

Haldane charge conjecture in one-dimensional multicomponent fermionic cold atoms

H. Nonne,¹ P. Lecheminant,¹ S. Capponi,² G. Roux,³ and E. Boulat⁴

¹Laboratoire de Physique Théorique et Modélisation, CNRS UMR 8089, Université de Cergy-Pontoise, Site de Saint-Martin, F-95300 Cergy-Pontoise Cedex, France

²Laboratoire de Physique Théorique, CNRS UMR 5152, Université Paul Sabatier, F-31062 Toulouse, France

³Laboratoire de Physique Théorique et Modèles Statistiques, Université Paris-Sud, CNRS UMR 8626, 91405 Orsay, France

⁴Laboratoire Matériaux et Phénomènes Quantiques, CNRS UMR 7162, Université Paris Diderot, 75013 Paris, France

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A Haldane conjecture is revealed for spin-singlet charge modes in $2N$ -component fermionic cold atoms loaded into a one-dimensional optical lattice. By means of a low-energy approach and density matrix renormalization group calculations, we show the emergence of gapless and gapped phases depending on the parity of N for attractive interactions at half-filling. The analog of the Haldane phase of the spin-1 Heisenberg chain is stabilized for $N=2$ with nonlocal string charge correlation and pseudo-spin-1/2 edge states. At the heart of this even-odd behavior is the existence of a spin-singlet pseudo-spin- $N/2$ operator which governs the low-energy properties of the model for attractive interactions and gives rise to the Haldane physics.

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I. INTRODUCTION

One of the major advances in the understanding of low-dimensional strongly correlated systems has been the so-called Haldane conjecture. In 1983, Haldane argued that the spin- S Heisenberg chain displays striking different properties depending on the parity of $2S$.¹ While half-integer Heisenberg spin chains have a gapless behavior, a finite gap from the singlet ground state to the first triplet excited states is found when $2S$ is even. The Haldane conjecture is now well understood and has been confirmed experimentally and numerically. On top of the existence of a gap, the spin-1 phase (the Haldane phase) has remarkable exotic properties. This phase displays nonlocal string long-range ordering which corresponds to the presence of a hidden Néel antiferromagnetic order.² One of the most remarkable properties of the Haldane phase is the liberation of fractional spin-1/2 edge states when the chain is doped by nonmagnetic impurities.³ The possibility of a similar hidden order has recently been proposed in a different context by studying the one-dimensional extended Bose-Hubbard model.⁴

In this Rapid Communication, we will reveal a Haldane conjecture for *spin-singlet* modes in a $2N$ -component fermionic chain at half-filling and for *attractive* interactions, with the emergence of gapless and gapped phases depending on the parity of N . The analog of the Haldane phase is stabilized for even N with all its well-known properties, while a gapless behavior occurs when N is odd. The Haldane physics with the alternating gapped or gapless behavior thus translates here directly into an insulating or metallic behavior depending on the parity of N . To exhibit this even-odd scenario, we will consider cold fermionic atoms with half-integer hyperfine spin $F=N-1/2$ at half-filling (N atoms per site) loaded into a one-dimensional optical lattice. Due to Pauli's principle, low-energy s -wave scattering processes of spin- F fermionic atoms are allowed in the even total spin $J=0, 2, \dots, 2N-2$ channels, so that the effective Hamiltonian with contact interactions reads as follows:⁵

$$\mathcal{H} = -t \sum_{i,\alpha} [c_{\alpha,i}^\dagger c_{\alpha,i+1} + \text{H.c.}] - \mu \sum_{i,\alpha} c_{\alpha,i}^\dagger c_{\alpha,i} + \sum_{i,J} U_J \sum_{M=-J}^J P_{JM,i}^\dagger P_{JM,i}, \quad (1)$$

where $c_{\alpha,i}^\dagger$ is the fermion creation operator corresponding to the $2N$ hyperfine states ($\alpha=1, \dots, 2N$) at the i th site of the optical lattice. The pairing operators in Eq. (1) are defined through the Clebsch-Gordan coefficients for spin- F fermions: $P_{JM,i}^\dagger = \sum_{\alpha\beta} \langle JM | F, F; \alpha\beta \rangle c_{\alpha,i}^\dagger c_{\beta,i}^\dagger$. In the general spin- F case, there are N couplings constants U_J in model (1) which are related to the N possible two-body scattering lengths of the problem. In the following, we will consider a simplified version of model (1) for $N \geq 2$ to reveal explicitly the Haldane charge conjecture. By fine tuning the different scattering lengths in channel $J \geq 2$, we will investigate model (1) with $U_2 = \dots = U_{2N-2}$,

$$\mathcal{H} = -t \sum_{i,\alpha} [c_{\alpha,i}^\dagger c_{\alpha,i+1} + \text{H.c.}] - \mu \sum_i n_i + \frac{U}{2} \sum_i n_i^2 + V \sum_i P_{00,i}^\dagger P_{00,i}, \quad (2)$$

with $U=2U_2$, $V=U_0-U_2$, and $n_i = \sum_\alpha n_{\alpha,i} = \sum_\alpha c_{\alpha,i}^\dagger c_{\alpha,i}$ is the density at site i . In Eq. (2), the singlet BCS pairing operator for spin- F fermions is $\sqrt{2N} P_{00,i}^\dagger = \sum_{\alpha\beta} c_{\alpha,i}^\dagger \mathcal{J}_{\alpha\beta} c_{\beta,i}^\dagger = -\sum_\alpha (-1)^\alpha c_{\alpha,i}^\dagger c_{2N+1-\alpha,i}^\dagger$, where the matrix \mathcal{J} is a $2N \times 2N$ antisymmetric matrix with $\mathcal{J}^2 = -I$. When $V=0$ ($U_0=U_2$), model (2) is nothing but the Hubbard model for $2N$ -component fermions with a $U(2N) = U(1) \times SU(2N)$ invariance. This symmetry is broken down to $U(1) \times Sp(2N)$ when $V \neq 0$.^{6,7} In the special $N=2$ case, i.e., $F=3/2$, there is no fine tuning and models (1) and (2) have an exact $U(1) \times SO(5)$ symmetry [$Sp(4) \sim SO(5)$].⁸ The zero-temperature phase diagram of model (2) away from half-filling has been recently investigated by means of a low-energy approach^{9,10} and large scale numerical calculations¹¹ for $F=3/2$. In this respect, the physics of $F > 1/2$ fermions is richer than in the standard spin-1/2

Hubbard chain.^{12,13} In particular, for $U < V < 0$ and at sufficiently low density, the leading superconducting instability is of a molecular type with charge $2Ne$.^{9–11} In this Rapid Communication, we will show by means of a low-energy approach and density matrix renormalization group (DMRG) calculations¹⁴ that a Haldane conjecture for *spin-singlet* charge modes emerges in model (2) at half-filling depending on the parity of N . In the $N=1$ case, it is well known that the half-filled SU(2) Hubbard chain displays a critical phase for attractive interaction. The analog of the Haldane phase of the spin-1 Heisenberg chain occurs for $N=2$ and attractive interactions.

II. STRONG-COUPLING ARGUMENT

We first give a simple physical explanation of the emergence of the Haldane conjecture for charge degrees of freedom. It stems from the existence of a pseudospin operator which carries charge: $S_i^+ = \sqrt{N/2} P_{00,i}^\dagger$ and $S_i^z = (n_i - N)/2$. This operator is a Sp(2N) spin singlet which is the generalization of the η -pairing operator introduced by Yang for the half-filled spin-1/2 (i.e., $N=1$) Hubbard model.¹⁵ It is easy to observe that \tilde{S}_i^+ satisfies the SU(2) commutation relations and generates a higher SU(2) \times Sp(2N) symmetry at half-filling along a very special line $V=NU$. The existence of such an extended SU(2) symmetry in the charge sector for $N=2$ has been first noticed in Ref. 8. In the general N case, one simple way to observe the emergence of this symmetry for $V=NU$ is to rewrite Hamiltonian (2) in absence of the hopping term [$\mu=U(N+1)$]: $\mathcal{H}(t=0) = 2U \sum_i [\tilde{S}_i^2 - N(N+2)/4]$. On top of the Sp(2N) symmetry, we thus deduce the existence of an extended SU(2) symmetry in the charge sector; moreover, for a strong attractive U , the pseudospin \tilde{S}_i^+ is a spin- $N/2$ operator, which acts on the degenerate low-lying even occupied states $(S_i^+)^k |\emptyset\rangle$,¹⁶ which one sketches here for $N=1, 2$:

$$\begin{array}{ccc}
 N=1 & & N=2 \\
 |\emptyset\rangle \leftrightarrow |S^z = -\frac{1}{2}\rangle & & |\emptyset\rangle \leftrightarrow |S^z = -1\rangle \\
 |\uparrow\uparrow\rangle \leftrightarrow |S^z = +\frac{1}{2}\rangle & & |\uparrow\uparrow\rangle - |\uparrow\downarrow\rangle \leftrightarrow |S^z = 0\rangle \\
 & & |\uparrow\downarrow\rangle \leftrightarrow |S^z = +1\rangle
 \end{array}$$

The next step of the approach is to derive an effective Hamiltonian in the strong-coupling regime $|U| \gg t$. At second order of perturbation theory and after a simple gauge transformation that changes the sign of the transverse exchange, we find a spin- $N/2$ antiferromagnetic SU(2) Heisenberg chain: $\mathcal{H}_{\text{eff}} = J \sum_i \tilde{S}_i \cdot \tilde{S}_{i+1}$ with $J = 4t^2/[N(2N+1)|U|]$. The Haldane conjecture for model (2) with attractive interactions thus becomes clear within this strong-coupling argument. When we deviate from the $V=NU$ line, the SU(2) charge symmetry is broken down to U(1) and in the strong-coupling regime the lowest correction is a single-ion anisotropy $D \sum_i (S_i^z)^2$ with $D = 2[U - V/N]$. The phase diagram of the resulting model for general N is known from the work of Schulz.¹⁷ For even N , on top of the Haldane phase, Néel and large- D singlet gapful phases appear while gapless (XY) and gapful (Ising) phases are stabilized for odd N in the vicinity of the SU(2) line.

We now turn to low-energy and numerical approaches to investigate the strong-weak coupling crossover and the de-

termination of the physical properties of the phases in the vicinity of the $V=NU$ line.

III. LOW-ENERGY APPROACH

We study here the low-energy approach in the simplest $F=3/2$ case with the emergence of the striking properties of a Haldane insulating (HI) phase. The general N case is highly technical and will be presented elsewhere. The low-energy procedure for $F=3/2$ cold fermions has already been presented away from half-filling.^{9,10,18} In the half-filled case, in sharp contrast to the $F=1/2$ case, there is no spin-charge separation for $F > 1/2$ since an umklapp process couples these degrees of freedom.¹⁹ The exact U(1) \times SO(5) continuous symmetry of model (2) is hidden in the bosonization description. However, it becomes explicit by a refermionization procedure as in the two-leg spin ladder.¹² To this end, we introduce eight right and left moving real (Majorana) fermions $\xi_{R,L}^A$, $A=1, \dots, 8$. The two Majorana fermions $\xi^{7,8}$ account for the U(1) charge symmetry, the five Majorana fermions $\xi^{1, \dots, 5}$ generate the SO(5) spin rotational symmetry, whereas the last one ξ^6 describes an internal discrete \mathbb{Z}_2 symmetry ($c_{1(4),i} \rightarrow ic_{1(4),i}$, $c_{2(3),i} \rightarrow -ic_{2(3),i}$) of model (2). Within this description, the interacting part of the low-energy Hamiltonian for the spin-3/2 model (2) at half-filling reads as follows:

$$\begin{aligned}
 \mathcal{H}_{\text{int}} = & \frac{g_1}{2} \left(\sum_{a=1}^5 \xi_R^a \xi_L^a \right)^2 + g_2 \xi_R^6 \xi_L^6 \sum_{a=1}^5 \xi_R^a \xi_L^a + \frac{g_3}{2} (\xi_R^7 \xi_L^7 + \xi_R^8 \xi_L^8)^2 \\
 & + (\xi_R^7 \xi_L^7 + \xi_R^8 \xi_L^8) \left(g_4 \sum_{a=1}^5 \xi_R^a \xi_L^a + g_5 \xi_R^6 \xi_L^6 \right), \quad (3)
 \end{aligned}$$

with $g_{1,2} = -a_0(U \pm V)$, $g_3 = a_0(3U + V)$, $g_4 = a_0U$, and $g_5 = a_0(U + 2V)$. The zero-temperature phase diagram of model (3) can then be derived by means of a one-loop renormalization group (RG) approach. By neglecting the velocity anisotropy, we find the one-loop RG equations,

$$\dot{g}_1 = 3g_1^2 + g_2^2 + 2g_4^2, \quad \dot{g}_2 = 4g_1g_2 + 2g_4g_5,$$

$$\dot{g}_3 = g_5^2 + 5g_4^2, \quad \dot{g}_4 = g_5g_2 + g_4g_3 + 4g_1g_4,$$

$$\dot{g}_5 = 5g_4g_2 + g_5g_3, \quad (4)$$

where $\dot{g}_a = \partial g_a / \partial l$, l being the RG time. The resulting phase diagram is presented in Fig. 1. As in two-leg electronic ladders, there is a special isotropic ray of the RG flow where an approximate SO(8) symmetry emerges in the far infrared limit.²⁰ Along the highly symmetric ray $g_a = g$ ($a=1, \dots, 5$), model (3) takes the form of the SO(8) Gross-Neveu model which is an integrable massive field theory for $g > 0$. The resulting gapful phase is twofold degenerate and corresponds to a spin-Peierls (SP) ordering, with lattice order parameter $\mathcal{O}_{\text{SP}} = \sum_{i,\alpha} (-1)^i [c_{\alpha,i}^\dagger c_{\alpha,i+1} + \text{H.c.}]$. A second massive phase is obtained from this SP phase by performing a duality transformation, $\xi_L^{7,8} \rightarrow -\xi_L^{7,8}$, which is an exact symmetry of Eq. (3) if $g_{4,5} \rightarrow -g_{4,5}$. This duality symmetry exchanges a SP phase with a long-ranged charge density-wave (CDW) phase

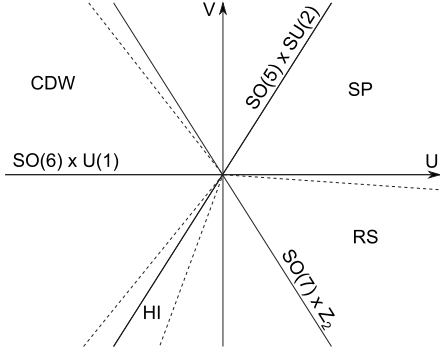


FIG. 1. Phase diagram obtained by the low-energy approach in the $N=2$ case (see text for definitions); the dotted lines stand for (second-order) quantum phase transitions.

with order parameter $\mathcal{O}_{\text{CDW}} = \sum_i (-1)^i \delta n_i$, where $\delta n_i = n_i - \langle n_i \rangle$. The quantum phase transition between the SP-CDW phases is found to belong to the $U(1)$ universality class. There is a second duality symmetry with $\xi_L^6 \rightarrow -\xi_L^6$ which is a symmetry of Eq. (3) if $g_{2,5} \rightarrow -g_{2,5}$. This duality symmetry is nonlocal in terms of the original lattice fermions $c_{\alpha,i}$ and gives rise to two nondegenerate fully gapped phases from SP and CDW phases. As it is seen in Fig. 1, a first nondegenerate phase contains the $V < 0$ axis. Its physical interpretation is a singlet-pairing phase which is the analog of the rung-singlet (RS) phase of the two-leg ladder. Upon doping, the singlet BCS pairing $P_{0,i}$ has a gapless behavior and becomes the dominant instability.¹¹ We need to introduce nonlocal string-order parameters to fully characterize the last nondegenerate phase. In this respect, we define two charge-string-order parameters: $\mathcal{O}_{c,i}^{\text{even}} = \cos(\frac{\pi}{2} \sum_{k < i} \delta n_k)$, $\mathcal{O}_{c,i}^{\text{odd}} = \delta n_i \mathcal{O}_{c,i}^{\text{even}}$, which are even or odd, respectively, under the particle-hole transformation $\delta n_i \rightarrow -\delta n_i$. Within the low-energy approach, we find the long-range ordering of odd (even respectively) charge-string operator in the second nondegenerate (RS respectively) phase. The phase with long-range ordering of $\mathcal{O}_c^{\text{odd}}$ is a HI phase similar to the Haldane phase of the spin-1 chain. Indeed, for attractive interactions $U, V < 0$, on general grounds, we expect that the $SO(5)$ spin gap (Δ_s) will be the largest scale of the problem. At energies lower than Δ_s , one can integrate out the $SO(5)$ spin degrees of freedom and the leading part of the effective Hamiltonian (3) simplifies as follows:

$$\mathcal{H}_{\text{int}} = -im_c \sum_{a=7}^8 \xi_R^a \xi_L^a - im_o \xi_R^6 \xi_L^6, \quad (5)$$

which is the well-known Majorana effective field theory of the spin-1 XXZ Heisenberg chain with a single-ion anisotropy D .²¹ Along the special line $V=2U$, the two masses $m_{c,o}$ are equal due to the presence of the extended $SU(2)$ symmetry which rotates the three Majorana fermions $\xi^{6,7,8}$. Within the spin-1 terminology, the interpretation of the phases for $U < 0$ of Fig. 1 reads as follow: the CDW phase is the Néel phase, the RS phase is the large- D singlet phase, and the HI phase is the Haldane phase. All the known quantum phase transitions in the spin-1 problem are consistent with the findings of the RG approach of model (3) with a $U(1)$ quantum

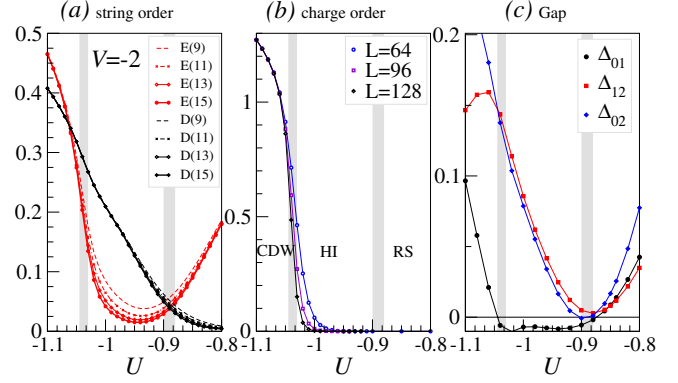


FIG. 2. (Color online) (a) and (b) Order parameters along the $V=-2$ line showing the three different phases CDW, HI, and RS. String orders are computed by taking i and j at equal distance from the center of the chain. (c) Various charge gaps Δ_{ab} (see text) extrapolated in the thermodynamic limit from data obtained on $L=16, 32$, and 64 . Quantum phase transitions are located in the gray regions.

criticality for the HI-RS transition and an Ising transition between the CDW and HI phases. The HI phase of Fig. 1 is characterized by a string-order $\mathcal{O}_c^{\text{odd}}$ which reveals its hidden order. We can also investigate the possible existence of edge states in the HI phase by considering a semi-infinite geometry. In that case, the low-energy effective Hamiltonian is still given by Eq. (5) with the boundary conditions: $\xi_L^{6,7,8}(0) = \xi_R^{6,7,8}(0)$. The situation at hand is very similar to the low-energy approach of the cut two-leg spin ladder.²² The resulting boundary model is integrable and three localized Majorana modes $\tilde{\eta}$ with zero energy inside the gap (midgap states) emerge in the HI phase. These three local fermionic modes give rise to a local pseudo-spin-1/2 operator \vec{S} , thanks to the identity:²³ $\vec{S} = -i\tilde{\eta} \wedge \tilde{\eta}/2$. We thus conclude on the existence of a spin-singlet pseudo-spin-1/2 edge state which is the main signature of the HI phase.

IV. DMRG CALCULATIONS

We now carry out numerical calculations, using DMRG, in order to validate this conjecture in the $N=2$ and $N=3$ cases. We keep up to 2000 states and use open boundary conditions. When $N=2$, we fix two quantum numbers for the spin part $S^z = \sum_{\alpha,i} (-)^{\alpha+1} n_{\alpha,i}/2$ and $T^z = \sum_i (n_{1,i} + n_{2,i} - n_{3,i} - n_{4,i})/2$ (the ground state lies in the $S^z = T^z = 0$ sector) and the total number of particles $N_f = 2L$. For $N=2$, we set $t=1$, $V=-2$ and we investigate order parameters showing the existence of the HI phase and its extension. In this respect, we define two string-order correlations: $E(|i-j|) = |\langle \exp[i\pi \sum_{i < k < j} (\delta n_k/2)] \rangle|$ and $D(|i-j|) = |\langle (\frac{\delta n_i}{2}) \exp[i\pi \sum_{i < k < j} (\frac{\delta n_k}{2})] (\frac{\delta n_j}{2}) \rangle|$. In Fig. 2, we plot these string correlations, the charge order parameter $\langle \mathcal{O}_{\text{CDW}}(L/2) \rangle$ in the bulk of the chain, and the pseudospin gaps which are defined by:

$$\Delta_{ab} = E_0(N_f = 2L + 2b) - E_0(N_f = 2L + 2a),$$

with $E_0(N_f)$ as the ground-state energy with N_f particles and $S^z = T^z = 0$. In the HI phase, because of the existence of edge

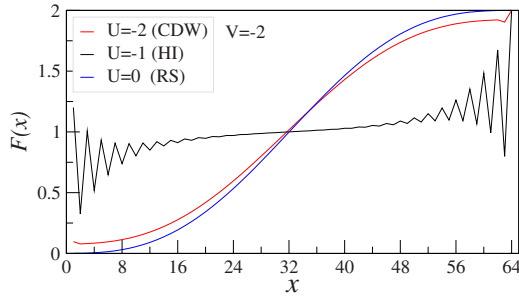


FIG. 3. (Color online) Integrated excess density $F(x)$ showing the edge states in the HI phase of the attractive model with $N=2$.

states (see below), the excited state with N_f+2 fermions falls onto the ground state (i.e., $\Delta_{01}=0$), so that the correct value for the gap in the bulk is given by $\Delta_{12}=\Delta_{02}$, similarly to what has been done for spin-1 chains. All these quantities lead to the conclusion of the existence of two gapful phases on top of the CDW phase. In particular, the data confirm the existence of the HI gapped phase with $\langle \mathcal{O}_{\text{CDW}} \rangle = 0$, $D(\infty) \neq 0$ while $E(\infty)$ scales to zero. On the contrary, $D(\infty)=0$ in the RS phase while $E(\infty)$ remains finite. In the CDW phase, both string orders are finite, which can be easily understood from the ground-state structure with alternating empty and fully occupied sites. One of the striking features of the HI phase are the edge states. As discussed above, these edge states are in the charge sector so one can observe them by adding two particles while staying in the $S^z = T^z = 0$ sector. In Fig. 3, we plot the integrated “excess density” defined as $F(x) = \int^x dy (n(y) - 2)$ for $U > -1$ and $F(x) = (-1)^x \int^x dy (n(y) - 2)$ if $U \leq -1$ to remove the typical CDW oscillations. We find that, in the HI phase, the added particles are pinned at the ends of the chains while in the RS and CDW phases, this excess lies in the bulk.

Finally, we discuss the case $N=3$, i.e., spin-5/2 fermions. As shown in Fig. 4, the system behaves *effectively* as a criti-

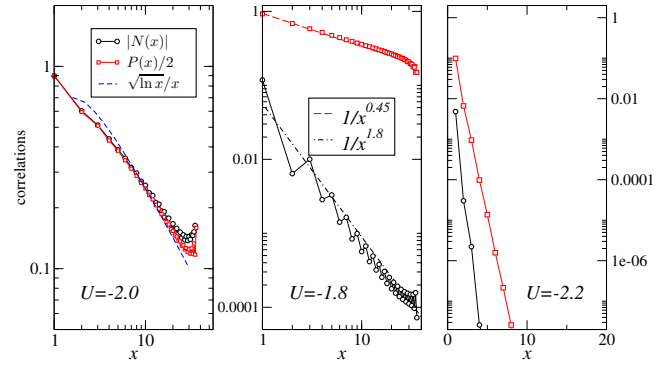


FIG. 4. (Color online) Correlation functions $|N(x)|$ and $P(x)$ for $N=3$, corresponding to the correlations of the S^z and S^+ pseudospin operators, as a function of distance x at $V=-6$ for $L=72$. For (a) $V=3U$, $SU(2)$ symmetry is manifest, while the system is XY -like if (b) $U > V/3$ or Ising-like if (c) $U < V/3$.

cal spin-3/2 $SU(2)$ chain on the line $V=3U$, with equal transverse and longitudinal pseudospin correlations given by the singlet-pairing $P(x) = \langle P_{00,L/2+x}^+ P_{00,L/2} \rangle$ and the charge correlations $N(x) = \langle \delta n_{L/2+x} \delta n_{L/2} \rangle$, respectively. In particular, we recover the same quantum critical behavior as a spin-1/2 chain as predicted.¹ Moving away from this line, we find in Fig. 4 the emergence of a Luttinger liquid phase with critical exponents close to the one of the XY model for $U \geq V/3$ and a gapped Ising phase with exponentially decaying correlations when $U < V/3$, in full agreement with the strong-coupling approach.

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