# The supersymmetric *t–J* model with a boundary

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**Abstract.** An open supersymmetric *t–J* chain with boundary fields is studied by means of the Bethe ansatz. Ground state properties for the case of an almost half-filled band and a bulk magnetic field are determined. Boundary susceptibilities are calculated as functions of the boundary fields. The effects of the boundary on excitations are investigated by constructing the exact boundary *S*-matrix. From the analytic structure of the boundary *S*-matrices one deduces that holons can form boundary bound states for sufficiently strong boundary fields.

## 1. Introduction

Recently there has been renewed interest in one-dimensional impurity problems and the related problem of one-dimensional Luttinger liquids with boundaries [1–8]. The main focus of these investigations has been the effects of Kondo-like impurities and effects due to potential scattering in Luttinger liquids. These impurity problems are closely related to open 1D systems with boundary fields. Some of these systems are integrable and can be solved exactly by Bethe ansatz [9–14]. In particular, in [1] an anisotropic Heisenberg chain with open boundary conditions was studied. It is the purpose of the present work extend the investigation of [1] to the case of the *t–J* model, which is a Luttinger liquid with both spin and charge degrees of freedom.

In [15] a trigonometric generalization of the supersymmetric *t–J* model with open boundaries was constructed by means of the quantum-inverse scattering method (see, e.g., [25]). This generalized the previous work by Förster and Karowski on the quantum-group invariant case [16]. Here we study this model at the rational point, for which it reduces to the supersymmetric *t–J* model with open boundaries and boundary fields. The reason for this restriction is that the trigonometric model in general leads to a non-Hermitian bulk Hamiltonian. The only exception is the hyperbolic regime, but there the spin excitations are gapped and thus irrelevant for the low-energy physics of the model. The Hamiltonian we consider in the grand canonical ensemble is given by

$$H = -\mathcal{P}\left(\sum_{j=1}^{L-1}\sum_{\sigma} c_{j,\sigma}^{\dagger} c_{j+1,\sigma} + c_{j+1,\sigma}^{\dagger} c_{j,\sigma}\right)\mathcal{P} + 2\sum_{j=1}^{L-1} \mathbf{S}_j \cdot \mathbf{S}_{j+1} - \frac{n_j n_{j+1}}{4}$$

$$+ \sum_{j=1}^{L-1} n_j + n_{j+1} - H S^z - \mu \hat{N} + H_{\alpha\beta} \tag{1}$$

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where $\mathcal{P}$ projects out double occupancies, $\boldsymbol{S}_j$ are spin operators at site $j$, $n_j = c_{j,\uparrow}^\dagger c_{j,\uparrow} + c_{j,\downarrow}^\dagger c_{j,\downarrow}$, and the four possible choices of boundary Hamiltonians $H_{\alpha\beta}$ compatible with integrability and conservation of total spin in the $z$-direction and particle number are given by

$$H_{aa} = h'_1 n_1 + h'_L n_L \qquad\qquad H_{ab} = h_1 \left( S_1^z - \frac{n_1^h}{2} \right) + h'_L n_L$$

$$H_{ba} = h'_1 n_1 + h_L \left( S_L^z - \frac{n_L^h}{2} \right) \qquad H_{bb} = h_1 \left( S_1^z - \frac{n_1^h}{2} \right) + \left( S_L^z - \frac{n_L^h}{2} \right).$$
(2)

Here $n_j^h = 1 - n_{j,\uparrow} - n_{j,\downarrow}$ is the number operator for holes (unoccupied sites) at site $j$. To simplify the computations we constrain ourselves to the regions $h \in (0, 2)$, $h' \in (0, 1)$. It is straightforward to extend the analysis below to other ranges of the fields. For later convenience we define the quantities

$$S_1 = \begin{cases} 2 - 2/h'_1 & \text{for } aa, ba \\ 1 - 2/h_1 & \text{for } ab, bb \end{cases} \qquad S_L = \begin{cases} 2 - 2/h'_L & \text{for } aa, ab \\ 1 - 2/h_L & \text{for } ba, bb. \end{cases}$$
(3)

In what follows we always assume that $S_1$ and $S_L$ are non-integer numbers. We note that for zero boundary fields equation (1) exhibits a global $sl(1|2)$ symmetry [16]. In the present work we perform a detailed study of the boundary effects in the model defined by (1), paying particular attention to the influence of the boundary fields. After some technical preliminaries we turn to an analysis of the ground state properties. We find that the zero-temperature susceptibilities exhibit some interesting singularities, which we argue to be related to the formation of bound states near the boundaries. We then study the interaction of elementary excitations with the boundaries by computing the exact boundary $S$-matrices. We find that boundary bound states can be formed for sufficiently strong boundary fields. We concentrate on the case of band fillings close to one (corresponding to the particularly interesting case of the lightly doped Mott–Hubbard insulator) for which it is possible to obtain explicit analytical results. However, it is straightforward to extend the present analysis to arbitrary band-fillings by solving the integral equations (14) numerically and then integrating (13) numerically.

Taking the rational limit of the Bethe ansatz equations derived in [15] we obtain

$$\eta_{\alpha\beta}(\lambda_k)\, (e_1(\lambda_k))^{2L} = \prod_{j\neq k}^{N_h+N_\downarrow} e_2(\lambda_k - \lambda_j) e_2(\lambda_k + \lambda_j) \prod_{l=1}^{N_h} e_{-1}(\lambda_k - \lambda_l^{(1)}) e_{-1}(\lambda_k + \lambda_l^{(1)})$$

$$1 = \zeta_{\alpha\beta}(\lambda_l^{(1)}) \prod_{j=1}^{N_h+N_\downarrow} e_1(\lambda_l^{(1)} - \lambda_j) e_1(\lambda_l^{(1)} + \lambda_j)$$
(4)

where $e_n(x) = (x + \frac{1}{2}in)/(x - \frac{1}{2}in)$ and $\alpha, \beta = a, b$. The boundary terms are given by

$$\eta_{aa}(\lambda) = 1 \qquad \eta_{ab}(\lambda) = -e_{-S_1}(\lambda) \qquad \eta_{ba}(\lambda) = -e_{-S_L}(\lambda) \qquad \eta_{bb}(\lambda) = \eta_{ab}(\lambda)\eta_{ba}(\lambda)$$

$$\zeta_{bb}(\lambda) = 1 \qquad \zeta_{ab}(\lambda) = -e_{-S_L}(\lambda) \qquad \zeta_{ba}(\lambda) = -e_{-S_1}(\lambda) \qquad \zeta_{aa}(\lambda) = \zeta_{ab}(\lambda)\zeta_{ba}(\lambda).$$
(5)

The restrictions imposed on $h$ and $h'$ are chosen such that in all these expressions the label $x$ on $e_x(\lambda)$ is positive with range $(0, \infty)$. The energy of a state corresponding to a solution of (4) is (up to an overall constant, which we drop)

$$E = E_{ij} - \sum_{j=1}^{N_h+N_\downarrow} \frac{1}{\frac{1}{4} + \lambda_j^2} + H(N_\downarrow + N_h) + \left( \mu - \frac{H}{2} \right) N_h - \left( \mu + \frac{H}{2} \right) L$$
(6)

where $E_{aa} = h'_1 + h'_L$, $E_{bb} = \frac{1}{2}(h_1 + h_L)$ and so on. The reference state used to derive (4) is the one with up-spin electrons at each site of the lattice. This leads to the constraint in (4) that the number $N_\downarrow$ of down-spins must be smaller than or equal to the number of up-spins $N_\uparrow$. Solutions of (4) violating this constraint can lead to vanishing wavefunctions and must be ignored. Eigenstates of (1) with $N_\downarrow > N_\uparrow$ must be constructed by switching the reference state to the state with down-spin electrons at all sites. This leads to the same Bethe equations (4) with $N_\downarrow \leftrightarrow N_\uparrow$ and different values for the quantities $S_j$:

$$
S_1 = \begin{cases} 2 - 2/h'_1 & \text{for } aa, ba \\ 1 + 2/h_1 & \text{for } ab, bb \end{cases} \qquad S_L = \begin{cases} 2 - 2/h'_L & \text{for } aa, ab \\ 1 + 2/h_L & \text{for } ba, bb. \end{cases} \tag{7}
$$

Below we will mainly deal with situations for which $N_\downarrow \leqslant N_\uparrow$. However, when considering excitations over the antiferromagnetic ground states we will also consider the case $N_\downarrow \geqslant N_\uparrow$, for which we will make use of the procedure outlined above.

In order to simplify (4) we make use of the 'string-hypothesis'†, which states that for $L \to \infty$ all solutions are composed of real $\lambda_\gamma^{(1)}$'s whereas the $\lambda$'s are distributed in the complex plane according to the description

$$
\lambda_\alpha^{n,j} = \lambda_\alpha^n + \mathrm{i}\left(\frac{n+1}{2} - j\right) \qquad j = 1, \ldots, n \tag{8}
$$

where $\alpha = 1, \ldots, M_n$ labels different 'strings' of length $n$. This string hypothesis is naturally identical to the one for the model with periodic boundary conditions. The imaginary parts of the $\lambda$'s can now be eliminated from (4) via (8). Taking the logarithm of the resulting equations (for $M_n$ strings (8) of length $n$ and $N_h$ $\lambda^{(1)}$'s (note that $\sum_{n=1}^{\infty} n M_n = N_\downarrow + N_h$) we arrive at

$$
\frac{2\pi}{L} I_\alpha^n = \left(2 + \frac{1}{L}\right)\theta\left(\frac{\lambda_\alpha^n}{n}\right) - \frac{1}{L}\sum_{(m\beta)}\theta_{mn}(\lambda_\alpha^n - \lambda_\beta^m) + \theta_{mn}(\lambda_\alpha^n + \lambda_\beta^m)
$$

$$
+ \frac{1}{L}\sum_{\gamma=1}^{N_h}\theta\left(\frac{\lambda_\alpha^n - \lambda_\gamma^{(1)}}{n}\right) + \theta\left(\frac{\lambda_\alpha^n + \lambda_\gamma^{(1)}}{n}\right) \tag{9}
$$

$$
+ \frac{1}{L}\kappa_{ij}^{(n)}(\lambda_\alpha^n) \qquad \alpha = 1, \ldots, M_n
$$

$$
\frac{2\pi}{L} J_\gamma = \frac{1}{L}\sum_{(n\alpha)}\theta(\lambda_\gamma^{(1)} - \lambda_\alpha^n) + \theta(\lambda_\gamma^{(1)} + \lambda_\alpha^n) + \frac{1}{L}\omega_{ij}(\lambda_\gamma^{(1)}) \qquad \gamma = 1, \ldots, M^{(1)}
$$

where $I_\alpha^n$ and $J_\gamma$ are integer numbers, $\theta(x) = 2\arctan(2x)$,

$$
\theta_{n,m}(x) = (1 - \delta_{m,n})\theta\left(\frac{x}{|n-m|}\right) + 2\theta\left(\frac{x}{|n-m|+2}\right) + \cdots
$$

$$
+ 2\theta\left(\frac{x}{n+m-2}\right) + \theta\left(\frac{x}{n+m}\right) \tag{10}
$$

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† As far as the present work is concerned we do not need to consider complex solutions of the Bethe equations explicitly and all of our results are really independent of the string hypothesis.

and the boundary contributions are given by

$$\kappa_{ab}^{(n)}(\lambda) = \sum_{l=1}^{n} \theta\left(\frac{\lambda}{n+1-2l-S_1}\right) \qquad \omega_{ab}(\lambda) = \theta\left(\frac{\lambda}{-S_L}\right)$$

$$\kappa_{ba}^{(n)}(\lambda) = \sum_{l=1}^{n} \theta\left(\frac{\lambda}{n+1-2l-S_L}\right) \qquad \omega_{ba}(\lambda) = \theta\left(\frac{\lambda}{-S_1}\right) \qquad (11)$$

$$\kappa_{bb}^{(n)}(\lambda) = \kappa_{ba}^{(n)}(\lambda) + \kappa_{ab}^{(n)}(\lambda) \qquad \omega_{bb}(\lambda) = 0$$

$$\kappa_{aa}^{(n)}(\lambda) = 0 \qquad \omega_{aa}(\lambda) = \omega_{ba}(\lambda) + \omega_{ab}(\lambda).$$

The ranges of integers $I_\alpha^n$ and $J_\gamma$ are

$$I_\alpha^n = 1, 2, \ldots, L + M_n - 2 \sum_{m=1}^{\infty} \min\{m, n\} M_m + N_h \qquad J_\gamma = 1, 2, \ldots, N_\downarrow + N_h - 1.$$

$$(12)$$

There are two differences compared with the case of periodic boundary conditions [17–24]: first there are additional $1/L$ terms (11), and second the integers $I_\alpha^n$ and $J_\gamma$ take different values. The allowed range of the integers $I_\alpha^n$ and $J_\gamma$ reflects the fact that all solutions of (4) with one or more roots $\lambda_j$ or $\lambda_k^{(1)}$ having vanishing real parts must be excluded as they lead to vanishing wavefunctions. This restriction leads to constraints on the allowed values of the integers $I_\alpha^n$ and $J_\gamma$: the $I_\alpha^n$ range from 1 to $L + M_n - 2\sum_{m=1}^{\infty} \min\{m, n\} M_m + N_h$, the solution with $I_\alpha^n = 0$ being excluded. Similarly $J_\gamma$ range from 1 to $N_\downarrow + N_h - 1$ and 0 is again excluded.

For zero boundary fields ($\kappa_{ij}^{(n)} = 0$, $\omega_{ij} = 0$) we can construct a complete set of $3^L$ states from the Bethe ansatz states defined in the above way: the model (1) with vanishing boundary fields is $sl(1|2)$-invariant and all Bethe states are highest-weight states of $sl(1|2)$ [15, 16]. Additional linearly independent eigenstates of (1) can be constructed by acting with the $sl(1|2)$ lowering operators on the highest-weight states. The total number of states obtained in this way is $3^L$ as can be proved in the same way as for the periodic $t$–$J$ chain [17] (the necessary combinatorics are identical). Thus we obtain a complete set of eigenstates of (1).

For non-vanishing boundary fields the situation is more complicated as the $sl(1|2)$ symmetry is broken by the boundary conditions. Therefore we cannot use the symmetry generators to construct additional states from the Bethe ansatz states and are left with the a priori incomplete set of eigenstates given by (9) and (12). For the present purposes this is inessential: the ground state is always a Bethe ansatz state, as are the states needed to extract the boundary $S$-matrices. The ground state and excitations can be constructed from (9) in a standard way (see, e.g., [25]). The ground state is obtained by filling all allowed vacancies of integers $I_\alpha^1$ and $J_\gamma$ up to maximal values $I_{max}$ and $J_{max}$, which corresponds to filling two Fermi seas of rapidities $\lambda_\alpha^1$ between 0 and $A$ and $\lambda_\gamma^{(1)}$ between 0 and $B$. The actual values of $A$, $B$ (and thus $I_{max}$ and $J_{max}$) depend on $H$ and $\mu$ and are determined below. We are interested in the case of a small magnetic field $H$ and a close to half-filled band ($\mu \approx 2\ln(2)$), for which $A \gg 1$ and $B \ll 1$. As is shown in appendix A, the ground-state energy per site (for the four possible sets of boundary fields) below half-filling is given by

$$\frac{E - \mu N_e - HS^z}{L} = \varepsilon_c(0) - 2\mu + \frac{1}{4\pi L}\int_{-A}^{A} d\lambda\, \varepsilon_s(\lambda)\kappa_{ij}'(\lambda) + \frac{1}{4\pi L}\int_{-B}^{B} d\lambda\, \varepsilon_c(\lambda)\omega_{ij}'(\lambda)$$

$$-\frac{1}{2L}\left[\varepsilon_s(0) + \mu - \frac{H}{2} - 2E_{ij}\right] + o(L^{-1}) \qquad (13)$$

where $i, j = a, b$ and where the dressed energies $\varepsilon_c(\lambda)$ and $\varepsilon_s(\lambda)$† are given in terms of the coupled integral equations

$$\varepsilon_s(\lambda) = -2\pi a_1(\lambda) + H - \int_{-A}^{A} d\mu \, a_2(\lambda - \mu)\varepsilon_s(\mu) + \int_{-B}^{B} d\mu \, a_1(\lambda - \mu)\varepsilon_c(\mu)$$

$$\varepsilon_c(\lambda) = \mu - \frac{H}{2} + \int_{-A}^{A} d\mu \, a_1(\lambda - \mu)\varepsilon_s(\mu) .$$

(14)

Here $a_n(\lambda) = (1/2\pi)n/(\lambda^2 + \frac{1}{4}n^2)$. For later use we define

$$G_x(\lambda) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \, \exp(-i\omega\lambda)\frac{\exp(-x|\omega/2|)}{2\cosh(\omega/2)} = \frac{1}{\pi} \text{Re}\left(\beta\left(\frac{1+x}{2} + i\lambda\right)\right)$$

(15)

where $x$ is real and where $\beta(z) = \frac{1}{2}\left[\psi((1+z)/2) - \psi(z/2)\right]$. Here $\psi(z)$ is the digamma function. The asymptotic behaviour of $G_x(\lambda)$ for large $l \gg 1$ and $\lambda \gg x$ is

$$G_x(\lambda) \sim \frac{1}{4\pi}\frac{x}{\lambda^2} + \mathcal{O}(\lambda^{-4}) .$$

(16)

Below we will also need the small-$\lambda$ asymptotics of $G_1(\lambda)$, which is given by

$$G_1(\lambda) = \frac{1}{2\pi}\left[2\ln(2) + 2\sum_{n=1}^{\infty}(-1)^n(1 - 2^{-2n})\zeta(2n + 1)\lambda^{2n}\right] \qquad |\lambda| < 1 .$$

(17)

## 2. Wiener–Hopf analysis for the dressed energies

In this section we analyse the coupled integral equations (14) by means of Wiener–Hopf techniques [30] (for detailed expositions see, e.g., [29, 31]). As equations (14) are similar to the analogous equations for the densities in the periodic $t$–$J$ chain the necessary steps are the same as in [19]. However, as we will need more explicit answers than are given in [19] for determining the boundary contribution to the ground-state energy we briefly summarize the most important steps below. After Fourier-transforming, the first equation of (14) can be turned into a Wiener–Hopf equation for $y(\lambda) = \varepsilon_s(\lambda + A)$:

$$y(\lambda) = -2\pi G_0(\lambda + A) + \frac{H}{2} + \int_0^{\infty} d\nu \, [G_1(\lambda - \nu) + G_1(\lambda + \nu + 2A)]y(\nu)$$

$$+ CG_0(\lambda + A)$$

(18)

where $C = \int_{-B}^{B} d\nu \, \exp(\pi\nu)\varepsilon_c(\nu)$. Here we have used the fact that $A \gg 1$ and $B \ll 1$ to approximate

$$\int_{-B}^{B} d\nu \, G_0(\lambda - \nu + A)\varepsilon_c(\nu) \approx G_0(\lambda + A)\int_{-B}^{B} d\nu \, \exp(\pi\nu)\varepsilon_c(\nu) .$$

The quantity $C$ is determined self-consistently below. Equation (18) can now be solved by iteration $y(\lambda) = y_1(\lambda) + y_2(\lambda) + \cdots$, where

$$y_1(\lambda) = -2\pi G_0(\lambda + A) + \frac{H}{2} + \int_0^{\infty} d\nu \, G_1(\lambda - \nu)y_1(\nu) + CG_0(\lambda + A)$$

(19)

$$y_2(\lambda) = \int_0^{\infty} d\nu \, G_1(\lambda + \nu + 2A) \, y_1(\nu) + \int_0^{\infty} d\nu \, G_1(\lambda - \nu) \, y_2(\nu) .$$

(20)

† These can be shown to be (minus) the energies of the order-one contributions to the elementary charge and spin excitations [22].

These equations can be solved in a standard way through a Wiener–Hopf factorization. The result for $y_1$ is obtained in complete analogy with, e.g., the appendix of [28]

$$\widetilde{y}_1^+(\omega) = G^+(\omega)\left\{\frac{\mathrm{i}HG^-(0)}{2}\frac{1}{\omega+\mathrm{i}0} - \mathrm{i}(2\pi - C)G^-(-\mathrm{i}\pi)\frac{\exp(-\pi A)}{\omega + \mathrm{i}\pi}\right\} + \mathcal{O}(\exp(-2\pi A)).\tag{21}$$

Here the Fourier transform $\widetilde{y}_1^+(\omega) = \int_0^\infty \mathrm{d}\lambda\, y(\lambda)\exp(\mathrm{i}\lambda\omega)$ is analytic in the upper half-plane and $G^\pm(\omega)$ are analytic functions in the upper/lower half-plane factorizing the kernel $1 + \exp(-|\omega|) = G^+(\omega)G^-(\omega)$

$$G^+(\omega) = G^-(-\omega) = \frac{\sqrt{2\pi}}{\Gamma(\frac{1}{2} - \mathrm{i}\omega/2\pi)}\left(\frac{-\mathrm{i}\omega}{2\pi}\right)^{-\mathrm{i}\omega/2\pi}\exp\left(\frac{\mathrm{i}\omega}{2\pi}\right).\tag{22}$$

The equation for $y_2(\lambda)$ is more difficult to solve. They key is to use the fact that $\lambda + \lambda' + 2A \gg 1$. Using the asymptotic behaviour (16) of $G_1(\lambda)$ in the expression for the driving term $D(\lambda) = \int_0^\infty \mathrm{d}\lambda'\, G_1(\lambda + \lambda' + 2A)y_1(\lambda')$ and then performing a Laplace transformation we obtain

$$D(\lambda) \sim \frac{1}{4\pi}\int_0^\infty \mathrm{d}x\,\exp(-2Ax)\exp(-|\lambda|x)\widetilde{y}_1^+(\mathrm{i}x)\left[x + \frac{x^3}{12} + \cdots\right]\tag{23}$$

where the expansion in $x$ corresponds to the asymptotic expansion of $G_1(\lambda + \lambda' + 2A)$. It is clear that due to the strongly decaying factor $\exp(-2Ax)$ the leading contribution to the integral comes from the small-$x$ region. Inserting the expression (23) for the driving term into (20) and then following through the same steps as in the analysis for $y_1$ we arrive at

$$\widetilde{y}_2^+(\omega) \sim G^+(\omega)\frac{\mathrm{i}}{4\pi}\int_0^\infty \mathrm{d}x\,\exp(-2Ax)\left[x + \frac{x^3}{12} + \cdots\right]\frac{G^+(\mathrm{i}x)\widetilde{y}_1^+(\mathrm{i}x)}{\omega + \mathrm{i}x}$$

$$\sim G^+(\omega)\frac{\mathrm{i}H\sqrt{2}}{4\pi}\int_0^\infty \mathrm{d}x\,\exp(-2Ax)\frac{1 + (x/2\pi)\ln(x) + \cdots}{\omega + \mathrm{i}x}.\tag{24}$$

By means of a similar analysis further corrections to $y(\lambda)$ can be determined. As far as the physical quantities determined below are concerned $y_3$, $y_4$, etc, give rise to contributions much smaller than those due to $y_1$ and $y_2$. We are now in a position to determine the limit of integration $A$ as a function of the magnetic field. By definition $\varepsilon_s(\pm A) = 0 = y(0)$, which leads to

$$A = -\frac{\ln(H)}{\pi} + \frac{\ln\left(\sqrt{2\pi/e}\,(2\pi - C)\right)}{\pi} + \frac{1}{4\pi\ln(H)} + \cdots.\tag{25}$$

Using equations (21) and (24) we can now solve the integral equation (14) for $\varepsilon_c(\lambda)$

$$\varepsilon_c(\lambda) = \varepsilon_0(\lambda) + \int_{-B}^{B}\mathrm{d}v\,[G_1(\lambda - v) + \frac{2a\cosh(\pi\lambda)}{2\pi}\exp(\pi v)]\varepsilon_c(v)\tag{26}$$

where $a = (\pi/e)\exp(-2\pi A)$, $\varepsilon_0(\lambda) = \mu - 2\pi G_1(\lambda) - 2a\cosh(\pi\lambda)$, and where we have neglected terms of order $o(\exp(-2\pi A))$. Here the term proportional to $a$ originates in the $C$-term in (21). Equation (26) can now be solved by iteration as $B \ll 1$ (corresponding to $|\bar{\mu}| = |2\ln(2) - \mu| \ll 1$) with the result

$$\varepsilon_c(\lambda) = \mu - (2\pi + g)G_1(\lambda) - 2a\cosh(\pi\lambda) + \mathrm{O}(\bar{\mu}a) + \mathcal{O}(\bar{\mu}^2) + \mathcal{O}(a^2)\tag{27}$$

where

$$a = \frac{H^2}{8\pi^2}\left(1 - \frac{1}{2\ln(H)} + \cdots\right) \qquad g = \frac{8}{3}\frac{1}{\sqrt{6\zeta(3)}}(\bar{\mu} + 2a)^{\frac{3}{2}}.\tag{28}$$

The boundary of integration $B$ defined via $\varepsilon_c(\pm B) = 0$ in this order is given by

$$B^2 = \frac{2}{3\zeta(3)} \left[ \bar{\mu} + 2a + \frac{8\ln(2)}{3\pi} \frac{1}{\sqrt{6\zeta(3)}} (\bar{\mu} + 2a)^{\frac{3}{2}} \right]. \tag{29}$$

$C$ is determined self-consistently to be $-2\zeta(3)B^3$. The higher-order (in $B$) contributions to $\varepsilon_c$ and $B$ do not contribute to the singularities in the thermodynamic quantities and therefore have been dropped.

## 3. Ground-state properties

We are now in a position to determine bulk and boundary contributions to the energy (13). The bulk energy per site is found to be

$$e_{\text{bulk}} = - \left[ \mu + 2\ln(2) + 2a + 2\ln(2)\frac{\zeta(3)}{\pi} B^3 \right] \tag{30}$$

from which we can determine the leading contributions to the zero-temperature magnetization per site, magnetic susceptibility, density and compressibility close to half-filling in a weak magnetic field

$$m_{\text{bulk}} = -\frac{\partial e_{\text{bulk}}}{\partial H} = \frac{H}{2\pi^2} \left( 1 - \frac{1}{2\ln(H)} \right) \left( 1 + \frac{\ln(2)}{\pi} \sqrt{\frac{8(\bar{\mu} + 2a)}{3\zeta(3)}} \right) + \cdots$$

$$\chi_{H,\text{bulk}} = \frac{1}{2\pi^2} \left( 1 - \frac{1}{2\ln(H)} \right) + \frac{2\ln(2)}{\pi} \frac{H^2}{4\pi^4} \left( 1 - \frac{1}{\ln(H)} \right) \frac{1}{\sqrt{6\zeta(3)(\bar{\mu} + 2a)}} + \cdots$$

$$D_{\text{bulk}} = -\frac{\partial e_{\text{bulk}}}{\partial \mu} = 1 - \frac{2\ln(2)}{\pi} \sqrt{\frac{2(\bar{\mu} + 2a)}{3\zeta(3)}} + \cdots \tag{31}$$

$$\chi_{c,\text{bulk}} = \frac{1}{D_{\text{bulk}}^2} \frac{\partial D_{\text{bulk}}}{\partial \mu} = \frac{2\ln(2)}{\pi} \frac{1}{\sqrt{6\zeta(3)[\bar{\mu} + 2a]}} + \cdots$$

in agreement with the expressions for periodic boundary conditions [19, 20]. We note that both the magnetic susceptibility and the compressibility diverge when we approach half-filling.

Contributions to the surface energy, i.e. all terms proportional to $L^{-1}$ in (13), can be divided into boundary-field dependent ones $E^{(\alpha\beta)}$ and contributions due to the 'geometry', i.e. the openness of the chain $E^0$ so that for the four permitted sets of boundary conditions we can write

$$E_{\text{boundary}} = E^0 + E^{(\alpha\beta)} \qquad \alpha, \beta = a, b. \tag{32}$$

The boundary field independent contributions are easily determined

$$E^0 = -\frac{1}{2} \left\{ -\frac{H}{2\ln(H)} \left( 1 + \frac{\ln(\ln(H))}{2\ln(H)} \right) + \mu - \pi - \sqrt{\frac{8}{27\zeta(3)}} (\bar{\mu} + 2a)^{\frac{3}{2}} + \cdots \right\}. \tag{33}$$

We note that for zero bulk magnetic field $H = 0$ and half-filling $\mu = 2\ln 2$ we obtain $E^0 = \frac{1}{2}\pi - \ln 2$, which is the correct result for the surface energy of the open $XXX$ Heisenberg chain [13, 35]. By differentiating the surface energy with respect to the thermodynamic parameters $H$ and $\mu$ we can evaluate the surface contributions to particle number and magnetization in analogy with, e.g., the treatment of the Kondo model [31] (see also [1]). It is reasonable to assume that these contributions are concentrated in the

boundary regions: e.g., we interpret the surface contribution to the particle number to lead to a depletion/increase of electrons in the 'vicinity' of the boundaries.

The leading contributions to the boundary magnetization, particle number and susceptibilities due to $E^0$ are

$$M^0 = -\frac{1}{4\ln(H)}\left(1 + \frac{\ln(\ln(H))}{2\ln(H)}\right) + \cdots \qquad \chi_H^0 = \frac{1}{4H(\ln(H))^2}\left(1 + \frac{\ln(\ln(H))}{2\ln(H)}\right) + \cdots$$

$$N^0 = \frac{1}{2}\left(1 + \sqrt{\frac{2(\bar{\mu} + 2a)}{3\zeta(3)}}\right) \qquad \chi_c^0 = -\frac{4\ln 2 + \pi}{2\pi\sqrt{6\zeta(3)(\bar{\mu} + 2a)}}. \tag{34}$$

We first note that boundary region exhibits a stronger magnetization compared with the bulk, i.e. $M^0/m_{\text{bulk}} = -\pi^2/2H\ln H$, which is much larger than one for the small magnetic fields considered here. The boundary magnetic susceptibility is seen to diverge for $H \to 0$. Following [1] we interpret this as an indication for the presence of a magnetic bound state in the boundary region. The magnetic behaviour is similar to the one for the $XXZ$ spin chain with an open boundary studied in [1].

The leading contribution to the boundary particle number is $\frac{1}{2}$. Because of the constraint of at most single occupancy at any site this increase in particle number (recall that we are very close to half-filling) must be spread out over large regions neighbouring the boundaries. This indicates that boundary effects spread deeply into the bulk. The boundary compressibility for zero boundary fields is seen to be negative and to diverge as we approach half-filling. The type of singularity is the same as for the bulk. Combining the results for magnetization and particle number we see that there is a tendency for spin-up electrons to get pushed towards the boundary.

The leading-order boundary-field dependent contributions $E^{(\alpha\beta)}$ are expressed (see equation (13)) in terms of the quantities

$$\epsilon_b(S) = \int_{-A}^{A} d\nu\, a_S(\nu)\varepsilon_s(\nu) \qquad \epsilon_a(S) = \int_{-B}^{B} d\nu\, a_S(\nu)\varepsilon_c(\nu). \tag{35}$$

where according to (13)

$$E^{(\alpha\beta)} = \frac{1}{2}\left[\epsilon_\beta(-S_1) + \epsilon_\alpha(-S_L)\right] + E_{\alpha\beta} \qquad \alpha, \beta = a, b \tag{36}$$

for the four possible sets of boundary conditions.

The leading contribution to the quantity $\epsilon_a(S)$ can be easily determined for the case $S \gg B$, in which we can expand $a_S(\nu)$ in a power series in $\nu$ and then perform the elementary integrations using expression (26) for $\varepsilon_c(\nu)$. For $S \ll B$ we instead expand $\varepsilon_c(\nu)$ in an infinite power series (using the fact that $G_1(\nu)$ is a smooth function around zero), then perform the integrations, resum the result, and then retain only the leading terms. This results in

$$\epsilon_a(S) = \begin{cases} -\dfrac{4\zeta(3)B^3}{\pi}\dfrac{1}{S} + \cdots & \text{if } S \gg B \\[3mm] \varepsilon_c(0) + \dfrac{2S}{\pi B}(\bar{\mu} + 2a + \cdots) + \cdots & \text{if } S \ll B. \end{cases} \tag{37}$$

The analogous computations for $\epsilon_b(S)$ are more involved, so that we give a brief summary of the necessary steps in appendix B. We find the following result for the leading behaviour:

$$\epsilon_b(S) = -G_S(0)(2\pi + 2\zeta(3)B^3) + \frac{H}{2} + \begin{cases} \dfrac{S-1}{2} \dfrac{H}{\ln(H)} + \cdots & \text{if } S \ll A \\[2ex] -\dfrac{H}{2} - \dfrac{2}{\pi^2 S} H \ln(H) + \cdots & \text{if } S \gg A. \end{cases}$$

(38)

### 3.1. Contributions due to small boundary fields of type a

The contribution to the boundary energy is given by $\frac{1}{2}\epsilon_a(2/h - 2)$ with $2/h - 2 \gg B = \sqrt{2(\bar{\mu} + 2a)/3\zeta(3)}$. (This defines what we mean with 'small' boundary field). Here $h$ is a boundary chemical potential. We define the quantity $\sigma = (h/(1-h))\sqrt{(\bar{\mu} + 2a)/6\zeta(3)}$, which in the present case is much smaller than one. We obtain the following contributions to boundary magnetization/particle number and susceptibilities

$$M^a = \frac{H}{\pi^3}\left(1 - \frac{1}{2\ln(H)}\right)\sigma \qquad N^a = -\frac{2}{\pi}\sigma$$

$$\chi_H^a = \frac{1}{\pi^3}\left(1 - \frac{1}{2\ln(H)}\right)\sigma + \frac{H^2}{4\pi^5}\left(1 - \frac{1}{2\ln(H)}\right)\sigma(\bar{\mu} + 2a)^{-1}$$

(39)

$$\chi_c^a = \frac{\sigma}{\pi}(\bar{\mu} + 2a)^{-1}.$$

We see that a small boundary chemical potential leads essentially to the same type of divergences as are present in the bulk. As expected electrons get pushed away from the boundary although the effect is small. By differentiation with respect to the boundary chemical potential we can evaluate the average number of electrons at the boundary site

$$\langle n_e \rangle = 1 - \frac{2\zeta(3)}{\pi} \frac{B^3}{(1-h)^2} \qquad h \to 0$$

(40)

where $B$ is given by (29). We see that the electron number is larger than the bulk value. This is consistent with the above observation that an open boundary without field leads to an increase in the elctron density in the boundary region.

### 3.2. Contributions due to large boundary fields of type a

Here the boundary chemical potential is taken large, by which we mean that $0 < 2/h - 2 \ll B$. We again use the notation $\sigma = (h/(1-h))\sqrt{(\bar{\mu} + 2a)/6\zeta(3)}$, but now $\sigma \gg 1$. We find

$$M^a = \frac{H}{4\pi^2}\left(1 - \frac{1}{2\ln(H)}\right)\left(1 - \frac{1}{\pi\sigma}\right)$$

$$N^a = -\frac{1}{2}\left(1 + \frac{2\ln(2)}{\pi}\sqrt{\frac{2(\bar{\mu} + 2a)}{3\zeta(3)}}\right) + \frac{1}{2\pi\sigma}$$

(41)

$$\chi_H^a = \frac{1}{4\pi^2}\left(1 - \frac{1}{2\ln(H)}\right)\left(1 - \frac{1}{\pi\sigma}\right) + \frac{1}{\pi\sigma}\frac{H^2}{(2\pi)^4}\left(1 - \frac{1}{\ln(H)}\right)(\bar{\mu} + 2a)^{-1} + \cdots$$

$$\chi_c^a = \frac{3\ln(2)}{\pi\sqrt{6\zeta(3)(\bar{\mu} + 2a)}} + \frac{1}{4\pi\sigma}(\bar{\mu} + 2a)^{-1}.$$

The magnetization is again proportional to $H$ and the magnetic susceptibility can only diverge at half-filling. The large boundary field yields, however, a contribution of $-\frac{1}{2}$ to the boundary particle number, which indicates a strong depletion of electrons in the boundary region. This is in accordance with the expectation based on a naive analysis of the Hamiltonian (1) that large boundary chemical potentials (with our choice of sign in (1)) should favour the presence of holes in the boundary region. The compressibility exhibits a stronger divergence than the bulk if we approach half-filling keeping $\sigma$ fixed. The average electron number at the boundary site is found to be

$$\langle n_{\mathrm{e}} \rangle = 1 - \frac{2}{\pi h^2} \sqrt{6 \zeta(3)(\bar{\mu} + 2a)} \qquad h \to 1 \tag{42}$$

which is less than the bulk value.

### 3.3. Contributions due to large boundary fields of type b

Let us first consider the region where $h|\ln H| \gg 2\pi$, which corresponds to the case $S \ll A$. By straightforward differentiation we find

$$M^b = -\frac{1}{4} + \frac{h-1}{2h \ln H} + \frac{HB}{4\pi^3}\left[\psi\left(\frac{1+h}{2h}\right) - \psi\left(\frac{1}{2h}\right)\right]$$

$$\chi_H^b = \frac{1-h}{2hH \ln^2 H} + \frac{1}{4\pi^3}\left[\psi\left(\frac{1+h}{2h}\right) - \psi\left(\frac{1}{2h}\right)\right]\left(B + \frac{H^2}{6\pi^2 \zeta(3)B}\right)$$

$$N^b = -\frac{1}{2\pi}\left[\psi\left(\frac{1+h}{2h}\right) - \psi\left(\frac{1}{2h}\right)\right]\sqrt{\frac{2(\bar{\mu}+2a)}{3\zeta(3)}} \tag{43}$$

$$\chi_c^b = \frac{1}{2\pi}\left[\psi\left(\frac{1+h}{2h}\right) - \psi\left(\frac{1}{2h}\right)\right]\frac{1}{\sqrt{6\zeta(3)(\bar{\mu}+2a)}}.$$

Thus the boundary field contributes to the singularity in the magnetic susceptibility for large boundary fields $h$. Furthermore there is a constant contribution $-\frac{1}{4}$ to the boundary magnetization, which indicates a surplus of spin-down electrons in the boundary region. The negative sign stems from the fact that the boundary field is antiparallel to the bulk magnetic field. The boundary particle number contribution is always small (and leads to a depletion of the electron number in the boundary region) and the compressibility exhibits the same type of divergence as the bulk. By differentiating with respect to the boundary field we can calculate the $\langle S^z - \frac{1}{2}n^h\rangle$ at site 1 ($L$) for $ab$ ($ba$) boundary conditions. The result is

$$\left\langle S^z - \frac{n^h}{2}\right\rangle = \frac{1}{2} - \int_0^\infty \mathrm{d}\omega\, \omega \frac{\exp(-\omega)}{1 + \exp(-h\omega)} - \frac{H}{2h^2 \ln H}. \tag{44}$$

This is always finite in the range of $h$ considered. To get a rough idea of the contribution of the integral we note its respective values for $h = 1$ and $h = 2$, which are $\frac{1}{12}\pi^2$ and $0.915\,97$ (Catalan's constant). The contribution proportional to $H$ is always small. The susceptibility is finite, which means that the spins and charges at the boundary itself do not contribute to the bound state responsible for the singularities in the susceptibilities.

### 3.4. Contributions due to small boundary fields of type b

Let us now turn to the region $h|\ln H| \ll 2\pi$ of vanishingly small boundary fields. We find

$$
M^b = \frac{h \ln(H)}{2\pi^2} \qquad \chi_H^b = \frac{h}{2\pi^2 H}
$$
$$
N^b = -\frac{h}{2\pi}\sqrt{\frac{2}{3\zeta(3)}}(\bar{\mu} + 2a) \qquad \chi_c^b = \frac{h}{2\pi\sqrt{6\zeta(3)(\bar{\mu} + 2a)}} \,.
\tag{45}
$$

Note that we cannot take $H \to 0$ without taking the boundary field to zero first. Thus the magnetization is always small. However, the boundary magnetic susceptibility may or may not diverge for $H \to 0$, depending on how fast we take take the boundary field to zero compared with the bulk field. The result for $\langle S^z - \frac{1}{2}n^h \rangle$ is now found to be

$$
\left\langle S^z - \frac{n^h}{2} \right\rangle = -\frac{H \ln(H)}{2\pi^2}\,.
\tag{46}
$$

This is again small and vanishes for half-filling and zero bulk field in accordance with [1]. The corresponding susceptibility is again finite and the spins/charges at the boundary site do not contribute to the bound state.

## 4. The boundary *S*-matrix

In this section we study the effects of the boundary on gapless excitations. For simplicity we set the bulk magnetic field $H$ to zero. As the elementary excitations in the bulk are the same for the periodic and the open chain we begin by giving a thorough discussion of the interpretation of the spectrum in terms of elementary excitations for the periodic system. After reviewing the known results of [17, 22] we present a conjecture concerning the $sl(1|2)$ descendants of the holon and spinon states obtained from the Bethe ansatz.

There are two kinds of gapless elementary excitations in the supersymmetric $t$–$J$ model, associated with spin and charge degrees of freedom, respectively. For the periodic chain they have been extensively studied in [21, 22] (see below for a discussion of the $sl(1|2)$ structure of the excitations). The spin excitations are called spinons and carry spin $\pm\frac{1}{2}$ and zero charge. They are very similar to the spin-waves in the Heisenberg $XXX$ chain [38]. The charge excitations are called holons and antiholons, carry zero spin and charge $\mp e$. Holons correspond to 'particles' in the charge Fermi sea of $\lambda^{(1)}$'s and are thus associated with a physical hole, whereas antiholons correspond to 'holes' (unoccupied $\lambda^{(1)}$'s) in the charge Fermi sea. At half-filling only holons can be excited as the charge Fermi sea is completely empty. The excitation energies are given by $\varepsilon_{s,c}(\lambda)$ (14), whereas their physical momenta (for the periodic chain) are given in terms of the quantities $\mathrm{p}_{s,c}(\lambda)$, which are solutions of the integral equations

$$
\mathrm{p}_s(\lambda) = -\theta(\lambda) - \int_{-A}^{A} \mathrm{d}\nu\, a_2(\lambda - \nu)\mathrm{p}_s(\nu) + \int_{-B}^{B} \mathrm{d}\nu\, a_1(\lambda - \nu)\,\mathrm{p}_c(\nu)
$$
$$
\mathrm{p}_c(\lambda) = \int_{-A}^{A} \mathrm{d}\nu\, a_1(\lambda - \nu)\,\mathrm{p}_s(\nu)\,.
\tag{47}
$$

The mometum of, e.g., a holon–antiholon excitation is given by $P_{c\bar{c}} = \mathrm{p}_c(\Lambda^p) - \mathrm{p}_c(\Lambda^h)$ where $\Lambda^p$ and $\Lambda^h$ are the spectral parameters of the holon and antiholon respectively.

We thus would define the physical holon momentum as $p_c(\Lambda^p) = \mathrm{p}_c(\Lambda^p) - \mathrm{p}_c(B)$. At half-filling the spinon ($p_s$) and holon ($p_c$) momenta are given by

$$p_s(\lambda) = 2\arctan(\exp(\pi\lambda)) - \pi$$

$$p_c(\lambda) = \frac{\pi}{2} + \mathrm{i}\ln\left(\frac{\Gamma(\frac{1}{2} - \frac{1}{2}\mathrm{i}\lambda)\,\Gamma(1 + \frac{1}{2}\mathrm{i}\lambda)}{\Gamma(\frac{1}{2} + \frac{1}{2}\mathrm{i}\lambda)\,\Gamma(1 - \frac{1}{2}\mathrm{i}\lambda)}\right). \tag{48}$$

The 'order one' contributions to the spinon and holon energies at half-filling take the simple form $\varepsilon_s(\lambda) = 2\pi G_0(\lambda)$ and $\varepsilon_c(\lambda) = 2\ln(2) - 2\pi G_1(\lambda)$. The spinon dispersion is thus of the Faddeev–Takhtajan form $\varepsilon_s(p) = \pi\sin(p)$. The holon dispersion cannot be written in closed form so easily.

So far we have not discussed the role played by the $sl(1|2)$ symmetry in the classification of eigenstates. As was shown in [17] all eigenstates of the Hamiltonian obtained from the Bethe ansatz are highest-weight states of the $sl(1|2)$ symmetry algebra of the model. Additional eigenstates of the Hamiltonian can be obtained by acting with the $sl(1|2)$ generators (recall that we are still discussing the periodic chain). This leads to the picture put forward in [17] for the structure of excitations over the antiferromagnetic ground state, i.e. spinon and holon/antiholon excitations are really only the highest-weight states of $sl(1|2)$ multiplets. However, all the additional excitations constructed by acting with the symmetry generators with the exception of the spin-$SU(2)$ descendants can be easily shown to have a gap proportional to the chemical potential (see also [26]). Therefore we can obtain a *complete* set of *gapless* excitations by taking into account spinon and holon states plus their spin-$SU(2)$ descendants. However, one can furthermore argue that in the thermodynamic limit (i.e. if we neglect all finite-size corrections) actually all the gapped $sl(1|2)$ descendants obtained by acting with the symmetry generators can be viewed as being incorporated in multiparticle spinon and holon/antiholon excitations. Let us first discuss the situation for a large finite chain. Here a complete set of states is given by first finding all sets of spectral parameters solving the Bethe equations (4). Each such solution yields the wavefunction of a highest-weight state of $sl(1|2)$ with a given fixed momentum, and a complete set of states is obtained by taking into account the $sl(1|2)$ descendants of the highest-weight state. As we approach the thermodynamic limit we identify one-parameter families of highest-weight states as elementary excitations, the free parameter being the rapidity (which is directly related to the momentum) of the particle. Thus in the thermodynamic limit we are interested in multiparameter families of excited states and the strict counting of states possible in the finite volume loses its meaning. This is the reason why the $sl(1|2)$ descendants of the spinon and holon/antiholon excitations do not have to be taken into account separately anymore in the thermodynamic limit. From the algebraic Bethe ansatz construction we know that the symmetry generators can be represented as the infinite spectral parameter limits of the elements of the monodromy matrix [17, 27]. On the level of the Bethe ansatz states this means that the action of the symmetry generators can be implemented by taking a spectral parameter in an appropriate Bethe ansatz state to infinity. If we therefore take $k$ rapidities of an $n$ parameter family of excited (highest-weight) states to infinity we produce an $n - k$ parameter family of exited states made of $sl(1|2)$ descendants! This means that the family of $sl(1|2)$ descendant states does not have to be taken into account separately anymore, as can equally well be interpreted as 'sitting on the boundary' of the $n$-parametric family of highest-weight states. In this way we obtain an equivalent yet different 'quasiparticle interpretation' in the spirit of McCoy *et al* [33].

As the simplest example let us consider the $sl(1|2)$ descendants of the antiferromagnetic ground state at half-filling, which sits in a multiplet of dimension four, the other three states

being $Q_\sigma|\mathrm{GS}\rangle$ ($\sigma =\uparrow, \downarrow$) with momentum zero and energy $E = 2\ln 2$ and $Q_\downarrow Q_\uparrow|\mathrm{GS}\rangle$ with momentum zero and $E = 4\ln 2$. The state $Q_\downarrow|\mathrm{GS}\rangle$ can be obtained from the spinon–holon scattering state (or more precisely the two-parametric family of states) by taking the spectral parameters of both the holon ($\Lambda^p$) and the spinon ($\lambda^h$) to infinity: indeed the quantum numbers match and $\varepsilon_s(\lambda^h) + \varepsilon_c(\Lambda^p) \to 2\ln 2$ and $p_s(\lambda^h) + p_c(\Lambda^p) \to 0$. The state $Q_\uparrow|\mathrm{GS}\rangle$ can then be obtained by acting with the spin raising operator $S^\dagger$. Similarly the state $Q_\downarrow Q_\uparrow|\mathrm{GS}\rangle$ is obtained from the (two-parametric) holon–holon scattering state by again taking both spectral parameters to infinity.

On the basis of the above discussion we therefore propose that the quasiparticle interpretation of the order one excitation spectrum in terms of two spinons with spin $\pm\frac{1}{2}$ and holon and antiholon excitations put forward in [22] does actually already incorporate the complete $sl(1|2)$ structure. For the half-filled band it is straightforward to show† by using the distribution of integers (12) and the highest-weight theorem that all gapless excitations are scattering states of two spinons and one holon with the superselection rule that the number of spinons plus the number of holons is even. Thus the excitation spectrum of the half-filled $t–J$ model is described by a $SU(2) \times U(1)$ scattering theory.

The scattering matrix has been determined by means of Korepin's method [25, 34] in [21, 22]. At half-filling the spinon-spinon $S$-matrix $S(\lambda)$ and the spinon–holon ($sc$) and holon–holon ($cc$) scattering phases are given by

$$S(\lambda) = \mathrm{i}\frac{\Gamma(\frac{1}{2} - \frac{1}{2}\mathrm{i}\lambda)\,\Gamma(1 + \frac{1}{2}\mathrm{i}\lambda)}{\Gamma(\frac{1}{2} + \frac{1}{2}\mathrm{i}\lambda)\,\Gamma(1 - \frac{1}{2}\mathrm{i}\lambda)}\left(\frac{\lambda}{\lambda - \mathrm{i}}I - \frac{\mathrm{i}}{\lambda - \mathrm{i}}P\right)$$

$$\exp(\mathrm{i}\varphi_{sc}(\lambda)) = -\mathrm{i}\frac{1 + \mathrm{i}\mathrm{e}^{\pi\lambda}}{1 - \mathrm{i}\mathrm{e}^{\pi\lambda}} \qquad \exp(\mathrm{i}\varphi_{cc}(\lambda)) = \frac{\Gamma(\frac{1}{2} + \frac{1}{2}\mathrm{i}\lambda)\,\Gamma(1 - \frac{1}{2}\mathrm{i}\lambda)}{\Gamma(\frac{1}{2} - \frac{1}{2}\mathrm{i}\lambda)\,\Gamma(1 + \frac{1}{2}\mathrm{i}\lambda)} \tag{49}$$

where $I$ and $P$ are the $4 \times 4$ identity and permutation matrices respectively. Below half-filling the $S$-matrices are given in terms of the solution of integral equations. This concludes our discussion of the excitation spectrum of the periodic $t–J$ model. For the case of the open chain the elementary excitations are identical as are the bulk $S$-matrices. What remains in order to completely specify the scattering of elementary excitations is to determine the phase-shifts acquired by the spinons and holons when reflecting from one of the boundaries. Note that due to the particular form of the boundary interactions (no particle production or transmutation) it is clear that the boundary $S$-matrices for holons and spinons are diagonal and thus reduce to phase-shifts for the physical states.

### 4.1. The boundary S-matrix for the exactly half-filled band

For the case of the exactly half-filled band the boundary $S$-matrix can be determined by the method introduced by the Miami group in [35] for the case of the spin $\frac{1}{2}$ $XXX$ Heisenberg chain, which generalizes the methods of Korepin [34] and Andrei *et al* [36, 37]. An alternative method was introduced in [4] and can be seen to lead to the same results. In order to determine the boundary phase shifts for spinons and holons we will study the spinon–holon scattering state. The method of [35] is based on the following quantization condition for factorized scattering of two particles with rapidities $\lambda_{1,2}$ on a line of length $L$ (see also [4])

$$\exp(2\mathrm{i}Lp(\lambda_1))S(\lambda_1 - \lambda_2)K_1(\lambda_1, h_1)S(\lambda_1 + \lambda_2)K_1(\lambda_1, h_L) = 1 \tag{50}$$

† The computation is analogous to the appendix of [32].

where $p(\lambda)$ is the expression for the physical momentum of the corresponding (infinite) periodic system, $S(\lambda)$ are the bulk scattering matrices for scattering of particles 1 and 2, and $K_1(\lambda, h)$ are the $K$-matrices describing scattering of particle 1 with rapidity $\lambda$ off a boundary with boundary field $h$. For the present case of spinon–holon scattering with boundary fields preserving the two $U(1)$ symmetries of spinon and holon numbers this condition turns into scalar equations for the scattering phases, which after taking the logarithm read

$$2Lp_s(\lambda^h) + \varphi_{sc}(\lambda^h - \Lambda^p) + \psi_s(\lambda^h, h_1) + \varphi(\lambda^h + \Lambda^p) + \psi_s(\lambda^h, h_L) = 0 \quad \mathrm{mod}\ 2\pi$$

$$2Lp_c(\Lambda^p) + \varphi_{sc}(\Lambda^p - \lambda^h) + \psi_c(\Lambda^p, h_1) + \varphi(\Lambda^p + \lambda^h) + \psi_c(\Lambda^p, h_L) = 0 \quad \mathrm{mod}\ 2\pi \,.$$

(51)

Here $\lambda^h$ and $\Lambda^p$ are the rapidities of the spinon and holon, respectively. Comparing these conditions with certain quantities ('counting functions') that can be calculated from the Bethe ansatz solution one can then read off the boundary phase-shifts $\psi_{s,c}$ [35]. Let us now discuss this program for the spinon–holon scattering state characterized by choosing $M_1 = L/2$, $N_h = 1$ in the Bethe equations (9). There are $\frac{1}{2}L + 1$ vacancies for the integers $I_\alpha^1$ and thus one hole in the Fermi sea of $\lambda_\alpha^1$. We denote the rapidity corresponding to this hole by $\lambda^h$. The rapidity corresponding to the holon is denoted by $\Lambda^p$. The Bethe equations read

$$\frac{2\pi}{L} I_\alpha = \left(2 + \frac{1}{L}\right)\theta(\lambda_\alpha) - \frac{1}{L}\sum_{\beta=1}^{\frac{1}{2}L+1} \theta\left(\frac{\lambda_\alpha - \lambda_\beta}{2}\right) + \theta\left(\frac{\lambda_\alpha + \lambda_\beta}{2}\right) + \frac{1}{L}\kappa_{ij}^{(1)}(\lambda_\alpha)$$

$$+ \frac{1}{L}\left[\theta\left(\frac{\lambda_\alpha - \lambda^h}{2}\right) + \theta\left(\frac{\lambda_\alpha + \lambda^h}{2}\right) + \theta(\lambda_\alpha - \Lambda^p) + \theta(\lambda_\alpha + \Lambda^p)\right]$$

$$\frac{2\pi}{L} J = \frac{1}{L}\sum_{\alpha=1}^{\frac{1}{2}L+1} \theta(\Lambda^p - \lambda_\alpha) + \theta(\Lambda^p + \lambda_\alpha) + \frac{1}{L}\omega_{ij}(\Lambda^p) - \frac{1}{L}\left[\theta(\Lambda^p - \lambda^h) + \theta(\Lambda^p + \lambda^h)\right].$$

(52)

We note that the ground state at half-filling is identical to the one of the $XXX$ Heisenberg chain and is obtained by filling the rapidities $\lambda_\alpha^1$ between $-\infty$ and $\infty$. In the limit $L \to \infty$ the distribution of roots $\lambda_\alpha$ is described by a single integral equation for the density of roots $\rho_s(\lambda)$, which is of the same structure as (3.28) of [13]. The main complication is that we need to take into account all contribution to order $1/L$ and thus must deal with the fact that the roots are distributed not between $-\infty$ and $\infty$ but between two finite, $L$-dependent values $-A$ and $A$. The integral equation is of Wiener–Hopf form but cannot be solved in a form sufficiently explicit for the purpose of determining the boundary phase-shifts. Following [35] and [4] we make the assumption that the contributions due to the shift of integration boundaries will be of higher order in $1/L$ as far as the boundary phase-shifts are concerned and take $A = \infty$ (the validity of this assumption is discussed at the end of the section). The integral equation then can be solved by Fourier transform with the result

$$\widetilde{\rho}_s(\omega) = 2\widetilde{G}_0(\omega) + \frac{1}{L}\left\{\widetilde{G}_1(\omega)[1 + 2\cos(\omega\lambda^h)] + \widetilde{G}_0(\omega)[1 + 2\cos(\omega\Lambda^p)] + f_{ij}(\omega)\right\} \quad (53)$$

where $\widetilde{G}_x(\omega) = \exp(-\frac{1}{2}x|\omega|)/2\cosh(\frac{1}{2}\omega)$ and where the contributions $f_{ij}$ due to the boundary fields are

$$f_{ab}(\omega) = \widetilde{G}_{-1-S_1}(\omega) \qquad f_{ba}(\omega) = \widetilde{G}_{-1-S_L}(\omega)$$

$$f_{bb}(\omega) = f_{ab}(\omega) + f_{ba}(\omega) \qquad f_{aa}(\omega) = 0\,.$$

(54)

For further analysis it is convenient to define the counting functions $z_s(\lambda)$ and $z_c(\lambda)$

$$
z_s(\lambda) = \frac{2L+1}{2\pi}\theta(\lambda) - \frac{1}{2\pi}\sum_{\beta=1}^{\frac{1}{2}L+1}\theta\left(\frac{\lambda-\lambda_\beta}{2}\right) + \theta\left(\frac{\lambda+\lambda_\beta}{2}\right) + \frac{1}{2\pi}\kappa_{ij}^{(1)}(\lambda)
$$

$$
+ \frac{1}{2\pi}\left[\theta\left(\frac{\lambda-\lambda^h}{2}\right) + \theta\left(\frac{\lambda+\lambda^h}{2}\right) + \theta(\lambda-\Lambda^p) + \theta(\lambda+\Lambda^p)\right]
$$

$$
z_c(\Lambda) = \frac{1}{2\pi}\sum_{\alpha=1}^{\frac{1}{2}L+1}\theta(\Lambda-\lambda_\alpha) + \theta(\Lambda+\lambda_\alpha) + \frac{1}{2\pi}\omega_{ij}(\Lambda) - \frac{1}{2\pi}\left[\theta(\Lambda-\lambda^h) + \theta(\Lambda+\lambda^h)\right].
$$

$$
(55)
$$

Note that for any root, e.g., $\lambda_\alpha$ of (52) the counting function takes the integer value $z_s(\lambda_\alpha) = I_\alpha$ by construction. In the thermodynamic limit $1/L$ times the derivative of $z_s(\lambda)$ yields the distribution function of rapidities $\rho_s(\lambda)$. Straightforward integration of the density $\rho_s(\lambda)$ yields the following results for the counting functions in the thermodynamic limit evaluated at the rapidities of the spinon and holon, respectively,

$$
2\pi z_s(\lambda^h) = 2Lp_s(\lambda^h) + \varphi_{sc}(\lambda^h - \Lambda^p) + \varphi_{sc}(\lambda^h + \Lambda^p) + \phi_s(\lambda^h) = 0 \mod 2\pi
$$

$$
-2\pi z_c(\Lambda^p) = 2Lp_c(\Lambda^p) + \varphi_{sc}(\Lambda^p - \lambda^h) + \varphi_{sc}(\lambda^h + \Lambda^p) + \phi_c(\Lambda^p) = 0 \mod 2\pi
$$

$$
(56)
$$

where $p_{s,c}(\lambda)$ are the spinon/holon momenta (48), $\varphi_{sc}(\lambda)$ is the bulk phase-shift for spinon–holon scattering (49), and

$$
\phi_s(\lambda) = -\int_{-\infty}^{\infty}\frac{d\omega}{i\omega}\left[\widetilde{G}_1(\omega)(1+\exp(-i\omega\lambda)) + \widetilde{G}_0(\omega) + f_{ij}(\omega)\right]\exp(-i\omega\lambda)
$$

$$
\phi_c(\lambda) = \int_{-\infty}^{\infty}\frac{d\omega}{i\omega}\left[\widetilde{G}_1(\omega)(1+\exp(-i\omega\lambda)) - \widetilde{G}_0(\omega) + f_{ij}(\omega)\exp\left(-|\frac{\omega}{2}|\right)\right]
$$

$$
\times \exp(-i\omega\lambda) - \omega_{ij}(\lambda).
$$

$$
(57)
$$

The last equalities in (56) hold due to the fact that evaluation of the counting function at a root of the Bethe equations yields an integer number. From these equations we can now infer the boundary phase shifts by comparing them with the quantization condition (51).

The scattering of spinons on a *b*-type boundary with boundary field $h$ is identical to the one in the $XXX$ spin chain and the results are the same as [35]: the phase for a spinon with spin-up and rapidity $\lambda$ is given by

$$
e^{i\psi_{s,\uparrow}^{(b)}(\lambda,h)} = \frac{\Gamma(\frac{1}{4}-\frac{1}{2}i\lambda)\,\Gamma(1+\frac{1}{2}i\lambda)\,\Gamma((2-h)/4h-\frac{1}{2}i\lambda)\,\Gamma((2+h)/4h+\frac{1}{2}i\lambda)}{\Gamma(\frac{1}{4}+\frac{1}{2}i\lambda)\,\Gamma(1-\frac{1}{2}i\lambda)\,\Gamma((2-h)/4h+\frac{1}{2}i\lambda)\,\Gamma((2+h)/4h-\frac{1}{2}i\lambda)}.
$$

$$
(58)
$$

The analogous phase for a spin-down spinon can be obtained in the following way [35]: as pointed out above switching to the reference state with all spins down leads to a redefinition of the quantities $S_j$. The excitation constructed in a way analogous to the one above over this reference state has spin quantum number $S^z = -\frac{1}{2}$. In order to study negative boundary fields we need to keep track of the modification in the quantities $S_{1,L}$, which are now always positive. Repeating the above analysis for this case we obtain the following boundary phase-shifts for spin-down spinons:

$$
e^{i\psi_{s,\downarrow}^{(b)}(\lambda,h)} = -\frac{\lambda+i(2-h)/2h}{\lambda-i(2-h)/2h}\,e^{i\psi_{s,\uparrow}^{(b)}(\lambda,h)}.
$$

$$
(59)
$$

The phases for scattering of spinons on $a$-type boundaries are very similar, e.g.,

$$\mathrm{e}^{i\psi_{s\uparrow}(\lambda,h')} = \frac{\Gamma(\frac{1}{4} - \frac{1}{2}\mathrm{i}\lambda)}{\Gamma(\frac{1}{4} + \frac{1}{2}\mathrm{i}\lambda)} \frac{\Gamma(1 + \frac{1}{2}\mathrm{i}\lambda)}{\Gamma(1 - \frac{1}{2}\mathrm{i}\lambda)}. \tag{60}$$

These expressions can be obtained from the $b$-type phases by setting the boundary fields to zero. Physically this means that the spinons do not 'see' the $a$-type boundary fields at half-filling.

The phases $\psi_c^{(a)}$ and $\psi_c^{(b)}$ accumulated by a holon scattering off a boundary of type $a$ or $b$ are given by

$$\mathrm{e}^{i\psi_c^{(a)}(\lambda,h)} = \left( \frac{1 - \mathrm{i}(h\lambda/(1-h))}{1 + \mathrm{i}(h\lambda/(1-h))} \right) \left( \frac{\Gamma(\frac{3}{4} + \frac{1}{2}\mathrm{i}\lambda)}{\Gamma(\frac{3}{4} - \frac{1}{2}\mathrm{i}\lambda)} \frac{\Gamma(1 - \frac{1}{2}\mathrm{i}\lambda)}{\Gamma(1 + \frac{1}{2}\mathrm{i}\lambda)} \right)$$

$$\mathrm{e}^{i\psi^{(b)}(\lambda,h)} = \frac{\Gamma((1+h)/2h - \frac{1}{2}\mathrm{i}\lambda)}{\Gamma((1+h)/2h + \frac{1}{2}\mathrm{i}\lambda)} \frac{\Gamma(1/2h + \frac{1}{2}\mathrm{i}\lambda)}{\Gamma(1/2h - \frac{1}{2}\mathrm{i}\lambda)} \left( \frac{\Gamma(\frac{3}{4} + \frac{1}{2}\mathrm{i}\lambda)}{\Gamma(\frac{3}{4} - \frac{1}{2}\mathrm{i}\lambda)} \frac{\Gamma(1 - \frac{1}{2}\mathrm{i}\lambda)}{\Gamma(1 + \frac{1}{2}\mathrm{i}\lambda)} \right).$$

$$\tag{61}$$

Thus scattering of holons off the boundaries is influenced by both types of boundary fields. Let us now investigate the analytic structure of the above phase-shifts. In [38] the physical strip for the spinon rapidity was defined by the condition $|\mathrm{Im}(\lambda)| < 1$ on the basis of periodicity of the expressions for momentum and energy. We propose the further constraint on the physical sheet that the imaginary part of the spinon momentum has to be positive (interpreting the spinons as *particles*). This implies that the spectral parameters should lie in the strip $0 \leqslant \mathrm{Im}(\lambda) < 1$. It now can be seen that the spinon boundary $S$-matrices have no poles on this strip (note that for $\mathrm{e}^{i\psi_{s\downarrow}}$ there is no pole at $\lambda = \mathrm{i}(2-h)/2h$). Therefore there are no boundary bound states in the region of boundary fields we consider here. Let us now turn to the holon boundary $S$-matrices. The physical strip for the holon rapidity is defined by $0 \leqslant \mathrm{Im}(\lambda) < 1$. This needs some explanation. First we impose the constraint $|\mathrm{Im}(\lambda)| < 1$ in order not to have a pole in the holon–holon $S$-matrix. We know that no pole may be present on the physical strip because holons and spinons form a *complete* set of excitations as can be shown by a counting argument based on the Bethe ansatz solution (see above). We then impose the constraint $\mathrm{Im}(\lambda) \geqslant 0$, which corresponds to $\mathrm{Im}(p_c(\lambda)) \leqslant 0$ as holons are not particles but physical holes. We now see that the holon boundary phase-shifts *can* have poles on the physical sheet. Before we continue we would like to recall the constraints $h \in (0, 2)$ and $h' \in (0, 1)$. The holon phase-shifts (61) have poles on the physical sheet for both $a$-type and $b$-type boundary conditions located at the positions $((1-h')/h')\mathrm{i}$ and $\mathrm{i}/h$, respectively. Thus boundary bound states exist in the regions $h' > \frac{1}{2}$ and $h > 1$. We see that a sufficiently strong boundary field is needed for a bound state to be formed.

Let us now dicuss the validity of our 'incomplete' $1/L$ analysis of the densities/counting functions. As pointed out above a complete analytical treatment encounters significant technical difficulties. However, our results can be checked numerically in the following way: if the shift in integration boundary would lead to an additional term of order $1/L$, equation (56) should be incorrect to order one. We performed an explicit numerical evaluation of $\Lambda^p$ and $\lambda^h$ corresponding to integers $L/n$ and $L/m$ with $n$ and $m$ fixed by solving the Bethe equations (52) for chains up to 600 sites. Through insertion of the numerical values of $\lambda^h$ and $\Lambda^p$ into (56) it is then possible to check whether the neglected finite-size effects contribute to order one in the counting functions. We found no evidence for any missing contribution to the boundary phase-shifts. We therefore conclude that for the half-filled band the shift in integration boundary can indeed be neglected.

*4.2. The boundary S-matrix for the less than half-filled band*

Let us now turn to the case of the less than half-filled band. It is a well known fact that below half-filling the scattering matrices are not functions of the differences of the rapidities of the scattering particles any longer. Therefore we need to replace (50) by an appropriately generalized prescription. This can be accomplished by following through the arguments used in [4] to derive (50): first of all the scattering considered below is diagonal in the sense that whenever a spinon or holon bounces off a wall, it merely changes its rapidity $\lambda$ to $-\lambda$ and acquires a phase-shift. Secondly the wavefunctions of the excitations on our finite interval with fixed boundary conditions are standing waves of states with opposite rapidities, which leads to the condition

$$\exp(iLp(\lambda_1))S(\lambda_1, \lambda_2)K_1(\lambda_1, h_1) = \exp(-iLp(\lambda_1))S(-\lambda_1, \lambda_2)K_1(-\lambda_1, h_L) \qquad (62)$$

where $p(\lambda)$ is again the physical momentum of the corresponding (infinite) periodic system and $S(\lambda, \nu)$ are the bulk scattering matrices. The extraction of the boundary phase-shifts from evaluating the counting functions at the spectral parameters of the holons/spinons is much more problematic than for the half-filled case as now the integration boundary $B$ corresponding to the charge Fermi sea is finite and the issue of how to treat the $1/L$ corrections to $B$ arises.

## 5. Conclusion

In this work we have studied zero-temperature boundary effects in an open supersymmetric $t–J$ chain with boundary fields. Surface contributions to ground state properties were evaluated as functions of the boundary fields and the phase-shifts acquired by holons and spinons scattering off a boundary were determined. It also would be interesting to extend the analysis to finite temperatures. This appears to be difficult as among other things the usual expression for the entropy [39] has to be modified in order to project out the spurious states. The best way to deal with these problems seems to be a thermal Bethe ansatz analysis [40].

The (sub-leading) finite-size corrections to the ground-state energy, and energies of low-lying excited states, can be evaluated by means of the Euler–Maclaurin sum formula as well. This was done for the case of the $aa$-boundary conditions and zero bulk magnetic field in [41]. That analysis, which can be straightforwardly extended to the other sets of integrable boundary conditions considered here, allows to make contact with conformal field theory in a geometry with boundary [42].

## Appendix A

In this appendix we derive the expression (13) for the ground state energy. The ground state for given magnetic field $H$ and chemical potential $\mu$ is obtained by filling all vacancies for the integers $I_\alpha^1$ from 1 to $I_{\max} = N_\downarrow + N_h$ and all vacancies for the integers $J_\gamma$ between 1 and $J_{\max} = N_h$. Inserting this description into the Bethe equations (9) and then subtracting

subsequent equations for $\alpha$ and $\alpha + 1$ and $\gamma$ and $\gamma + 1$ we obtain the following equations for the densities $\varrho_s(\lambda_\alpha) = 1/L(\lambda_{\alpha+1} - \lambda_\alpha)$ and $\varrho_c(\lambda_\gamma^{(1)}) = 1/L(\lambda_{\gamma+1}^{(1)} - \lambda_\gamma^{(1)})$:

$$\varrho_s(\lambda_\alpha) = 2a_1(\lambda_\alpha) - \frac{1}{L} \sum_\beta a_2(\lambda_\alpha - \lambda_\beta) + a_2(\lambda_\alpha + \lambda_\beta)$$

$$+ \frac{1}{L} \sum_\gamma a_1(\lambda_\alpha - \lambda_\gamma^{(1)}) + a_1(\lambda_\alpha + \lambda_\gamma^{(1)}) + \frac{1}{L}\left(\frac{\kappa_{ij}'(\lambda_\alpha)}{2\pi} + a_1(\lambda_\alpha)\right) \qquad \text{(A1)}$$

$$\varrho_c(\lambda_\gamma^{(1)}) = \frac{1}{L} \sum_\alpha a_1(\lambda_\gamma^{(1)} - \lambda_\alpha) + a_1(\lambda_\gamma^{(1)} + \lambda_\alpha) + \frac{1}{2\pi L}\omega_{ij}'(\lambda_\gamma^{(1)}).$$

Here $\kappa_{ij}'(\lambda)$ and $\omega_{ij}'(\lambda)$ are the derivatives of $\kappa_{ij}^{(1)}(\lambda)$ and $\omega_{ij}(\lambda)$ defined in (11), respectively. Now we follow [4] and rewrite (A1) in terms of a set of 'doubled' variables

$$\nu_\alpha = \begin{cases} -\lambda_{N_\downarrow + H_h - \alpha} & \alpha = 0, \dots, N_\downarrow + N_h \\ \lambda_{\alpha - N_\downarrow - N_h} & \alpha = N_\downarrow + N_h + 1, \dots, 2(N_\downarrow + N_h) \end{cases}$$

$$\nu_\gamma^{(1)} = \begin{cases} -\lambda_{N_h - \gamma}^{(1)} & \gamma = 0, \dots, N_h \\ \lambda_{\gamma - N_h} & \gamma = N_h + 1, \dots, 2N_h \end{cases} \qquad \text{(A2)}$$

where we defined $\lambda_0 = 0$ and $\lambda_0^{(1)} = 0$. Now we take the thermodynamic limit of the equations (A1) written in the new variables. This is done by using the Euler–Maclaurin sum formula to turn sums into integrals (see, e.g, [13, 43, 44]). Care has to be exercised in order to take into account the fact that terms depending on the spectral parameters located at zero must be subtracted explicitly. After some manipulations we arrive at following coupled integral equations for the densities $\rho_s(\nu_\alpha) = 1/L(\nu_{\alpha+1} - \nu_\alpha)$ and $\rho_c(\nu_\gamma^{(1)}) = 1/L(\nu_{\gamma+1}^{(1)} - \nu_\gamma^{(1)})$:

$$\rho_s(\lambda) = 2a_1(\lambda) - \int_{-A^+}^{A^+} d\mu\, a_2(\lambda - \mu)\, \rho_s(\mu) + \int_{-B^+}^{B^+} d\mu\, a_1(\lambda - \mu)\rho_c(\mu)$$

$$+ \frac{1}{L}\left(\frac{\kappa_{ij}'(\lambda)}{2\pi} + a_2(\lambda)\right) \qquad \text{(A3)}$$

$$\rho_c(\lambda) = \int_{-A^+}^{A^+} d\mu\, a_1(\lambda - \mu)\, \rho_s(\mu) + \frac{1}{L}\left(\frac{\omega_{ij}'(\lambda)}{2\pi} - a_1(\lambda)\right)$$

where $A^+$ and $B^+$ are the spectral parameters corresponding to the maximal taken integers $I_\alpha^1$ and $J_\gamma$ plus $\frac{1}{2}$. Higher order terms in the Euler–Maclaurin expansion have been dropped as they turn out to not contribute to the surface energy.

The energy per site (6) in the thermodynamic limit can be expressed in terms of the densities $\rho_{s,c}$ as†

$$\frac{E}{L} = - \int_{-A^+}^{A^+} d\nu \left[\pi a_1(\nu) - \frac{H}{2}\right] \rho_s(\nu) + \int_{-B^+}^{B^+} d\nu \left[\frac{\mu}{2} - \frac{H}{4}\right] \rho_c(\nu)$$

$$+ \frac{1}{L}\left(-\frac{\mu}{2} - \frac{H}{4} + E_{ij} + 2\right) - \mu - \frac{H}{2}. \qquad \text{(A4)}$$

Note that we have divided the bare energies by two due to the fact that we are working with the densities of the doubled variables. We also explicitly subtracted a term

† We again turn the sums into integrals by means of the Euler–Maclaurin formula.

$(1/L)(\mu/2 + H/4 - 2)$ to compensate for the spurious roots at zero. To proceed further we rewrite (A3) as an operator equation:

$$\begin{pmatrix} I - \widehat{K}_{ss} & -\widehat{K}_{sc} \\ -\widehat{K}_{cs} & I - \widehat{K}_{cc} \end{pmatrix} * \begin{pmatrix} \rho_s \\ \rho_c \end{pmatrix} = \begin{pmatrix} \rho_s^{(0)} \\ \rho_c^{(0)} \end{pmatrix}$$

(A5)

where $I$ is the identity operator and $*$ denotes convolution with the appropriate kernel, e.g., $-\widehat{K}_{ss} * \rho_s\big|_\lambda = \int_{-A^+}^{A^+} \mathrm{d}\mu\, a_2(\lambda - \mu)\rho_s(\mu)$ and where

$$\rho_s^{(0)} = 2a_1(\lambda) + \frac{1}{L}\left(\frac{\kappa'_{ij}(\lambda)}{2\pi} + a_2(\lambda)\right) \qquad \rho_c^{(0)} = \frac{1}{L}\left(\frac{\omega'_{ij}(\lambda)}{2\pi} - a_1(\lambda)\right).$$

(A6)

We note that the above integral kernels are all symmetric. In what follows we use the shorthand notation $(id - \widehat{K})_{ab}\rho_b = \rho_a^{(0)}$ for (A5). Let us now define quantities $\varepsilon_s(\lambda)$ and $\varepsilon_c(\lambda)$ through the integral equations $(id - \widehat{K})_{ab}\varepsilon_b = \varepsilon_a^{(0)}$, where $\varepsilon_s^{(0)}(\lambda) = -2\pi a_1(\lambda) + H$ and $\varepsilon_c^{(0)}(\lambda) = \mu - H/2$. With $\chi = -\mu/2 - H/4 + E_{ij} + 2$ the energy per site can now be written as

$$\begin{aligned}
\frac{E}{L} &= \frac{1}{2}\sum_{b=s,c}\int_{-C_b^+}^{C_b^+} \mathrm{d}\mu\, \varepsilon_b^{(0)}(\mu)\rho_b(\mu) - \mu - \frac{H}{2} + \frac{\chi}{L} \\
&= \frac{1}{2}\sum_{a,b=s,c}\int_{-C_b^+}^{C_b^+} \mathrm{d}\mu\, \varepsilon_b^{(0)}(\mu)(id - \widehat{K})_{ba}^{-1} * \rho_a^{(0)}\bigg|_\mu - \mu - \frac{H}{2} + \frac{\chi}{L} \\
&= \frac{1}{2}\sum_{a=s,c}\int_{-C_a^+}^{C_a^+} \mathrm{d}\mu\, \varepsilon_a(\mu)\rho_a^{(0)}(\mu) - \mu - \frac{H}{2} + \frac{\chi}{L}
\end{aligned}$$

(A7)

where $C_s^+ = A^+$ and $C_c^+ = B^+$. In the thermodynamic limit the ground state is obtained by minimizing $E$ with respect to the integration boundaries $A^+$ and $B^+$ (see, e.g., [44]), i.e. $\partial E/\partial C_a^+\big|_{C_a^+ = C_a} = 0$, where $C_s = A$, $C_c = B$. From this fact it follows that the integration boundaries $C_a^+$ in (A7) can be replaced by $C_a$ with error of $\mathcal{O}(L^{-2})$, which does not affect the surface energy we are after. In other words we can replace $C_a^+$ by $C_a$ (up to $\mathcal{O}(L^{-2})$) due to the fact that the dressed energies vanish at the integration boundaries. This finally establishes (13).

## Appendix B

In this appendix we outline how to evaluate the integral (38). We first note that via Fourier transform the following equality can be established:

$$\int_{-A}^{A} \mathrm{d}\mu\, a_S(\mu)\, \varepsilon_s(\mu) = -2\pi G_S(0) + \frac{H}{2} + 2\int_0^\infty \mathrm{d}\mu\, \big[G_{1+S}(\mu + A) - a_S(\mu + A)\big] y(\mu)$$

$$+ \int_{-B}^{B} G_S(\mu)\varepsilon_c(\mu).$$

(B1)

The last term on the right-hand side is readily evaluated by using the fact that $G_S(\mu)$ is smooth around zero and thus can be Taylor expanded

$$\int_{-B}^{B} G_S(\mu)\varepsilon_c(\mu) = -2\zeta(3)B^3 G_S(0).$$

(B2)

The second term on the right-hand side (which will be denoted by $R_2$ in the following) is more difficult to treat. In the region where $S \ll A$ we can use the asymptotic expansions

$G_{1+S}(\mu + A) \sim (1 + S)/4\pi(\mu + A)^2$ and $a_S(\mu + A) \sim S/2\pi(\mu + A)^2$ to determine the leading contribution to the integral. We then Laplace transform $1/(\mu + A)^2$ and after some manipulations arrive at

$$\int_0^\infty d\mu \, \frac{1}{(A + \mu)^2} \, y(\mu) = \int_0^\infty dx \, x e^{-Ax} \widetilde{y}^+(ix) \, . \tag{B3}$$

Due to the strongly decaying factor $e^{-Ax}$ the leading contribution to this integral clearly comes from the region around $x = 0$. Expanding $\widetilde{y}^+(ix)$ around $x = 0$ we finally obtain

$$R_2 = \frac{S - 1}{2} \frac{H}{\ln H} + \text{ subleading terms} \, . \tag{B4}$$

In the region $S \gg A$ the above strategy for determining $R_2$ is not applicable. Instead we Fourier transform and arrive at

$$R_2 = -\frac{1}{2\pi A} \int_0^\infty d\omega \, \frac{e^{-((S-1)/2A)\omega}}{\cosh(\omega/2A)} \left\{ \cos\omega \left( \widetilde{y}^+\left(\frac{\omega}{A}\right) + \widetilde{y}^+\left(-\frac{\omega}{A}\right) \right) \right.$$

$$\left. + i\sin\omega \left( \widetilde{y}^+\left(\frac{\omega}{A}\right) - \widetilde{y}^+\left(-\frac{\omega}{A}\right) \right) \right\} \, . \tag{B5}$$

We again have a strongly decaying factor in the integrand (recall that $(S - 1)/2A \gg 1$) so that we can expand the other terms around $\omega = 0$. The problem we run into now is that the subleading terms in the expansion of $y(\lambda)$ contribute in an important way. The leading contribution of $y_1$ to $R_2$ is found to be (after expanding $\widetilde{y}_1^+$ around $\omega = 0$ only elementary integrals are encountered)

$$-\frac{H}{2} + \frac{H}{\pi^2} \frac{\ln(S - 1)}{S - 1} - \frac{2H \ln H}{\pi^2(S - 1)} \, . \tag{B6}$$

The second term is precisely cancelled by the leading contribtuion from $y_2$ to $R_2$, whereas the further terms are all small compared with $-2H \ln H/\pi^2(S - 1)$.

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