Entanglement of Free Fermions

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1 Analytical Results

Due to Pauli exclusion, momentum ket of different fermions must be different. So for n free fermions there has to be n different momentum states $e^{ik_j r}$ that are mutually orthogonal. For simplicity, I denote them as $|k_j\rangle_{r_j}$, which means j-th particle at position r_j whose unique (w.r.t. other particles) momentum is k_j. Then the wavefunction of n free fermions is the Slater determinant:

$$|\Psi_n\rangle = \mathcal{A}(|k_1\rangle_{r_1}|k_2\rangle_{r_2}\dots|k_n\rangle_{r_n}) = \det\begin{pmatrix} |k_1\rangle_{r_1} & |k_1\rangle_{r_2} & \dots & |k_1\rangle_{r_n} \\ |k_2\rangle_{r_1} & |k_2\rangle_{r_2} & \dots & |k_2\rangle_{r_n} \\ \vdots & \vdots & \vdots & \vdots \\ |k_n\rangle_{r_1} & |k_n\rangle_{r_2} & \dots & |k_n\rangle_{r_n} \end{pmatrix} \tag{1.1}$$

where $\mathcal{A}$ is the anti-symmetrizer which is equivalent to the Slater determinant. To evaluate the determinant we expand it in terms of n-permutation group S_n:

$$|\Psi_n\rangle = \sum_{\sigma\in S_n} sgn(\sigma)\bigotimes_{i=1}^{n}\left|k_{\sigma(i)}\right\rangle_{r_i} \tag{1.2}$$

where $sgn(\sigma)$ is $+1$ for even permutations, and -1 for odd permutations. In this representation the density matrix is

$$\rho = |\Psi_n\rangle\langle\Psi_n| = \sum_{\sigma,\sigma'\in S_n} sgn(\sigma)\, sgn(\sigma')\bigotimes_{i,j=2}^{n}\left|k_{\sigma(i)}\right\rangle_{r_i}\left\langle k_{\sigma'(i')}\right|_{r_{i'}} \tag{1.3}$$

Now we'd like to find the reduced density matrix of the first m particles, that is, we want to trace out momentum kets which are identified by $r_j,\ j \geq m+1$.

$$\begin{aligned}\rho_s &= \sum_{\tilde\sigma}\bigotimes_{j=m+1}^{n} {}_{r_j}\left\langle k_{\tilde\sigma(j)}\middle|\Psi_n\right\rangle\langle\Psi_n|\bigotimes_{j=m+1}^{n}\left|k_{\tilde\sigma(j)}\right\rangle_{r_j} \\ &= \sum_{\sigma\in S_n}\bigotimes_{i=1}^{m}\left|k_{\sigma(i)}\right\rangle\bigotimes_{i'=1}^{m}\left\langle k_{\sigma(i')}\right|_{r_{i'}}\end{aligned} \tag{1.4}$$

where we ignored the constant $sgn^2(\sigma) = 1$. Details are attached in Appendix.

In the simplest case, where the system is assigned only with the first particle i.e. $m = 1$, all the rest (from $i = 2$ to n) are environment to be traced out. The single fermion reduced density matrix becomes

$$\rho_s^{(1)} = \sum_{\sigma\in S_n}\left|k_{\sigma(1)}\right\rangle\left\langle k_{\sigma(1)}\right| \tag{1.5}$$

upto a global normalization factor. It's readily to see that the reduced density matrix is diagonal in this basis. Also all diagonal elements are equally weighed, since the number of configurations $\mathbb{N} \ni \forall i = \sigma(1)$ are the same. After normalization, all diagonal elements becomes $1/n$. So the entanglement entropy for n free fermions is:

$$\boxed{S_E^{(1)}(n) = -\sum_i^n \frac{1}{n} \log\left(\frac{1}{n}\right) = \log(n)} \tag{1.6}$$

For $m > 1$, reduced density matrix reads

$$\rho_s^{(m)} = \sum_{\sigma \in S_n} \left(\bigotimes_{i=1}^m |k_{\sigma(i)}\rangle \right) \left(\bigotimes_{i'=1}^m \langle k_{\sigma(i')}| \right) \tag{1.7}$$

This is still diagonal with equal elements $1/d$. However the dimension of matrix is dependent on both n and m. The dimension d of this $d \times d$ square matrix is determined by

$$d = C_n^m = \frac{n!}{m!(n-m)!} \tag{1.8}$$

Hence

$$S_E^{(m)} = -\sum_i^d \frac{1}{d} \log\left(\frac{1}{d}\right) = \log[\frac{n!}{m!(n-m)!}] = \log(n!) - \log(m!) - \log[(n-m)!] \tag{1.9}$$

By Stirling's approximation $\log(n!) \approx n \log n - n$, this becomes

$$\begin{aligned} S_E^{(m)} &\approx n \log n - n - m \log m + m - [(n-m)\log(n-m) - (n-m)] \\ &= n \log n - m \log m - n \log(n-m) + m \log(n-m) \\ &= m\Big[\log(n-m) - \log m\Big] + n\Big[\log n - \log(n-m)\Big] \\ &= m \log\left(\frac{n}{m} - 1\right) + n \log\left(\frac{n}{n-m}\right) \\ &\approx m \log\left(\frac{n}{m}\right) - n \log\left(1 - \frac{m}{n}\right) \\ &\approx m \log\left(\frac{n}{m}\right) + m \\ &\approx m \log\left(\frac{n}{m}\right) \end{aligned} \tag{1.10}$$

where we assumed $n \gg m \gg 1$. This result is consistent with former result on $m = 1$.

Here I make a very rougth estimation of EE scaling: suppose there is a macroscopic amount of free fermions uniformly distributed in d-dimensional space. Assuming particle density $\rho = 1$ i.e. 1 per unit volumn, and use the length scale of universe as the measure, then $n \gg m$ indicates the length scale of system is $\mathcal{L} \to 0$. So the EE of system is approximated by

$$S_E^{(m)}(\mathcal{L}) \approx \mathcal{L}^d \log\left(\frac{1}{\mathcal{L}}\right)^d \sim \mathcal{L}^d \log\left(\frac{1}{\mathcal{L}}\right) \tag{1.11}$$

$\log(1/\mathcal{L})$ above is large for small system size, nonetheless it is bounded by

$$\log\left(\frac{1}{\mathcal{L}}\right) < \frac{1}{\mathcal{L}} \tag{1.12}$$

so we have

$$S_E(\mathcal{L}) < \mathcal{L}^{d-1} \tag{1.13}$$

This result holds for uniformly distributed free fermions and $n \gg m \gg 1$ (universe $\gg$ system size).

2 Numerical Results

In this section I present the numerical results on the Slater determinant of 2-7 free fermions. First Linear-Linear scale, then Exp-Linear scale. From the Exp-Linear plot it's readily to see that the results are in good agreement with Eq.(1.6).

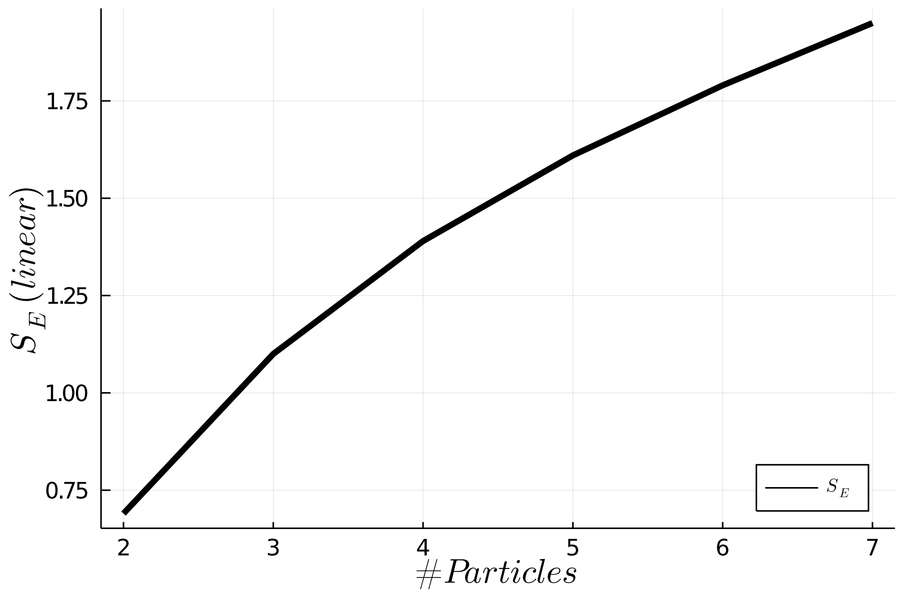

Figure 1: Number of fermions vs. Entanglement entropy (Linear-Linear). Results obtained by tracing all but the 1st particle

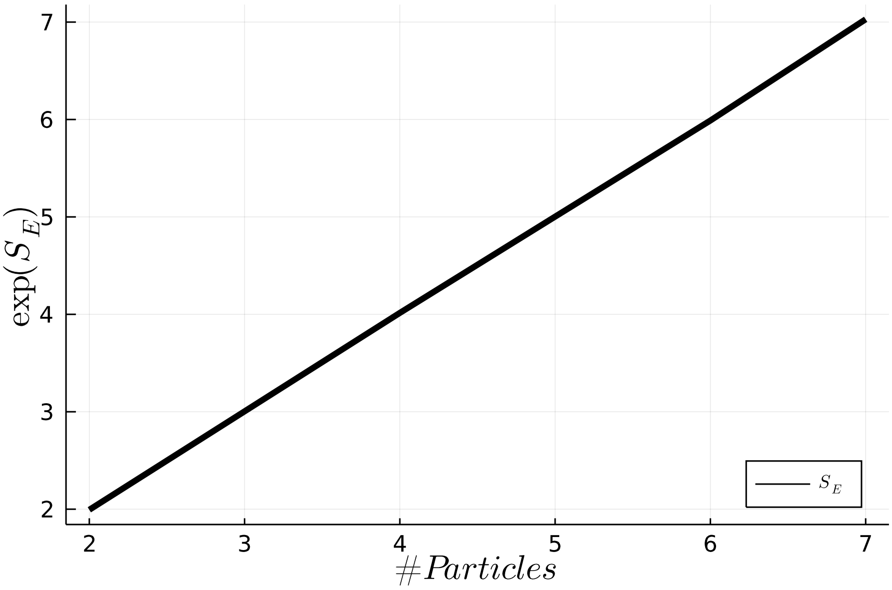

Figure 2: Number of fermions vs. Entanglement entropy (Exp-Linear). Results obtained by tracing all but the 1st particle

3 Appendix

Here I present the detailed derivation. In order to evaluate:

$$\rho_s = \sum_{\tilde{\sigma}} \bigotimes_{j=m+1}^{n} {}_{r_j}\left\langle k_{\tilde{\sigma}(j)} \middle| \Psi_n \right\rangle \left\langle \Psi_n \right| \bigotimes_{j=m+1}^{n} \left| k_{\tilde{\sigma}(j)} \right\rangle_{r_j} \tag{3.1}$$

Let's first look at the right-most braket:

$$\begin{aligned} \left\langle \Psi_n \right| \bigotimes_{j=m+1}^{n} \left| k_{\tilde{\sigma}(j)} \right\rangle_{r_j} &= \sum_{\sigma' \in S_n} sgn(\sigma') \bigotimes_{i'=1}^{m} {}_{r_{i'}}\left\langle k_{\sigma'(i')} \right| \left(\bigotimes_{i',j=m+1}^{n} {}_{r_{i'}}\left\langle k_{\sigma'(i')} \middle| k_{\tilde{\sigma}(j)} \right\rangle_{r_j} \right) \\ &= \sum_{\sigma' \in S_n} sgn(\sigma') \bigotimes_{i'=1}^{m} {}_{r_{i'}}\left\langle k_{\sigma'(i')} \right| \delta_{\sigma',\tilde{\sigma}} \end{aligned}$$

The left-most braket of Eq.(3.1) is

$$\begin{aligned} \bigotimes_{j=m+1}^{n} {}_{r_j}\left\langle k_{\tilde{\sigma}(j)} \middle| \Psi_n \right\rangle &= \sum_{\sigma \in S_n} sgn(\sigma) \left(\bigotimes_{i,j=m+1}^{n} {}_{r_j}\left\langle k_{\tilde{\sigma}(j)} \middle| k_{\sigma(i)} \right\rangle_{r_i} \right) \bigotimes_{i=1}^{m} \left| k_{\sigma(i)} \right\rangle_{r_i} \\ &= \sum_{\sigma \in S_n} sgn(\sigma) \bigotimes_{i=1}^{m} \left| k_{\sigma(i)} \right\rangle_{r_i} \delta_{\tilde{\sigma},\sigma} \end{aligned} \tag{3.2}$$

so Eq.(3.1) becomes

$$\begin{aligned}\rho_s &= \sum_{\tilde{\sigma},\sigma,\sigma'\in S_n} sgn(\sigma)sgn(\sigma') \bigotimes_{i,i'=1}^{m} \left|k_{\sigma(i)}\right\rangle_{r_i} \left\langle k_{\sigma'(i')}\right|_{r_{i'}} \delta_{\tilde{\sigma},\sigma}\delta_{\sigma',\tilde{\sigma}} \\ &= \sum_{\sigma\in S_n} \bigotimes_{i=1}^{m} \left|k_{\sigma(i)}\right\rangle \bigotimes_{i'=1}^{m} \left\langle k_{\sigma(i')}\right|_{r_{i'}}\end{aligned} \tag{3.3}$$