We can now define the reduced density matrix for subsystem A to be the partial trace of $\rho_{A\cup B}$ over the degrees of freedom in B
$= |\psi\rangle\langle\psi|$

$$\rho_A = \mathrm{Tr}_B \; \rho_{A\cup B}$$

and similarly for the reduced density matrix ρ_B. Therefore, if we observe only subsystem A, it is in a mixed state defined by the reduced density matrix ρ_A.

Using the Schmidt decomposition (*) we can write the reduced density matrix ρ_A as

$$\rho_A = \sum_n^D |\lambda_n|^2 \; |n\rangle_A \langle n|_A$$

Hence, the quantities $p_n \equiv |\lambda_n|^2$ represent the probabilities of observing the subsystem A in state $|n\rangle_A$. In fact, ρ_A and ρ_B have the same non-zero eigenvalues.

Entanglement entropies

quantitative measure

The von Neumann entanglement entropy S_A for subsystem A is defined to be the entropy of the reduced density matrix

$$S_A = -\mathrm{Tr}_A \left(\rho_A \cdot \ln \rho_A \right)$$

It can also be written as

$$S_A = -\mathrm{Tr}_A (\rho_A \cdot \ln \rho_A) = -\sum_n^D |\lambda_n|^2 \cdot \ln |\lambda_n|^2 = -\mathrm{Tr}_B (\rho_B \cdot \ln \rho_B) = S_B \, .$$

In other words, the entanglement entropy is symmetric in the two entangled subsystems.

The von Neumann entropy is the first representative of the family of Rényi entropies defined as

$$S_n(\rho_A) = \frac{1}{1-n} \log \left(\mathrm{Tr}_A (\rho_A^n) \right) .$$

In numerical simulations, one often considers the second $(n=2)$ Renyi entropy

$$S_2(\rho_A) = -\log \left(\mathrm{Tr}_A (\rho_A^2) \right) .$$

Example

Let us consider a system of two spins that we bipartition into two systems A and B of a single spin each. The wavefunction of the composite system shall be

$\alpha = 0 \quad |\uparrow\rangle|\downarrow\rangle$

$\alpha = \frac{\pi}{4} \quad \frac{1}{\sqrt{2}}\left(|\uparrow\rangle|\downarrow\rangle + |\downarrow\rangle|\uparrow\rangle\right)$

$$|\psi\rangle = \cos\alpha\, |\uparrow\rangle_A |\downarrow\rangle_B + \sin\alpha\, |\downarrow\rangle_A |\uparrow\rangle_B$$

Tracing over subsystem B we obtain the reduced density matrix for subsystem A

$$\hat{\rho}_A = |\psi\rangle_A \langle\psi|_A = \mathrm{Tr}_B\left(|\psi\rangle\langle\psi|\right)$$

$$= \sum_{\beta_B = \downarrow,\uparrow} \langle \beta_B | \psi \rangle\langle \psi | \beta_B \rangle$$

which gives

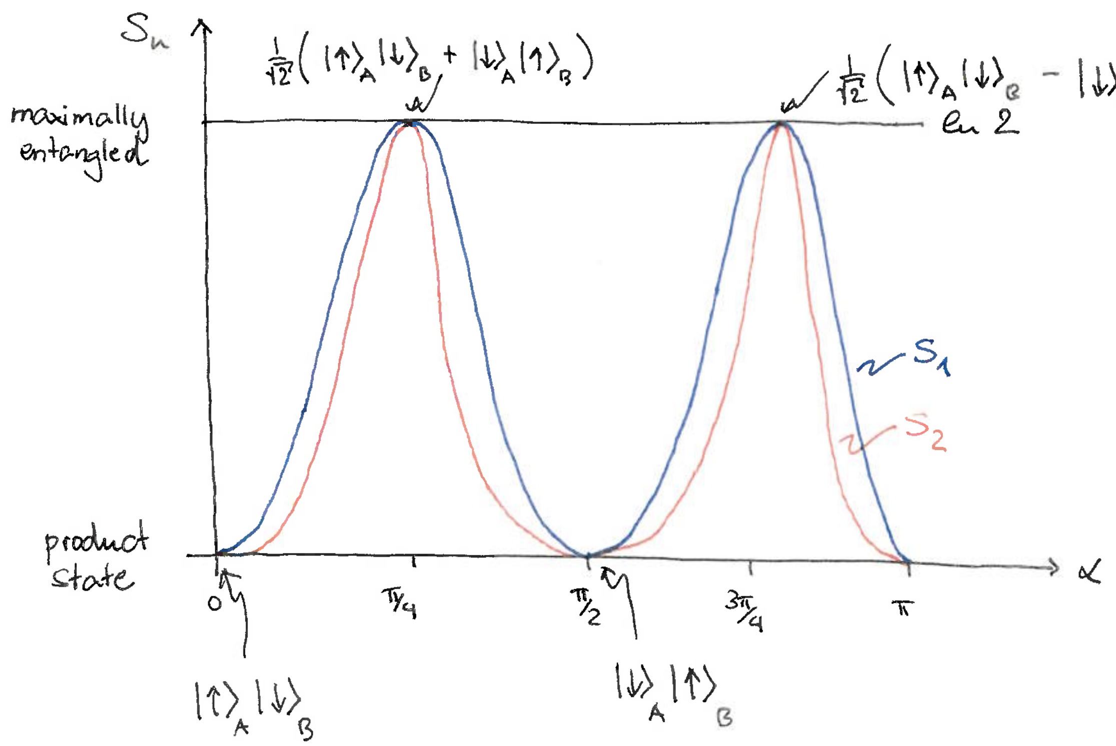
$$\hat{\rho}_A = \cos^2\alpha\, |\uparrow\rangle_A \langle\uparrow|_A + \sin^2\alpha\, |\downarrow\rangle_A \langle\downarrow|_A$$

$$= \begin{pmatrix} \cos^2\alpha & 0 \\ 0 & \sin^2\alpha \end{pmatrix}$$

$\alpha = 0 \quad \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad S_A = 0$

$\alpha = \frac{\pi}{2} \quad \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} \quad S_A = -\left(\frac{1}{2}\ln\frac{1}{2} + \frac{1}{2}\ln\frac{1}{2}\right) = \ln 2$

Calculating the entanglement entropies from this given density matrix we obtain the following qualitative behavior as a function of the angle α



For this two-dimensional arrangement we see that the entanglement entropy scales with the number of dimers being cut along the bipartition of the system into parts A and B. As such the entanglement entropy is primarily sensitive to the length of the boundary between A and B. This dependence is often referred to as boundary law or area law*.

* The term area law goes back to the first discussion of the scaling of entanglement entropies by Bekenstein and Hawking who considered the entanglement entropy of a black hole.

different from thermal entropies which are always extensive.

The two-dimensional state constructed above, a valence bond crystal, could well be the ground state of some spin Hamiltonian. This ground state would obey the boundary law

$$S \sim \ell = \partial A = \partial B$$

In fact, this statement generalizes to arbitrary ground states of local Hamiltonians (i.e. Hamiltonians with only local = short-ranged interaction terms), though some subleading corrections might occur – the latter turn out to be of utmost interest as they allow to classify quantum ground states.

Examples:

$S = a + b \cdot \ell$ for a topologically ordered state in 2D

$S \sim \ell \cdot \ln \ell$ for a gapless state with Fermi line in 2D

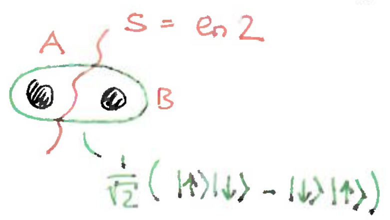
⋮

As such the quantum information perspective has provided us with a very powerful tool to positively identify e.g. topologically ordered states and to conceptually classify quantum ground states. This in turn has lead to novel computational [illegible]

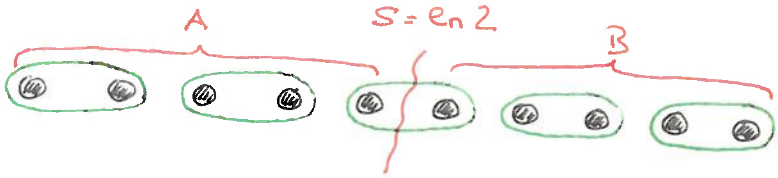
Entanglement in quantum many-body systems

Our quantum information approach has provided us with a first insight – entanglement is the key distinction between quantum and classical systems. We can quantitatively measure entanglement by calculating the entanglement entropy. Before asking how we can use entanglement to perform elementary quantum computations, we want to learn how we can use entanglement as a resource in describing quantum many-body states (which we might think of as a collection of many qubits if we want to stick to the quantum information perspective).

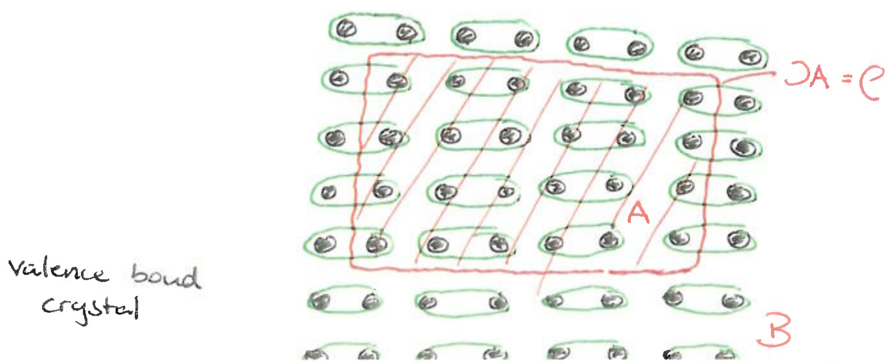
So far, we considered a two-spin system and realized that a singlet state is a maximally entangled state



Let us now construct an extended one-dimensional arrangement of such dimers



We see that for this many-spin state the entanglement is still $S = \ln 2$.
Now let us look at a two-dimensional arrangement of such dimers



$S \sim \ell \cdot \ln 2$

Entanglement entropies in QMC simulations

Let us recapitulate that we can write the density matrix for a quantum many-body system in its ground state as

$$\rho = |\psi\rangle\langle\psi| = \frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle} = \frac{\rho'}{\mathcal{N}}$$

where we have introduced an explicit normalization constant $\mathcal{N}$ in the denominator, which not only ensures that the trace of the so-defined density matrix is 1, but will also play an important conceptual role in the following.

In our numerical formulation of Rényi entropies we will concentrate on the second Renyi entropy S_n with $n=2$ defined as

$$S_2(A) = S_2(\rho_A) = -\log\left(\mathrm{Tr}_A (\rho_A)^2\right)$$

Using the above notation for the density matrix we can thus write

$$S_2(A) = S_2(\rho_A) = -\log\left(\frac{\mathrm{Tr}_A(\rho_A')^2}{\mathcal{N}^2}\right) \qquad (*)$$

To make the calculation of $S_2(A)$ amenable to QMC techniques, we want to formulate both the nominator and denominator as world-line representations of partition functions. Let us first look at the denominator and note that

$$\mathcal{N}^2 = (\mathrm{Tr}\,\rho)^2 = Z^2 ,$$

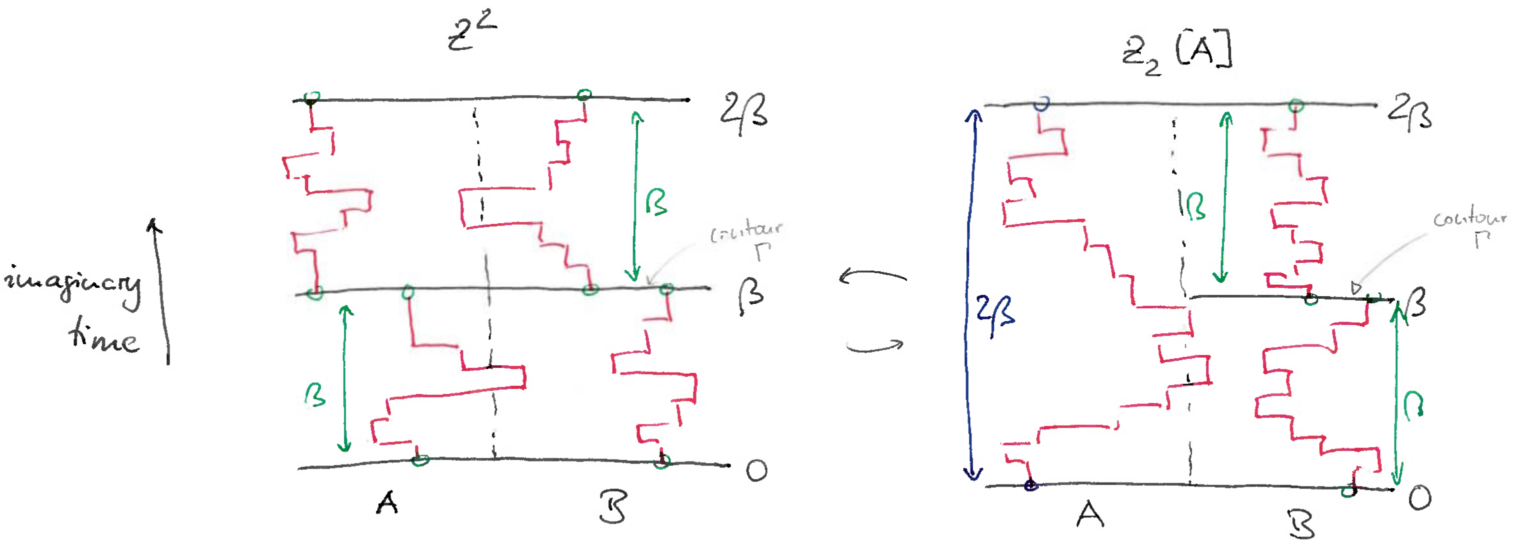
i.e. the normalization $\mathcal{N}^2$ is equal to the square of the usual partition sum. The nominator is a bit more involved

$$\mathrm{Tr}_A(\rho_A')^2 = \sum_{A,A',B,B'} \langle \psi_A \phi_{B'} | \rho' | \psi_{A'} \phi_{B'} \rangle\langle \psi_{A'} \phi_B | \rho' | \psi_A \phi_B \rangle \equiv Z_2[A]$$

So, we have

$$S_2(A) = S_2(\rho_A) = -\log \frac{Z_2[A]}{Z^2}$$

Let us translate these two partition sums into their world-line representations



We see that we can sample both of these replicated partition functions in world-line QMC approaches or within the context of the stochastic series expansion. To evaluate the ratio of the two partition functions we sample Z^2 and count the number of sampled world-line configurations that would also match the boundary conditions of $Z_2[A]$ (which is entirely included in Z^2). The ratio of these counted incidences and the total number of sampled world-line representations is the desired ratio.

Interestingly, this world-line representation of the Rényi entropies allows us to understand a very important aspect of the scaling behavior of these entropies. To see this let us introduce the free energies

$$F_1 = -\log Z \quad \text{and} \quad F_2 = -\log Z_2[A]$$

In terms of these free energies the Rényi entropy is given by

$$S_2(A) = F_2 - 2 \cdot F_1 \qquad S_n(A) = \frac{F_n - nF_1}{n-1} \text{ more generally}$$

The free energy of a physical system in d spatial dimensions with a well-defined thermodynamic limit has a leading extensive term, e.g. for $d = 2$ spatial dimensions we have

$$F = f \cdot L^2 + \beta \cdot L + a \cdot \ln L + b + \mathcal{O}(L^{-1})$$

Since the copies in the replicated system are identical away from the contour Γ, which can be viewed as a "defect" in the replicated system, it is clear that the extensive terms (proportional to the free energy density f) must be the same for F_n and $n \cdot F_1$ and hence must cancel out exactly. Therefore in the limit $L \gg \ell$ we expect the Rényi entropies to have the form

$$S_2(A) = \alpha \cdot \ell + C_1 \cdot \ln\left(\frac{\ell}{a}\right) + \phi\left(\frac{\ell}{L}\right) + \mathcal{O}(\ell^{-1})$$

where the first term describes a "boundary law" with a non-universal prefactor α, C_1 is a constant, and $\phi(x)$ is a dimensionless function of the aspect ratio ℓ/L.

In three spatial dimensions, this "boundary law" or "area law" was first derived by Bekenstein and Hawking ('73 & '75) describing the physics of black holes. In spite of their origin in a classical theory of gravity, i.e. the general theory of relativity, black holes behave as if they were thermodynamic objects that have entropy and temperature. A fundamental result in black-hole physics is the expression for the black-hole entropy by Bekenstein and Hawking

$$S_{BH} = \frac{1}{4\ell_p^2} \cdot \mathcal{A}$$

where $\mathcal{A}$ is the area of the event horizon of the black hole, ℓ_p is the Planck length. This formula is most intriguing – it is one of the motivations for the holographic principle.

~~Entanglement entropies in QMC simulations~~ Replica trick

Let us recapitulate that we can write the density matrix for a quantum many-body system in its ground state as

$$\rho = |\psi\rangle\langle\psi| = \frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle} = \frac{\rho'}{\mathcal{N}}$$

where we have introduced an explicit normalization constant $\mathcal{N}$ in the denominator, which not only ensures that the trace of the so-defined density matrix is 1, but will also play an important conceptual role in the following.

In our numerical formulation of Rényi entropies we will concentrate on the second Renyi entropy S_n with $n=2$ defined as

$$S_2(A) = S_2(\rho_A) = -\log\left(\mathrm{Tr}_A\,(\rho_A)^2\right)$$

Using the above notation for the density matrix we can thus write

$$S_2(A) = S_2(\rho_A) = -\log\left(\frac{\mathrm{Tr}_A\,(\rho'_A)^2}{\mathcal{N}^2}\right) \qquad (*)$$

To make the calculation of $S_2(A)$ amenable to QMC techniques, we want to formulate both the nominator and denominator as world-line representations of partition functions. Let us first look at the denominator and note that

$$\mathcal{N}^2 = (\mathrm{Tr}\,\rho)^2 = Z^2 \quad ,$$

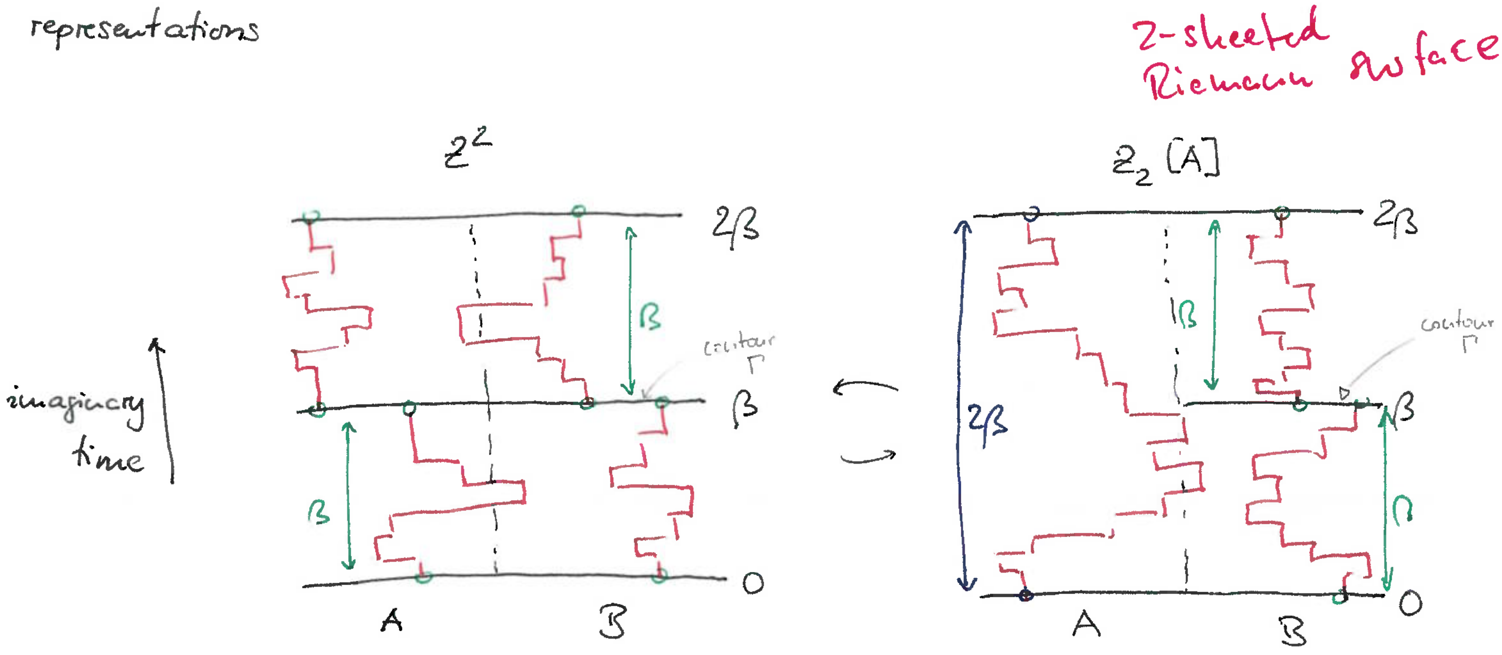
i.e. the normalization $\mathcal{N}^2$ is equal to the square of the usual partition sum. The nominator is a bit more involved

$$\mathrm{Tr}_A(\rho'_A)^2 = \sum_{A,A',B,B'} \langle \psi_A \psi_{B'} | \rho' | \psi_{A'} \phi_{B'} \rangle\langle \psi_{A'} \phi_B | \rho' | \psi_A \phi_B \rangle \equiv Z_2[A]$$

So, we have

$$S_2(A) = S_2(\rho_A) = -\log\frac{Z_2[A]}{Z^2}$$

Let us translate these two partition sums into their world-line representations



We see that we can sample both of these replicated partition functions in world-line QMC approaches or within the context of the stochastic series expansion. To evaluate the ratio of the two partition functions we sample Z^2 and count the number of sampled world-line configurations that would also match the boundary conditions of $Z_2[A]$ (which is entirely included in Z^2). The ratio of these counted incidences and the total number of sampled world-line representations is the desired ratio. snap!

Interestingly, this world-line representation of the Rényi entropies allows us to understand a very important aspect of the scaling behavior of these entropies. To see this let us introduce the free energies

$k_B T = 1$

$$F_1 = -\log Z \quad \text{and} \quad F_2 = -\log Z_2[A]$$

In terms of these free energies the Rényi entropy is given by

$$S_2(A) = F_2 - 2 \cdot F_1 \qquad S_n(A) = \frac{F_n - nF_1}{n-1} \text{ more generally}$$

The free energy of a physical system in d spatial dimensions with a well-defined thermodynamic limit has a leading extensive term, e.g. for $d = 2$ spatial dimensions we have

$$F = f \cdot L^2 + \beta \cdot L + a \cdot \ln L + b + \mathcal{O}(L^{-1})$$

Since the copies in the replicated system are identical away from the contour Γ, which can be viewed as a "defect" in the replicated system, it is clear that the extensive terms (proportional to the free energy density f) must be the same for F_n and $n \cdot F_1$ and hence must cancel out exactly.

Therefore in the limit $L \gg \ell$ we expect the Rényi entropies to have the form

$$S_2(A) = \alpha \cdot \ell + c_1 \cdot \ln\left(\frac{\ell}{a}\right) + \phi\left(\frac{\ell}{L}\right) + \mathcal{O}(\ell^{-1})$$

where the first term describes a "boundary law" with a non-universal prefactor α, c_1 is a constant, and $\phi(x)$ is a dimensionless function of the aspect ratio ℓ/L.

At finite temperatures, the mutual information provides the appropriate analog of the entanglement entropy (measuring info between one part of the system and another.)

$$I_2(A:B) = S_2(A) + S_2(B) - S_2(AB).$$