

Entanglement Entropy of Fermions in Any Dimension and the Widom Conjecture

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We show that entanglement entropy of free fermions scales faster than area law, as opposed to the scaling L^{d-1} for the harmonic lattice, for example. We also suggest and provide evidence in support of an explicit formula for the entanglement entropy of free fermions in any dimension d , $S \sim c(\partial\Gamma, \partial\Omega)L^{d-1} \log L$ as the size of a subsystem $L \rightarrow \infty$, where $\partial\Gamma$ is the Fermi surface and $\partial\Omega$ is the boundary of the region in real space. The expression for the constant $c(\partial\Gamma, \partial\Omega)$ is based on a conjecture due to Widom. We prove that a similar expression holds for the particle number fluctuations and use it to prove a two sided estimate on the entropy S .

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In recent years a number of parallel findings have emphasized the importance of entanglement entropy [1–10]. Although originally studied in the context of black hole physics [1], this quantity also plays an important role in quantum information as a measure of the number of maximally entangled pairs that can be extracted from a given quantum state [2].

The behavior of entanglement entropy is closely related to the criticality behavior of quantum systems: for a gapped system one expects an area scaling law due to a finite correlation length ξ . In the 1D case [3], this behavior changes drastically near criticality where the absence of gap leads to long range correlations, and so the entanglement does not saturate. Many interesting results have been obtained for 1D models. For classes of critical models, where conformal field theory (CFT) methods are applicable, the entropy was found to exhibit a logarithmic behavior, with a coefficient depending on the central charge of the CFT models [4,5]; recently a modification of these results in case of strong disorder was found [6]. The bipartite structure of the ground state of Fermion models was studied in several works [7–9]. A connection between the entropy of spin chains and random matrix theory was established in [10].

Fewer results were obtained in dimensions $d > 1$, although from the field theoretic point of view these are very interesting. Indeed, initial investigation of the entropy as a correction to the Bekenstein-Hawking entropy, suggested that the entropy of a scalar field is proportional to the boundary area for spherical or half-space regions [1,11]. Recently, it has been rigorously proved [12] for a harmonic lattice model, that the entropy of a cube with side L behaves as the boundary area, i.e., as L^{d-1} .

In this Letter we examine the dependence of entanglement entropy on dimension and geometry in a simple case of a gapless system consisting of free fermions.

Let us summarize our main results: First, we prove that $S \sim L^{d-1} \log L$ [13] for cubelike domains [(3) below]. We then present a heuristic argument for the more explicit

formula $S \sim \frac{d}{3} L^{d-1} \log L$. We note that results which are derived for cubes do not necessarily describe the scaling for general boundaries: indeed we find that $S \geq L^{d-\beta}$ for fractal-like boundaries, where $\beta \in (0, 1)$ (described below) characterizes regularity of the boundary. However, the results for cubelike domains should reflect the correct scaling for regions with sufficiently regular boundaries. For general piecewise smooth boundaries we prove $O(L^{d-1} \log L) \leq S \leq O[L^{d-1}(\log L)^2]$, see (6) and (9), (this estimate was independently derived in [9] for d dimensional cubes in the lattice case).

Finally, making a connection with a conjecture of Widom [14], we suggest an explicit geometric formula for the entropy as $L \rightarrow \infty$:

$$S \sim \frac{L^{d-1} \log L}{(2\pi)^{d-1}} \frac{1}{12} \int_{\partial\Omega} \int_{\partial\Gamma} |n_x \cdot n_p| dS_x dS_p, \quad (1)$$

where $\partial\Gamma$, $\partial\Omega$ are the boundaries of the Fermi sea and the region considered, n_p , n_x are the unit normals to these boundaries. We present evidence supporting this conjecture and prove a similar formula for the fluctuations in particle number in the subsystem, which also gives bounds on S . Recently the formula (1) was checked numerically for 2D and 3D [15] and a perfect agreement concerning both the order and the coefficient was found. Widom's conjecture is closely related to the problem of recovering data from a measurement during a finite time interval and in a finite frequency set. This problem, known as *time-frequency limiting*, is of basic importance in signal theory, and it was studied extensively [16]. It turns out that operators appearing in calculations of entanglement entropy for free fermions are exactly the same as the ones studied in [16], which is natural since one studies the properties of a field in restricted sets of real space and momentum space.

The ground state of a translation invariant Hamiltonian describing a noninteracting fermion field (on a lattice or in the continuum), with dispersion relation $\epsilon(k)$, is $\prod_{\epsilon(k) \leq \epsilon_F} a_k^\dagger |0\rangle$. Here ϵ_F is the Fermi energy. This defines

the Fermi sea region $\Gamma = \{k | \epsilon(k) \leq \epsilon_F\}$ in momentum space. We also assume that the system is gapless [17]. The bipartite structure of the ground state can be studied by fixing a region Ω in real space and computing the reduced density matrix $\rho_\Omega = \text{Tr}_{[\mathcal{F}(\mathbb{R}^d \setminus \Omega)]} \rho$ where $\mathcal{F}(\Omega)$ is the fermion Fock space associated with the region Ω (see Fig. 1). The entanglement entropy $S = -\text{Tr}_{[\mathcal{F}(\Omega)]} \rho_\Omega \log \rho_\Omega$ is given in this case [8] by $S(L) = \text{Tr} h(PQP)$, where $h = h_1 + h_2$ with $h_1(t) = -t \log t$ and $h_2(t) = -(1-t) \log(1-t)$. Here P is a projection operator on the modes inside the Fermi sea Γ , and Q is a projection on the region Ω scaled by a factor L . The operator PQP is related to the fermion correlation function $g(x-x') = \langle a_x^\dagger a_{x'} \rangle = \langle x | P | x' \rangle$ so that $\langle x | PQP | x' \rangle = \int_\Omega g(x-x'') g(x''-x') dx''$. The density of particles is $n = \text{vol}(\Gamma)$, and one may rescale L appropriately, as to set $n = 1$, which we will assume from now on.

Results for cubic domains.—Consider the case of a rectangular box with sides L_j , i.e., $\Omega = [0, L_1] \times \dots \times [0, L_d]$ and $\Gamma = [0, 1]^d$. Let $S_1(L)$ be the entropy in the 1D case and let S be the entropy corresponding to Ω , Γ as above. Then we have the following:

Theorem.—Under the above assumptions

$$\frac{1}{2d} \sum_{j=1}^d S_1(L_j) \prod_{i \neq j} N(L_i) \leq S \leq \sum_{j=1}^d S_1(L_j) \prod_{i \neq j} N(L_i), \quad (2)$$

where $N(L_j)$ is the average number of particles. Note, in particular, that for $\Omega = [0, L]^d$

$$\frac{1}{2} \left(\frac{L}{2\pi} \right)^{d-1} S_1(L) \leq S \leq d \left(\frac{L}{2\pi} \right)^{d-1} S_1(L). \quad (3)$$

Proof: Note that we can make separation of variables $Q = \otimes_1^d Q_j$ where Q_j is a projection on coordinate j , and P factors in a similar way. Hence $PQP = \otimes_1^d T_j$ where $T_j = P_j Q_j P_j$. Note the following:

Lemma.—For $a_i \in [0, 1]$ one has

$$\frac{1}{2d} G(a_1, \dots, a_d) \leq h_2 \left(\prod_{i=1}^d a_i \right) \leq G(a_1, \dots, a_d), \quad (4)$$

where $G(a_1, \dots, a_d) = \sum_{j=1}^d h_2(a_j) \prod_{i \neq j} a_i$. To prove (4), one has to check it for two variables a_1, a_2 and then proceed by induction.

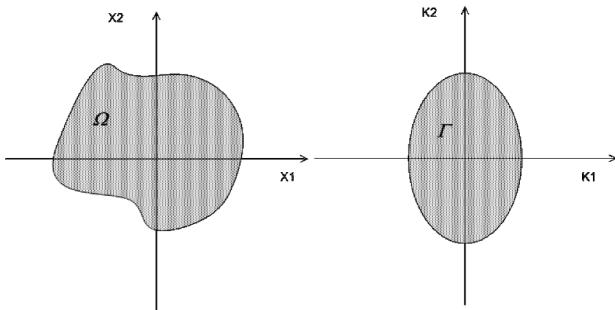


FIG. 1. The Fermi sea Γ in momentum space, and a region Ω in real space.

We observe that the eigenvalues of PQP are of the form $a_{i,1} \dots a_{i,d}$ with $a_{i,j}$ being some eigenvalue of T_j . Writing the entropy S as $\sum h(a_{i,1} \dots a_{i,d})$, using (4) and $h_1(\prod_{i=1}^d a_i) = \sum_{j=1}^d h_1(a_j) \prod_{i \neq j} a_i$, and recalling that the average number of particles [8] $N = \text{Tr} T_j$, (2) follows.

Result (2) shows that the entropy may be evaluated using the 1D expressions. This reflects the compatibility of Γ , Ω with factorizing the fermionic modes into the different coordinates. It is now a matter of substituting the numerous results obtained in the 1D case. For the lattice case, it follows from the many works on the subject that for fermions on a 1D lattice, or equivalently for an XX spin chain (via the Jordan-Wigner transformation), $S_1(L) = \frac{1}{3} \log L + o(\log L)$, see in particular [18]. In the continuous case the same expression is obtained by formally substituting $h(t)$ in the 1D result of [19,20].

For any body composed of a union of cubes C_i of side L_i we have, using the subadditivity of entropy [21], $S(\bigcup C_i) \leq \sum S(C_i)$, thus we have an upper bound that depends on the number of cubes needed to describe the body: using (3) we find $S(\bigcup C_i) \leq \frac{d}{3} \left(\frac{1}{2\pi} \right)^{d-1} \times \sum L_i^{d-1} \log(L_i) + o(L_M^{d-1} \log L_M)$, $L_M = \max_i L_i$. A lower bound proportional to $L_m^{d-1} \log L_m$, $L_m = \min_i L_i$ follows from (6) and (9), below.

Scaling coefficient.—Here we derive heuristically

$$S = \frac{d}{3} \left(\frac{L}{2\pi} \right)^{d-1} \log L + o(L^{d-1} \log L) \quad (5)$$

for $\Omega = \Gamma = [0, L]^d$. Since the eigenvalues of T_j are strictly less than one, the series $\text{Tr} h_2(PQP) = \text{Tr}(\otimes_1^d T_j) - \sum_{n=2}^{\infty} \frac{1}{n(n-1)} \text{Tr}(\otimes_1^d T_j^n)$ converges. By [19] [see (11) below for $d=1$ and $f(t) = t^n$], as $L \rightarrow \infty$, $\text{Tr} T_j^n = \frac{L}{2\pi} + \frac{\log L}{\pi^2} \times \sum_{k=1}^n \frac{1}{k} + o(\log L)$. Hence $\text{Tr}(\otimes_1^d T_j^n) = \left(\frac{L}{2\pi} \right)^d + \left(\frac{L}{2\pi} \right)^{d-1} \times \frac{\log L}{\pi^2} \left(\sum_{k=1}^n \frac{1}{k} \right) + o(L^{d-1} \log L)$. Substituting the latter in the series for h_2 and calculating the sums involved we find $\text{Tr} h_2(PQP) = \frac{d}{6} \left(\frac{L}{2\pi} \right)^{d-1} \log L + o(L^{d-1} \log L)$. Adding this to $\text{Tr} h_1(PQP)$, which is computed directly and gives the same value, (5) follows [22]. Further control of the remainder term in $\text{Tr} T_j^n$ as $L \rightarrow \infty$ is required to make this calculation rigorous [23].

Results for general boundaries.—We now turn to the case of general bounded Fermi sea Γ and region Ω . It is known [8] that the variance in particle number, given by $(\Delta N)^2 = \text{Tr} PQP(1 - PQP)$ can be used to obtain a lower bound on S .

Theorem.—For general sets Ω one has

$$4(\Delta N)^2 \leq S \leq O(\log L)(\Delta N)^2. \quad (6)$$

We derive also an explicit formula (9) which implies, in particular, that $(\Delta N)^2 = O(L^{d-1} \log L)$.

The proof of (6) in the lattice case is immediate using the inequalities of the form $4t(1-t) \leq h(t) \leq \epsilon - Ct(1-t) \log \epsilon$, valid for $\epsilon > 0$, with C being a constant [24]. One substitutes the operators PQP instead of t and calcu-

lates the trace. Note that $\text{tr}(\epsilon) \sim \epsilon L^d$ for a finite lattice of size L , thus taking $\epsilon < \frac{\log L}{L}$, (6) follows. The proof of (6) in the continuous case is new: note first that the kernel of the operator PQP is given by

$$\langle p|PQP|p' \rangle = \chi_\Gamma(p)\chi_\Gamma(p') \left(\frac{L}{2\pi}\right)^d \int_\Omega e^{iL(p-p') \cdot x} dx, \quad (7)$$

where χ_A is defined for any set A as $\chi_A(x) = 1$ if $x \in A$ and $\chi_A(x) = 0$, otherwise. For the continuous case the mentioned inequality [24] is not helpful, since the Hilbert space associated with any set Ω is infinite dimensional, so $\text{Tr}\epsilon = \infty$. We proceed as follows: write instead

$$h(t) \leq \epsilon \sqrt{t(1-t)} - Ct(1-t) \log \epsilon, \quad (8)$$

valid for small enough ϵ (with a different constant C). We then take the trace of both sides. It remains to estimate $\text{Tr}\sqrt{PQP(1-PQP)}$. We have the following: $\text{Tr}\sqrt{PQP(1-PQP)} \leq \text{Tr}\sqrt{PQ_\square P}$ where Q_\square is a projection on a box containing Ω , and we have used operator monotonicity of $t \rightarrow t^{1/2}$ (see, e.g., [25]), and that $PQ_\square P \geq PQP$ (as operators). Next we note that the operators $PQ_\square P$ and $Q_\square PQ_\square$ have the same positive eigenvalues counted with multiplicities [26]. Thus, we have $\text{Tr}\sqrt{PQP(1-PQP)} \leq \text{Tr}\sqrt{Q_\square PQ_\square} \leq \text{Tr}\sqrt{Q_\square P_\square Q_\square}$, where we have used the monotonicity again. It remains to evaluate $\text{Tr}\sqrt{Q_\square P_\square Q_\square}$: this can be done using bounds on the singular values of the operator $Q_\square P_\square Q_\square$, which in this case are also the respective eigenvalues. It follows from [27] that for any $\alpha > d/2$ the eigenvalues of $Q_\square P_\square Q_\square$ satisfy $\lambda_n \leq Cn^{-1/2-\alpha/d}L^{d/2+\alpha}$. Taking $\alpha > 3d/2$ we find $\text{Tr}\sqrt{Q_\square P_\square Q_\square} < L^{d+\delta}$ for any $\delta > 0$, and thus we can choose, e.g., $\epsilon < L^{-\delta-1}$, and (6) follows.

Having established $(\Delta N)^2$ as a way of obtaining bounds we proceed to evaluate it. Our next result is as follows:

Theorem.—Let Ω, Γ be two compact sets in \mathbb{R}^d , $d \geq 1$, with smooth boundaries $\partial\Omega, \partial\Gamma$. Then

$$(\Delta N)^2 = \frac{L^{d-1} \log L}{(2\pi)^{d-1}} \frac{\ln 2}{4\pi^2} \int_{\partial\Omega} \int_{\partial\Gamma} |n_x \cdot n_p| dS_x dS_p + o(L^{d-1} \log L), \quad (9)$$

where n_x, n_p are unit normals to $\partial\Omega, \partial\Gamma$, respectively. The full proof is too technical to be included here, and will appear elsewhere (see, however, [28]). It starts by observing that

$$\text{Tr}(PQP)^2 = \left(\frac{L}{2\pi}\right)^{2d} \int_{\mathbb{R}^d} A_\Omega(z) \hat{A}_\Gamma(Lz) dz, \quad (10)$$

where $A_\Omega(z) \equiv \int_{\mathbb{R}^d} \chi_\Omega(x) \chi_\Omega(x-z) dx$ is the volume of the set Ω intersected with Ω shifted by z [i.e., $\Omega \cap (\Omega + z)$], and proceeds with an asymptotic analysis of this integral.

Note the geometric nature of the coefficient in (9): for a spherical Fermi sea Γ , and a convex region Ω this coefficient is just the average cross section of Ω over all directions. In the more general case the coefficient depends on the two surfaces and their mutual orientations. Thus (6)

with (9) establish the scaling $O(L^{d-1} \log L) \leq S \leq O[L^{d-1}(\log L)^2]$ when Γ, Ω have smooth boundaries.

Fractal boundaries.—A very interesting enhancement in the scaling of S occurs if the sets Ω, Γ are allowed to have fractal-like boundaries. Physically, this means that making the boundaries less regular, makes the typical momentum states more incompatible with the shape of the region Ω , and hence contributes to enhanced entropy when integrating the external modes. More precisely, it was shown in [28] that if $C_1 \|h\|^{\beta_\Omega} < \text{Vol}[\Omega \setminus (\Omega + h)] < C_2 \|h\|^{\beta_\Omega}$ for small $\|h\|$ and some $0 < \beta_\Omega \leq 1$, and the same holds for Γ with β_Γ , then $(\Delta N)^2$ is bounded above and below by $\tilde{C}_{1,2} L^{d-\min(\beta_\Omega, \beta_\Gamma)}$ if $\beta_\Omega \neq \beta_\Gamma$ and $\tilde{C}_{1,2} L^{d-\beta_\Omega} \log L$ if $\beta_\Omega = \beta_\Gamma$. In particular this and (6) imply that $S > 4\tilde{C}_1 L^{d-\beta_\Omega} \log L$ if $\beta_\Omega = \beta_\Gamma$ and $S > 4\tilde{C}_1 L^{d-\min(\beta_\Omega, \beta_\Gamma)}$ if $\beta_\Omega \neq \beta_\Gamma$ [29].

Connection to Widom's conjecture.—It turns out that the result (9) is a special case of a well-known conjecture by Widom [14,30]. The problem of time-frequency limiting mentioned in the introduction leads to a study of the spectrum of the operator PQP where Q is a time window scaled by L , and P represents a frequency window. One way of studying the eigenvalues of PQP is to study the asymptotic behavior of $\text{Tr}f(PQP)$, as $L \rightarrow \infty$, for some general class of f . It is conjectured in [14] that for a function $f(t)$, analytic on a disc of radius > 1 with $f(0) = 0$, the following holds as $L \rightarrow \infty$

$$\begin{aligned} \text{Tr}f(PQP) &= \left(\frac{L}{2\pi}\right)^d f(1) \int_\Omega \int_\Gamma dx dp + \left(\frac{L}{2\pi}\right)^{d-1} \frac{\ln 2 \log L}{4\pi^2} \\ &\times U(f) \int_{\partial\Omega} \int_{\partial\Gamma} |n_x \cdot n_p| dS_x dS_p \\ &+ o(L^{d-1} \log L), \end{aligned} \quad (11)$$

where n_x, n_p are unit normals to $\partial\Omega, \partial\Gamma$, respectively, and $U(f) = \int_0^1 \frac{f(t)-tf(1)}{t(1-t)} dt$. The formula (11) and a generalized form of it were proved for $d = 1$ in [14,19]. For $d \geq 2$ only special cases were proved [28,30]. Note finally that (9) is a verification of Widom's conjecture for the special case $f(t) = t(1-t)$.

In a broader context one may think of Widom's conjecture (11) as a generalization of the strong (two-term) Szegő limit theorem (SSLT) for the *continuous* setting. The SSLT plays a special role in entanglement entropy [18,31]. The SSLT was initially used by Onsager in his celebrated computation of the spontaneous magnetization for the 2D Ising model (see, e.g., [32]). It is interesting to note that in Onsager's computation (and also in [18]) the leading asymptotic term vanishes, and one needs to compute the subleading term. This is exactly the situation that we have in the continuous version of the Szegő theorem (11): the leading term should vanish since $h(1) = 0$.

Widom's conjecture suggests the explicit geometric expression for the entropy (1). Note that if $\Omega = \Gamma = [0, 1]^d$ then the double integral in (1) equals $4d$ (twice the number of faces), so that (1) and (5) are consistent. Note also that

the coefficient $\frac{\ln 2}{4\pi}$ in the expression for the number variance (9) gives a lower estimate for S in (6) within 16% of the conjectured $\frac{1}{2}$ in (1).

Finite temperature.—From the semiclassical point of view one expects the entropy to be extensive, $S \sim L^d$, for $T > 0$. This suggests to look for a transition temperature between the L^d and $L^{d-1} \log L$ regimes. Let $\beta = 1/T$ and introduce the Fermi-Dirac function $k(p) = 1/(1 + e^{\beta(p^2 - \mu)})$ (we take $\hbar = k_B = 1$ and $m = 1/2$). The expression for the entanglement entropy at finite temperatures [8] is given by $\text{Tr} h(QKQ)$, where K is the operator of multiplication by $k(p)$ in momentum space. Semiclassically, integrating over the phase space one finds [33]

$$\text{Tr} h(QKQ) = \left(\frac{L}{2\pi}\right)^d \text{Vol}(\Omega) \int_{\mathbb{R}^d} h[k(p)] dp + O(L^{d-1}).$$

Introducing polar variables and scaling out β gives

$$S = \left(\frac{L}{2\pi}\right)^d \text{Vol}(\Omega) |\mathbb{S}^{d-1}| \frac{\mu^{-1+d/2}}{\beta} \int_{e^{-\beta\mu}}^{\infty} \frac{du}{u} h\left(\frac{1}{1+u}\right) \times \left(1 + \frac{\log u}{\beta\mu}\right)^{-1+d/2} + O(L^{d-1}), \quad (12)$$

which scales as $L^d \beta^{-1} \mu^{-1+d/2}$ for $\beta \rightarrow \infty$. Comparing this with the $T = 0$ results above we see that for the zero temperature effect $L^{d-1} \log L$ to be seen, the transition temperature should satisfy $T \mu^{-1+d/2} \sim \frac{\log L}{L}$, $L \rightarrow \infty$.

Summary and discussion.—In systems with finite correlation length ξ , one expects quantities such as the entropy S and the number variance $(\Delta N)^2$ to scale like the area of the boundary of the region. The system studied here does not behave this way. Here, the correlation function $\langle a_x^\dagger a_{x'} \rangle$ decays slowly and the fermion momentum modes are spread over the entire system and are highly sensitive to localization in space and consequently the area law is violated.

Let us summarize the concrete results of this Letter: We prove that the scaling is of the form $L^{d-1} \log L$ for cubelike domains. We find a connection between the scaling behavior of S and a well-known conjecture due to Widom (11), which suggests the explicit geometric formula (1) for S in any d . Finally, while Widom's conjecture is far from being proven, we find that it holds for $(\Delta N)^2$, and use this to obtain lower and upper bounds on S . We also find an enhanced scaling of S for fractal-like boundaries and at finite temperatures.

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