On single-copy entanglement

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The largest eigenvalue of the reduced density matrix for quantum chains is shown to have a simple physical interpretation and power-law behaviour in critical systems. This is verified numerically for XXZ spin chains.

In a recent paper Eisert and Cramer [1] investigated the following problem from quantum information theory: Given an initial state of a total system, what maximally entangled state between two subsystems can be obtained from it by local transformations in both parts, together with classical communication ? The general answer is that the spectrum of the reduced density matrix for the new state must majorize that of the initial one [2]. If the final state is maximally entangled, it is the superposition of M product states which all have the same weight, and the reduced density matrix ρ then has M non-zero eigenvalues with magnitude $1/M$. To reach this state, the largest density-matrix eigenvalue w_1 in the initial state must therefore be smaller than $1/M$. This lead the authors to study this eigenvalue and the associated quantity $S_1 = -\ln w_1$ for free-fermion chains. For critical systems, they found a logarithmic behaviour $S_1 \sim \ln L$ if the length L of the smaller subsystem diverges. This is the same behaviour as for the entanglement entropy $S = -\mathrm{tr}(\rho \ln \rho)$. Moreover, the factor of proportionality for the XX chain was $1/6$ which is just half the value one finds for S. In the following we show that this can be understood very easily and generalize the result to arbitrary conformally invariant models.

Consider an infinitely long quantum chain in its ground state and an interval of L consecutive sites. The reduced density matrix can be written in the form

$$\rho = \frac{1}{Z} \exp(-H) \tag{1}$$

where $Z = \mathrm{tr}(\exp(-H))$ such that ρ is normalized to one, $\mathrm{tr}(\rho) = 1$. Then the largest eigenvalue of ρ is given by

$$w_1 = \frac{1}{Z} \exp(-E_0) \tag{2}$$

where E_0 denotes the smallest eigenvalue of H. Therefore one has

$$S_1 = \ln Z + E_0 \tag{3}$$

Now consider

$$\ln \mathrm{tr}(\rho^n) = \ln \mathrm{tr}(\exp(-nH)) - n \ln Z \tag{4}$$

in the limit of large n. Then only the smallest eigenvalue of H contributes to the first term and one has

$$\ln \mathrm{tr}(\rho^n) = -nE_0 - n \ln Z \tag{5}$$

Therefore the quantity S_1 is given by the limit

$$S_1 = -\lim_{n\to\infty} \frac{1}{n} \ln \mathrm{tr}(\rho^n) \tag{6}$$

By comparison, the entanglement entropy can be expressed as

$$S = \ln Z + < H > \tag{7}$$

and follows from values n near one via

$$S = -\frac{d}{dn}\mathrm{tr}(\rho^n)|_{n=1} \tag{8}$$

Thus both S and S_1 are determined by $\mathrm{tr}(\rho^n)$, or equivalently $\mathrm{tr}(\exp(-nH))$. The latter quantity has a simple meaning in terms of the classical two-dimensional system associated with the quantum chain [3, 4]. For this system, $\exp(-H)$ is the partition function for a plane with a cut of length L along which the variables are held fixed. Thus $\mathrm{tr}(\exp(-nH))$ gives the partition function of a system on a n-sheeted Riemann plane which has the topology of a double winding staircase. Therefore S_1 is the difference between the dimensionless free energies of one section of the Riemann surface and of a normal plane. The entropy S, on the other hand, is obtained from an almost planar system of conical shape, and its logarithmic behaviour can be traced back to the critical free energy of such systems [4, 5, 6, 7].

To determine S_1 for a critical system, one can now use the conformal result [4]

$$\mathrm{tr}(\rho^n) = b_n \, (\frac{L}{a})^{-\frac{c}{6}(n-\frac{1}{n})} \tag{9}$$

where c is the central charge in the conformal classification and a denotes the radius of small circles around the branch points which one has to exclude in the continuum model. The constant b_n is not determined from the conformal considerations but independent of L. Inserting (9) into (6) one obtains immediately

$$S_1 = \frac{c}{6} \ln(\frac{L}{a}) + k_1 \tag{10}$$

where a non-universal constant k_1 has been added. The logarithmic term is exactly one-half of the one appearing in S. For the XX chain, $c = 1$ and one recovers the result found in [1]. In the same way one can obtain S_1 for the other situations which have been studied. If the subsystem forms the end of a half-infinite chain, the prefactor of the logarithm is reduced by 2 and if one considers a chain of length L which is divided into two sections of length l and $L - l$, the result is [4]

$$S_1 = \frac{c}{12} \ln[\frac{2L}{\pi a} \sin(\frac{\pi l}{L})] + k_1 \tag{11}$$

Although the conformal results give the general answer to the problem, it is still instructive to look at the free-fermion case once again. Then the operator H in (1) is also fermionic and has the diagonal form

$$H = \sum_k \varepsilon_k c_k^\dagger c_k \tag{12}$$

where the single-particle eigenvalues ε_k follow from the correlation functions in the considered state [8, 9]. For a half-filled chain of fermions, corresponding to an XX model, these quantities have been studied before [10, 11] and appear in pairs $(\varepsilon, -\varepsilon)$ if L is even. Then one can express S in the form

$$S = 2 \sum_{\varepsilon_k > 0} \left[\ln[1 + \exp(-\varepsilon_k)] + \frac{\varepsilon_k}{\exp(\varepsilon_k) + 1} \right] \tag{13}$$

whereas S_1 is given only by the first sum. For odd L, an additional eigenvalue $\varepsilon_k = 0$ appears and gives a contribution $\ln 2$ to both S and S_1. This is valid for arbitrary L. In the limit $L \to \infty$, however, the situation simplifies as the spectrum of the ε_k then becomes linear and dense. For even L it is given by

$$\varepsilon_k = \frac{\pi^2}{2 \ln L}(2k+1); \quad k = 0, 1, 2, ... \tag{14}$$

One can then go over to integrals in (13) and finds that the two contributions to S are exactly the same (and proportional to $\ln L$). This gives directly $S_1 = S/2$ for the leading logarithmic terms. The argument can be extended to non half-filled systems, where the spectrum of the ε_k is shifted.

In the free-fermion case one can also make use of the results for the ε_k obtained for non-critical XY spin chains and for the Ising model in a transverse field [3, 12, 13] to calculate S_1. The same holds for the XXZ model for $\Delta > 1$. As the entanglement entropy, S_1 is then finite and diverges only as one approaches the critical point. Using the formulae in [12], it can be expressed in closed form. For example, a transverse Ising chain divided into two halves gives in the disordered region

$$S_1 = \frac{1}{24}\left[\ln(\frac{16}{k^2 k'^2}) - \pi \frac{I(k')}{I(k)}\right] \tag{15}$$

where k measures the coupling, $k'^2 = 1 - k^2$ and $I(k)$ is the complete elliptic integral of the first kind. Near criticality ($k \to 1$) this has the expansion

$$S_1 = \frac{1}{24}\left[\ln(\frac{8}{1-k}) - \frac{\pi^2}{2}\frac{1}{\ln(\frac{8}{1-k})}\right] \tag{16}$$

The logarithms can be expressed in terms of the correlation length, since $\xi \sim 1/(1-k)$. This expansion differs from that for S, where the second term does not appear. For the XY chain one obtains similar results.

Returning to w_1 itself, the results imply that it varies as a power in $1/L$ for critical systems. Its vanishing for $L \to \infty$ is connected with the fact that the spectrum of ρ, as well-known from DMRG calculations, flattens more and more as L becomes larger. The power-law behaviour can also be seen in numerical calculations. This is shown in Fig.1 where results for XXZ spin chains with anisotropies Δ between -1 and $+1$ are presented. They were obtained from DMRG calculations on open chains of odd total length up to 801 sites, keeping m=500 states but using no sweeps. The division was into subsystems of L and $L-1$ sites with L odd. Thus one is dealing with the situation described by the formula (11). The odd length was chosen because then the convergence is better. As one can see, the curves in the double-logarithmic plot become rather straight for large L and differ by additive constants. The resulting values of c are shown in the right part of the figure as function of $1/\ln L$. They clearly tend to the value 1, but the convergence is relatively slow and dependent on the value of Δ, as well as on the chosen expression for the slope of S_1. A second order extrapolation in $1/\ln L$ gives c-values which deviate from 1 by at most 5%. By contrast, the values for c determined from the entanglement entropy S lie much closer to 1 and converge faster. One could associate this with the different behaviour of the two quantities near criticality mentioned above.

Summing up, we have shown that the largest density-matrix eigenvalue for a quantum chain can be interpreted as a difference of two free energies. Correspondingly, it shows universal features if the system is critical. For the problem cited at the beginning, this means that the rank M of the maximally entangled state grows unlimited with the subsystem size (although the power is relatively small) and the central charge c appears again in the field of quantum information.

Note added: The conformal result for S_1 was given independently also by Orús et al.[14] with an additional subleading term.

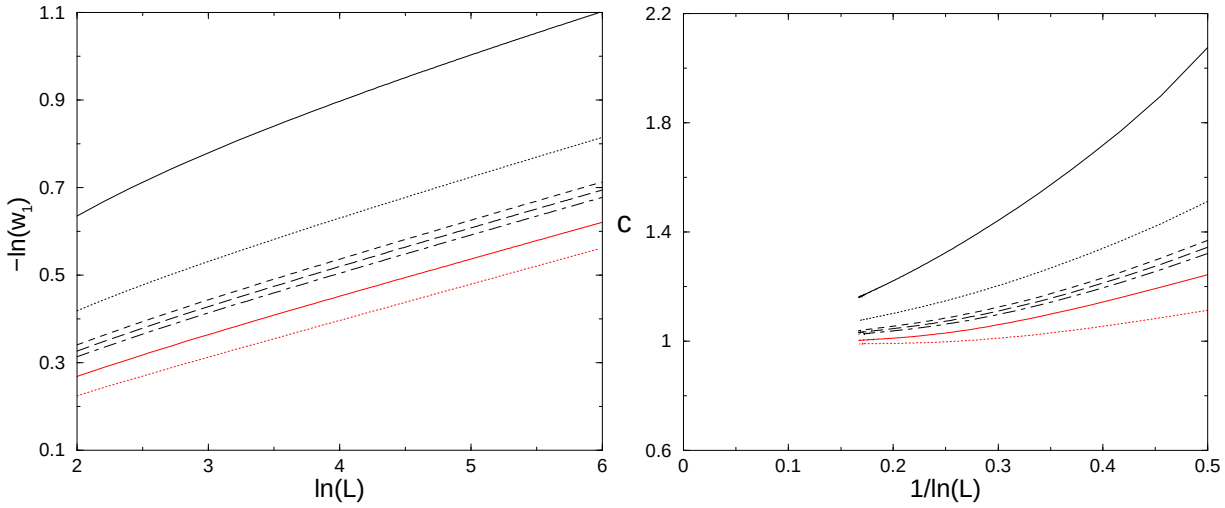

FIG. 1: Left: Largest eigenvalue of ρ for XXZ chains with half-length L. Right: Central charge c determined from the slopes in the left figure multiplied by 12. The curves correspond to the anisotropies $\Delta = -0.9; -0.5; -0.1; 0; 0.1; 0.5; 0.9$, from top to bottom.

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