Entanglement entropies in free-fermion gases for arbitrary dimension

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Abstract – We study the entanglement entropy of connected bipartitions in free-fermion gases of \( N \) particles in arbitrary dimension \( d \). We show that the von Neumann and Rényi entanglement entropies grow asymptotically as \( N^{(d-1)/d} \ln N \), with a prefactor that is analytically computed using the Widom conjecture both for periodic and open boundary conditions. The logarithmic correction to the power-law behavior is related to the area-law violation in lattice free fermions. These asymptotic large-\( N \) behaviors are checked against exact numerical calculations for \( N \)-particle systems.

The study of the entanglement properties of many-body quantum systems has attracted much attention in recent years, mainly in relation with the critical behavior displayed at quantum phase transitions [1–3]. In particular, lots of studies have been devoted to quantify the highly nontrivial connections between different parts of an extended quantum system, by computing von Neumann (vN) or Rényi entanglement entropies of the reduced density matrix \( \rho_A = \text{Tr}_B \rho \) of a subsystem \( A \) with respect to its complement \( B \).

While a good understanding of the entanglement has been achieved in one-dimensional (1D) systems, where a leading logarithmic behavior has been established at conformal invariant quantum critical points [4–6], in higher dimensions the scaling behavior of the bipartite entanglement entropy is generally more complicated, without a definite general scenario for the universal behavior at a quantum phase transition, despite an enormous effort on the problem. Earlier investigations in the black-hole physics [7] proposed the general validity of the so-called area law [2]: for \( d \geq 1 \) the entanglement entropy is asymptotically proportional to the surface of the area separating the two subsystems \( A \) and \( B \). The area law has been generally proven for gapped systems [8], independently of the statistics of the microscopical constituents. This result is corroborated by exact and numerical calculations for systems with topological order [9], at 2D quantum Lifshitz points [10], and some explicit field-theoretical computations [11]. The situation is less clear for critical systems. On the one hand, the area law holds in bosonic systems [2,12,13]. Quantum critical points described by a Landau-Ginzburg action satisfy the area law [14], which is also supported by holographic calculations by means of AdS/CFT [15] with subleading logarithmic corrections. Even in some disordered systems the area law is confirmed by analytical and numerical calculations and the presence of universal subleading term has been shown [16]. On the other hand, the simplest condensed-matter models, i.e. free fermions on a lattice, show multiplicative logarithmic corrections to the area law [13,17–24], i.e. for a large subsystem \( A \) of linear size \( \ell \) in an infinite \( d \)-dimensional lattice the entanglement entropies scale like

\[
S^{(\alpha)}(A) \sim \ell^{d-1} \ln \ell,
\]

where \( S^{(\alpha)}(A) \) are the Rényi entropies defined as

\[
S^{(\alpha)}(A) = \frac{1}{1-\alpha} \ln \text{Tr} \rho_A^\alpha.
\]

For \( \alpha \to 1 \), one recovers the vN definition \( S(A) \equiv S^{(1)}(A) \equiv -\text{Tr}[\rho_A \ln \rho_A] \). It has been argued that these logarithmic corrections should also appear for interacting fermions with a finite Fermi surface [17–24].

In this paper we investigate the entanglement properties of free-fermion gases of \( N \) particles in arbitrary dimensions, focussing on the large-\( N \) asymptotic behavior of the entanglement entropies of connected spatial bipartitions. Analogously to lattice models, an interesting issue concerns the existence of multiplicative logarithmic corrections to the large-\( N \) power-law behavior corresponding to the area law. A related question is whether these logarithmic corrections are due to the presence of corners in the
area separating $A$ and $B$, or they are also present for a smooth surface.

The entanglement entropies of continuous free-fermion gases for a finite number of particles $N$ can be computed in a framework based on the overlap matrix described below. This method has been already applied to 1D systems [25–27], but it allows also computations in higher dimensions. We consider systems of $N$ particles in a finite volume of arbitrary dimension $d$, and focus on the large-$N$ scaling behavior of the spatial entanglement entropies of connected bipartitions, finding a general $N(d−1)/d \ln N$ behavior for large $N$. This multiplicative logarithmic correction to the large-$N$ power law is related to the logarithmic correction to the area law in lattice models. Combined with simple scaling arguments, this result allows us to conclude that multiplicative logarithmic corrections to the area law are general features of free-fermion systems both on the lattice and in the continuum.

**The method.** – The ground-state wave function of a gas of $N$ noninteracting spinless fermions $\Psi(\mathbf{x}_1,\ldots,\mathbf{x}_N) = \det[\psi_i(\mathbf{x}_j)]/\sqrt{N!}$, where $\psi_i$ are the normalized wave functions of the one-particle problem with lowest energies. Explicit expressions of the one-particle eigensolutions are products of eigenfunctions of corresponding 1D Schrödinger problems, i.e.

$$\psi_{n_1,n_2,\ldots,n_d}(\mathbf{x}) = \prod_{i=1}^{d} \phi_{n_i}(x_i),$$

where the $n_i$ label the eigenfunctions along the $d$ directions which are solution of $-\partial^2_{x_i}\phi_{n}(x_i) = e_n\phi_{n}(x_i)$, so that the energy of the $d$-dimensional problem is $E_{n_1,n_2,\ldots,n_d} = \sum_{i=1}^{d} e_{n_i}$. Note that, although the spatial dependence of the one-particle eigenfunctions is essentially decoupled along the various directions, fermion gases in different dimensions present notable differences due to the nontrivial filling of the lowest $N$ states to obtain the ground state of the $N$-particle system.

In the following we consider hypercubic systems of linear size $L$ with periodic boundary conditions (PBC) and Dirichlet (open) boundary conditions (OBC). The corresponding normalized 1D eigensolutions are $\phi^\text{PBC}_k(x) = L^{-1/2}e^{2\pi ikx/L}$ for PBC and $\phi^\text{OBC}_k(x) = (2/L)^{1/2} \sin k\pi x/L$ for OBC, with $k \in \mathbb{Z}$ and $x \in [0, L]$.

The spatial entanglement entropies of connected bipartitions can be computed using the method developed in refs. [25,26] (to which we refer for details). For this purpose, we consider the $N \times N$ overlap matrix $A$ [25,28] with elements

$$A_{nm} = \int_A d^d z \psi^*_m(z)\psi_n(z), \quad n, m = 1, \ldots, N,$$

where the integration is over the spatial region $A$, and involves the lowest $N$ energy levels. Then, in analogy with well-known lattice models [29], the Rényi entanglement entropies are derived from the formula

$$S^{(\alpha)}(A) = \sum_{n=1}^{N} e_{\alpha}(a_n),$$

where $a_n$ are the eigenvalues of $A$, and

$$e_{\alpha}(\lambda) = \frac{1}{1-\alpha} \ln[\lambda^\alpha + (1-\alpha)^\alpha].$$

The vN entropy is obtained by the limit $\alpha \to 1$. The knowledge of the $S^{(\alpha)}(A)$ for different $\alpha$ characterizes the full spectrum of nonzero eigenvalues of $\rho_A$ [30], and gives more information about the entanglement than the single vN entropy. Furthermore, numerical stochastic methods such as classical [31] and quantum Monte Carlo [32] can measure only Rényi entropies with integer $\alpha$.

For systems with both PBC and OBC, the form of the overlap matrix is analogous to that of the two-point correlation of free spinless fermions on the lattice. Indeed, taking as simpler example the PBC case, the two-point function is

$$G_{\text{lat}}(\mathbf{x},\mathbf{y}) = \int_{\Gamma(\mu)} \frac{d^dk}{(2\pi)^d} e^{ik(\mathbf{x}-\mathbf{y})},$$

where $\Gamma(\mu)$ is the volume limited by the Fermi surface $\partial \Gamma(\mu)$, and $\mathbf{x}, \mathbf{y}$ are the positions of the sites of the lattice in unit of the lattice spacing, thus $x \in \mathbb{Z}^d$. On the other hand, after inserting the one-particle eigensolutions, the overlap matrix (3) reads

$$A_{nm} = \frac{1}{L^d} \int_{A} d^d x \ e^{i2\pi(k_m-k_n)x/L}.$$
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\[
S(N) = \frac{1}{2} c(\mu) \ell^{d-1} \ln \ell + o(\ell^{d-1} \ln \ell),
\]

where \( \mu \) is the chemical potential, \( \Omega \) is the real-space region \( A \) rescaled by \( \ell \) so that its volume equals one. \( \mathbf{n}_x \) and \( \mathbf{n}_k \) denote the normal vectors on the spatial surface \( \partial \Omega \) and the Fermi surface \( \partial \Gamma(\mu) \), respectively. The validity of these predictions has been also supported by numerical results [13,19].

Calculations based on the Widom conjecture allow us to derive an analogous result for the large-\( N \) asymptotic behavior of the entanglement entropy in fermion gases defined in the continuum, as already suggested by the above-mentioned correspondence between the overlap matrix \( a \) and the lattice two-point function. For a \( d \)-dimensional cubic volume of size \( L \) with PBC, containing \( N \) fermions, the corresponding Fermi surface is a \( d \)-dimensional sphere of radius \( k_F \), which is related to the particle number \( N \) by

\[
V_T = v_d k_F^d = N, \quad v_d = \frac{\pi^{d/2}}{\Gamma(d/2 + 1)},
\]

We want to compute the vN entanglement entropy of a space region \( A \), which may be given by the volume \([0, z_1 L] \times [0, z_2 L] \times \ldots \times [0, z_d L]\) with \( z_i \leq 1 \). Using the Widom conjecture as in ref. [18], we obtain the asymptotic large-\( N \) behavior,

\[
S(A) = cN^{(d-1)/d} \ln N + o(N^{(d-1)/d} \ln N),
\]

and specifically

\[
c = \begin{cases} 
\frac{1}{3}, & d = 1, \\
\frac{1}{3\sqrt{\pi}} (z_1 + z_2), & d = 2, \\
\frac{1}{6} \left( \frac{\pi}{6} \right)^{1/3} (z_1 z_2 + z_1 z_3 + z_2 z_3), & d = 3.
\end{cases}
\]

Using the Widom conjecture, one can also derive analogous formulas for generic shapes of the connected space region \( A \). Note that the factor \( 2^{d-1} \prod_{j=1}^{d} z_i \) is just the area of the surface separating \( A \) and \( B \) in units of \( L = 1 \). This could lead to the erroneous conclusion that the area law is satisfied in these systems, but eq. (11) is just an asymptotic expansion in \( N \) and the size-dependent multiplicative logarithmic correction to the area law is a subleading term of the form \( N^{1-1/d} \) times the logarithm of the area (see the conclusions for a discussion of this issue).

Note that eq. (13) is not valid when one \( z_i \) is one, because the terms at the edge do not contribute to the area, i.e. the approach to the asymptotic large-\( N \) behavior (11) is not uniform as a function of \( z_i \). In particular, when all \( z_i = 1 \) except one (let us say \( z_1 \)), the area separating \( A \) and \( B \) is just 2 (in units of \( L \)) and we have

\[
\mathcal{E}_S = \frac{1}{6} \frac{\Gamma \left( \frac{d}{2} \right)}{\Gamma \left( \frac{d+1}{2} \right) \Gamma \left( \frac{d}{2} + 1 \right)} \frac{\Gamma \left( \frac{d}{2} + 1 \right)}{\Gamma \left( \frac{d}{2} + 1 \right)},
\]

independently of \( z_1 \). In this case, the subsystem \( A \) is a \( d \)-dimensional strip without corners (because of PBC). Note that the approach to the asymptotic large-\( N \) behavior...
The asymptotic behaviors predicted by eqs. (11), (12) are definitely supported by calculations of the bipartite vN entanglement entropy, as shown by fig. 1. To be more quantitative, in fig. 2 we report the difference

$$N^{-1/2}S(A) - c \ln N$$

for 2D systems, with $c$ given by eq. (12). This difference appears limited, although presenting sizable oscillations which enlarge with increasing $z_1$ and $z_2$. Its large-$N$ behavior provides information on the subleading behavior of $N^{-1/2}S$, which appears to be $O(1)$, supporting eq. (16).

The amplitude of the oscillations modulating the difference (17) appears to decrease. However, it is not clear how they decrease and whether the amplitude of the oscillations gets suppressed in the large-$N$ limit. Oscillating corrections to the leading behavior have been observed also for 1D systems, but in the case of PBC only for Rényi entropies with $\alpha \neq 1$ [26,35]. Their origin can be traced back to the presence of relevant operators localized at the borders of the region $A$ [36]. However, the ones observed in $d > 1$ are present also for $\alpha = 1$ and their structure (periods, amplitudes etc.) appears very different from the 1D ones. For these reasons both the general structure and their physical origin remain unclear and this issue would deserve further investigations.

For the Rényi entropies, the application of the Widom conjecture leads to

$$S(\alpha) = \frac{1 + \alpha^{-1}}{2} S(A) + o(N^{(d-1)/d} \ln N),$$

analogously to lattice models [21]. This is supported by the data shown in fig. 3, where we plot the difference $N^{-1/2}(S^{(2)} - 3S/4)$ between the $\alpha = 2$ Rényi and vN entropies of spatial regions $A = [0, z_1 L] \times [0, z_2 L]$ for some values of $z_1, z_2$. The data appear to approach a constant, with large oscillations that make difficult to extract the rate of convergence.

In fig. 4 we report analogous results in $d = 3$. Again, the subtracted quantity $N^{-2/3}S(\alpha) - c_0 \ln N$ turns out to be limited, indicating that it is $O(1)$ (in agreement with eq. (16)), with sizable oscillating corrections whose qualitative features are again unclear.

Open boundary conditions. – The results for the asymptotic large-$N$ behavior of the entanglement entropy can be extended to OBC. For simplicity, we consider only 2D systems. We first study the half-space entanglement entropy, i.e. $A$ corresponds to the region $z_1 < L/2$. The
We plot the quantity $S/N$ vs. $N$ for a system with OBC, up to entropy of space regions $W$. Widom conjecture gives

$$S_{\text{HS}}(\alpha) = N^{1/2} \left[ \frac{1 + \alpha^{-1}}{12\pi^{1/2}} \ln N + O(1) \right],$$

(19)

where the coefficient of the leading term is half of the one for PBC, due to the fact that the boundary between the half-spaces is half of the one of stripes. Figure 5 shows results at fixed $N$ up to $N \approx 10^4$, for the half-space entanglement entropies $S_{\text{HS}}(\alpha)$ showing agreement with the prediction (19) and the presence of sizable oscillating corrections as for PBC.

The presence of boundaries breaks translational invariance. Thus, the entanglement entropy depends on the location of the subsystem $A$. We consider the case when $A$ corresponds to the region limited by an hyperplane parallel to one axis and at distance $x + L/2$ from the boundary. We denote the corresponding entanglement entropy by $S_B^{(\alpha)}(x)$ (with $S_{\text{HS}} = S_B^{(0)}(0)$). Figure 6 reports the quantity

$$S_B^{(\alpha)}(x) = S_{\Delta}^{(\alpha)}(x) - S_B^{(\alpha)}(0) = N^{1/2}[f_{\Delta}^{(\alpha)}(x) + o(1)],$$

(20)

where the function $f_{\Delta}(x)$ is a $O(1)$ contribution and cannot be obtained from Widom conjecture. Figure 6 shows clearly that, despite the oscillating corrections, the data for many different $N$ collapse on the same master curve supporting the scaling ansatz.

We also consider the case of a subsystem $A$ enclosed by two parallel hyperplanes at the same distance $x < L/2$ from the center, both parallel to one of the cubic axes. The corresponding entanglement entropies are denoted by $S_B^{(\alpha)}(x)$. Using again the Widom conjecture for the leading large-$N$ behavior, we expect

$$S_B^{(\alpha)}(x) = N^{1/2} \left[ \frac{1 + \alpha^{-1}}{6\pi^{1/2}} \ln N + f_{\Delta}^{(\alpha)}(x) + o(1) \right],$$

(21)

where the coefficient of the leading term equals the one for PBC. Again the functions $f_{\Delta}(x)$ cannot be obtained from the Widom conjecture, but the validity of this ansatz is supported by the data reported in fig. 6.

Conclusions. – We have studied the vN and Rényi entanglement entropies of a system of $N$ particles in a volume $L^d$ with periodic and open boundary conditions. The large-$N$ asymptotics of these entanglement entropies can be obtained by means of the Widom conjecture [33].
and can be written in the simple form

$$S^{(\alpha)} = \frac{1 + \alpha^{-1}}{2} c_{S} A_{\alpha} N^{1-1/d} \ln N,$$

(22)

where the coefficient $c_{S}$ is given in eq. (15) while $A_{\alpha}$ is the area between $A$ and $B$ in units where $L = 1$.

This large-$N$ asymptotic behaviors can be also turned into an asymptotic size dependence of the entanglement entropies for connected bipartitions of fermion gases in a cubic box of volume $L^d$, in the thermodynamic limit when $N, L \to \infty$ and $N/L^d \to \rho$ with $\rho$ the particle density. Equation (22) can be written as

$$\frac{4S^{(\alpha)}}{1 + \alpha^{-1}} \approx A_{\alpha} c_{S} \rho^{1-1/d} L^{d-1} \ln L \approx \frac{dc_{S}}{d-1} \rho^{1-1/d} A \ln A,$$

where we used $L^{d-1} A_{\alpha} = A$ with $A$ being the area separating $A$ and $B$. This confirms the presence of logarithmic corrections to the area law in free-fermion gases.

While the leading asymptotic behavior in $N$ of $S^{(\alpha)}$ is understood from our analysis, the numerical data show the presence of oscillating subleading corrections to the scaling whose structure and origin are still not clear.

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