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Boundary states and edge singularities in the degenerate Hubbard chain

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Abstract. Using the Bethe ansatz we study the spectrum of boundary bound states of the $SU(N)$ generalization of the one-dimensional Hubbard model with open boundaries and applied boundary potentials. The number of electrons bound by the boundary field is found from the surface contribution to the energy. Finite size corrections to the low-lying energies in this system and use of the predictions of boundary conformal field theory allows us to study the exponents related to the orthogonality catastrophe and absorption edges.

1. Introduction

Boundary conformal field theory (BCFT) [1–3] and the formulation of Bethe ansatz soluble models on open lattices with potentials applied on the boundary sites [4–7] provide new tools for studies of problems such as the orthogonality catastrophe [8, 9] and edge singularities in optical absorption experiments [10–12] in the framework of microscopic models.

The bulk critical behaviour of $(1 + 1)$-dimensional systems of correlated electrons has been studied successfully in the Tomonaga–Luttinger model [13–15]. Further insights, for example on the influence of external fields and lattice effects (back scattering, Mott transition), have been obtained from exact solutions of integrable lattice models [16–18]. Similarly, studies of lattice models with open boundaries [4, 19, 20] contribute to the understanding of the impurity effects mentioned above. A feature of these lattice models not easily included in the field theoretical approach is the generation of a sequence of localized levels due to a boundary potential (see, for example, [21, 22]). The effect of the occupation of such bound states on the critical properties of the boundary has been studied in various one-dimensional electronic models [22–24] and opens new possibilities for the experimental observation of Luttinger liquid behaviour in quasi-one-dimensional materials.

In addition, the presence of the boundary field gives rise to one of the rare possibilities to compute certain *local* expectation values for a Bethe ansatz soluble model. The structure of the Bethe states complicates direct evaluation of the corresponding matrix elements (see [25]). In lattice models with an external potential coupled to a density at the boundary site, however, the expectation value of this density can be obtained from the surface terms to the ground-state energy. This allows us to gain additional information on the physical properties of the bound states identified from the Bethe ansatz solution. Furthermore, for a model given only in terms of its spectrum, as is the one considered later, the dependence

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of the local density on the system parameters may provide new insights into the nature of the microscopic interactions.

The one-dimensional degenerate Hubbard model studied in this paper is an extension of the Bethe ansatz solution [26] of the usual Hubbard model ($N = 2$) to an arbitrary number N of bands with $SU(N)$ symmetry. More general models with degeneracies due to spin or orbital degrees of freedom have been introduced to describe the Mott transition [27] or itinerant ferromagnetism [28]. The interaction terms in the system discussed here are parametrized by a single parameter, namely the Hubbard interaction $4u$ (see [29] for a comprehensive review). Although the corresponding Hamiltonian can be identified in certain limits [30] its precise form for arbitrary degeneracy N and strength of the Hubbard interaction is unknown [31]. In this paper we use the fact that in the sector with less than three populated bands the model reduces to the $N = 2$ model. The resulting Hamiltonian on a chain of L sites subject to an additional chemical potential p at the first one is given by†

$$\mathcal{H}|_{N=2} = -\sum_{j=1}^{L-1}\sum_{\alpha=1,2}(c_{j\alpha}^{\dagger}c_{j+1\alpha} + \mathrm{HC}) + 4u\sum_{j=1}^{L} n_{j,1}n_{j,2} + \mu\hat{N} - p_1\hat{N}_1 - p_L\hat{N}_L. \tag{1.1}$$

$c_{j\alpha}$ ($c_{j\alpha}^{\dagger}$) are annihilation (creation) operators for electrons with $SU(N)$-spin α on site j obeying canonical anticommutation rules, $n_{j\alpha} = c_{j\alpha}^{\dagger}c_{j\alpha}$, and $\hat{N}_1 = \sum_{\alpha=1}^{N} n_{1\alpha}$, and $\hat{N} = \sum_j \hat{N}_j$ are number operators. The $N = 2$ model (1.1) is soluble by means of the Bethe ansatz for arbitrary values of the boundary potentials $p_{1,L}$ [4, 19]. Due to the fact, that p_i couples to the charge sector only, the extension of the Bethe ansatz to the N-band case is completely analogous to that for the periodic chain [32–35]. In addition, the result can be checked against the corresponding continuum model studied in [36].

Our paper is organized as follows: in the following section we introduce the extension of the Bethe ansatz equations for the $N = 2$ model [19] to those for the degenerate $SU(N)$ Hubbard model in the presence of a boundary chemical potential p at site 1. Assuming that the coupling of p to the electrons is still of the form given in (1.1) we compute the occupation of the first site of the lattice as a function of the boundary potential and the Coulomb repulsion u in section 3. We find that—depending on p—up to N electrons can be localized on this site. The position of the corresponding thresholds is determined by the Coulomb splitting which gives new information on the interaction part of the complete $SU(N)$ symmetric Hamiltonian. In section 4 we determine the $1/L$ corrections to the ground-state energy and the low-lying excitations. BCFT results allow us to extract the scaling dimensions of boundary changing operators from those spectra which we use to study the effect of the band filling and coupling constant on the orthogonality and x-ray edge exponents. We find that the number of channels available to the electrons has a profound effect on these exponents: as a function of N the edge exponents become negative leading to the disappearance of observable singularities for any $N > 2$.

2. Bethe ansatz for the open degenerate Hubbard model

In the $SU(N)$ generalization of the Hubbard model the N_e-particle eigenstates are parametrized by one set of quasi-momenta $\{k_j\}_{j=1}^{N_e}$ related to the charge degree of freedom

† Here we have chosen the hopping amplitude as our unit of energy ($t = 1$). For technical reasons the strength of the on-site Coulomb interaction is given by $4u$.

and $N-1$ sets of spin rapidities $\{\lambda_\alpha^{(r)}\}_{\alpha=1}^{M_r}$, $r=1,\ldots,N-1$ [32–35]. The extension of (1.1) to electrons with an internal $SU(N)$ degree of freedom itself is defined through the set of all possible solutions to the Bethe ansatz equations (BAE) for these parameters (see also [36])

$$\mathrm{e}^{\mathrm{i}k_j 2(L+1)} B_c(k_j;\, p) = \prod_{\beta=1}^{M_1} e_1(\eta_j - \lambda_\beta^{(1)}) e_1(\eta_j + \lambda_\beta^{(1)}) \qquad j = 1,\ldots,N_e$$

$$B_s^{(r)}(\lambda_\alpha^{(r)};\, p) \prod_{\beta=1}^{M_{r-1}} e_1(\lambda_\alpha^{(r)} - \lambda_\beta^{(r-1)}) e_1(\lambda_\alpha^{(r)} + \lambda_\beta^{(r-1)}) \prod_{\beta=1}^{M_{r+1}} e_1(\lambda_\alpha^{(r)} - \lambda_\beta^{(r+1)}) e_1(\lambda_\alpha^{(r)} + \lambda_\beta^{(r+1)})$$
$$= \prod_{\substack{\beta=1 \\ \beta\neq\alpha}}^{M_r} e_2(\lambda_\alpha^{(r)} - \lambda_\beta^{(r)}) e_2(\lambda_\alpha^{(r)} + \lambda_\beta^{(r)}) \qquad \alpha = 1,\ldots,M_r$$
$$r = 1,\ldots,N-1 \qquad M_0 = N_e \geqslant M_1 \geqslant \cdots \geqslant M_{N-1} \geqslant M_N \equiv 0 \tag{2.1}$$

with $e_n(x) = (x + \mathrm{i}nu)/(x - \mathrm{i}nu)$ and $\lambda_j^{(0)} \equiv \eta_j = \sin k_j$. In the absence of any fields breaking the $SU(N)$ symmetry the energy of the corresponding state is

$$E = \sum_{j=1}^{N_e} (\mu - 2\cos k_j). \tag{2.2}$$

In the case considered here, namely a boundary chemical potential p at one end of the lattice as in (1.1), only the charge quasi-momenta k_j are affected by p and the boundary phase shifts in (2.1) read

$$B_c(k;\, p) = \left(\frac{1 - p\,\mathrm{e}^{-\mathrm{i}k}}{1 - p\,\mathrm{e}^{\mathrm{i}k}}\right) \qquad B_s^{(r)}(\lambda;\, p) \equiv 1. \tag{2.3}$$

With these equations (2.1) reduce to those found for the $SU(2)$ invariant case for $N=2$ [4, 19].

For a sufficiently strong attractive boundary potential one expects the formation of localized states for the quasi-particles of the system. Their identification among the Bethe ansatz many-particle wavefunctions corresponding to solutions of (2.1) is next to impossible; however, from comparison with analytically accessible occupation numbers (see later) and with numerical results the creation of bound states due to the boundary potential can be traced back to the appearance of purely imaginary solutions to the BAE. In the thermodynamic limit they are of the form (with exponential accuracy)

$$\sin(\tilde{k}_j) = \mathrm{i}t(p) - 2\mathrm{i}u(j-1) \qquad j = 1,\ldots,\tilde{N}_c$$
$$\tilde{\lambda}_\beta^{(r)} = \mathrm{i}t(p) - \mathrm{i}u(2\beta + r - 2) \qquad r = 1,\ldots,N-1, \qquad \beta = 1,\ldots,\tilde{N}_r \tag{2.4}$$

with

$$\tilde{N}_r = \min\left\{N - r, \max\left\{0, \left\lfloor \frac{t(p)}{2u} - \frac{r}{2} \right\rfloor + 1\right\}\right\} \qquad \tilde{N}_c = \tilde{N}_0 \qquad t(p) = \frac{p}{2} - \frac{1}{2p}.$$

In the ground state for attractive boundary potentials all accessible bound states (2.4) are occupied; configurations with some of these missing can be identified with sectors of the Hilbert space containing states with bound holons and spinons.

In the analysis of the BAE the imaginary roots (2.4) should be treated separately from those associated with bulk modes [22]. This leads to a modification of the boundary phase

factors in the equations for the latter

$$
\begin{aligned}
B_c(k) &= e_{-t/u}(\sin(k_j))e_{t/u-2\tilde{N}_1}(\sin(k_j))\\
B_s^{(r)}(\lambda) &= e_{2\tilde{N}_{r-1}-r+2-t/u}(\lambda_\alpha^{(r)})e_{2\tilde{N}_{r+1}-r-t/u}(\lambda_\alpha^{(r)})e_{t/u-2\tilde{N}_r-r}(\lambda_\alpha^{(r)})e_{t/u-2\tilde{N}_r-r+2}(\lambda_\alpha^{(r)})\\
&\qquad r=1,\ldots,N-2\\
&= e_{2\tilde{N}_{N-2}+N-3-t/u}(\lambda_\alpha^{(N-1)})e_{t/u-4\tilde{N}_{N-1}-N+3}(\lambda_\alpha^{(N-1)}) \qquad r=N-1. \qquad (2.5)
\end{aligned}
$$

In the thermodynamic limit ($L\to\infty$ with N_e/L, N_r/L kept fixed) the ground state and the low-lying states for filling $N_e \leqslant L$ are parametrized by real quasi-momenta $0<k_j<\pi$ and spin rapidities $\lambda_\alpha^{(r)}>0$ apart from the imaginary roots (2.4) associated with bound states. Using standard methods we can rewrite the BAE into a set of linear integral equations for the corresponding densities $\rho_c(k)$ and $\rho_r(\lambda^{(r)})$ of the real roots. Symmetrizing the resulting equations by means of the identification $\rho_i(x)=\rho_i(-x)$ one obtains

$$
\begin{aligned}
\rho_c(k) &= \frac{1}{\pi}+\frac{1}{L}\tau_c^{(0)}(k)+\cos k\int_{-\Lambda_1}^{\Lambda_1}\mathrm{d}\mu\, a_1(\sin k-\mu)\rho_1(\mu)\\
\rho_1(\lambda) &= \frac{1}{L}\tau_1^{(0)}(\lambda)+\int_{-k_0}^{k_0}\mathrm{d}k'\, a_1(\lambda-\sin k')\rho_c(k')-\int_{-\Lambda_{r-1}}^{\Lambda_r}\mathrm{d}\mu\, a_2(\lambda-\mu)\rho_r(\mu)\\
&\quad+\int_{-\Lambda_{r+1}}^{\Lambda_{r+1}}\mathrm{d}\mu\, a_1(\lambda-\mu)\rho_{r+1}(\mu)\\
\rho_r(\lambda) &= \frac{1}{L}\tau_r^{(0)}(\lambda)+\int_{-\Lambda_{r-1}}^{\Lambda_{r-1}}\mathrm{d}\mu\, a_1(\lambda-\mu)\rho_{r-1}(\mu)-\int_{-\Lambda_{r-1}}^{\Lambda_r}\mathrm{d}\mu\, a_2(\lambda-\mu)\rho_r(\mu)\\
&\quad+\int_{-\Lambda_{r+1}}^{\Lambda_{r+1}}\mathrm{d}\mu\, a_1(\lambda-\mu)\rho_{r+1}(\mu) \qquad r=2,\ldots,N-1 \qquad (2.6)
\end{aligned}
$$

with $a_n(x)=(nu/\pi)/(x^2+(nu)^2)$ and $\Lambda_N\equiv 0$. The boundary phase shifts (2.5) give rise to the terms of order $1/L$

$$
\begin{aligned}
\tau_c^{(0)}(k) &= \frac{1}{\pi}-\cos k\; a_1(\sin k)-\frac{\mathrm{i}}{2\pi}\partial_k\ln B_c(k;\,p)\\
\tau_r^{(0)}(\lambda) &= a_2(\lambda)-(1-\delta_{r,N-1})a_1(\lambda)-\frac{\mathrm{i}}{2\pi}\partial_\lambda\ln B_s^{(r)}(\lambda;\,p) \qquad r=1,\ldots,N-1. \qquad (2.7)
\end{aligned}
$$

In terms of the solutions to (2.6) the charge and spin-quantum numbers are given as

$$
n_e\equiv\frac{N_e}{L}=\frac{1}{2}\int_{-k_0}^{k_0}\mathrm{d}k\,\rho_c(k)-\frac{1}{2L} \qquad m_r\equiv\frac{M_r}{L}=\frac{1}{2}\int_{-\Lambda_r}^{\Lambda_r}\mathrm{d}\mu\,\rho_r(k)-\frac{1}{2L}. \qquad (2.8)
$$

(The contribution $-1/2L$ is a consequence of the symmetrization of the equations mentioned above.)

Further simplifications are possible in the case of unbroken $SU(N)$-symmetry considered here. In this case the ground state of the system is an $SU(N)$ singlet with $M_r=N_e(N-r)/N$ spin rapidities at level r which corresponds to $\Lambda_1=\cdots=\Lambda_N=\infty$. As a consequence, the densities $\rho_r(\lambda)$, $r=1,\ldots,N-1$, can be eliminated from (2.6) by Fourier transformation. The result is a scalar integral equation for the density of quasi-momenta ($\psi(x)$ is the Digamma function)

$$
\begin{aligned}
\rho_c(k) &= \rho_c^{(0)}(k)+\frac{1}{L}\tau_c^{(0)}+\frac{\cos k}{2\pi}\int_{-k_0}^{k_0}\mathrm{d}k'\,h_N(\sin k-\sin k')\rho_c(k')\\
h_N(x) &= \frac{1}{Nu}\,\mathrm{Re}\left\{\psi\left(1+\frac{\mathrm{i}x}{2Nu}\right)-\psi\left(\frac{1}{N}+\frac{\mathrm{i}x}{2Nu}\right)\right\}. \qquad (2.9)
\end{aligned}
$$

The driving terms in (2.9) are $\rho_c^{(0)}(k) = 1/\pi$ and

$$\tau_c^{(0)}(k) = \frac{1}{\pi} + \frac{\cos(k)}{2\pi u N}\,\mathrm{Re}\left\{\Psi\left(\frac{1}{N}+\alpha\right)+\Psi\left(\frac{1}{2N}+\alpha\right)-\Psi\left(\frac{1}{2}+\alpha\right)-\Psi\left(\frac{N+1}{2N}+\alpha\right)\right\}$$
$$+\frac{p\cos(k)-p^2}{\pi(1+p^2-2p\cos(k))}+\Theta(t)\frac{\cos(k)}{2\pi u N}\,\mathrm{Re}\left\{\Psi(\gamma_+)-\Psi(\beta_+)+\Psi(\gamma_-)\right.$$
$$\left.-\Psi\left(\beta_- + \frac{N_b}{N}\right)+\Psi\left(\beta_+ + \frac{1-N_b}{N}\right)-\Psi\left(\beta_+ + \frac{1}{N}\right)\right\} \tag{2.10}$$

with $\alpha = \mathrm{i}\sin(k)/2uN$, $\beta_\pm = \alpha \pm (t(p)/2uN)$, $\gamma_\pm = 1+\beta_\pm$ and $N_b = \min\{N, \max\{0, 1+\lfloor t(p)/2u \rfloor\}\}$ bound charges at site 1.

For the discussion of the thermodynamic properties of the system it is convenient to introduce the dressed energy of holon excitations $\varepsilon_c(k)$, which is given in terms of the equation

$$\varepsilon_c(k) = \mu - 2\cos k + \frac{1}{2\pi}\int_{-k_0}^{k_0} \mathrm{d}k'\cos k' h_N(\sin k - \sin k')\varepsilon_c(k'). \tag{2.11}$$

The condition $\varepsilon_c(\pm k_0) = 0$ gives an alternative definition of the integration boundary k_0 as a function of the chemical potential. From (2.2) we obtain the bulk and surface contribution to the ground-state energy in terms of the quantities introduced above:

$$E = L\varepsilon_\infty + f_\infty + o(L^{-1})$$
$$= \frac{L}{2\pi}\int_{-k_0}^{k_0}\mathrm{d}k\,\varepsilon(k) + \left(\int_{-k_0}^{k_0}\mathrm{d}k\,\varepsilon(k)\tau_c^{(0)}(k) + \sum_{j=1}^{\tilde{N}_c}(\mu - 2\cos\tilde{k}_j)\right) + o(L^{-1}). \tag{2.12}$$

Note that the bulk properties of the system are determined completely by the $o(L^0)$-terms in the integral equation which coincide with those for the periodic system (see [29]). From this, we conclude that the low-lying excitations of the system for densities $n_e < 1$ are holon and $SU(N)$-spinon excitations with group velocities

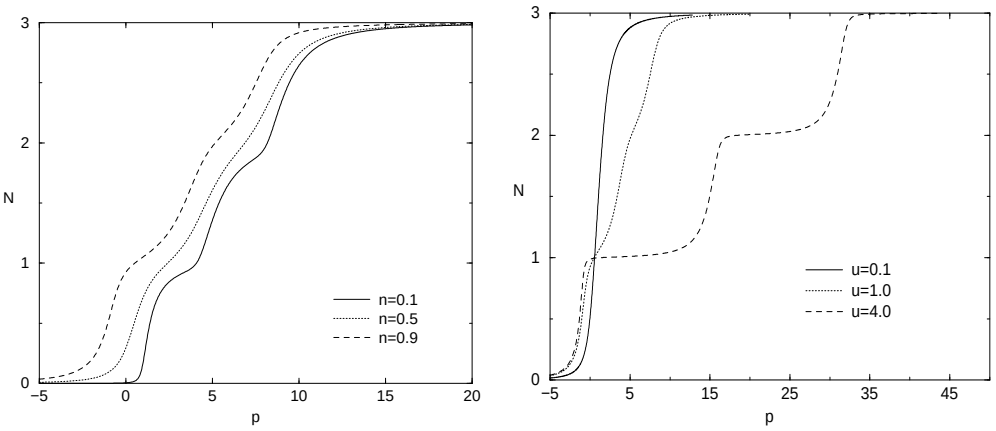
$$v_c = \frac{1}{\pi\rho_c(k_0)}\partial_k\varepsilon_c(k)|_{k=k_0} \qquad v_s = -\frac{1}{Nu}\frac{\int_{-k_0}^{k_0}\mathrm{d}k\cos k\;\varepsilon_c(k)\,\mathrm{e}^{\pi\sin k/Nu}}{\int_{-k_0}^{k_0}\mathrm{d}k\;\rho_c(k)\,\mathrm{e}^{\pi\sin k/Nu}} \tag{2.13}$$

respectively. At filling $n_e = 1$ the system undergoes a Mott transition to an insulating state at $u = u_c$, above which excitations in the charge sector have a gap [37, 38]. The critical coupling strength u_c is determined by the condition $\rho_c(\pi) = 0$ or equivalently $\int_{-\pi}^{\pi}\mathrm{d}k\,h_N(\sin k) = 2\pi$.

3. Occupation of boundary sites and Friedel's sum rule

Assuming that the coupling of the boundary potential to the charges in the degenerate Hubbard model is of the same form as in the $SU(2)$ case (1.1), i.e. via a local potential $-p\sum_{\alpha=1}^{r} n_{1\alpha}$, the expectation value $\langle\hat{N}_1\rangle$ of the occupation of the boundary site can be determined from the ground-state energy (2.12) by differentiation with respect to p

$$\langle\hat{N}_1\rangle = -\partial_p E_0 = -\sum_{j=1}^{N_b}\partial_p\tilde{E}_j - \frac{1}{2}\int_{-k_0}^{k_0}\mathrm{d}k\,\epsilon_c(k)\left(\frac{p^2\cos(k)+\cos(k)-2p}{\pi(p^2+1-2p\cos(k))^2}\right.$$
$$+\cos(k)\partial_p\,\mathrm{Re}\,\{\Psi(\gamma_+)-\Psi(\beta_+)+\Psi(\gamma_-)-\Psi(\beta_- + (N_b/N))$$
$$\left.+\Psi(\beta_+ + ((1-N_b)/N)) - \Psi(\beta_+ + (1/N))\}/2\pi u N\right) \tag{3.1}$$



(*a*) (*b*)

Figure 1. Boundary occupation $\langle \hat{N}_1 \rangle$ in the ground state of the $N = 3$ model as a function of the boundary potential p for (*a*) $u = 1$ and varying n_e and (*b*) $n_e = 0.9$ and varying u.

with $\tilde{E}_j = -\cos \tilde{k}_j = -2\sqrt{1-(t(p)+2u(j-1))^2}$. For $p \to \infty$ only the sum in (3.1) contributes, which indicates an occupation of the first site by N charges in the limit of infinitely strong attraction—the maximum number possible for fermions with an internal $SU(N)$ degree of freedom. In figure 1 we present results on $\langle \hat{N}_1 \rangle$ as a function of boundary potential for different fillings and coupling constants from numerical solutions of (3.1).

The underlying assumption of a local impurity potential of strength p can be checked by comparison of $\langle \hat{N}_1 \rangle$ with Friedel's sum rule [39]: the number of charges N_F attracted by a local scattering potential is directly related to the phase shift $\delta(\epsilon_F)$ at the Fermi surface, namely $N_F = \delta(\epsilon_F)/\pi$. Although these quantities are defined within a system of non-interacting fermions, Friedel's sum rule can be applied to the solution of the degenerate Hubbard model. In the Bethe ansatz solution the phase shift is given by $\pi\Theta_c(p)$ where

$$\Theta_c(p) = \frac{1}{2}\int_{-k_0}^{k_0} \mathrm{d}k\, \tau_c(k) + \tilde{N}_c - \frac{1}{2}. \tag{3.2}$$

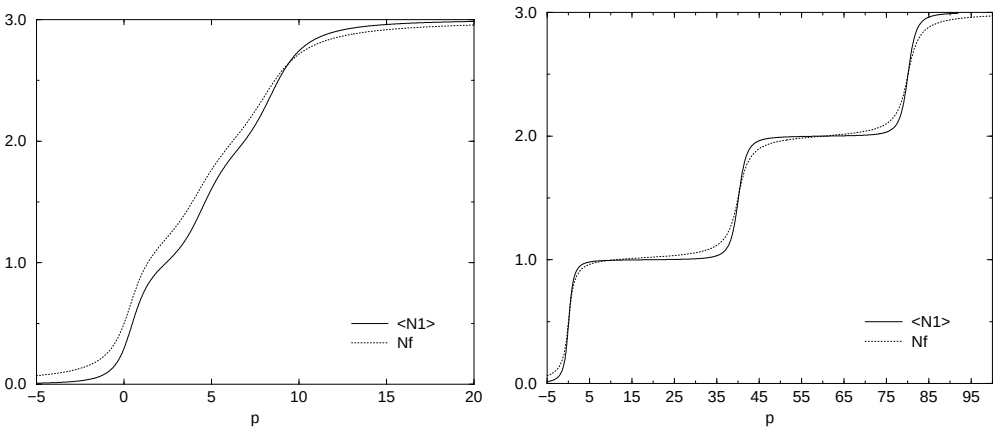
($\tau_c(k)$ is the $o(L^{-1})$ contribution to the density (2.9).) Taking the number of particles at site 1 for $p \to -\infty$ as a reference we obtain

$$N_F = \Theta_c(p) - \Theta_c(p \to -\infty). \tag{3.3}$$

In figures 2 and 3 we present numerical data on the p dependence of N_F and $\langle \hat{N}_1 \rangle$ in the ground state and the state with the local levels unoccupied ($N_b = 0$). One should note N_F describes the integrated effect of the local scatterer on the particle density. Since a newly added bound state is only weakly localized near the threshold this explains the difference between N_F and $\langle \hat{N}_1 \rangle$ in these regions.

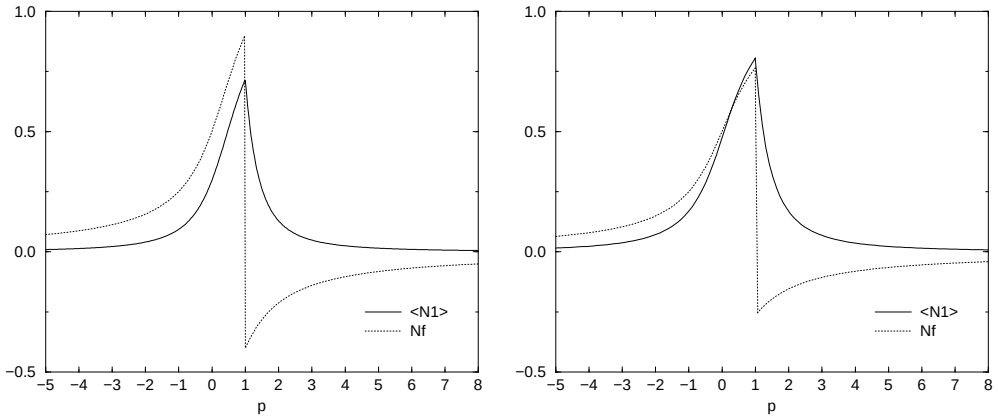
4. Finite size spectra and critical exponents

Following [18] the $o(L^{-1})$ terms for the ground state (2.12) and the low-lying excitations of the degenerate Hubbard model can be obtained. Restricting ourselves to the $SU(N)$



(*a*) (*b*)

Figure 2. Comparison of $\langle \hat{N}_1 \rangle$ and N_F in the ground state of the $N = 3$ model as a function of the boundary potential p for $u = 1$ (*a*), $u = 10$ (*b*) at $n_e = 0.5$.



(*a*) (*b*)

Figure 3. As in figure 2 but in the lowest state with all bound states empty, i.e. without imaginary roots in the BAE (2.1).

symmetric case again we obtain (see also [36])

$$E - L\epsilon_\infty = f_\infty + \frac{\pi v_c}{L}\left\{-\frac{1}{24} + \frac{1}{2}\left(\frac{\Delta N_e - \Theta_c(p)}{z_c}\right)^2 + N_e^+\right\} + \frac{\pi v_s}{L}\left\{-\frac{1}{24}(N-1) + \frac{1}{2}\Delta\widetilde{M}_r\,(\mathcal{C}_N)_{rs}\,\Delta\widetilde{M}_s + N_r^+\right\}. \tag{4.1}$$

Here the numbers ΔN_e and $\Delta\widetilde{M}_r = \Delta M_r - (1 - r/N)\Delta N_e$ describe the change in the total number of electrons and electrons with colour r with respect to the ground state for which $\Delta N_e = \Theta_c(p)$, $\Delta\widetilde{M} = 0$ at a given value of p and occupation of the bound states. N_e^+, N_r^+ count the number of particle hole excitations, $z_c = \xi(k_0)$ is a function of filling and the coupling constant is related to the compressibility of the electron gas. It is defined in terms

of the equation

$$\xi(k) = 1 + \frac{1}{2\pi}\int_{-k_0}^{k_0} \mathrm{d}k' \cos k' h_N(\sin k - \sin k')\xi(k'). \tag{4.2}$$

For fixed particle density, z_c decreases from $\sqrt{N}$ for non-interacting particles to 1 in the limit $u \to \infty$. $\mathcal{C}_N$ is the Cartan matrix for the Lie algebra $SU(N)$ (see [18]).

From the finite size corrections in the low-lying energies of a gapless $(1 + 1)$-dimensional quantum system subject to various boundary conditions one can obtain the scaling dimensions of certain boundary changing operators with the predictions of boundary conformal field theory. These relations can be used to study phenomena such as Anderson's orthogonality catastrophe and the related edge singularities in Luttinger liquids [2, 12, 22–24, 36]. Of particular interest in the context of the present system is the dependence of the associated critical exponents on the number N of channels available to the electrons and the consequences of the presence of bound states. Furthermore, it is possible to study the behaviour of these quantities in the vicinity of the Mott transition at $n_e = 1$, $u = u_c$.

As noted by Anderson [8] the overlap between the ground state $|p\rangle$ of a Fermi gas in the presence of a local perturbation of strength p and the unperturbed state $|0\rangle$ decreases as a power of the system size, namely $|\langle p|0\rangle| \propto L^{-x}$. For the one-dimensional system considered here x can be related to the difference between the L^{-1}-terms in the ground-state energies (4.1) for the same numbers of particles N_e and spin M_r but different values of p computed with respect to the same reference state [9, 12, 22]. Since p enters the finite size corrections in (4.1) in the charge contribution only, there is no spinon contribution to the orthogonality exponent and we find

$$x = \frac{1}{2z_c^2}(\Theta_c(p) - \Theta_c(p=0))^2. \tag{4.3}$$

In figure 4 we present numerical results on the p-dependence of x for various values of particle density n_e and coupling strengths.

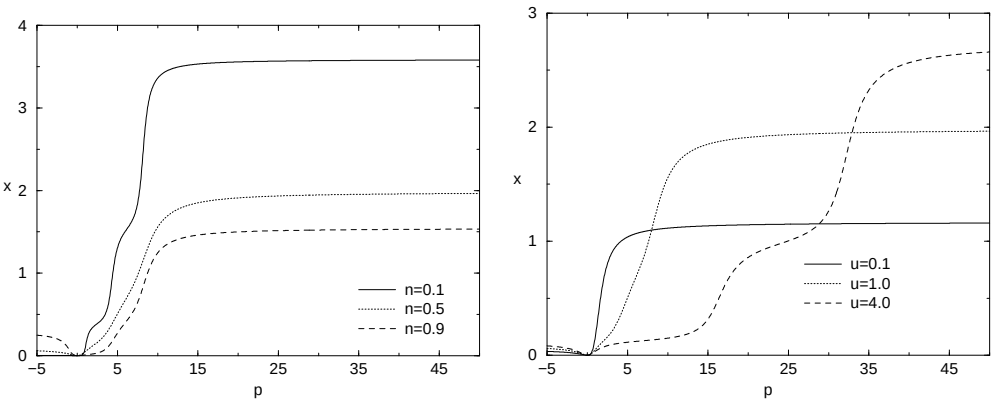


Figure 4. Orthogonality exponent for the overlap between ground states $\langle 0|p\rangle$ for the $N = 3$ model against p for (*a*) $u = 1$ and varying n_e and (*b*) $n_e = 0.5$ and varying u.

Closely related to Anderson's orthogonality catastrophe, but of greater relevance for possible observation of Luttinger liquid properties in an experiment, are edge singularities arising in transport measurements involving tunnelling through localized states or x-ray

absorption profiles in quasi-one-dimensional electronic systems. A simple model describes the photo-absorption process through the sudden switching of the local electrostatic potential V due to the creation of a core hole by the x-ray photon [10]. Within this model a characteristic power-law singularity

$$I(\omega) \propto \frac{1}{|\omega - \omega_0|^{\alpha}} \tag{4.4}$$

is observed in the vicinity of the absorption threshold ω_0 and the exponent α can be related to the phase shift $\delta(\epsilon_F)$ due to the local potential [10, 11]. If V is strong enough to bind one or more conduction electrons this will give additional thresholds at energy $\omega_0^{(n)}$ with different edge exponents $\alpha^{(n)}$.

Again, the absorption intensity (4.4) can be considered as a correlation function of boundary changing operators in a $(1+1)$-dimensional quantum system and it is possible to extract the exponents α by comparing the finite size scaling behaviour of the low-lying states of the unperturbed system (with *periodic* boundary conditions) with those of the system with a local scatterer described through an *open* boundary and boundary potentials $p_1 = p_L = p$ [2, 23]. The finite size corrections to the ground-state energy of the degenerate Hubbard model with periodic boundary conditions have been obtained in [18]:

$$E - L\epsilon_{\infty} = -\frac{\pi v_c}{6L} - \frac{\pi v_s}{6L}(N-1). \tag{4.5}$$

The difference in the universal scaling behaviour of the ground-state energies (4.1) and (4.5) leads to an upper bound $1 - N/8$ for the the exponents α arising in all possible processes. The quantum numbers ΔN_e and ΔM_r in (4.1) have to be adjusted depending on whether one considers photo-emission or photo-absorption with simultaneous occupation of some of the bound states of V. For photo-emission the particle numbers in the system are unchanged resulting in

$$\alpha_{photo} = 1 - \frac{N}{8} - \frac{1}{2z_c^2}\Theta_c^2(p) \tag{4.6}$$

where p is the strength of the core potential. Similarly, one should choose $\Delta N_c = 1$, $\Delta M_r = 0$ for absorption of the core electron into the conduction band (leaving possible bound states unoccupied). The corresponding edge exponent is found to be

$$\alpha_{band} = 2 - \frac{5}{8}N - \frac{1}{2N} - \frac{1}{2z_c^2}\left(\Theta_c(p) - 1\right)^2. \tag{4.7}$$

Note that this exponent is always negative for $N > 2$ leading to a shoulder in the absorption profile rather than a singularity. This observation puts a strong constraint on the possibility of observing edge singularities in quasi-one-dimensional systems of the type discussed here: in selecting or preparing the material much care should be devoted to reduce the number of channels participating in the transport of the system. In addition, the strength of the impurity potential p should—if possible—be tuned to the region $-t < p < t$ where the largest exponents are found (see figure 5).

Finally, we consider the edge exponent α_{abs} associated with the absolute threshold for absorption, namely all bound states occupied in the final state. Formally, this exponent is given again by (4.7), although $\Theta_c(p)$ has to be computed for the state with maximal number of bound particles. This leads to the same conditions for pronounced singularities as discussed above. In figure 6 numerical results on this exponent are shown for $N = 3$.

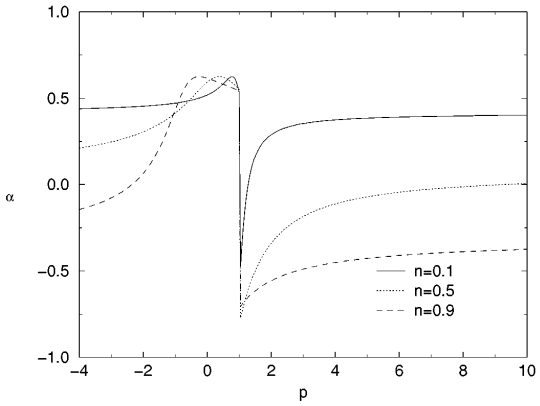
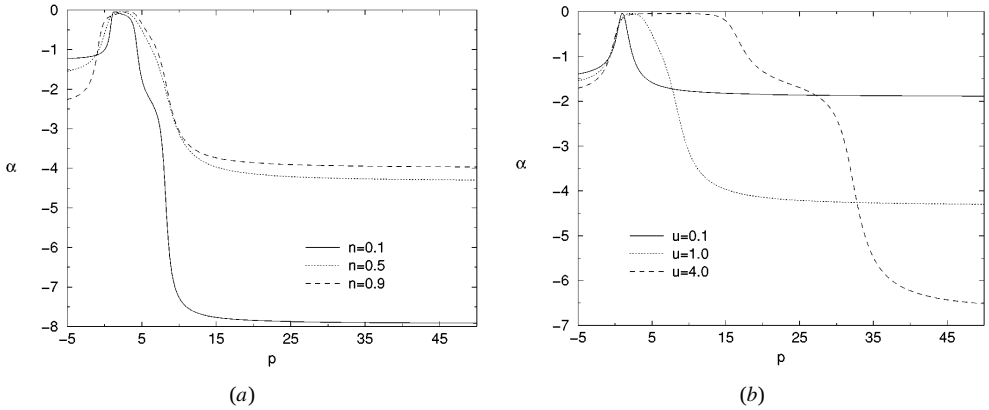


Figure 5. Edge exponent α_{photo} for photoemission into the state without bound charges against p in the $N = 3$ model for $u = 1$ and varying n_e.



(*a*) (*b*)

Figure 6. Edge exponent α_{abs} at the absolute threshold for x-ray absorption against p in the $N = 3$ model for (*a*) $u = 1$ and varying densities and (*b*) $n_e = 0.5$ and various values of u.

5. Conclusion

We have studied the spectrum of bound states and boundary critical properties of an integrable $SU(N)$-symmetric Hubbard chain. From its low-energy properties this model is known to be described by a $U(1)$ Gaussian model in the charge sector and the level-one $SU(N)$ Wess–Zumino–Witten model in the spin sector. These symmetries give rise to a rich structure of boundary states associated with the holon and spinon excitations of the bulk system. The spectrum of these bound states gives rise to a sequence of thresholds which should be observable in absorption profiles or tunnelling rates of quasi-one-dimensional compounds. The associated edge singularities are found to be most pronounced for $N = 2$. This restricts the possibility of their observation in systems where many channels contribute to the transport properties.

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Appendix. Explicit expressions in the strong coupling limit

For general values of the system parameters the Bethe ansatz integral equations (2.9), (2.11) and (4.2) have to be solved numerically. Simplifications allowing us to obtain the relevant quantities in closed form occur in the strong coupling limit $u \to \infty$. In this case the kernel function can be replaced by a constant $h_N \to (\psi(1) - \psi(1/N))/Nu$ to leading order and we obtain the following expressions for the boundary phase shifts with maximum number of bound charges at site 1 ($p_1 = p$, $p_L = 0$) (3.2):

$$\begin{aligned}\Theta_c(p) = \frac{1}{\pi}\arctan\left(\frac{p-\cos(\pi n_c)}{\sin(\pi n_c)}\right) + \frac{\Theta(p-1)}{\pi}\Bigg(\pi(N_b-1) + \arctan\left(\frac{\sin(\pi n_c)}{t(p)}\right) \\ - \arctan\left(\frac{\sin(\pi n_c)}{2uN - t(p)}\right) + \arctan\left(\frac{\sin(\pi n_c)}{2uN_b - t(p)}\right) \\ - \arctan\left(\frac{\sin(\pi n_c)}{t(p) + 2u - 2uN_b}\right)\Bigg).\end{aligned} \tag{A.1}$$

Similarly we obtain for the orthogonality exponent (4.3)

$$\begin{aligned}x = \frac{1}{2}\Bigg(\frac{1}{\pi}\arctan\left(\frac{p-\cos(\pi n_c)}{\sin(\pi n_c)}\right) - n_c + \frac{1}{2} + \frac{\Theta(p-1)}{\pi}\Bigg(\pi(N_b-1) \\ + \arctan\left(\frac{\sin(\pi n_c)}{t(p)}\right) - \arctan\left(\frac{\sin(\pi n_c)}{2uN - t(p)}\right) + \arctan\left(\frac{\sin(\pi n_c)}{2uN_b - t(p)}\right) \\ - \arctan\left(\frac{\sin(\pi n_c)}{t(p) + 2u - 2uN_b}\right)\Bigg)\Bigg)^2 \\ \longrightarrow \begin{cases} \frac{1}{2}n_c^2 & p \to -\infty \\ \frac{1}{2}(N_b - n_c)^2 & 1 \ll p = 2u + 4un,\ n \in \mathbb{N} \ \text{(plateau value)}\end{cases}\end{aligned} \tag{A.2}$$

and the edge exponents ($p_1 = p_L = p$)

$$\alpha_{photo} = 1 - \frac{N}{8} - \frac{1}{2}\left(\frac{2}{\pi}\arctan\left(\frac{1+p}{1-p}\tan\left(\frac{\pi n_c}{2}\right)\right) - \frac{1}{2}\right)^2$$

$$\longrightarrow \begin{cases} 1 - \dfrac{N}{8} - \dfrac{(\frac{1}{2}+n_c)^2}{2} & p \to \pm\infty \\ \dfrac{7-N}{8} & p \to 1 \ \text{ from below} \\ -\dfrac{1+N}{8} & p \to 1 \ \text{ from above}\end{cases}$$

$$\alpha_{band} = 2 - \frac{5N}{8} - \frac{1}{2N} - \frac{1}{2}\left(\frac{2}{\pi}\arctan\left(\frac{1+p}{1-p}\tan\left(\frac{\pi n_c}{2}\right)\right) - \frac{3}{2}\right)^2$$

$$\longrightarrow \begin{cases} 2-\dfrac{5N}{8}-\dfrac{1}{2N}-\dfrac{(n_c+\frac{3}{2})^2}{2} & p\to\pm\infty \\ \dfrac{15-5N}{8}-\dfrac{1}{2N} & p\to 1 \text{ from below} \\ -\dfrac{9+5N}{8}-\dfrac{1}{2N} & p\to 1 \text{ from above} \end{cases}$$

$$\begin{aligned} \alpha_{abs} = 2-\frac{5N}{8}-\frac{1}{2N}-\frac{1}{2}\Bigg(&\frac{2}{\pi}\arctan\left(\frac{p-\cos(\pi n_c)}{\sin(\pi n_c)}\right)-\frac{1}{2}-n_c \\ &+2\frac{\Theta(p-1)}{\pi}\Bigg(\pi(N_b-1)+\arctan\left(\frac{\sin(\pi n_c)}{t(p)}\right) \\ &-\arctan\left(\frac{\sin(\pi n_c)}{2uN-t(p)}\right)+\arctan\left(\frac{\sin(\pi n_c)}{2uN_b-t(p)}\right) \\ &-\arctan\left(\frac{\sin(\pi n_c)}{t(p)+2u-2uN_b}\right)\Bigg)\Bigg)^2 \end{aligned}$$

$$\longrightarrow 2-\frac{5N}{8}-\frac{1}{2N}-\frac{1}{2}\begin{cases} (n_c+\frac{3}{2})^2 & p\to-\infty \\ (n_c-\frac{3}{2})^2 & p=0 \\ (2N_b-n_c-\frac{3}{2})^2 & 1\ll p=2u+4un, \\ & n\in\mathbb{N} \text{ (plateau value).} \end{cases} \tag{A.3}$$

Comparison with the numerical results shows good quantitative agreement of these expressions for $u \gtrapprox 10$.

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