Large-scale behaviour of local and entanglement entropy of the free Fermi gas at any temperature‡

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Abstract. The leading asymptotic large-scale behaviour of the *spatially bipartite entanglement entropy* (EE) of the free Fermi gas infinitely extended in multidimensional Euclidean space at zero absolute temperature, $T = 0$, is by now well understood. Here, we present and discuss the first rigorous results for the corresponding EE of thermal equilibrium states at $T > 0$. The leading large-scale term of this *thermal* EE turns out to be twice the first-order finite-size correction to the infinite-volume thermal entropy (density). Not surprisingly, this correction is just the thermal entropy on the interface of the bipartition. However, it is given by a rather complicated integral derived from a semiclassical trace formula for a certain operator on the underlying one-particle Hilbert space. But in the zero-temperature limit $T \downarrow 0$, the leading large-scale term of the thermal EE considerably simplifies and displays a $\ln(1/T)$-singularity which one may identify with the known logarithmic enhancement at $T = 0$ of the so-called area-law scaling.

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In memory of Enrico Fermi (1901–1954)
on the occasion of the 90th birthday of the ideal Fermi gas

1. Introduction and main results.

In recent years, entanglement entropy has turned out to be a useful and much studied quantifier of nonclassical correlations between subsystems in composite quantum systems [1]. In particular, given the (pure) ground state of a spatially large many-particle system and reducing (or localising) it to a spatial subregion Ω, we denote the von Neumann entropy of the resulting (mixed) substate by $S(0, \Omega)$ and call it the local

ground-state entropy. The *spatially bipartite entanglement entropy* (EE), defined for a *bounded* Ω as the (quantum) mutual information relative to the complement of Ω and denoted by $H(0, \Omega)$, then simply equals $2S(0, \Omega)$ by the purity of the ground state. This (ground-state) EE quantifies, to some extent, how strongly all particles within Ω are correlated with all those outside Ω. It is thus, for example, well suited to detect long-range correlations near the critical point of a quantum phase transition by enlarging Ω, see [2, 3, 4, 5].

For a many-particle system without long-range interactions the ground-state EE

$$H(0, L\Omega) = 2S(0, L\Omega), \quad L \geq 1 \tag{1}$$

is widely believed [6, 7] to grow to leading order proportional to the area $|\partial\Omega|L^{d-1}$ of the boundary surface $\partial(L\Omega)$ of the scaled region $L\Omega$ as the (dimensionless) scaling parameter L tends to infinity, $L \to \infty$. Here, $d = 1, 2, 3, \ldots$ is the spatial dimension of Ω. If the particles are fermions and if there is no spectral gap above their ground-state energy in the infinite-volume limit, the effective long-range correlations lurking in the (Pauli–)Fermi–Dirac statistics are expected to slightly enhance the large-scale growth of $H(0, L\Omega)$ by a logarithmic factor $\ln(L)$. Indeed, for the free Fermi gas infinitely extended in d-dimensional Euclidean space $\mathbb{R}^d$ such a large-scale growth of the ground-state EE with a precise and rather explicit prefactor has been proved with full mathematical rigour [8], thereby confirming a stimulating conjecture by Gioev and Klich [9].

In this note, we present and discuss the first rigorous results on the EE of the free Fermi gas in $\mathbb{R}^d$ in the state of thermal equilibrium at nonzero temperature, $T > 0$, and chemical potential $\mu \in \mathbb{R} := \mathbb{R}^1$. The latter we mostly suppress for notational simplicity, but also because we often consider thermal quantities for fixed (mean) particle-number density $\rho > 0$. In contrast with the ground-state or $T = 0$ case, the EE at $T > 0$, denoted by $H(T, \Omega)$, must not be expected to be just twice the local thermal entropy $S(T, \Omega) < \infty$, since thermal states are mixed ones. However, in trying to define $H(T, \Omega)$ as the mutual information

$$H(T, \Omega) = S(T, \Omega) + \text{``}S(T, \mathbb{R}^d \setminus \Omega) - S(T, \mathbb{R}^d)\text{''} \tag{2}$$

of the bipartition, we are confronted with the two infinities $S(T, \mathbb{R}^d \setminus \Omega) = S(T, \mathbb{R}^d) = \infty$ due to the additivity of macroscopic thermal entropy. We solve this problem by rewriting the right-hand side of (2) in a mathematically and physically reasonable way as a sum of two finite (that is, not infinite) differences, see (19) and (20) below. By construction, $H(T, L\Omega)$ is then well-defined and exhibits a leading term proportional to L^{d-1} as $L \to \infty$. Given that, our general line of arguments is similar to that of Ref. [10] devoted to noninteracting fermions in the d-dimensional simple cubic lattice $\mathbb{Z}^d$ with emphasis on the case $d = 1$.

Our main results may be summarised as follows. For the (spinless) free Fermi gas in $\mathbb{R}^d$ at any $T > 0$ we find the following two asymptotic large-scale expansions: the *local thermal entropy* satisfies

$$S(T, L\Omega) = s(T)|\Omega|L^d + \eta(T, \partial\Omega)L^{d-1} + \ldots \tag{3}$$

and the *thermal* EE satisfies

$$H(T, L\Omega) = 2\eta(T, \partial\Omega)L^{d-1} + \dots, \tag{4}$$

up to terms growing slower than L^{d-1} as $L \to \infty$. Here, the bounded subregion $\Omega \subset \mathbb{R}^d$ may be rather general except that its boundary surface $\partial\Omega$ (if $d \geq 2$) should be sufficiently smooth. For further assumptions see our theorem in Sec. 3 below. There we also make the definitions of the entropies $S(T, \Omega)$ and $H(T, \Omega)$ more precise and express the coefficient $\eta(T, \partial\Omega)$ in terms of a multiple integral. Nevertheless, in this Letter we concentrate on the physical aspects and publish the somewhat lengthy mathematical details in separate papers [11, 12, 13]. In the next section we just identify $s(T)$ and offer some explanations and comments.

2. Physical meanings of the asymptotic coefficients and their dependence on temperature.

Not surprisingly, the leading asymptotic coefficient $s(T)|\Omega|$ in (3) is nothing but the thermal entropy contained in Ω and $s(T) \geq 0$ is the (infinite-volume) *thermal entropy density* or mean entropy. The latter is given by the thermodynamic relation

$$s(T) = \frac{\partial}{\partial T}\mathsf{p}(T), \quad \mathsf{p}(T) := \int_{\mathbb{R}} dE\, \mathcal{N}(E)f_T(E - \mu), \tag{5}$$

where the integral is the pressure of the free Fermi gas as a function of T (and μ). The quantity $\mathcal{N}(E) := (2\pi\hbar)^{-d} \int_{\mathbb{R}^d} dp\, \Theta(E - \varepsilon(p))$ defines the integrated density of states $\mathcal{N} : \mathbb{R} \to [0, \infty[$ of the energy-momentum dispersion relation $\varepsilon : \mathbb{R}^d \to [0, \infty[$ which characterises the translation-invariant one-particle Hamiltonian of the free Fermi gas.§ Here, $2\pi\hbar$ is Planck's constant and Θ is Heaviside's unit-step function. The second factor of the integrand in (5) involves the Fermi function, $f_T : \mathbb{R} \to [0, 1]$, $f_T(E) := [1 + \exp(E/T)]^{-1}$, where from now on we put Boltzmann's constant $k_B = 1$. From (5) and Sommerfeld's asymptotic low-temperature expansion,

$$f_T(E) = \Theta(-E) - (\pi^2/6)\, T^2\Theta''(E) + \dots \tag{6}$$

(in distributional sense), we get the well-known formula

$$s(T) = (\pi^2/3)\, \mathcal{N}'(\mu)T + \dots \tag{7}$$

up to terms vanishing faster than T as $T \downarrow 0$. Eq. (7) holds, as it stands, at fixed chemical potential $\mu \in \mathbb{R}$. If instead of μ the particle density $\rho > 0$ is kept fixed, one has to invert the thermodynamic relation $\rho = \partial\mathsf{p}/\partial\mu$ between ρ and μ. By (6), one thus finds at low temperatures another well-known formula

$$\mu(T, \rho) = \varepsilon_F - (\pi^2/6)\big[\mathcal{N}''(\varepsilon_F)/\mathcal{N}'(\varepsilon_F)\big]T^2 + \dots, \tag{8}$$

§ For convenience, we have assumed $\varepsilon(p) \geq 0$ for all $p \in \mathbb{R}^d$ so that $\mathcal{N}(E) = 0$ if $E < 0$. This is no loss of generality as long as ε is bounded from below.

where $\varepsilon_F := \lim_{T \downarrow 0} \mu(T, \rho) > 0$ is the Fermi energy which satisfies $\rho = \mathcal{N}(\varepsilon_F)$. Consequently, Eq. (7) implies that $s(T) = (\pi^2/3)\mathcal{N}'(\varepsilon_F)T + \dots$ for fixed $\rho > 0$. For the *ideal* (non-relativistic, free) Fermi gas [14], corresponding to the prime example $\varepsilon(p) = p^2/(2\mathsf{m})$ with $\mathsf{m} > 0$ being the mass of each particle, we recall the explicit formula

$$\mathcal{N}(E) = \Theta(E) \left[\mathsf{m}E/(2\pi\hbar^2) \right]^{d/2}/(d/2)! \tag{9}$$

for its integrated density of states. Quantum effects dominate at low temperatures and become weaker at higher temperatures. Accordingly, the properties of the ideal Fermi gas approach those of the ideal Maxwell–Boltzmann gas in the high-temperature limit, $T \to \infty$. For example, in this limit the thermal entropy density of the ideal Fermi gas grows, to leading order, proportional to $T^{d/2}$ at fixed μ and proportional to $\ln(T)$ for fixed ρ, in symbols,

$$s(T) \sim (T/T_0)^{d/2} \qquad (\mu \text{ fixed}), \tag{10a}$$

$$s(T) \sim \ln(T/T_0) \qquad (\rho \text{ fixed}). \tag{10b}$$

Here, the constant $T_0 > 0$ is an arbitrary comparison temperature.

   Returning to the expansions (3) and (4), we note that the other asymptotic coefficient, $\eta(T, \partial\Omega)$, is also positive. On the one hand, it represents the thermal entropy on the boundary surface $\partial\Omega$ and determines the first-order finite-size correction to the infinite-volume entropy (density). On the other hand, $\eta(T, \partial\Omega)L^{d-1}$ is half the thermal EE to leading order in L. Consequently, Eq. (3) shows that the local entropy at $T > 0$ displays a leading large-scale behaviour in agreement with a "volume law" as it should be. In contrast, Eqs. (3) and (4) show that the EE at $T > 0$ obeys a strict "area law": although the two subregions $L\Omega$ and its complement $\mathbb{R}^d \setminus L\Omega$ carry (contrary to the case $T = 0$) extremely different local entropies (namely $S(T, L\Omega) < \infty$ and $S(T, \mathbb{R}^d \setminus L\Omega) = \infty$), on their common boundary $\partial(L\Omega)$, or interface, the entropies are equal and proportional to L^{d-1} as $L \to \infty$. Roughly phrased, the logarithmic enhancement $\ln(L)$ present [8, 9] in the large-scale behaviour of the ground-state EE, see (1) and (13) below, disappears when the temperature is raised from $T = 0$ to $T > 0$ because the Fermi surface "grows soft". Incidentally, we note that $\eta(T, \partial\Omega)$ does not depend on the choice of a condition imposed on the domain of the (quantum) Hamiltonian at the boundary $\partial\Omega$, because we work from the outset in the infinitely extended position space $\mathbb{R}^d$ and view all operators to act *self-adjointly* on the associated one-particle Hilbert space $\mathrm{L}^2(\mathbb{R}^d)$ of square-integrable functions $\psi : \mathbb{R}^d \to \mathbb{C}, q \mapsto \psi(q)$.

   The coefficient $\eta(T, \partial\Omega)$ is given by a rather complicated integral (see (22–24) below), which, fortunately, is well-known in the theory of semiclassical expansions for traces of certain (truncated) Wiener–Hopf type operators, see Refs. [15, 16, 17, 18]. Interestingly, in the limit $T \downarrow 0$ the coefficient $\eta(T, \partial\Omega)$ simplifies, displays a logarithmic singularity and takes (at fixed $\mu > 0$ ‖) the rather explicit form

$$\eta(T, \partial\Omega) = (1/12) \, J(\partial\Gamma_\mu, \partial\Omega) \, \ln(T_0/T) + \dots \tag{11}$$

‖ If $\mu < 0$, then $\eta(T, \partial\Omega)$ vanishes as $T \downarrow 0$.

up to terms remaining bounded as $T \downarrow 0$. Here, the level set $\partial\Gamma_\mu := \{p \in \mathbb{R}^d : \varepsilon(p) = \mu\}$ in momentum space is the (effective) Fermi surface corresponding to μ. The factor $J(\partial\Gamma_\mu, \partial\Omega)$ is defined as in Ref. [8] and for $d \geq 2$ given by the twofold surface integral

$$J(\partial\Gamma_\mu, \partial\Omega) := (2\pi\hbar)^{1-d} \int_{\partial\Gamma_\mu \times \partial\Omega} \mathrm{d}\sigma(p)\mathrm{d}\tau(q) \left| m(p) \cdot n(q) \right|. \tag{12}$$

The vectors $m(p), n(q) \in \mathbb{R}^d$ denote the exterior unit normals at the points $p \in \partial\Gamma_\mu$ and $q \in \partial\Omega$, respectively. The canonical $(d-1)$-dimensional area measures on the surfaces $\partial\Gamma_\mu$ and $\partial\Omega$ are denoted by σ and τ, respectively. If we fix the particle density $\rho > 0$ and use (8) in (11), we arrive at (11) with μ replaced by ε_F.

By identifying the large ratio T_0/T inside the logarithm in (11) with the scaling parameter L, Eqs. (3) and (7) give

$$S(0, L\Omega) = (1/12) \, J(\partial\Gamma_\mu, \partial\Omega) \, L^{d-1} \ln(L) + \ldots \tag{13}$$

in agreement with the result for $T = 0$ in Refs. [8, 9] (resp. the corresponding expression with μ replaced by ε_F). For an isotropic dispersion relation ε we know from Ref. [8] that $J(\partial\Gamma_\mu, \partial\Omega)$ is proportional to the area $|\partial\Omega|$.¶ This is even true for $\eta(T, \partial\Omega)$ itself, at arbitrary $T > 0$. However, the emerging prefactor, the thermal entropy surface density, remains to be given by a multiple integral, see the remarks below the subsequent Eq. (24).

As for the entropy density $s(T)$, the leading high-temperature behaviour of the coefficient $\eta(T, \partial\Omega)$ of the ideal Fermi gas depends on whether μ or ρ is kept fixed. More precisely, it follows from (24) that

$$\eta(T, \partial\Omega) \sim (T/T_0)^{(d-1)/2} \qquad (\mu \text{ fixed}), \tag{14a}$$
$$\eta(T, \partial\Omega) \sim (T_0/T)^{1/2} \qquad (\rho \text{ fixed}), \tag{14b}$$

as $T \to \infty$. Eq. (14b) reflects the fact that the particles become effectively uncorrelated for fixed particle density at sufficiently high temperature.

3. Precise definitions and formulations of results.

In order to define the local thermal entropy and the thermal EE precisely we first recall that the infinite-volume equilibrium state of the free Fermi gas at temperature $T > 0$ and chemical potential $\mu \in \mathbb{R}$ is quasi-Gaussian (in other words, quasi-free) and uniquely determined by its reduced one-particle density operator $f_T(\varepsilon(P) - \mu\mathbb{1})$ on $\mathrm{L}^2(\mathbb{R}^d)$. Here, $P := -i\hbar\partial/\partial q$ is the canonical-momentum operator, $\varepsilon(P) \geq 0$ the one-particle quantum Hamiltonian and $\mathbb{1}$ the identity operator. The local (or truncated) version

$$D(f_T, \Omega) := \mathbb{1}_\Omega \, f_T(\varepsilon(P) - \mu\mathbb{1}) \, \mathbb{1}_\Omega \tag{15}$$

¶ In particular, for the ideal Fermi gas in $\mathbb{R}^d$ one simply has $J(\partial\Gamma_\mu, \partial\Omega) = 2\mathcal{N}_{d-1}(\mu)|\partial\Omega|$, where $\mathcal{N}_{d-1}(E)$ is given by the right-hand side of (9) with d replaced by $d-1$.

of the density operator then characterises the quasi-Gaussian substate obtained from the equilibrium state by spatial reduction to $\Omega \subseteq \mathbb{R}^d$. Here, $\mathbb{1}_\Omega : \mathrm{L}^2(\mathbb{R}^d) \to \mathrm{L}^2(\mathbb{R}^d)$ denotes the projection operator associated with the indicator function of Ω, that is, $(\mathbb{1}_\Omega \psi)(q) := \psi(q)$ if $q \in \Omega$ and 0 otherwise for all $\psi \in \mathrm{L}^2(\mathbb{R}^d)$. Next we recall the *binary entropy function* $h : [0,1] \to [0, \ln(2)]$ defined by

$$h(0) := h(1) := 0 \quad \text{and} \quad h(t) := -t \ln(t) - (1-t) \ln(1-t) \quad \text{if} \quad t \in]0,1[. \tag{16}$$

The positivity

$$\widetilde{h}(\lambda, r, t) := h\big((1-\lambda)r + \lambda t\big) - (1-\lambda)h(r) - \lambda h(t) \geq 0 \tag{17}$$

for all $\lambda, r, t \in [0,1]$ is equivalent to the concavity of h. In fact, h is even operator-concave [19]. The *local thermal* (von Neumann) *entropy* is now given as the trace

$$S(T, \Omega) := \mathrm{Tr}[\mathbb{1}_\Omega \, h(D(f_T, \Omega))\mathbb{1}_\Omega] = \mathrm{Tr}[\, h(D(f_T, \Omega))], \tag{18}$$

see, for example, [20]. The second equality in (18) follows from $h(0) = 0$.

The definition of the thermal (von Neumann) EE requires two steps. In the first step we introduce the "entropic" operator difference

$$\Delta(T, \Omega) := \mathbb{1}_\Omega h(D(f_T, \Omega))\mathbb{1}_\Omega - D(h \circ f_T, \Omega). \tag{19}$$

Here, the operator $D(h \circ f_T, \Omega)$ is obtained from (15) by replacing the Fermi function f_T with the composed function $h \circ f_T$ defined by $(h \circ f_T)(E) := h(f_T(E))$ for all $E \in \mathbb{R}$. From the operator concavity of the function h and from Refs. [19, 21] we get the operator positivity $\Delta(T, \Omega) \geq 0$. In the second step we define the *thermal* EE for a *bounded* $\Omega \subset \mathbb{R}^d$ as the sum of two positive traces

$$H(T, \Omega) := \mathrm{Tr}\,\Delta(T, \Omega) + \mathrm{Tr}\,\Delta(T, \mathbb{R}^d \setminus \Omega). \tag{20}$$

This is the precise version of (2). Arguments as in Ref. [22] show that even the second trace is finite, although the (positive) minuend and the (positive) subtrahend of $\Delta(T, \mathbb{R}^d \setminus \Omega)$ have both an infinite trace. Therefore, we arrive at the (in)equalities

$$0 \leq H(T, \Omega) = H(T, \mathbb{R}^d \setminus \Omega) < \infty. \tag{21}$$

Moreover, in the limit $T \downarrow 0$ we get back to Eq. (1) by observing that $h \circ f_0 = 0$, confer (6).

To explain the coefficient $\eta(T, \partial\Omega)$ of the subleading asymptotic behaviour of $S(T, L\Omega)$ and of the leading behaviour of $H(T, L\Omega)$ as $L \to \infty$, we need some auxiliary definitions. In contrast to the well-known leading "volume term" in (3) the subleading "area term" is new and rather complicated. It cannot be obtained from simple heuristic considerations, not even for $d = 1$. But it can be derived from the semiclassical "area coefficient" in Refs. [15, 16, 17, 18] by observing that the traces in (18) and (20), with Ω replaced by $L\Omega$, depend on Planck's constant $2\pi\hbar$ and the scaling parameter

L only via the ratio $\hbar/L$ which can be seen by a (unitary) dilatation. In order to recall this "area coefficient" from the mentioned literature we first define the function $U : [0,1] \times [0,1] \rightarrow [0,\infty[,\ (r,t) \mapsto U(r,t)$ by

$$U(r,t) := \frac{1}{8\pi^2} \int_0^1 \mathrm{d}\lambda\, \frac{\widetilde{h}(\lambda, r, t)}{\lambda(1-\lambda)}, \tag{22}$$

see (16) and (17) for the definition of $\widetilde{h}$. Then we consider the integral

$$\mathcal{U}[g] := \lim_{\delta \downarrow 0} \int_{\mathbb{R} \times \mathbb{R}} \mathrm{d}v\, \mathrm{d}w\, \Theta(|v-w|-\delta)\, \frac{U\big(g(v), g(w)\big)}{(v-w)^2} \tag{23}$$

defined, in the principal-value sense, for smooth functions $g : \mathbb{R} \rightarrow [0,1]$. We observe that $\mathcal{U}[g] \geq 0$ since $U(r,t) \geq 0$ due to the concavity of h. If the function h were smooth, then $\mathcal{U}[g]$ could be defined as a standard Riemannian integral, whose finiteness could be easily checked (for smooth g). For the function (16) however, as well as for certain other functions (such as $t \mapsto t^\alpha(1-t)^\alpha$, $\alpha \in]0,1[$) being continuous but not differentiable at the points $t = 0$ and $t = 1$, the finiteness of $\mathcal{U}[g]$ is a non-trivial matter. This and other relevant properties of the integral (23) are investigated in [11].

If $d \geq 2$, then we consider for g at given $T > 0$ the $2(d-1)$-parameter family of functions $f_{T;(p,q)} : \mathbb{R} \rightarrow [0,1]$ defined in terms of the Fermi function by $f_{T;(p,q)}(v) := f_T\big(\varepsilon(p + v\,n(q)) - \mu\big)$, where $v \in \mathbb{R}, q \in \partial\Omega$ and $p \in \mathsf{T}_q^*(\partial\Omega)$ with $\mathsf{T}_q^*(\partial\Omega) \cong \mathbb{R}^{d-1}$ being the dual space of the $(d-1)$-dimensional tangent space of $\partial\Omega$ at the point q. The vector $n(q) \in \mathbb{R}^d$ and the subsequent area measure τ have the same meanings as in (12). Finally, we define

$$\eta(T, \partial\Omega) := (2\pi\hbar)^{1-d} \int_{\partial\Omega} \mathrm{d}\tau(q) \int_{\mathsf{T}_q^*(\partial\Omega)} \mathrm{d}p\, \mathcal{U}[f_{T;(p,q)}]. \tag{24}$$

If the dispersion relation ε is isotropic, then the functions $f_{T;(p,q)}$ do not depend on the parameter $q \in \partial\Omega$ due to the orthogonality of $p \in \mathsf{T}_q^*(\partial\Omega)$ and $n(q)$. Consequently, the surface area $|\partial\Omega|$ can be factored out on the right-hand side of (24). Nevertheless, the multiple integral underlying $\eta(T, \partial\Omega)$ remains to be a fourfold one for $d \geq 2$. For $d = 1$ the set $\Omega \subset \mathbb{R}$ is the union of finitely many pairwise disjoint bounded intervals, according to an assumption in the subsequent theorem. Then $|\partial\Omega|$ equals the (even) number of all endpoints of the constituent intervals and one has $\eta(T, \partial\Omega) = \mathcal{U}[f_T \circ (\varepsilon - \mu)]\,|\partial\Omega|$, which still involves a threefold integral.

Now we are prepared to state our central "technical" result as the following

Theorem. *For any temperature $T > 0$, for any bounded subregion $\Omega \subset \mathbb{R}^d$ with finitely many connected components and (if $d \geq 2$) piecewise smooth boundary surface $\partial\Omega$ (see Ref. [23]) and for any smooth and polynomially bounded dispersion relation ε the trace of $\Delta(T, \Lambda)$ is finite and positive for $\Lambda = \Omega$ or $\Lambda = \mathbb{R}^d \setminus \Omega$ with the same leading term in both large-scale expansions*

$$\mathrm{Tr}\,\Delta(T, L\Lambda) = \eta(T, \partial\Omega)\, L^{d-1} + \dots, \tag{25}$$

up to terms growing slower than L^{d-1} as $L \rightarrow \infty$.

Our proof goes as follows. At first we "smooth out" the function h, which enables us to refer for the formula (25) directly to available literature, notably to [15] or [17] (see, in particular, Chap. I and V in [17]). To return to the original non-smooth function h, we then "close" the asymptotics using the estimates obtained in [22] for non-smooth functions of operators of the type $D(f, \Omega)$. This strategy is similar to the one applied in [8]. Full mathematical details will be published elsewhere [12, 13]. There we also establish the validity of formula (25) even if $L \to \infty$ and $T \downarrow 0$ *simultaneously* provided that $LT/T_0 \geq 1$ throughout. In our view, these observations provide a deeper insight into the low-temperature behaviour of the thermal EE.

Combining (20) and (25) immediately gives the claimed large-scale behaviour (4) of the thermal EE. From (25) we also infer the claimed two-term large-scale behaviour (3) of the local thermal entropy (18) by observing

$$
\begin{aligned}
S(T, L\Omega) &= \operatorname{Tr} D(h \circ f_T, L\Omega) + \operatorname{Tr} \Delta(T, L\Omega) \\
&= s(T)|\Omega|L^d + \operatorname{Tr} \Delta(T, L\Omega) \\
&= s(T)\,|\Omega|\,L^d + \eta(T, \partial\Omega)\,L^{d-1} + \dots ,
\end{aligned}
\tag{26}
$$

where we have used the identities

$$
(2\pi\hbar)^{-d} \int_{\mathbb{R}^d} \mathrm{d}p\, h\big(f_T(\varepsilon(p) - \mu)\big) = \int_{\mathbb{R}} \mathrm{d}E\, \mathcal{N}'(E) h\big(f_T(E - \mu)\big) = s(T)
\tag{27}
$$

in the second equality. The leading large-scale behaviour of the local entropy $S(T, L\Omega)$ at $T > 0$ was first proved in [24, 25]. The subleading correction of the order L^{d-1} in (26) is new.

4. Summary, discussion and an open problem.

For the free Fermi gas in multidimensional continuous space $\mathbb{R}^d$ in thermal equilibrium at temperature $T > 0$ and for a given bounded subregion $\Omega \subset \mathbb{R}^d$ we carefully distinguish between the *local thermal entropy* $S(T, \Omega) \geq s(T)|\Omega|$ and the *thermal spatially bipartite entanglement entropy* $H(T, \Omega) \geq 0$. Their large-scale behaviours (3) and (4) contain the thermal entropy density $s(T) \geq 0$ and the new asymptotic coefficient $\eta(T, \partial\Omega) \geq 0$ as two characteristics of the rather old free Fermi-gas model [14]. The results (3) and (4) are physically even more relevant than the corresponding ground-state results (13) and (1), because in real gases the temperature is never strictly zero. Furthermore, the new results (3) and (4) deepen our understanding of the older ones (13) and (1) by observing that $s(0) = 0$ and that $\eta(T, \partial\Omega)$ diverges logarithmically as $T \downarrow 0$ according to (11). A result similar to (11) for noninteracting fermions in the one-dimensional lattice $\mathbb{Z}^1$ was derived in [10], but without an explicit prefactor. As in [8, 10], many of our present results extend to the whole one-parameter family of (quantum) Rényi entropies, see [12, 13].

Finally, we check whether the exact asymptotic results (13), (3), (7) and (11) for the local thermal entropy $S(T, L\Omega)$ can be descibed consistently by a so-called universal

crossover formula as obtained in [26, 27, 28, 29, 30, 31] by arguments from a suitable conformal field theory, at least for $d = 1$. Such a formula has the appealing form

$$S(T, L\Omega) = L^{d-1}A\ln\left[\frac{T_0}{T}\sinh\left(L\frac{T}{T_0}\right)\right] \tag{28}$$

with suitable constants $A \geq 0$ and $T_0 > 0$ not depending on L and T. Remarkably, if we choose $A = (1/12)\,J(\partial\Gamma_\mu, \partial\Omega)$ and $T_0 = 3A/[\pi^2\mathcal{N}'(\mu)|\Omega|]$, then we find consistency, provided that $L \gg 1$ and $T \ll T_0$. We conclude that (28) correctly reflects asymptotic properties of the free Fermi gas in $\mathbb{R}^d$ if L is large and T is small, but does, for example, not reproduce the large-T behaviours (10) and (14) (of the ideal Fermi gas). However, Eq. (28) suggests the scaling-type formula

$$\lim_{L\to\infty}\frac{1}{L^{d-1}}\left[S\left(\frac{xT_0}{L}, L\Omega\right) - S(0, L\Omega)\right] = A\ln\left[\frac{\sinh(x)}{x}\right] \tag{29}$$

for *any* $x > 0$. Although we have a result for the simultaneous limits $L \to \infty$ and $T \downarrow 0$ with $x = LT/T_0 \ (> 1)$ kept fixed, see a remark below the above theorem, at present we do not know whether (29) or a similar formula follows from the "microscopic" definition (18), not even for $d = 1$.

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References

[1] R. Horodecki, P. Horodecki, M. Horodecki, and K. Horodecki. Quantum entanglement. *Rev. Mod. Phys.*, 81:865–942, 2009.

[2] S. Sachdev. *Quantum Phase Transitions, 2nd edition.* Cambridge University Press, Cambridge, United Kingdom, 2011.

[3] G. Vidal, J.I. Latorre, E. Rico, and A. Kitaev. Entanglement in quantum critical phenomena. *Phys. Rev. Lett.*, 90:227902, 2003.

[4] S. Chakravarty. Scaling of von Neumann entropy at the Anderson transition. *Int. J. Mod. Phys. B*, 24:1823–1840, 2010.

[5] L. Pastur and V. Slavin. Area law scaling for the entropy of disordered quasifree fermions. *Phys. Rev. Lett.*, 113:150404, 2014.

[6] J. Eisert, M. Cramer, and M.B. Plenio. Area laws for the entanglement entropy – a review. *Rev. Mod. Phys.*, 82:277–306, 2010.

[7] M.B. Hastings. Entropy and entanglement in quantum ground states. *Phys. Rev. B*, 76:035114, 2007.

[8] H. Leschke, A.V. Sobolev, and W. Spitzer. Scaling of Rényi entanglement entropies of the free Fermi-gas ground state: a rigorous proof. *Phys. Rev. Lett.*, 112:160403, 2014.

[9] D. Gioev and I. Klich. Entanglement entropy of fermions in any dimension and the Widom conjecture. *Phys. Rev. Lett.*, 96:100503, 2006.

[10] H. Bernigau, M.J. Kastoryano, and J. Eisert. Mutual information area laws for thermal free fermions. *J. Stat. Mech.: Theory and Experiment*, 2015:P02008, 2015.

[11] A.V. Sobolev. On a coefficient in trace formulas for Wiener–Hopf operators. *arXiv:1601.00463 [math.SP]*, 2016.

[12] H. Leschke, A.V. Sobolev, and W. Spitzer. Trace formulas for Wiener–Hopf operators with applications to entropies of free fermionic equilibrium states. *arXiv: 1605.04429 [math.SP]*, 2016.

[13] A.V. Sobolev. Trace formula for multidimensional Wiener–Hopf operators. *In preparation*, 2016.

[14] E. Fermi. Zur Quantelung des idealen einatomigen Gases. *Z. Physik*, 36:902–912, 1926.

[15] H. Widom. Szegő's limit theorem: the higher-dimensional matrix case. *J. Funct. Anal.*, 39:182–198, 1980.

[16] H. Widom. A trace formula for Wiener–Hopf operators. *J. Operator Theory: Adv. Appl.*, 8:279–298, 1982.

[17] H. Widom. *Asymptotic Expansions for Pseudodifferential Operators on Bounded Domains.* Springer–Verlag, Berlin, 1985.

[18] R. Roccaforte. Asymptotic expansions of traces for certain convolution operators. *Trans. Amer. Math. Soc.*, 285:581–602, 1984.

[19] T. Ando. Concavity of certain maps on positive definite matrices and applications to Hadamard products. *Lin. Alg. and Appl.*, 26:203–241, 1979.

[20] R. Helling, H. Leschke, and W. Spitzer. A special case of a conjecture by Widom with implications to fermionic entanglement entropy. *Int. Math. Res. Notices*, 2011:1451–1482, 2011.

[21] C. Davis. A Schwarz inequality for convex operator functions. *Proc. Amer. Math. Soc.*, 8:42–44, 1957.

[22] A.V. Sobolev. Functions of self-adjoint operators in ideals of compact operators. *arXiv: 1504.07261 [math.SP]*, 2015.

[23] A.V. Sobolev. Wiener–Hopf operators in higher dimensions: the Widom conjecture for piece-wise smooth domains. *Integr. Equ. Oper. Theory*, 81:435–449, 2015.

[24] Y.M. Park and H.H. Shin. Dynamical entropy of space translations of CAR and CCR algebras with respect to quasi-free states. *Commun. Math. Phys.*, 152:497–537, 1993.

[25] F. Benatti, T. Hudetz, and A. Knauf. Quantum chaos and dynamical entropy. *Commun. Math. Phys.*, 198:607–688, 1998.

[26] V.E. Korepin. Universality of entropy scaling in one dimensional gapless models. *Phys. Rev. Lett.*, 92:096402, 2004.

[27] B. Swingle. Conformal field theory approach to Fermi liquids and other highly entangled states. *Phys. Rev. B*, 86:035116, 2012.

[28] B. Swingle and T. Senthil. Universal crossover between entanglement entropy and thermal entropy. *Phys. Rev. B*, 87:045123, 2013.

[29] P. Calabrese and J. Cardy. Entanglement entropy and quantum field theory. *J. Stat. Mech.: Theory and Experiment*, 2004:P06002, 2004.

[30] P. Calabrese and J. Cardy. Entanglement entropy and conformal field theory. *J. Phys. A: Math. Theor.*, 42:504005, 2009.

[31] P. Calabrese, J. Cardy, and E. Tonni. Finite temperature entanglement negativity in conformal field theory. *J. Phys. A: Math. Theor.*, 48:015006, 2015.