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The one-dimensional Hubbard model with open ends: universal divergent contributions to the magnetic susceptibility

Michael Bortz[1] **and Jesko Sirker**[2]

[1] Department of Theoretical Physics, Research School of Physics and Engineering, Australian National University, Canberra ACT 0200, Australia

[2] Department of Physics and Astronomy, University of British Columbia, Vancouver, BC V6T 1Z1, Canada

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Abstract

The magnetic susceptibility of the one-dimensional Hubbard model with open boundary conditions at arbitrary filling is obtained from field theory at low temperatures and small magnetic fields, including leading and next-leading orders. Logarithmic contributions to the bulk part are identified as well as algebraic–logarithmic divergences in the boundary contribution. As a manifestation of spin–charge separation, the result for the boundary part at low energies turns out to be independent of filling and interaction strength and identical to the result for the Heisenberg model. For the bulk part at zero temperature, the scale in the logarithms is determined exactly from the Bethe ansatz. At finite temperature, the susceptibility profile as well as the Friedel oscillations in the magnetization are obtained numerically from the density-matrix renormalization group applied to transfer matrices. Agreement is found with an exact asymptotic expansion of the relevant correlation function.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

The one-dimensional Hubbard model plays a central role in the understanding of interacting electrons in one dimension. The Hamiltonian,

$$H = -\sum_{j=1}^{L-1}\sum_{a=\uparrow,\downarrow}\left(c_{j,a}^{\dagger}c_{j+1,a} + c_{j+1,a}^{\dagger}c_{j,a}\right) + 4u\sum_{j=1}^{L} n_{j,\uparrow}n_{j,\downarrow} - \frac{h}{2}\sum_{j=1}^{L}(n_{j,\uparrow} - n_{j,\downarrow}), \tag{1}$$

arises naturally in the tight-binding approximation of electrons on a chain with L sites. In (1), the magnetic field h couples to the z-component of the total spin. The interaction parameter

$u = U/|t| > 0$ is the ratio between the on-site Coulomb repulsion U and the hopping amplitude t. Note that the eigenvalues of H are invariant under a sign change $t \to -t$ [1]. Furthermore, H is invariant under reversal of all spins and under a particle–hole transformation (the so-called Shiba transformation) [1]. Therefore we restrict ourselves here to positive magnetization and lattice filling less than or equal to 1.

The appealing simplicity of the Hamiltonian, combined with its Bethe ansatz (BA) solvability and its adequateness for field-theoretical studies are the reasons for its wide popularity.

Recent experimental achievements in two areas additionally motivate our studies: on the one hand, the fabrication and characterization of carbon nanotubes have shown that these can be considered as realizations of one-dimensional Hubbard models [2]. Especially, kinks in these quantum wires have been realized experimentally [3, 4]. A kink locally weakens the hopping amplitude at one specific lattice site in the Hamiltonian. Such a modification is known to be a relevant perturbation, which, at $u > 0$, is governed by a fixed point with zero conductance through the kink [5]. Thus at low energies the chain is effectively cut into two pieces.

On the other hand, ultracold fermionic atoms in optical lattices can be described by a one-band Hubbard model [6]. Given the recent progress in realizing quasi one-dimensional bosonic quantum gases [7], it is likely that similar experimental progress will be made with fermions.

In order to model these situations, we consider open boundary conditions in (1). Compared to the case with periodic boundary conditions, an additional surface contribution f_B to the free energy occurs, defined as

$$f_B = \lim_{L\to\infty} (F_{obc} - F_{pbc}), \tag{2}$$

where F_{obc} (F_{pbc}) is the total free energy for open (periodic) boundary conditions. In this work, we will focus on the magnetic susceptibility per lattice site $\chi = \chi_{bulk} + \chi_B/L$ both at $T = 0, h \geqslant 0$ and $T \geqslant 0, h = 0$, at arbitrary fillings.

For half-filling, the bulk contribution χ_{bulk} at $T = h = 0$ has first been given by Takahashi [8], where the existence of logarithmic contributions at finite h is also mentioned. Later on, Shiba [9] calculated χ_{bulk} at $T = h = 0$ for general filling. The free energy at finite temperatures was given by Takahashi (for an overview and original literature, cf the book [10]), and later by Klümper (the book [11] contains a detailed account of this work). However, it seems as if the explicit behaviour of χ_{bulk} at $T = 0, h \gtrsim 0$ and $T \gtrsim 0, h = 0$ has not been derived so far. In this work, this gap will be filled.

Although the boundary quantity χ_B is only an $\mathcal{O}(1)$-correction to the total bulk contribution, it may become important in experiments if it shows a divergence with respect to the temperature T or magnetic field h. Indeed, such divergences have been discovered and analysed in the tJ-chain [12] spin-1/2 Heisenberg chain [13–17]. Since the isotropic spin-1/2 Heisenberg chain is obtained from (1) in the limit $u \to \infty$, related divergences are also expected to occur in (1). In the case of half-filling for $T = 0$, it has been shown in [15, 18] that the boundary magnetic susceptibility is divergent, $\chi_B \sim 1/(h \ln^2 h)$, for $h \to 0$. In addition, due to the OBCs translational invariance is broken. Therefore quantities such as the magnetization or the density become position dependent. Local measurements of such quantities then provide a way to obtain information about the impurity making theoretical predictions about the behaviour of such one-point correlation functions desirable.

In section 2 we give the functional forms of both the bulk and the boundary contributions by using a field-theoretical argument. Leading and next-leading logarithmic contributions to the finite bulk susceptibility are found both at finite T and finite h. On the other hand, the boundary contribution diverges in a Curie-like way with logarithmic terms, where again we give both the leading and next-leading divergences. These results depend each on two constants, which are the spin velocity and the scale involved in the logarithms. At magnetic fields or temperatures much smaller than this scale the result for the boundary susceptibility becomes independent of the spin velocity and the scale and therefore completely universal. This is a manifestation of spin–charge separation as will become clear in the next section. For the bulk susceptibility, on the other hand, only the functional dependence on field or temperature will be universal for low energies. The value at zero field and zero temperature, however, is a non-universal constant which does depend on filling and interaction strength via the spin velocity.

The spin velocity has been determined previously from the Bethe ansatz solution [9]. In section 3, for $T = 0$, the scale in the logarithms will be determined exactly as well. The calculation of boundary effects at $T > 0$ based on the Bethe ansatz solution still remains an open problem, as for all Yang–Baxter integrable models (reasons for that are given in [16, 19] for the special case of the spin-1/2 XXZ chain). In section 4 we therefore calculate the susceptibility profile $\chi(x, T)$ and magnetization profile $s(x, T)$ in the asymptotic low-energy limit (that is, for large distances and small temperatures) by making use of conformal invariance. Due to the open boundaries, $s(x, T)$ shows the characteristic Friedel oscillations [20–22]. To test the field-theory predictions, we perform numerical calculations in the framework of the density matrix renormalization group applied to transfer matrices, which is particularly suited for impurity and open-boundary models. In the final section, we will present our conclusions and discuss in which experimental situations the calculated boundary effects might become important.

2. The low-energy effective Hamiltonian

First, we briefly review the effective field theory for the Hubbard model following in large parts [11, 23]. From the effective Hamiltonian we then obtain the magnetic susceptibility at small magnetic field and low temperature.

Let a be the lattice spacing. We introduce fermionic fields $\psi(x)$ in the continuum by

$$c_{j\sigma} \to \sqrt{a}\psi(x) = \sqrt{a}(\mathrm{e}^{\mathrm{i}k_{\mathrm{F}\sigma}x} R_\sigma(x) + \mathrm{e}^{-\mathrm{i}k_{\mathrm{F}\sigma}x} L_\sigma(x)) \tag{3}$$

where $x = j \cdot a$ and the usual splitting into left- and right-moving parts has been performed. The Fermi momentum depends on both the density n and the magnetization s as $k_{\mathrm{F}\uparrow} = \pi(n+2s)/(2a)$, $k_{\mathrm{F}\downarrow} = \pi(n-2s)/(2a)$ (the magnetization is defined as $s = (m_\uparrow - m_\downarrow)/2$, with $m_\sigma = M_\sigma/L$ being the density of particles with spin σ). In the following, we will consider the zero-field case where $k_{\mathrm{F}\uparrow} = k_{\mathrm{F}\downarrow} = \pi n/(2a)$. Equation (3) allows it to introduce a Hamiltonian density $\mathcal{H}(x)$, such that $H = \int \mathcal{H}\,\mathrm{d}x$. In terms of the right- and left-movers in (3) the kinetic part of the Hamiltonian (1) in a lowest order expansion in a becomes

$$\mathcal{H}_0 = -\mathrm{i}v_{\mathrm{F}} \sum_\sigma \left(R_\sigma^\dagger \partial_x R_\sigma - L_\sigma^\dagger \partial_x L_\sigma\right) \tag{4}$$

and the interaction part

$$\begin{aligned}\mathcal{H}_{\mathrm{int}} = 4ua\big\{&:\!\left(R_\uparrow^\dagger R_\uparrow + L_\uparrow^\dagger L_\uparrow\right)\left(R_\downarrow^\dagger R_\downarrow + L_\downarrow^\dagger L_\downarrow\right)\!: - :\!R_\uparrow^\dagger R_\downarrow L_\downarrow^\dagger L_\uparrow\!: - :\!R_\downarrow^\dagger R_\uparrow L_\uparrow^\dagger L_\downarrow\!: \\ &- \left(\mathrm{e}^{4\mathrm{i}k_F x} L_\uparrow^\dagger L_\downarrow^\dagger R_\uparrow R_\downarrow + \mathrm{h.c.}\right)\big\}.\end{aligned} \tag{5}$$

Here ':' denotes normal ordering. For brevity, the x-dependence of the operators has been dropped. The Fermi velocity is given by $v_{\mathrm{F}} := 2a\sin(k_{\mathrm{F}}a)$. The second term in (5) represents backward scattering processes whereas the last term is due to Umklapp scattering. Only in the half-filled case, where $k_F = \pi/(2a)$, is the Umklapp term non-oscillating and has to be kept in the low-energy effective theory. For all other fillings it can be dropped.

To make the Hamiltonian manifestly $SU(2)$ invariant under spin-rotations one can also express $\mathcal{H}$ in terms of the following currents [11, 24, 25]:

$$J = \sum_\sigma : R_\sigma^\dagger R_\sigma :, \qquad \overline{J} = \sum_\sigma : L_\sigma^\dagger L_\sigma :,$$

$$J^a = \frac{1}{2}\sum_{\alpha,\beta} : R_\alpha^\dagger \sigma_{\alpha\beta}^a R_\beta :, \qquad \overline{J}^a = \frac{1}{2}\sum_{\alpha,\beta} : L_\alpha^\dagger \sigma_{\alpha\beta}^a L_\beta :.$$

The free part (4) then reads

$$\mathcal{H}_0 = v_F\left[\frac{\pi}{2}(: J^2 : + : \overline{J}^2 :) + \frac{2\pi}{3}(: \mathbf{J}\cdot\mathbf{J} : + : \bar{\mathbf{J}}\cdot\bar{\mathbf{J}} :)\right]. \tag{6}$$

As far as the interaction part (5) is concerned, we first consider the case $n \neq 1$, that is away from half-filling. Then Umklapp scattering can be ignored leading to

$$\mathcal{H}_{\rm int} = g_c[: J^2 : + : \overline{J}^2 :] + g_s[: \mathbf{J}\cdot\mathbf{J} : + : \bar{\mathbf{J}}\cdot\bar{\mathbf{J}} :] + \lambda_c : J\overline{J} : + \lambda : \mathbf{J}\cdot\bar{\mathbf{J}} : \tag{7}$$

and coupling constants $g_c = ua$, $g_s = -4ua/3$, $\lambda_c = 2ua$ and $\lambda = -8ua$.

Taking equations (6) and (7) together, we see that the Hamiltonian is a sum of two terms: one depending on the scalar currents $J, \overline{J}$ only (corresponding to charge excitations) and the second depending on the vector currents $\mathbf{J}, \bar{\mathbf{J}}$ (associated with spin excitations).

$$\mathcal{H}_c = \left(\frac{\pi v_F}{2} + g_c\right) : [J^2 + \overline{J}^2] : + \lambda_c : J\overline{J} :, \tag{8}$$

$$\mathcal{H}_s = \left(\frac{2\pi v_F}{3} + g_s\right) : [\mathbf{J}\cdot\mathbf{J} + \bar{\mathbf{J}}\cdot\bar{\mathbf{J}}] : + \lambda : \mathbf{J}\cdot\bar{\mathbf{J}} :. \tag{9}$$

The charge and spin parts commute, $[\mathcal{H}_c, \mathcal{H}_s] = 0$.

Let us first focus on $\mathcal{H}_c$. The term with coefficient g_c gives rise to a renormalization of v_F, yielding the charge velocity

$$v_c = v_F + 2ua/\pi. \tag{10}$$

Upon bosonizing, the charge currents are written as [23]

$$J = -\frac{1}{\sqrt{4\pi}}(\Pi + \partial_x\varphi), \qquad \overline{J} = \frac{1}{\sqrt{4\pi}}(\Pi - \partial_x\varphi)$$

where the boson field φ and the corresponding momentum Π satisfy the canonical commutation relation $[\varphi(x), \Pi(x')] = \mathrm{i}\delta(x - x')$. Then

$$\mathcal{H}_c = \frac{v_c}{4}\left[\Pi^2\left(1 - \frac{\lambda_c}{\pi v_c}\right) + (\partial_x\varphi)^2\left(1 + \frac{\lambda_c}{\pi v_c}\right)\right]. \tag{11}$$

By scaling $\varphi' = \varphi\sqrt{K_c}$, $\Pi' = \Pi/\sqrt{K_c}$,

$$K_c = 1 - \frac{\lambda_c}{\pi v_c} \approx 1 - \frac{2ua}{\pi v_F}, \tag{12}$$

this Hamiltonian is written as $\mathcal{H}_c = \frac{v_c}{4}[\Pi'^2 + (\partial_x\varphi')^2]$, which describes noninteracting fields. Note that in this field-theoretical approach the Luttinger parameter K_c is calculated only up to the linear order in u. The same is true for $v_{c,s}$. Contributions in higher u-order would occur if the perturbational approach is pursued further. Fortunately, the Bethe ansatz solvability of the model allows it to calculate $v_{c,s}$, K_c exactly [11]. We will come back to this point in the next section.

In $\mathcal{H}_s$, the g_s-term leads to a renormalization of the spin velocity

$$v_s = v_F - 2ua/\pi. \tag{13}$$

The remaining interaction of vector currents is a marginal perturbation. By setting up the corresponding renormalization group equations, it turns out that it is marginally irrelevant (relevant) for $\mathrm{sgn}(\lambda) < 0$ ($\mathrm{sgn}(\lambda) > 0$) [23, 26]. In our case, $\lambda = -8ua < 0$. The remarkable point about this is that the spin part of the low-energy effective Hubbard model is identical to the corresponding expression for the *XXX*-Heisenberg chain [27, 28], whereas the charge part is described by free bosons (away from half-filling). For this case, field theory has been employed [26–28] to obtain the bulk contribution to the magnetic susceptibility in the form

$$\chi_{\mathrm{bulk}}(E) = \chi_0 \left(1 + \frac{1}{2\ln E_0/E} - \frac{\ln\ln E_0/E}{4\ln^2 E_0/E} + \frac{\gamma_E}{\ln^2 E_0/E} + \cdots\right) \tag{14}$$

$$\chi_0 = \frac{1}{2\pi v_s}, \tag{15}$$

where $E = h, T$ (magnetic field or temperature), $E_0 = h_0, T_0$ is some scale and $\chi_0 := \chi(T = 0, h = 0)$ is given by the inverse of the spin velocity. For the open *XXX*-chain, the boundary contributions have been found to be [13, 14, 17]

$$\chi_B(T) = \frac{1}{12T\ln T_0^{(B)}/T}\left(1 - \frac{\ln\ln T_0^{(B)}/T}{2\ln T_0^{(B)}/T} + \frac{\gamma_T^{(B)}}{\ln T_0^{(B)}/T} + \cdots\right) \tag{16}$$

$$\chi_B(h) = \frac{1}{4h\ln^2 h_0^{(B)}/h}\left(1 - \frac{\ln\ln h_0^{(B)}/h}{\ln\left(h_0^{(B)}/h\right)} + \frac{\gamma_h^{(B)}}{\ln h_0^{(B)}/h} + \cdots\right). \tag{17}$$

From the above considerations we conclude that the bulk and boundary contributions to the magnetic susceptibility in the Hubbard model are also of the form (14)–(17), where, compared to the *XXX*-model, χ_0, T_0, h_0, $\gamma_{T,h}$, $\gamma_{T,h}^{(B)}$ are renormalized by the charge part.

Most interestingly, the pre-factor of χ_B remains unaffected by the charge channel. The divergent boundary contribution for $T \ll T_0^{(B)}$ or $h \ll h_0^{(B)}$ is therefore completely universal

$$\chi_B\left(T \ll T_0^{(B)}\right) = -\frac{1}{12T\ln T}\left(1 + \frac{\ln|\ln T|}{2\ln T}\right) \tag{18}$$

$$\chi_B\left(h \ll h_0^{(B)}\right) = \frac{1}{4h\ln^2 h}\left(1 + \frac{\ln|\ln h|}{\ln h}\right). \tag{19}$$

This can be understood as follows: as the charge- and spin-part of the Hamiltonian separate at low energies, the only way how the charge channel can affect the spin channel is by a renormalization of v_s and K_s. The Luttinger parameter K_s in the spin sector, however, is fixed to $K_s \equiv 1$ due to the $SU(2)$ symmetry and cannot renormalize. The explicit calculations of the pre-factor of χ_B for the *XXX*-model in [13, 14, 17] show, on the other hand, that it does not depend on the spin-velocity v_s. It therefore remains completely independent of the filling factor and the interaction strength.

Let us now comment on the scales involved in equations (14), (16) and (17). Including the order $\mathcal{O}(\ln^{-2} E)$ in equation (14), this equation can be written as

$$\chi_{\mathrm{bulk}}(E) = \chi_0\left(1 - \frac{1}{2\ln E} - \frac{\ln|\ln E|}{4\ln^2 E} + \frac{\gamma_E - (\ln E_0)/2}{\ln^2 E} + \cdots\right). \tag{20}$$

It is convenient to define a new scale $E_0 = \widetilde{E}_0\,\mathrm{e}^{2\gamma_E}$. Then, again up to the order $\mathcal{O}(\ln^{-2} E)$, we have

$$\chi_{\mathrm{bulk}}(E) = \chi_0 \left(1 + \frac{1}{2\ln \widetilde{E}_0/E} - \frac{\ln\ln \widetilde{E}_0/E}{4\ln^2 \widetilde{E}_0/E} + \cdots\right),$$

where the term $\sim\ln^{-2}E$ has been absorbed in the term $\sim\ln^{-1}E$ by the redefinition of the scale. This procedure fixes the scale uniquely [26].

One proceeds analogously with equations (16) and (17) and obtains

$$T_0^{(\mathrm{B})} = \widetilde{T}_0^{(\mathrm{B})}\,\mathrm{e}^{\gamma_T^{(\mathrm{B})}}, \qquad h_0^{(\mathrm{B})} = \widetilde{h}_0^{(\mathrm{B})}\,\mathrm{e}^{\gamma_h^{(\mathrm{B})}} \tag{21}$$

$$\chi_{\mathrm{B}}(T) = \frac{1}{12T\ln \widetilde{T}_0^{(\mathrm{B})}/T}\left(1 - \frac{\ln\ln \widetilde{T}_0^{(\mathrm{B})}/T}{2\ln \widetilde{T}_0^{(\mathrm{B})}/T} + \cdots\right) \tag{22}$$

$$\chi_{\mathrm{B}}(h) = \frac{1}{4h\ln^2 \widetilde{h}_0^{(\mathrm{B})}/h}\left(1 - \frac{\ln\ln \widetilde{h}_0^{(\mathrm{B})}/h}{\ln \widetilde{h}_0^{(\mathrm{B})}/h} + \cdots\right). \tag{23}$$

Let us now turn to the half-filled case $n = 1$. The additional Umklapp term in (5) can also be bosonized and is proportional to $\cos\sqrt{8\pi}\varphi$. When we now again rescale the field $\varphi' = \varphi\sqrt{K_c}$ we obtain a relevant interaction $\sim\cos\sqrt{8\pi/K_c}\varphi'$ for any finite $u > 0$ because $K_c < 1$ in this case. This means that the charge sector will be massive. Indeed, at $u \to \infty$, the excitations of the Hubbard model at half-filling are exactly those of the *XXX*-chain [11]. Formulae (14), (16) and (17) remain valid at half-filling as well. The leading term in equation (17), including the constant h_0, was given in [18]. There, a phenomenological argument was found that generalizes this result to arbitrary filling. The constant h_0 was left undetermined in the arbitrary filling case.

3. Bethe ansatz

In the framework of the BA solution, the energy eigenvalues of (1) are given in terms of certain quantum numbers, the Bethe roots. These roots have to be calculated from a set of coupled algebraic equations. In the thermodynamic limit, these algebraic equations can be transformed into linear integral equations for the densities of roots, with the energy being given by an integral over these densities. In this section, the Bethe ansatz solution is first used to verify the small-coupling expressions for v_c, v_s, K_c; cf equations (10), (12) and (13).

Afterwards, we obtain the magnetic susceptibility at $T = 0$. Therefore, we first analyse the integral equations in the small-field limit, thereby determining the constants in equation (14) (for $T = 0$). The pre-factor χ_0 has been calculated by Shiba [9]. Our essential new results are twofold: on the one hand, the leading h-dependence of the bulk-susceptibility is calculated exactly at small fields, including the scale, for arbitrary fillings. On the other hand, the result for the boundary susceptibility (17) is confirmed within the exact solution. However, due to cumbersome calculations, the constant $\gamma_h^{(\mathrm{B})}$ in equation (17) is left undetermined here. Finally, we consider some special cases and present numerical results.

In order to introduce our notation, we shortly state the main results of the BA solution. For any further details, the reader is referred to [11], which also contains an extensive list of the original literature. The BA solution for the one-dimensional Hubbard model with open boundary conditions has been found by Schulz [29], based on the coordinate Bethe ansatz.

The algebraic BA for this model has been performed in [30]. The BA equations read

$$e^{2ik_j(L+1)} = \prod_{l=1}^{M_\downarrow} \frac{\lambda_l - \sin k_j - iu}{\lambda_l - \sin k_j + iu} \frac{\lambda_l + \sin k_j + iu}{\lambda_l + \sin k_j - iu}, \qquad j = 1, \ldots, N \tag{24}$$

$$\prod_{j=1}^{N} \frac{\lambda_l - \sin k_j - iu}{\lambda_l - \sin k_j + iu} \frac{\lambda_l + \sin k_j - iu}{\lambda_l + \sin k_j + iu} = \prod_{m=1, m\neq l}^{M_\downarrow} \frac{\lambda_l - \lambda_m - 2iu}{\lambda_l - \lambda_m + 2iu} \frac{\lambda_l + \lambda_m - 2iu}{\lambda_l + \lambda_m + 2iu},$$
$$l = 1, \ldots, M_\downarrow, \tag{25}$$

and the energy is given by

$$E = -2 \sum_{j=1}^{N} \cos k_j. \tag{26}$$

Here, we analyse the ground state, where the N-many k_js and the $M_\downarrow$-many λ_ls lie on one half of the real axis, *except the origin*. Although $k = 0, \lambda = 0$ *are* solutions of the system (24) and (25), they must not be counted in (26): these solutions correspond to zero-momentum excitations, which have to be excluded due to the broken translational invariance in the open system[3]. However, one can show that if k_j, λ_l solve (24) and (25), then the same is true for $-k_j, -\lambda_l$. One then 'symmetrizes' equations (24) and (25) by setting up those equations for the sets $\{p_1, \ldots, p_{2N+1}\} := \{-k_N, \ldots, -k_1, 0, k_1, \ldots, k_N\}$ and $\left\{v_1, \ldots, v_{2M_\downarrow+1}\right\} := \left\{-\lambda_{M_\downarrow}, \ldots, -\lambda_1, 0, \lambda_1, \ldots, \lambda_{M_\downarrow}\right\}$:[4]

$$e^{2ip_j(L+1)} \frac{\sin p_j + iu}{\sin p_j - iu} = \prod_{l=1}^{2M_\downarrow+1} \frac{v_l - \sin p_j - iu}{v_l - \sin p_j + iu}, \qquad j = 1, \ldots, 2N+1 \tag{27}$$

$$\frac{v_l + 2iu}{v_l - 2iu} \prod_{j=1}^{2N+1} \frac{v_l - \sin p_j + iu}{v_l - \sin p_j - iu} = \prod_{m=1, m\neq l}^{2M_\downarrow+1} \frac{v_l - v_m + 2iu}{v_l - v_m - 2iu}, \qquad l = 1, \ldots, 2M_\downarrow + 1. \tag{28}$$

These equations can be solved analytically in the small coupling limit; cf appendix A. However, this solution has to be treated with care. It has been shown in [31] that a small-coupling expansion of the ground-state energy *in the thermodynamic limit* has zero radius of convergence. This does not come as a surprise when considering again the low-energy effective theory presented in section 2: at $u = 0$ the interaction of vector currents in equation (9) changes from marginally relevant to marginally irrelevant. Thus in the following we perform the thermodynamic limit before considering any small-field or small-coupling approximations and compare with the results of appendix A afterwards.

In the thermodynamic limit, one can set up equations equivalent to (27) and (28), by introducing the density of ps, $\rho(k)$, and the density of λs, $\sigma(v)$. These densities are solutions to the following set of coupled linear integral equations [15, 29]

$$\rho(k) = \frac{1}{\pi} + \frac{1}{L}\left(\frac{1}{\pi} - \cos k\, a_1(\sin k)\right) + \cos k \int_{-B}^{B} a_1(\sin k - v)\sigma(v)\, dv \tag{29}$$

$$\sigma(v) = \frac{1}{L} a_2(v) + \int_{-Q}^{Q} a_1(v - \sin k)\rho(k)\, dk - \int_{-B}^{B} a_2(v - w)\sigma(w)\, dw, \tag{30}$$

[3] The wavefunction constructed from the coordinate BA [29] would vanish identically for $k = 0, \lambda = 0$.

[4] $k = 0, \lambda = 0$ are included here to introduce homogeneous densities of roots. Their contribution is then subtracted later on; see equations (32) and (33).

where

$$a_n(x) = nu/(\pi(n^2u^2 + x^2)). \tag{31}$$

The integration boundaries are determined from the particle density n and the density of particles with spin down $m_\downarrow$,

$$n = \frac{1}{2}\int_{-Q}^{Q} \rho(k)\,\mathrm{d}k - \frac{1}{2L}, \qquad m_\downarrow = \frac{1}{2}\int_{-B}^{B} \sigma(v)\,\mathrm{d}v - \frac{1}{2L}. \tag{32}$$

Once these equations are solved, the energy density e is obtained from

$$e = -\int_{-Q}^{Q} \cos k\rho(k)\,\mathrm{d}k + \frac{1}{L}. \tag{33}$$

3.1. Velocities and Luttinger parameter

Before proceeding further, we first make contact with the field-theoretical results (10), (12) and (13) in the previous section. Since these concern only bulk-quantities, we discard the $1/L$-corrections in this subsection. We also set the lattice parameter $a \equiv 1$ here.

Furthermore, the results (10), (12) and (13) have been obtained for densities $n \neq 1$ (such that both the charge and spin channels are massless). Analogously, we restrict ourselves here to densities away from half-filling. Within the BA, charge- and spin-velocities are calculated as

$$v_{\mathrm{c,s}} = \frac{\partial\epsilon_{\mathrm{c,s}}}{\partial p_{\mathrm{c,s}}} = \left.\frac{\partial_\lambda\epsilon_{\mathrm{c,s}}(\lambda)}{\partial_\lambda p_{\mathrm{c,s}}(\lambda)}\right|_{\lambda=B,Q} = \left.\frac{1}{\pi}\frac{\partial_\lambda\epsilon_{\mathrm{c,s}}(\lambda)}{(\rho,\sigma)}\right|_{\lambda=B,Q} \tag{34}$$

where $\epsilon_{\mathrm{c,s}}$ is the energy of the lowest possible (i.e. at the Fermi surface) elementary charge/spin excitation and $p_{\mathrm{c,s}}$ the corresponding momentum. After the second equality sign, these quantities are parametrized by the spectral parameter $\lambda = k, v$. Then $p_{\mathrm{c,s}}$ is expressed by the densities ρ, σ. The derivatives of the elementary excitations with respect to the spectral parameter are given by ($\epsilon_{\mathrm{c}}'(k) = \partial_k\epsilon_{\mathrm{c}}(k)$, $\epsilon_{\mathrm{s}}'(v) = \partial_v\epsilon_{\mathrm{s}}(v)$)

$$\epsilon_{\mathrm{c}}'(k) = 2\sin k + \cos k\int_{-B}^{B} a_1(\sin k - v)\epsilon_{\mathrm{s}}'(v)\,\mathrm{d}v \tag{35}$$

$$\epsilon_{\mathrm{s}}'(v) = \int_{-Q}^{Q} a_1(v - \sin k)\epsilon_{\mathrm{c}}'(k)\,\mathrm{d}k - \int_{-B}^{B} a_2(v - w)\epsilon_{\mathrm{s}}'(w)\,\mathrm{d}w. \tag{36}$$

Furthermore, from $\mathcal{H}_{\mathrm{c}}$ in equation (11) it follows that the Luttinger liquid parameter K_{c} is obtained from the charge susceptibility χ_{c} at zero field,

$$\chi_{\mathrm{c}} = \frac{2K_{\mathrm{c}}}{\pi v_{\mathrm{c}}}. \tag{37}$$

The susceptibility $\chi_{\mathrm{c}} = \partial_\mu n$ in turn can be expressed by $\epsilon'(k)|_{k=B}$, $\rho(\mathrm{B})$ and a related function [32]. Although the analytical solution of the integral equations in the limit $u \to 0$ is difficult to obtain due to singular integration kernels, these equations can be solved numerically to high accuracy. Figures 1 and 2 show the velocities and the Luttinger parameter at different fillings as a function of u, together with the analytical predictions (10), (12) and (13) for small u. Agreement is found in all cases.

Once v_{s} is calculated, χ_0 is also known by virtue of equation (15). In the next section we describe how to obtain the h-dependent corrections.

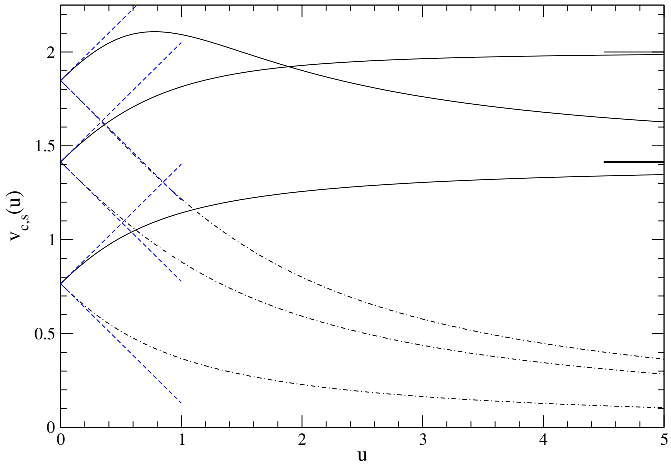

Figure 1. Spin- (black point-dashed lines) and charge- (black full lines) velocities at fillings $n = 1/4, 1/2, 3/4$ (pairs from bottom to top). The dashed lines on the left are the low-u results equations (10) and (13). The horizontal bars on the right indicate the limiting value $v_c|_{u\to\infty} = 2\sin(\pi n)$ [33]. Note that this asymptotic value is the same for both $n = 1/4, 3/4$. By comparing $v_c|_{u=0} = v_F = 2\sin(\pi n/2)$ with $v_c|_{u\to\infty}$, one concludes that $v_c(u)$ is maximal at a finite u for $2/3 < n < 1$.

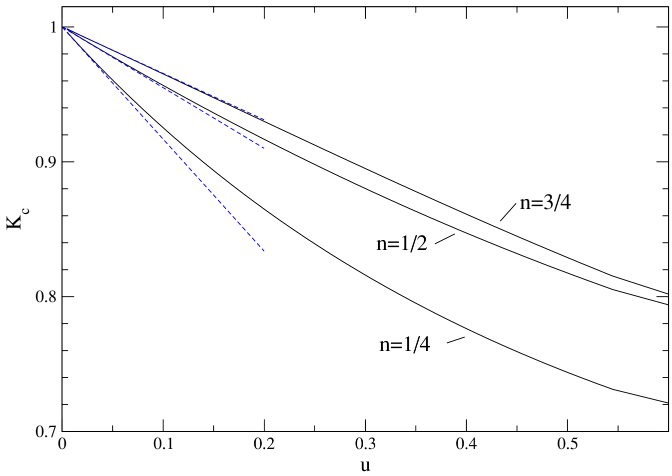

Figure 2. Luttinger parameter K_c at fillings $n = 1/4, 1/2, 3/4$. The blue dashed lines are the low-u results equation (12).

3.2. Spin susceptibility

An analytical solution of equations (29) and (30) is a challenging task due to the finite integration boundaries Q, B. To gain a first insight, consider the integral of equation (30) over the whole real axis, yielding $\int_{-\infty}^{\infty} \sigma(v)\,\mathrm{d}v = 2(n - m_\downarrow) + 1/L$ and therefore the magnetization

$$s := \frac{n}{2} - m_\downarrow = \frac{1}{2}\int_B^\infty \sigma(v)\,\mathrm{d}v. \tag{38}$$

Our aim is to perform a low-field expansion, i.e. an expansion around $s = 0$. From equation (38), this corresponds to an asymptotic expansion of $\sigma(v > B \gg 0)$. This expansion is done by generalizing Shiba's approach [9], who calculated χ_0 for pbc in a different way than via the spin velocity.

Substitute equation (29) into equation (30) to obtain

$$\sigma(v) = \frac{1}{L}\left(g_Q^{(0)}(v) + S_Q(v,0)\right) + g_Q^{(0)}(v) - \int_{-B}^{B} S_Q(v,v')\sigma(v')\,\mathrm{d}v'$$
$$S_Q(v,v') := a_2(v-v') - \int_{-Q}^{Q} a_1(v-\sin k)a_1(\sin k - v')\cos k\,\mathrm{d}k. \tag{39}$$

Here $g_Q^{(0)}$ is the $\nu = 0$-case of $g_Q^{(\nu)}$, defined by

$$g_Q^{(\nu)}(v) := \int_{-Q}^{Q} \frac{1}{\pi} a_1(v-\sin k)\cos^\nu k\,\mathrm{d}k. \tag{40}$$

Furthermore,

$$\sigma^{(\nu)}(v) := \frac{1}{L}\left(g_Q^{(\nu)}(v) + S_Q(v,0)\right) + g_Q^{(\nu)}(v) - \int_{-\infty}^{\infty} S_Q(v,v')\sigma^{(\nu)}(v')\,\mathrm{d}v'. \tag{41}$$

Equation (41) can be solved for $\sigma^{(\nu)}$, at the expense of introducing a new unknown function $\mathcal{M}_Q(v,v')$:

$$\mathcal{M}_Q(v,v') = S_Q(v,v') - \int_{-\infty}^{\infty} S_Q(v,v'')\mathcal{M}_Q(v'',v')\,\mathrm{d}v'' \tag{42}$$

$$\sigma^{(\nu)}(v) = \frac{1}{L}\left(g_Q^{(\nu)}(v) + S_Q(v,0)\right) + g_Q^{(\nu)}(v)$$
$$- \int_{-\infty}^{\infty} \mathcal{M}_Q(v,v')\left[\frac{1}{L}\left(g_Q^{(\nu)}(v') + S_Q(v',0)\right) + g_Q^{(\nu)}(v')\right]\mathrm{d}v'. \tag{43}$$

We consider now $\int_{-\infty}^{\infty} \mathcal{M}_Q(v,v')\sigma(v')\,\mathrm{d}v'$, where $\sigma(v')$ is given by the rhs of equation (39). Making use of equation (43) with $\nu = 0$, one obtains

$$\sigma(v) = \sigma^{(0)}(v) + \int_{|v'|>B} \mathcal{M}_Q(v,v')\sigma(v')\,\mathrm{d}v'. \tag{44}$$

Similarly, starting from $\int_{-B}^{B} \sigma(v)\sigma^{(\nu)}(v)\,\mathrm{d}v$ (where $\sigma^{(\nu)}(v)$ is given by equation (41), one gets

$$\int_{|v|>B} \sigma(v)\sigma^{(\nu)}(v)\,\mathrm{d}v = \int_{-\infty}^{\infty}\left[g_Q^{(0)}(v) + \frac{1}{L}\left(g_Q^{(0)}(v) + S_Q(v,0)\right)\right]\sigma^{(\nu)}(v)\,\mathrm{d}v$$
$$- \int_{-B}^{B}\left\{\frac{1}{L}\left[g_Q^{(0)}(v) + S_Q(v,0)\right] + g_Q^{(\nu)}(v)\right\}\sigma(v)\,\mathrm{d}v. \tag{45}$$

Let us now express the energy and the particle density in terms of these functions. By use of definition (40), and recalling equations (32) and (33), one arrives at

$$e - e_0 = -\pi\int_{-B}^{B} g_Q^{(2)}(v)\sigma(v)\,\mathrm{d}v + \pi\int_{-\infty}^{\infty} g_Q^{(2)}(v)\sigma^{(0)}(v)\,\mathrm{d}v \tag{46}$$

$$n - n_0 = \frac{\pi}{2}\int_{-B}^{B} g_Q^{(1)}(v)\sigma(v)\,\mathrm{d}v - \frac{\pi}{2}\int_{-\infty}^{\infty} g_Q^{(1)}(v)\sigma^{(0)}(v)\,\mathrm{d}v, \tag{47}$$

where e_0, n_0 are the energy and particle densities at $B = \infty$, i.e. zero magnetic field. Note that e, n are functions of both Q, B. First, we hold Q fixed so that both e and n change with varying B. At the end, we will account for the change in n and calculate the susceptibility at fixed n.

Let us now distinguish between the bulk and boundary parts in the auxiliary function $\sigma^{(\nu)}$ (an index $_{\rm B}$ denotes the boundary contribution and should not be confused with the integration boundary B),

$$\sigma^{(\nu)} =: \sigma^{(\nu)}_{\rm bulk} + \frac{1}{L}\sigma^{(\nu)}_{\rm B}. \tag{48}$$

Then with the help of equation (41) the second term in equation (46) is written as

$$\int_{-\infty}^{\infty} g_Q^{(2)}(v)\sigma^{(0)}(v)\,{\rm d}v = \int_{-\infty}^{\infty}\left[g_Q^{(0)}(v)\left(1+\frac{1}{L}\right)+\frac{1}{L}S_Q(v,0)\right]\sigma^{(2)}_{\rm bulk}(v)\,{\rm d}v. \tag{49}$$

The first term in equation (46) is reformulated with the aid of equation (45). Analogous calculations are done for equation (47). Putting everything together allows us to write

$$e - e_0 = \pi\int_{|v|>B}\sigma(v)\sigma^{(2)}(v)\,{\rm d}v - \frac{\pi}{L}\int_{|v|>B}\left[g_Q^{(2)}(v)+S_Q(v,0)\right]\sigma_{\rm bulk}(v)\,{\rm d}v \tag{50}$$

$$n - n_0 = -\frac{\pi}{2}\int_{|v|>B}\sigma(v)\sigma^{(1)}(v)\,{\rm d}v + \frac{\pi}{2L}\int_{|v|>B}\left[g_Q^{(1)}(v)+S_Q(v,0)\right]\sigma_{\rm bulk}(v)\,{\rm d}v. \tag{51}$$

We thus have to evaluate $\sigma(v)$, $\sigma^{(1,2)}(v)$ asymptotically. From equation (41),

$$\begin{aligned}
\sigma^{(\nu)}(v) &= d_Q^{(\nu)}(v) + \int_{-\infty}^{\infty}\int_{-Q}^{Q}\frac{a_1(\sin k - v')\cos k}{4u\cosh\frac{\pi}{2u}(v-\sin k)}\sigma^{(\nu)}(v')\,{\rm d}k\,{\rm d}v' \\
d_Q^{(\nu)}(v) &:= \left(1+\frac{1}{L}\right)\frac{1}{\pi}\int_{-Q}^{Q}\frac{\cos^{\nu}k}{4u\cosh\frac{\pi}{2u}(v-\sin k)}\,{\rm d}k \\
&\quad + \frac{1}{L}\left(\kappa^{(1)}(v) - \int_{-Q}^{Q}\frac{a_1(\sin k)\cos k}{4u\cosh\frac{\pi}{2u}(v-\sin k)}\,{\rm d}k\right).
\end{aligned} \tag{52}$$

Here the integration kernel

$$\kappa^{(\mu)}(p) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{{\rm e}^{-\mu u|\omega|}}{2\cosh\omega u}\,{\rm e}^{{\rm i}\omega p}\,{\rm d}\omega$$

has been defined. Equation (52) can be solved for $\sigma^{(\nu)}$, at the expense of introducing an unknown function $L_Q(t,t')$,

$$\begin{aligned}
L_Q(t,t') &= \delta(t-t') + \int_{-\sin Q}^{\sin Q}\kappa(t-t'')L_Q(t'',t')\,{\rm d}t'' \\
\sigma^{(\nu)}(v) &= d_Q^{(\nu)}(v) + \int_{-\sin Q}^{\sin Q}{\rm d}t\int_{-\sin Q}^{\sin Q}{\rm d}t'\frac{L_Q(t,t')}{4\pi u\cosh\frac{\pi}{2u}(v-t)} \\
&\quad\times\left[\left(1+\frac{1}{L}\right)\int_{-Q}^{Q}\cos^{\nu}p\,\kappa^{(1)}(\sin p - t')\,{\rm d}p\right. \\
&\quad\left. - \frac{\pi}{L}\int_{-Q}^{Q}a_1(\sin p)\cos p\,\kappa^{(1)}(\sin p - t')\,{\rm d}p + \frac{\pi}{L}\kappa^{(2)}(t')\right].
\end{aligned} \tag{53}$$

From expression (53), the $v\to\infty$ asymptotic behaviour of $\sigma^{(\nu)}(v)$ can be read off, namely:

$$\sigma^{(\nu)}(v) \overset{|v|\to\infty}{\sim} \frac{1}{u}\,{\rm e}^{-\frac{\pi}{2u}|v|}I_Q^{(\nu)} + \frac{1}{L}\kappa^{(1)}(v), \tag{54}$$

with an algebraic decay $\kappa^{(1)}(|v|\to\infty)\sim 1/(4v^2)$. The quantity $I_Q^{(\nu)}$ is defined as

$$I_Q^{(\nu)} = \left(1+\frac{1}{L}\right)\int_{-Q}^{Q}\frac{\cos^\nu k}{2\pi}\,\mathrm{e}^{\frac{\pi}{2u}\sin k}\,\mathrm{d}k - \frac{1}{2L}\int_{-Q}^{Q} a_1(k)\cos k\,\mathrm{e}^{\frac{\pi}{2u}\sin k}\,\mathrm{d}k$$
$$+\int_{-\sin Q}^{\sin Q}\mathrm{d}t\int_{-\sin Q}^{\sin Q}\frac{\mathrm{d}t'}{2\pi}\,\mathrm{e}^{\frac{\pi}{2u}t}L_Q(t,t')\left[\left(1+\frac{1}{L}\right)\int_{-Q}^{Q}\cos^\nu p\kappa^{(1)}(\sin p - t')\,\mathrm{d}p\right.$$
$$\left.-\frac{1}{L}\int_{-Q}^{Q}\pi a_1(\sin p)\cos p\kappa^{(1)}(\sin p - t')\,\mathrm{d}p + \frac{\pi}{L}2\pi\kappa^{(2)}(t')\right]. \tag{55}$$

For later purposes, let us also separate this function into bulk and boundary parts,

$$I_Q^{(\nu)} = I_{Q,\mathrm{bulk}}^{(\nu)} + \frac{1}{L}I_{Q,B}^{(\nu)}.$$

From equation (44), we now calculate $\sigma(v)$ in the asymptotic limit. Therefore it is helpful first to reformulate equation (44) by writing

$$\mathcal{M}_Q(v,v') = \kappa^{(1)}(v-v') - \int_{-Q}^{Q}\frac{a_1(\sin k - v')\cos k}{4u\cosh\frac{\pi}{2u}(v-\sin k)}\,\mathrm{d}k + \int_{-\sin Q}^{\sin Q}\mathrm{d}t$$
$$\times\int_{-\sin Q}^{\sin Q}\mathrm{d}t'\frac{1}{8\pi u\cosh\frac{\pi}{2u}(v-t)}L_Q(t,t')\int_{-Q}^{Q}\cos^\nu p\kappa^{(1)}(\sin p - t')\,\mathrm{d}p.$$

From this we conclude

$$\mathcal{M}_Q(v+B,v'+B) + \mathcal{M}_Q(v+B,-v'-B) \approx \kappa^{(1)}(v-v') + \kappa^{(1)}(v+v'+2B). \tag{56}$$

Therefore the equation

$$\sigma(v+B) = \sigma^{(0)}(v+B) + \int_0^\infty[\mathcal{M}_Q(v+B,v'+B) + \mathcal{M}_Q(v+B,-v'-B)]\sigma(v'+B)\,\mathrm{d}v' \tag{57}$$

can be approximated by

$$\sigma(v+B) \overset{B\to\infty}{\sim} \frac{1}{u}\,\mathrm{e}^{-\frac{\pi}{2u}(v+B)}I_Q^{(0)} + \frac{1}{L}\kappa^{(1)}(v+B)$$
$$+\int_0^\infty[\kappa^{(1)}(v-v') + \kappa^{(1)}(v+v'+2B)]\sigma(v'+B)\,\mathrm{d}v'$$
$$=: \frac{1}{u}\,\mathrm{e}^{-\frac{\pi}{2u}(v+B)}I_Q^{(0)}P_1(v+B) + \frac{1}{L}\frac{1}{2u}P_2(v+B) \tag{58}$$

$$P_1(v) =: \mathrm{e}^{-\frac{\pi}{2u}v} + \int_0^\infty[\kappa^{(1)}(v-v') + \kappa^{(1)}(v+v'+2B)]P_1(v')\,\mathrm{d}v' \tag{59}$$

$$P_2(v) =: 2u\kappa^{(1)}(v) + \int_0^\infty[\kappa^{(1)}(v-v') + \kappa^{(1)}(v+v'+2B)]P_2(v')\,\mathrm{d}v'. \tag{60}$$

Let us estimate the error involved in the above approximations. We will see later that $B\sim -\ln h$ for small magnetic fields h. Corrections to the first term in equation (54) are higher order exponentials and thus would add terms $\sim h^{2n}$ to the susceptibility (the term taken into account here yields a constant contribution $\sim h^0$). In the second term, higher order algebraic terms have been dropped. These would contribute in order $\sim 1/(h\ln^n h)$, $n>3$, to the boundary susceptibility. The expected result (17) shows that all these terms are negligible for our purposes. The same holds for equation (57).

We continue and treat the bulk and boundary contributions separately.

3.3. Bulk contribution

For the bulk, the quantities $I^{(\nu)}_{Q,\mathrm{bulk}}$ $(\nu = 1, 2)$ and the function $P_1(v)$ have to be calculated. The crucial observation is that equation (59), which determines P_1, is well known in the study of the spin-1/2 *XXX*-Heisenberg chain: exactly the same function determines the $T = 0$ susceptibility in that model; cf [10] and references therein. Equation (59) is solved iteratively by the Wiener–Hopf method. The solution reads [17] in terms of the Fourier transform $\widetilde{\mathcal{P}}(k)$ of the function $\mathcal{P}(v) := P(2uv)$:

$$\widetilde{\mathcal{P}}(k) = G_+(k) \times \begin{cases} \dfrac{\beta_0}{k\widetilde{B}^2}, & k \neq 0 \\ \dfrac{\beta_1}{\widetilde{B}} + \beta_2 \dfrac{\ln \widetilde{B}}{\widetilde{B}^2} + \dfrac{\beta_3}{\widetilde{B}^2}, & k = 0 \end{cases} \tag{61}$$

with $\widetilde{B} := B/(2u)$ and

$$\beta_0 = \frac{\mathrm{i}G_+(\mathrm{i}\pi)G_-^2(0)}{16\pi^2}, \qquad \beta_1 = \frac{G_+(\mathrm{i}\pi)}{4\pi^2},$$

$$\beta_2 = -\frac{G_+(\mathrm{i}\pi)}{8\pi^3}, \qquad \beta_3 = \frac{G_+(\mathrm{i}\pi)}{8\pi^3}(-\ln \pi + 1).$$

The function $G_+(k)$ is given by

$$G_+(k) = \sqrt{2\pi} \frac{(-\mathrm{i}k)^{-\mathrm{i}k/(2\pi)}}{\Gamma(1/2 + \mathrm{i}k/(2\pi))} \mathrm{e}^{-\mathrm{i}ak} \qquad a = -\frac{1}{2\pi} - \frac{\ln(2\pi)}{2\pi}.$$

Combining equations (50) and (51) with equations (54) and (58) yields the bulk magnetization and energy in terms of the auxiliary function $\mathcal{P}(v)$:

$$e - e_0 = \frac{4\pi}{u} \mathrm{e}^{-\frac{\pi}{u}B} I^{(0)}_{Q,\mathrm{bulk}} I^{(2)}_{Q,\mathrm{bulk}} \int_0^\infty \mathcal{P}(v)\, \mathrm{e}^{-\pi v}\, \mathrm{d}v \tag{62}$$

$$n - n_0 = -\frac{2\pi}{u} \mathrm{e}^{-\frac{\pi}{u}B} I^{(0)}_{Q,\mathrm{bulk}} I^{(1)}_{Q,\mathrm{bulk}} \int_0^\infty \mathcal{P}(v)\, \mathrm{e}^{-\pi v}\, \mathrm{d}v. \tag{63}$$

Furthermore, from equation (38),

$$s = \mathrm{e}^{-\frac{\pi B}{2u}} I^{(0)}_{Q,\mathrm{bulk}} \int_0^\infty \mathcal{P}(v)\, \mathrm{d}v. \tag{64}$$

We now successively substitute $\mathcal{P}(v)$ from (61) into (64), (62) and (63). From the substitution of (61) into (64), one obtains

$$\widetilde{B} = -\frac{1}{\pi} \ln \frac{s}{s_0} \tag{65}$$

$$s_0 := I^{(0)}_{Q,\mathrm{bulk}} G_+(0) \frac{G_+(\mathrm{i}\pi)}{\pi}. \tag{66}$$

Thus $e - e_0$ and $n - n_0$ are obtained as functions of s:

$$e - e_0 = b_Q \left(\frac{s}{s_0}\right)^2 \left(1 + \frac{b_1}{\ln s/s_0} + b_2 \frac{\ln|\ln s/s_0|}{\ln^2 s/s_0} + \frac{b_3}{\ln^2 s/s_0}\right) \tag{67}$$

$$
\begin{aligned}
&n - n_0 = c_Q \left(\frac{s}{s_0}\right)^2 \left(1 + \frac{b_1}{\ln s/s_0} + b_2 \frac{\ln|\ln s/s_0|}{\ln^2 s/s_0} + \frac{b_3}{\ln^2 s/s_0}\right) \\
&b_Q := \frac{4\pi}{u} I^{(0)}_{Q,\mathrm{bulk}} I^{(2)}_{Q,\mathrm{bulk}} \frac{G_+^2(0)}{2\pi} G_+^2(\mathrm{i}\pi) \\
&c_Q := -\frac{2\pi}{u} I^{(0)}_{Q,\mathrm{bulk}} I^{(1)}_{Q,\mathrm{bulk}} \frac{G_+^2(0)}{2\pi} G_+^2(\mathrm{i}\pi) \\
&b_1 := 2\beta_1\pi/\alpha; \qquad b_2 := b_1/2 \\
&b_3 := \frac{G_-(0)}{4} - \frac{2\pi^2}{\alpha}\left(\beta_3 - \frac{\beta_1^2}{\alpha}\right) + 2\beta_2\pi^2 \frac{\ln\pi}{\alpha} \\
&\alpha := G_+(\mathrm{i}\pi)G_+(0)/\pi = \sqrt{\frac{2}{\pi\,\mathrm{e}}}.
\end{aligned}
\tag{68}
$$

The Q-dependence enters only through b_Q, c_Q. Since we want to calculate the susceptibility at constant density, we have to adjust Q such that the density is not altered by the finite B-value. This adjustment is done by setting $Q = Q_0 + \Delta$, where Q_0 corresponds to $B = \infty$:

$$
e = e_0 + (\partial_Q e_0)\Delta + b_Q f(s/s_0) \qquad n = n_0 + (\partial_Q n_0)\Delta + c_Q f(s/s_0),
$$

and $f(s/s_0)$ contains the whole s-dependence of equations (67) and (68). From this it follows

$$
\Delta = -\frac{c_Q}{\partial_Q n_0} f(s/s_0) \qquad e = e_0 + \left[b_Q - \frac{\partial_Q e_0}{\partial_Q n_0} c_Q\right] f(s/s_0).
$$

Now the magnetic field $h = -\partial_s e$ and the susceptibility $\chi^{-1} = \partial_s^2 e$ are calculated, where χ is expressed as a function of h. This calculation is equivalent to considering B as a variational parameter and requiring $\partial_B(e - hs) = 0$, from which one obtains a relation $B = B(h)$, analogous to equation (65). This is then substituted into equation (64) to get $s = s(h)$ and therefrom $\chi = \chi(h)$. This second approach has been chosen in [17]. We end up with

$$
\chi_{\mathrm{bulk}}(h) = \frac{s_0}{h_0}\left(1 - \frac{1}{2\ln h/h_0} - \frac{\ln|\ln h/h_0|}{4\ln^2 h/h_0} + \frac{5}{16\ln^2 h/h_0}\right) \tag{69}
$$

$$
h_0 = \left[b_Q - \frac{\partial_Q e_0}{\partial_Q n_0} c_Q\right] \Big/ s_0. \tag{70}
$$

The constant s_0 is given in equation (66). Equation (69) is the key result of this section for $\chi_{\mathrm{bulk}}(h)$. Note that it is of the form (14) (with $E = h$ there), with specified constants. Especially, an alternative expression for v_{s} has been obtained; cf equation (15):

$$
\frac{h_0}{s_0} = 2\pi v_{\mathrm{s}}. \tag{71}
$$

To complement our discussion of the bulk susceptibility, we are going to express h_0 in terms of the dressed energy functions (35) and (36) by combining equations (34) and (71). From equations (34)–(36), it is not difficult to show that at zero magnetic field,

$$
2\pi v_{\mathrm{s}} = \frac{\int_{-Q}^{Q} \mathrm{e}^{\frac{\pi}{2u}\sin k} \epsilon_{\mathrm{c}}'(k)\,\mathrm{d}k}{\int_{-Q}^{Q} \mathrm{e}^{\frac{\pi}{2u}\sin k} \rho(k)\,\mathrm{d}k}. \tag{72}
$$

An expression for $I^{(\nu)}_{Q,\mathrm{bulk}}$ equivalent to equation (55) is as follows:

$$I^{(\nu)}_{Q,\mathrm{bulk}} = \int_{-Q}^{Q} \frac{\cos^{\nu} k}{2\pi} \psi(k)\,\mathrm{d}k \tag{73}$$

$$\psi(k) = \mathrm{e}^{\frac{\pi}{2u}\sin k} + \int_{-Q}^{Q} \cos k' \kappa^{(1)}(\sin k - \sin k')\psi(k')\,\mathrm{d}k'. \tag{74}$$

Thus, by comparing with (35) and (36) at $h = 0$,

$$I^{(0)}_{Q,\mathrm{bulk}} = 2u\left[\sigma(v)\,\mathrm{e}^{\frac{\pi}{2u}v}\right]_{v\to\infty} = \int_{-Q}^{Q} \mathrm{e}^{\frac{\pi}{2u}\sin k}\epsilon_{\mathrm{c}}'(k)\,\mathrm{d}k. \tag{75}$$

We now insert equation (66) into equation (71), making use of equation (75). Then we obtain

$$h_0 = \sqrt{\frac{2}{\mathrm{e}\pi}} \int_{-Q}^{Q} \mathrm{e}^{\frac{\pi}{2u}\sin k}\epsilon_{\mathrm{c}}'(k)\,\mathrm{d}k, \tag{76}$$

which is an expression equivalent to equation (70).

3.4. Boundary contribution

Let us go back to equations (54) and (58). The boundary contribution is calculated by plugging these equations into equations (50) and (51). The resulting expression is lengthy and we do not write it down here. We rather apply the approximation to neglect terms of the order

$$\mathrm{e}^{-\pi B/(2u)}/B^2 \sim \frac{s}{\ln^2 s} \sim \frac{h}{\ln^2 h}$$

in the ground-state energy. These terms would yield a contribution $\sim 1/(h\ln^3 h)$ to the susceptibility; cf equation (17). Neglecting these terms means not fixing the scale $h_0^{(\mathrm{B})}$ in (17) uniquely. However, the algebraic $1/h$ divergence in (17) dominates such terms. Then the boundary contributions read

$$[e - e_0]_{\mathrm{B}} = 2\pi \int_0^{\infty} \sigma_{\mathrm{bulk}}(v+B)\sigma^{(2)}_{\mathrm{bulk}}(v+B)\,\mathrm{d}v \tag{77}$$

$$[n - n_0]_{\mathrm{B}} = -\pi \int_0^{\infty} \sigma_{\mathrm{bulk}}(v+B)\sigma^{(1)}_{\mathrm{bulk}}(v+B)\,\mathrm{d}v \tag{78}$$

$$s_{\mathrm{B}} = \frac{1}{4u}\int_0^{\infty} P_2(v)\,\mathrm{d}v, \tag{79}$$

where P_2 is given by equation (60). Note that the only difference with respect to the bulk is the different dependence of s on B; cf equation (79). Instead of $s_{\mathrm{bulk}} \sim \exp[-\pi B/(2u)]$ we now have $s_{\mathrm{B}} \sim 2u/B$, which will, according to equation (65), cause a logarithmic divergence in the magnetization: $1/B \sim 1/\ln(h)$, yielding the divergence indicated in equation (17). Terms neglected in (79) are $\sim \exp[-B] \sim h + 1/(\ln h)$, and consequently they will yield a contribution to the boundary susceptibility which is of the bulk form, equation (14). These finite terms are negligible compared to the divergent terms given in (17). We thus have to insert the expressions for $\sigma_{\mathrm{bulk}}(v)$, $\sigma^{(1,2)}_{\mathrm{bulk}}(v)$ from the previous section into equations (77) and (78). The Fourier transform $\widetilde{\mathcal{P}}_2(k)$ of the function $\mathcal{P}_2(v) := P(2uv)$ is given in [17], namely

$$\widetilde{\mathcal{P}}_2(k) = \begin{cases} G_+(0)(\alpha_1/B + \alpha_2(\ln B)/B^2) & k = 0 \\ \mathrm{i}\alpha_1 G_+(k)/(kB^2), & k \neq 0 \end{cases}$$

$$\alpha_1 = \frac{1}{\sqrt{2\pi}}, \qquad \alpha_2 = -\frac{\sqrt{2}}{4\pi^2}.$$

We now go through the same steps as in the previous subsection: calculate $[e - e_0]_B$, $[n - n_0]_B$, s_B as functions of the integration boundary B, and derive therefrom the boundary susceptibility as a function of h. This results in

$$\chi_B(h) = \frac{1}{4h\ln^2(h_0/h)}\left(1 - \frac{\ln\ln h_0/h}{\ln(h_0/h)}\right) \tag{80}$$

with the scale h_0 given in equation (70).

3.5. Explicit expressions in special cases

We consider three special cases: half-filling for arbitrary coupling, as well as weak and strong coupling for arbitrary filling.

At half-filling, $Q = \pi$, $I^{(1)}_{Q,\mathrm{bulk}} = 0$ and

$$I^{(2)}_{Q,\mathrm{bulk}} = \frac{1}{\pi}\int_0^{\pi} \sin^2 k\, \mathrm{e}^{\frac{\pi}{2u}\sin k}\, \mathrm{d}k \qquad h_0 = \frac{2\pi}{u}\sqrt{\frac{2\pi}{\mathrm{e}}}\, I^{(2)}_{Q,\mathrm{bulk}}. \tag{81}$$

This expression coincides with that given by Asakawa *et al* [18]. For strong coupling, $Q = \pi n$ and

$$h_0 \overset{u\to\infty}{\to} \frac{n}{u}\sqrt{\frac{2\pi^3}{\mathrm{e}}}\left[1 - \frac{\sin(2\pi n)}{2\pi n}\right] =: h_{0,2} \tag{82}$$

$$\chi_0 \overset{u\to\infty}{\to} \frac{u}{\pi^2}\left[1 - \frac{\sin(2\pi n)}{2\pi n}\right]^{-1}. \tag{83}$$

The latter result has also been obtained in [9]. It is interesting to note that

$$h_{0,2} = \sqrt{\frac{2\pi^3}{\mathrm{e}}}\, h_c,$$

where h_c is the critical field above which the system is fully polarized, $s_{\mathrm{bulk}}(h \geqslant h_c) = n/2$, [11]. Thus in the strong coupling limit, the logarithmic corrections are confined to fields $h \ll h_c \sim 1/u$. In the special case $n = 1$ (half-filling), equations (82) and (83) are consistent with known results for the *XXX*-chain with coupling constant $J = 1/u$: for this model, $\chi_0^{(XXX)} = 1/(J\pi^2)$ [10], and the scale $h_0^{(XXX)} = \sqrt{2\pi^3/\mathrm{e}}$, without taking account of the term $\sim\ln^{-2} h$ in (14) [17].

The small coupling limit is technically more involved: the integration kernels in the integral equations become singular. A numerical evaluation of $\chi_0(u)$ (see section 3.6) confirms the field-theoretical prediction equation (A.15). As far as the scale h_0 is concerned, it is clear that it must diverge for $u \to 0$: exactly at the free-fermion point $u = 0$, the logarithmic corrections in equation (14) vanish altogether; corrections to χ_0 at $u = 0$ are algebraic with integer powers. The leading contributions $\sim h^2, T^2$ for $u = 0$ are calculated in the appendix; cf equations (B.1), (B.2), (B.5) and (B.6).

To describe the divergence of $h_0|_{u\to 0}$ quantitatively, consider first the half-filling case where $h_0 \sim \mathrm{e}^{\mathrm{const}/u}$. From the general expressions of $I^{(1,2)}_{Q,\mathrm{bulk}}$ (equation (55)), it is clear that this is the case for arbitrary filling. Thus in the small-coupling limit, the finite-field susceptibility is obtained from equation (14) with $|\ln h| \ll |\ln h_0|$, i.e. $h_0 \gg h \gg 1/h_0 \sim \exp[-1/u]$:

$$\chi_{\mathrm{bulk}}(u \to 0, h_0 \gg h \gg 1/h_0) = \chi_0\left(1 + \frac{1}{2\ln h_0}\right) + \mathcal{O}\left(\frac{\ln h}{\ln^2 h_0}\right). \tag{84}$$

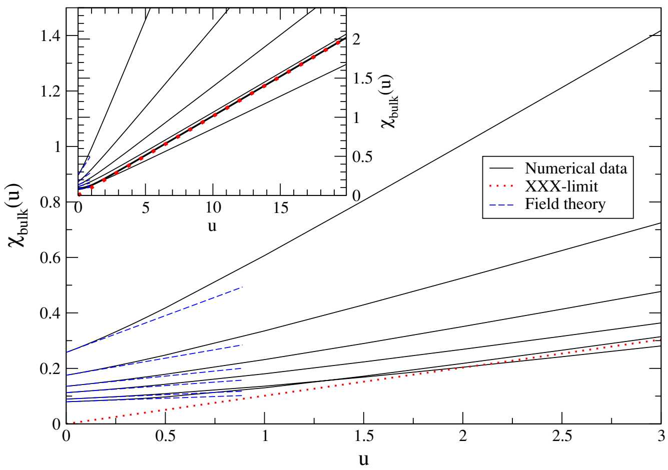

Figure 3. The susceptibility χ_{bulk} over u at densities $n = 0.2, 0.3, 0.4, 0.5, 0.7, 1$ (from top to bottom at $u = 0$). A similar figure has been shown by Shiba [9]. Here, we additionally compare with the field-theory result at small u (A.15) (blue dashed lines) and with the *XXX*-limit (for better comparison the inset shows the same figure on a larger scale; the $n = 1$-line is printed bold here).

This has to be understood such that the limit $u \to 0$ is considered at small but finite and fixed h. Then the h-dependent terms are next-leading and can be neglected in a first approximation. On the other hand, $\chi_{\text{bulk}}(u \to 0, h > 0)$ has been calculated in appendix A (equation (A.14),

$$\chi_{\text{bulk}}(u \to 0, h > 0) = \frac{1}{2\pi v_{\text{F}}} + \frac{2u}{\pi^2 v_{\text{F}}^2} \tag{85}$$

with the Fermi velocity $v_{\text{F}} = 2\sin(\pi n/2)$. Equations (84) and (85) match provided that

$$h_0 = \text{const}\exp\left[\frac{\pi}{4u} v_{\text{F}}\right]. \tag{86}$$

We will confirm numerically this behaviour in section 3.6.

3.6. Numerical results

In order to compare the low-field expansion equations (69) and (80) to the outcome of the non-approximated integral equations (29) and (30), we first compute χ_0, h_0 numerically. To do so, we follow Shiba [9] and rewrite the quantities $\partial_Q e_0$, $\partial_Q n_0$ as solutions of linear integral equations. Namely, from equations (33) and (32),

$$\partial_Q e_0 = -4\cos Q\rho(Q) - 2\int_{-Q}^{Q} \cos k\,\partial_Q\rho(k)\,\mathrm{d}k$$

$$\partial_Q n_0 = 2\rho(Q) + \int_{-Q}^{Q} \partial_Q\rho(k)\,\mathrm{d}k,$$

where $\partial_Q\rho(k)$ is obtained from equations (29) and (30) at $h = 0$ (i.e. $B = \infty$):

$$\partial_Q\rho(k) = \cos k[\kappa(\sin k - \sin Q) + \kappa(\sin k + \sin Q)]\rho(Q) + \cos k\int_{-Q}^{Q} \kappa(\sin k - \sin p)\partial_Q\rho(p)\,\mathrm{d}p.$$

These linear integral equations, together with equations (73) and (74), are solved numerically. The result for χ_0 as a function of u for different fillings is given in figure 3, together with

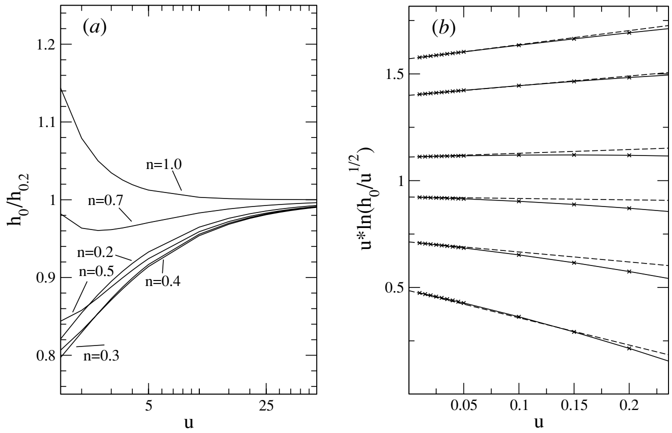

Figure 4. The scale h_0 over u for $n = 0.2, 0.3, 0.4, 0.5, 0.7, 1.0$ (from bottom to top). In (*a*, the large-coupling result equation (82) is verified; in (*b*), the small-coupling formula equation (87) is visualized (dashed lines).

the small-u expansion (A.15) and the *XXX*-limit. We checked numerically that this way of obtaining χ_0 is equivalent to calculating v_s from equation (34) and then using equation (15). The scale h_0 as a function of u at different fillings is depicted in figure 4. Besides confirming the small-coupling result equation (86), we observe that the numerical data are well described by assuming the following form of the constant of proportionality in equation (86):

$$h_0 = \left[\frac{4}{\pi^2}\sqrt{\frac{2\pi}{e}}\right]^{1/n} \pi\sqrt{u}\,\mathrm{e}^{\frac{\pi}{2u}\sin\frac{\pi n}{2}}. \tag{87}$$

The exponent is exact (cf equation (86), the constant is conjectured from observing good agreement with the numerics; cf figure 4. Having calculated h_0, χ_0, the next step consists in finding $\chi(h)$ numerically and comparing with equations (69) and (80). The calculation of $\chi_{\mathrm{bulk}}(h)$ is described in [11, appendix to chapter 6]. The idea is to rewrite the energy in terms of dressed energy functions (rather than in terms of dressed density functions like in equations (29) and (30). The magnetic field enters the linear integral equations for the dressed energy functions. Once these equations are solved, both the field and the magnetization are determined. By varying slightly the integration boundaries while keeping the density fixed, one performs a numerical derivative $\Delta s/\Delta h$ to obtain χ. The results shown in the following demonstrate that this procedure is highly accurate.

Figure 5 shows χ_{bulk} for densities $n = 0.2, 1$ at different couplings, together with the analytical result (69). The boundary contribution $\chi_B(h)$ can be calculated similarly to $\chi_{\mathrm{bulk}}(h)$ as sketched above, because the equations are linear in the $1/L$ contribution. Results for $u = 1, 10$ and densities $n = 0.2, 1$ are shown in figure 6.

4. Friedel oscillations

Due to the open boundary conditions, translational invariance is broken. This means that one-point correlation functions such as the density or the magnetization will no longer be just constants but rather become position dependent. In particular, they will show characteristic oscillations near the boundaries, the so-called *Friedel oscillations* [22]. These oscillations are expected to decay algebraically with distance x from the boundary, finally reaching the

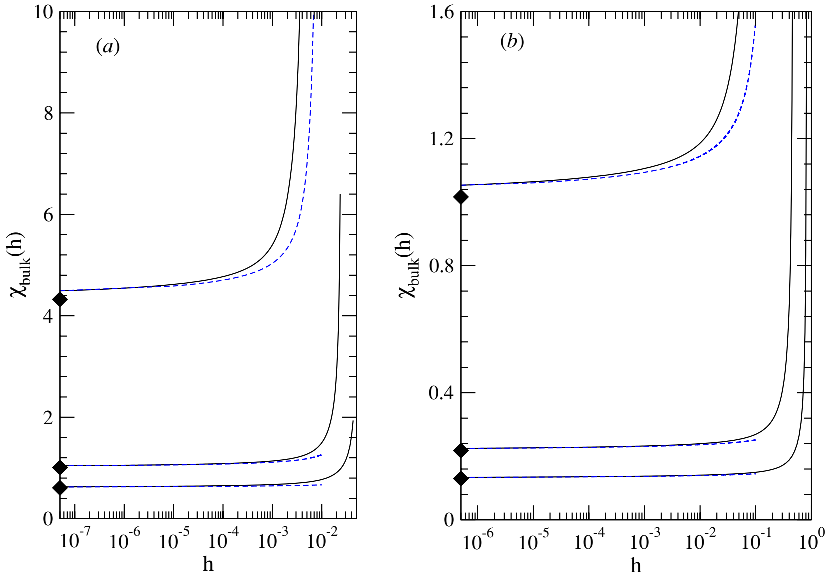

Figure 5. The bulk susceptibility for $n = 0.2$ in (*a*) and for $n = 1$ in (*b*) at $u = 1, 2, 10$ (from bottom to top). The dashed blue curves are the analytical result (69). The diamonds indicate χ_0, showing the decrease of the scale h_0 with increasing u.

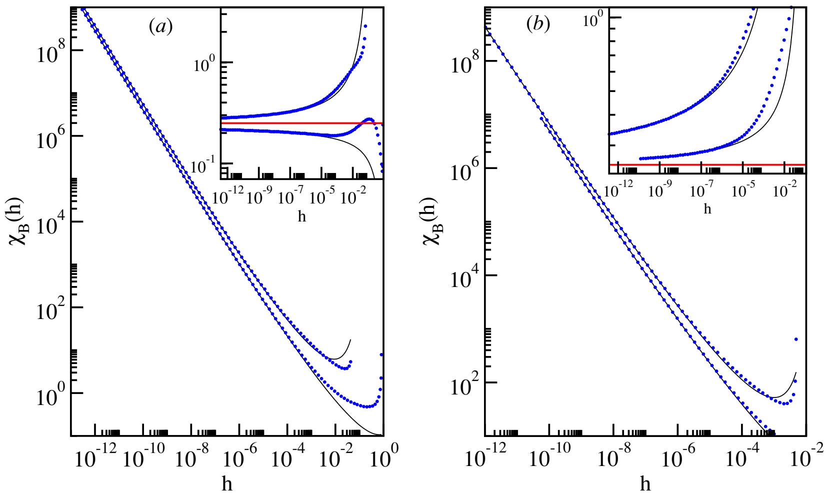

Figure 6. The boundary susceptibility $\chi_B(h)$ for $u = 1$ in (*a*) and for $u = 10$ in (*b*) with $n = 0.2, 1$ (from top to bottom). The dots are the numerical data, the lines the asymptotic form (17) where $h_0^{(B)}$ has been determined by a fit. The insets show $\chi_B \cdot h \cdot \ln^2 h$, the red horizontal line denotes the asymptotic value $1/4$.

mean density or magnetization, respectively, for $x \to \infty$. From a field-theoretical point of view, such a one-point correlation function can be obtained from the holomorphic part of the corresponding two-point function [34]. We therefore first recall here the asymptotics of two-point functions in the Hubbard model according to [11, 35]. After that, we will derive the one-point correlation functions for the density $n(x)$ and the magnetization $s^z(x)$. This will then allow us to obtain the local susceptibility $\chi(x)$. By a conformal mapping, we will generalize our results to small finite temperatures. As nuclear magnetic resonance Knight shift experiments yield direct access to $\chi(x)$, the predictions obtained here about its position, temperature as well as density dependence should be valuable for experiments on one-dimensional itinerant electron systems. To test our conformal field theory results, we present some numerical data based on the density-matrix renormalization group applied to transfer matrices (TMRG).

4.1. Two-point functions

In the following, we content ourselves with stating the results for the asymptotics of pair-correlation functions, without giving any derivations. For any further details, the reader is referred to [11, 35]. We also restrict ourselves to the case $n \neq 1$, i.e., we do not consider half-filling. The reason to do so, is that at half-filling the charge sector is massive and the correlation functions will be identical to those of the Heisenberg model up to the amplitudes and the spin velocity which do depend on u. The local magnetization and susceptibility for this case, however, have already been discussed in [16, 36].

The Hubbard model away from half-filling has two critical degrees of freedom with different velocities and the low-energy effective theory outlined in section 2 is therefore not Lorentz-invariant. As the spin and charge excitations are independent from each other we can, however, still apply conformal field theory in this situation on the basis of a critical theory which is a product of two Virasoro algebras both with central charge $c = 1$. Due to conformal invariance, the exponents of the correlation functions of primary fields can then be obtained from the finite-size corrections of low-lying excitation energies for the finite system. These in turn can be calculated exactly *via* Bethe ansatz. Then the remaining challenge is to relate the primary fields to the original fields of the model. This goal can be achieved by considering the selection rules for the form factors involved and by using additional restrictions obtained from the Bethe ansatz solution for the finite size spectrum [35].

In this situation, the correlation function of two primary fields at zero temperature is given by (we include here the dependence on the imaginary time τ)

$$\langle \phi_{\Delta^\pm}(\tau,x)\phi_{\Delta^\pm}(0,0)\rangle = \frac{\mathrm{e}^{2\mathrm{i}D_c k_{F\uparrow}x}\,\mathrm{e}^{2\mathrm{i}(D_c+D_s)k_{F\downarrow}x}}{(v_c\tau+\mathrm{i}x)^{2\Delta_c^+}(v_c\tau-\mathrm{i}x)^{2\Delta_c^-}(v_s\tau+\mathrm{i}x)^{2\Delta_s^+}(v_c\tau-\mathrm{i}x)^{2\Delta_s^-}}$$

with the scaling dimensions

$$2\Delta_c^\pm(\Delta\mathbf{N},\mathbf{D}) = \left(\xi_{cc}D_c + \xi_{sc}D_s \pm \frac{\xi_{cc}\Delta N_c - \xi_{cs}\Delta N_s}{2\det\hat{\xi}}\right)^2 + 2N_c^\pm$$

$$2\Delta_s^\pm(\Delta\mathbf{N},\mathbf{D}) = \left(\xi_{cs}D_c + \xi_{ss}D_s \pm \frac{\xi_{cc}\Delta N_s - \xi_{sc}\Delta N_c}{2\det\hat{\xi}}\right)^2 + 2N_s^\pm.$$

Let us explain the symbols used. The entries of the vector $\Delta\mathbf{N}$ are integers ΔN_c, ΔN_s, which denote the change of charges and down spins with respect to the ground state. The $N_{c,s}^\pm$ denote non-negative integers, and $\mathbf{D} = (D_c, D_s)$ depends on the parity of $\Delta N_{c,s}$:

$$D_c = \tfrac{1}{2}(\Delta N_c + \Delta N_s) \bmod 1 \tag{88}$$

$$D_s = \tfrac{1}{2}\Delta N_c \bmod 1. \tag{89}$$

Therefore D_c, D_s are either integers are half-odd integers. The matrix $\hat{\xi}$ has entries

$$\hat{\xi} := \begin{pmatrix} \xi_{cc} & \xi_{cs} \\ \xi_{sc} & \xi_{ss} \end{pmatrix} := \begin{pmatrix} Z_{cc}(B) & Z_{cs}(Q) \\ Z_{sc}(B) & Z_{ss}(Q) \end{pmatrix}. \tag{90}$$

These entries are obtained from the following system of linear integral equations

$$Z_{cc}(k) = 1 + \int_{-B}^{B} Z_{cs}(v) a_1(\sin k - v)\,\mathrm{d}v$$
$$Z_{cs}(v) = \int_{-Q}^{Q} \cos k a_1(v - \sin k) Z_{cc}(k)\,\mathrm{d}k - \int_{-B}^{B} a_2(v - v') Z_{cs}(v')\,\mathrm{d}v'.$$
$$Z_{sc}(k) = \int_{-B}^{B} a_1(\sin k - v) Z_{ss}(v)\,\mathrm{d}v$$
$$Z_{ss}(v) = 1 + \int_{-Q}^{Q} \cos k a_1(v - \sin k) Z_{sc}(k)\,\mathrm{d}k - \int_{-B}^{B} a_2(v - v') Z_{ss}(v')\,\mathrm{d}v'.$$

The integration kernels are given by equation (31). The integration boundaries B, Q are obtained from the linear integral equations for the root densities, equations (29) and (30).

Let us now focus onto $\langle \hat{O}(\tau, x)\hat{O}(0, 0)\rangle$ with $\hat{O} = n, s^z$, respectively. Since the operator $\hat{O}$ does neither change the particle density nor the magnetization, we have $\Delta N_c = 0 = \Delta N_s$. Consequently, according to (88) and (89), $D_c = 0, \pm 1, \pm 2, \ldots, D_s = 0, \pm 1, \pm 2, \ldots$. Then

$$\begin{aligned}
&\langle \hat{O}(\tau, x)\hat{O}(0, 0)\rangle - \langle \hat{O}\rangle^2 \\
&\quad = \frac{A_1 \cos(2k_{F\uparrow}x)}{(v_c\tau + \mathrm{i}x)^{(\xi_{cc}-\xi_{sc})^2}(v_c\tau - \mathrm{i}x)^{(\xi_{cc}-\xi_{sc})^2}(v_s\tau + \mathrm{i}x)^{(\xi_{cs}-\xi_{ss})^2}(v_s\tau - \mathrm{i}x)^{(\xi_{cs}-\xi_{ss})^2}} \\
&\qquad + \frac{A_2 \cos(2k_{F\downarrow}x)}{(v_c\tau + \mathrm{i}x)^{\xi_{sc}^2}(v_c\tau - \mathrm{i}x)^{\xi_{sc}^2}(v_s\tau + \mathrm{i}x)^{\xi_{ss}^2}(v_s\tau - \mathrm{i}x)^{\xi_{ss}^2}} \\
&\qquad + \frac{A_3 \cos 2(k_{F\uparrow} + k_{F_\downarrow})x}{(v_c\tau + \mathrm{i}x)^{\xi_{cc}^2}(v_c\tau - \mathrm{i}x)^{\xi_{cc}^2}(v_s\tau + \mathrm{i}x)^{\xi_{cs}^2}(v_s\tau - \mathrm{i}x)^{\xi_{cs}^2}} \\
&\qquad + \frac{A_4 \cos 2(k_{F\uparrow} + 2k_{F\downarrow})x}{(v_c\tau + \mathrm{i}x)^{(\xi_{cc}+\xi_{sc})^2}(v_c\tau - \mathrm{i}x)^{(\xi_{cc}+\xi_{sc})^2}(v_s\tau + \mathrm{i}x)^{(\xi_{cs}+\xi_{ss})^2}(v_s\tau - \mathrm{i}x)^{(\xi_{cs}+\xi_{ss})^2}} \\
&\qquad + A_5 \frac{x^2 - v_c^2\tau^2}{\left(x^2 + v_c^2\tau^2\right)^2} + A_6 \frac{x^2 - v_s^2\tau^2}{\left(x^2 + v_s^2\tau^2\right)^2} + \cdots,
\end{aligned} \tag{91}$$

where the amplitudes A_i are different for the density–density and the longitudinal spin–spin correlation function. The oscillating terms on the right-hand side correspond to $\mathbf{D} = (\pm 1, \mp 1), (0, \pm 1), (\pm 1, 0), (\pm 1, \pm 1)$ with $\mathbf{N} = \left(N_c^+, N_c^-, N_s^+, N_s^-\right) = 0$ and the non-oscillating to $\mathbf{N} = (1, 0, 0, 0), (0, 1, 0, 0), (0, 0, 1, 0), (0, 0, 0, 1)$ with $\mathbf{D} = 0$.

4.2. One-point functions in the open system

From the two-point function $\langle \hat{O}(z_1, \bar{z}_1)\hat{O}(z_2, \bar{z}_2)\rangle$ in equation (91) with $z = v_{c,s}\tau + \mathrm{i}x$ we can read of the one-point correlation function in the presence of an open boundary by considering it as a function of (z_1, z_2) only and identifying $z_2 = \bar{z}_1$ afterwards [34].

$$\begin{aligned}
\langle \hat{O}(x)\rangle - \langle \hat{O}(x)\rangle_{x\to\infty} &= A_1 \frac{\cos(2k_{F\uparrow}x + \phi_1)}{(2x)^{(\xi_{cc}-\xi_{sc})^2}(2x)^{(\xi_{cs}-\xi_{ss})^2}} + A_2 \frac{\cos(2k_{F\downarrow}x + \phi_2)}{(2x)^{\xi_{sc}^2}(2x)^{\xi_{ss}^2}} \\
&\quad + A_3 \frac{\cos[2(k_{F\uparrow} + k_{F_\downarrow})x + \phi_3]}{(2x)^{\xi_{cc}^2}(2x)^{\xi_{cs}^2}} + A_4 \frac{\cos[2(k_{F\uparrow} + 2k_{F\downarrow})x + \phi_4]}{(2x)^{(\xi_{cc}+\xi_{sc})^2}(2x)^{(\xi_{cs}+\xi_{ss})^2}} + \frac{A_5 + A_6}{(2x)^2},
\end{aligned} \tag{92}$$

with unknown amplitudes A_i and phases ϕ_i where x now denotes the distance from the boundary.

By the usual mapping of the complex plane onto a cylinder we can generalize (92) to finite temperatures:

$$\langle\hat{O}(x)\rangle - \langle\hat{O}(x)\rangle_{x\to\infty} = A_1 \frac{\cos(2k_{F\uparrow}x+\phi_1)}{\left(\frac{v_c}{\pi T}\sinh\frac{2\pi T x}{v_c}\right)^{(\xi_{cc}-\xi_{sc})^2}\left(\frac{v_s}{\pi T}\sinh\frac{2\pi T x}{v_s}\right)^{(\xi_{cs}-\xi_{ss})^2}}$$
$$+ A_2 \frac{\cos(2k_{F\downarrow}x+\phi_2)}{\left(\frac{v_c}{\pi T}\sinh\frac{2\pi T x}{v_c}\right)^{\xi_{sc}^2}\left(\frac{v_s}{\pi T}\sinh\frac{2\pi T x}{v_s}\right)^{\xi_{ss}^2}} + A_3 \frac{\cos\left[2(k_{F\uparrow}+k_{F_\downarrow})x+\phi_3\right]}{\left(\frac{v_c}{\pi T}\sinh\frac{2\pi T x}{v_c}\right)^{\xi_{cc}^2}\left(\frac{v_s}{\pi T}\sinh\frac{2\pi T x}{v_s}\right)^{\xi_{cs}^2}}$$
$$+ A_4 \frac{\cos[2(k_{F\uparrow}+2k_{F\downarrow})x+\phi_4]}{\left(\frac{v_c}{\pi T}\sinh\frac{2\pi T x}{v_c}\right)^{(\xi_{cc}+\xi_{sc})^2}\left(\frac{v_s}{\pi T}\sinh\frac{2\pi T x}{v_s}\right)^{(\xi_{cs}+\xi_{ss})^2}} + \frac{A_5}{\left(\frac{v_c}{\pi T}\sinh\frac{2\pi T x}{v_c}\right)^2} + \frac{A_6}{\left(\frac{v_s}{\pi T}\sinh\frac{2\pi T x}{v_s}\right)^2}. \tag{93}$$

The magnetic susceptibility at zero field is obtained by taking the derivative with respect to h:[5] here $k_{F\uparrow} = \pi(n+2s)/2a$, $k_{F\downarrow} = \pi(n-2s)/2a$ and $s = \chi_0 h$ for $|h| \ll 1$ (without taking account of the logarithmic corrections). Furthermore, the exponents and the amplitudes depend on h. However, we neglect this h-dependence here since it gives rise to higher-order contributions in $\chi(x)$. In the $h = 0$-case,

$$\xi_{cc} =: \xi, \qquad \xi_{ss} = 1/\sqrt{2}, \qquad \xi_{cs} = 0, \qquad \xi_{sc} = \xi/2,$$

leading to

$$\chi(x) - \chi_0 = 2\pi\chi_0 x \frac{-A_1\sin(\pi n x+\phi_1) + A_2\sin(\pi n x+\phi_2)}{(2x)^{\xi^2/4}(2x)^{1/2}} + 2\pi\chi_0 x \frac{A_4\sin(3\pi n x+\phi_4)}{(2x)^{9\xi^2/4}(2x)^{1/2}}. \tag{94}$$

Note that the $k_{F\uparrow} + k_{F\downarrow}$-term in equation (92) is h-independent in lowest order and therefore does not contribute to the susceptibility.

Again we generalize this to finite temperatures:

$$\chi(x) - \chi_0 = 2\pi\chi_0 x \frac{-A_1\sin(\pi n x+\phi_1) + A_2\sin(\pi n x+\phi_2)}{\left(\frac{v_c}{\pi T}\sinh\frac{2\pi T x}{v_c}\right)^{\xi^2/4}\left(\frac{v_s}{\pi T}\sinh\frac{2\pi T x}{v_s}\right)^{1/2}}$$
$$+ 2\pi\chi_0 x \frac{A_4\sin(3\pi n x+\phi_4)}{\left(\frac{v_c}{\pi T}\sinh\frac{2\pi T x}{v_c}\right)^{9\xi^2/4}\left(\frac{v_s}{\pi T}\sinh\frac{2\pi T x}{v_s}\right)^{1/2}}. \tag{95}$$

Note that we have ignored logarithmic corrections to the algebraic decay of the correlation functions throughout this section. Multiplicative logarithmic corrections will be present due to the marginal operator in (9). These corrections have been discussed for the leading term in (91) in [37].

4.3. Numerical results

To calculate numerically the local magnetization $s^z(x)$ and susceptibility $\chi(x)$ at finite temperatures we use the density-matrix renormalization group applied to transfer matrices (TMRG). The advantage of this method compared to quantum Monte Carlo algorithms is that the thermodynamic limit can be performed exactly. This is particularly helpful in the present situation where we want to study boundary effects, i.e., corrections which are of order $1/L$ compared to bulk quantities. The method is explained in detail in [16, 38, 39]. Here we concentrate on the local magnetization for $h \neq 0$ and on the local susceptibility for $h = 0$, both times for generic filling $n \neq 1$. In figure 7 TMRG data for $\langle s^z(x)\rangle$ are shown in comparison

[5] In the same way the compressibility can be obtained by taking derivatives with respect to a chemical potential μ.

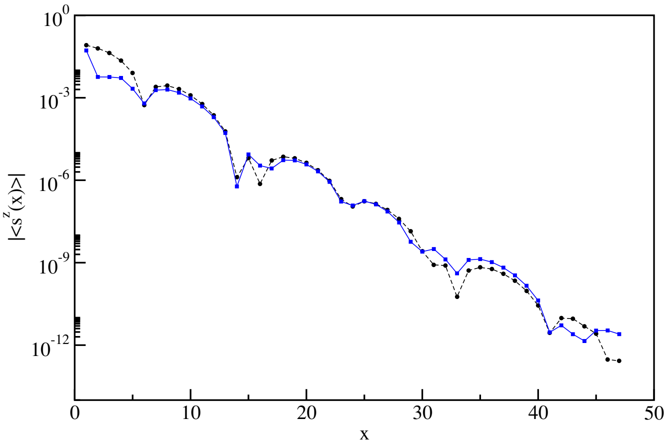

Figure 7. TMRG data (black circles) for the local magnetization $\langle s^z(x)\rangle$ where $u = 1.0, T = 0.131, s = 0.037$ and $n = 0.886$. In comparison the field theory result (93) is shown (blue squares) where the amplitudes and phases have been determined by a fit.

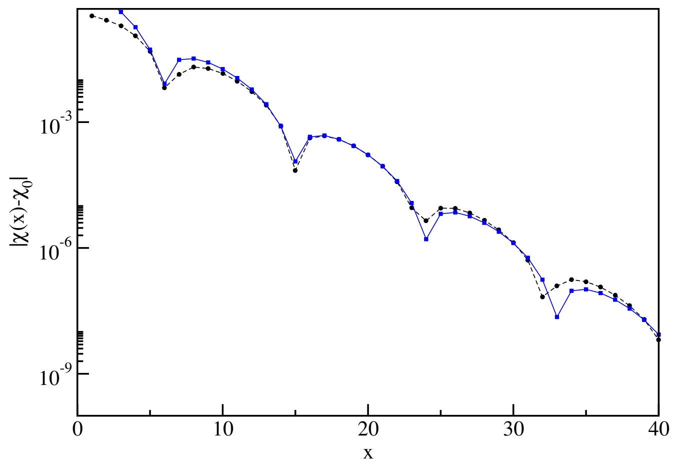

Figure 8. TMRG data (black circles) for the local susceptibility $\chi(x)$ where $u = 1.0, T = 0.131, s = 0.0$ and $n = 0.886$. In comparison the field theory result (95) is shown (blue squares) where the amplitudes and phases have been determined by a fit.

to the field theory result (93). Here the exponents and velocities have been determined exactly by the Bethe ansatz solutions equations (90) and (34) whereas the amplitudes and phases have been used as fitting parameters. The agreement is very good. In particular, the exponential decay of the correlation function is correctly described by the exponents and velocities obtained by Bethe ansatz. The surprisingly rich structure of $\langle s^z(x)\rangle$ is caused by a competition between the first three terms in (93) which oscillate with different wave vectors but have similar correlation lengths given by $\xi_1 = 1.906, \xi_2 = 1.903$ and $\xi_3 = 1.708$ (the correlation lengths ξ_i should not be confused with the matrix $\hat{\xi}$ in (90).

In figure 8, the local susceptibility for the same set of parameters as in figure 7 but zero magnetization is shown. The TMRG data are again compared to the field theory result (95) and good agreement is found. Here only the first term of (95) has been taken into account because the correlation length belonging to the second term is small compared to that of the first one.

5. Conclusions

We studied the low-energy thermodynamic and ground-state properties of the one-dimensional Hubbard model with open ends. In particular, we concentrated on the bulk and boundary parts of the magnetic susceptibility. On the basis of the low-energy effective theory for this model, we argued that the functional form of $\chi_{\mathrm{bulk,B}}(h, T = 0)$ and $\chi_{\mathrm{bulk,B}}(h = 0, T)$ is universal, i.e., does not depend on filling n or interaction strength u. For the bulk susceptibility only the zero temperature and zero-field value $\chi_0 = (2\pi v_s)^{-1}$ depends on n, u via the spin-wave velocity v_s as does the scale E_0 appearing in the logarithms. For $E \ll E_0$ with $E = T, h$, however, the scale is not important and the bulk susceptibility becomes

$$\chi_{\mathrm{bulk}} = \frac{1}{2\pi v_s}\left(1 - \frac{1}{2\ln E} - \frac{\ln|\ln E|}{\ln^2 E}\right).$$

For the boundary part we even find that the result for $T = 0, h \ll h_0$

$$\chi_{\mathrm{B}} = \frac{1}{4h\ln^2 h}\left(1 + \frac{\ln|\ln h|}{\ln h}\right)$$

as well as the result for $h = 0, T \ll T_0$

$$\chi_{\mathrm{B}} = -\frac{1}{12T\ln T}\left(1 + \frac{\ln|\ln T|}{2\ln T}\right)$$

are completely universal. In particular, they are identical to the results obtained for the Heisenberg model [13, 14]. The universal behaviour of χ_{B} at low energies has nothing to do with the special properties making the Hubbard model integrable. Instead, the universal behaviour will hold for any system whose low-energy effective theory is identical to that for the Hubbard model described in section 2. Therefore even in a generic itinerant electron system, non-magnetic impurities or structural defects can give rise to a Curie-like contribution to the magnetic susceptibility. This has profound consequences for experiments on such systems, where a Curie term in the susceptibility is often assumed to be directly related to the concentration of magnetic impurities in the sample. In the light of the results presented here a more sophisticated analysis is necessary. In particular, the temperature dependence of the Curie constant has to be analysed carefully—in the case of a boundary considered here the Curie constant will show a logarithmic dependence on temperature. In addition, it might be useful to investigate if the Curie contribution can be reduced by annealing as one would expect if it is caused by structural defects.

On the basis of the Bethe ansatz solution for the Hubbard model at zero temperature, we have been able to calculate χ_{bulk} exactly beyond the limit $h \ll h_0$ by determining the scale h_0 for arbitrary filling. In addition, the exact solution has confirmed that the bulk and boundary parts show indeed the universal functional dependence on magnetic field which has been obtained by the low-energy effective theory.

For the Friedel oscillations in magnetization and density caused by the open boundaries, we have derived an asymptotic expansion by making use of conformal invariance. We have also calculated the local susceptibility near the boundary which is a quantity directly measurable in nuclear magnetic resonance Knight shift experiments. We confirmed our results by comparing with numerical data obtained by the density-matrix renormalization group applied to transfer matrices.

Acknowledgments

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Appendix A. Small-u expansion

The Bethe ansatz equations for a finite system are expanded with respect to the coupling constant at small couplings, in analogy to the model of an interacting Fermi gas [40]. Before turning to the open boundary case, we first perform this expansion for periodic boundary conditions. The comparison with open boundary conditions yields the surface energy in this approximation.

A.1. Periodic boundary conditions

The energy eigenvalues are given by

$$E_{\mathrm{pbc}} = -2\sum_{j=1}^{N} \cos k_j \tag{A.1}$$

where the k_j are obtained through

$$\mathrm{e}^{\mathrm{i}k_j L} = \prod_{l=1}^{M_\downarrow} \frac{\lambda_l - \sin k_j - \mathrm{i}u}{\lambda_l - \sin k_j - \mathrm{i}u}, \qquad j = 1, \ldots, N \tag{A.2}$$

$$\prod_{j=1}^{N} \frac{\lambda_l - \sin k_j + \mathrm{i}u}{\lambda_l - \sin k_j - \mathrm{i}u} = \prod_{m=1, m\neq l}^{M_\downarrow} \frac{\lambda_l - \lambda_m + 2\mathrm{i}u}{\lambda_l - \lambda_m - 2\mathrm{i}u}, \qquad l = 1, \ldots, M_\downarrow. \tag{A.3}$$

For $u = 0, 2M_\downarrow$-many of the $k_j^{(0)}$ are grouped in pairs at $2\pi l/L, l = 1, \ldots, M_\downarrow$, and the $M_\downarrow$-many $\lambda_l^{(0)}$s lie at $\sin(2\pi l/L)$. The rest of the $k_j^{(0)}$s (namely $N - 2M_\downarrow$ many) are not paired, they are at $\pm 2\pi j/L$, $j = -(N - M_\downarrow - 1)/2, \ldots, -(M_\downarrow + 1)/2$. We make the following ansatz, distinguishing between paired (unpaired) momenta $k_j^{(p)}$ $\left(k_j^{(u)}\right)$:

$$k_j^{(p)} = k_j^{(p,0)} \pm \beta_j + \delta_j^{(p)} \qquad k_j^{(u)} = k_j^{(u,0)} + \delta_j^{(u)} \tag{A.4}$$

$$\lambda_l = \lambda_l^{(0)} + \epsilon_l. \tag{A.5}$$

This ansatz is motivated by evaluating numerically the BA equations (A.2) and (A.3) and it is justified *a posteriori* by observing that the quantities $\delta_j^{(u,p)}$, β_j, ϵ_l can be obtained in a closed form. Equation (A.4) means that two paired momenta are centred around their 'centre of mass' $k_j^{(p,0)} + \delta_j^{(p)}$. It can be verified that $\epsilon_l = \delta_j^{(p)}$ only for $N = 2M_\downarrow$ (no magnetization). Expanding the BA equations (A.2) and (A.3) and comparing coefficients of the imaginary and real parts yields

$$\beta_j^2 = 2\frac{u}{L} \cos k_j^{(p,0)} \tag{A.6}$$

$$\delta_j^{(p)} = 2\frac{u}{L} \cos k_j^{(p,0)} \left[\sum_{l\neq j} \frac{1}{\lambda_j^{(0)} - \lambda_l^{(0)}} + \frac{1}{2} \sum_{l} \frac{1}{\lambda_j^{(0)} - \sin k_l^{(u,0)}} \right] - \frac{u}{L} \frac{\sin k_j^{(0)}}{\cos k_j^{(0)}} \tag{A.7}$$

$$\delta_j^{(u)} = -2\frac{u}{L}\cos k_j^{(u,0)} \sum_l \frac{1}{\lambda_l^{(0)} - \sin k_l^{(u,0)}}. \tag{A.8}$$

Note that β_j^2 may be positive or negative, depending on the value of $\cos k_j^{(0)}$. The quantity ϵ_l in (A.5) may be obtained similarly; however, it will be of no further importance for our purposes. Inserting (A.6)–(A.8) into (A.1) results in

$$E_{\rm pbc} = -4\frac{\sin\frac{\pi}{L}\frac{N}{2}\cos\frac{\pi}{L}S}{\sin\frac{\pi}{2}} + \frac{u}{L}(N^2 - 4S^2), \tag{A.9}$$

where $S = \frac{N}{2} - M_\downarrow$.

Now, with $n := N/L$, $s =: S/L$,

$$e_{\rm pbc} = -\frac{4}{\pi}\sin\frac{\pi n}{2}\cos\pi s + u(n^2 - 4s^2) - \frac{4\pi}{6L^2}\sin\frac{\pi n}{2}\cos\pi s. \tag{A.10}$$

At $s = 0$ (that is, for zero magnetic field), we obtained the charge and spin velocities at small u from the low-energy effective Hamiltonian in section 2,

$$v_{\rm c,s} = 2\sin\frac{\pi n}{2} \pm \frac{2u}{\pi}.$$

This provides a consistency check on the leading finite-size correction of the ground-state energy, as obtained from conformal field theory [41]

$$e_{\rm pbc} := \frac{E_{\rm pbc}}{L} = {\rm e}^{(\infty)} - \frac{\pi}{6L^2}(v_{\rm c} + v_{\rm s}). \tag{A.11}$$

At finite magnetic field

$$h = -\partial_s e_{\rm pbc} = -4\sin\frac{\pi n}{2}\sin\pi s + 2us, \tag{A.12}$$

the susceptibility is derived from equation (A.10),

$$\chi_{\rm bulk}(u \to 0, h) = \frac{1}{4\pi\sin\frac{\pi n}{2}\cos\pi s}\left(1 + \frac{2u}{\pi\sin\frac{\pi n}{2}\cos\pi s}\right). \tag{A.13}$$

It is important to note that equation (A.13) has been derived at finite s, in the limit of vanishing u. In the limit of small fields, $s \propto h$, and thus the small-field expansion of (A.13) reads

$$\chi_{\rm bulk}(u \to 0, h > 0) = \frac{1}{2\pi v_{\rm F}} + \frac{2u}{\pi^2 v_{\rm F}^2}, \tag{A.14}$$

with $s = s(h)$. The order of the limits is important here: the small-coupling limit has been taken *before* the small h-limit. That is, equation (A.14) is valid at small but still finite fields, where the field-dependent terms have been neglected (in the main part (cf equation (84), a lower bound on the field is given in terms of the scale h_0, namely $h \gg 1/h_0$). These singular limits are due to the non-analytic behaviour of $\chi_{\rm bulk}$ as a function of the magnetic field in the thermodynamic limit; cf equation (17).

The result for $\chi_{\rm bulk}(h \to 0, u > 0)$, that is, with interchanged limits compared to equation (A.14), is obtained from the low-energy effective Hamiltonian given in section 2:

$$\chi_{\rm bulk}(h \to 0, u > 0) \equiv \chi_0 = \frac{1}{2\pi v_{\rm s}}$$
$$= \frac{1}{2\pi v_{\rm F}} + \frac{u}{\pi^2 v_{\rm F}^2} \tag{A.15}$$

where the result for $v_{\rm s}$, given in equation (13), has been inserted. The origin of the difference between (A.14) and (A.15) is clarified in section 3.3.

A.2. Open boundary conditions

For open boundary conditions, the BA equations are given in (24) and (25). The remarks from A.1 apply similarly to this case, with the modification that all roots are on one half of the real axis. Furthermore, the above expansion procedure can be repeated with the results

$$\beta_j^2 = \frac{u}{L+1}\cos k_j^{(p,0)} \tag{A.16}$$

$$\delta_j^{(p)} = \frac{u}{L+1}\cos k_j^{(p,0)}\left[\sum_{l\neq j}\frac{1}{\lambda_j^{(0)}-\lambda_l^{(0)}}+\frac{1}{2}\sum_l\frac{1}{\lambda_j^{(0)}-\sin k_l^{(u,0)}}\right]-\frac{u}{2(L+1)}\frac{\sin k_j^{(0)}}{\cos k_j^{(0)}} \tag{A.17}$$

$$\delta_j^{(u)} = -\frac{u}{L+1}\cos k_j^{(u,0)}\sum_l\frac{1}{\lambda_l^{(0)}-\sin k_l^{(u,0)}}. \tag{A.18}$$

Here the sums run over the symmetrized sets of BA-numbers. We now obtain the energy

$$E_{\text{obc}} = -2\frac{\sin\frac{\pi(N+1)}{2(L+1)}\cos\frac{\pi S}{L+1}}{\sin\frac{\pi}{2(L+1)}}+2+\frac{u}{L+1}(N^2-4S^2+N-2S). \tag{A.19}$$

Expanding (A.19) in powers of $1/L$ yields the boundary contribution to the energy in this weak-coupling approximation

$$\begin{aligned} e_{\text{B}} = \sin\frac{n\pi}{2}\left(-4s\sin s\pi-\frac{4}{\pi}\cos s\pi\right)+2(n-1)\cos s\pi\cos\frac{n\pi}{2} \\ +2+u(2s-n)(2s+n-1). \end{aligned} \tag{A.20}$$

If the boundary susceptibility is derived from this expression as in the previous section, one would obtain a constant depending on n and u only. This result cannot be related to equation (17), showing again the non-commutativity of diverse limits at $u \neq 0$.

Appendix B. Free fermions

In this section we give $\chi_{\text{bulk}}, \chi_{\text{B}}$ for free fermions ($u = 0$) in the low-energy limit. The corresponding quantities are marked by an index $^{(\text{ff})}$.

At $T = 0$, $\chi^{(\text{ff})}(h)$ is directly obtained from equations (A.10) (the bulk part) and (A.20), both at $u = 0$, with the magnetic field given by $h = -\partial_{\text{s}} e$. In the small-field limit, one obtains

$$\chi_{\text{bulk}}^{(\text{ff})}(h) = \frac{1}{2\pi v_{\text{F}}}+\frac{1}{16\pi v_{\text{F}}^3}h^2+\mathcal{O}(h^4) \tag{B.1}$$

$$\chi_{\text{B}}^{(\text{ff})}(h) = \frac{1}{2\pi v_{\text{F}}}+\frac{(n-1)\cos\frac{n\pi}{2}}{2v_{\text{F}}^2}+\frac{h^2}{16\pi}\left(\frac{1}{v_{\text{F}}^3}+\frac{\pi(n-1)\cos\frac{\pi n}{2}}{v_{\text{F}}^4}\right)+\mathcal{O}(h^4). \tag{B.2}$$

Note that $\chi_{\text{bulk}}^{(\text{ff})}(h) = \chi_{\text{B}}^{(\text{ff})}(h)$ only for $n = 1$.

To calculate the susceptibility at finite temperatures, one starts with the free energy per lattice site $f^{(\text{ff})}$,

$$-\beta f^{(\text{ff})} = \frac{1}{L}\sum_{j=1}^{L}\left[\ln\left(1+\exp\left[-\beta\left(-2\cos\frac{\pi j}{L+1}-\mu-h/2\right)\right]\right)+(h\leftrightarrow -h)\right], \tag{B.3}$$

where the chemical potential μ is to be determined from $n = -\partial_\mu f^{(\mathrm{ff})}$. Applying the Euler–MacLaurin formula to equation (B.3) yields

$$-\beta f^{(\mathrm{ff})} = \left(1+\frac{1}{L}\right)\frac{1}{\pi}\int_0^{\pi} \ln(1+\mathrm{e}^{-\beta(-2\cos k-\mu-h/2)})\,\mathrm{d}k - \frac{1}{2L}[\ln(1+\mathrm{e}^{-\beta(-2-\mu-h/2)})(1+\mathrm{e}^{-\beta(2-\mu-h/2)})] + (h\leftrightarrow -h). \tag{B.4}$$

In the $T = 0$ limit, the results equation (B.1) and (B.2) are recovered. By performing a saddle-point approximation around the two Fermi points in the integral in (B.4), one obtains the first T-dependent correction to the zero-field susceptibility,

$$\chi_{\mathrm{bulk}}^{(\mathrm{ff})}(T) = \frac{1}{2\pi v_{\mathrm{F}}} + \left[\frac{2\pi}{3v_{\mathrm{F}}^5}\left(1-\frac{1}{4}v_{\mathrm{F}}^2\right) + \frac{\pi}{12v_{\mathrm{F}}^3}\right]T^2 + \mathcal{O}(T^4) \tag{B.5}$$

$$\chi_{\mathrm{B}}^{(\mathrm{ff})}(T) = \frac{1}{2\pi v_{\mathrm{F}}} + \frac{(n-1)\cos\frac{n\pi}{2}}{2v_{\mathrm{F}}^2} + \left[\frac{2\pi}{3v_{\mathrm{F}}^5}\left(1-\frac{1}{4}v_{\mathrm{F}}^2\right) + \frac{\pi}{12v_{\mathrm{F}}^3} + \frac{\pi^2}{3}(n-1)(7+3\cos n\pi)\frac{\cos n\pi}{v_{\mathrm{F}}^6} + \frac{\pi^2(n-1)\cos\frac{n\pi}{2}}{3v_{\mathrm{F}}^4}\right]T^2 + \mathcal{O}(T^4). \tag{B.6}$$

As in the $T = 0$ case, $\chi_{\mathrm{bulk}}^{(\mathrm{ff})} = \chi_{\mathrm{B}}^{(\mathrm{ff})}$ for $n = 1$ only.

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