod_{j=1}^{N_e-1} e_{2u}(\lambda_\alpha - \eta_j) e_{2u}(\lambda_\alpha + \eta_j) = e_{2t-2u}(\lambda_\alpha) e_{6u-2t}(\lambda_\alpha) \prod_{\substack{\beta=1 \\ \beta\neq\alpha}}^{N_\downarrow - 1} e_{4u}(\lambda_\alpha - \lambda_\beta) e_{4u}(\lambda_\alpha + \lambda_\beta) \qquad (2.2)$$

$$\alpha = 1, \ldots, N_\downarrow - 1.$$

Again, this state can be interpreted as that of a charge bound to the surface. The physical excitations in the spin sector—so-called *spinons*—correspond to *holes* in the distribution of spin rapidities λ which are still real.

III. $p > p2$

For boundary potentials larger than the Hubbard interaction $p'4u$ a pair of electrons forming a singlet is bound to the surface, parametrized by $\lambda_{N_\downarrow} = \sin k_{N_e} - \mathrm{i}u = \sin k_{N_e-1} + \mathrm{i}u = \mathrm{i}(t-u)$. The resulting BAE are

$$\mathrm{e}^{\mathrm{i}k_j 2(L+1)} s_p(k_j) e_{2t-4u}(\eta_j) = e_{2t}(\eta_j) \prod_{\beta=1}^{N_\downarrow - 1} e_{2u}(\eta_j - \lambda_\beta) e_{2u}(\eta_j + \lambda_\beta) \qquad j = 1, \ldots, N_e - 2$$

$$\prod_{j=1}^{N_e-2} e_{2u}(\lambda_\alpha - \eta_j) e_{2u}(\lambda_\alpha + \eta_j) = \prod_{\substack{\beta=1 \\ \beta\neq\alpha}}^{N_\downarrow - 1} e_{4u}(\lambda_\alpha - \lambda_\beta) e_{4u}(\lambda_\alpha + \lambda_\beta) \qquad \alpha = 1, \ldots, N_\downarrow - 1. \qquad (2.3)$$

The energy of the second complex solution k_{N_e-1} is given by $E_2 = -2\sqrt{1+(t-2u)^2} + \mu - \frac{h}{2}$.

Note that region I is already realized in the ferromagnetic case with spin-$\uparrow$ electrons only. As $t = u$ ($p = p_1$) the index of the first factor in the λ-equation of (2.1) changes

the sign, allowing for the complex λ-solution. A similar change occurs in (2.1) for $t = 2u$ ($p = p2$) leading to the second complex k-solution. No such point exists in (2.3), hence no further complex solutions are expected in the ground state—in perfect agreement with the physical intuition.

Recently, the BAE for the model with a boundary magnetic field ($-p_1(n_{1\uparrow} - n_{1\downarrow})$) applied at the first site have been constructed [28, 29]. This field induces an additional phase factor $-e_{2u-2t}(\lambda_\alpha)$ in the second equation of (1.2) which cancels the first factor in (2.1) (up to a sign). As a consequence, we do not expect another complex solution to exist in the ground state besides the first one for this case.

Using standard procedures the BAE for the ground state and low-lying excitations can be rewritten as linear integral equations for the densities $\rho_c(k)$ and $\rho_s(\lambda)$ of real (positive) quasimomenta k_j and spin rapidities λ_α, respectively. Identification of positive and negative k and λ allows us to symmetrize the resulting equations with the usual result

$$\begin{pmatrix} \rho_c \\ \rho_s \end{pmatrix} = \begin{pmatrix} \frac{1}{\pi} + \frac{1}{L}\hat{\rho}_c^0 \\ \frac{1}{L}\hat{\rho}_s^0 \end{pmatrix} + \begin{pmatrix} 0 & \cos k a_{2u}(\eta - \lambda') \\ a_{2u}(\lambda - \eta') & -a_{4u}(\lambda - \lambda') \end{pmatrix} * \begin{pmatrix} \rho_c \\ \rho_s \end{pmatrix}. \tag{2.4}$$

Here we have introduced $a_y(x) = \frac{1}{2\pi}\frac{y}{y^2/4+x^2}$ and $f * g$ denotes the convolution $\int_{-A}^{A} \mathrm{d}y\, f(x-y)g(y)$ with the boundaries k_0 and λ_0 in the charge and spin sector, respectively. The latter are fixed by the conditions

$$\begin{aligned} \int_{-k_0}^{k_0} \mathrm{d}k\, \rho_c &= \frac{2\left[N_e - \theta(p-1) - \theta(p-p_2)\right] + 1}{L} \\ \int_{-\lambda_0}^{\lambda_0} \mathrm{d}\lambda\, \rho_s &= \frac{2\left[N_\downarrow - \theta(p-p_1)\right] + 1}{L} \end{aligned} \tag{2.5}$$

where $\theta(x)$ is the Heaviside step function. The driving terms of the $1/L$-corrections in the different regions are given by

$$\hat{\rho}_c^0(k) = \frac{1}{\pi} - \cos k a_{2u}(\eta) + \frac{\cos kp - p^2}{\pi(p^2 + 1 - 2p\cos k)} + \theta(p - p1)\cos k[a_{2t}(\eta) + a_{4u-2t}(\eta)] \tag{2.6}$$

for the charge sector† and

$$\hat{\rho}_s^0(\lambda) = a_{4u}(\lambda) + \begin{cases} 0 & p < 1 \\ a_{2u-2t}(\lambda) + a_{2u+2t}(\lambda) & \mathrm{I} \\ -a_{2t-2u}(\lambda) - a_{6u-2t}(\lambda) & \mathrm{II} \\ 0 & \mathrm{III} \end{cases} \tag{2.7}$$

for the spin sector. In terms of the dressed energies ε_c and ε_s which satisfy the same integral equations as in the Hubbard model with periodic boundary conditions:

$$\begin{pmatrix} \varepsilon_c \\ \varepsilon_s \end{pmatrix} = \begin{pmatrix} \mu - \frac{h}{2} - 2\cos k \\ h \end{pmatrix} + \begin{pmatrix} 0 & a_{2u}(\eta - \lambda') \\ a_{2u}(\lambda - \eta')\cos k' & -a_{4u}(\lambda - \lambda') \end{pmatrix} * \begin{pmatrix} \varepsilon_c \\ \varepsilon_s \end{pmatrix} \tag{2.8}$$

the energy of the state can be expressed as:

$$\begin{aligned} \frac{E}{L} = e_\infty + \frac{1}{L}f_\infty + \mathrm{o}\left(\frac{1}{L}\right) &= \frac{1}{2}\int_{-k_0}^{k_0} \mathrm{d}k\, \frac{\varepsilon_c(k)}{\pi} \\ &+ \frac{1}{2L}\left[\int_{-k_0}^{k_0} \mathrm{d}k\, \varepsilon_c(k)\hat{\rho}_c^0(k) + \int_{-\lambda_0}^{\lambda_0} \mathrm{d}\lambda\, \varepsilon_s(\lambda)\hat{\rho}_s^0(\lambda)\right] \end{aligned}$$

† Note that the index of a_{4u-2t} changes sign at $p = p_2$.

$$+\frac{1}{2L}\left[-(\mu+\frac{h}{2}-2)+2\theta(p-1)E_1+2h\theta(p-p_1)+2\theta(p-p_2)E_2\right]$$
$$+\mathrm{o}\left(\frac{1}{L}\right). \tag{2.9}$$

3. Ground-state expectation value of N_1

The ground-state expectation values for the occupation of the boundary site $\langle N_1\rangle$ can be calculated from the identity $\langle N_1\rangle = -\partial E/\partial p$. With (2.9) we obtain

$$\langle N_1\rangle = -\frac{1}{2}\Bigg[\int_{-k_0}^{k_0}\mathrm{d}k\,\varepsilon_c(k)\frac{\partial\hat{\rho}_c^0(k)}{\partial p}+\int_{-\lambda_0}^{\lambda_0}\mathrm{d}\lambda\,\varepsilon_s(\lambda)\frac{\partial\hat{\rho}_s^0(\lambda)}{\partial p}$$
$$+2\theta(p-1)\frac{\partial E_1}{\partial p}+2\theta(p-p_2)\frac{\partial E_2}{\partial p}\Bigg]. \tag{3.1}$$

In absence of a bulk magnetic field h the ground state of the Hubbard model is known to be a singlet (for even particle number) corresponding to $\lambda_0=\infty$. In this case the system of integral equations (2.8) can be reduced to a scalar one

$$\varepsilon_c(k)=\mu-2\cos k+\int_{-k_0}^{k_0}\mathrm{d}k'\,G_{2u}^{2u}(\eta-\eta')\cos k'\varepsilon_c(k') \tag{3.2}$$

with ($y>0$, $y+z>0$)

$$G_y^z(\lambda)=\frac{1}{2\pi y}\,\mathrm{Re}\left\{\Psi\left(\frac{3}{4}+\frac{z}{4y}+\mathrm{i}\frac{\lambda}{2y}\right)-\Psi\left(\frac{1}{4}+\frac{z}{4y}+\mathrm{i}\frac{\lambda}{2y}\right)\right\}$$
$$G_y^z(\omega)=\frac{\mathrm{e}^{-\frac{z}{2}|\omega|}}{2\cosh\left(\frac{y}{2}\omega\right)} \tag{3.3}$$

(Ψ is the digamma function). We obtain

$$\langle N_1\rangle = -\theta(p-1)\frac{\partial E_1}{\partial p}-\theta(p-p_2)\frac{\partial E_2}{\partial p}$$
$$-\frac{1}{2}\int_{-k_0}^{k_0}\mathrm{d}k\,\varepsilon_c(k)\begin{cases}\gamma_p(k) & p<1\\ \gamma_p(k)+\dfrac{\partial}{\partial p}\left(G_{2u}^{2u-2t}(\eta)+G_{2u}^{2u+2t}(\eta)\right)\cos k & \text{I, II}\\ \gamma_p(k)+\dfrac{\partial}{\partial p}\left(a_{2t}(\eta)-a_{2t-4u}(\eta)\right)\cos k & \text{III}\end{cases} \tag{3.4}$$

with $\gamma_p(k)=\frac{\cos kp^2+\cos k-2p}{\pi(p^2+1-2\cos kp)^2}$. In the limit of $p\to\infty$ only the the first two parts survive and we get the expected result $\langle N_1\rangle=2$. Some numerical results are shown in figure 1.

4. Finite size corrections

Following [30] we can calculate the finite size spectrum of the model, reproducing the result of [19]:

$$E=Le_\infty+f_\infty+\frac{\pi v_c}{L}\left\{-\frac{1}{24}+\frac{1}{2\det^2(Z)}[(\Delta N_c^0-\theta_p^c)Z_{ss}-(\Delta N_s^0-\theta_p^s)Z_{cs}]^2+N_c^+\right\}$$
$$+\frac{\pi v_s}{L}\left\{-\frac{1}{24}+\frac{1}{2\det^2(Z)}[(\Delta N_s^0-\theta_p^s)Z_{cc}-(\Delta N_c^0-\theta_p^c)Z_{sc}]^2+N_s^+\right\}. \tag{4.1}$$

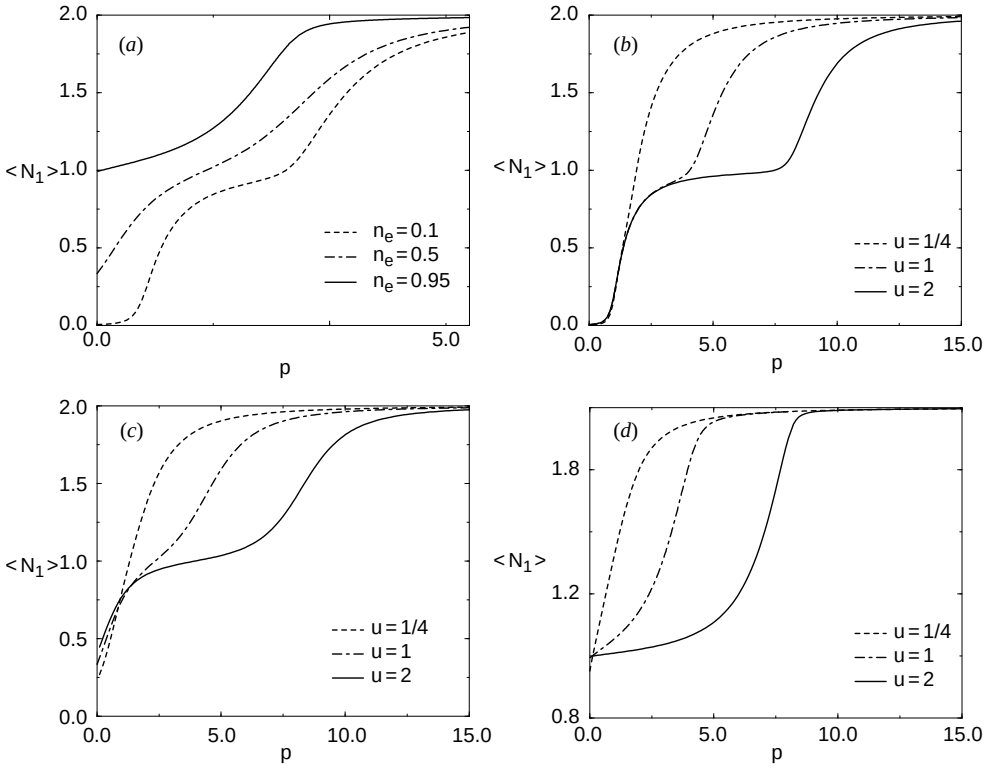

Figure 1. Ground-state expectation value of N_1 as a function of the boundary potential p for $u = 1$ and several electron densities n_e; (*a*) fixed density $n_e = 0.1$, (*b*) $n_e = 0.5$, (*c*) $n_e = 0.95$ and (*d*) several values of u.

Here $N^+_{c,s}$ are non-negative integers counting the number of particle hole excitations at the Fermi points, the Fermi velocities are given by $v_c = \frac{\varepsilon_c'(k_0)}{\pi\rho_c(k_0)}$ and $v_s = \frac{\varepsilon_s'(\lambda_0)}{\pi\rho_s(\lambda_0)}$. Z is the dressed charge matrix

$$Z = \begin{pmatrix} Z_{cc} & Z_{cs} \\ Z_{sc} & Z_{ss} \end{pmatrix} = \begin{pmatrix} \xi_{cc}(k_0) & \xi_{sc}(k_0) \\ \xi_{cs}(\lambda_0) & \xi_{ss}(\lambda_0) \end{pmatrix}^{\top} \tag{4.2}$$

given in terms of the integral equation

$$\begin{pmatrix} \xi_{cc}(k) & \xi_{sc}(k) \\ \xi_{cs}(\lambda) & \xi_{ss}(\lambda) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} 0 & a_{2u}(\eta - \lambda') \\ a_{2u}(\lambda - \eta')\cos k' & -a_{4u}(\lambda - \lambda') \end{pmatrix} * \begin{pmatrix} \xi_{cc}(k') & \xi_{sc}(k') \\ \xi_{cs}(\lambda') & \xi_{ss}(\lambda') \end{pmatrix}. \tag{4.3}$$

The $\Delta N^0_{c,s}$ are given by $\Delta N^0_c = N_e - Ln_e$ and $\Delta N^0_s = N_\downarrow - Ln_\downarrow$, where n_e and $n_\downarrow$ denote the total density of electrons and spin-$\downarrow$ electrons of the reference state which we define through

$$n_e = \tfrac{1}{2}\int_{-k_0}^{k_0} \mathrm{d}k\, \rho_c^{(0)}(k) \qquad n_\downarrow = \tfrac{1}{2}\int_{-\lambda_0}^{\lambda_0} \mathrm{d}\lambda\, \rho_s^{(0)}(\lambda). \tag{4.4}$$

Here $\rho_{cs}^{(0)}$ should be computed from (2.4) *without* the $1/L$ terms, i.e. $\hat{\rho}^0_{cs} \equiv 0$ (note that this choice differs from that used in [19]). This choice implies that for a given boundary

condition $\Delta N^0_{c,s} = \theta^{c,s}_p$ are non-zero in the corresponding ground state. The shifts $\theta^{c,s}_p$ are due to the $\frac{1}{L}$-terms in (2.4):

$$\begin{aligned}\theta^c_p &= \tfrac{1}{2}\left(\int_{-k_0}^{k_0} \mathrm{d}k\, \hat{\rho}_c - 1 + 2\theta(p-1) + 2\theta(p-p2)\right)\\ \theta^s_p &= \tfrac{1}{2}\left(\int_{-\lambda_0}^{\lambda_0} \mathrm{d}\lambda\, \hat{\rho}_s - 1 + 2\theta(p-p1)\right)\end{aligned} \tag{4.5}$$

with $\hat{\rho}_c$ and $\hat{\rho}_s$ denoting the solution of (2.4) without the $\frac{1}{\pi}$ driving term. Hence, the finite size spectrum (4.1) determining the bulk correlation functions [16] can be written in a manifestly particle-hole symmetric form by introducing $\Delta\tilde{N}^0_{c,s} = \Delta N^0_{c,s} + \theta^{c,s}_p$, where $\Delta\tilde{N}^0_{c,s}$ denotes the change in charge and spin as compared with the ground state (see also [31, 32]):

$$\begin{aligned}E = Le_\infty + f_\infty &+ \frac{\pi v_c}{L}\left\{-\frac{1}{24} + \frac{1}{2\det^2(Z)}[\Delta\tilde{N}^0_c Z_{ss} - \Delta\tilde{N}^0_s Z_{cs}]^2 + N^+_c\right\}\\ &+ \frac{\pi v_s}{L}\left\{-\frac{1}{24} + \frac{1}{2\det^2(Z)}[\Delta\tilde{N}^0_s Z_{cc} - \Delta\tilde{N}^0_c Z_{sc}]^2 + N^+_s\right\}.\end{aligned} \tag{4.6}$$

These expressions simplify in certain limits (see also the corresponding discussion for the periodic model in [16, 17]):

4.1. Zero magnetic field ($\lambda_0 = \infty$)

The spin part of the equations can be eliminated by a Fourier transformation with the result that the matrix Z depends on the scalar dressed charge $\xi = \xi(k_0)$ only [30]:

$$Z = \begin{pmatrix} Z_{cc} & Z_{cs} \\ Z_{sc} & Z_{ss}\end{pmatrix} = \begin{pmatrix} \xi & 0 \\ \frac{1}{2}\xi & \frac{\sqrt{2}}{2}\end{pmatrix} \tag{4.7}$$

which is defined as the solution of

$$\xi(k) = 1 + \int_{-k_0}^{k_0} \mathrm{d}k'\, \cos k' G^{2u}_{2u}(\eta - \eta')\xi(k'). \tag{4.8}$$

Furthermore, one finds the relation $\theta^s_p = \frac{1}{2}\theta^c_p$, which allows us to rewrite the finite size spectrum (4.1) as

$$\begin{aligned}E = Le_\infty + f_\infty &+ \frac{\pi v_c}{L}\left\{-\frac{1}{24} + \frac{1}{2\xi^2}(\Delta N^0_c - \theta^c_p)^2 + N^+_c\right\}\\ &+ \frac{\pi v_s}{L}\left\{-\frac{1}{24} + \left(\Delta N^0_s - \frac{1}{2}\Delta N^0_c\right)^2 + N^+_s\right\}.\end{aligned} \tag{4.9}$$

The function $\hat{\rho}_c$ in (4.5) satisfies the integral equation $\hat{\rho}_c(k) = \tilde{\rho}_c(k) + \cos k \int_{-k_0}^{k_0} \mathrm{d}k'\, G^{2u}_{2u}(\eta - \eta')\hat{\rho}_c(k')$ with driving term

$$\begin{aligned}\tilde{\rho}_c(k) = \frac{1}{\pi} &+ \frac{\cos kp - p^2}{\pi(p^2 + 1 - 2p\cos k)} - G^0_{2u}(\eta)\cos k\\ &+ \cos k \begin{cases} 0 & p < 1\\ G^{2u-2t}_{2u}(\eta) + G^{2u+2t}_{2u}(\eta) & \text{I, II}\\ a_{2t}(\eta) - a_{2t-4u}(\eta) & \text{III.}\end{cases}\end{aligned} \tag{4.10}$$

4.2. The ferromagnetic case ($\lambda_0 = 0$)

In view of the ferromagnetic case with only spin-↑ electrons, the finite size spectrum is given by

$$E = Le_\infty^\uparrow + f_\infty^\uparrow + \frac{\pi v_c}{L}\left\{-\frac{1}{24} + \frac{1}{2}(\Delta N_c^0 - \theta_{\uparrow,p}^c)^2 + N_c^+\right\} \tag{4.11}$$

and the shift $\theta_{\uparrow,p}^c$ can be given explicitly as a function of the boundary field and the electron density (the Hubbard interaction is not relevant in this state):

$$\theta_{\uparrow,p}^c = -\frac{1}{2} - \frac{1}{\pi}\arctan\left(\frac{p+1}{p-1}\tan\frac{\pi n_e}{2}\right) + \theta(p-1). \tag{4.12}$$

5. Orthogonality exponent

Recently, the predictions of boundary conformal field theory regarding the relation of the finite size corrections in the spectrum of a gapless $(1+1)$-dimensional quantum system with various boundary conditions and scaling dimensions of certain boundary changing operators have been applied to various problems such as Fermi edge singularities in Luttinger liquids and the related problem of Anderson's orthogonality catastrophe in these systems [2, 12, 31, 27]. Here we want to apply these ideas to study the second problem, namely the system size dependence of the overlap of the many-particle ground states corresponding to different choices of the boundary potential. For this we have to consider the operator $\mathcal{O}_p$ switching on the boundary chemical potential p. Following [12] we apply the conformal transformation $z = L\mathrm{e}^{\frac{\pi\omega}{L}}$ to obtain a relation between the correlation functions in the infinite strip $\omega = u + \mathrm{i}v$ ($0 \leqslant v \leqslant L$ will be identified with the spatial and u with the (complex) time variable, the Fermi velocity is set to unity for this argument) with those on the half plane $z = \tau + \mathrm{i}r$, $r \geqslant 0$. The correlation function of the primary boundary operator $\mathcal{O}_p$ in the half plane is:

$$\langle AA|\mathcal{O}_p(\tau_1)\mathcal{O}_p^\dagger(\tau_2)|AA\rangle = \frac{1}{(\tau_1-\tau_2)^{2x_p}}. \tag{5.1}$$

Applying the conformal transformation we obtain the correlation function on the strip which is given by

$$\langle AA|\mathcal{O}_p(u_1)\mathcal{O}_p^\dagger(u_2)|AA\rangle \sim \left(\frac{\pi}{L}\right)^{2x_p}\mathrm{e}^{-\frac{\pi x_p \Delta u}{L}} \tag{5.2}$$

for large $\Delta u = u_2 - u_1$. Above we denoted the ground state of the system with vanishing boundary fields by $|AA\rangle$. The last expression can be evaluated by inserting a complete set of eigenstates $|BA; n\rangle$ of the system with chemical potential p at the first site (boundary condition 'B') giving:

$$\sum_n |\langle AA|\mathcal{O}_p|BA; n\rangle|^2 \mathrm{e}^{-[E_n^{BA}-E_0^{AA}]\Delta u} \sim \left(\frac{\pi}{L}\right)^{2x_p}\mathrm{e}^{-\frac{\pi x_p \Delta u}{L}}. \tag{5.3}$$

For the operator considered here the form factor $\langle AA|\mathcal{O}_p|BA; 0\rangle$ is non-zero and the exponent x_p can be read off to be

$$x_p = \frac{L}{\pi}(E_0^{BA} - E_0^{AA}). \tag{5.4}$$

From (5.3) we can identify x_p as the orthogonality exponent:

$$|\langle AA|\mathcal{O}_p|BA; 0\rangle| = |\langle p|0\rangle| \sim \left(\frac{1}{L}\right)^{x_p} \tag{5.5}$$

where $|p\rangle$ is the ground state of the system with boundary chemical potential p.

Using the results of the previous section we can now calculate this exponent from the finite size spectrum (the necessary generalization from (5.4) to the present case of a two-component Luttinger liquid with different Fermi velocities in the respective sectors is completely analogous to the one in the periodic Hubbard model [16]). The key to the correct identification of the orthogonality exponent is the correct choice of $\Delta N^0_{c,s}$ in (4.1): as discussed above the ground-state energy E^{AA}_0 is obtained by taking $\Delta N^0_{c,s} = \theta^{c,s}_{p=0}$. If we compare this energy with E^{AB}_0 it is crucial to compute the finite size corrections with respect to the *same* reference state. Since $|0\rangle$ and $|p\rangle$ need to be states with the same particle numbers N_e and $N_\downarrow$ this implies that the correct choice of $\Delta N^0_{c,s}$ in E^{AB}_0 is again $\theta^{c,s}_{p=0}$.

The easiest way to check that this choice gives the desired answer is to use the ferromagnetic case: From (4.11) we obtain

$$x_p = \frac{1}{2}(\theta^c_{\uparrow,p=0} - \theta^c_{\uparrow,p})^2 = \frac{1}{2}\left(\frac{1}{\pi}\arctan\left(\frac{p+1}{p-1}\tan\frac{\pi n_e}{2}\right) + \frac{n_e}{2} - \theta(p-1)\right)^2 \tag{5.6}$$

approaching $x_p = \frac{1}{2}(n_e - 1)^2$ in the limit $p \to \infty$. In this ferromagnetic case the many-particle wavefunction is simply a later determinant of the one-particle functions $\Psi_k(x) \propto \sin(kx) - p\sin(k(x-1))$. The product $\langle p|0\rangle$ can be evaluated numerically for finite systems leading to exponents which are in perfect agreement with (5.6).

For the case of vanishing bulk magnetic field the finite size corrections are given by (4.9). Choosing $\Delta N^0_c = \theta^c_{p=0} = 2\theta^s_{p=0} = 2\Delta N^0_s$ we find that there are no corrections from the spinon sector and the orthogonality exponent becomes

$$x_p = \frac{1}{2\xi^2}(\theta^c_{p=0} - \theta^c_p)^2 \tag{5.7}$$

with θ^c_p given in (4.5). For very large $p \to \infty$ we obtain $x_p = \frac{1}{2\xi^2}(2-n_e)^2$. As we approach half filling $n_e \to 1$ the exponent becomes $x_p = \frac{\theta(p-p_2)}{2}$. In figure 2 we present numerical data for x_p as a function of p for several values of n_e and $u = 1$.

In the general case of non-vanishing magnetic fields the exponent is given as the sum of the respective charge and spin part $x_p = x_c + x_s$ with

$$\begin{aligned} x_c &= \frac{1}{2\det^2(Z)}[(\theta^c_{p=0} - \theta^c_p)Z_{ss} - (\theta^s_{p=0} - \theta^s_p)Z_{cs}]^2 \\ x_s &= \frac{1}{2\det^2(Z)}[(\theta^s_{p=0} - \theta^s_p)Z_{cc} - (\theta^c_{p=0} - \theta^c_p)Z_{sc}]^2. \end{aligned} \tag{5.8}$$

Again, this expression simplifies for $p \to \infty$:

$$\lim_{p\to\infty} x_p = \frac{((2-n_e)Z_{ss} - Z_{cs})^2 + (Z_{cc} - (2-n_e)Z_{sc})^2}{2\det^2(Z)}. \tag{5.9}$$

In figure 3 the exponent x_p is shown as a function of p for several magnetic fields h.

Finally, let us remark on the effect of a second boundary potential p_L at site L: the BAE (1.2) are modified by another factor $s_{p_L}(k)$ leading to additional shifts $\theta^{c,s}_{p_L} - \theta^{c,s}_{p_L=0}$ in the expressions for the finite size spectrum (4.1). In this case the orthogonality exponent $x_{p_1 p_L}$

$$\langle p_1 p_L|00\rangle \sim \left(\frac{1}{L}\right)^{x_{p_1 p_L}} \tag{5.10}$$

cannot be obtained by simply adding the new shifts. Instead, numerical studies of the ferromagnetic case (see figure 4) suggest that the exponent $x_{p_1 p_L}$ is given by

$$x_{p_1 p_L} = x_{p_1} + x_{p_L} \tag{5.11}$$

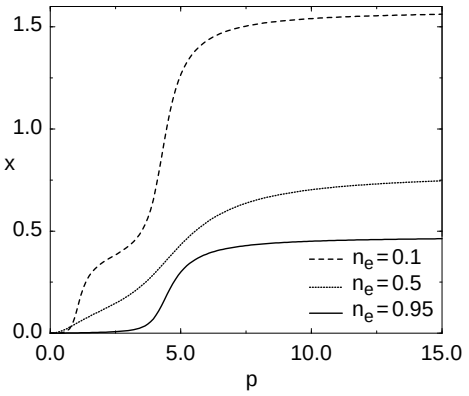

Figure 2. Orthogonality exponent x as a function of the boundary potential p for several electron densities and $u = 1$.

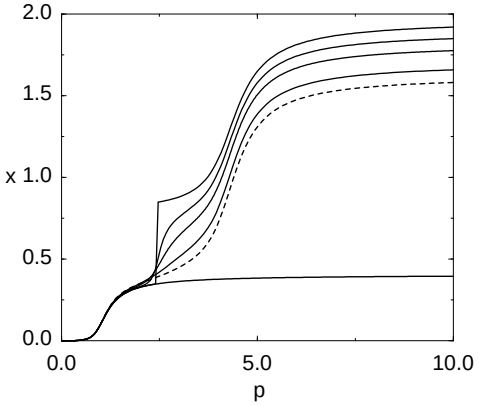

Figure 3. Orthogonality exponent x as a function of the boundary potential p for electron density $n_e = 0.1$ and $u = 1$. The heavy curve is the exponent for the ferromagnetic case. The other ones have different magnetic fields h, starting with $h = 0$ (broken curve) up to the critical magnetic field h_c (largest exponent for $p \to \infty$).

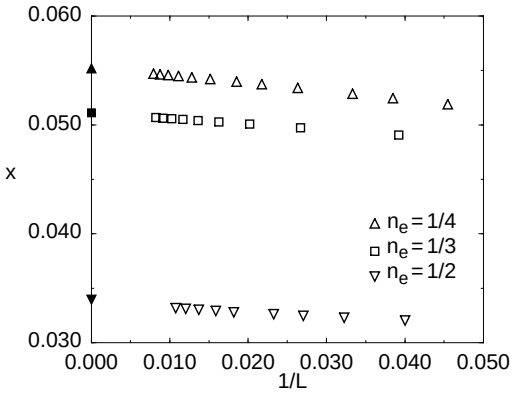

Figure 4. Numerical results for the exponent $x_{0.8,0.5}$ in the ferromagnetic case for three electron densities and $u = 1$ as a function of $1/L$. The plotted exponent is calculated from the ratio $\langle p_1 p_L|00\rangle|_L / \langle p_1 p_L|00\rangle|_{L+1/n_e}$.

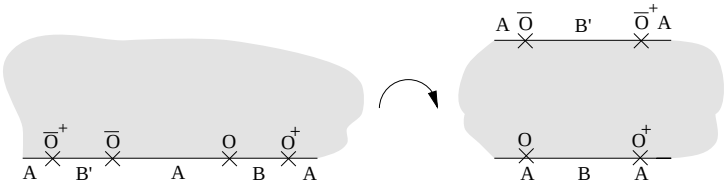

Figure 5. Conformal mapping of the infinite half plane with $\omega = \frac{L}{\pi} \ln(\frac{z}{L})$ to the strip.

i.e. the effects from the two boundaries are additive. In the framework of boundary conformal field theory this result is a consequence of the fact that changing the potential at *both* boundaries is not possible by the action of a single boundary changing operator $\mathcal{O}_{p_1 p_L}$ but rather two operators $\mathcal{O}_{p_1}$ and $\overline{\mathcal{O}}_{p_L}$ as becomes obvious when one switches back from the system on the strip to that on the half plane (see figure 5). Hence, the correlation function

considered is

$$|\langle AA|\mathcal{O}_{p_1}(\tau_1')\overline{\mathcal{O}}_{p_L}(\tau_1)\overline{\mathcal{O}}^{\dagger}_{p_L}(\tau_2)\mathcal{O}^{\dagger}_{p_1}(\tau_2')|AA\rangle| \tag{5.12}$$

which gives (provided that $|\tau_i - \tau_i'| \ll |\tau_1 - \tau_2|$)

$$|\langle AA|\mathcal{O}_{p_1}(\tau_1')\mathcal{O}^{\dagger}_{p_1}(\tau_2')|AA\rangle||\langle AA|\overline{\mathcal{O}}_{p_L}(\tau_1)\overline{\mathcal{O}}^{\dagger}_{p_L}(\tau_2)|AA\rangle| = \frac{1}{(\tau_1' - \tau_2')^{2x_{p_1}}}\frac{1}{(\tau_1 - \tau_2)^{2x_{p_L}}} \tag{5.13}$$

for the leading asymptotic of the correlator in the semi-infinite plane. Conformal mapping of this expression to the strip results in (5.11).

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