Notes on Entanglement and Computational Complexity

M. B. Hastings

Outline

— Lecture 1: What is entanglement entropy?

— Lecture 1: What we know about entanglement in many-body quantum systems—using entanglement as a computational tool to determine properties of a given system

— Lecture 2: Computing entanglement

— Lecture 2: Relationship between entanglement and computational complexity

1 What is Entanglement Entropy?

We will NOT discuss entanglement of mixed states....this is a mess and one could spend many lectures on it! We will talk about pure states. Any pure state that is not a product is entangled.

We write a state of a bipartite system as:

$$|\psi\rangle = \sum_{ij} \psi_{ij} |i\rangle |j\rangle. \tag{1}$$

Recall SVD from White's lecture: can pick orthonormal basis $|\alpha_L\rangle, |\alpha_R\rangle$ for left and right such that

$$|\psi\rangle = \sum_{\alpha} \lambda_\alpha |\alpha_L\rangle |\alpha_R\rangle. \tag{2}$$

Rank λ_α in order so that $\lambda_1 \geq \lambda_2 \geq ...$

Given sequence of λ_α, we extract an entropy:

$$S = -\sum_{\alpha} \lambda_\alpha^2 \ln(\lambda_\alpha^2). \tag{3}$$

Express this through reduced density matrix:

$$\rho_L = \sum_\alpha \lambda_\alpha^2 |\alpha_L\rangle\langle\alpha_L|. \tag{4}$$

$$S(\rho) = -\mathrm{Tr}(\rho \ln(\rho)). \tag{5}$$

This is called the **von Neumann entropy**.

More generally define **Renyi entropies**:

$$S_\alpha(\rho) = \frac{1}{1-\alpha}\mathrm{Tr}(\rho^\alpha). \tag{6}$$

Some comments:

— $S_1(\rho) = S$ (check by taking a limit as $\alpha \to 1$).

— Sorry about using α both as a subscript in λ_α and in S_α. This is the standard notation (so you just have to get used to it) and it is unfortunate that α is re-used. The two different alphas means very different things.

— The various Renyi entropies are ways to take the sequence of numbers λ_α and extract useful information. S_α is more sensitive to the largest Schmidt coefficients for $\alpha > 1$ and more sensitive to the small ones (the tail of the distribution) for $\alpha < 1$.

1.1 Some useful inequalities

Monotonicity If $\alpha > \beta$ then $S_\alpha \leq S_\beta$. This implies that S_α is bounded by the log of the number of states (since S_0 is just the log of the rank of the density matrix).

Subadditivity Let A and B be subsystems of a large system. Then:

$$S(\rho_{AB}) \leq S(\rho_A) + S(\rho_B). \tag{7}$$

Strong Subadditivity Let A, B, C be subsystems of a large system. Then:

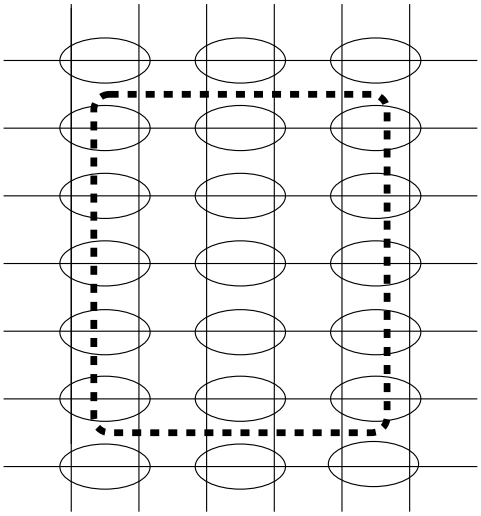
$$S(\rho_{AB}) + S(\rho_{BC}) - S(\rho_B) - S(\rho_{ABC}) \geq 0. \tag{8}$$

Note: the last two only hold for the von Neumann entropy (S_1). Also, we will use strong subadditivity when talking about topological entropy later.

2 Entanglement in Quantum Many-Body Systems

2.1 Toy Model in Valence Bond State

Consider a "valence bond solid state". Ovals denote spins in a singlet.



Region A in dashed line. Entropy is $log(2)$ times number of bonds cut.

$$H = \sum_{<i,j>} \vec{S}_i \cdot \vec{S}_j \tag{9}$$

Results: entropy proportional to area. This is called an "area law" and is prototypical behavior for a gapped system. Area law in 1D means entropy is system size independent.

2.2 Free Systems in 1d

Define 1-particle density matrix:

$$\rho_{ij} = \langle \psi_i^\dagger \psi_j \rangle. \tag{10}$$

Let p_α denote the eigenvalues of reduced ρ_{ij} on region A. Entropy of many-body state:

$$S(\rho_A) = -\sum_\alpha \Big(\log(p_\alpha) p_\alpha + \log(1-p_\alpha)(1-p_\alpha) \Big). \tag{11}$$

Easy to compute numerically. We find that for a free fermi chain,

$$H = \sum_i \psi_i^\dagger \psi_{i+1} + h.c., \tag{12}$$

that $S(\rho_A)$ scales logarithmically. If we take chain of length L, let A denote half the chain, then we get

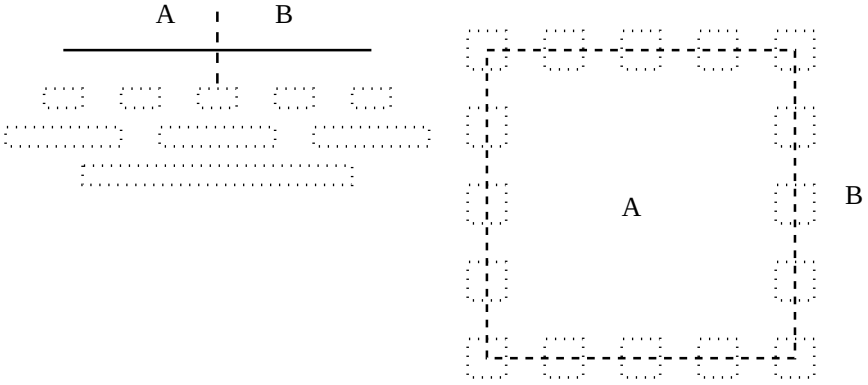
$$S_{OBC}(\rho_A) = (1/6)\log(L) \tag{13}$$

$$S_{PBC}(\rho_A) = (1/3)\log(L) \tag{14}$$

for open and periodic boundary conditions respectively.

2.3 Heuristic Arguments

Heuristic argument for the log by counting modes.



In 1d, we get

$$1 + 1 + 1 + ... \sim \log(L) \tag{15}$$

In 2d, we get

$$L + L/2 + L/4 + ... \sim L \tag{16}$$

2.4 Conformal Field Theory

Consider two copies of the free fermion system (spin-up and down):

$$H = \sum_i \sum_{\sigma=\uparrow,\downarrow} \psi^\dagger_{i,\sigma}\psi_{i+1,\sigma} + h.c. \tag{17}$$

Entropy is doubled compared to previous result:

$$S_{OBC}(\rho_A) = (2/6)\log(L) \tag{18}$$

In general, n copies give an entropy n times as large.

We write

$$S_{OBC}(\rho_A) = \frac{c}{6}\log(L), \tag{19}$$

$$S_{PBC}(\rho_A) = \frac{c}{6}\log(L), \tag{20}$$

where c is called the "central charge". It measures number of gapless modes.

$c = n$ for n free fermions (or for a fermion ladder system with n different k_y values).

Interestingly, there exist nontrivial systems with fractional central charge. For example, the Ising model has $c = 1/2$.

For Renyi entropies we find

$$S_{OBC} = \frac{c}{12}(1 + \frac{1}{\alpha})\log(L). \tag{21}$$

Perturbed CFT: open a gap, entropy $\sim \log(\xi)$, where ξ is the correlation length.

2.5 Free Fermions in $D > 1$

Free fermions for $D > 1$ gives $S \sim L\log(L)$ if they have a fermi surface and $S \sim L$ if they are gapped or have a Dirac cone.

You can see the $S \sim L\log(L)$ behavior by considering a ladder as a model $2d$ system. Note that this violates an area law. So, some gapless systems in 2d have an area law (recall heuristic argument) and some do not.

2.6 Subleading corrections and topological entanglement entropy

For a gapped system in 2d, there can be additive corrections to the entropy depending on the number of corners and on the topology of the region A:

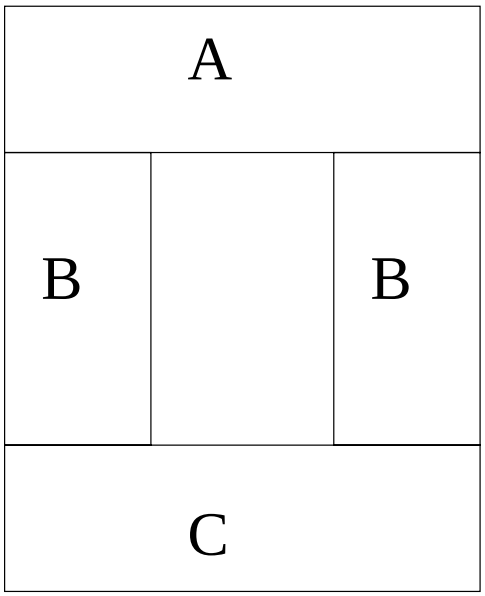
$$S = \text{const} \times L - c_1 \times (number\, of\, corners) - c_2 \times (number\, of\, surfaces). \quad (22)$$

The corner term may depend on the angle of the corner, but is the same for a 90 degree or 270 degree corner.

The second constant is called the topological entanglement entropy and one typically writes

$$c_2 = \log(D). \quad (23)$$

It can be measured by considering a sum and difference of entropies.



Compute:

$$S_{\text{topo}} = S_{AB} + S_{BC} - S_{ABC} - S_B \geq 0. \quad (24)$$

One can check that the area terms (in L) cancel as do the corner terms. The result is $2c_2$.

Note, we use strong subadditivity to show that c_2 is positive. We can similarly show that c_1 is positive.

3 Computing Entanglement

Exact Diagonalization: Compute the wavefunction, then compute the reduced density matrix ρ_A on A, then diagonalize ρ_A and get entropy from its eigenvalues. Note: always choose A to be the smaller subsystem and use the fact that $S(\rho_A) = S(\rho_B)$ in a pure state or else the memory costs can become too much.

DMRG: the DMRG wavefunction truncates the smallest Schmidt cooefficients. So, it can accurately compute S_α for α which is not too small. For example, it will get S_0 (the log of the rank) completely wrong.

3.1 The Replica Trick

Compute Renyi entropies S_α for integer $\alpha = 2, 3, ...$ by computing $Tr(\rho_A^\alpha)$. This can be done in Field Theory or in QMC.

We can consider modified boundary conditions in imaginary time (periodic with period β for sites in B and with period $\alpha\beta$ for sites in A) to compute this.

Also, we can study expectation value of a $Swap$ operator (for $\alpha = 2$) or a $Permute$ operator (for $\alpha \geq 3$). Consider two copies of the systme. Let $Swap_A$ swap the state in region A. Then,

$$\mathrm{Tr}(\rho_A^2) = \langle \psi_0 \otimes \psi_0 | Swap_A | \psi_0 \otimes \psi_0 \rangle. \tag{25}$$

4 Entanglement And Computational Complexity

4.1 Truncation Error

Let us look at error in truncating a general bipartite state to a state of Schmidt rank k. The closest state we can find is

$$\Psi_k = \sum_{\alpha=1}^{k} \lambda_\alpha |\alpha_L\rangle |\alpha_R\rangle. \tag{26}$$

The norm-squared truncation error

$$|\Psi - \Psi_k|^2 = \sum_{\alpha \geq k+1} |\lambda_\alpha^2| \equiv \epsilon(k). \tag{27}$$

If we know something about the Renyi entropy we can estimate the truncation error. We have for any $0 \leq \alpha \leq 1$

$$\log(\epsilon(k)) \leq \frac{1-\alpha}{\alpha}\Big(S_\alpha(\rho) - \log(\frac{k}{1-\alpha})\Big). \tag{28}$$

Proof: consider distribution that maximizes error for given entropy (this is obtained by picking a certain λ_1^2, then picking $\lambda_2 = \lambda_3 = ...\lambda_n$ for some n and choosing constants λ_1, n that maximize the error).

4.2 Matrix Product State Truncation Error

In fact, we can prove an error in approximating a state with given $\epsilon(k)$ across every cut by a matrix product state. The error is at most twice the sum of $\epsilon(D)$ across each cut. Proof: apply projectors in sequence.

4.3 Complexity

DMRG: complexity scales polynomially with bond dimension. Bond dimension needs to scale exponentially with entropy. Entropy scales logarithmically with system size for a system descibed by conformal field theory. So: such gapless systems can be simulated with polynomial cost (in system size). But, see next section for more pessimistic cases!

4.4 Rigourous Results

Rigourous results on possible entanglement:

In 1d, a gap does imply an area law (not yet proven in 2d). This implies that gapped systems in 1d are in "NP" (see Nayak's lectures on complexity classes) since there is an efficient representation of the ground state. However, finding that representation may be very hard. It has been proven also that there are Hamiltonians with exact matrix product states ground states of polynomial

bond dimension for which finding the MPS is NP-hard (however, it has not yet been shown for Hamiltonians with a gap that finding the MPS can be NP-hard).

Entropy can diverge more rapidly than the conformal field theory prediction of $\log(1/(gap))$ however.

There exist so-called "QMA-complete" Hamiltonians such that determining their ground state energy to an accuracy which is only polynomially small is a very hard problem. (This is a quantum analogue of NP, and is hard even for a quantum computer). This holds even in one dimension.

5 Some Interesting Examples From the Literature

5.1 Measurement of Central Charge of a System

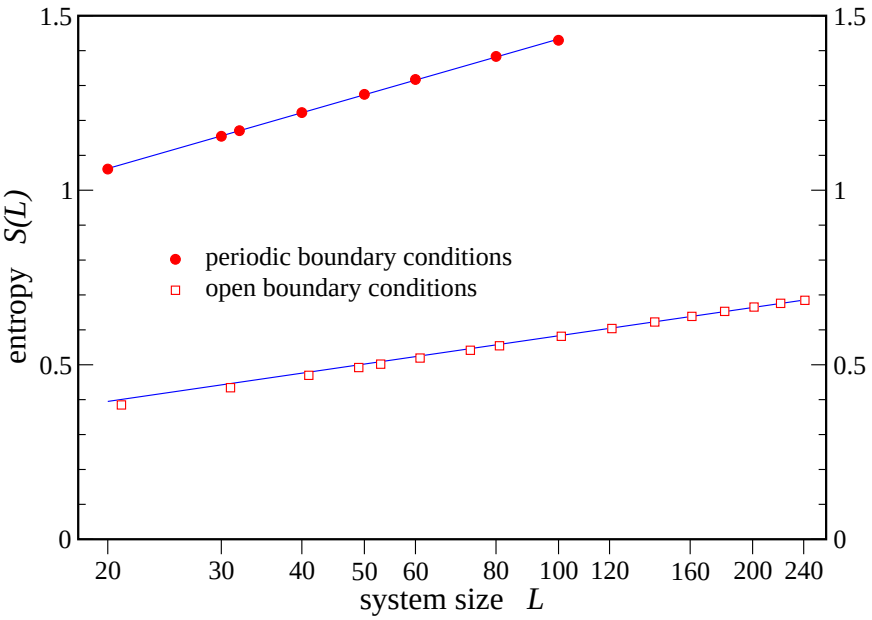
A. Feiguin et. al., Phys. Rev. Lett. 98, 160409 (2007).

The authors were studying a one dimensional model consisting of interacting anyons. They wished to identify the effective field theory of the model and compare it so numerical results. Variety of techniques used, including exact diagonalization (to compute spectra) and DMRG. DMRG used to compute entanglement entropy of half of the system with the rest, and fit to the forms

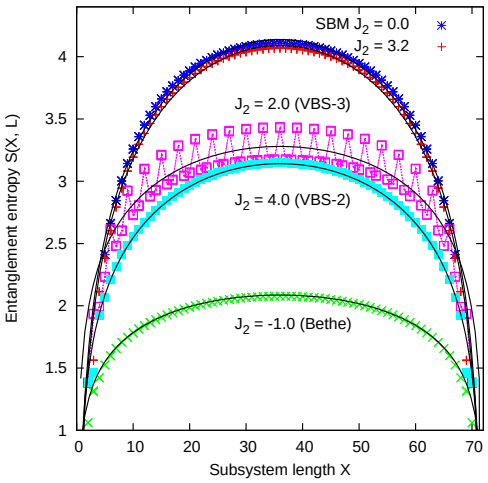
$$S_{PBC} = \frac{c}{3} c \log(L), \tag{29}$$

$$S_{OBC} = \frac{c}{6} c \log(L), \tag{30}$$

The fits gave $c = .701$, matching the field theory $c = 7/10$.



More recently, Sheng, Motrunich, Fisher were studying a ladder system, again facing the same problem. Various values of c obtained at different parameter values. Note oscillation (due to presence of VBS order in VBS-3 case).

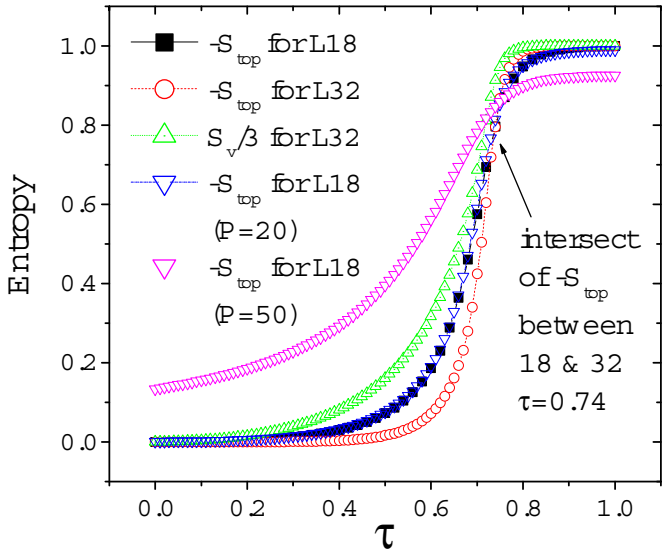


In this case, fit is done by considering entropy of subsystem of size x in length $L = 2$ chain, fitting to form

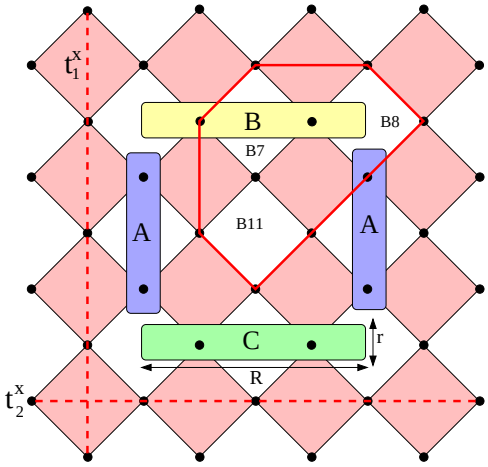
$$S(x, L) = \frac{c}{3} \log(\frac{L}{\pi} \sin(\frac{x\pi}{L})) + \text{const.} \tag{31}$$

5.2 Determining a Topological Phase Transition

The Kitaev toric code is an interesting model with a nontrivial topological entanglement entropy. Hamma et. al. wanted to study the stability of the model to disorder and to perturbation. They considered a random model with a parameter τ that drove from the "trivial" phase to the "topologically ordered" phase using exact diagonalization. They detected the existence of a phase transition with other methods (such as energy as a function of τ), but then confirmed the topological character of the phase using topological entanglment entropy:



However, this was a very small system (32 sites) so the regions A, B, C were not very big:


t_1^x
B
B8
B7
A
B11
A
C
r
R
t_2^x

5.3 Area Laws in Two Dimensions

Kallin, MBH, Gonzalez, and Melko, wanted to study the entanglement entropy in a 2d system and check the area law prediction from heuristic calculation. See below. Ladder calculations of S_{vN} are from DMRG. Free fermi clearly shows area law in contrast.

Geometry used was an N-by-$4N$ system, and entropy of an N-by-$2N$ subsystem was computed (or, in some plots, we consider and N-by-100 subsystem). This way, region A had an even number of spins, reducing even-odd oscillations. Entropy was divided by N to check the area law.