Entropy and Entanglement Bounds for Reduced Density Matrices of Fermionic States

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Introduction

Bosons are sometimes thought to be more complicated than fermions because they can 'condense'. But condensed bosons that are in a product, or 'coherent', state $\Psi = \phi(x_1)\,\phi(x_2)\cdots\phi(x_N)$ are *not* entangled in any way (by usual definitions of entanglement) whereas fermions are *always* entangled, by the Pauli principle. Our goal was to quantify the minimum possible entanglement and, as folklore might suggest, show that pure Slater determinant states give the minimum entanglement. If this is the case then

Slaters can be said to be the fermionic analog of boson condensation!

We study the bipartite density matrix of 2 fermions embedded in a sea of N fermions. Some results depend on N, while others do not. A subtle, but signifcant question, then, is *What is N?* It is the number of particles in a 'container' under observation. But any electron, in or out of the container, is (Pauli principle) entangled with all the electrons in the universe, so is $N = \infty$?

Remark about N

The reason N is finite is that a physical state is really a state on a physically relevant algebra of observables, which, in this case, is the algebra of observables *in the container.* In statistical mechanics one must always use the lowest possible dimensionality of a density matrix, and not add superfluous degrees of freedom like color or flavor, which might exist, but are not observable, to artificially increase entropy.

Entanglement Reminder

Consider a bipartite quantum system on $\mathcal{H}_1 \otimes \mathcal{H}_2$. A density matrix (state) ρ_{12} on $\mathcal{H}_1 \otimes \mathcal{H}_2$ is separable if it is convex combination of tensor product states:

$$\rho_{12} = \sum_{j=1}^{n} \lambda_j \rho_1^{(j)} \otimes \rho_2^{(j)} \ .$$

Otherwise, it is entangled – by definition.
The fundamental example of an entangled state is the ebit $\rho_{12} := |\phi\rangle\langle\phi|$,
where $|\phi\rangle \in \mathbb{C}^2 \otimes \mathbb{C}^2$ is the (pure) Bell state

$$|\phi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \ .$$

The ebit is the basic 'currency of the realm' in quantum information. Given a bipartite state ρ_{12} one can ask: 'How many ebits does it take to construct ρ_{12}' or 'How many ebits can one extract from ρ_{12}'? These questions can be partially answered by certain entropically based *entanglement measures*, which will be the subject of this talk.

THEOREM #1

We all know subadditivity of entropy (positivity of mutual information): $S_1 + S_2 - S_{12} \geq 0$, and that equality occurs only when $\rho_{12} = \rho_1 \otimes \rho_2$. Equality can happen for bosons but not for fermions!

Mutual Information of fermionic ρ_{12}:

$$S_1 + S_2 - S_{12} \geq \ln \left(\frac{2}{1 - \mathrm{Tr}\rho_1^2} \right),$$

and *there is equality if and only if the N-particle fermionic state is a pure-state Slater determinant.* (not a convex combination of Slaters)

Recall that for N fermions $\rho_1 = \rho_2 \leq \frac{1}{N} \mathbb{1}$, and equality occurs only for an N-particle Slater. For a Slater $S_1 = S_2 = \ln N$ and $S_{12} = \ln \binom{N}{2}$.

Proof of Theorem #1

First we prove a new, general, non-fermionic, theorem

THM: [Quantitative subadditivity]

$$S_1 + S_2 - S_{12} \geq -2\ln\left(1 - \tfrac{1}{2}\mathrm{Tr}\left[\sqrt{\rho_{12}} - \sqrt{\rho_1 \otimes \rho_2}\right]^2\right) \geq \mathrm{Tr}\left[\sqrt{\rho_{12}} - \sqrt{\rho_1 \otimes \rho_2}\right]^2$$

In particular, $S_1 + S_2 - S_{12} \geq 0$ with equality if and only if $\rho_{12} = \rho_1 \otimes \rho_2$.

Proof: Peierls-Bogoliubov inequality: If H and A are self adjoint operators and $\mathrm{Tr} e^{-H} = 1$,

$$\mathrm{Tr}\left(e^{-H+A}\right) \geq \exp\{\mathrm{Tr}\, A\, e^{-H}\}\ .$$

Apply this with $H = -\log\rho_{12}$ and $A = \frac{1}{2}(\log\rho_1 + \log\rho_2 - \log\rho_{12})$. Then with $\Delta := \frac{1}{2}(S_{12} - S_1 - S_2)$ (Note the $1/2$!). By the Peierls-Bogoliubov inequality and the Golden-Thompson inequality, we have:

$$
\begin{aligned}
e^{\Delta} &= \exp\left[\mathrm{Tr}\,\rho_{12}\ \left\{\tfrac{1}{2}(\log\rho_1 + \log\rho_2 - \log\rho_{12})\right\}\right] \\
&\le \mathrm{Tr}\exp\left[\tfrac{1}{2}(\log\rho_{12} + \log(\rho_1\otimes\rho_2)\right] \\
&\le \mathrm{Tr}\exp\left[\tfrac{1}{2}\log\rho_{12}\right]\exp\left[\tfrac{1}{2}\log(\rho_1\otimes\rho_2)\right] \\
&= \mathrm{Tr}\left[\rho_{12}^{1/2}(\rho_1\otimes\rho_2)^{1/2}\right]\ .
\end{aligned}
$$

Since

$$
\mathrm{Tr}\left[\rho_{12}^{1/2}(\rho_1\otimes\rho_2)^{1/2}\right] = \left(1 - \tfrac{1}{2}\mathrm{Tr}\left[\rho_{12}^{1/2} - (\rho_1\otimes\rho_2)^{1/2}\right]^2\right)\ , \qquad (1)
$$

the quantitative subadditivity theorem is proved. QED

Now we prove that for fermions $S_1 + S_2 - S_{12} \ge \ln\left(\frac{2}{1-\mathrm{Tr}\rho_1^2}\right)$. We use Schwarz on the left side of (1), but remember to insert P_f the projector onto 2-particle antisymmetric states. Thus, since $\mathrm{Tr}\rho_{12} = 1$, $\mathrm{Tr}\left[\rho_{12}^{1/2}(\rho_1\otimes\rho_2)^{1/2}\right] \le \mathrm{Tr}\left[P_f(\rho_1\otimes\rho_2)^{1/2}P_f\right]^2$.

By introducing a spectral resolution for ρ_1, and antisymmetrizing, and fiddling around, one gets Theorem #1. QED

Theorem #2

Entanglement of Formation of ρ_{12}:

$$E_f(\rho_{12}) := \inf_{\lambda,\omega} \left\{ \sum_{j=1}^{n} \lambda_j S(\mathrm{Trace}_2\, \omega^j) \ :\ \rho_{12} = \sum_{j=1}^{n} \lambda_j \omega^j \right\}.$$

Then, $\boxed{E_f(\rho_{12}) \geq \ln(2) \text{ for fermions}}$

and there is equality *if and only if ρ_{12} is a convex combination of pure-state Slater determinants; i.e., the state is fermionic separable.* In other words,

$$E_f^{antisymmetric}(\rho_{12}) := E_f(\rho_{12}) - \ln(2)$$

is a faithful measure of fermionic entanglement.

Proof of Theorem #2

Recall that $E_f(\rho_{12}) := \inf_{\lambda,\omega}\left\{\sum_{j=1}^n \lambda_j S(\mathrm{Tr}_2\ \omega^j)\right\}$. To prove $E_f \geq \ln(2)$ it suffices to prove that if ρ_{12} is any fermionic density matrix on $\mathcal{H}\wedge\mathcal{H}$ and $\rho_1 = \mathrm{Tr}_2\rho_{12}$, then

$$S(\rho_1) \geq \ln 2\ . \tag{2}$$

Any pure Slater has $S(\rho_1) \geq \ln 2$, and so does a convex combination of pure Slaters. So Slaters would minimize if we can prove (2).

By theorem #1 (subadditivity) and by $S(\rho_{12}) \geq 0$, and by $S(\rho_1) = S(\rho_2)$, we have

$$2S(\rho_1) \geq S(\rho_1) + \tfrac{1}{2}\left\{\ln 2 - \ln[1 - \mathrm{Tr}\,\rho_1^2]\right\}\ . \tag{3}$$

By Jensen, $e^{-S(\rho_1)} \leq \mathrm{Tr}\,\rho_1^2$. Therefore, letting $x := \mathrm{Tr}\,\rho_1^2$, we can deduce from (3) that

$$2S(\rho_1) \geq \inf_{0\leq x\leq 1/2}\left\{-\ln x - \tfrac{1}{2}\ln(1-x) + \tfrac{1}{2}\ln 2\right\}\ .$$

A simple calculation shows the minimum is achieved at $x = 1/2$, which yields (2). QED

Theorem #3

Consider the entropy $S(\rho_{12}) = S_{12}$ of the two-particle density matrix of an N-particle fermion state. For a Slater we easily find that ρ_{12} has $\binom{N}{2}$ eigenvalues $1/\binom{N}{2}$, and thus $S_{12} = \ln\binom{N}{2} \approx 2\ln N - \ln(2)$ for a Slater.

We *believe* that a Slater minimizes S_{12}. What we *can prove* is:

The 2-particle reduced density matrix of any N-particle fermionic state satisfies

$$S(\rho_{12}) \geq 2\ln N + \mathcal{O}(1) \ .$$

and, therefore, a Slater is at least *asymptotically* close to the minimum.

Theorem #3 continued

To summarize: The entropy of a single fermion satisfies

$$S_1 \geq \ln N \quad \text{with equality only for a Slater}$$

and the entropy of two fermions satisfies

$$S_{12} \geq 2\ln N + \mathcal{O}(1) \quad \text{which is satisfied by any Slater.}$$

The N dependence and the factor of 2 is very interesting for the following reason: Recall that while the eigenvalues of a fermionic ρ_1 are characterized by $\lambda \leq 1/N$, there is no simple characterization of the eigenvalues of a fermionic ρ_{12}. Yang showed that the upper bound is not $\binom{N}{2}^{-1}$, as one might think, but rather $\lambda \leq 2/(N-1)$. If the eigenvalues were mostly of this magnitude one could get an entropy $S_{12} \approx \ln N - \ln(2)$.

But our result says that this cannot happen. There must be many much smaller eigenvalues because $S_{12} \geq 2\ln N + \mathcal{O}(1)$.

Topic#4

Squashed Entanglement of ρ_{12}:

$$E_{sq}(\rho_{12}) = \frac{1}{2} \inf_{\rho_{123}} \{-S_{123} - S_3 + S_{13} + S_{23}\} \geq 0,$$

where 3 refers to an extra Hilbert space (of arbitrary dimension) and $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3$, and $\mathrm{Tr}_3\, \rho_{123} = \rho_{12}$.

In general, $E_{sq} > 0$ unless ρ_{12} is separable, (which a fermionic ρ_{12} is not) and $E_f \geq E_{sq}$.

We cannot find the minimum of E_{sq} over all fermionic states but

We conjecture that the minimum E_{sq} occurs for Slaters

We conjecture that E_{sq} for a Slater is given by:

$$E_{sq}(\rho_{12}) = \begin{cases} \frac{1}{2} \ln \frac{N+2}{N-2} & \text{if } N \text{ is even} \\ \frac{1}{2} \ln \frac{N+3}{N-1} & \text{if } N \text{ is odd} \end{cases}$$

Squashed entanglement continued

At first we thought that the minimum was the same as for the entanglement of formation E_f, namely, $\ln(2)$. This is grossly incorrect! The mininimum is at least as small as the value just mentioned, i.e.,

$$Esq(\rho_{12}) = \begin{cases} \frac{1}{2}\ln\frac{N+2}{N-2} & \text{if } N \text{ is even} \\ \frac{1}{2}\ln\frac{N+3}{N-1} & \text{if } N \text{ is odd.} \end{cases}$$

This upper bound shows that E_{sq} for a Slater depends heavily on N, namely $\approx 2/N$.

We obtain it by starting with an N-particle Slater (which is pure and which gives us the required ρ_{12}) and then taking ρ_{123} to be the (mixed) $N/2$-particle reduced density matrix of this Slater state. Thus, $\dim \mathcal{H}_3 = \binom{N}{N/2-\ 2}$. Then

$$S_{123} = \ln\binom{N}{N/2}, \quad S_3 = \ln\binom{N}{N/2-2}, \quad S_{13} = S_{23} = \ln\binom{N}{N/2-1}$$

and $\frac{1}{2}(S_{13} + S_{23} - S_{123} - S_3)$ is as above. (Also found by Christandl-Schuch-Winter.)

Monotonicity of Relative Entropy

Finally, let me mention an inequality, which is not related to entanglement, but which is proved similarly to the previous ones (using the Peierls-Bogoliubov inequality) – except for one thing! The Golden-Thompson inequality used before is not strong enough for this purpose and one has to use the triple matrix inequality, which was at the basis of the proof of strong subadditivity of entropy (with Ruskai).

$$\mathrm{Tr}\exp\{\ln A + \ln B - \ln C\} \leq \mathrm{Tr}\int_0^\infty A\frac{1}{t+C}B\frac{1}{t+C}\mathrm{d}t$$

Remainder term for the monotonicity of relative entropy: $D(\rho||\sigma) := \mathrm{Tr}\,\rho[\ln\rho - \ln\sigma]$.

$$\boxed{D(\rho_{12}||\sigma_{12}) - D(\rho_1||\sigma_1) \geq \mathrm{Tr}\left[\sqrt{\rho}_{12} - \exp\left\{\tfrac{1}{2}\ln\sigma_{12} - \tfrac{1}{2}\ln\sigma_1 + \tfrac{1}{2}\ln\rho_1\right\}\right]^2.} \qquad (4)$$

Thus, we rederive a theorem of Ruskai that there is equality if and only if

$$\rho_{12} - \ln\sigma_{12} = (\ln\rho_1 - \ln\sigma_1)\otimes I_2.$$

TwoParticle Entropy of the Pairing State

Recall the pairing state of Yang (1962), which is at the basis of the BCS theory of superconductivity. Take an O.N. set of M vectors $u_1, \ldots, u_M$, let $m = M/2$, $n = N/2$, and consider the m pairs of vectors $\pi_j = u_{2j},\ u_{2j+1}$. We can make $\binom{m}{n}$ Slater determinants using these pairs. Finally, let $|\psi\rangle$ be the sum of all these $\binom{m}{n}$ determinants and let ρ_{12} be the 2-particle reduced density matrix (normalized to $\mathrm{Tr}\rho_{12} = 1$).

It turns out that ρ_{12} has one huge eigenvalue close to $1/N$, namely

$$\lambda_{\max} = \frac{m^2 - mn + n - 1}{(2n-1)m(m-1)}. \tag{5}$$

TwoParticle Entropy of the Pairing State (continued)

The entropy of ρ_{12} can be computed to be

$$S(\rho_{12}) = 2\ln(M) + \text{lower order terms (for } M \gg N \gg 1). \tag{6}$$

Thus, S can be *much larger* than $O(\ln(N)$, as it is for a determinant. It could even be infinite! One can also compute that

$$E_f(\rho_{12}) - \ln(2) = \frac{1}{N}\ln(M) + \text{lower order}, \tag{7}$$

and one can use the variational principle to compute (for $M \gg N \gg 1$) that

$$E_{sq}(\rho_{12}) \leq \frac{1}{N}\ln(M) + \text{lower order}. \tag{8}$$

Moral of the story: Here is a fermionic state with a 2-body eigenvalue close to $1/N$. If it had many eigenvalues close to this order we might expect it to have low entropy and entanglement. Instead, it has only one eigenvalue of this kind and many tiny eigenvalues (of order M^{-2}), which gives it a large entropy and, possibly, large entanglement!

THANKS FOR LISTENING!