Entanglement entropy

Paolo Stornati

1 Von-Neumann entanglement entropy

Let us suppose we have the ground state of a gapped model on a lattice V described by the density matrix ρ. The von Neumann entropy is defined as:

$$S(\rho) = -Tr(\rho \log(\rho)) \tag{1}$$

The entropy of the ground-state is zero since it is a product state. We can not state this for subset of the system. We define a subset A of V suche that $B := V/A$. We define the reduced density matrix of the sub-system as:

$$\rho_A = Tr_B(\rho) \tag{2}$$

We define the von-Neumann entropy of the subsystem A as:

$$S(\rho_A) = -Tr(\rho_A \log_2(\rho_A)) \tag{3}$$

Now, the entropy $S(\rho_A)$ is null if the subsystems A and B are product states. This is not true if there is quantum correlations between A and B. Quantum correlations can lead to non-vanishing values of $S(\rho_A)$. In fact, the von-Neumann entropy is a index of the entanglement for pure states. This is also why the von-Neumann entropy is also called entanglement entropy.

2 Matrix product states

We define the wavefunction of a quantum state as [1]:

$$|\psi\rangle = \sum j_1, ..., j_n c_{j_1,...,j_n} |j_1\rangle \otimes ... \otimes |j_n\rangle \tag{4}$$

The matrix product state (MPS) Ansatz defines $c_{j_1,...,j_n}$ as:

$$c_{j_1,...,j_n} = \sum_{\alpha,\beta,\dots,\gamma} A^1_{\alpha,\beta,j_1} A^2_{\beta,\delta,j_2} \dots A^N_{\gamma,\alpha,j_n} \tag{5}$$

We can now make a comparison between the number of parameters there are in the exact description and the MPS Ansatz. If we have a system of n spin physical dimension d we have $\mathcal{O}(d^n)$

parameters in the exact description. If we decide to truncate the dimension of the greek(i.e. $\alpha\,\beta\,...$) to be at most D (D is usually called *bond dimension* in the literature) indexes in the definition of the MPS Ansatz we have $\mathcal{O}(ndD^2)$ parameters.

2.1 Gauge degree of freedom

A MPS is defined univocally but the tensors $A^{(i)}$. On the other the set of tensors $A^{(i)}$ that define a generic Ψ is not unique. Ψ is defined as the contraction of the tensors $A^{(i)}$. Given a element of $Gl_D(\mathbb{C})$ M, a MPS is invariant under the insertions:

$$A^{(i)}_{\alpha,\,\beta}A^{(i+1)}_{\beta,\,\gamma} = A^{(i)}_{\alpha,\,\beta}M_{\beta,\,\delta}M^{-1}_{\delta,\,\xi}A^{(i+1)}_{\xi,\,\gamma} \tag{6}$$

At this point it is very important to remind the reader a fundamental too in linear algebra: The singular value decomposition (SVD). Given.a generic rectangular matrix N is is always possible to find matrices U, S, V such that:

$$N = U\,S\,V^\dagger \tag{7}$$

U is a matrix containing the left singular vectors of N. Since U has orthonormal columns it is also unitary $UU^\dagger = U^\dagger U = 1$. S is a diagonal matrix with non-negative entries. Those numbers s_a are called the singular values of N. The number of non-zero singular values is the rank of N. $V^\dagger$ is a matrix that contains the right singular vectors. In the same way as U, $V^\dagger$ has orthonormal columns it is also unitary $VV^\dagger = V^\dagger V = 1$. The sigular values contained in S has lot of interesting properties. Let us suppose we have a state $|\psi\rangle$. For any partition A and B of the Hilbert space in which $|\psi\rangle$ is defined it is always possible to write:

$$|\psi\rangle = \sum_{\alpha,\,\beta} c_{\alpha,\,\beta}\,|\alpha\rangle_A\,|\beta\rangle_B \tag{8}$$

If perform a SVD of the matrix c in Equation 8, we can write:

$$|\psi\rangle = \sum_{\alpha,\,\beta}\sum_{s_a} U_{\alpha,\,s_a}S_{s_a,\,s_a}V^\dagger_{s_a,\,\beta}\,|\alpha\rangle_A\,|\beta\rangle_B \tag{9}$$

We can absorb U and V in A and B due to their orthonormality in those spaces write:

$$|\psi\rangle = \sum_{s_a} s_a\,|\alpha\rangle_A\,|\beta\rangle_B \tag{10}$$

In this decoposition it is trivial to derive the reduced density matrix for the sub-system A in Equation 2:

$$\rho_A = \sum_{s_a} s_a^2\,(|\alpha\rangle\,\langle\alpha|)_A \tag{11}$$

The von-Neumann entanglement entropy can be computed directly from here:

$$S(\rho_A) = -Tr(\rho_A\log_2(\rho_A)) = -\sum_a s_a^2\log_2 s_a^2 \tag{12}$$

2.2 Canonical form

Fixing those matrices M or, more generally, fixing M such that the MPS satisfies certain relations is referred to as *fixing a gauge.* Two particular gauge, called *canonical forms* are particularly useful when computing expectation values of operators (i.e. the Hamiltonian H of a quantum system). Those gauge consist into choosing the matrices M such that the tensors $A^{(i)}$ satisfy the following relations:

$$\sum_{\beta=1}^{D}\sum_{s=1}^{d}\left(A^{[s](i)}_{\alpha,\beta}\right)^{*}A^{[s](i)}_{\beta,\gamma}=\delta_{\alpha,\gamma} \tag{13}$$

$$\sum_{\beta=1}^{D}\sum_{s=1}^{d}A^{[s](i)}_{\alpha,\beta}\left(A^{[s](i)}_{\beta,\gamma}\right)^{*}=\delta_{\alpha,\gamma} \tag{14}$$

If a MPS satisfies the relation in Equation 13 it is called to be in the *left canonical form.* If a MPS satisfies the relation in Equation 14 it is called to be in the *right canonical form.*

There is also a very useful notation introduced by [2] that highlights the singular values of the matrices of a MPS:

$$|\psi\rangle=\sum_{s_1,\,\dots,\,s_N}U^{s_1}S_1U^{s_2}S_2\dots U^{s_N}S_N\,|s_1,\,\dots,\,s_N\rangle \tag{15}$$

2.3 Computation of the Von-Neumann entropy in the MPS formalism

Let us suppose we have a spin chain of local Physical dimension d and N sites described by a MPS in the *left canonical form.* The partition function ρ is defined as:

$$\rho=\sum_{s_1,\dots,s_N}^{d}\sum_{s_1',\dots,s_N'}^{d}Tr\left[M^{1,s_1,s_1'}M^{2,s_2,s_2'}\dots M^{N,s_N,s_N'}\right]|s_1,\,\dots,\,s_N\rangle\left\langle s_1',\,\dots,\,s_N'\right| \tag{16}$$

where:

$$M^{i,s_i,s_i'}=A^{[s_i](i)}\otimes\left(A^{[s_i'](i)}\right)^{\dagger} \tag{17}$$

We now partition the system in two sub-system A and B. A includes all the sites up to k and B its complementary. $\rho(A)$, defined as in Equation 2, can now be written as:

$$\tilde{\rho}^{[l]}_{A}=Tr_B(\rho)=\sum_{s_1,\dots,s_l}^{d}\sum_{s_1',\dots,s_l'}^{d}A^{1,s_1}\dots A^{l,s_l}\rho^{(l)}_{[A]}\left(A^{1,s_1'}\right)^{\dagger}\dots\left(A^{l,s_l'}\right)^{\dagger}|s_1,\,\dots,\,s_l\rangle\left\langle s_1',\,\dots,\,s_l'\right| \tag{18}$$

where $\rho^l_{[A]}$ is defined as:

$$\rho^{(l)}_{[A]} = \sum_{s_{l+1},\,\dots\,,s_N}^{d} \sum_{s'_{l+1},\,\dots\,,s'_N}^{d} A^{l+1,\,s_{l+1}} ... A^{N,\,s_N} \left(A^{l+,\,s'_{l+1}}\right)^{\dagger} ... \left(A^{N,\,s'_N}\right)^{\dagger} \tag{19}$$

Equation 19 denotes a recursive relation:

$$\rho^{(l+1)}_{[A]} = A^{l+1,\,s_{l+1}} \rho^{(l)}_{[A]} \left(A^{l+,\,s'_{l+1}}\right)^{\dagger} \tag{20}$$

We can always rewrite a MPS such in the form of Equation 15. From this form it is trivial to derive the von-Neumann entanglement entropy in the same fashion as in Equation 12. We just need to identify:

$$|\alpha\rangle_A = \sum_{s_1,\,\dots\,,\,s_l} U^{s_1} S_1 U^{s_2} S_2 \dots S_{l-1} U^{s_l} \left|s_1,\,\dots\,,\,s_l\right\rangle \tag{21}$$

$$|\alpha\rangle_B = \sum_{s_1,\,\dots\,,\,s_N} U^{s_{l+1}} S_{l+1} U^{s_{l+2}} S_{l+2} \dots U^{s_N} S_N \left|s_{l+1},\,\dots\,,\,s_N\right\rangle \tag{22}$$

At this point we can write:

$$\rho_A = \sum_{s_a} s_a^2 \left(|\alpha\rangle\langle\alpha|\right)_A = \sum_a \left(S_l\right)_{a,\,a} \left(|\alpha\rangle\langle\alpha|\right)_A \tag{23}$$

Since we have the coefficients of the reduced density matrix ρ_A we can compute the von-Neumann entropy as:

$$S(\rho_A) = -Tr(\rho_A \log_2(\rho_A)) = -\sum_a \left(S_l\right)^2_{a,\,a} \log_2 \left(S_l\right)^2_{a,\,a} \tag{24}$$

References

[1] Ulrich Schollwöck. The density-matrix renormalization group in the age of matrix product states. *Annals of Physics*, 326(1):96–192, Jan 2011.

[2] Guifré Vidal. Efficient classical simulation of slightly entangled quantum computations. *Physical Review Letters*, 91(14), Oct 2003.