Entanglement entropy of free fermions

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- Model of free fermions
- Rényi entropy, localization, entanglement entropy
- Zero-temperature case: logarithmically enhanced area-law
- Positive-temperature case: area-law
- See Phys. Rev. Lett. **112** 160403 (2014) and arXiv: 1501.03412 and references therein

Motivation: Entanglement entropy (EE) is a much studied concept in condensed matter physics and quantum information theory. Originally, EE was introduced in mid 80's (and independently early 90's) to explain Bekenstein-Hawking entropy of black holes. Here, this entropy grows with the surface area rather than with the volume as in usual thermodynamics.

EE is a purely quantum mechanical effect. Like non-commutativity, it is easy to formulate mathematically but it may be hard to understand physically. For instance, you may have complete information (0 entropy) on a given system but less (> 0 entropy) on part of this system.

Rigorous mathematical results on EE of many-particle systems are sparse. Here, I discuss *spatial* EE for one of the simplest physical system, namely of free fermions in $\mathbb{R}^d$ in equilibrium.

Consider spinless free (pairwise non-interacting and no exterior fields) fermions in d-dimensional Euclidean space, $\mathbb{R}^d$. One-particle Hilbert space is $\mathrm{L}^2(\mathbb{R}^d)$. Consider translation-invariant one-particle Hamiltonian, that is, $\varepsilon(P)$ with momentum operator $P := -i\hbar\nabla$ and energy-dispersion relation $\varepsilon : \mathbb{R}^d \to [0, \infty)$. E.g., $\varepsilon(p) = p^2/(2m)$.

For given chemical potential $\mu \in \mathbb{R}$, temperature $T > 0$ and Fermi-function $f_T : \mathbb{R} \to [0, 1], f_T(E) := 1/(1 + \exp(E/T))$, we define one-particle density operator

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

on $\mathrm{L}^2(\mathbb{R}^d)$. At zero temperature $T = 0$ and with $\mu > 0$, let $\Gamma := \{p \in \mathbb{R}^d : \varepsilon(p) \leq \mu\}$ be the Fermi-sea. Then, with $\mathbf{1}_\Gamma$ the indicator function of Γ we define the Fermi-projection

$$D(0, \mu) := \mathbf{1}_\Gamma(P)\,. \tag{2}$$

$D(T,\mu)$ determines (all correlations of) free Fermi-gas equilibrium state, $\omega = \omega(T,\mu)$, at temperature T and chemical potential μ: ω is state on Fermi-algebra, $\mathcal{A}(\mathbb{R}^d)$, so that for $f_j, g_k \in \mathrm{L}^2(\mathbb{R}^d)$:

$$\omega\big(a^*(f_1)\cdots a^*(f_n)a(g_1)\cdots a(g_m)\big) = \begin{cases} 0 & \text{if } n \neq m \\ \det\langle g_k, Df_j\rangle & \text{if } n = m \end{cases} \tag{3}$$

For any one-particle density operator $0 \leq \widetilde{D} \leq \mathbb{1}$ on $\mathrm{L}^2(\mathbb{R}^d)$ define the (quasi-free) Fermi state $\omega_{\widetilde{D}}$ as in (3). For any (Rényi index) $\alpha > 0$ define Rényi-entropy function $h_\alpha : [0,1] \to [0, \ln(2)]$:

$$h_\alpha(t) := \begin{cases} \frac{1}{1-\alpha} \ln\left[t^\alpha + (1-t)^\alpha\right] & \text{if } \alpha \neq 1 \\ -t\ln(t) - (1-t)\ln(1-t) & \text{if } \alpha = 1 \end{cases} . \tag{4}$$

Define the α-Rényi entropy of $\omega_{\widetilde{D}}$:

$$S_\alpha(\omega_{\widetilde{D}}) := \operatorname{tr} h_\alpha(\widetilde{D}) \,. \tag{5}$$

Spatial localization of quasi-free Fermi-state ω on $\mathcal{A}(\mathbb{R}^d)$: Fix some spatial (measurable) region $\Omega \subset \mathbb{R}^d$. Let $\mathrm{L}^2(\Omega)$ and $\mathrm{L}^2(\Omega^c)$ be one-particle Hilbert spaces for fermions inside Ω respectively outside Ω. Fermi-algebra $\mathcal{A}(\mathbb{R}^d) \cong \mathcal{A}(\Omega) \otimes \mathcal{A}(\Omega^c)$.

Define locally reduced (marginal) states ω_1 and ω_2 of ω by taking partial traces

$$\begin{aligned} \omega_1(A_1) &:= \omega(A_1 \otimes \mathbb{1})\,, \quad A_1 \in \mathcal{A}(\Omega)\,, \\ \omega_2(A_2) &:= \omega(\mathbb{1} \otimes A_2)\,, \quad A_2 \in \mathcal{A}(\Omega^c)\,. \end{aligned}$$

E.g. $A_1 = a^*(f)a(f), f \in \mathrm{L}^2(\Omega)$.

If $\omega = \omega_D$ is quasi-free then the reduced states $\omega_{1,2}$ are also quasi-free. Moreover, $\omega_1 = \omega_{D_\Omega}$ and $\omega_2 = \omega_{D_{\Omega^c}}$ with

$$D_\Omega = \mathbf{1}_\Omega(Q)\, D\, \mathbf{1}_\Omega(Q)\,, \quad D_{\Omega^c} = \mathbf{1}_{\Omega^c}(Q)\, D\, \mathbf{1}_{\Omega^c}(Q)\,, \tag{6}$$

and Q usual position multiplication operator on $\mathrm{L}^2(\mathbb{R}^d)$.

Define α-Rényi EE (or mutual information) of quasi-free state $\omega = \omega_D$ with respect to the spatial bi-partition $\mathbb{R}^d = \Omega \cup \Omega^c$:

$$\begin{aligned} H_\alpha(\omega, \Omega) &:= S_\alpha(\omega_1) + S_\alpha(\omega_2) - S_\alpha(\omega) \\ &= \operatorname{tr} h_\alpha(D_\Omega) + \text{``}\operatorname{tr} h_\alpha(D_{\Omega^c}) - \operatorname{tr} h_\alpha(D)\text{''}\,. \end{aligned}$$

Zero-temperature case: Here, one-particle density operator, $D = D(0,\mu) = \mathbf{1}_\Gamma(P)$, of the free Fermi ground-state ($\omega = \omega_D$) is a projection. Hence, its eigenvalues λ_j are 0 and 1 so that with $h_\alpha(0) = h_\alpha(1) = 0$,

$$S_\alpha(\omega) = \operatorname{tr} h_\alpha(D) = \sum_j h_\alpha(\lambda_j) = 0\,.$$

The locally reduced density operators $D_1 = D_\Omega = \mathbf{1}_\Omega(Q)\, D\, \mathbf{1}_\Omega(Q)$ and $D_2 = D_{\Omega^c} = \mathbf{1}_{\Omega^c}(Q)\, D\, \mathbf{1}_{\Omega^c}(Q)$ are no longer projections so that $S_\alpha(D_{1,2}) > 0$. Not difficult to see $S_\alpha(D_1) = S_\alpha(D_2)$.

But it is non-trivial to show that $S_\alpha(D_1) < \infty$. Therefore,

$$H_\alpha(\omega, \Omega) = 2S_\alpha(\omega_1) = 2\,\mathrm{tr}\, h_\alpha(D_\Omega) \, < \, \infty\,.$$

Goal is to describe local entropy $S_\alpha(\omega_1)$ for large Ω. To this end, we fix Ω, introduce a scaling parameter $L > 0$ and study the asymptotics of $\mathrm{tr}\, h_\alpha(D_{L\Omega})$ as $L \to \infty$.

Heuristics: Since the entropy of inside $L\Omega$ = entropy of outside $L\Omega^c$, one expects entropy $\propto L^{d-1}|\partial\Omega|$. This is called an area-law. Motivation for black-hole entropy.

Such an area-law seems indeed true for gapped system (with proofs by Hastings et al) but it is not quite true for this gapless model.

Theorem (Leschke-Sobolev-S). *Let $\Gamma \subset \mathbb{R}^d$ be bounded with piece-wise C^3-boundary $\partial\Gamma$, $D = \mathbf{1}_\Gamma(P)$ the zero temperature Fermi-projection, $\Omega \subset \mathbb{R}^d$ be bounded with piece-wise C^1-boundary $\partial\Omega$, $\alpha > 0$. Let $\omega_1 = \omega_{D_{L\Omega}}$ be the quasi-free state ω_D locally reduced to $L\Omega$. Then, as $L \to \infty$*

$$
\begin{aligned}
S_\alpha(\omega_1) &= \operatorname{tr} h_\alpha\big(\mathbf{1}_{L\Omega}(Q)\,\mathbf{1}_\Gamma(P)\,\mathbf{1}_{L\Omega}(Q)\big) \\
&= h_\alpha(1)\,|\Omega|\,|\Gamma/(2\pi\hbar)|\,L^d \\
&+ \frac{1+\alpha}{24\alpha}\,(2\pi\hbar)^{1-d}\int_{\partial\Gamma\times\partial\Omega} \mathrm{d}\tau(p)\mathrm{d}\sigma(q)\,|n_p\cdot n_q|\,L^{d-1}\ln(L) \\
&+ o(L^{d-1}\ln(L))\,.
\end{aligned}
$$

n_p and n_q are unit normal vectors at $p \in \partial\Gamma$ resp. $q \in \partial\Omega$, and $\tau(p)$ and $\sigma(q)$ are the surface measures on $\partial\Gamma$ resp. $\partial\Omega$.

Since $h_\alpha(1) = 0$ the "leading" (volume) Weyl-term vanishes and leading term of entropy is $O(L^{d-1}\ln(L))$.

If energy dispersion relation ε is radial resp. if Fermi-surface $\partial\Gamma = p_F\,\mathbb{S}^{d-1}$ then

$$(2\pi\hbar)^{1-d}\int_{\partial\Gamma\times\partial\Omega}\mathrm{d}\tau(p)\mathrm{d}\sigma(q)\,|n_p\cdot n_q| = \frac{2}{\left(\frac{d-1}{2}\right)!}\left(\frac{p_F^2}{4\pi\hbar^2}\right)^{\frac{d-1}{2}}\,|\partial\Omega|\,.$$

This proves a logarithmically enhanced area-law for entropy of free fermions in ground states.

• For $\alpha = 1$, Gioev-Klich conjectured this formula in PRL **96**, 100503 (2006) based on a conjecture by H. Widom in 1982. Widom's formula (simple version): $g \in C^\infty(\mathbb{R}), g(0) = 0$. Let

$$U(g) := \frac{1}{4\pi^2} \int_0^1 \mathrm{d}\lambda \, \frac{g(\lambda) - \lambda g(1)}{\lambda(1-\lambda)}$$

and

$$\mathcal{I}(\partial\Gamma, \partial\Omega) := (2\pi\hbar)^{1-d} \int_{\partial\Gamma \times \partial\Omega} \mathrm{d}\tau(p) \mathrm{d}\sigma(q) \, |n_p \cdot n_q|$$

Then,

$$\begin{aligned} \operatorname{tr} g\big(\mathbf{1}_{L\Omega}(Q)\, \mathbf{1}_\Gamma(P)\, \mathbf{1}_{L\Omega}(Q)\big) \quad &= \quad g(1)\, |\Omega|\, |\Gamma/(2\pi\hbar)|\, L^d \\ &+ \quad U(g)\, \mathcal{I}(\partial\Gamma, \partial\Omega)\, L^{d-1} \ln(L) \\ &+ \quad o(L^{d-1} \ln(L))\,. \end{aligned}$$

Using $U(h_\alpha) = \frac{1+\alpha}{24\alpha}$ leads to formula conjectured by Gioev-Klich ($\alpha = 1$).

• In IMRN **2011** (2011), Helling-Leschke-S proved Widom formula for $t \mapsto t^2$. Using entropy particle-fluctuation inequality $h_\alpha(t) \geq g_2(t) := 4\ln(2)\, t(1-t)$ for $\alpha \geq 1$ this implies

$$S_\alpha(\omega_{L\Omega}) \geq U(g_2)\,\mathcal{I}(\partial\Gamma, \partial\Omega)\, L^{d-1}\ln(L) + o(L^{d-1}\ln(L))\,.$$

• In Mem. AMS. **222**, 1043 (2013), Sobolev proved Widom's formula for smooth functions and smooth spatial domains Ω and Γ. Extended in 2013 to piece-wise C^1, resp. C^3-smooth domains.

• We extended Widom-Sobolev formula to non-smooth h_α. Proof is based on an approximation of h_α by a smooth function and a trace estimate to control error term. We write $h_\alpha = h_\alpha(1-\varphi_\delta) + h_\alpha\varphi_\delta$ with $\varphi_\delta \in C^\infty(\mathbb{R}), 0 \leq \varphi \leq 1$ localized near endpoints 0 and 1 of width δ.

Define

$$
\begin{aligned}
D_L &:= \mathbf{1}_{L\Omega}(Q)\,\mathbf{1}_{\Gamma}(P)\,\mathbf{1}_{L\Omega}(Q) \\
A &:= \operatorname{tr} h_\alpha(D_L) \\
A^{sc} &:= U(h_\alpha)\,\mathcal{I}(\partial\Gamma,\partial\Omega)\,L^{d-1}\ln(L) \\
A_\delta &:= \operatorname{tr}\left[h_\alpha(1-\varphi_\delta)(D_L)\right] \\
A^{sc}_\delta &:= U(h_\alpha(1-\varphi_\delta))\,\mathcal{I}(\partial\Gamma,\partial\Omega)\,L^{d-1}\ln(L)
\end{aligned}
$$

One can find $0 < \gamma < \alpha, \gamma < 1$ and constant C so that

$$(h_\alpha\varphi_\delta)(t) \le C\,\delta^{\alpha-\gamma}\,t^\gamma(1-t)^\gamma\,.$$

Then Schatten von-Neumann (quasi) norm estimate (Sobolev, JFA **226**, 2014) shows

$$
\begin{aligned}
|A - A_\delta| &= \operatorname{tr}(h_\alpha \varphi_\delta)(D_L) \\
&\leq C\delta^{\alpha-\gamma} \operatorname{tr}\left[D_L^\gamma (1 - D_L)^\gamma\right] \\
&\leq C\delta^{\alpha-\gamma}\, C_\gamma\, L^{d-1} \ln(L)\,.
\end{aligned}
$$

Using Widom-Sobolev formula for A_δ and simple estimates on integrals we obtain

$$
\begin{aligned}
|A - A^{sc}| &\leq |A - A_\delta| + |A_\delta - A_\delta^{sc}| + |A_\delta^{sc} - A^{sc}| \\
&= o_\delta(1) L^{d-1} \ln(L) + o(L^{d-1} \ln(L)) + o_\delta(1) L^{d-1} \ln(L)\,.
\end{aligned}
$$

Divide by $L^{d-1} \ln(L)$, let $L \to \infty$ and finally, let $\delta \to 0$:

$$
\frac{|A - A^{sc}|}{L^{d-1} \ln(L)} = o_\delta(1)\,.
$$

Positive-temperature case: Recall, one-particle density operator,

$$D = D(T,\mu) = f_T(\varepsilon(P) - \mu\mathbb{1}) = \frac{1}{1 + \exp((\varepsilon(P) - \mu)/T)} \,,$$

locally reduced one-particle density operators,

$$D_\Omega = \mathbf{1}_\Omega(Q)\, D\, \mathbf{1}_\Omega(Q)\,, \quad D_{\Omega^c} = \mathbf{1}_{\Omega^c}(Q)\, D\, \mathbf{1}_{\Omega^c}(Q)\,,$$

and definition of EE of state ω_D (dropping Rényi-index α) ,

$$\begin{aligned} H(T,\Omega) &:= S(\omega_1) + S(\omega_2) - S(\omega) \\ &= \operatorname{tr} h(D_\Omega) + \text{“}\operatorname{tr} h(D_{\Omega^c}) - \operatorname{tr} h(D)\text{”}\,. \end{aligned}$$

Immediate problem: $S(\omega) = \operatorname{tr} h(D) = \infty$ since ω is translation invariant. But, for bounded Ω, also $S(\omega_2) = \operatorname{tr} h(D_{\Omega^c}) = \infty$ and there is a chance that their difference is finite.

Split contribution of $S(\omega) = \operatorname{tr} h(D)$, introduce for $\Lambda = \Omega$ or $\Lambda = \Omega^c$ the operator $(D = D(T, \mu))$

$$\Delta(T, \Lambda) := h\big(\mathbf{1}_\Lambda(Q)\, D\, \mathbf{1}_\Lambda(Q)\big) - \mathbf{1}_\Lambda(Q)\, h(D)\, \mathbf{1}_\Lambda(Q)\,,$$

and write

$$\begin{aligned} H(T, \Omega) &= \operatorname{tr}\left[h(\mathbf{1}_\Omega(Q)\, D\, \mathbf{1}_\Omega(Q)) - \mathbf{1}_\Omega(Q)\, h(D)\, \mathbf{1}_\Omega(Q)\right] \\ &+ \operatorname{tr}\left[h(\mathbf{1}_{\Omega^c}(Q)\, D\, \mathbf{1}_{\Omega^c}(Q)) - \mathbf{1}_{\Omega^c}(Q)\, h(D)\, \mathbf{1}_{\Omega^c}(Q)\right] \\ &= \operatorname{tr} \Delta(T, \Omega) + \operatorname{tr} \Delta(T, \Omega^c)\,. \end{aligned}$$

A-priori estimate for $\Lambda = \Omega$ or Ω^c bounded (under smoothness conditions on $\partial\Omega$ and conditions on ε and "smooth" h):

$$\operatorname{tr} \Delta(T, L\Lambda) \le C L^{d-1}\,. \tag{7}$$

This implies an area-law bound for EE. To determine its precise scaling we need another Widom formula for smooth symbols f_T and some more definitions.

For $\{r, t\} \subset [0,1]$ define

$$U(r,t) := \int_0^1 \mathrm{d}\lambda \, \frac{h((1-\lambda)r + \lambda t) - (1-\lambda)h(r) - \lambda h(t)}{\lambda(1-\lambda)} \, .$$

Then, for a function $g : \mathbb{R} \to [0,1]$, let

$$\mathcal{U}[g] := \frac{1}{8\pi^2} \int_{\mathbb{R}^2} \mathrm{d}u\mathrm{d}v \, \frac{U(g(u), g(v))}{(u-v)^2} \, .$$

In $d = 1$, set $\eta(T, \partial\Omega) := \mathcal{U}[f_T \circ (\varepsilon - \mu)] \, |\partial\Omega|$. If $d \geq 2, q \in \partial\Omega$ and $p \in \mathrm{T}^*_q(\partial\Omega) \cong \mathbb{R}^{d-1}$ then define first 1d symbol $f_{T;(q,p)} : \mathbb{R} \to \mathbb{R}$

$$f_{T;(q,p)}(v) := f_T(\varepsilon(p + v \cdot n_q) - \mu) \, .$$

Finally, let

$$\eta(T, \partial\Omega) := (2\pi\hbar)^{1-d} \int_{\partial\Omega} \mathrm{d}\sigma(q) \int_{\mathbb{R}^{d-1}} \mathrm{d}p \, \mathcal{U}[f_{T;(q,p)}] \, . \tag{8}$$

Theorem (Leschke-Sobolev-S, Sobolev)**.** *Under some conditions on* ε *and* Ω *and with* $\Lambda = \Omega$ *or its complement, as* $L \to \infty$

$$\operatorname{tr} \Delta(T, L\Lambda) = \eta(T, \partial\Omega) L^{d-1} + o(L^{d-1})\,. \tag{9}$$

Area-law scaling of EE in equilibrium state at $T > 0$, as $L \to \infty$

$$H(T, L\Omega) = 2\,\eta(T, \partial\Omega) L^{d-1} + o(L^{d-1}) \tag{10}$$

and a two-term asymptotic expansion of local entropy,

$$\begin{aligned} S(T, L\Omega) &= \operatorname{tr}\big[h(\mathbf{1}_{L\Omega}(Q)\, f_T(\varepsilon(P) - \mu\mathbb{1})\, \mathbf{1}_{L\Omega}(Q))\big] \\ &= \operatorname{tr}\big[\mathbf{1}_{L\Omega}(Q)\,(h \circ f_T)(\varepsilon(P) - \mu\mathbb{1})\, \mathbf{1}_{L\Omega}(Q)\big] + \operatorname{tr}\Delta(T, L\Omega) \\ &= s(T)|\Omega| L^d + \eta(T, \partial\Omega) L^{d-1} + o(L^{d-1})\,, \end{aligned}$$

with the thermal entropy density

$$s(T) = (2\pi\hbar)^{-d} \int_{\mathbb{R}^d} \mathrm{d}p\, h\big[1 + \exp((\varepsilon(p) - \mu)/T)\big]^{-1}\,. \tag{11}$$

The leading $s(T)|\Omega|L^d$ behavior was proved by Park and Shin in 1993. The next-to-leading term of order L^{d-1} is new.

As $T \downarrow 0$, the coefficient $s(T)$ goes to zero but $\eta(T, \partial\Omega)$ displays a logarithmic singularity,

$$\eta(T, \partial\Omega) = \ln(1/T)\, \frac{1}{12}\, \mathcal{I}(\partial\Gamma, \partial\Omega) + O_T(1)$$

with $\Gamma := \{p \in \mathbb{R}^d : \varepsilon(p) \leq \mu\}$ being the Fermi-sea. So if we identify $1/T$ with L we recover the logarithmically enhanced area-law scaling at zero temperature.