Entanglement Spectroscopy and its Application to Topological Phases

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August 7, 2014

Contents

This is a preliminary version of the lecture notes. Comments, corrections and feedback are welcome.

1 Entanglement spectrum and entanglement entropy

As a first step, we discuss the concept of entanglement spectroscopy in some simple cases. We also briefly cover the definition and the relevant properties of the entanglement entropy. We introduce the Li-Haldane conjecture in the case of the AKLT spin chain. We discuss the important situation where the number of reduced density matrix non-zero eigenvalues is massively reduced. In particular, we show the relation between the latter property and the matrix product state representation.

1.1 Definitions

Let consider a generic n-body quantum state $|\Psi\rangle$ that can be decomposed on the orthonormal basis $\{|\lambda\rangle\}$. We now assume that this basis can be written as the tensor product of two orthonormal basis $\{|\mu_A\rangle\}$ and $\{|\mu_B\rangle\}$ i.e. $\{|\lambda\rangle = |\mu_A\rangle \otimes |\mu_B\rangle\}$, providing a natural bipartition of the system into A and B. The decomposition of the state $|\Psi\rangle$ reads

$$|\Psi\rangle \quad = \quad \sum_{\mu_A,\mu_B} c_{\mu_A,\mu_B} |\mu_A\rangle \otimes |\mu_B\rangle \tag{1}$$

The entanglement matrix M is defined such that its matrix elements are given by $M_{\mu_A,\mu_B} = c_{\mu_A,\mu_B}$. The size of M is given by the dimension of the subspaces A and B that we denote respectively $\dim_A$ and $\dim_B$. Note that we do not assume that $\dim_A = \dim_B$, and thus M is generically a rectangular matrix. One can perform a singular value decomposition (SVD) of M. The SVD allows to write a rectangular matrix

$$M \quad = \quad UDV^\dagger \tag{2}$$

where U is a $\dim_A \times \min(\dim_A, \dim_B)$ matrix which satisfies $U^\dagger U = 1$ (i.e. has orthonormalized columns), V is a $\dim_B \times \min(\dim_A, \dim_B)$ matrix which satisfies $VV^\dagger = 1$ (i.e. has orthonormalized rows). D is a diagonal square of dimension $\min(\dim_A, \dim_B)$ where all entries are non-negative and can be expressed as $\{e^{-\xi_i/2}\}$.

Using the SVD, one can derive the Schmidt decomposition of $|\Psi\rangle$

$$|\Psi\rangle \quad = \quad \sum_i e^{-\xi_i/2} |A:i\rangle \otimes |B:i\rangle \tag{3}$$

where

$$|A:i\rangle = \sum_{\mu_A} U^\dagger_{i,\mu_A} |\mu_A\rangle \tag{4}$$

$$\text{and} \qquad |B:i\rangle = \sum_{\mu_B} V^\dagger_{i,\mu_B} |\mu_B\rangle \tag{5}$$

To be a Schmidt decomposition, the states $|A:i\rangle$ and $|B:i\rangle$ have to obey $\langle A:i|A:j\rangle = \langle B:i|B:j\rangle = \delta_{i,j}$. This property is trivially verified using the identities on U and V. The Schmidt decomposition provides a nice and numerically efficient way to compute the spectrum of the reduced density matrix. Consider the density matrix of the pure state $\rho = |\Psi\rangle \langle\Psi|$, we compute the reduced density matrix of A by tracing out the degree of freedom related to B, i.e. $\rho_A = \mathrm{Tr}_B \rho$. Using Eq. 3, we deduce that

$$\rho_A \quad = \quad \sum_i e^{-\xi_i} |A:i\rangle \langle A:i| \tag{6}$$

Thus the spectrum of ρ_A can be obtained from the coefficient of the Schmidt decomposition or the SVD of the entanglement matrix and is given by the set $\{e^{-\xi_i}\}$. From a numerical perspective, getting the spectrum of ρ_A is more accurate using the SVD of M than a brute force calculation of ρ_A in the $\{|\mu_A\rangle\}$ basis followed by its diagonalization. In a similar way, we can obtain the reduced density matrix of B

$$\rho_B = \mathrm{Tr}_A \rho = \sum_i e^{-\xi_i} |B:i\rangle \langle B:i| \tag{7}$$

Note that ρ_A and ρ_B have the same spectrum. While these two square matrices might have different dimensions (respectively $\dim_A$ and $\dim_B$), they both have the same number of non-zero eigenvalues. This number has to be lower than or equal to $\min(\dim_A, \dim_B)$. Thus studying the properties of ρ_A for various partitions (i.e. choices of A and B) can be restricted to the cases where $\dim_A \leq \dim_B$.

With these tools and properties, we can now define the entanglement spectrum. The latter corresponds to the set $\{\xi_i\}$, the logarithm of the reduced density matrix eigenvalues. The key idea of the original article of

Li and Haldane[1] was not only to look at this whole spectrum, but at a specific subset of these values (or a block of ρ_A) with well defined quantum numbers. Assume an operator $\mathcal{O}$ that can be decomposed as $\mathcal{O}_A+\mathcal{O}_B$ where $\mathcal{O}_A$ (resp. $\mathcal{O}_B$) only acts on the A (resp. B) subspace. One can think about $\mathcal{O}$ as the projection of the spin operator or the momentum. If $[\mathcal{O},\rho]=0$, we also have $0=\mathrm{Tr}_B[\mathcal{O}_A,\rho]+\mathrm{Tr}_B[\mathcal{O}_B,\rho]=[\mathcal{O}_A,\mathrm{Tr}_B\rho]=[\mathcal{O}_A,\rho_A]$ as the trace over the B degrees of freedom of a commutator operator in the B part vanishes. If $|\Psi\rangle$ is an eigenstate of $\mathcal{O}$, then the latter commutes with ρ. We can simultaneously diagonalize ρ_A and $\mathcal{O}_A$,and label the $\{\xi_i\}$ according to the quantum number of $\mathcal{O}_A$.

1.2 A simple example: Two spin-$\frac{1}{2}$

To exemplify the previous notations and concepts, we consider a system of two spin-$\frac{1}{2}$ as depicted in Fig. 1a. Any state $|\Psi\rangle$ can be decomposed onto the four basis states:

$$|\Psi\rangle = c_{\uparrow\uparrow}|\uparrow\uparrow\rangle + c_{\uparrow\downarrow}|\uparrow\downarrow\rangle + c_{\downarrow\uparrow}|\downarrow\uparrow\rangle + c_{\downarrow\downarrow}|\downarrow\downarrow\rangle \tag{8}$$

A natural way to cut this system into two parts consists of the A (resp. B) part being the left (resp. right) spin. The entanglement matrix is given by

$$M = \begin{array}{c} \begin{array}{cc} |B:\uparrow\rangle & |B:\downarrow\rangle \end{array} \\ \begin{pmatrix} c_{\uparrow\uparrow} & c_{\uparrow\downarrow} \\ c_{\downarrow\uparrow} & c_{\downarrow\downarrow} \end{pmatrix} \end{array} \begin{array}{l} |A:\uparrow\rangle \\ |A:\downarrow\rangle \end{array} \tag{9}$$

where we have explicitly written which states were associated with each row and column of M. We consider three examples: A product state $|\Psi_1\rangle=|\uparrow\uparrow\rangle$, a maximally entangled state $|\Psi_2\rangle=\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle-|\downarrow\uparrow\rangle)$ and a generic entangled state $|\Psi_3\rangle=\frac{1}{2}|\uparrow\downarrow\rangle+\frac{\sqrt{3}}{2}|\downarrow\uparrow\rangle$. The entanglement matrices for these three states are

$$M_1=\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix},\quad M_2=\begin{pmatrix} 0 & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & 0 \end{pmatrix},\quad M_3=\begin{pmatrix} 0 & \frac{1}{2} \\ \frac{\sqrt{3}}{2} & 0 \end{pmatrix} \tag{10}$$

Performing the SVD on the first state $|\Psi_1\rangle$ is trivial: Being a product state, it is already written as a Schmidt decomposition. For $|\Psi_2\rangle$, we can do the SVD

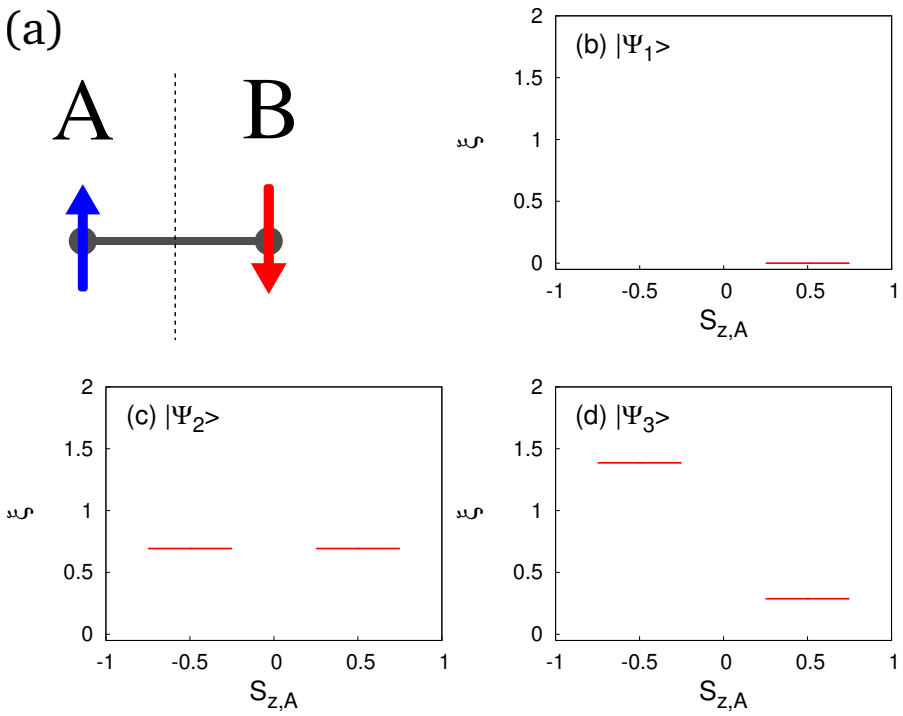

Figure 1: *From left to right:* (a) schematic picture of the two spin-$\frac{1}{2}$ system. (b) Entanglement spectrum for the state $|\Psi_1\rangle = |\uparrow\uparrow\rangle$. (c) Entanglement spectrum for the state $|\Psi_2\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$. (d) Entanglement spectrum for the state $|\Psi_3\rangle = \frac{1}{2}|\uparrow\downarrow\rangle + \frac{\sqrt{3}}{2}|\downarrow\uparrow\rangle$.

$$M_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \quad (11)$$

such that the Schmidt decomposition is

$$\begin{aligned} |\Psi_2\rangle &= \frac{1}{\sqrt{2}} (+|\uparrow\rangle) \otimes (+|\downarrow\rangle) \\ &\quad + \frac{1}{\sqrt{2}} (+|\downarrow\rangle) \otimes (-|\uparrow\rangle) \end{aligned} \quad (12)$$

S similar calculation can be performed for $|\Psi_3\rangle$.

The projection of the total spin along the z axis S_z is the sum of individual components $S_{z,A}$ and $S_{z,B}$. Thus, when performing the cut into the two parts A and B, $S_{z,A}$ is a good quantum number that can be used to label the eigenvalues of the entanglement spectrum according to the discussion in Sec. 1.1. The entanglement spectra for the three states $|\Psi_1\rangle$, $|\Psi_2\rangle$ and $|\Psi_3\rangle$ are shown in Figs. 1b-d. For the product state $|\Psi_1\rangle$, there is a single level appearing since the reduced density matrix has a single non-zero eigenvalue. For the two other examples, there are two levels, each with a given $S_{z,A}$ value. The calculation of the entanglement entropy, which is a measure of the entanglement, directly tells that $|\Psi_1\rangle$ is a product state. We can derive the same conclusion from the number of levels in the entanglement spectrum. While this example is rather a trivial result obtained from the entanglement spectrum, it stresses one of strong points of this technique. Some properties of the states can be deduced just by counting the non-zero eigenvalues of reduced density matrix.

1.3 Entanglement entropy

They are several ways to quantify the entanglement between two parts of a system and there is an extensive literature on this topic (see Ref. [2] for an extensive review). The goal of these lectures is not to give a detailed introduction to entanglement entropies. So we will restrict to a few useful examples in the context of topological phases. Perhaps the most common measure of entanglement is the Von Neumann entanglement entropy

$$\mathcal{S}_A = -\mathrm{Tr}_A \left[\rho_A \ln \rho_A\right] \quad (13)$$

From a practical point of view, the calculation of the Von Neumann entanglement entropy can be easily obtained once the Schmidt decomposition or the spectrum of the reduced density matrix has been obtained.

$$\mathcal{S}_A = -\sum_i \lambda_i \ln \lambda_i = \sum_i \xi_i e^{-\xi_i} \tag{14}$$

Similarly, we can define the entanglement entropy for the B part of the system $S_B = -\mathrm{Tr}_B [\rho_B \ln \rho_B]$. Using Eq. 7, we immediately see that $S_A = S_B$. If A and B are not entangled (i.e. $|\Psi\rangle = |\Psi_A\rangle \otimes |\Psi_B\rangle$), we get $S_A = 0$. For the full system $A+B$, the entanglement entropy is also zero. As a consequence, we get in general that $S_A + S_B \neq S_{A+B}$ (the entanglement entropy is actually strongly subadditive)

We will now turn to the entanglement entropy of some specific systems. In many situations, it is useful to look at the case of a random state. Especially for people interested in numerical simulations, it is always a good idea to compare with what a random output would give. For example, consider the calculation of the overlap (the simplest way to compare two wavefunctions). Let's take two random states $|\Psi_1\rangle$ and $|\Psi_2\rangle$ defined in a Hilbert space of dimension $\mathcal{D}$. Then the average overlap $|\langle\Psi_1|\Psi_2\rangle|^2 \simeq \frac{1}{\mathcal{D}}$. This result gives a simple bound for what is a bad overlap in finite systems (note that one should not cheat and define $\mathcal{D}$ as the dimension of the Hilbert space with all the symmetries the system has).

For the entanglement entropy, we remind the notations $\dim_A$ for the dimension of the Hilbert associated to the A part and $\dim_B$ for the dimension of the Hilbert space of the B part. In the limit $\dim_B \geq \dim_A \gg 1$, it was shown[3] that

$$S_A \simeq \ln(\dim_A) - \frac{\dim_A}{2\dim_B} \tag{15}$$

In particular when $\dim_B \gg \dim_A \gg 1$, we obtain that $S_A \simeq \ln(\dim_A)$.

To get a more physical picture of this foumla, we can consider that the system is made of spin-$\frac{1}{2}$, V_A spin-$\frac{1}{2}$ for A and V_B spin-$\frac{1}{2}$ for B. We get for the Hilbert space dimensions $\dim_A = 2^{V_A}$ and $\dim_B = 2^{V_B}$, leading to $S_A \simeq V_A \ln 2$. Thus for a random state, the entanglement entropy is proportional to the volume of the subsystem A, meaning the entanglement entropy obeys a volume law.

We can now move to the case of gapped phases. We note η the correlation length. We consider a geometrical bipartition of the system into A and B

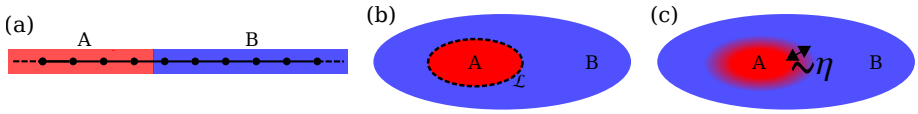

Figure 2: A schematic description of the bipartite geometrical partition for a one dimensional system (a) and for a two dimensional system (b). The righmost panel (c) illustrates the small region around the boundary between A and B (with a thickness of the order of the correlation length η) that is relevant in the entanglement entropy when considering a gapped phase.

as depicted in Fig. 2. For one dimensional gapped systems, if the size of A in large enough compared to η, the entanglement entropy does not depend on the length V_A, i. e. S_A is constant. This statement can be proved and an upper bound on the constant can be found[4].

For higher dimensional systems, it is conjectured that the entanglement entropy satisfies

$$\mathcal{S}_A \simeq \alpha\mathcal{L} \tag{16}$$

$\mathcal{L} \gg \eta$ denotes the area of the surface that separates A from B and α is a constant. Thus the entanglement entropy for a gapped system satisfies an area law (as opposed to the volume law of the random state). In two dimension, $\mathcal{L}$ is just the perimeter of the boundary between A and B (see Fig. 2b). Here we should make two remarks. First one dimensional gapped systems also obey the area law (just set $\mathcal{L}$ to 1, the boundary being just a point). Second, this is a major difference with a random state where one gets a volume law for the entanglement entropy. Intuitively, if one has a finite correlation length, we expect that only the region around the boundary between A and B, whose thickness is of the order of a few η's (as shown in Fig. 2c) should matter in the entanglement between A and B.

For two dimensional topological phases, we can go beyond the area law contribution. Refs. [5] and [6] showed that the first correction to this area law is a constant term γ

$$\mathcal{S}_A \sim \alpha\mathcal{L} - \gamma \tag{17}$$

While α is non-universal, this is not the case the sub-leading term γ. This latest is called the topological entanglement entropy: It is a constant for a given topologically ordered phase

$$\gamma \;=\; \ln\left(\frac{\mathcal{D}}{d_a}\right) \tag{18}$$

For a given type of excitations a, the quantum dimension d_a defines how the Hilbert space dimension exponentially increases with the number of such excitations. Each type of excitations corresponds to a topological sector. Abelian excitations have a quantum dimension equal to 1 while non-abelian ones have $d_a > 1$. The total quantum dimension is given by $\mathcal{D} = \sqrt{\sum_a d_a^2}$. These quantum dimensions characterize the topological field theory describing the phase and thus the nature of the system excitations. Note that in Eq. 18, the a of the d_a term corresponds to the topological sector of the wavefunction $|\Psi\rangle$ whose entanglement entropy is computed.

The topological entanglement entropy appears as a way to characterize the topological order of a phase. However, its practical calculation depends on scaling arguments, which might be hard to obtain to sufficient accuracy from numerical calculations[7, 8]. Moreover, it does not uniquely determine the topological order in the state. For that reason, it is interesting to look at the full spectrum of the reduced density matrix and not to reduce it to a single number.

References

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