Quantum fluctuations of one-dimensional free fermions and Fisher–Hartwig formula for Toeplitz determinants

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Abstract
We revisit the problem of finding the probability distribution of a fermionic number of one-dimensional spinless free fermions on a segment of a given length. The generating function for this probability distribution can be expressed as a determinant of a Toeplitz matrix. We use the recently proven generalized Fisher–Hartwig conjecture on the asymptotic behavior of such determinants to find the generating function for the full counting statistics of fermions on a line segment. Unlike the method of bosonization, the Fisher–Hartwig formula correctly takes into account the discreteness of charge. Furthermore, we numerically check the precision of the generalized Fisher–Hartwig formula, find that it has a higher precision than rigorously proven so far and conjecture the form of the next-order correction to the existing formula.

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(Some figures may appear in colour only in the online journal)

1. Introduction
The problem of finding the fermion-number fluctuation on a segment for free one-dimensional spinless fermions is a classical textbook problem. It is related to a variety of topics in the theory of one-dimensional quantum systems and in mathematical physics, such as quantum spin chains \([1, 2]\), bosonization \([3]\), full counting statistics (FCS) \([4, 5]\), random-matrix theory \([6]\), theory of Toeplitz determinants \([7, 8]\), etc. Remarkably, some helpful results related to this simple problem have been obtained only recently: a generalized version of the Fisher–Hartwig conjecture on Toeplitz determinants has been proven \([9]\). These mathematical results were further used in a non-equilibrium bosonization approach in \([10, 11]\).

In this paper, we use the generalized Fisher–Hartwig formula to calculate the generating function for FCS of free fermions on a one-dimensional line segment. Unlike the bosonization
approach, the generalized Fisher–Hartwig formula treats correctly the discreteness of particles. As a result, we obtain a quantitative description of the development of the singularity in the FCS generating function in the limit of a large segment length (an FCS phase transition, in the definition of [12]).

Furthermore, we investigate numerically the precision of the existing generalized Fisher–Hartwig formula and come to the conclusion that it is more precise than formally proven. In addition, our numerical results allow us to extract the next-order correction to the existing formula and to conjecture its analytic form.

The paper is organized as follows. In section 2, we define the problem of counting free fermions on a one-dimensional line segment. In section 3, we briefly review the existing analytical approaches to the problem and apply the generalized Fisher–Hartwig formula to obtain a good approximation for the FCS generating function. In section 4, we analyze the precision of the obtained expression numerically and conjecture its improvement by including a higher order correction. Finally, in section 5 we summarize our findings. Some technical details are presented in the appendices.

2. Formulation of the problem: counting fermions on a 1D line segment

Consider free spinless fermions in one dimension (either on a line or on a one-dimensional lattice) at zero temperature. We study the fluctuations of the fermion number on a segment of a large length $L$. The system is considered at zero temperature, with the fermionic levels filled for wavevectors $-k_F < k < k_F$. Thus, the Fermi wave vector $k_F$ is the only parameter defining the state, and the form of the energy spectrum is irrelevant.

One can easily find (using either Wick’s theorem or bosonization) that

$$\langle (Q^2) \rangle \equiv \langle (Q - \langle Q \rangle)^2 \rangle \sim \frac{1}{\pi^2} \ln(L/l_0)$$  \hspace{1cm} (1)

in the limit of a large segment length $L \gg l_0$. Here, $Q = \int_0^L dx \, c^\dagger c$ is the operator of the total number of fermions (total charge) on the segment ($c^\dagger$ and $c$ are the fermionic creation and annihilation operators). The ultraviolet cutoff $l_0$ is given by $l_0 \sim k_F^{-1}$ on the line and by $l_0 \sim (\sin k_F)^{-1}$ on the lattice (here and below we set the lattice constant equal to 1, in order to shorten the formulas). The average charge on the segment is given exactly by

$$\langle Q \rangle = Lk_F/\pi$$  \hspace{1cm} (2)

(so that the average density of fermions is $k_F/\pi$).

A more complicated problem is to find all moments of charge $\langle Q^k \rangle$ or, equivalently, the full distribution of probabilities of having a given charge $q$ on a segment. Instead of calculating all moments separately, it is convenient to introduce the characteristic function

$$\chi(\lambda) \equiv \langle e^{i\lambda Q} \rangle = \sum_{q=0}^\infty P_q e^{i\lambda q}$$  \hspace{1cm} (3)

also known as the FCS generating function. The charge cumulants may be expressed as its logarithmic derivatives:

$$\langle (Q^k) \rangle = (-i\partial_{\lambda})^k \log \chi(\lambda)|_{\lambda=0}.$$  \hspace{1cm} (4)

It is obvious from the definition of (3) that (i) $\chi(\lambda)$ is normalized so that $\chi(0) = 1$, (ii) $\chi(-\lambda) = \chi^*(\lambda)$ and (iii) it is periodic $\chi(\lambda + 2\pi) = \chi(\lambda)$. The latter property follows from the fact that the charge operator is integer-valued (all charges are integer numbers). Our goal is to find a good approximation for $\chi(\lambda)$ in the limit of large $L$. 

2
3. From bosonization to generalized Fisher–Hartwig conjecture: early approaches and new results

The simplest approach to calculating \( \chi(\lambda) \) is bosonization, which is equivalent to assuming that the density fluctuations are Gaussian. This assumption leads immediately to the following result:

\[
\ln \chi(\lambda) \approx \frac{i}{2} \lambda \langle Q \rangle - \frac{\lambda^2}{2} \langle \langle Q^2 \rangle \rangle
\]  

with the average charge and the variance given by (2) and (1), respectively (see appendix A for a brief review of the bosonization calculation).

One can notice two obvious drawbacks of this approximation. First, the bosonization method does not allow us to calculate the numerical coefficient for the ultraviolet cut-off \( l_0 \). This problem can be partly solved by a direct calculation of the second moment in the original fermionic representation using Wick’s theorem. Such a calculation (see appendix D) reproduces the result (1) with \( l_0^{-1} = 2e^{\gamma_E} \sin k_F \) in the lattice problem and \( l_0^{-1} = 2e^{\gamma_E} k_F \) in the continuous case (note that the formulas for the continuous case may be obtained from the results on the lattice by taking the limit \( k_F \to 0 \) while keeping the product \( k_F L \) fixed). Here, \( \gamma_E = 0.57721\ldots \) is the Euler–Mascheroni constant.

Nevertheless, even after fixing the numerical coefficient in \( l_0 \), the bosonization result for \( \chi(\lambda) \) is only precise up to a numerical \( \lambda \)-dependent coefficient of order 1. These \( \lambda \)-dependent corrections may be interpreted as cumulants of order higher than 2, which are not captured by bosonization. If we include those corrections, we arrive at the following expansion:

\[
\ln \chi(\lambda) = \frac{i k_F}{\pi} L - \frac{\lambda^2}{2\pi^2} \ln \frac{L}{l_0} + F_0(\lambda) + o(1)
\]

as \( L \to \infty \). The function \( F_0(\lambda) \) may, in principle, be reconstructed from the cumulants \( \langle \langle Q^k \rangle \rangle \) calculated with the help of Wick’s theorem. Such calculations appear to be very tedious. Fortunately, the exact expression for \( F_0(\lambda) \) can be obtained using the determinant representation of (3) and the Fisher–Hartwig formula for Toeplitz determinants (see appendix B for details and references):

\[
F_0(\lambda) = 2 \ln \left| G \left( 1 + \frac{\lambda}{2\pi} \right) G \left( 1 - \frac{\lambda}{2\pi} \right) + \frac{\lambda^2}{2\pi^2} (\gamma_E + 1) \right|
\]

where \( G(z) \) is the Barnes G-function [13]. Remarkably, \( F_0(\lambda) \) does not depend on \( k_F \), even in the lattice version 4.

The second deficiency of the bosonization approximation is that \( \chi(\lambda) \) does not obey the periodicity property. This is due to the nature of the bosonization approximation, which treats the fermionic density as a continuous field and thus ignores the discreteness of the fermionic charge. This problem was addressed in [7], where a phenomenological formula was proposed to restore the periodicity (taking into account umklapp processes in the bosonization language). Aristov’s ansatz in [7] corresponds to neglecting the correction \( F_0(\lambda) \) with its nontrivial \( \lambda \) dependence.

3 One can restore the dimensionful lattice constant \( a \) by replacing \( k_F \to k_F a \) and \( L \to L/a \) in all our formulas. Then the continuous case corresponds to the conventional limit \( a \to 0 \).

4 In the continuum limit this expression is identical to equations (4.6) and (4.19) of [14] obtained from the asymptotics of a Fredholm determinant.
In this work, we show that a rigorous formula restoring the periodicity of $\chi(\lambda)$ can be obtained by an application of the recently proven generalized Fisher–Hartwig conjecture [9]. It turns out that the correct recipe for the periodic extension of equation (7) is simply to add two such expressions with shifted values of $\lambda$ in the vicinity of the ‘switching points’ $\lambda = (2k + 1)\pi$:

$$\chi(\lambda) \approx \chi_0(\lambda - 2k\pi) + \chi_0(\lambda - 2[k+1]\pi),$$

where $\ln \chi_0(\lambda)$ is given on the right-hand side of equation (7). The two terms are of the same order of magnitude at the ‘switching point’ $\lambda = (2k+1)\pi$, but one of them becomes subleading (in $L$) away from this point. For the same reason, only two shifted values of $\lambda$ are of relevance at each ‘switching point’: shifts by higher multiples of $2\pi$ produce terms decaying as higher powers of $L$ and therefore may be neglected. The details of the application of the Fisher–Hartwig formula to our problem are presented in appendix B.2.

4. Improving the generalized Fisher–Hartwig formula: numerical analysis

In the proof of the generalized Fisher–Hartwig conjecture in [9], its precision is only estimated as a relative $o(1)$ as $L \to \infty$. This implies that, in the approximation (9), both terms are within the proven precision only exactly at the switching point (and therefore, at the switching point, the expansion (7) fails). Away from the switching point, the subleading term is already beyond the rigorously proven precision (and thus the expansion (7) is the best-proven estimate).

In order to rectify this situation, we perform a numerical analysis of the generalized Fischer–Hartwig formula (9) based on exact evaluation of Toeplitz determinants of sizes up to 5000. We claim that the formula (9) has a higher precision than that rigorously proven: the subleading of the two terms in equation (9) provides the main correction to the asymptotic behavior (7). Moreover, the next-order correction may be captured with the use of the following conjectured formulas (to simplify notation, we specify to the interval $\lambda \in [0, 2\pi]$):

$$\chi(\lambda) = \chi_1(\lambda) + \chi_1(\lambda - 2\pi) + \varepsilon,$$

where

$$\chi_1(\lambda) = \exp\left[i\lambda\frac{k_F}{\pi} - \frac{\lambda^2}{2\pi^2} \ln \frac{L + F_0(\lambda) + F_1(k_F, \lambda)}{l_0}L^{-1}\right],$$

and the higher order correction $\varepsilon$ is of the relative order $L^{-2}$. More precisely, it can be estimated as

$$\varepsilon = ((|\chi_1(\lambda)| + |\chi_1(\lambda - 2\pi)|) \cdot O(L^{-2}).$$

We confirm this conjecture numerically by extracting the coefficient $F_1(k_F, \lambda)$ and verifying the estimate (12) for the deviation from the fit. As a result of the fit, we find that the coefficient $F_1(k_F, \lambda)$ is purely imaginary and an odd function of $\lambda$. Moreover, we observe that, to a very high precision, $F_1(k_F, \lambda)$ can be described by a simple formula

$$F_1(k_F, \lambda) = -\frac{i}{4} \left(\frac{\lambda}{\pi}\right)^3 \cot k_F$$

(see appendix C for details of the numerical calculations). We therefore conjecture that this formula is analytically exact for our expansion (10)–(12).

To support this conjecture, we have calculated the second and the third cumulants to the order $L^{-1}$ (see appendix D). While $\langle\langle Q^2\rangle\rangle$ does not produce any contribution at the order $L^{-1}$, the third cumulant, to the leading order, is given by

$$\langle\langle Q^3\rangle\rangle \sim \frac{3}{2\pi^3 L} \cot k_F,$$

(14)
which is consistent with equation (13). Furthermore, if there are corrections to equation (13), then they are of the order higher than $\lambda^3$. Since the relative deviation of the numerically extracted $F_1(k_F, \lambda)$ from the formula (13) does not exceed $10^{-4}$–$10^{-5}$ in the range of $\lambda = 0.3, \ldots, 1.3$ (error bars are higher for $\lambda$ close to zero and to $\pi$), we conclude that the numerical coefficients at such corrections, if nonzero, would be below $10^{-4}$ (at least, for the values of $k_F$ tested). It seems therefore likely that such corrections vanish identically and our suggested expression (13) is exact. It would be interesting to verify or disprove this conjecture by the methods of [9], and we leave this for future studies.

5. Summary and discussion

The results of this work are twofold. First, we apply the recently proven generalized Fisher–Hartwig conjecture to describe the asymptotic behavior of the FCS problem of counting free fermions on a line segment. Second, we analyze numerically the precision of the generalized Fisher–Hartwig formula and find that, at least in our case, it is more accurate than rigorously proven. Furthermore, we numerically extract the next-order correction to the generalized Fisher–Hartwig formula and conjecture a simple analytical expression for it.

We hope that our results will be useful in several respects. On the mathematical side, we hope that they will stimulate further studies of the asymptotic behavior of Toeplitz determinants. In particular, it seems plausible that our formulas (10) and (11) are the beginning of a more general exact expansion in powers of $L^{-1}$, see equations (E.1) and (E.2) of appendix E. Another interesting question would be extending the Fisher–Hartwig prescription (9) to block-Toeplitz determinants [15–17]. Such an extension would be relevant for various FCS problems with noninteracting fermions, where the generating function is given by the Levitov–Lesovik determinant formula [4, 5] related to block-Toeplitz matrices.

On the physical side, the example we consider in this work is probably the simplest quantum example of the ‘nonanalytic’ FCS phase, as defined in [12], where the thermodynamic limit ($L \to \infty$) can be studied in detail. Remarkably, the ‘sum prescription’ (9), which describes the development of the singularity in the generating function, is the same as in FCS phase transitions in classical Markov processes (see, e.g., the discussion of the ‘weather model’ in [12]). It would thus be interesting to explore the extent of universality of the formula (9), in particular in the case of interacting quantum models.

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Appendix A. Bosonization calculation of FCS for free fermions

Here, we briefly derive (5) (together with (2) and (1)) using the bosonization technique (see, e.g., [3]). In the simplest version of the bosonization approach, the density of one-dimensional fermions is given by

$$\rho(x) \approx \rho_0 - \frac{1}{\pi} \partial_x \phi(x),$$

where $\phi(x)$ is a free bosonic field with the correlation function

$$\langle [\phi(x) - \phi(0)]^2 \rangle \approx \ln \frac{|x|}{\ell_0}$$

(A.2)
with $l_0$ being an ultraviolet cutoff (of the order of lattice constant). Expression (A.2) is good at $|x| \gg l_0$. The number of fermions on a segment of length $L$ is obtained from (A.1) as
\[ Q = \int_0^L dx \rho(x) = \rho_0 L - \frac{1}{\pi} (\phi(L) - \phi(0)). \] (A.3)

Upon substituting this bosonized form in (3), we find
\[ \chi(\lambda) = e^{i \lambda \rho_0 L} \left( e^{-i \lambda (\phi(L) - \phi(0))} \right) = e^{i \lambda \rho_0 L} e^{-i \lambda^2 (\phi(L) - \phi(0))^2} = e^{i \lambda \rho_0 L / l_0} \left( L / l_0 \right)^{-\lambda^2 / (2 \pi^2)}, \] (A.4)
which gives us (5).

This calculation misses the most important property of $\chi(\lambda)$: its periodicity in $\lambda$. This is due to the approximation (A.1), which treats particles as a continuous medium. In fact, the full density operators also contain terms of higher conformal dimensions oscillating with the wavevector $2k_F$ and its multiples [18]. The inclusion of such terms would, in principle, restore the periodicity of $\chi(\lambda)$. However, the coefficients at those terms are non-universal (depending on the short-range structure of the theory), and we are not aware of any consistent way to calculate them for our problem without resorting to the theory of Toeplitz determinants.

At a phenomenological level, the effects of those higher order terms were taken into account in [7], which resulted in a qualitatively (but not quantitatively) correct approximation. The ansatz of [7] can also be reproduced in a different way: suppose we calculate the probabilities of different particle numbers as the Fourier transform of the bosonization result (A.4) and then restrict the particle number to be integer. This prescription produces the particle-number probabilities
\[ P_q \propto e^{-\frac{(q - \langle Q \rangle)^2}{2 \langle Q^2 \rangle}}, \] (A.5)
which result in the generating function
\[ \chi(\lambda) = \sum_{q=-\infty}^{+\infty} P_q e^{i \lambda q} \propto \sum_{j=-\infty}^{+\infty} e^{i (\lambda - 2\pi j) (\langle Q \rangle - \frac{\langle Q^2 \rangle}{\langle Q \rangle} (\langle Q \rangle^2))}, \] (A.6)
where we used Poisson’s summation formula (the overall coefficient being determined from the normalization condition $\chi(\lambda = 0) = 1$). Remarkably, this ansatz coincides with Aristov’s conjecture in [7]. It is only qualitatively correct (the errors being of relative order $O(L^{1/2})$), as can be seen from the exact results based on the Fisher–Hartwig formula.

Appendix B. Fisher–Hartwig formula for FCS of free fermions

In this appendix, we review the Toeplitz-determinant approach to the problem and apply the generalized Fisher–Hartwig formula.

B.1. Toeplitz-determinant representation for $\chi(\lambda)$

We start by reproducing the Toeplitz-determinant representation of $\chi(\lambda)$ following [1]. We consider lattice fermions hopping on an infinite one-dimensional lattice with sites labeled by integer numbers. The single-particle states are parameterized by the wave vector $k$ from the Brillouin zone, $k \in [-\pi, \pi]$. We assume that the ground state consists of the filled states with wavevectors $-k_F < k < k_F$, where $k_F$ is the Fermi wavevector. We do not specify Hamiltonian here, as we are interested in the static problem, where the correlator (3) is determined only by
the ground state of the system. The one-particle Green’s function in the coordinate space is given by

$$g_{ij} = g_{i-j} \equiv \langle c^\dagger_i c_j \rangle = \int_{-\pi}^{\pi} \frac{dk}{2\pi} g(k) e^{-i k (i-j)}, \quad (B.1)$$

where Green’s function in momentum space is the step function equal to 1 for $|k| < k_F$ and 0 otherwise:

$$g(k) = \Theta(k_F - |k|). \quad (B.2)$$

Explicitly combining (B.1) and (B.2), we obtain

$$g_{i-j} = \frac{\sin(k_F (i-j))}{\pi (i-j)} \quad (B.3)$$

with $g_0 = k_F / \pi$. The operator of the number of fermions on the segment $1 \leq j \leq L$ is given by

$$Q = \sum_{i=1}^{L} c^\dagger_i c_i. \quad (B.4)$$

Then, we can rewrite (3) as

$$\chi(\lambda) = \langle \sum_{i=1}^{L} e^{i \lambda i} c_i c_i \rangle = \left\langle \prod_{i=1}^{L} (1 + (e^{i \lambda} - 1)c^\dagger_i c_i) \right\rangle. \quad (B.5)$$

Here, we used the projector property $(c^\dagger_i c_i)^2 = c^\dagger_i c_i$. Applying Wick’s theorem to (B.5) we obtain

$$\chi(\lambda) = \det T_L = \det(1 + (e^{i \lambda} - 1)g)_{L \times L}, \quad (B.6)$$

where $1$ is the unit $L \times L$ matrix and $g$ is the $L \times L$ matrix with the matrix elements $g_{ij} = g_{i-j}$ given by (B.3).

The determinant (B.6) is that of the Toeplitz matrix $T_L$ (its matrix elements $(T_L)_{ij}$ depend only on the difference of the row and column indices $i-j$). It is said that this Toeplitz matrix $T_L$ has the symbol $f(e^{i \theta})$ with

$$f(e^{i \theta}) = 1 + (e^{i \lambda} - 1)\Theta(k_F - |\theta|), \quad (B.7)$$

so that the matrix elements are given by

$$(T_L)_{ij} = \int \frac{d\theta}{2\pi} e^{i \theta (i-j)} f(e^{i \theta}). \quad (B.8)$$

The formulas (B.6) and (B.3) express the FCS $\chi(\lambda)$ as the determinant of a given $L \times L$ Toeplitz matrix. As we are interested in the limit of large length of a segment, we need to find the asymptotics of the Toeplitz determinant (B.6) as $L \to \infty$.

**B.2. The Fisher–Hartwig conjecture**

Let us calculate the asymptotics of the Toeplitz determinant (B.6) as $L \to \infty$ using the Fisher–Hartwig conjecture [19, 9]. This appendix is not self-contained. We explicitly refer to the notations and the results of [9] (except for the matrix size denoted $L$ in our paper and $n$ in [9]).

5 For a recent similar application of the Fisher–Hartwig conjecture see [20, 11].
The symbol (B.7) of the Toeplitz matrix has two singularities. In the notation of [9], one of the singularities must be at \( \theta = 0 \), so if one follows the notation of that paper, one needs to consider an equivalent problem with the symbol

\[
f(e^{i\theta}) = \begin{cases} 
  e^{ik} & \text{for } 0 < \theta < 2kF \\
  1 & \text{for } 2kF < \theta < 2\pi.
\end{cases}
\]  

(B.9)

The two point singularities (Fisher–Hartwig singularities) on the unit circle are located at \( z_0 = 1 \) and \( z_1 = e^{2ik}\). These are pure phase discontinuities characterized by \( \alpha_0 = \alpha_1 = 0 \) and \( \beta_1 = -\beta_0 = \lambda/2\pi \) (for notations see [9]). The regular part of the symbol \( f(z) \) is given by \( V_L = 0 \) for \( k \neq 0 \) and by \( V_0 = i2kF \frac{z}{\pi} \). Then, theorem 1.1 of [9] (due to Ehrhardt [8]) gives

\[
\chi(\lambda) \sim e^{2ik_0\lambda L}(2L\sin kF)^{-2k_0} [G(1 + \kappa_0)G(1 - \kappa_0)]^2.
\]  

(B.10)

Here, \( \kappa_0 \equiv \frac{\lambda}{2\pi} \) and the result (B.10) is valid for \(-\pi < \lambda < \pi \) in the asymptotic sense as \( L \to \infty \). The relative accuracy of (B.10) is \( o(1) \).

The Barnes \( G \) function used in (B.10) is defined as [13]

\[
G(1 + z) \equiv (2\pi)^{z/2} e^{-\left(\frac{\pi(1 + z)}{2}\right)^2} \prod_{k=1}^{\infty} \left(1 + \frac{z}{k}\right)^{k} e^{-z+\frac{z^2}{2}}.
\]  

(B.11)

where \( \gamma_E \approx 0.57721 \ldots \) is the Euler–Mascheroni constant. We have from (B.11)

\[
G(1 + z)G(1 - z) \approx e^{-\gamma_E z^2} \prod_{k=1}^{\infty} \left(1 - \frac{z^2}{k^2}\right)^k e^{\frac{z^2}{4}}.
\]  

(B.12)

To extend the result (B.10) to \( \lambda \) outside the interval \((-\pi, \pi)\), one has to introduce the realizations of the symbol [9]. In our particular case, it amounts to using (B.10) with \( \kappa_0 \) replaced by

\[
k_j = \frac{\lambda}{2\pi} - j
\]  

(B.13)

for \(-\pi + j < \lambda < \pi + j, \ j = 0, \pm 1, \pm 2, \ldots \). In other words, for a given \( \lambda \), one should replace in (B.10) \( \kappa_0 \to k_j \) with the value \( j \) minimizing \( k_j \). It is important that for \( \lambda \) being an odd multiple of \( \pi \) there are two such values of \( j \) minimizing \( k_j \). In these cases, one should replace (B.10) by the sum over corresponding realizations. In particular, according to theorem 1.13 of [9] we have for \( \lambda = \pi \)

\[
\chi(\lambda) \sim \sum_{j=0,1} e^{2ik_0\lambda L}(2L\sin kF)^{-2k_0} [G(1 + \kappa_j)G(1 - \kappa_j)]^2.
\]  

(B.14)

Here \( \kappa_{0,1} = \pm 1/2 \). We argue in the main text that in fact, the accuracy of this formula is \( O(1/L) \). Moreover, the prescription of adding the most relevant realizations produces correct subleading terms even away from \( \lambda = \pi \).

B.3. Limits \( \lambda \to 0 \) and \( \lambda = \pi \)

For completeness, we present here the two limiting cases: \( \lambda \to 0 \) and \( \lambda = \pi \).

For small \( \lambda \), the leading realization in (B.14) is given by \( j = 0 \) (with the term \( j = 1 \) suppressed compared to \( j = 0 \) by about \( 1/L^2 \)). We have

\[
\chi(\lambda \ll \pi) \approx e^{\lambda e^{L} - \frac{\lambda^2}{\pi^2} \ln(2Le^{\pi^2 + 0.5}) - \frac{\lambda}{\pi^2}}' (3).
\]  

(B.15)

where we have expanded in small \( \lambda \),

\[
G(1 + z)G(1 - z) \approx e^{-\gamma_E z^2 - \frac{1}{2}z^4 + \cdots}.
\]  

(B.16)

6 A similar improvement of the Fisher–Hartwig formula was shown to work numerically for some Toeplitz determinants in [20] and was also suggested in [11].
We extract from (B.15)
\[ \langle Q \rangle = \frac{k_F}{\pi} L = \rho_0 L, \]  \hfill (B.17)

\[ \langle\langle Q^2 \rangle\rangle = \frac{1}{\pi^2} \ln[2L e^{i\pi+1} \sin k_F] + o(1), \]  \hfill (B.18)

\[ \langle\langle Q^4 \rangle\rangle = -\frac{3}{2\pi^2} \zeta(3) + o(1). \]  \hfill (B.19)

\[ \langle\langle Q^{2n+1} \rangle\rangle = o(1), \quad n = 1, 2, \ldots. \]  \hfill (B.20)

Let us now consider the case \( \lambda = \pi \). Then, the dominating parametrizations are \( j = 0, 1 \) (or, equivalently, \( \kappa = \pm 1/2 \)). We sum over these parametrizations in (B.14) and obtain
\[ \chi(\lambda = \pi) \sim 2[G(1/2)G(3/2)]^2 \cos(k_F L) \sqrt{2L \sin k_F}. \]  \hfill (B.21)

**Appendix C. Details of numerical calculations**

Numerical calculations of the Toeplitz determinant (B.6), up to \( L = 5000 \), were performed using the superfast algorithm of [21] implemented in C++ and, independently, with the help of Wolfram Mathematica [22] (the two methods agree within the error bars, which range from \( 10^{-9} \) to \( 10^{-12} \), depending on the method). For our computations, we took three values of \( k_F \) (\( k_F/\pi = 1/30, 3/17, \) and \( 8/17 \)) and various values of \( \lambda \) (in multiples of \( 0.1\pi \)). The obtained determinants were then fitted according to equation (11), and the coefficients \( F_1(k_F, \lambda) \) were extracted for each pair of the parameters \( k_F \) and \( \lambda \) used. This fitting procedure involved splitting the whole range of values of \( L \) into intervals of an adjustable length and fitting within each interval (using \( F_1(k_F, \lambda) \) and \( F_1(k_F, \lambda - 2\pi) \) as the two fitting parameters). Then, the fit parameters were extrapolated to \( L \to \infty \) using quadratic or cubic polynomials in \( L^{-1} \). This fitting procedure allowed us to obtain a very good precision for \( F_1(k_F, \lambda) \).

The resulting values of \( F_1(k_F, \lambda) \) are presented in table C1. Within the error bars, \( F_1(k_F, \lambda) \) is purely imaginary, which, in combination with the reality condition \( F_1(k_F, -\lambda) = F_1(k_F, \lambda)^* \), implies that \( F_1(k_F, \lambda) \) is odd in \( \lambda \).

We further observe that thus the extracted function \( F_1(k_F, \lambda) \) can be described by the formula (13) to a very high precision. The ratio of the numerically extracted \( F_1(k_F, \lambda) \) to the analytical conjecture (13) is plotted in figure C1.

Finally, we calculate the error \( \varepsilon \) of our expansion at the order \( L^{-1} \), as defined in equation (10). In figure C2, we show a typical plot of the ratio \( |\varepsilon| L^2 \langle\langle \chi(\lambda) \rangle\rangle + |\chi(\lambda - 2\pi)\rangle^{-1} \). The plot suggests that this quantity remains finite at \( L \to \infty \), which supports our conjecture (12). In principle, the precision of our numerics should be sufficient for continuing the expansion in \( L^{-1} \) (the next term being of the order \( L^{-2} \)). This possibility is also connected to the question about the precision of the ‘sum prescription’ (9): whether this decomposition into a sum (involving all shifts of \( \lambda \) by multiples of \( 2\pi \)) is exact to all (perturbative) orders in \( L \) (see appendix E) or breaks down at a certain order. We leave this interesting mathematical question for future studies.
Figure C1. The ratio of the numerically found value of $F_1(k_F, \lambda)$ (reported in table C1) to the analytical conjecture (13).

Table C1. Numerical values of $iF_1(k_F, \lambda)$ extracted from the fits. For most of the data, the determinants were calculated with the precision $10^{-9}$. For several sets of data (marked by the asterisks), a higher precision ($10^{-12}$) was used, with the help of Mathematica [22]. Using higher precision results in reducing the error bars for the fitting parameters. The dashes in the last lines of the table correspond to the values of $\lambda$, for which $F_1(k_F, \lambda)$ could not be reliably determined from our computations.

| $\lambda/\pi$ | $k_F = \pi/30$ | $k_F = 3\pi/17$ | $k_F = 8\pi/17$ |
|---------------|-----------------|-----------------|-----------------|
| 0.1           | 0.002 382(9)    | 0.000 4043(4)   | 0.000 023 16(3)*|
| 0.2           | 0.019 04(1)     | 0.003 2315(6)   | 0.000 1858(3)   |
| 0.3           | 0.064 23(1)     | 0.010 9030(7)   | 0.000 6259(6)   |
| 0.4           | 0.152 24(1)     | 0.025 8409(4)*  | 0.001 4840(8)   |
| 0.5           | 0.297 34(2)     | 0.050 472(2)    | 0.002 8957(4)*  |
| 0.6           | 0.513 78(3)     | 0.087 217(3)    | 0.005 0038(1)*  |
| 0.7           | 0.815 86(5)     | 0.138 495(3)    | 0.007 947(1)    |
| 0.8           | 1.217 83(9)     | 0.206 731(4)    | 0.011 862(1)    |
| 0.9           | 1.7340(2)       | 0.294 348(5)    | 0.016 889(2)    |
| 1.0           | 2.3785(3)       | 0.403 763(7)    | 0.023 166(3)    |
| 1.1           | 3.1658(5)       | 0.537 40(1)     | 0.030 832(5)    |
| 1.2           | 4.1100(9)       | 0.697 70(4)     | 0.040 03(1)     |
| 1.3           | 5.225(2)        | 0.8870(1)       | 0.050 88(5)     |
| 1.4           | 6.525(4)        | 1.1078(3)       | 0.063 57(3)*    |
| 1.5           | 8.025(9)        | 1.362(2)        | 0.0782(2)*      |
| 1.6           | 9.74(3)         | 1.654(1)*       | 0.095(4)        |
| 1.7           | 11.6(3)         | 1.99(2)         | 0.12(2)         |
| 1.8           | 13(3)           | 2.3(1)          | –               |
| 1.9           | –               | –               | –               |

Appendix D. Second and third cumulants of the fermionic number on a line segment

In this appendix, we calculate analytically $\langle Q^2 \rangle$ and $\langle Q^3 \rangle$ up to the orders $L^{-2}$ and $L^{-1}$, respectively. Wick’s theorem expresses those cumulants in terms of the Green function.
Figure C2. A plot of $|\varepsilon| L^2 (|\chi_1(\lambda)| + |\chi_1(\lambda - 2\pi)|)^{-1}$ for $k_F = \pi/30$ and $\lambda/\pi = 0.8$. Here, $\varepsilon$ is the deviation from our conjectured formula, as defined by equations (10) and (11), with the values of $F_1(k_F, \lambda)$ obtained from the numerical fit (as reported in table C1). The plotted quantity remains finite in the limit $L \to \infty$, which supports our estimate (12).

We further denote the set of lattice sites belonging to the segment considered by $[L] = \{1, 2, \ldots, L\}$.

For the second cumulant, one obtains

$$\langle \langle Q^2 \rangle \rangle = \sum_{i,j \in [L]} g_{ij} \bar{g}_{ij},$$

where

$$\bar{g}_{ij} = \langle c_i c_j^\dagger \rangle = \delta_{ij} - g_{ji}. \tag{D.2}$$

Using the relation

$$\sum_{j = -\infty}^{\infty} g_{ij} g_{jk} = g_{ik}, \tag{D.3}$$

one can re-express

$$\langle \langle Q^2 \rangle \rangle = \sum_{i,j \in [L]} \bar{g}_{ij} \bar{g}_{ji}. \tag{D.4}$$

Collecting together all terms with the same distances between the pair of sites, we arrive at

$$\langle \langle Q^2 \rangle \rangle = 2 \sum_{x=1}^{\infty} (g_x)^2 s(x), \tag{D.5}$$

where we define the function $s(x) = \min(x, L)$. Using the explicit expression (B.3), we find

$$\langle \langle Q^2 \rangle \rangle = \frac{1}{\pi^2} \ln L + \frac{1}{\pi^2} \ln \left| \sin k_F L \right| + 1 + 1 + \frac{1}{2 \pi^2 L^2} + \frac{1}{\pi^2} \frac{\cos(2k_F L)}{(2L \sin k_F)^2} + O(L^{-3}) \tag{D.6}$$

(note that there are no terms of the order $L^{-1}$).
Repeating the same procedure for the third cumulant, we find
\[
\langle \langle Q^3 \rangle \rangle = \sum_{i,j,k \in [L]} \left( g_{ij} \bar{g}_{jk} \bar{g}_{ik} - g_{ij} g_{jk} \bar{g}_{ik} \right),
\]  
(D.7)
which, using relation (D.3), can be converted to
\[
\langle \langle Q^3 \rangle \rangle = \sum_{i \in [L]} \bar{g}_{i} \bar{g}_{j} \bar{g}_{j} / \sum_{i \in [L]} \bar{g}_{i} \sum_{j \in [L]} \bar{g}_{j} g_{ji} \bar{g}_{j} - \sum_{i \in [L]} \bar{g}_{i} \sum_{j \in [L]} \bar{g}_{j} \sum_{k \in [L]} \bar{g}_{k} \bar{g}_{ik}.
\]  
(D.8)
Again, collecting together all terms with the same relative positions of points, we arrive at
\[
\langle \langle Q^3 \rangle \rangle = 6 \sum_{x,y > 0} [s(x) + s(y) - s(x+y)] x y g_{xy} g_{xy} g_{xy} + y / x y,
\]  
(D.9)
Note that there is no contribution to this sum from small \( x \) and \( y \) for which \( x + y \leq L \). At large \( L \), the main contribution to this sum is determined by the two boundary pieces: \( y = 0, x > L \) and \( x = 0, y > L \). The easiest technique to extract these contributions is summation ‘by parts’. If we re-factorize
\[
\langle \langle Q^3 \rangle \rangle = 6 \sum_{x,y > 0} x y g_{xy} g_{x+y} [s(x) + s(y) - s(x+y)] / x y,
\]  
(D.10)
then we can associate the leading contribution with the jumps of the function \( [s(x) + s(y) - s(x+y)] / (x y) \) at the boundary. The contributions from the two pieces of the boundary are equal, and, after a simple calculation, one arrives at
\[
\langle \langle Q^3 \rangle \rangle \approx 3 \pi^3 \sum_{j=0}^{\infty} \sin(2k_F y) / x (x+y)
\]  
(D.11)
to the leading order in \( L \) (in the calculation, we neglected the terms oscillating in \( x \) in \( g_{xy} g_{x+y} \), as they produce contributions of higher orders).

**Appendix E. Charge cumulants from the generalized Fisher–Hartwig formula**

In this appendix, we try to push our conjecture about the precision of the generalized Fisher–Hartwig formula even further than in the main body of the paper. Namely, we assume that the generalized Fisher–Hartwig ‘sum prescription’ is exact to all orders of \( L^{-1} \), if all possible realizations (B.13) are included:
\[
\chi(\lambda) = \sum_{j=-\infty}^{+\infty} \chi_s(\lambda - 2\pi j),
\]  
(E.1)
where
\[
\chi_s(\lambda) = \exp \left[ i \lambda k_F L / \pi - \frac{\lambda^2}{2\pi^2} \ln L / l_0 + \sum_{m=0}^{\infty} F_m(k_F, \lambda) L^{-m} \right],
\]  
(E.2)
(we assume that the sum in the exponent contains only \( L^{-m} \), but no logarithms)\(^7\). The series (E.1) may be, in general, divergent at a fixed \( L \) and should be understood as an asymptotic

\(^7\) A similar expression with the sum over all realizations was suggested in [11]. However, in that work only the leading terms in \( \chi_s(\lambda) \) were kept. We conjecture here a stronger statement that equation (E.1) is asymptotically exact to all orders in \( L^{-1} \) with a suitable choice of the coefficients \( F_m(k_F, \lambda) \).
expansion at $L \to \infty$. Such a conjecture may, in principle, be verified by comparing with the charge cumulants (4). In particular, for the first several cumulants, we find from equations (E.1) and (E.2)\footnote{Here $F_m^{(k)}$ means $\partial^i F_m|_{k=0}$.}

$$\langle Q \rangle = \frac{1}{\pi} k_F L.$$ \hspace{1cm} (E.3)

$$\langle Q^2 \rangle = \frac{1}{\pi^2} \ln(e^{\pi/4} 2 L \sin k_F) - \frac{1}{\pi^2} \frac{\cos(2 k_F L)}{(2 L \sin k_F)^2} - F_1'' L^{-1} - F_2'' L^{-2} + o(L^{-2}),$$ \hspace{1cm} (E.4)

$$\langle Q^3 \rangle = \frac{6}{\pi^3} \frac{\sin(2 k_F L)}{(2 L \sin k_F)^2} \ln(e^{\pi/4} 2 L \sin k_F) + i F_1^{(3)} L^{-1} + i F_2^{(3)} L^{-2} + o(L^{-2}),$$ \hspace{1cm} (E.5)

$$\langle Q^4 \rangle = -\frac{3}{2 \pi^4} \zeta(3) + \frac{24}{\pi^4} \frac{\cos(2 k_F L)}{(2 L \sin k_F)^2} \left[ \ln(e^{\pi/4} 2 L \sin k_F) \right]^2 + F_1^{(4)} L^{-1} + F_2^{(4)} L^{-2} + o(L^{-2}).$$ \hspace{1cm} (E.6)

In other words, the coefficients in the expansions of the cumulants $\langle Q^n \rangle$ in $L^{-1}$ may be related to the expansions of $F_m(k_F, \lambda)$ in $\lambda$ (at $\lambda = 0$). These relations may, in principle, be verified against direct calculations of the cumulants using Wick’s theorem (along the lines of appendix D).

In this work, we have only calculated analytically the cumulant $\langle Q^2 \rangle$ to the order $L^{-2}$ and the cumulant $\langle Q^3 \rangle$ to the order $L^{-1}$ (see equations (D.6) and (D.11), respectively). This implies $F_1'' = 0$, $F_2'' = -(1/(12 \pi^2))$ and $F_1^{(3)} = -(3i/2 \pi^3 L \cot k_F$ (in agreement with our conjecture (13)). Furthermore, numerical studies of the third and fourth cumulants indicate that $F_1^{(3)} = F_1^{(4)} = 0$ and $F_2^{(4)} \neq 0$. In other words, if our conjecture in equations (E.1) and (E.2) is correct, then $F_2(k_F, \lambda)$ has the form

$$F_2(k_F, \lambda) = -\frac{\lambda^2}{24 \pi^2} + O(\lambda^4)$$ \hspace{1cm} (E.7)

in its expansion around $\lambda = 0$. It seems likely that further analytical progress is possible in these questions, and we leave them for future studies.

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