Current fidelity susceptibility and conductivity in one-dimensional lattice models with open and periodic boundary conditions

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We study, both numerically and analytically, the finite size scaling of the fidelity susceptibility χJ with respect to the charge or spin current in one-dimensional lattice models, and relate it to the low-frequency behavior of the corresponding conductivity. It is shown that in gapless systems with open boundary conditions the leading dependence on the system size L stems from the singular part of the conductivity and is quadratic, with a universal form χJ = 7KL^2ζ(3)/2π^4 where K is the Luttinger liquid parameter. In contrast to that, for periodic boundary conditions the leading system size dependence is directly connected with the regular part of the conductivity (giving alternative possibility to study low frequency behavior of the regular part of conductivity) and is subquadratic, χJ ∝ L^(γ(K)), (γ being a K dependent constant) in most situations linear, γ = 1. For open boundary conditions, we also study another current-related quantity, the fidelity susceptibility to the lattice tilt χP and show that it scales as the quartic power of the system size, χP = 3KLζ(5)/8u^2π^6, where u is the sound velocity. We comment on the behavior of the current fidelity susceptibility in gapped phases, particularly in the topologically ordered Haldane state.

I. INTRODUCTION

The ground state fidelity susceptibility (FS) has established itself as a useful computational tool for locating quantum phase transitions in many-body systems for a general Hamiltonian,

\[ \hat{H}(\lambda) = \hat{H}_0 + \lambda \hat{W} \]

with a phase transition driven by the coupling to a certain operator \( \hat{W} \), the fidelity \( F(\lambda, \delta \lambda) = \langle \psi_0(\lambda) | \psi_0(\lambda + \delta \lambda) \rangle \) measures the change in the ground state wave function \( | \psi_0(\lambda) \rangle \) with the infinitesimal change of the coupling \( \lambda \), and the fidelity susceptibility \( \chi_W \) with respect to the “perturbation” \( \hat{W} \) is defined as

\[ \chi_W(\lambda) = \lim_{\delta \lambda \to 0} \frac{1 - |F(\lambda, \delta \lambda)|^2}{\delta \lambda^2} = \sum_{n \neq 0} \frac{|\langle \psi_0(\lambda) | \hat{W} | \psi_n(\lambda) \rangle|^2}{(E_n(\lambda) - E_0(\lambda))^2}, \]

where second equality is derived, in the second order of perturbation theory, assuming that the ground state is unique. Summation in (2) is over all eigenstates \( | \psi_n(\lambda) \rangle \) of the Hamiltonian \( \hat{H}(\lambda) \) with the eigenvalues \( E_n(\lambda) \), except the ground state \( | \psi_0(\lambda) \rangle \).

Typically, in thermodynamic limit the FS would diverge at the point \( \lambda_c \) corresponding to a quantum phase transition \( \chi_W \propto L/(\lambda - \lambda_c)\alpha \) and for systems of a finite size \( L \) the analysis of the scaling behavior of

\[ \chi_W(\lambda_c) \propto L^\nu \]

allows one to extract the critical exponent \( \nu \) of the correlation length, \( \nu = (\mu - 1)/\alpha \) and thus to determine the universality class of the transition.

One of the most advanced unbiased numerical method for analyzing lattice models in reduced spatial dimensions is the density matrix renormalization group (DMRG), which is best suited for systems with open boundary conditions at least along one of the directions. In one dimension (1d), systems with open boundaries consisting of \( L \sim 10^2-10^3 \) sites can be efficiently analyzed by DMRG. Hence, it is crucial to understand the dependence of the FS on the boundary conditions. For many types of the “perturbation” \( \hat{W} \), the FS depends only weakly on the boundary conditions for large systems.

In the present paper, we show that if \( \hat{W} \) is charge or spin current operator \( \hat{J} \), or the “polarization” operator \( \hat{P} \) (which physically corresponds to introducing the external electric field for charged particles, or to tilting the lattice for neutral particles, or to a magnetic field gradient for spins), the situation is very special. We study the current FS in several model systems, including spin chains, the Hubbard model for spinful fermions, and the Bose-Hubbard model. It is shown that in gapless 1d systems with open boundary conditions (o.b.c.) the leading terms in the \( L \) dependence are given by \( \chi_J \propto KL^2 \) and \( \chi_P \propto KL^4/u^2 \) respectively, where \( K \) is the Luttinger liquid parameter, \( u \) is the characteristic “sound” velocity, and the numerical prefactors are universal. We show, by means of relating \( \chi_J \) and \( \chi_P \) to the behavior of the positive frequency conductivity \( \sigma_+(\omega) \), that those superextensive terms in the FS originate from the low-frequency behavior of the singular part of the conductivity. Since those terms are universal, they can mask the diverging part of the FS at a phase transition point between two gapless regions.

In contrast to that, for gapless systems with periodic boundary conditions (p.b.c.) the leading system size dependence of the current FS is linear, \( \chi_J \propto L \), in a wide range of the Luttinger liquid parameter \( K \), and may
change to a subquadratic one, $\chi_J \propto L^\gamma$ with $\gamma$ depending on $K$, $1 \leq \gamma < 2$. At Kosterlitz-Thouless (KT) metal-insulator transition point $\chi_J \propto (L/\ln L)^2$.

As a byproduct of this study, we establish the general properties of the low-frequency behavior of the conductivity in systems with open and periodic boundary conditions. We emphasize a crucial difference in the behavior of conductivity in systems with p.b.c. and o.b.c., which is responsible for the peculiar difference in the current FS properties.

In gapped phases the current FS is generically extensive, independent of boundary conditions, $\chi_J \propto L$, but it may again acquire the quadratic system size dependence for topologically ordered states in systems with open boundary conditions, for example in the singlet ground state of the open Haldane chain, due to non-locally entangled edge spins.

The structure of the paper is as follows: in Sec. II we consider the main properties of the current fidelity susceptibility, its relation to the conductivity, and the dependence on boundary conditions, on the simplest example of the spin-$1/2$ XXZ chain in its gapless phase (which is equivalent to nearest-neighbor interacting spinless fermions). We present two ways of calculating the current FS for open systems: one is based on the free-fermion picture and involves bosonization arguments for a generalization to the interacting case, and the other way is based on applying a unitary twist transformation and reducing the problem to calculating certain integrals of the (spin) density correlation function. We also present an example of how the presence of universal quadratic terms in the current FS can hinder the detection of a phase transitions between two gapless phases of the 1d Bose-Hubbard model. In Sec. III we consider the properties of the current FS in the fermionic Hubbard model. Sec. IV comments on the behavior of the current FS in gapped phases, and Sec. V contains a brief summary. In appendix we provide details of bosonization calculations used throughout paper for open chains.

II. SPIN-CURRENT FIDELITY SUSCEPTIBILITY AND CONDUCTIVITY OF SPIN-$1/2$ XXZ CHAIN

We start by considering a spin-$1/2$ XXZ chain with the additional Dzyaloshinskii-Moriya (DM) coupling, described by the Hamiltonian

$$\hat{H} = \hat{H}_{XXZ} + \hat{H}_{DM},$$

with

$$\hat{H}_{XXZ} = J \sum_l (S^x_l S^x_{l+1} + S^y_l S^y_{l+1} + \Delta S^z_l S^z_{l+1}),$$

$$\hat{H}_{DM} = d \hat{J}, \quad \hat{J} = \sum_l J_l = \sum_l (\hat{S}_l \times \hat{S}_{l+1})^z,$$

where $S^a_l$ are spin-$1/2$ operators acting at site $l$ of the chain. In what follows, we set the Planck constant $\hbar$ and the lattice spacing $a$ to unity and measure energy in units of $J = 1$.

We will study the current fidelity susceptibility (CFS) $\chi_J(d)$ that describes the response of the ground state to an infinitesimal change of the DM coupling $d$. In the following, we study separately the cases of open and periodic boundary conditions. We will use the upper index $o$ and $p$ to distinguish the FS for those two cases.

Consider first the CFS at $d = 0$ (the alternative derivation, valid for finite $d$ and for arbitrary half-integer spin $S$, is presented later in Sec. III). At $d = 0$, the quantity $\hat{J}$ has the meaning of the total spin current, because the local currents $J_l$ satisfy the continuity equation $\partial_t S^x_l = J_l - J_{l+1}$.

It is worthwhile to note, that the CFS is identical to the so-called stiffness FS $\chi_o$, which describes the response of the ground state to a uniform infinitesimal twist $\varphi$ on every link:

$$\hat{H} \mapsto \hat{H}(\varphi) = \sum_j \left[ \frac{1}{2} S^+_j S^-_{j+1} e^{i\varphi} + \text{h.c.} \right] + \Delta S^z_j S^z_{j+1}. \quad (6)$$

The second derivative of the ground state energy with respect to $\varphi$ defines the spin stiffness $\rho$; for spin-$1/2$ XXZ chain and the Hubbard model, exact results for $\rho$ are available. Note, even though $\chi_J = \chi_o$ the second derivative of the ground state energy with respect to $d$ and $\varphi$ differ. Following the results of the second order perturbation theory in Ref. [3],

$$\frac{1}{L} \frac{\partial^2 E_0}{\partial \varphi^2} \bigg|_{\varphi=0} = \frac{1}{L} \left( \frac{-T_k > -2 \sum_{n \neq 0} | < \psi_0 | \hat{J} | \psi_n > |^2}{E_n - E_0} \right)$$

$$= 2 \rho \quad (7)$$

gives twice the spin stiffness $\rho$ as already mentioned and $T_k = \sum_j \left[ \frac{1}{2} S^+_j S^-_{j+1} + \text{h.c.} \right]$ is kinetic energy. Similarly the second order perturbation theory gives,

$$\frac{\partial^2 E_0}{\partial d^2} \bigg|_{d=0} = -2 \sum_{n \neq 0} | < \psi_0 | \hat{J} | \psi_n > |^2 \quad (8)$$

In particular, for p.b.c. $\partial^2 E_0/\partial d^2 = 0$ for $\Delta = 0$ as current commutes with kinetic energy in periodic chains and $\rho = 1/\pi$.

For the systems with o.b.c. the uniform twist can be completely absorbed by unitary transformation for any $\Delta$ (equivalently due to the $f-$sum rule for any $\Delta$),

$$\frac{\partial^2 E_0}{\partial \varphi^2} \bigg|_{\varphi=0} = 0 \quad (9)$$

and

$$\frac{\partial^2 E_0}{\partial d^2} \bigg|_{d=0} = < T_k >, \quad (10)$$

hence $\partial^2 E_0/\partial d^2 \neq 0$ even for $\Delta = 0$ ($< T_k >= -1/\pi$ for free case) as current does not commute with kinetic energy for o.b.c.
Note also that if one performs a twist by $L \varphi \ll 1$ only on one link of a periodic chain (twisting the boundary conditions) the energies will not change as compared to uniform twist of every link with $\varphi$ angle, but the FS with respect to the twist in one link will be different from $\chi_{\varphi}$ of Eq. (4). The reason is that twisting the single link (twisting the boundary condition) breaks translational symmetry and thus makes the situation similar to that in the o.b.c. case. As a result, the response of the ground state wavefunction to the infinitesimal twist on a single link is non-zero independent of boundary conditions, even for the non-interacting case ($\Delta = 0$).

Instead of the spin-$\frac{1}{2}$ XXZ chain with the DM coupling, described by the Hamiltonian \([4]\), we may have in mind interacting lattice fermions or hard-core bosons, under the action of some “field” $d$ that couples to the total particle current,

$$
\tilde{H} = \frac{-1}{2} \sum_j \left[ c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j \right] + \Delta \sum_j n_j n_{j+1}
- \frac{i}{2} d \sum_j \left[ c_j^\dagger c_{j+1} - c_{j+1}^\dagger c_j \right],
$$

(11)

which is equivalent to the spin-$\frac{1}{2}$ XXZ chain by the well-known Jordan-Wigner transformation. At $d = 0$ CFS $\chi_J$ defines the response of the ground state of such a system to the infinitesimal uniform change of current through nearest-neighbor links.

A. Relation between the CFS and the conductivity

According to \([2]\), the CFS can be written as

$$
\chi_J(d = 0) = \sum_{n \neq 0} \frac{\left| \langle \psi_0 | J | \psi_n \rangle \right|^2}{(E_n - E_0)^2},
$$

(12)

where $E_n$ are the eigenvalues of $\tilde{H}_{\text{XXZ}}$ and summation is over all excited states. Comparing the above expression to the definition of the positive frequency real part of the spin current conductivity\([9,11–13]\),

$$
\sigma_1(\omega) \equiv \left. \text{Re} \right|_{\omega > 0} \sigma(\omega) = \frac{\pi}{L \omega} \sum_{n \neq 0} \left| \langle \psi_0 | J | \psi_n \rangle \right|^2 \delta(\omega - (E_n - E_0)),
$$

(13)

one obtains the following relation between the CFS and the integrated conductivity:

$$
\chi_J = \frac{L}{\pi} \int_0^\infty \omega \sigma_1(\omega) d\omega.
$$

(14)

It is important that for p.b.c. systems the definition \([13]\) does not include the Drude weight term $K u \delta(\omega)$. The Drude weight is concentrated at $\omega = 0$, while the sum in Eq. (13) is over the energy eigenstates with the lower bound $E_n - E_0 \sim 1/L > 0$, so it does not account for the zero mode\([2]\).

In contrast to that, in systems with o.b.c. the total current does not commute with the Hamiltonian even in the noninteracting case ($\Delta = 0$). Its zero mode vanishes identically (see Eq. (62) in the Appendix), hence the singular part of the conductivity (the Drude weight term) is included in $\sigma_1(\omega)$. As we will see below, it is due to this reason that the finite-size scaling of $\chi_J$ is quite different for systems with periodic and open boundary conditions.

B. Periodic boundary conditions

For a periodic chain

$$
\sigma_1^p(\omega) = \sigma_{\text{reg}}(\omega),
$$

(15)

where $\sigma_{\text{reg}}(\omega)$ is a regular part of conductivity; as mentioned above, the total real part of the conductivity (including zero mode) is

$$
\text{Re} \sigma^p(\omega) = K u \delta(\omega) + \sigma_{\text{reg}}(\omega),
$$

(16)

where $u = \frac{K}{2K - 1} \sin \frac{\pi}{2K}$ has the meaning of the spin-wave velocity of the XXZ chain. The total conductivity satisfies the $\tilde{f}$-sum rule\([11,13]\)

$$
\frac{1}{\pi} \int_0^\infty \sigma(\omega) d\omega = -\frac{1}{2L} \langle T_k \rangle,
$$

(17)

where $\langle T_k \rangle$ is the average kinetic energy which in the case of the XXZ chain can be evaluated exactly from the dependence of the ground state energy on anisotropy parameter $\Delta$,

$$
\langle T_k \rangle = E_0(\Delta) - \Delta \partial_{\Delta} E_0(\Delta).
$$

(18)

One can observe that for the XXZ chain with $-1 < \Delta \lesssim 1/4$ the product $K u$ is well approximated by

$$
K u \simeq \pi \langle -T_k \rangle / L,
$$

(19)
so the r.h.s. of \( \text{(17)} \) is, in a rather wide region \(-1 < \Delta \leq 1/4\), well approximated by \( Ku/(2\pi) \) and thus in this region the sum rule \( \text{(17)} \) is exhausted to a high accuracy by the Drude term (using \( \int_0^\infty \delta(x)dx = 1/2 \)).

For weak interaction \( \Delta \), a perturbative calculation\(^4\) yields \( \sigma_{\text{reg}}(\omega) \sim \Delta^2 \omega^{-5/2} \). Then for \( K > 5/8 \) (which corresponds to \( \Delta < \frac{1+\sqrt{5}}{4} \approx 0.8 \) and strictly speaking is outside the perturbative in \( \Delta \) regime) the integral in \( \text{(14)} \) is \( O(1) \), so the CFS has a usual extensive dependence on the system size,

\[
\chi_J \propto L + \cdots, \quad K > \frac{5}{8},
\]

where dots stand for subleading contributions in the system size. The situation is different for periodic chains with \( 1/2 < K < 5/8 \), where the relation \( \text{(14)} \) suggests the following non-trivial dependence on the system size:

\[
\chi^p_J \propto L^{6-8K} + \cdots, \quad \frac{1}{2} < K < \frac{5}{8}.
\]

It can be obtained by replacing the lower integration limit in Eq. \( \text{(14)} \) by a quantity of the order of \( u/L \).

The KT phase transition point \( \Delta = 1 \), where \( K = 1/2 \), must be treated separately, since at this point the conductivity gets logarithmic corrections\(^3\), \( \sigma_{\text{reg}}(\omega) \sim 1/\omega \log^2(\omega) \), and hence

\[
\chi^p_J \sim (L/\ln L)^2 + \cdots, \quad \Delta = 1.
\]

It should be remarked that our results Eqs. \( \text{(20)-(22)} \) disagree with the conclusions of Ref. \( \text{[8]} \) who have studied the stiffness FS \( \chi_\rho \) that is equal to our current FS \( \chi_J \) as already mentioned. First, Eq. \( \text{(20)} \) and Figs. 1 and 2 of Ref. \( \text{[8]} \) create the impression that the leading contribution to the \( \chi_\rho \) scales generically as \( L^2 \) in periodic systems. We believe this is a mistake in the presentation, since we have perfectly reproduced Figs. 1 and 2 of Ref. \( \text{[8]} \) for the quantity \( \chi_\rho \) (and not for \( \chi_\rho/L \) as it stands in the original paper). Second, in view of the intimate connection between the CFS and the regular part of conductivity established by us above, the subleading corrections to the finite-size scaling of \( \chi_\rho \), as proposed in Ref. \( \text{[8]} \) and derived on the basis of analyzing the scaling dimensions of operators\(^4\) perturbing the Luttinger liquid in the bosonization framework, contradict Giamarchi’s result\(^4\) for the conductivity.

Fig. 2 shows the DMRG results for \( \chi^p_J \) in periodic XXZ chains with different values of the interaction \( \Delta \). For \( \Delta \lesssim 0.5 \), a good convergence to the linear scaling \( \chi^p_J \propto L \) is achieved already at \( L = 100 \). However, for larger values of \( \Delta \) (especially for \( \Delta \rightarrow 1 \)) the value \( \chi^p_J/L \) does not seem to converge to a constant at \( L \gg 1 \), though to make a definitive claim one has to study much larger system sizes. For the range of \( L \) studied here, \( L \leq 100 \), fitting with \( \chi^p_J \sim (L/\ln L)^2 \) as well as with \( \chi^p_J \sim L^{6-8K} \) seems equally reasonable.

At \( SU(2) \) symmetric point \( \Delta = 1 \) it is worthwhile to mention effect of the next-nearest-neighbor antiferromagnetic (as well \( SU(2) \) symmetric) interaction \( J_2 \),

\[
\tilde{H} = \sum_j \left( \hat{S}_j \hat{S}_{j+1} + J_2 \hat{S}_j \hat{S}_{j+2} \right).
\]

Observe that due to \( J_2 \) coupling expression of current operator changes as follows,

\[
\tilde{J} \rightarrow \frac{i}{2} \sum_j \left[ \hat{S}^+_j \hat{S}^-_{j+1} + J_2 \hat{S}^+_j \hat{S}^-_{j+2} \right] + \text{(h.c.)}
\]

At a special point, \( J_2 = J^*_2 \simeq 0.241 \) (that in thermodynamic limit corresponds to a phase transition point between Luttinger liquid and dimerized phases) the amplitude of the basic (marginal) Umklapp term vanishes in effective bosonization formulation and hence low frequency behavior of the regular part of conductivity changes to \( \sigma_1(\omega) \sim \omega^{8nK-5} \), where \( K = 1/2 \) due to \( SU(2) \) symmetry and \( n \) is some integer \( n > 1 \) so that in any case \( \int \sigma_1(\omega)/\omega d\omega \) converges at \( \omega = 0 \). Hence at \( J_2 = J^*_2 \) the CFS \( \chi^p_J \sim L \), even though this is a phase transition point between gapless and gapped regions. This agrees well with the data on Fig. 4 of Ref. \( \text{[8]} \) namely ratio \( \chi^p_J/L \) becomes nearly system size independent at \( J^*_2 \). The form of the current operator \( \text{(24)} \) explains why infinitesimal twist must be the same (and not factor of 2 different) in both nearest-neighbor and next-nearest-neighbor links to observe the flat curve \( \chi^p_J/L \) vs \( L \) at \( J_2 = J^*_2 \).
C. Open boundary conditions

Let us start our discussion of the CFS for open chains from the non-interacting case $\Delta = 0$ (free spinless fermions or hardcore bosons). At low excitation energies, the spectrum is approximately linear, $E_m - E_0 \simeq u m/L$. The expression (13), which for o.b.c. represents the entire conductivity, can be rewritten as

$$\sigma_1^o = \frac{\pi}{\omega L} \sum_{m>0} \rho(m) |\langle \psi_0 | J | \psi_m \rangle|^2 \delta(\omega - (E_m - E_0)) \quad (25)$$

where the matrix element of the current (see the Appendix) is

$$|\langle \psi_0 | J | \psi_m \rangle| = \left[ \frac{1 - (-1)^m}{m \pi} \right] u$$

where according to our conventions for free fermions $u(\Delta = 0) = 1$ and the degeneracy

$$\rho(m) = m \quad (27)$$

is the number of different particle-hole excitations with the same energy $E_m$ as is illustrated in Fig. 3 (excited states with more than one particle-hole pair do not contribute, since they cannot be created by the current operator from the ground state). Note that the matrix element satisfies the parity selection rule and is nonzero only for odd $m = 2k + 1$.

Putting everything together, we obtain the following low-frequency behavior for the conductivity of free fermions (the XY model, $\Delta = 0$) in an open chain:

$$\sigma_1^o = \frac{\pi u^2}{L \omega} \sum_{k=0}^{\infty} 4 \frac{(2k+1)}{2(2k+1)^2 \pi^2} \delta(\omega - (E_{2k+1} - E_0))$$

$$= \sum_{k=0}^{\infty} 4 u \frac{(2k+1)^2 \pi^2}{(2k+1)^2 \pi^2} \delta(\omega - \frac{(2k+1)u \pi}{L}). \quad (28)$$

Note that this low-frequency behavior is singular, $L \sigma_1^o(\omega) \propto 1/\omega^2$ at $\omega \to 0$. This is the form, into which the Drude peak transforms in the open chain.

For the interacting case, we divide the conductivity of the open chain into the Drude part $D(\omega)$, and the “regular” contribution,

$$\sigma_1^o(\Delta) = D(\omega) + \sigma_{\text{reg}}^o \quad (29)$$

We calculate the Drude part within the Luttinger liquid (LL) approximation (i.e., we neglect umklapp processes). For the interacting case, the expression for the current operator does not change, since the interaction commutes with the local density operator, but the matrix elements of the current Eq. (25) do change. To separate the Drude contribution, we estimate the matrix element of the current for the interacting case. Introducing a bosonic field $\phi$ and its conjugate momentum $\Pi$, which satisfy the commutation relations $[\phi(x), \Pi(y)] = i \delta(x - y)$, we get the following Gaussian model as the effective bosonic Hamiltonian of free fermions:

$$\tilde{H}(\Delta = 0) = \frac{u(\Delta = 0)}{2} \int_0^L dx \left[ (\partial_x \phi)^2 + \Pi^2 \right]. \quad (30)$$

In the LL approach, the presence of the interaction $\Delta$ leads simply to the rescaling of the bosonic field $\phi \rightarrow \sqrt{K} \phi$, having the following rescaling effect on the current:

$$\tilde{J} \rightarrow \frac{1}{\sqrt{K}} \int_0^L dx \partial_x \phi$$

and the effective LL Hamiltonian of interacting fermions is

$$\tilde{H}_{XXZ} = \tilde{H}(\Delta = 0) + \Delta \sum_i S_i^x S_{i+1}^x$$

$$\rightarrow \tilde{H}_{LL} = \frac{u}{2} \int_0^L (\partial_x \phi)^2 + \Pi^2 \right] dx.$$\]

The matrix element of $\int_0^L \Pi dx$ between the ground state and excited states is calculated in the Appendix.

Thus, the effect of interactions on the Drude weight (the singular contribution) boils down to rescaling of the matrix elements of the total current for the free case Eq. (20) by the factor $\sqrt{K}$, and of course the sound velocity $u$ is also renormalized by the interaction:

$$D(\omega) = \frac{\pi}{L \omega} \sum_{k=0}^{\infty} \frac{4 K u^2}{(2k+1)^2 \pi^2} \delta(\omega - \frac{(2k+1)u \pi}{L}). \quad (31)$$

The integral of the Drude part $D(\omega)$ is exactly equal to that of the Drude weight in a periodic chain:

$$\int_0^\infty D(\omega) d\omega = \sum_K \frac{4 K u}{(2k+1)^2 \pi^2} = \frac{K u}{2}. \quad (32)$$

Needless to say, as in periodic chains, the singular part $D(\omega)$ almost exhausts the sum rule (14) for $K \lesssim 1/4$. The regular part of the conductivity in open and periodic
chains can, generally speaking, be different, but the sum rule requires that
\[ \lim_{L \to \infty} \frac{1}{L} \int_0^\infty \frac{\sigma_{\text{reg}}^0 - \sigma_{\text{reg}}}{d \omega} \, d\omega \to 0. \]

Importantly, the leading size dependence of the CFS comes from the singular part \( D(\omega) \), and thus in an open chain the CFS scales quadratically with the system size:
\[ \chi_j^0 = \frac{L}{\pi} \int_0^\infty \frac{D(\omega)}{\omega} = \sum_{k=0}^{\infty} \frac{4KL^2}{\pi^4(2k+1)^3} = \frac{7\zeta(3)}{2\pi^4} KL^2, \]
where \( \zeta(x) \) is the Riemann zeta-function. This result prominently illustrates the difference between the periodic and open chains, and shows that one has to be careful when applying the CFS for detecting phase transitions: unless the transition involves some divergences in the current correlators, the leading contribution will be “blind” to it, so the divergence of \( \chi_j \) at the phase transition will be hidden in the subleading terms (usually, the exponent \( \mu \) that determines the finite-size scaling of the divergent part of the FS at the phase transition (see Eq. (33) is some number between 1 and 2).

We illustrate such “masking” on the example of the attractive single-component Bose-Hubbard model with the additional 3-body occupation constraint:
\[
H = -\frac{t}{2} \sum_j \left[ b_j^\dagger b_{j+1} + b_{j+1}^\dagger b_j \right] - \frac{id}{2} \sum_j \left[ b_j^\dagger b_{j+1} - b_{j+1}^\dagger b_j \right] + \frac{U}{2} \sum_j n_j(n_j - 1) + U_3 \sum_j n_j(n_j - 1)(n_j - 2),
\]
where \( b_j^\dagger, b_j \) are the bosonic creation/annihilation operators of particles at site \( j \), \( n_j = b_j^\dagger b_j \), and the three-body coupling constant \( U_3 \to \infty \) forbids sites with more than double occupancy. Fig. 4 presents the DMRG results for the FS study of the Ising phase transition between the single-particle superfluid and pair superfluid states (see the phase diagram in Ref. 13). The transition is easily detected by looking at the FS with respect to the hopping part (changing \( t \)), but when it is studied by looking at the current FS (i.e., the parameter \( d \) is changed), it is masked for chains with o.b.c. as seen in the lower panel of Fig. 4.

### D. Alternative derivation of the CFS scaling for open boundary conditions

The CFS behavior in spin-\( S \) XXZ chain with arbitrary half-integer \( S \) can be analyzed with the help of a different approach, valid at any \( d \) as well as at finite magnetization \( M \) (i.e., in presence of some external magnetic field). Consider a unitary transformation defined by the twist operator
\[
\hat{U}[\phi(d)] = e^{i\phi(d)\hat{\mathcal{P}}}, \quad \hat{\mathcal{P}} = \sum_j j S_j^z,
\]
where \( \phi(d) = \arctan(d) \) and \( \hat{\mathcal{P}} \) is the “polarization” operator, or the “spin center of mass”. Applied to the Hamiltonian Eq. (3), it removes the DM interaction, for the price of changing the anisotropy. Performing two such transformations, \( U(d) \) and \( U(d + \delta d) \), one can transform the fidelity \( F(d, \delta d) \) into the matrix element of the form
\[
F(d, \delta d) = \langle \psi_0(M, \Delta_d) | e^{i[\phi(d+\delta d)-\phi(d)]\hat{\mathcal{P}}} | \psi_0(M, \Delta_{d+\delta d}) \rangle.
\]
where $\bar{\Delta}_d = \Delta / \sqrt{1 + d^2}$. Expanding the fidelity up to quadratic terms in $\delta d$, one obtains

$$F(d, \delta d) \approx 1 - \frac{1}{2} \delta \Delta^2 \chi_{\Delta}$$

$$+ i \delta \phi \langle \psi_0(M, \bar{\Delta}_d) | \hat{P} | \psi_0(M, \bar{\Delta}_d + \delta d) \rangle$$

$$- \frac{1}{2} \delta \phi^2 \langle \psi_0(M, \bar{\Delta}_d) | \hat{P}^2 | \psi_0(M, \bar{\Delta}_d + \delta d) \rangle,$$

where $\delta \phi = \delta d / (1 + d^2)$ and $\delta \Delta = -\frac{1}{2} \Delta (1 + d^2)^{-3/2} \delta d$, and $\chi_{\Delta}$ is the FS with respect to the anisotropy,

$$\chi_{\Delta} = \lim_{\delta \Delta \to 0} \frac{1 - |F(\Delta, \delta \Delta)|^2}{\delta \Delta^2}.$$

$\chi_{\Delta}$ scales with the system size $L$ in a standard way, i.e., linearly, so it can be neglected if we are interested only in the leading $L$ dependence of $\chi_{j}$ which, as we can already guess, is quadratic.

We will further assume that the total $z$-projection of the spin $S_{\text{tot}}^z = \sum_j S_j^z = ML$ is a good quantum number, then even at finite magnetization the ground state wave function $|\psi_0(M, \bar{\Delta}_d)\rangle$ can be made real, so that the geometric connection term

$$\langle \psi_0(M, \bar{\Delta}_d) | \hat{P} | \psi_0(M, \bar{\Delta}_d + \delta d) \rangle \sim (\text{h.c.})$$

vanishes. Then the leading term in the current FS can be written as

$$\chi_j^0(d, M) \approx \frac{1}{(1 + d^2)^2} \left( \langle \hat{P}^2 \rangle - \langle \hat{P} \rangle^2 \right),$$

where the averages here and in what follows are taken in the ground state $|\psi_0(M, \bar{\Delta}_d)\rangle$. This in turn leads to the formula

$$\chi_j^0(d, M) = \frac{1}{2(1 + d^2)^2} \sum_{j', j''} (j - j')^2 \left( \langle S_j^z S_{j'}^z \rangle - \langle S_j^z \rangle \langle S_{j'}^z \rangle \right),$$

where we have again used the assumption that $S_{\text{tot}}$ is conserved and hence

$$\sum_{j', j''} j^2 \left( \langle S_j^z S_{j'}^z \rangle - \langle S_j^z \rangle \langle S_{j'}^z \rangle \right) = 0.$$

Note that the evaluation of the CFS is simplified drastically for open boundary conditions, since it is reduced to the task of calculating the spin-spin correlation functions in the ground state.

Only the smooth part of the correlation function $\langle S_j^z S_{j'}^z \rangle$ contributes to the leading size dependence of $\chi_j^0$. This smooth part has the following universal behavior [6] (see also Ref. 25, where exact correlation functions for an open spin-$1/2$ XY chain have been calculated):

$$\langle S_j^z S_{j'}^z \rangle = \langle S_j^z \rangle \langle S_{j'}^z \rangle$$

$$\frac{K}{2 \pi^2} \left[ \frac{2(L + 1)}{\pi} \sin \frac{\pi x}{2(L + 1)} \right]^2 \cdot$$

$$f_2(x) = \left[ \frac{2(L + 1)}{\pi} \sin \frac{\pi x}{2(L + 1)} \right]^2,$$

where $\chi_{\text{CFS}}(d, M)$ denotes oscillating terms, and $K = K(M, \bar{\Delta})$ is the Luttinger liquid parameter that depends on the effective anisotropy $\bar{\Delta}$ and the magnetization per site $M$.

For $S = 1/2$ and $M = 0$, it is given by

$$K(M = 0, \bar{\Delta}) = \frac{\pi}{2 \arccos(-\bar{\Delta})}, \quad \bar{\Delta} = \frac{\Delta}{(1 + d^2)^{1/2}}.$$

In the limit $L \to \infty$ one can transform the sums into integrals. Introducing the relative and center of mass coordinates, $r = j - j'$ and $R = (j + j')/2$, we get,

$$\sum_{j, j'} (j - j')^2 \int_0^{L-r} \frac{dr}{2} \int_0^{L} \frac{dr}{f_2(r)} \int_0^{L} \frac{dy}{f_2(r)} \int_0^{L} \frac{dy}{f_2(r)}$$

$$= 2 \int_0^{L} \frac{dr}{f_2(r)} \int_0^{L} \frac{dr}{f_2(r)}$$

$$= \frac{4L^2}{\pi^2} \int_0^{\pi/2} dy \frac{(1 - 2y/\pi)y^2}{\sin^2 y}$$

$$= \frac{4L^2}{\pi^2} \left[ \frac{1}{2} \pi^2 \ln 2 + \frac{21}{4} \zeta(3) \right]$$

and

$$\sum_{j, j'} (j - j')^2 \int_0^{L/2} \frac{dr}{f_2(R)} \int_0^{2R} \frac{dr}{f_2(2R)}$$

$$= \frac{4L}{\pi^2} \int_0^{\pi/2} dy \frac{y^3}{\sin^2 y}$$

$$= \frac{8L^2}{3\pi^2} \int_0^{\pi/2} dy \frac{y^3}{\sin^2 y}$$

$$= \frac{L^2}{\pi^2} (2 \pi^2 \ln 2 - 7 \zeta(3)).$$

We obtain the final result for the system size dependence of the current FS in the gapless spin-$1/2$ XXZ chain with open boundaries, in the following form:

$$\chi_{\text{CFS}}^0(d, M) = \frac{7 \zeta(3)}{2 \pi^4 (1 + d^2)^{3/2}} K(M, \bar{\Delta}) + O \left( \frac{1}{L} \right).$$

For $S = 1/2$ chain at zero magnetization, one can use the formula [31] for the LL parameter to obtain a closed expression for the CFS; it is easy to see that $\chi_{\text{CFS}}^0(d = 0, M = 0)$ has a singular behavior at $\Delta = 1$.

The $L^2$ dependence of the current FS is a generic feature for gapless models with o.b.c. and conserved $S^z$, where one can eliminate the current term (the DM interaction) by means of a unitary “twist” operator [33], and where the smooth part of the $\langle S_j^z S_{j'}^z \rangle$ correlator decays like $1/(j - j'^2)$.

E. Relation to the tilt fidelity susceptibility

In a spin chain with open boundaries, one can study another quantity, which is, as we will show, related to the
current FS, namely, the fidelity susceptibility $\chi_F$ with respect to the “polarization” operator $\hat{P} = \sum_j j S_j^z$. For a spin-$\frac{1}{2}$ chain, this physically means a response to the gradient of the external magnetic field. For the equivalent system of spinless fermions this could be a response to the the “lattice tilt”, or, if one assumes that the particles are electrically charged, then this is a response to the external electric field. The tilt FS is given by

$$\chi_F = \sum_{n \neq 0} \frac{|\langle \psi_0 | \hat{P} | \psi_n \rangle|^2}{(E_n - E_0)^2}. \quad (45)$$

It is easy to see that the tilt FS is related to the “dynamic polarizability” $\alpha(\omega)$

$$\alpha(\omega) = \frac{1}{L} \sum_{n \neq 0} |\langle \psi_0 | \hat{P} | \psi_n \rangle|^2 \delta(\omega - (E_n - E_0)) \quad (46)$$

by the following formula:

$$\chi_F = \frac{L}{\pi} \int_0^\infty d\omega \frac{\alpha(\omega)}{\omega^2}. \quad (47)$$

On the other hand, one has

$$i[\hat{H}_{XXZ}, \hat{P}] = \sum_i l(J_i - J_{i+1}) = \hat{J},$$

and thus $\sigma_1(\omega) = \omega \alpha(\omega)$, which leads to the following relation between the tilt FS and the conductivity:

$$\chi_F = \frac{L}{\pi} \int_0^\infty d\omega \frac{\sigma_1(\omega)}{\omega^3}. \quad (48)$$

Thus, the leading term in the finite size scaling of $\chi_F$, similarly to the CFS $\chi_J$, will be determined just by the low-frequency behavior of the conductivity. Using the formulas for the conductivity (49) and (50), one arrives at the following result:

$$\chi_F = \frac{31KL^4\zeta(5)}{8u^2\pi^6}. \quad (49)$$

For free fermions ($\Delta = 0$), the above result can be also reproduced directly in the same way as it has been done in Eqs. (24)–(25) for the conductivity, using the “density of states” (27) and the explicit expression for the matrix element (see the Appendix),

$$|\langle \psi_0 | \hat{P} | \psi_m \rangle| = \frac{L[1 - (-1)^m]}{(m\pi)^2}. \quad (50)$$

Indeed, using the perturbative expression

$$\chi_F = \sum_{m > 0} \rho(m) \frac{|\langle \psi_0 | \hat{P} | \psi_m \rangle|^2}{(E_m - E_0)^2} \quad (51)$$

with the linearized spectrum $E_m - E_0 \approx u\pi m/L$, one obtains for free fermions

$$\chi_F(\Delta = 0) = \sum_{k=0}^{\infty} \frac{4(2k + 1) L^2}{(E_{2k+1} - E_0)^2(2k + 1)^4\pi^4} \approx \frac{31L^4\zeta(5)}{8u^2\pi^6}. \quad (52)$$

For interacting fermions $S^z$ gets the additional factor of $\sqrt{K}$ (see the Appendix), hence bringing us back to the general result (49).

For the ratio of the current FS and the tilt FS in open chains one obtains the universal result

$$\frac{L^2 \chi_I}{\chi_F} = \frac{28u^2\pi^2\zeta(3)}{31\zeta(5)} \approx 10.3341u^2. \quad (53)$$

### III. CURRENT FS IN THE FERMIONIC HUBBARD MODEL

Consider the Hubbard model for spin-$\frac{1}{2}$ fermions (attractive or repulsive), at arbitrary filling:

$$\hat{H}_0 = - \sum_{j, \sigma} (c_j^{\dagger} \sigma c_{j+1,\sigma} + \mathrm{H.c.}) + U \sum_j n_j^2, \quad (54)$$

where $c_{j,\sigma}$ annihilates a fermion at site $j$ with the spin $\sigma = \{\uparrow, \downarrow\}$, and $n_j = \sum_\sigma c_j^{\dagger} \sigma c_{j,\sigma}$ is the fermion density at the site. We assume open boundary conditions, and study the FS $\chi_F$ with respect to the total current, $\vec{I} = \vec{I}_0 + \lambda \vec{I}_{\text{tot}}$, with

$$\vec{I}_{\text{tot}} = -i \sum_{j, \sigma} (c_j^{\dagger} \sigma c_{j+1,\sigma} - c_{j+1,\sigma}^{\dagger} c_{j,\sigma}). \quad (55)$$

The CFS can be calculated using the method of the unitary twist operator, as described in Sect. II D for spin chains, with the replacement of $S_j^z$ by $n_j$. One can closely follow all the steps of the calculation presented above for a spin chain, and express the CFS through the density-density correlation function of the Hubbard model. Assuming that its smooth part has the form similar to Eq. (10), with $K$ now being the charge Luttinger parameter $K_c$ of the Hubbard model, we obtain the leading term in the finite-size scaling of the CFS as follows:

$$\chi_F^2 = \frac{7\zeta(3)}{\pi^4} K_c \nu, M + O(\frac{1}{L}), \quad (56)$$

where $\nu$ is the lattice filling and $M$ is the magnetization. Fig. 4 shows the theoretical curve corresponding to Eq. (50) for the repulsive Hubbard model at $M = 0$, versus numerical results obtained by means of the density matrix renormalization group (DMRG) technique for open chains of up to $L = 128$ sites. The agreement between the analytical expression and numerical results is quite good, especially taking into account the fact that our analytical result (56) concerns only the $\sim L^2$ contribution.

Similar to the case of spin chains, one can study the tilt FS $\chi_F$ (i.e., the response to the perturbation determined by $\check{W} = \sum_j j n_j$) of the fermionic Hubbard model with gapless charge excitations. Physically, such a perturbation can be either the lattice tilt (for atoms in optical lattices), or simply the external electric field (for charged
corresponds to the analytical expression (56).

Finally, a few remarks are in order concerning the behavior of Hubbard chains with p.b.c. One can again use the general connection between the current FS and the conductivity, as we have done for spin chains, but now it is the charge current and the charge conductivity, respectively. In the repulsive Hubbard model at half-filling and at any magnetization, the charge excitations are gapped, so we expect the linear scaling of CFS independent of boundary conditions. Away from the half-filling, using the low frequency result for the conductivity of doped Mott insulators $\sigma_{\text{reg}}(\omega) \sim \omega^{12}$, one again obtains a linear finite-size scaling, $\chi^p_\ell \sim L$, for any filling $\nu$ and magnetization $M$. The same behavior (linear scaling of the CFS) we expect for the attractive case away from half-filling as well, at any filling and magnetization.

At half filling, however, provided the perturbative result $\sigma_{\text{reg}}(\omega) \sim U^2\omega^{4K_c-5}$ holds for the Hubbard model, one obtains

$$\chi^p_\ell \sim L, \quad K_c > 5/4,$$

$$\chi^p_\ell \sim L^{6-4K_c}, \quad K_c < 5/4. \quad (58)$$

The point $K_c = 1$ is special in Hubbard model, as it corresponds to $U = 0$ and hence $\chi^p_\ell = 0$ there.

### IV. CURRENT FS IN GAPPED SYSTEMS

Up to now, we have dealt with systems that have gapless excitation spectrum, apart of the comment on Hubbard model at half-filling in the previous section. It is easy to see that the system size dependence of the CFS in gapped systems is generically linear, $\chi^p_\ell \propto L$, independent of boundary conditions. The reason is that Drude part disappears in gapped phases and conductivity vanishes at energies below excitation gap $\omega_0$ (no excited states are available below gap), $\sigma_\ell(\omega) \sim \Theta(\omega - \omega_0)$, where $\Theta(x)$ is a step function. Alternatively for systems with o.b.c., the unitary transformation approach of Sec. III D (which is applicable in case of a pure chain geometry, i.e., in absence of next-nearest-neighbor and longer range hoppings) can be utilized for gapped spin chains as well, and leads to the formulas (58) and (59) connecting the CFS and the reduced longitudinal spin-spin correlator. In a gapped system (for example, in the Néel state of the spin-$\frac{1}{2}$ XXZ chain at $\Delta > 1$, or in the Néel and rung-singlet phases of the spin-$\frac{1}{2}$ XXZ ladder, see below), this correlator decays exponentially, so the sum in (59) will be proportional to $L$. A similar argument can be applied for fermionic or bosonic models.

Numerically, if the gap is extremely small, it may be difficult to distinguish exponential decay from algebraic one; for the FS this would mean distinguishing the linear scaling $\chi^p_\ell \propto CL$ with a large prefactor $C$ from the quadratic scaling, $\chi^p_\ell \propto L^2$.

We illustrate the generic behavior of the CFS in gapped systems on the example of the spin-$\frac{1}{2}$ antiferromagnetic spin ladder defined by the Hamiltonian

$$\hat{H}_{\text{Lad}} = \sum_{l,\alpha} \left[ S^x_{l,\alpha} S^x_{l+1,\alpha} + S^y_{l,\alpha} S^y_{l+1,\alpha} + \Delta S^z_{l,\alpha} S^z_{l+1,\alpha} \right] + J_R \sum_l \vec{S}_{l,1} \cdot \vec{S}_{l,2} + d \sum_{l,\alpha} (\vec{S}_{l,\alpha} \times \vec{S}_{l+1,\alpha})^2, \quad (59)$$

where $\alpha = 1, 2$ denotes the two legs of the ladder. In Fig. 6 we show the DMRG results for the CFS in the vicinity of the Ising quantum phase transition between the Néel and rung-singlet states. Ordinary quadratic scaling of the CFS peak at transition and linear scaling of the wings is observed.

However, there are peculiar cases when the CFS may have a nontrivial finite size scaling in a gapped system with open boundaries. Namely, in a topologically ordered system, the presence of entangled edge spins localized at the boundaries may render the sum in (59) $\propto L^2$, despite the exponentially decaying correlation function. Let us take the spin-1 Haldane chain as an example. The topologically ordered ground state of the open Haldane chain is “nearly” fourfold degenerate due to the presence of spin-$\frac{1}{2}$ edge spins localized at the boundaries: the lowest state is a singlet, which is split from the Kennedy-Tasaki triplet by the exponentially small “boundary gap” $\propto e^{-L/\xi}$, where $\xi \sim 6$ is the bulk correlation length. In the singlet ground state, the reduced correlator between the edge spins remains finite, so, according to (59), $\chi^p_\ell \propto L^2$. It is clear that this behavior will be typical for any state characterized by the presence of edge spins that are non-locally entangled with each other.

The scaling of $\chi^p_\ell$ will be very sensitive to the numer-
Combining numerical simulations with analytical arguments based on bosonization, we have studied the finite size scaling of the current fidelity susceptibility \( \chi_J \) with respect to the charge or spin current in gapless one-dimensional lattice models. We related it to the low-frequency behavior of the regular part of the conductivity, while in open systems \( \chi_J \) is determined by the singular part of the conductivity that is essentially the smeared Drude peak.

For the systems with o.b.c. we obtained the universal quadratic scaling \( \chi_J \propto L^2 \), which obscures the detection of quantum phase transitions between two gapless regions from the finite-size scaling of the peak in \( \chi_J \). Furthermore, for open chains we related \( \chi_J \) with the “tilt” fidelity susceptibility that describes the response to the gradient of the chemical potential.

In the future studies, it would be interesting to perform numerical calculations of \( \chi_J \) for large periodic spin-\( \frac{1}{2} \) XXZ chains \( L > 100 \), to confirm the nontrivial low-frequency behavior of the regular conductivity predicted by Giamarchi for \( \Delta \lesssim 1 \). It would also be interesting to study 1d models with iTEBD method and determine the scaling of \( \chi_j \) with matrix dimension. Similar studies in higher dimensions can also be interesting.

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Appendix

In this Appendix, we derive analytical expressions for matrix elements of the total momentum \( \int_0^L \Pi dx \) and the ‘center-of-mass’ operator \( \int_0^L x \partial_x \phi(x) dx \) between the vacuum and excited states of the Gaussian bosonic model, for the case of zero boundary conditions.

We start with the total momentum operator. It is convenient to expand the bosonic fields in the Fourier modes of the open string,

\[
\tilde{\phi}(x) = \sqrt{\frac{2}{L}} \sum_{n=1}^{\infty} \sin \frac{\pi nx}{L} \phi_n
\]

\[
\tilde{\Pi}(x) = \sqrt{\frac{2}{L}} \sum_{n=1}^{\infty} \sin \frac{\pi nx}{L} \pi_n,
\]

which guarantees the boundary conditions \( \tilde{\phi}, \tilde{\Pi} = 0 \) at the chain ends. The inverse relations,

\[
\phi_n = \sqrt{\frac{2}{L}} \int_0^L \sin \frac{\pi nx}{L} \tilde{\phi}(x) dx
\]

\[
\pi_n = \sqrt{\frac{2}{L}} \int_0^L \sin \frac{\pi nx}{L} \tilde{\Pi}(x) dx
\]

imply that zero modes for open chain do not exist,

\[
\phi_0 \equiv 0 , \quad \pi_0 \equiv 0 .
\]

Commutation relations of the Fourier modes are canonical,

\[
[\phi_n , \pi_m ] = i \delta_{n,m} .
\]

The total momentum operator in terms of the Fourier components can be rewritten as

\[
\int_0^L \tilde{\Pi} \, dx = \int_0^L \sqrt{\frac{2}{L}} \sum_{n=1}^{\infty} \sin \frac{\pi nx}{L} \pi_n \, dx
\]

\[
= \sqrt{2L} \sum_{n=1}^{\infty} \frac{1 - (-1)^n}{\pi n} \pi_n ,
\]
and the Luttinger liquid Hamiltonian reads

\[ \hat{H}_{LL} = \frac{u}{2} \int_0^L \left[ (\partial_x \hat{\phi})^2 + \hat{\Pi}^2 \right] \, dx \]

\[ = \frac{u}{2} \sum_{n=1}^{\infty} \left[ \frac{\pi^2 n^2}{L^2} + \frac{\pi n}{L} \phi_n^2 \right] \]

\[ = \frac{\pi u}{L} \sum_{n>0} \left[ \hat{a}_n^\dagger \hat{a}_n + \frac{1}{2} \right] = \sum_{n>0} \omega_n \hat{a}_n^\dagger \hat{a}_n + E_0. \]

Here

\[ \hat{a}_n^\dagger = \sqrt{\frac{L}{2\pi n}} \hat{\pi}_n + i \sqrt{\frac{\pi n}{2L}} \hat{\phi}_n \]

\[ \hat{a}_n = \sqrt{\frac{L}{2\pi n}} \hat{\pi}_n - i \sqrt{\frac{\pi n}{2L}} \hat{\phi}_n \]

(65)

are the standard bosonic creation and annihilation operators, \( \hat{a}_n |0\rangle = 0 \), satisfying the commutation relations \( [\hat{a}_n, \hat{a}_{m}^\dagger] = \delta_{n,m} \), and defining the eigenstates \( \hat{H}_{LL} \hat{a}_n^\dagger |0\rangle = (\omega_n + E_0) \hat{a}_n^\dagger |0\rangle \).

The total momentum in this basis obtains the following form:

\[ \int_0^L \hat{\Pi} \, dx = L \sum_{n} \frac{1 - (-1)^n}{\sqrt{\pi n}} \left[ \hat{a}_n + \hat{a}_n^\dagger \right]. \]

(66)

Hence,

\[ \langle n | \int_0^L \hat{\Pi} \, dx | 0 \rangle = L \frac{1 - (-1)^n}{\sqrt{\pi n}}. \]

(67)

The matrix elements of the fermionic total current are obtained from the relation,

\[ \hat{J} \rightarrow \frac{\sqrt{K u}}{\sqrt{\pi}} \int_0^L \hat{\Pi} \, dx. \]

so that,

\[ \rho(n) | \langle \psi_n | \hat{J} | \psi_0 \rangle |^2 = \frac{K u^2}{\pi} | \langle n | \int_0^L \hat{\Pi} \, dx | 0 \rangle |^2 \]

\[ = \frac{K L u^2 [1 - (-1)^n]^2}{\pi^2 n^3}. \]

(68)

Note that in the bosonized formulation each eigenstate with the energy \( E_n = u \pi n / L + E_0 \), obtained from the vacuum by acting with the total momentum operator, involves a single state \( \hat{a}_n^\dagger |0\rangle \); in other words, the bosonic density of states is \( \rho_{bosonic}(n) = 1 \), as opposed to the fermionic picture where \( \rho(n) = n \).

In a similar way, we can calculate the matrix elements of the polarization (center of mass) operator

\[ \hat{P} = \sum_j j S_j^z \rightarrow - \sqrt{\frac{K}{\pi}} \int_0^L x \partial_x \hat{\phi}(x) \, dx. \]

One obtains

\[ - \int_0^L x \partial_x \hat{\phi}(x) \, dx = - \sum_n \frac{\sqrt{2L}}{\pi n} \int_0^{\pi n} y \cos y \, \phi_n \]

\[ = \sqrt{2L} \sum_n \frac{1 - (-1)^n}{\pi n} \phi_n. \]

(69)

On the other hand,

\[ \phi_n = \frac{\sqrt{2L} a_n^\dagger - a_n}{2i} \]

(70)

hence,

\[ - \int_0^L x \partial_x \hat{\phi}(x) \, dx = L \sum_n \frac{1 - (-1)^n}{\pi n} \frac{a_n^\dagger - a_n}{i}. \]

(71)

In a full similarity to Eq. (65), we arrive at the generalization of Eq. (60) to the interacting case:

\[ \rho(n) | \langle \psi_n | \hat{P} | \psi_0 \rangle |^2 = \frac{K L^2 [1 - (-1)^n]^2}{\pi^4 n^3}. \]

(72)

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