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Threshold singularities in the one-dimensional Hubbard model

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We consider excitations with the quantum numbers of a hole in the one-dimensional Hubbard model below half-filling. We calculate the finite-size corrections to the energy. The results are then used to determine threshold singularities in the single-particle Green's function for commensurate fillings. We present the analogous results for the Yang-Gaudin model (electron gas with δ-function interactions).

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I. INTRODUCTION

The Hubbard model constitutes a key paradigm for strong correlation effects in one-dimensional (1D) electron systems.[1] Its Hamiltonian is

$$H=-t\sum_{j,\sigma}c^{\dagger}_{j,\sigma}c_{j+1,\sigma}+c^{\dagger}_{j+1,\sigma}c_{j,\sigma}+U\sum_{j}n_{j,\uparrow}n_{j,\downarrow}-\mu\sum_{j}n_j - B\sum_{j}[n_{j,\uparrow}-n_{j,\downarrow}], \quad (1)$$

where $n_{j,\sigma}=c^{\dagger}_{j,\sigma}c_{j,\sigma}$ and $n_j=n_{j,\uparrow}+n_{j,\downarrow}$. In the following discussion, the magnetic field B will be set to zero, but we will reinstate it in the calculations in Secs. III A, IV, and V. The Hubbard model is solvable by Bethe Ansatz[2] and many exact results are available in the literature.[1] Of particular interest in view of experimental applications are dynamical response functions such as the single-particle spectral function

$$A(\omega,q)=-\frac{1}{\pi}\mathrm{Im}\;G_{\rm ret}(\omega,q),$$

$$G_{\rm ret}(\omega,q)=-i\int_0^{\infty}dt e^{i\omega t}\sum_l e^{-iqla_0}\langle 0|\{c_{j+l,\sigma}(t),c^{\dagger}_{j,\sigma}\}|0\rangle. \quad (2)$$

The spectral function is measured in angle-resolved photoemission experiments. Such measurements on the quasi-1D organic conductor TTF-TCNQ have been interpreted in terms of $A(\omega,q)$ of the 1D Hubbard model.[3,4] While high-quality numerical results are available from dynamical density matrix renormalization group computations,[4,5] it is so far not possible to calculate Eq. (2) analytically from the exact solution. However, using a field theory approach it is possible to determine low-energy properties exactly. In particular, the singularity as a function of ω at the Fermi wave number can be obtained using Luttinger liquid theory.[6] The low-energy physics of the Hubbard model in zero magnetic field is described by a spinful Luttinger liquid with Hamiltonian $H=H_c+H_s$, where[1,7]

$$H=\sum_{\alpha=c,s}\frac{v_\alpha}{2\pi}\int dx\left[\frac{1}{K_\alpha}\left(\frac{\partial\Phi_\alpha}{\partial x}\right)^2+K_\alpha\left(\frac{\partial\Theta_\alpha}{\partial x}\right)^2\right] + \text{irrelevant operators}. \quad (3)$$

Here, $K_s=1$ (we are concerned with the $B=0$ case for the time being) and the spin and charge velocities $v_{c,s}$ as well as the Luttinger parameter K_c are known functions of the density and interaction strength.[1] The Bose fields Φ_α and the dual fields Θ_α fulfill the commutation relations

$$\left[\Phi_\alpha(x),\frac{\partial\Theta_\beta(y)}{\partial y}\right]=i\pi\delta_{\alpha\beta}\delta(x-y). \quad (4)$$

The spectrum of low-lying excitations (relative to the ground state) in a large but finite system of size L is given by[1,8]

$$\Delta E=\frac{2\pi v_c}{L}\left[\frac{(\Delta N_c)^2}{4\xi^2}+\xi^2\left(D_c+\frac{D_s}{2}\right)^2+N_c^++N_c^-\right]+\frac{2\pi v_s}{L}\left[\frac{\left(\Delta N_s-\frac{\Delta N_c}{2}\right)^2}{2}+\frac{D_s^2}{2}+N_s^++N_s^-\right],$$

$$\Delta P=\frac{2\pi}{L}[\Delta N_cD_c+\Delta N_sD_s+N_c^+-N_c^-+N_s^+-N_s^-]+2k_F(2D_c+D_s), \quad (5)$$

where ΔN_α, D_α, and $N_\alpha^{\pm}$ are integer or half-odd integer "quantum numbers" subject to the selection rules

$$N_\alpha^{\pm}\in\mathbb{N}_0,\quad \Delta N_\alpha\in\mathbb{Z},\quad D_c=\frac{\Delta N_c+\Delta N_s}{2}\mathrm{mod}\;1,\quad D_s=\frac{\Delta N_c}{2}\mathrm{mod}\;1. \quad (6)$$

We note that the form of the finite-size corrections implies that in the finite volume the spin and charge sectors are not independent but are in fact coupled through the boundary conditions of the fields Φ_α, Θ_α. Neglecting the effects of the irrelevant operators in Eq. (3) makes it possible to calculate $A(\omega,q)$ at low energies.[1,6,7] The spectral function is found to exhibit singularities following the dispersions of the collective spin ("spinon") and charge ("holon") excitations. The exponents characterizing these singularities are given in terms of the quantum numbers ΔN_α, D_α and $N_\alpha^{\pm}$.

In a series of recent works[9–20] it was demonstrated for the case of a spinless fermions, that neglecting the irrelevant operators perturbing the Luttinger liquid Hamiltonian leads in general to incorrect results for singularities in response functions. Using a mapping to a Luttinger liquid coupled to a mobile impurity and taking the leading irrelevant operators into account nonperturbatively it is possible to determine the

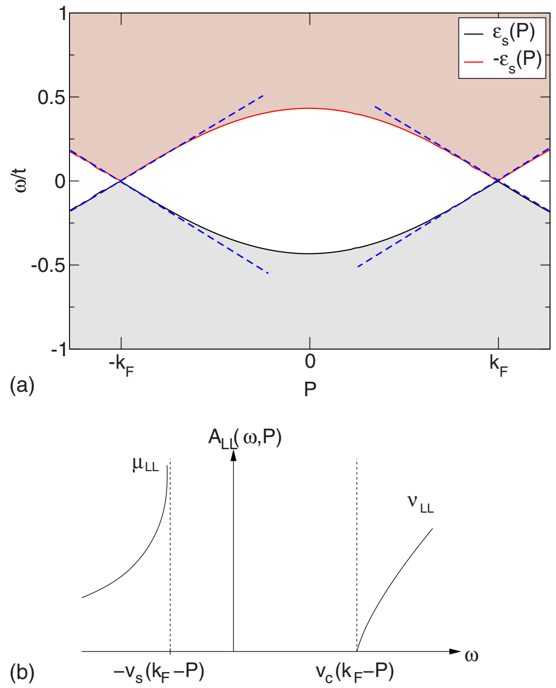

FIG. 1. (Color online) (a) Support of the single-particle spectral function. $A(\omega,P)$ is nonvanishing in the shaded areas. $\epsilon_s(P)$ is the dispersion relation of the collective spin excitations ("spinons"). The blue lines depict the linearized dispersions $\pm v_s(P-k_F)$ and $\pm v_s(P+k_F)$ that underlie the Luttinger liquid approximation. (b) Structure of the single-particle spectral function in the Luttinger liquid approximation for momenta close to k_F and $P<k_F$. There is a singularity at negative frequencies $\omega=-v_s(k_F-P)$ and a power-law "shoulder" at positive frequencies $\omega=v_c(k_F-P)$.

exact singularities in response functions.[9–21] Crucially, these singularities are generally *momentum dependent* (Fig. 1). Two recent preprints have addressed the generalization to spinful fermions.[22,23] In particular, Ref. 23 derives expressions for the exponents $\mu_{n,\pm}$ characterizing the singularities of the single-particle spectral function (2). The resulting spectral function is depicted in Fig. 2.

Our goal is to provide an exact expression for the threshold exponents $\mu_{0,-}$ in terms of the microscopic parameters

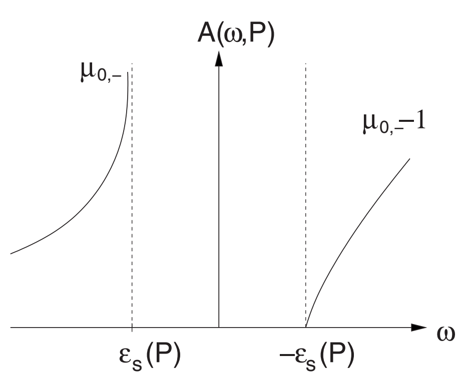

FIG. 2. Power-law singularity in the single-hole spectral function for $|P|<k_F$. There is a singularity at negative frequencies $\omega=\epsilon_s(P)$ with a momentum-dependent exponent $\mu_{0,-}$ and a power-law "shoulder" at positive frequencies $\omega=-\epsilon_s(P)$.

entering the Hamiltonian, i.e., U, μ, and B in the case of the Hubbard model. This is achieved by determining the finite-size corrections to low-lying energy levels *in presence of a high-energy excitation*. Comparing the results obtained from the Bethe Ansatz solution of the Hubbard model as well as the closely related Yang-Gaudin model to field theory predictions, we are able to derive explicit expressions for the threshold exponents. In the Yang-Gaudin case our explicit results agree with the relations of spectrum and exponents proposed in Ref. 23 for Galilei-invariant models.[24]

There is one caveat for the case of the Hubbard model. As for any lattice model it is possible to generate low-lying excitations for any momentum by combining multiple Umklapp processes if the band filling is incommensurate. A completely analogous situation is encountered for spinless fermions.[19] Hence for incommensurate fillings no thresholds exist. While we would still expect the spectral function to feature peaks associated with the thresholds of particular excitations, in particular those involving small numbers of holons and spinons, these peaks will no longer correspond to singularities. In order to circumvent this problem we will consider only the case of commensurate fillings in the Hubbard model.

The outline of this paper is as follows. In Sec. II, we briefly review the Bethe Ansatz description of the ground state of the Hubbard model. In Sec. III, we present the excitations that give rise to low-energy thresholds around the Fermi momentum in the Hubbard model. In Secs. IV and V, we determine the finite-size spectrum of excited states describing these thresholds. In Sec. VI, we relate these results to the field theory treatment of the threshold problem and extract threshold exponents. In Sec. VII, we summarize the analogous results for the Yang-Gaudin model.

II. BETHE ANSATZ EQUATIONS FOR THE HUBBARD MODEL

The logarithmic form of the Bethe ansatz equations of the Hubbard model for N electrons out of which M have spin down (for real solutions only) is

$$k_jL = 2\pi I_j - \sum_{\alpha=1}^{M} \theta\left(\frac{\sin k_j - \Lambda_\alpha}{u}\right), \quad j=1,\ldots,N,$$

$$\sum_{j=1}^{N} \theta\left(\frac{\Lambda_\alpha - \sin k_j}{u}\right) = 2\pi J_\alpha + \sum_{\beta=1}^{M} \theta\left(\frac{\Lambda_\alpha - \Lambda_\beta}{2u}\right),$$
$$\alpha = 1,\ldots,M. \tag{7}$$

Here

$$u = \frac{U}{4t}, \tag{8}$$

the length of the lattice L is taken to be even, $\theta(x) = 2\arctan(x)$ and I_j, J_α are integer or half-odd integer numbers that arise due to the multivaluedness of the logarithm. They are subject to the "selection rules"

$$I_j \text{ is} \begin{cases} \text{integer} & \text{if } M \text{ is even} \\ \text{half-odd integer} & \text{if } M \text{ is odd,} \end{cases} \tag{9}$$

$$J_\alpha \text{ is} \begin{cases} \text{integer} & \text{if } N-M \text{ is odd} \\ \text{half-odd integer} & \text{if } N-M \text{ is even,} \end{cases} \tag{10}$$

$$-\frac{L}{2} < I_j \le \frac{L}{2}, \quad |J_\alpha| \le \frac{1}{2}(N-M-1). \tag{11}$$

The energy (in units of t) and momentum of such Bethe ansatz states are

$$E = uL + 2BM - \sum_{j=1}^{N} [2\cos(k_j) + \mu + 2u + B],$$
$$P = \sum_{j=1}^{N} k_j \equiv \frac{2\pi}{L}\left[\sum_{j=1}^{N} I_j + \sum_{\alpha=1}^{M} J_\alpha\right]. \tag{12}$$

Ground state below half-filling

Following Sec. 7.7 of Ref. 1we now take consider the ground state below half-filling. We have

$$N = N_{\mathrm{GS}}, \quad M = M_{\mathrm{GS}}, \tag{13}$$

where we take $N_{\mathrm{GS}}=2\times\text{odd}$ and $M_{\mathrm{GS}}=\text{odd}$. We note that in zero magnetic field we have $M_{\mathrm{GS}}=\frac{N_{\mathrm{GS}}}{2}$. Our choice for N and M implies that I_j are half-odd integers and J_α are integers. In the ground state all vacancies are filled symmetrically around zero

$$I_j = j - \frac{N_{\mathrm{GS}}+1}{2}, \quad j = 1, \ldots, N_{\mathrm{GS}},$$

$$J_\alpha = \alpha - \frac{M_{\mathrm{GS}}+1}{2}, \quad \alpha = 1, \ldots, M_{\mathrm{GS}}. \tag{14}$$

It follows from Eq. (12) that the ground-state momentum is zero. The bulk ground state energy can be expressed in terms of the solution of the following set of coupled integral equations

$$\rho_c(k) = \frac{1}{2\pi} + \cos k \int_{-A}^{A} d\Lambda a_1(\sin k - \Lambda)\rho_s(\Lambda), \tag{15}$$

$$\rho_s(\Lambda) = \int_{-Q}^{Q} dk a_1(\Lambda - \sin k)\rho_c(k) - \int_{-A}^{A} d\Lambda' a_2(\Lambda - \Lambda')\rho_s(\Lambda'), \tag{16}$$

where

$$a_n(x) = \frac{1}{2\pi}\frac{2nu}{(un)^2 + x^2}. \tag{17}$$

The integrated densities yield the total number of electrons per site and the number of electrons with spin down per site, respectively

$$\int_{-Q}^{Q} dk\rho_c(k) = \frac{N_{\mathrm{GS}}}{L} \equiv n_c, \quad \int_{-A}^{A} d\Lambda\rho_s(\Lambda) = \frac{M_{\mathrm{GS}}}{L} = \frac{N_\downarrow}{L} \equiv n_s. \tag{18}$$

The integration boundaries Q and A can be fixed in terms of N_{GS} and M_{GS} by these equations. Alternatively one can define *dressed energies* by

$$\epsilon_c(k) = -2\cos k - \mu - 2u - B + \int_{-A}^{A} d\Lambda a_1(\sin k - \Lambda)\epsilon_s(\Lambda),$$

$$\epsilon_s(\Lambda) = 2B + \int_{-Q}^{Q} dk \cos(k) a_1(\sin k - \Lambda)\epsilon_c(k) - \int_{-A}^{A} d\Lambda' a_2(\Lambda - \Lambda')\epsilon_s(\Lambda'). \tag{19}$$

Here, the integration boundaries $\pm Q$ and $\pm A$ are by definition the points at which the dressed energies switch sign, so that they are determined as functions of the chemical potential and the magnetic fields via the conditions

$$\epsilon_c(\pm Q) = 0, \quad \epsilon_s(\pm A) = 0. \tag{20}$$

The bulk ground-state energy per site is

$$e_{\mathrm{GS}} = \int_{-Q}^{Q} dk(-2\cos k - \mu - B - 2u)\rho_c(k) + 2Bn_s + u$$
$$= \int_{-Q}^{Q} \frac{dk}{2\pi}\epsilon_c(k) + u. \tag{21}$$

III. EXCITATIONS WITH CHARGE $-e$ AND SPIN $\frac{1}{2}$

We now consider an excitation over the ground state with the quantum numbers of a hole with spin down. As the total charge must be one less than in the ground state we must have

$$N = N_{\mathrm{GS}} - 1. \tag{22}$$

Recalling that the z component of total spin quantum number is $S^z=\frac{N-2M}{2}$ we see that relative to the ground state we must have

$$\delta S^z = \frac{2l+1}{2}, \quad l \in \mathbb{N}_0. \tag{23}$$

Equation (23) requires an explanation. As shown in[25] the Bethe ansatz states only provide *highest-weight states* of the SO(4) symmetry[26] of the Hubbard model. The corresponding SO(4) multiplet is then obtained by acting with lowering operators. As a result, for any excitation given by the Bethe ansatz with $\delta S^z=\frac{2l+1}{2}$ for non-negative integers l we can construct an excited state with $\delta S^z=\frac{1}{2}$ by acting with the spin lowering operator. In presence of a magnetic field this shifts the energy by $-2Bl$.

A. Holon-spinon excitation

The simplest excitation with the quantum numbers [Eq. (23)], Eq. (22) is *two parametric*[1] and obtained by setting

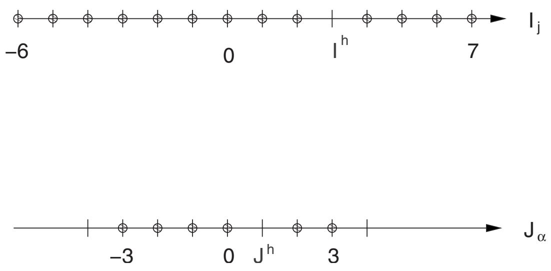

FIG. 3. Distribution of integers for the holon-spinon excitation for $N_{GS}=14$, $M_{GS}=7$. The positions of the two holes are I^h and Λ^h respectively. We have shown the configuration where the I_j range from $\frac{N_{GS}}{2}-1$ to $\frac{N_{GS}}{2}$, but we equally well can choose them $\frac{N_{GS}}{2}\le I_j \le \frac{N_{GS}}{2}-1$. The two possibilities give rise to the two signs in Eq. (27).

$$N=N_{GS}-1,\quad M=M_{GS}-1, \tag{24}$$

in the Bethe ansatz Eq. (7). It then follows from Eqs. (9) and (10) that both I_j and J_α are integers. In order to see that we are dealing with a two-parametric excitation we consider the number of vacancies for the integers I_j and J_α [Eq. (11)]. As

$$-\frac{L}{2}<I_j\le\frac{L}{2}, \tag{25}$$

there is the same number of vacancies for the I_j's as in the ground state, but we have one fewer integer, i.e., one additional "hole." Similarly we have

$$|J_\alpha|\le\frac{1}{2}(N_{GS}-M_{GS}-1), \tag{26}$$

which tells us that we have the same number of vacancies as in the ground state but one root less, which leaves one hole. It is useful to plot the distribution of integers. This is done in Fig. 3.

The energy and momentum of the "holon-spinon" excitation described above are determined in Chap. 7 of Ref. 1

$$E_{hs}=-\epsilon_c(k^h)-\epsilon_s(\Lambda^h),$$

$$P_{hs}=-p_c(k^h)-p_s(\Lambda^h)\pm\pi n_c, \tag{27}$$

where the dressed energies are defined in Eq. (19) and the dressed momenta are

$$p_c(k)=2\pi\int_0^k dk'\rho_c(k'),$$

$$p_s(\Lambda)=\pi(n_c-n_s)-2\pi\int_\Lambda^\infty d\Lambda\rho_s(\Lambda). \tag{28}$$

The extra contribution $\pm\pi n_c$ in Eq. (27) arises as the distribution of I_j's is asymmetric with respect to the origin. In zero magnetic field the equation for $p_s(\Lambda)$ can be simplified

$$p_s(\Lambda)|_{B=0}=\frac{\pi n_c}{2}-2\int_{-Q}^{Q}dk\arctan\left[\exp\left(-\frac{\pi}{2u}(\Lambda-\sin(k)\right)\right]\rho_c(k). \tag{29}$$

In Fig. 4, we plot the upper and lower boundaries of the holon-spinon continuum for two different band fillings in zero magnetic field. We see that as expected there are soft modes around $\pm k_F=\frac{\pi n_c}{2}$.

B. Holon–3 spinon excitation

Other kinds of excitations with the quantum numbers [Eq. (23)], Eq. (22) involve more than two "elementary" excitations. As we are interested in the threshold of the spectral function, we focus on excitations that lead to the smallest possible energy for a given momentum. This leads us to consider holon–3 spinon excitations characterized by a solution of the Bethe ansatz Eq. (7) with

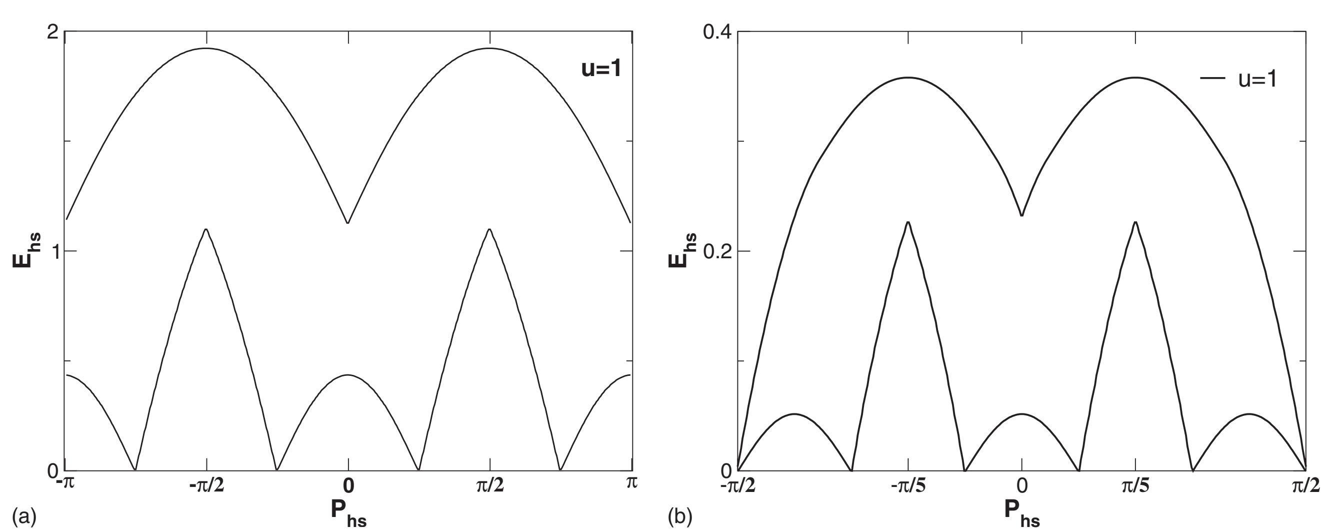

FIG. 4. Boundaries of the holon-spinon excitation continuum in zero magnetic field for (a) $u=1$ and density $n_c=0.5$ and (b) for $u=1$ and $n_c=0.2$.

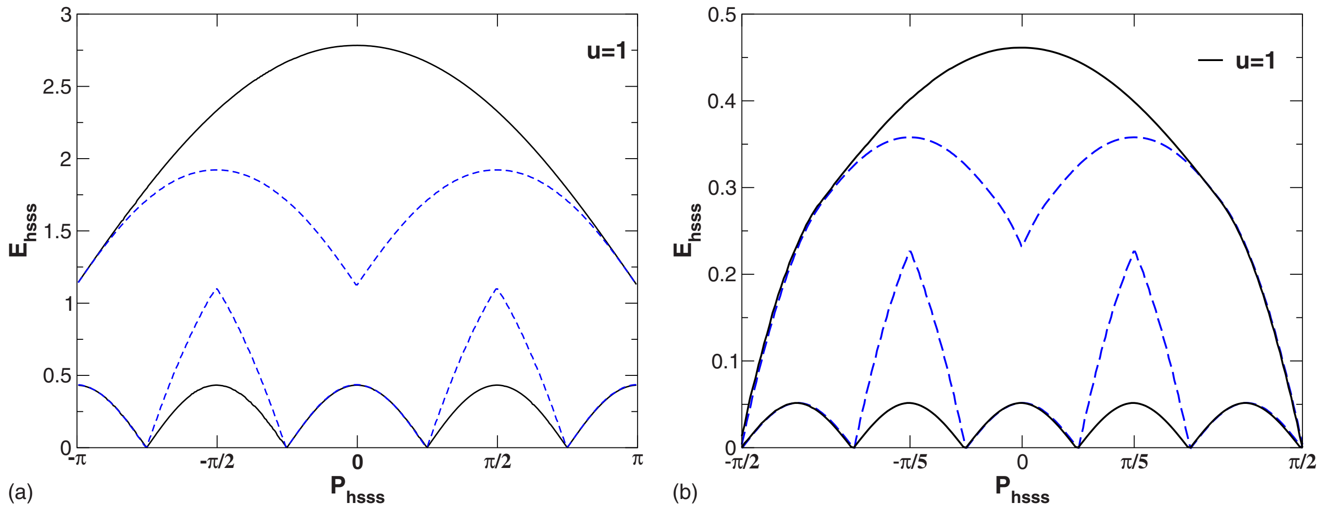

FIG. 5. (Color online) Boundaries of the holon–3 spinon excitation continuum in zero magnetic field for (a) $u=1$ and density $n_c=0.5$ and (b) for $u=1$ and $n_c=0.2$. The boundaries of the holon-spinon continua are depicted by the dashed blue lines.

$$N=N_{\mathrm{GS}}-1,\quad M=M_{\mathrm{GS}}-2. \tag{30}$$

It follows from Eqs. (9) and (10) that both I_j and J_α are half-odd integers. In order to see that we are dealing with a four-parametric excitation we consider the number of vacancies for the integers I_j and J_α [Eq. (11)]. As

$$-\frac{L}{2}<I_j\le\frac{L}{2}, \tag{31}$$

there is the same number of vacancies for the I_j's as in the ground state, but we have one fewer integer, i.e., one additional hole. Similarly we have

$$|J_\alpha|\le\frac{1}{2}(N_{\mathrm{GS}}-M_{\mathrm{GS}}), \tag{32}$$

which tells us that we have one more vacancy than in the ground state but two roots less, which amounts to three holes. The energy and momentum of this excitation are

$$E_{hsss}=-\epsilon_c(k^h)-\sum_{j=1}^{3}\epsilon_s(\Lambda_j^h),$$

$$P_{hsss}=-p_c(k^h)-\left(\sum_{j=1}^{3}p_s(\Lambda_j^h)\right), \tag{33}$$

where the dressed energies and momenta are defined in Eqs. (19) and (28), respectively. We note that there is no additional constant contribution to the momentum because both the I_j and J_α are half-odd integers, leading to symmetric distributions of roots in the absence of holes. In Fig. 5, we plot the upper and lower boundaries of the holon–3 spinon continuum for two different band fillings in zero magnetic field. We see that in part of the Brillouin zone the holon–3 spinon threshold is lower in energy than the holon-spinon continuum.

C. Thresholds in zero magnetic field

We are now in a position to determine the lower boundaries of the holon-spinon and holon–3 spinon continua in the vicinity of k_F. We find that the lower boundary is obtained as follows:

$$0<P_{hs}<k_F.$$

Here the threshold is identical for both types of excitation considered above. The leading singularity of the spectral function is given by contribution of the holon-spinon continuum. The threshold is obtained as follows: we choose the plus sign in Eq. (27) and place the holon at its right "Fermi point," i.e.,

$$I^h=\frac{N_{\mathrm{GS}}}{2},\quad k^h=Q. \tag{34}$$

It therefore carries zero energy and momentum $-\pi n_c$. For $P_{hs}=k_F$ the spinon has rapidity $\Lambda^h=-\infty$, which corresponds to momentum $k_F=\frac{\pi n_c}{2}$. Taking the spinon rapidity from $\Lambda^h=-\infty$ to $\Lambda^h=0$ then traces out the lower boundary of the holon-spinon continuum for $0<P_{hs}<k_F$.

$$2k_F>P_{hs}>k_F.$$

Here, the threshold is given by the holon–3 spinon continuum. It is obtained by placing the holon at its left "Fermi point"

$$I^h=-\frac{N_{\mathrm{GS}}-1}{2},\quad k^h=-Q. \tag{35}$$

It therefore carries zero energy and momentum $\pi n_c=2k_F$. Two of the spinons are placed at their left and right Fermi points, respectively

$$J_{1,2}^h=\pm\frac{M_{\mathrm{GS}}}{2},\quad \Lambda_{1,2}^h=\pm\infty. \tag{36}$$

Their contributions to the total momentum cancel. To obtain total momentum $P_{hsss}=k_F$ the third spinon is taken to have rapidity $\Lambda^h=\infty$, which corresponds to momentum $-k_F=-\frac{\pi n_c}{2}$. Taking the spinon rapidity from $\Lambda^h=\infty$ to $\Lambda^h=0$ then traces out the lower boundary of the holon–3 spinon continuum for $k_F<P_{hsss}<2k_F$.

At this point an obvious question to ask is whether other excitations may lead to even lower thresholds. As we have restricted ourselves to commensurate band fillings and zero-magnetic field the answer close to k_F is negative. This follows from the general expression for the low-energy part of the spectrum Eq. (5). This strongly suggests that the threshold of the spectral function is given by the two excitations given above and we will assume this to be the case in what follows.

D. Holon-spinon threshold in zero magnetic field

It is conceivable that the spectral function $A(\omega,q)$ could exhibit features associated with the threshold of the holon-spinon excitation in the momentum range where the threshold of $A(\omega,q)$ occurs at a lower frequency. We therefore determine the threshold of the holon-spinon excitation in zero field in the momentum range $2k_F>P_{hs}>k_F$. It is obtained by choosing the plus sign in Eq. (27) and place the spinon at its Fermi point, i.e.,

$$J^h=-\frac{N_{\rm GS}-2}{4},\quad \Lambda^h=-\infty. \tag{37}$$

It therefore carries zero energy and momentum $\frac{\pi n_c}{2}$. For $P_{hs}=k_F$ the holon has rapidity $k^h=Q$, which corresponds to momentum $-\pi n_c$. Reducing the holon rapidity from $k^h=Q$ traces out the lower boundary of the holon-spinon continuum for $k_F<P_{hs}<2k_F$.

IV. THRESHOLD AT $0<P<k_F$ FOR THE HOLON-SPINON EXCITATION

In the following, we consider the threshold at $0<P<k_F$ for the holon-spinon excitation. By virtue of Eq. (34) we are dealing with a distribution of integers I_j that is symmetric around zero. The free parameter is then the spinon rapidity Λ^h. More precisely, the distributions of integers are

$$I_j=-\frac{N_{\rm GS}}{2}+j,\quad 1\le j\le N_{\rm GS}-1,$$

$$J_\alpha=\begin{cases}-\dfrac{M_{\rm GS}+1}{2}+\alpha & \text{if } 1\le\alpha<\dfrac{M_{\rm GS}+1}{2}+J^h\\[2mm] -\dfrac{M_{\rm GS}+1}{2}+\alpha+1 & \text{if } \dfrac{M_{\rm GS}+1}{2}+J^h\le\alpha\le M_{\rm GS}-1\end{cases}. \tag{38}$$

Our goal is to determine the finite-size corrections to the energy of this excitation in the limit

$$L,J^h,N_{\rm GS},M_{\rm GS}\to\infty,\quad \frac{J^h}{L},\frac{N_{\rm GS}}{L},\frac{M_{\rm GS}}{L}\text{fixed}. \tag{39}$$

A. Finite-size corrections

Our starting point are the Bethe ansatz Eq. (7) for the holon-spinon excitation where the holon sits at the Fermi momentum of the k_j's. It is convenient to write them in terms of *counting functions*

$$z_c(k)=k+\frac{1}{L}\sum_{\alpha=1}^{M}\theta\left(\frac{\sin k-\Lambda_\alpha}{u}\right), \tag{40}$$

$$z_s(\Lambda)=\frac{1}{L}\sum_{j=1}^{N}\theta\left(\frac{\Lambda-\sin k_j}{u}\right)-\frac{1}{L}\sum_{\beta=1}^{M}\theta\left(\frac{\Lambda-\Lambda_\beta}{2u}\right). \tag{41}$$

The Bethe Ansatz equations then read

$$z_c(k_j)=\frac{2\pi I_j}{L},\quad z_s(\Lambda_\alpha)=\frac{2\pi J_\alpha}{L}. \tag{42}$$

We now turn these into integral equations by means of the Euler-Maclaurin sum formula

$$\frac{1}{L}\sum_{n=n_1}^{n_2}f\left(\frac{n}{L}\right)=\int_{n_-/L}^{n_+/L}dxf(x)+\frac{1}{24L^2}\left[f'\left(\frac{n_-}{L}\right)-f'\left(\frac{n_+}{L}\right)\right]+\dots, \tag{43}$$

where

$$n_+=n_2+\frac{1}{2},\quad n_-=n_1-\frac{1}{2}. \tag{44}$$

For the specific excitation we are considering we have

$$I_\pm=\pm\frac{N_{\rm GS}-1}{2},\quad J_\pm=\pm\frac{M_{\rm GS}}{2}. \tag{45}$$

Using Eq. (43) in Eq. (41) and then changing variables from x (i.e., integers divided by L) to the rapidities we arrive at

$$z_c(k)=k+\int_{A_-}^{A_+}d\Lambda\rho_s(\Lambda)\theta\left(\frac{\sin k-\Lambda}{u}\right)-\frac{1}{L}\theta\left(\frac{\sin k-\Lambda_L^h}{u}\right)+\frac{1}{24L^2}\left[\frac{a_1(\sin k-A_+)}{\rho_s(A_+)}-\frac{a_1(\sin k-A_-)}{\rho_s(A_-)}\right]+o(L^{-2}), \tag{46}$$

$$z_s(\Lambda)=\int_{Q_-}^{Q_+}dk\theta\left(\frac{\Lambda-\sin k}{u}\right)\rho_c(k)-\int_{A_-}^{A_+}d\Lambda'\rho_s(\Lambda')\theta\left(\frac{\Lambda-\Lambda'}{2u}\right)+\frac{1}{L}\theta\left(\frac{\Lambda-\Lambda_L^h}{2u}\right)+\frac{1}{24L^2}\left[\frac{a_1(\Lambda-\sin Q_+)\cos Q_+}{\rho_c(Q_+)}-\frac{a_1(\Lambda-\sin Q_-)\cos Q_-}{\rho_c(Q_-)}-\frac{a_2(\Lambda-A_+)}{\rho_s(A_+)}+\frac{a_2(\Lambda-A_-)}{\rho_s(A_-)}\right]+o(L^{-2}). \tag{47}$$

Here $a_n(x)$ is given in Eq. (17), the integration boundaries are fixed by

$$z_c(Q_\pm)=\frac{2\pi I_\pm}{L},\quad z_s(A_\pm)=\frac{2\pi J_\pm}{L}, \tag{48}$$

and the root densities are defined by

$$2\pi\rho_s(\Lambda)=\frac{dz_s(\Lambda)}{d\Lambda},\quad 2\pi\rho_c(k)=\frac{dz_c(k)}{dk}. \tag{49}$$

In addition there is the equation fixing the position of the hole

$$z_s(\Lambda_L^h)=\frac{2\pi J^h}{L}. \tag{50}$$

Here our notation makes the L-dependence of the rapidity of the hole explicit. Taking derivatives of Eq. (47) we obtain coupled linear integral equations for the root densities $\rho_{c,s}$

$$\begin{aligned}\rho_c(k)&=\frac{1}{2\pi}+\cos(k)\int_{A_-}^{A_+}d\Lambda\rho_s(\Lambda)a_1(\sin k-\Lambda)\\&\quad-\frac{a_1(\sin k-\Lambda_L^h)\cos k}{L}+\frac{\cos k}{24L^2}\left[\frac{a_1'(\sin k-A_+)}{\rho_s(A_+)}\right.\\&\quad\left.-\frac{a_1'(\sin k-A_-)}{\rho_s(A_-)}\right],\end{aligned} \tag{51}$$

$$\begin{aligned}\rho_s(\Lambda)&=\int_{Q_-}^{Q_+}a_1(\Lambda-\sin k)\rho_c(k)-\int_{A_-}^{A_+}d\Lambda'\rho_s(\Lambda')a_2(\Lambda-\Lambda')\\&\quad+\frac{1}{L}a_2(\Lambda-\Lambda_L^h)+\frac{1}{24L^2}\left[\frac{a_1'(\Lambda-\sin Q_+)\cos Q_+}{\rho_c(Q_+)}\right.\\&\quad-\frac{a_1'(\Lambda-\sin Q_-)\cos Q_-}{\rho_c(Q_-)}-\frac{a_2'(\Lambda-A_+)}{\rho_s(A_+)}\\&\quad\left.+\frac{a_2'(\Lambda-A_-)}{\rho_s(A_-)}\right].\end{aligned} \tag{52}$$

In shorthand notations these can be written as

$$\rho_\alpha=\rho_\alpha^{(0)}+\hat{K}_{\alpha\beta}*\rho_\beta, \tag{53}$$

where $*$ denotes convolution on the interval $[Q_-,Q_+]$ ($[A_-,A_+]$) if $\beta=c$ ($\beta=s$). The components of the matrix kernel are

$$K_{cc}(k,k')=0,\quad K_{cs}(k,\Lambda)=\cos(k)a_1(\sin k-\Lambda),$$

$$K_{sc}(\Lambda,k)=a_1(\sin k-\Lambda),\quad K_{ss}(\Lambda,\Lambda')=-a_2(\Lambda-\Lambda'). \tag{54}$$

It is useful to introduce a unified notation for the integration boundaries

$$X_\pm^\alpha=\begin{cases}Q_\pm & \text{if } \alpha=\text{c}\\ A_\pm & \text{if } \alpha=\text{s}.\end{cases} \tag{55}$$

Using the Euler-MacLaurin sum formula on the expression for the energy (12) we obtain

$$\begin{aligned}E&=Lu+L\sum_\alpha\int_{X_-^\alpha}^{X_+^\alpha}dz\epsilon_\alpha^{(0)}(z)\rho_a(z)-\epsilon_s^{(0)}(\Lambda_L^h)\\&\quad-\frac{1}{24L}\sum_\alpha\frac{\epsilon_\alpha^{(0)\prime}(X_+^\alpha)}{\rho_\alpha(X_+^\alpha)}-\frac{\epsilon_\alpha^{(0)\prime}(X_-^\alpha)}{\rho_\alpha(X_-^\alpha)},\end{aligned} \tag{56}$$

where the prime denotes the derivative with respect to the argument and $\epsilon_\alpha^{(0)}$ are the *bare energies*, i.e., the driving terms in Eq. (19)

$$\epsilon_c^{(0)}(k)=-2\cos(k)-\mu-2u-B,\quad \epsilon_s^{(0)}(\Lambda)=2B. \tag{57}$$

Now we have to solve the system of Eq. (52) with boundary conditions (49) in by expanding both the densities and the integration boundaries in inverse powers of L. As the integral equations are linear we may proceed by first keeping the integration boundaries general and only expanding the densities as

$$\rho_\alpha(z)=\rho_{\alpha,0}(z)+\frac{1}{L}\rho_{\alpha,1}(z)+\frac{1}{24L^2}\sum_{\beta,\sigma=\pm}\frac{f_{\alpha\beta}^{(\sigma)}(z)}{\rho_\beta(X_\sigma^\beta)}. \tag{58}$$

The various parts then fulfill the integral equations

$$\rho_{\alpha,a}=\rho_{\alpha,a}^{(0)}+\hat{K}_{\alpha\beta}*\rho_{\beta,a},\quad a=0,1, \tag{59}$$

$$f_{\alpha\beta}^{(\sigma)}=d_{\alpha\beta}^{(\sigma)}+\hat{K}_{\alpha\gamma}*f_{\gamma\beta}^{(\sigma)}, \tag{60}$$

where the driving terms are given by

$$\rho_{\alpha,0}^{(0)}(z)=\frac{\delta_{\alpha c}}{2\pi}, \tag{61}$$

$$\rho_{\alpha,1}^{(0)}(z)=-K_{\alpha s}(z,\Lambda_L^h), \tag{62}$$

$$d_{\alpha\beta}^{(\sigma)}(z)=-\sigma\left.\frac{\partial}{\partial z'}\right|_{z'=X_\sigma^\beta}K_{\alpha\beta}(z,z'). \tag{63}$$

The integral equations for the f's are solved by formal (matrix) Neumann series and using this we can bring the expression for the energy in the form

$$\begin{aligned}E&=Lu+L\sum_\alpha\int_{X_-^\alpha}^{X_+^\alpha}dz\epsilon_\alpha^{(0)}(z)\rho_{a,0}(z)-\epsilon_s^{(0)}(\Lambda_L^h)\\&\quad+\sum_\alpha\int_{X_-^\alpha}^{X_+^\alpha}dz\epsilon_\alpha^{(0)}(z)\rho_{\alpha,1}(z)-\frac{\pi}{6L}(v_s+v_c),\end{aligned} \tag{64}$$

where the spin and charge velocities are

$$v_\alpha=\frac{\epsilon_\alpha'(X^\alpha)}{2\pi\rho_{\alpha,0}(X^\alpha)},\quad \alpha=c,s. \tag{65}$$

Let us denote the first two terms in Eq. (64) as $Le_{\text{GS}}(\{X_\pm^\alpha\})$. We consider it as a functional of the integration boundaries and expand it to second order around $\pm X^a$, i.e.,

$$e_{\rm GS}(\{X^\alpha_\pm\}) = e_{\rm GS}(\{X^\alpha\}) + \sum_{\beta,\sigma}\left[\frac{\delta}{\delta X^\beta_\sigma}\bigg|_{X^\beta_\sigma=\sigma X^\beta} e_{\rm GS}(\{X^\alpha_\pm\})\right](X^\beta_\sigma - \sigma X^\beta)$$
$$+\frac{1}{2}\sum_{\beta,\sigma,\gamma,\tau}\left[\frac{\delta^2}{\delta X^\beta_\sigma \delta X^\gamma_\tau}\bigg|_{\substack{X^\beta_\sigma=\sigma X^\beta\\ X^\gamma_\tau=\tau X^\gamma}} e_{\rm GS}(\{X^\alpha_\pm\})\right](X^\beta_\sigma - \sigma X^\beta)(X^\gamma_\tau - \tau X^\gamma). \quad (66)$$

We find that the linear term vanishes by virtue of the Eq. (19) for the dressed energies. For the quadratic term we find after some calculations

$$\frac{\delta^2}{\delta X^\beta_\sigma \delta X^\gamma_\tau}\bigg|_{\substack{X^\beta_\sigma=\sigma X^\beta\\ X^\gamma_\tau=\tau X^\gamma}} e_{\rm GS}(\{X^\alpha_\pm\}) = \delta_{\alpha\beta}\delta_{\sigma\tau}2\pi v_\alpha[\rho_{\alpha,0}(X^\alpha)]^2. \quad (67)$$

The third and fourth terms in Eq. (64) can be simplified using the integral equations for the dressed energies. Introducing the shift of the hole rapidity in the finite volume by

$$\Lambda^h_L = \Lambda^h + \frac{1}{L}\delta\Lambda^h, \quad (68)$$

we can express the finite-size energy as

$$E = Le_{\rm GS}(\{X^\alpha\}) - \epsilon_s(\Lambda^h) + L\pi\sum_\alpha v_\alpha\{[\rho_{\alpha,0}(X^\alpha)(X^\alpha_+ - X^\alpha)]^2 + [\rho_{\alpha,0}(X^\alpha)(X^\alpha_- + X^\alpha)]^2\} - \frac{\pi}{6L}(v_s+v_c) - \frac{1}{L}\epsilon_s'(\Lambda^h)\delta\Lambda^h. \quad (69)$$

We may calculate $\delta\Lambda^h$ from the equation

$$z_s(\Lambda^h_L) = \frac{2\pi J^h}{L} = \int_{Q_-}^{Q_+} dk\rho_{c,0}(k)\theta\left(\frac{\Lambda^h_L - \sin k}{u}\right) - \int_{A_-}^{A_+} d\Lambda\rho_{s,0}(\Lambda)\theta\left(\frac{\Lambda^h_L-\Lambda}{2u}\right) + \frac{1}{L}\int_{-Q}^{Q} dk\rho_{c,1}(k)\theta\left(\frac{\Lambda^h_L - \sin k}{u}\right) - \frac{1}{L}\int_{-A}^{A} d\Lambda\rho_{s,1}(\Lambda)\theta\left(\frac{\Lambda^h_L-\Lambda}{2u}\right) + o(L^{-1}). \quad (70)$$

Using the definition (68) we obtain

$$\delta\Lambda^h = -\frac{L}{2\pi\rho_{s,0}(\Lambda^h)}\sum_{\beta,\sigma}\Psi^{(\sigma)}_\beta(\Lambda^h)[X^\beta_\sigma - \sigma X^\beta] - \frac{L}{2\pi\rho_{s,0}(\Lambda^h)}\left[\frac{1}{L}\int_{-Q}^{Q} dk\rho_{c,1}(k)\theta\left(\frac{\Lambda^h - \sin k}{u}\right) - \frac{1}{L}\int_{-A}^{A} d\Lambda\rho_{s,1}(\Lambda)\theta\left(\frac{\Lambda^h-\Lambda}{2u}\right)\right]. \quad (71)$$

Here

$$\Psi^{(\sigma)}_\beta(\Lambda^h) = \left[\sigma\rho_{\beta,0}(X^\beta)g_{\beta,\sigma}(\Lambda^h) + \int_{-Q}^{Q} dk r^{(\sigma)}_{c\beta}(k)\theta\left(\frac{\Lambda^h - \sin k}{u}\right) - \int_{-A}^{A} d\Lambda r^{(\sigma)}_{s\beta}(\Lambda)\theta\left(\frac{\Lambda^h-\Lambda}{2u}\right)\right], \quad (72)$$

where $g_{c,\sigma}(\Lambda^h)=\theta(\frac{\Lambda^h-\sigma\sin(Q)}{u})$, $g_{s,\sigma}(\Lambda^h)=-\theta(\frac{\Lambda^h-\sigma A}{2u})$ and the functions $r^{(\sigma)}_{\alpha\beta}$ fulfill the integral equations

$$r^{(\sigma)}_{\alpha\beta}(z_\alpha) = \sigma\rho_{\beta,0}(X^\beta)K_{\alpha\beta}(z_\alpha,\sigma X^\beta) + \hat{K}_{\alpha\gamma} * r^{(\sigma)}_{\gamma\beta}\big|_{z_\alpha}. \quad (73)$$

B. Relating $X^\alpha_\sigma - \sigma X^\alpha$ to quantum numbers

In the next step we want to express the deviations of the integration boundaries from their thermodynamic values through appropriate quantum numbers. We define $N_{c,s}$ by

$$n_c = \frac{N_c}{L} = \frac{I_+ - I_-}{L} = \int_{Q_-}^{Q_+} dk\rho_c(k),$$
$$n_s = \frac{N_s}{L} = \frac{J_+ - J_-}{L} = \int_{A_-}^{A_+} d\Lambda\rho_s(\Lambda). \quad (74)$$

We note that the number of down spins is $N_s - 1$ rather than N_s as we have one "deep" hole in the distribution of Λ's. The other quantities we want to use are

$$2D_c = I_+ + I_- = \frac{L}{2\pi}[z_c(Q_+) + z_c(Q_-)],$$

$$2D_s = J_+ + J_- = \frac{L}{2\pi}[z_s(A_+) + z_s(A_-)]. \tag{75}$$

Using the integral Eq. (47) for the counting functions $z_{c,s}$ we can rewrite these as

$$\frac{2D_s}{L} = 2d_s = \int_{-\infty}^{A_-} d\Lambda \rho_s(\Lambda) - \int_{A_+}^{\infty} d\Lambda \rho_s(\Lambda),$$

$$\frac{2D_c}{L} = 2d_c = \int_{-\pi}^{Q_-} dk \rho_c(k) - \int_{Q_+}^{\pi} dk \rho_c(k) - \frac{1}{\pi}\int_{A_-}^{A_+} d\Lambda\, \theta\left(\frac{\Lambda}{u}\right)\rho_s(\Lambda) + \frac{1}{\pi L}\theta\left(\frac{\Lambda^h}{u}\right). \tag{76}$$

We have to order $1/L$

$$n_\alpha = \int_{X_-^\alpha}^{X_+^\alpha} dz \rho_{\alpha,0}(z) + \frac{1}{L}\int_{-X^\alpha}^{X^\alpha} dz \rho_{\alpha,1}(z). \tag{77}$$

The second term no longer depends on X_σ^α and is denoted by

$$N_c^{\text{imp}} = \int_{-Q}^{Q} dk \rho_{c,1}(k),$$

$$N_s^{\text{imp}} = \int_{-A}^{A} dk \rho_{s,1}(\Lambda). \tag{78}$$

The variation of the integration boundaries X_σ^α with n_β is now easily calculated to leading order in L^{-1}

$$\frac{\partial X_\pm^\alpha}{\partial n_\beta} = \pm \frac{1}{2}\frac{Z_{\alpha\beta}^{-1}}{\rho_{\alpha,0}(X^\alpha)}. \tag{79}$$

Here the dressed charge matrix Z

$$Z = \begin{pmatrix} \xi_{cc}(Q) & \xi_{cs}(A) \\ \xi_{sc}(Q) & \xi_{ss}(A) \end{pmatrix}, \tag{80}$$

is given by $Z_{\alpha\beta}=\xi_{\alpha\beta}(X^\beta)$, where $\xi_{\alpha\beta}$ fulfill the set of coupled integral equations

$$\xi_{\alpha\beta}(z_\beta) = \delta_{\alpha\beta} + \xi_{\alpha\gamma} * \hat{K}_{\gamma\beta}|_{z_\beta}. \tag{81}$$

Similarly we have

$$2d_s = \int_{-\infty}^{A_-} d\Lambda \rho_{s,0}(\Lambda) - \int_{A_+}^{\infty} d\Lambda \rho_{s,0}(\Lambda) + \frac{2}{L}D_s^{\text{imp}},$$

$$2d_c = \int_{-\pi}^{Q_-} dk \rho_{c,0}(k) - \int_{Q_+}^{\pi} dk \rho_{c,0}(k) - \frac{1}{\pi}\int_{A_-}^{A_+} d\Lambda\, \theta\left(\frac{\Lambda}{u}\right)\rho_{s,0}(\Lambda) + \frac{2}{L}D_c^{\text{imp}}, \tag{82}$$

where

$$2D_s^{\text{imp}} = \int_{-\infty}^{-A} d\Lambda \rho_{s,1}(\Lambda) - \int_{A}^{\infty} d\Lambda \rho_{s,1}(\Lambda),$$

$$2D_c^{\text{imp}} = \int_{-\pi}^{-Q} dk \rho_{c,1}(k) - \int_{Q}^{\pi} dk \rho_{c,1}(k) - \frac{1}{\pi}\int_{-A}^{A} d\Lambda\, \theta\left(\frac{\Lambda}{u}\right)\rho_{s,1}(\Lambda) + \frac{1}{\pi}\theta\left(\frac{\Lambda^h}{u}\right). \tag{83}$$

These allows us calculate the dependence of the integration boundaries on d_α

$$\frac{\partial X_\pm^\alpha}{\partial d_\beta} = \frac{Z_{\beta\alpha}}{\rho_{\alpha,0}(X^\alpha)}. \tag{84}$$

Combining Eq. (79) with Eq. (84), we obtain the described relationship between the change in integration boundaries and the quantum numbers n_α, d_α

$$X_\pm^\alpha \mp X^\alpha = \pm \frac{1}{2}\frac{Z_{\alpha\beta}^{-1}}{\rho_{\alpha,0}(X^\alpha)}\left[\Delta n_\beta - \frac{1}{L}N_\beta^{\text{imp}}\right] + \frac{Z_{\alpha\beta}^T}{\rho_{\alpha,0}(X^\alpha)} \times\left[\Delta d_\beta - \frac{1}{L}D_\beta^{\text{imp}}\right]. \tag{85}$$

Here $\Delta n_{c,s}$ and $\Delta d_{c,s}$ are the changes in the quantum numbers [Eq. (74)], Eq. (76) compared to the ground state.

C. Result for the finite-size energy

Putting everything together we then arrive at

$$E = Le_{\text{GS}}(\{X^\alpha\}) - \epsilon_s(\Lambda^h) + \frac{1}{L}\Bigg\{-\frac{\pi}{6}(v_s + v_c) - \epsilon_s'(\Lambda^h)\delta\Lambda^h + 2\pi\left[\frac{\Delta\tilde{N}_\gamma}{4}(Z^T)^{-1}_{\gamma\alpha}v_\alpha Z^{-1}_{\alpha\beta}\Delta\tilde{N}_\beta + \tilde{D}_\gamma Z_{\gamma\alpha}v_\alpha Z^T_{\alpha\beta}\tilde{D}_\beta\right]\Bigg\}. \tag{86}$$

Here we have defined

$$\Delta\tilde{N}_\alpha = \Delta N_\alpha - N_\alpha^{\text{imp}},$$

$$\tilde{D}_\alpha = D_\alpha - D_\alpha^{\text{imp}}. \tag{87}$$

In writing Eq. (87) we have used that for the ground-state $D_\alpha=0$. The first term in Eq. (86) is the ground-state energy, the second term the excitation energy in the thermodynamic limit and the remaining contributions give the L^{-1} corrections. For our case, we have

$$N_c = I_+ - I_- = N_{\text{GS}} - 1, \quad N_s = J_+ - J_- = M_{\text{GS}},$$
$$D_c = \frac{I_+ + I_-}{2} = 0, \quad D_s = \frac{J_+ + J_-}{2} = 0. \tag{88}$$

For the ground state, we have

$$N_c = N_{\text{GS}}, \quad N_s = M_{\text{GS}}, \tag{89}$$

which gives

$$\Delta N_c = -1, \quad \Delta N_s = 0. \tag{90}$$

D. Relation of $N_\alpha^{\rm imp}$ to the spectrum

The quantities $N_\alpha^{\rm imp}$ are given in terms of the solutions to the coupled integral Eq. (59). It is possible to relate them to properties of the dispersions of the elementary excitations as follows. The integral equations for $\rho_{\alpha,1}$ are formally solved by

$$\rho_{\alpha,1} = (1-\hat{K})^{-1}_{\alpha\beta} * \rho^{(0)}_{\beta,1} = -(1-\hat{K})^{-1}_{\alpha\beta} * K_{\beta s}. \tag{91}$$

Substituting this into the equations for $N_\alpha^{\rm imp}$ we obtain

$$N_c^{\rm imp} = -\int_{-Q}^{Q} dk (1-\hat{K})^{-1}_{c\beta} * K_{\beta s} = -\int_{-Q}^{Q} dk (1-\hat{K})^{-1}_{cs}(k,\Lambda^h),$$

$$N_s^{\rm imp} = -\int_{-A}^{A} d\Lambda (1-\hat{K})^{-1}_{s\beta} * K_{\beta s}$$

$$= 1 - \int_{-A}^{A} d\Lambda (1-\hat{K})^{-1}_{ss}(\Lambda,\Lambda^h). \tag{92}$$

Here we have used e.g.

$$(1-\hat{K})^{-1}_{c\beta} * K_{\beta s} = (1-\hat{K})^{-1}_{c\beta} * (\hat{K}-1+1)_{\beta s} = (1-\hat{K})^{-1}_{cs}. \tag{93}$$

On the other hand, by differentiating the integral Eq. (19) for the dressed energies we obtain

$$\frac{\partial \epsilon_\alpha}{\partial \mu} = \frac{\partial \epsilon_\beta}{\partial \mu} * \hat{K}_{\beta\alpha} - \delta_{\alpha c}, \tag{94}$$

which are solved by

$$\frac{\partial \epsilon_\alpha}{\partial \mu} = -\int_{-Q}^{Q} dk (1-\hat{K})^{-1}_{c\alpha}(k,z_\alpha). \tag{95}$$

This gives us our first relation

$$N_c^{\rm imp} = \frac{\partial \epsilon_s(\Lambda^h)}{\partial \mu}. \tag{96}$$

By comparing Eq. (94) to Eq. (81) we observe that

$$\frac{\partial \epsilon_\alpha}{\partial \mu}(z_\alpha) = -\xi_{c\alpha}(z_\alpha), \tag{97}$$

which in conjunction with Eq. (96) allows us to relate $N_c^{\rm imp}$ to the dressed charge matrix as $N_c^{\rm imp} = -\xi_{cs}(\Lambda^h)$. This generalizes the analogous relation for the spin-1/2 *XXZ* chain found in Ref. 19. A second relation is obtained by considering

$$\frac{\partial \epsilon_\alpha}{\partial B} = \frac{\partial \epsilon_\beta}{\partial B} * \hat{K}_{\beta\alpha} + 2\delta_{\alpha s} - \delta_{\alpha c}. \tag{98}$$

Comparing this to Eq. (81) and using the linearity of the integral equation we observe that

$$\frac{\partial \epsilon_\alpha}{\partial B} = 2\xi_{s\alpha} - \xi_{c\alpha}. \tag{99}$$

The formal solution of Eq. (98) is

$$\frac{\partial \epsilon_\alpha}{\partial B} = \frac{\partial \epsilon_\alpha}{\partial \mu} + 2\int_{-A}^{A} d\Lambda (1-\hat{K})^{-1}_{s\alpha}. \tag{100}$$

Our second relation is then

$$N_s^{\rm imp} = 1 - \frac{1}{2}\left[\frac{\partial \epsilon_s(\Lambda^h)}{\partial B} - \frac{\partial \epsilon_s(\Lambda^h)}{\partial \mu}\right] = 1 - \xi_{ss}(\Lambda^h). \tag{101}$$

E. Simplification for zero magnetic field

In the absence of a magnetic field we have $A=\infty$ which allows us to simplify our results for the finite-size corrections to the energy Eq. (86). The dressed charge matrix takes the form[1]

$$Z = \begin{pmatrix} \xi & 0 \\ \frac{\xi}{2} & \frac{1}{\sqrt{2}} \end{pmatrix}, \tag{102}$$

where $\xi = \xi(Q)$ is obtained from the solution of the integral equation

$$\xi(k) = 1 + \int_{-Q}^{Q} dk' \cos(k') R(\sin(k) - \sin(k'))\xi(k'). \tag{103}$$

Here, the function $R(x)$ is

$$R(x) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{e^{i\omega x}}{1+\exp(2u|\omega|)}, \tag{104}$$

and can be expressed in terms of the Digamma function. The integral equations for the dressed energies and root densities simplify to[1]

$$\epsilon_c(k) = -2\cos(k) - \mu - 2u + \int_{-Q}^{Q} dk' \cos(k') R[\sin(k) - \sin(k')]\epsilon_c(k'),$$

$$\epsilon_s(\Lambda) = \int_{-Q}^{Q} dk \cos(k)\, s[\Lambda - \sin(k)]\epsilon_c(k),$$

$$\rho_c(k) = \frac{1}{2\pi} + \cos(k)\int_{-Q}^{Q} dk' R[\sin(k) - \sin(k')]\rho_c(k'),$$

$$\rho_s(\Lambda) = \int_{-Q}^{Q} dk\, s[\Lambda - \sin(k)]\rho_c(k), \tag{105}$$

where $s(x) = \frac{1}{4u\cosh(\frac{\pi x}{2u})}$. The finite-size energy can be expressed as

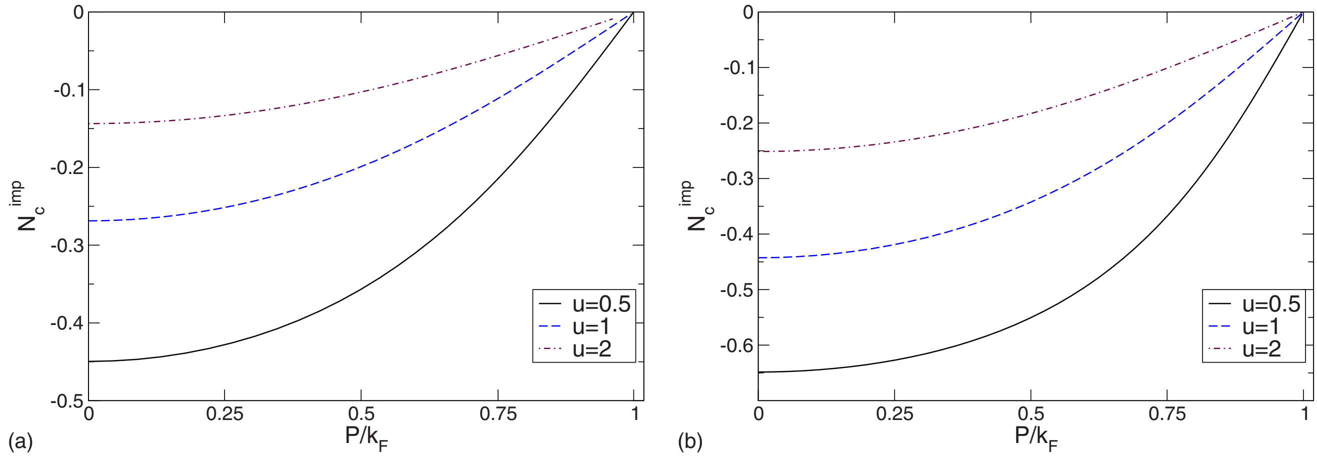

FIG. 6. (Color online) N_c^{imp} as a function of momentum for $u=0.5,1,2$ and densities (a) $n_c=0.2$ and (b) $n_c=0.5$.

$$E = Le_{\text{GS}}(\{X^\alpha\}) - \epsilon_s(\Lambda^h) - \frac{\pi}{6L}(v_s+v_c) - \frac{1}{L}\epsilon_s'(\Lambda^h)\delta\Lambda^h + \frac{2\pi v_c}{L}\left[\frac{(\Delta N_c - N_c^{\text{imp}})^2}{4\xi^2} + \xi^2\left(D_c - D_c^{\text{imp}} + \frac{D_s}{2}\right)^2\right] + \frac{2\pi v_s}{L}\left[\frac{1}{2}\left(\Delta N_s - \frac{\Delta N_c}{2} - \frac{1}{2}\right)^2 + \frac{D_s^2}{2}\right], \tag{106}$$

where

$$N_c^{\text{imp}} = 2N_s^{\text{imp}} - 1 = \int_{-Q}^{Q} dk\rho_{c,1}(k), \tag{107}$$

$$D_s^{\text{imp}} = 0, \tag{108}$$

$$2D_c^{\text{imp}} = \int_Q^\pi dk[\rho_{c,1}(-k) - \rho_{c,1}(k)] + \frac{1}{\pi}\theta\left[\tanh\left(\frac{\pi\Lambda^h}{4u}\right)\right] - \frac{1}{\pi}\int_{-Q}^{Q} dk\rho_{c,1}(k)i\ln\left[\frac{\Gamma\left(\frac{1}{2}+i\frac{\sin k}{4u}\right)}{\Gamma\left(\frac{1}{2}-i\frac{\sin k}{4u}\right)}\frac{\Gamma\left(1-i\frac{\sin k}{4u}\right)}{\Gamma\left(1+i\frac{\sin k}{4u}\right)}\right]. \tag{109}$$

Here $\rho_{c,1}$ is the solution to the integral equation

$$\rho_{c,1}(k) = -\frac{\cos(k)}{4u\cosh\left[\frac{\pi(\Lambda^h - \sin k)}{2u}\right]} + \cos(k)\int_{-Q}^{Q} dk' R(\sin k - \sin k')\rho_{c,1}(k'). \tag{110}$$

The fact that $D_s^{\text{imp}}=0$ is established in Appendix A. The relation Eq. (96) of N_c^{imp} to the dressed energy of spin excita-

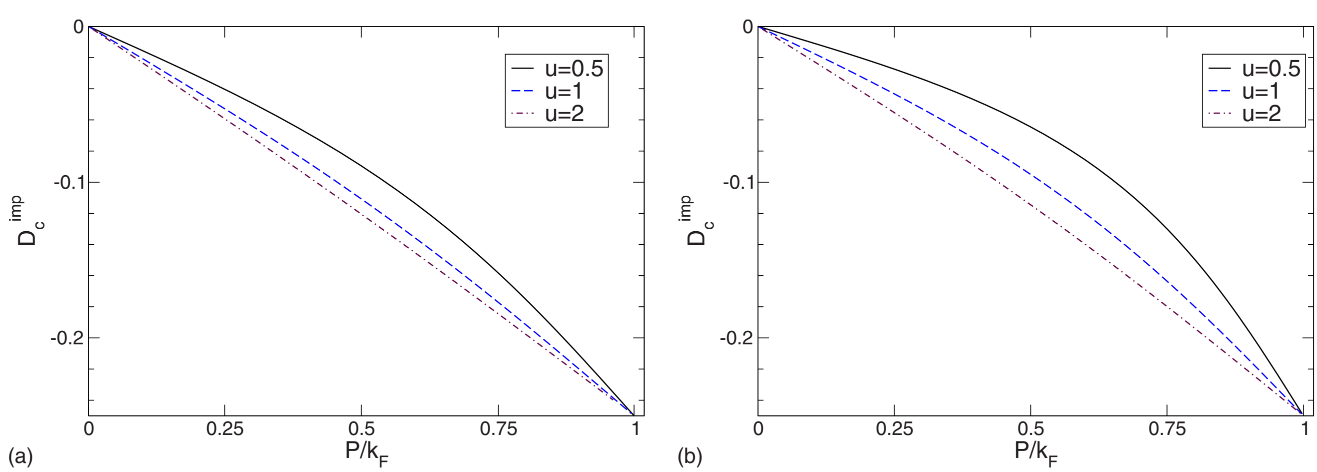

FIG. 7. (Color online) D_c^{imp} as a function of momentum for $u=0.5,1,2$ and densities (a) $n_c=0.2$ and (b) $n_c=0.5$.

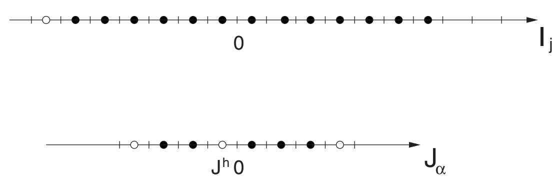

FIG. 8. Distribution of integers for the threshold of the holon–3 spinon excitation. The hole in the distribution of I_j is at $-(N_{GS}-1)/2$ and the three holes in the distribution of J_α occur at $\pm M_{GS}/2$ and J^h, respectively.

tions remains valid for zero magnetic field, i.e., we have that $N_c^{imp} = \frac{\partial \epsilon_s(\Lambda^h)}{\partial \mu}$. The quantum numbers ΔN_α, D_α for the holon-spinon excitation in zero magnetic field are

$$D_c = D_s = 0, \quad \Delta N_c = -1, \quad \Delta N_s = 0. \tag{111}$$

This shows that there are no L^{-1} corrections to the excitation energy in the spin sector. In terms of the field theory picture (see Sec. VI) of a deep hole interacting with the gapless Luttinger liquid degrees of freedom this shows that the interaction of the deep hole with the gapless spin sector is indeed irrelevant. Due to the presence of the marginally irrelevant interaction of spin currents we expect logarithmic corrections, but these are beyond the accuracy of our finite-size calculation.

Explicit values for the quantities N_c^{imp} and D_c^{imp} are readily obtained from a numerical solution of the linear integral Eq. (110). We present results for several values of u and two band fillings in Figs. 6 and 7.

Large-u limit

In the strong interaction limit $u \gg 1$ we can solve the integral Eq. (110) by iteration and obtain explicit results. To leading order we find

$$D_c^{imp} \approx \frac{p_s(\Lambda^h)}{2\pi n_c} = -\frac{P_{hs}}{4k_F}, \quad N_c^{imp} \approx -\frac{\sin(Q)}{2u\cosh(\pi\Lambda^h/2u)}. \tag{112}$$

V. THRESHOLD AT $k_F < P < 2k_F$ FOR THE HOLON–3 SPINON EXCITATION

We now want to determine the finite-size corrections to the energy of the holon–3 spinon excitation along the low-energy threshold in the momentum range $k_F < P < 2k_F$. The threshold of this excitation is described by the Bethe Ansatz Eqs. (7) with $N = N_{GS}-1$, $M = M_{GS}-2$ and half-odd integer numbers

$$I_j = -\frac{N_{GS}-1}{2} + j, \quad 1 \le j \le N_{GS}-1,$$

$$J_\alpha = \begin{cases} -\dfrac{M_{GS}}{2} + \alpha & \text{if } 1 \le \alpha < \dfrac{M_{GS}}{2} + J^h \\ -\dfrac{M_{GS}}{2} + \alpha + 1 & \text{if } \dfrac{M_{GS}}{2} + J^h \le \alpha \le M_{GS}-2 \end{cases}. \tag{113}$$

The corresponding distributions of half-odd integers are shown in Fig. 8.

The calculation on the finite-size corrections to the energy now proceeds just like for the holon-spinon excitation. The result is given by Eqs. (86), (87), (78), and (83) where now

$$N_c = I_+ - I_- = N_{GS} - 1, \quad N_s = J_+ - J_- = M_{GS} - 1,$$

$$D_c = \frac{I_+ + I_-}{2} = \frac{1}{2}, \quad D_s = \frac{J_+ + J_-}{2} = 0. \tag{114}$$

Recalling that in the ground state the $N_{c,s}$ quantum numbers are

$$N_c = N_{GS}, \quad N_s = M_{GS}, \tag{115}$$

we conclude that for the holon–3 spinon excitation we have

$$\Delta N_c = -1, \quad \Delta N_s = -1, \quad D_c = \frac{1}{2}, \quad D_s = 0. \tag{116}$$

The reduction in the zero-magnetic field case is completely analogous to the holon-spinon excitation. Hence, the energy is again given by Eqs. (106), (109), and (110), but the quantum numbers $N_{c,s}$, $D_{c,s}$ are now given by Eq. (116).

VI. FIELD THEORY

We now relate our results to the field theory treatment of Ref. 23 for the threshold singularity problem. There it was shown that a high-energy excitation in a spinful Luttinger liquid can be mapped to a mobile impurity in a Luttinger liquid. The corresponding Hamiltonian is $H = \Sigma_{\alpha=c,s} H_\alpha + H_d + H_{int}$, where

$$H_\alpha = \frac{v_\alpha}{2\pi}\int dx \left[\frac{1}{K_\alpha}\left(\frac{\partial \Phi_\alpha}{\partial x}\right)^2 + K_\alpha\left(\frac{\partial \Theta_\alpha}{\partial x}\right)^2\right],$$

$$H_d = \int dx d^\dagger(x)[\varepsilon_s(P) - iu\partial_x]d(x),$$

$$H_{int} = \int dx \left[\frac{V_R - V_L}{2\pi}\partial_x\Theta_c - \frac{V_R + V_L}{2\pi}\partial_x\Phi_c\right] d(x)d^\dagger(x). \tag{117}$$

Here the Bose fields Φ_α and the dual fields Θ_α fulfill the commutation relations (4), $d(x)$ and $d^\dagger$ are annihilation and creation operators of the mobile impurity, which carries momentum P and travels at velocity u. The parameters $V_{R,L}$ characterize the interaction of the impurity with the low-energy charge degrees of freedom. The parameters of $H_{c,s}$ and H_d in Eq. (117) are readily identified with quantities obtained from the Bethe Ansatz. The spin and charge velocities $v_{s,c}$ are given by Eq. (65) and the Luttinger parameters are

$$K_s = 1, \quad K_c = \frac{\xi^2}{2}, \tag{118}$$

where ξ is given by Eq. (103). The velocity of the impurity is expressed in terms of the solutions to the integral Eq. (105) as

$$u = \frac{\epsilon_s'(\Lambda^h)}{2\pi\rho_s(\Lambda^h)}. \tag{119}$$

The chemical potential of the impurity is $\epsilon_s(\Lambda^h)$, where the position Λ^h of the hole is fixed by the requirement

$$P_{hs}(\Lambda^h) = P. \tag{120}$$

The parameters $V_{R,L}$ entering the expression for $H_{\rm int}$ are determined as follows. Following Refs. 19 and 23, we remove the interaction term $H_{\rm int}$ through the unitary transformation on the fields

$$U = \exp\left\{ - i \int dx \left[\sqrt{K_c}\frac{\Delta\delta_{+,c} - \Delta\delta_{-,c}}{2\pi}\Theta_c(x) - \frac{\Delta\delta_{+,c} + \Delta\delta_{-,c}}{2\pi\sqrt{K_c}}\Phi_c(x) \right] d(x)d^\dagger(x) \right\}, \tag{121}$$

where

$$- (V_L \mp V_R)K_c^{\mp 1/2} = (v_c + u)\Delta\delta_{-,c} \pm (v_c - u)\Delta\delta_{+,c}. \tag{122}$$

In the resulting Hamiltonian, the impurity no longer interacts explicitly with the charge part of Luttinger liquid, but it does affect the boundary conditions of the charge boson. In particular we find that

$$\partial_x\hat{\Phi}_c = U^\dagger\partial_x\Phi_c U = \partial_x\Phi_c - \frac{\sqrt{K_c}}{2}(\Delta\delta_{+,c} - \Delta\delta_{-,c})dd^\dagger,$$

$$\partial_x\hat{\Theta}_c = U^\dagger\partial_x\Theta_c U = \partial_x\Theta_c + \frac{1}{2\sqrt{K_c}}(\Delta\delta_{+,c} + \Delta\delta_{-,c})dd^\dagger. \tag{123}$$

Taking the expectation value of Eq. (123) with respect to a state with a high-energy hole we find that

$$\int dx\langle\partial_x\Theta_c\rangle = \int dx\langle\partial_x\hat{\Theta}_c\rangle - \frac{1}{2\sqrt{K_c}}(\Delta\delta_{+,c} + \Delta\delta_{-,c}),$$

$$\int dx\langle\partial_x\Phi_c\rangle = \int dx\langle\partial_x\hat{\Phi}_c\rangle + \frac{\sqrt{K_c}}{2}(\Delta\delta_{+,c} - \Delta\delta_{-,c}). \tag{124}$$

Denoting by $\rho_{c,R}$ and $\rho_{c,L}$ the charge densities at the right and left Fermi wave numbers respectively we have that the numbers ΔN and D of low-energy charge and current excitations is

$$\Delta N = \int dx\sqrt{2}[\rho_{c,R} + \rho_{c,L}] = -\frac{\sqrt{2}}{\pi}\int dx\langle\partial_x\Phi_c\rangle,$$

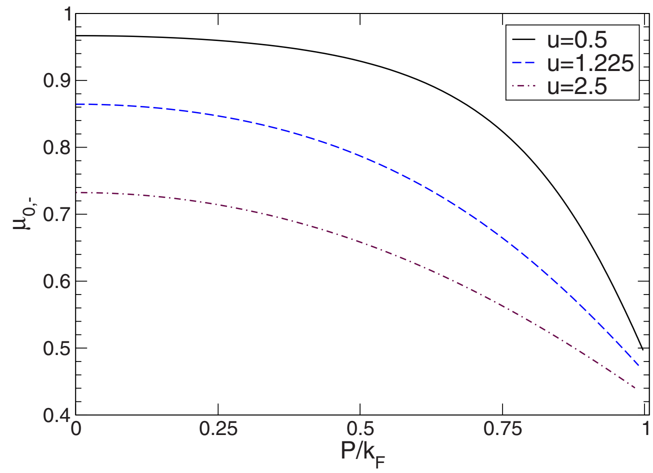

FIG. 9. (Color online) Threshold singularity exponent $\mu_{0,-}$ as a function of momentum for n_c=0.6.

$$4D = \sqrt{2}\int dx[\rho_{c,R} - \rho_{c,L}] = \frac{\sqrt{2}}{\pi}\int dx\langle\partial_x\Theta_c\rangle. \tag{125}$$

We are now in a position to identify the additional contributions in Eq. (124) that arise from the interaction of the Luttinger liquid with the mobile impurity with the quantities $N_c^{\rm imp}$ and $D_c^{\rm imp}$.

A. Holon-spinon excitation

Taking into account that for the holon-spinon excitation we have

$$-\frac{\sqrt{2}}{\pi}\int dx\langle\partial_x\Phi_c\rangle = -1, \quad \frac{\sqrt{2}}{\pi}\int dx\langle\partial_x\Theta_c\rangle = -1, \tag{126}$$

we conclude that the quantities $N_c^{\rm imp}$ and $2D_c^{\rm imp}$ are related to the phases $\Delta\delta_{\pm,c}$ by

$$N_c^{\rm imp} = -\sqrt{2K_c}\frac{\Delta\delta_{+,c} - \Delta\delta_{-,c}}{2\pi},$$

$$2D_c^{\rm imp} = \frac{1}{2} - \frac{1}{\sqrt{2K_c}}\frac{\Delta\delta_{+,c} + \Delta\delta_{-,c}}{2\pi}. \tag{127}$$

In Ref. 23 it was shown that in the momentum range $|P| < k_F$ the single particle spectral function exhibits a threshold singularity of the form

$$A(\omega,P) \propto [\omega - \epsilon_s(P)]^{-\mu_{0,-}}, \tag{128}$$

where the exponent is expressed in terms of the phase-shifts $\Delta\delta_{\pm,c}$ by

$$\mu_{0,-} = 1 - \frac{1}{2}\left[- \sqrt{\frac{K_c}{2}} + \frac{\Delta\delta_{+,c} + \Delta\delta_{-,c}}{2\pi}\right]^2 - \frac{1}{2}\left[\frac{1}{\sqrt{2K_c}} - \frac{\Delta\delta_{+,c} - \Delta\delta_{-,c}}{2\pi}\right]^2 = 1 - K_c(2D_c^{\rm imp})^2 - \frac{1}{4K_c}(1 + N_c^{\rm imp})^2. \tag{129}$$

We note that Eq. (129) differs from the Luttinger liquid result[6,8]

$$\mu_{LL} = 1 - \frac{K_c}{4} - \frac{1}{4K_c}. \tag{130}$$

However, in the zero energy limit $P \to k_F$ the Luttinger liquid result is recovered. Explicit results for $\mu_{0,-}$ are obtained by solving the integral Eq. (110) numerically. In Fig. 9 we present results for density $n_c=0.6$ and three different values of u.

1. Large-u limit

For $u \gg 1$ we have $K_c \approx \frac{1}{2}$ and using Eq. (112) we find

$$\mu_{0,-} \approx \frac{1}{2} - \frac{1}{8}\left[\frac{P}{k_F}\right]^2. \tag{131}$$

This suggests that the singularity is only weakly momentum dependent and is close to a square root. The result Eq. (131) agrees with the exponent computed by exploiting the factorization of the wave function into spin and charge parts.[27–29]

2. Comparison to DMRG results

In Ref. 4 the single particle spectral function for parameter values $u=1.225$ and $n_c=0.6$ was computed by the dynamical density matrix renormalization group method.[5] The following two exponents were reported based on a scaling analysis of the low-energy peak heights

$$\mu_{0,-} \approx 0.86 \ \text{for}\ P=0, \quad \mu_{0,-} \approx 0.78 \ \text{for}\ P=\frac{\pi}{10}. \tag{132}$$

The Luttinger liquid parameter and Luttinger liquid threshold exponent are $K_c=0.6851$ and $\mu_{LL}=0.4638$, respectively. Our results are

$$\mu_{0,-} \approx 0.864 \ \text{for}\ P=0, \quad \mu_{0,-} \approx 0.832 \ \text{for}\ P=\frac{\pi}{10}. \tag{133}$$

The agreement for $P=0$ is excellent, but the $P=\frac{\pi}{10}$ values are very different. One possible explanation for this discrepancy is as follows. The frequency range over which the power-law Eq. (129) holds can *a priori* be quite small and furthermore is expected to narrow as P increases from zero to k_F. Extracting the threshold exponent from the scaling of the peak height could then require very small values of the parameter η in Ref. 4.

B. Holon–3 spinon excitation

The threshold of the holon–3 spinon excitation can also be analyzed in terms of a mobile impurity field theory model.[13,23] The threshold behavior in the range $k_F < P < 3k_F$ is no longer singular but describes a power law shoulder. The exponent can be expressed in terms of the quantities D_c^{imp}, N_c^{imp} derived above.

VII. ELECTRON GAS

The analysis for the electron gas[30] is completely analogous to the one for the Hubbard model. The Hamiltonian is

$$H = -\sum_{j=1}^{N} \frac{\partial^2}{\partial x_j^2} + 4u\sum_{i<j} \delta(x_i - x_j) - \mu N + B(2M - N). \tag{134}$$

The Bethe Ansatz equations read[30,31]

$$k_j L = 2\pi I_j - \sum_{\alpha=1}^{M} \theta\left(\frac{k_j - \Lambda_\alpha}{u}\right), \quad j=1,\ldots,N, \tag{135}$$

$$\sum_{j=1}^{N} \theta\left(\frac{\Lambda_\alpha - k_j}{u}\right) = 2\pi J_\alpha + \sum_{\beta=1}^{M} \theta\left(\frac{\Lambda_\alpha - \Lambda_\beta}{2u}\right), \quad \alpha=1,\ldots,M. \tag{136}$$

For the ground state and the excitations we are interested in we only need to consider real roots of Eqs. (135) and (136). For these the "quantum numbers" I_j, J_α fulfill the restrictions

$$I_j \ \text{is} \begin{cases} \text{integer} & \text{if } M \text{ is even} \\ \text{half-odd integer} & \text{if } M \text{ is odd,} \end{cases} \tag{137}$$

$$J_\alpha \ \text{is} \begin{cases} \text{integer} & \text{if } N-M \text{ is odd} \\ \text{half-odd integer} & \text{if } N-M \text{ is even,} \end{cases} \tag{138}$$

The energy and momentum of such Bethe ansatz states are

$$E = 2BM + \sum_{j=1}^{N} [k_j^2 - \mu - B],$$

$$P = \sum_{j=1}^{N} k_j \equiv \frac{2\pi}{L}\left[\sum_{j=1}^{N} I_j + \sum_{\alpha=1}^{M} J_\alpha\right]. \tag{139}$$

A. Ground state and excitations in the thermodynamic limit

In the thermodynamic limit the ground state is described by the solution of the integral equations

$$\rho_{c,0}(k) = \frac{1}{2\pi} + \int_{-A}^{A} d\Lambda \mathcal{K}_{cs}(k-\Lambda)\rho_{s,0}(\Lambda),$$

$$\rho_{s,0}(\Lambda) = \int_{-Q}^{Q} dk K_{sc}(\Lambda - k)\rho_{c,0}(k) + \int_{-A}^{A} d\Lambda' \mathcal{K}_{ss}(\Lambda-\Lambda')\rho_{s,0}(\Lambda'), \tag{140}$$

where we have defined integral kernels as

$$\mathcal{K}_{cc}(k,k') = 0, \quad \mathcal{K}_{cs}(k,\Lambda) = a_1(k-\Lambda),$$

$$\mathcal{K}_{sc}(\Lambda,k) = a_1(k-\Lambda), \quad \mathcal{K}_{ss}(\Lambda,\Lambda') = -a_2(\Lambda-\Lambda'). \tag{141}$$

Density and magnetization per site are given by n_c and $\frac{n_c}{2} - n_s$, respectively, where

$$n_c = \int_{-Q}^{Q} dk \rho_{c,0}(k), \quad n_s = \int_{-A}^{A} d\Lambda \rho_{s,0}(\Lambda). \tag{142}$$

The dressed energies of elementary charge and spin excitations in the thermodynamic limit at finite density and magnetization are given in terms of the solutions to the coupled integral equations

$$\epsilon_c(k) = k^2 - \mu - B + \int_{-A}^{A} d\Lambda \mathcal{K}_{cs}(k-\Lambda)\epsilon_s(\Lambda),$$

$$\epsilon_s(\Lambda) = 2B + \int_{-Q}^{Q} dk \mathcal{K}_{sc}(\Lambda - k)\epsilon_c(k) + \int_{-A}^{A} d\Lambda' \mathcal{K}_{ss}(\Lambda-\Lambda')\epsilon_s(\Lambda'), \tag{143}$$

where the integration boundaries are fixed by the requirements

$$\epsilon_c(\pm Q) = 0, \quad \epsilon_s(\pm A) = 0. \tag{144}$$

The holon-spinon excitation is constructed in complete analogy with the Hubbard model. In the thermodynamic limit its energy and momentum are expressed as

$$E_{hs} = -\epsilon_c(k^h) - \epsilon_s(\Lambda^h), \quad P_{hs} = -p_c(k^h) - p_s(\Lambda^h) \pm \pi n_c. \tag{145}$$

B. Finite-size corrections for threshold excitations at $|P_{hs}| < k_F$

Following through the same steps as for the Hubbard model we obtain

$$E = L e_{\rm GS}(\{X^\alpha\}) - \epsilon_s(\Lambda^h) - \frac{\pi}{6L}(v_s + v_c) + \frac{2\pi}{L}\left[\frac{1}{4}\Delta\tilde{N}_\gamma (Z^T)^{-1}_{\gamma\alpha} v_\alpha Z^{-1}_{\alpha\beta}\Delta\tilde{N}_\beta + \tilde{D}_\gamma Z_{\gamma\alpha} v_\alpha Z^T_{\alpha\beta}\tilde{D}_\beta\right] - \frac{1}{L}\epsilon_s'(\Lambda^h)\delta\Lambda^h + o(L^{-1}). \tag{146}$$

Here $e_{\rm GS}(\{X^\alpha\})$ is the ground-state energy per site in the thermodynamic limit (and we again use notations where $X_c = Q$ and $X_s = A$), $-\epsilon_s(\Lambda^h)$ is the $\mathcal{O}(1)$ contribution of the spinon excitation in the thermodynamic limit and v_s and v_c are the velocities of the gapless elementary spin and charge excitations. They are given in terms of the solutions of the integral Eqs. (140) and (143) by

$$v_c = \frac{\epsilon_c'(Q)}{2\pi\rho_{c,0}(Q)}, \quad v_s = \frac{\epsilon_s'(A)}{2\pi\rho_{s,0}(A)}. \tag{147}$$

The dressed charge matrix Z in Eq. (146) is defined as

$$\mathbf{Z} = \begin{bmatrix} \xi_{cc}(Q) & \xi_{cs}(A) \\ \xi_{sc}(Q) & \xi_{ss}(A) \end{bmatrix}, \tag{148}$$

where $\xi_{\alpha\beta}$ fulfill the set of coupled integral equations

$$\xi_{\alpha\beta}(z_\beta) = \delta_{\alpha\beta} + \sum_{\gamma=c,s}\int_{-X_\gamma}^{X_\gamma} dz_\gamma \xi_{\alpha\gamma}(z_\gamma)\mathcal{K}_{\gamma\beta}(z_\gamma - z_\beta). \tag{149}$$

The quantities $\Delta\tilde{N}_\alpha$ and $\tilde{D}_\alpha$ are defined as in the case of the Hubbard model

$$\Delta\tilde{N}_\alpha = \Delta N_\alpha - N_\alpha^{\rm imp}, \quad \tilde{D}_\alpha = D_\alpha - D_\alpha^{\rm imp}, \tag{150}$$

where now

$$N_c^{\rm imp} = \int_{-Q}^{Q} dk \rho_{c,1}(k), \quad N_s^{\rm imp} = \int_{-A}^{A} d\Lambda \rho_{s,1}(\Lambda), \tag{151}$$

$$2D_c^{\rm imp} = \int_{-\infty}^{-Q} - \int_{Q}^{\infty} dk \rho_{c,1}(k),$$

$$2D_s^{\rm imp} = \int_{-\infty}^{-A} - \int_{A}^{\infty} d\Lambda \rho_{s,1}(\Lambda). \tag{152}$$

Note that these are different from what we had for the Hubbard model. The root densities $\rho_{c,1}$ and $\rho_{s,1}$ fulfill the coupled integral equations

$$\rho_{c,1}(k) = -a_1(k - \Lambda^h) + \int_{-A}^{A} d\Lambda \mathcal{K}_{cs}(k-\Lambda)\rho_{s,1}(\Lambda), \tag{153}$$

$$\rho_{s,1}(\Lambda) = a_2(\Lambda - \Lambda^h) + \int_{-Q}^{Q} dk \mathcal{K}_{sc}(\Lambda - k)\rho_{c,1}(k) + \int_{-A}^{A} d\Lambda' \mathcal{K}_{ss}(\Lambda - \Lambda')\rho_{s,1}(\Lambda'). \tag{154}$$

Finally, $\epsilon_s'(\Lambda)$ is the derivative of the dressed energy Eq. (143) and $\delta\Lambda^h/L$ is the shift in the hole rapidity due to the finite volume quantization conditions. It is obtained from a set of equations completely analogous to Eqs. (71)–(73).

C. Simplification for zero magnetic field

In the absence of a magnetic field we have $A = \infty$, which again allows us to simplify all expressions. The integral equations for the dressed energies can be written in the form

$$\epsilon_c(k) = k^2 - \mu + \int_{-Q}^{Q} dk' R(k' - k)\epsilon_c(k'),$$

$$\epsilon_s(\Lambda) = \int_{-Q}^{Q} dk\, s(\Lambda - k)\epsilon_c(k), \tag{155}$$

where the integration boundary Q is fixed as a function of the chemical potential μ by the requirement $\epsilon_c(\pm Q) = 0$. The dressed charge matrix takes the form Eq. (102), where $\xi = \xi(Q)$ is obtained from the integral equation

$$\xi(k) = 1 + \int_{-Q}^{Q} dk' R(k-k')\xi(k'). \qquad (156)$$

The expression for the finite-size energy simplifies to

$$E = Le_{GS}[(X^\alpha)] - \epsilon_s(\Lambda^h) - \frac{\pi}{6L}(v_s + v_c) - \frac{1}{L}\epsilon_s'(\Lambda^h)\delta\Lambda^h + \frac{2\pi v_c}{L}\left[\frac{(\Delta N_c - N_c^{imp})^2}{4\xi^2} + \xi^2\left(D_c - D_c^{imp} + \frac{D_s}{2}\right)^2\right] + \frac{2\pi v_s}{L}\left[\frac{\left(\Delta N_s - \frac{1}{2}\Delta N_c - \frac{1}{2}\right)^2}{2} + \frac{D_s^2}{2}\right] + o(L^{-1}). \qquad (157)$$

The expressions for N_α^{imp} and D_α^{imp} become

$$N_c^{imp} = 2N_s^{imp} - 1 = \int_{-Q}^{Q} dk \rho_{c,1}(k), \qquad (158)$$

$$2D_c^{imp} = \int_{Q}^{\infty} dk[\rho_{c,1}(-k) - \rho_{c,1}(k)], \quad D_s^{imp} = 0, \qquad (159)$$

where $\rho_{c,1}$ is the solution to the integral equation

$$\rho_{c,1}(k) = -\frac{1}{4u\cosh\left[\frac{\pi(\Lambda^h - k)}{2u}\right]} + \int_{-Q}^{Q} dk' R(k-k')\rho_{c,1}(k'). \qquad (160)$$

Here $R(x)$ is given by Eq. (104). We note that our expression for N_c^{imp} is related to the dressed energies Eq. (143) by

$$N_c^{imp} = \frac{\partial \epsilon_s(\Lambda^h)}{\partial \mu}. \qquad (161)$$

For the holon-spinon excitation we have

$$\Delta N_c = N_c - N_{GS} = (N_{GS} - 1) - N_{GS} = -1,$$

$$\Delta N_s = N_s - \frac{N_{GS}}{2} = 0. \qquad (162)$$

Like for the Hubbard model the corrections in the low-energy spin sector vanish, which in terms of the field theory description implies that the interaction of the high-energy spinon with the low-energy spin sector is irrelevant.

D. Threshold exponent

As for the Hubbard model the spectral function exhibits a threshold singularity of the form

$$A(\omega,P) \propto [\omega - \epsilon_s(P)]^{-\mu_{0,-}}, \qquad (163)$$

where the exponent $\mu_{0,-}$ is expressed both in terms of the phase-shifts $\delta_{\pm,c}$ arising in the field theory treatment Eq. (121) and in terms of the quantities N_c^{imp}, D_c^{imp} in Eq. (159)

$$\mu_{0,-} = 1 - \frac{1}{2}\left[-\sqrt{\frac{K_c}{2}} + \frac{\delta_{+,c} + \delta_{-,c}}{2\pi}\right]^2 - \frac{1}{2}\left[\frac{1}{\sqrt{2K_c}} - \frac{\delta_{+,c} - \delta_{-,c}}{2\pi}\right]^2 = 1 - K_c(2D_c^{imp})^2 - \frac{1}{4K_c}(1 + N_c^{imp})^2. \qquad (164)$$

In Ref. 23 the phase-shifts $\delta_{\pm,c}$ were expressed in terms of properties of the excitation spectrum. We have verified the relations given there by numerically solving the relevant integral equations for the Yang-Gaudin model.

VIII. SUMMARY AND CONCLUSIONS

In this work, we have determined the $\mathcal{O}(L^{-1})$ corrections to energies of excited states in the Hubbard and Yang-Gaudin models for the case where in addition to any finite number of low-energy excitations, high-energy excitations are present as well. This extends the work of Woynarovich,[8] which considered exclusively low-lying excited states. We have focused on the case of a single high-energy holon or spinon, but the method is easily extended to other cases. There are several contributions to the $\mathcal{O}(L^{-1})$ energy corrections. One of these arises from the quantization of the momentum for the high-energy particle in the finite volume. More interestingly, we find that the presence of a high-energy particle leads to a modification of the low-energy part of the spectrum. This effect can be understood by a mapping to a model of a mobile impurity coupled to the spin-charge separated Luttinger liquid that describes the low-energy degrees of freedom.[23] By matching the finite-size spectrum of the mobile impurity model to the one obtained from the exact solution, we have obtained explicit results for threshold singularities in the spectral function $A(\omega,q)$. In the momentum range $|P|<k_F$ the negative frequency part exhibits a singularity at $\omega=\epsilon_s(P)$ of the form

$$A(\omega,P) \propto [\omega - \epsilon_s(P)]^{-\mu_{0,-}}, \qquad (165)$$

while the positive frequency part vanishes in a characteristic power-law fashion above $\omega=-\epsilon_s(P)$ as

$$A(\omega,P) \propto [\omega + \epsilon_s(P)]^{1-\mu_{0,-}}. \qquad (166)$$

Expression (129) for $\mu_{0,-}$ is the main result of this work. The resulting spectral function is depicted in Fig. 2.

There have been a number of previous studies of the single-particle spectral function of the one dimensional Hubbard model below half-filling. Ref. 4 reports dynamical density matrix renormalization group results for density $n_c=0.6$ and $U/t=4.9$. We found that the threshold exponent Eq. (129) is only in partial agreement with Ref. 4. A possible explanation is that smaller values for the imaginary part of the energy are required in the DMRG computation in order to extract the singularity reliably. It would be interesting to test this conjecture. In the large-u limit the single-particle spectral function has been computed[27] by exploiting the factorization of the wave function into spin and charge parts.[28] The behavior obtained by this method was reported in Ref. 29 and agrees with Eq. (131). Finally, singularity exponents obtained by completely different methods have been reported in Ref. 29. We have checked that the numerical results for the exponent $\mu_{0,-}$ in the range $|P|<k_F$, density $n_c=0.59$ and several values of $u(u=0.25,1.225,2.5)$ are in agreement with ours. It would be interesting to demonstrate the equivalence of the expressions for the exponents of Ref. 29 and our results analytically.

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APPENDIX A: ZERO-FIELD LIMIT

In this appendix we consider the zero-magnetic field limit for the quantity D_s^{imp} Eq. (83). By definition we have

$$D_s^{\mathrm{imp}}=\int_A^\infty d\Lambda[\rho_{s,1}(-\Lambda)-\rho_{s,1}(\Lambda)]=-\int_0^\infty d\Lambda f(\Lambda), \tag{A1}$$

where

$$f(\Lambda)=\rho_{s,1}(\Lambda+A)-\rho_{s,1}(-\Lambda-A). \tag{A2}$$

After Fourier transforming the integral equation for $\rho_{s,1}$ we obtain the following set of equations for $f(\Lambda)$ and $\rho_{c,-}(k)=\rho_{c,1}(k)-\rho_{c,1}(-k)$

$$\begin{aligned}f(\Lambda)=&-R(\Lambda+A+\Lambda^h)+R(\Lambda+A-\Lambda^h)\\&+\int_{-Q}^{Q}dk s(\Lambda+A-\sin k)\rho_{c,-}(k)+\int_0^\infty d\Lambda'[R(\Lambda-\Lambda')\\&-R(\Lambda+\Lambda'+2A)]f(\Lambda'),\end{aligned} \tag{A3}$$

$$\begin{aligned}\rho_{c,-}(k)=&-\cos(k)[s(\Lambda^h-\sin k)-s(\Lambda^h+\sin k)]\\&+\cos(k)\int_{-Q}^{Q}dk' R(\sin k-\sin k')\rho_{c,-}(k')\\&-\cos(k)\int_0^\infty d\Lambda[s(\Lambda+A-\sin k)\\&-s(\Lambda+A+\sin k)]f(\Lambda).\end{aligned} \tag{A4}$$

We now observe that for large A and $|\Lambda^h|\ll\Lambda+A$ the driving term in Eq. (A3) is small

$$R(\Lambda+A+\Lambda^h)-R(\Lambda+A-\Lambda^h)\approx-\frac{2u}{\pi}\frac{\Lambda^h}{(\Lambda+A)^3}. \tag{A5}$$

Iterating the integral equations in this limit then shows that D_s^{imp} vanishes when A tends to ∞.

APPENDIX B: FINITE-SIZE CORRECTIONS FOR A HIGH-ENERGY HOLON EXCITATION

Our starting point are the Bethe ansatz Eqs. (7) for the holon-spinon excitation where the spinon sits at the Fermi momentum of the Λ_α's. The hole in the distribution of k_j's is denoted by k^h and the corresponding integer in the logarithmic form of the Bethe Ansatz Eq. (7) by I^h. Expressing the Bethe Ansatz equations in terms of counting functions (41) we have

$$z_c(k_j)=\frac{2\pi I_j}{L},\quad z_s(\Lambda_\alpha)=\frac{2\pi J_\alpha}{L}, \tag{B1}$$

where the integers I_j and J_α are given by

$$J_\alpha=-\frac{M_{\mathrm{GS}}}{2}+\frac{1}{2}+\alpha,\quad \alpha=1,\ldots,M_{\mathrm{GS}}-1,$$

$$I_j=\begin{cases}-\frac{N_{\mathrm{GS}}}{2}+j & \text{if } 1\le j<\frac{N_{\mathrm{GS}}}{2}+I^h\\ -\frac{N_{\mathrm{GS}}}{2}+j+1 & \text{if } \frac{N_{\mathrm{GS}}}{2}+I^h\le j<N_{\mathrm{GS}}\end{cases}. \tag{B2}$$

1. Finite-size corrections

As before we turn these into integral equations by means of the Euler-Maclaurin sum formula (43). This results in

$$\begin{aligned}z_c(k)=&k+\int_{A_-}^{A_+}d\Lambda\rho_s(\Lambda)\theta\left(\frac{\sin k-\Lambda}{u}\right)\\&+\frac{1}{24L^2}\left[\frac{a_1(\sin k-A_+)}{\rho_s(A_+)}-\frac{a_1(\sin k-A_-)}{\rho_s(A_-)}\right]+o(L^{-2}),\end{aligned} \tag{B3}$$

$$\begin{aligned}z_s(\Lambda)=&\int_{Q_-}^{Q_+}dk\theta\left(\frac{\Lambda-\sin k}{u}\right)\rho_c(k)-\frac{1}{L}\theta\left(\frac{\Lambda-\sin(k_L^h)}{u}\right)\\&-\int_{A_-}^{A_+}d\Lambda'\rho_s(\Lambda')\theta\left(\frac{\Lambda-\Lambda'}{2u}\right)\\&+\frac{1}{24L^2}\left[\frac{a_1(\Lambda-\sin Q_+)\cos Q_+}{\rho_c(Q_+)}\right.\\&\left.-\frac{a_1(\Lambda-\sin Q_-)\cos Q_-}{\rho_c(Q_-)}-\frac{a_2(\Lambda-A_+)}{\rho_s(A_+)}+\frac{a_2(\Lambda-A_-)}{\rho_s(A_-)}\right]\\&+o(L^{-2}),\end{aligned} \tag{B4}$$

where $a_n(x)$ is given in Eq. (17), the root densities $\rho_{c,s}$ are given in terms of the counting functions by Eq. (49), and the integration boundaries are fixed by

$$z_c(Q_\pm)=\frac{2\pi I_\pm}{L},\quad z_s(A_\pm)=\frac{2\pi J_\pm}{L}. \tag{B5}$$

Here

$$I_\pm=\pm\frac{N_{\mathrm{GS}}}{2}+\frac{1}{2},\quad J_+=\frac{M_{\mathrm{GS}}}{2},\quad J_-=-\frac{M_{\mathrm{GS}}}{2}+1. \tag{B6}$$

The equation fixing the position of the hole is

$$z_c(k_L^h) = \frac{2\pi I^h}{L} = \text{fixed}. \tag{B7}$$

Here our notation makes the L-dependence of the rapidity of the hole explicit. Following through the same steps as in Sec. IV, we find that the finite-size energy is expressed as

$$E = Le_{\rm GS}(\{X^\alpha\}) - \epsilon_c(k^h) + \frac{1}{L}\Bigg\{ -\frac{\pi}{6}(v_s+v_c) + 2\pi\left[\frac{1}{4}\Delta\tilde{N}_\gamma (Z^T)^{-1}_{\gamma\alpha} v_\alpha Z^{-1}_{\alpha\beta}\Delta\tilde{N}_\beta + \tilde{D}_\gamma Z_{\gamma\alpha} v_\alpha Z^T_{\alpha\beta}\tilde{D}_\beta\right] - \epsilon_c'(k^h)\,\delta k^h\Bigg\}, \tag{B8}$$

where $e_{\rm GS}(\{X^\alpha\})$ and $-\epsilon_c(k^h)$ are, respectively, the ground state energy per site and the dressed energy of the holon in the thermodynamic limit, $Z_{\alpha\beta}$ are the elements of the dressed charge matrix Eq. (80) and $\Delta\tilde{N}_\alpha$, $\Delta\tilde{D}_\alpha$ are defined by Eq. (87), where

$$N_c^{\rm imp} = \int_{-Q}^{Q} dk \rho_{c,1}(k), \quad N_s^{\rm imp} = \int_{-A}^{A} dk \rho_{s,1}(\Lambda),$$

$$2D_s^{\rm imp} = \int_{-\infty}^{-A} d\Lambda \rho_{s,1}(\Lambda) - \int_{A}^{\infty} d\Lambda \rho_{s,1}(\Lambda),$$

$$2D_c^{\rm imp} = \int_{-\pi}^{-Q} dk \rho_{c,1}(k) - \int_{Q}^{\pi} dk \rho_{c,1}(k) - \frac{1}{\pi}\int_{-A}^{A} d\Lambda\, \theta\!\left(\frac{\Lambda}{u}\right)\rho_{s,1}(\Lambda). \tag{B9}$$

Here, the root densities $\rho_{\alpha,1}$ fulfill the coupled integral equations

$$\rho_{c,1}(k) = \cos(k)\int_{-A}^{A} d\Lambda a_1[\Lambda - \sin(k)]\rho_{s,1}(\Lambda),$$

$$\rho_{s,1}(k) = -a_1[\Lambda - \sin(k^h)] + \int_{-Q}^{Q} dk a_1(\Lambda - \sin k)\rho_{c,1}(k) - \int_{-A}^{A} d\Lambda' a_2(\Lambda - \Lambda')\rho_{s,1}(\Lambda'). \tag{B10}$$

The quantum numbers D_α, ΔN_α are

$$D_c = D_s = \frac{1}{2}, \quad \Delta N_c = 0, \quad \Delta N_s = -1. \tag{B11}$$

Like for the spinon threshold it is possible to express $N_{c,s}^{\rm imp}$ in terms of the dressed energies. We find that

$$N_c^{\rm imp} = 1 + \frac{\partial \epsilon_c(k^h)}{\partial \mu}, \quad N_s^{\rm imp} = -\frac{1}{2}\left[\frac{\partial \epsilon_c(k^h)}{\partial B} - \frac{\partial \epsilon_c(k^h)}{\partial \mu}\right]. \tag{B12}$$

2. Simplification for zero magnetic field

In zero-magnetic field the expression for the energy simplifies to

$$E = Le_{\rm GS}(\{X^\alpha\}) - \epsilon_c(k^h) - \frac{\pi}{6L}(v_s+v_c) - \frac{1}{L}\epsilon_c'(k^h)\,\delta k^h + \frac{2\pi v_c}{L}\left[\frac{(\Delta N_c - N_c^{\rm imp})^2}{4\xi^2} + \xi^2\left(D_c - D_c^{\rm imp} + \frac{D_s}{2}\right)^2\right] + \frac{2\pi v_s}{L}\left[\frac{\left(\Delta N_s - \frac{\Delta N_c}{2} - \frac{1}{2}\right)^2}{2} + \frac{D_s^2}{2}\right], \tag{B13}$$

where

$$N_c^{\rm imp} = 2N_s^{\rm imp} + 1 = \int_{-Q}^{Q} dk \rho_{c,1}(k), \quad D_s^{\rm imp} = 0, \tag{B14}$$

$$2D_c^{\rm imp} = \int_{Q}^{\pi} dk[\rho_{c,1}(-k) - \rho_{c,1}(k)] - \frac{1}{\pi}\int_{-Q}^{Q} dk[\rho_{c,1}(k) - \delta(k-k^h)] \times i\ln\left[\frac{\Gamma\left(\frac{1}{2} + i\frac{\sin k}{4u}\right)\Gamma\left(1 - i\frac{\sin k}{4u}\right)}{\Gamma\left(\frac{1}{2} - i\frac{\sin k}{4u}\right)\Gamma\left(1 + i\frac{\sin k}{4u}\right)}\right]. \tag{B15}$$

Here, $\rho_{c,1}$ is the solution to the integral equation

$$\rho_{c,1}(k) = -\cos(k)R[\sin(k) - \sin(k^h)] + \cos(k)\int_{-Q}^{Q} dk' R(\sin k - \sin k')\rho_{c,1}(k'). \tag{B16}$$

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