



# On numerical calculation of Rényi entropy for a sphere



Nakwoo Kim

Department of Physics and Research Institute of Basic Science, Kyung Hee University, Seoul 130-701, Republic of Korea

## ARTICLE INFO

### Article history:

Received 23 March 2014

Accepted 28 April 2014

Available online 1 May 2014

Editor: M. Cvetič

### Keywords:

Rényi entropy

Conformal field theory

## ABSTRACT

We numerically compute the Rényi entropy for four-dimensional free scalar field theory with a spherical entangling surface. As is well known, the Rényi entropy as a function of the boundary area exhibits linear dependence in the leading order. The coefficient of the subleading logarithmic term from our numerical data, as a function of the Rényi order  $q$ , agrees nicely with the general prediction of conformal field theory computation. The motivation of this work is also partly to see how the efficiency of numerical computation changes as a function of  $q$ . For  $q < 1$  the summation over eigenvalues of reduced density matrix takes longer since the series converges more slowly than for  $q = 1$ . For  $q > 1$  the convergence is faster, but the relative error becomes large as a general trend.

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## 1. Introduction

In this paper we largely follow the prescription of Srednicki [1] and apply it to compute the Rényi entropy numerically for a scalar field in four dimensions. For simplicity, like in [1] we will choose a spherical surface of radius  $R$  as the entangling surface.

The definition of entanglement entropy involves dividing the space into two disjoint subsets. For a given density matrix of the entire system, we first eliminate the quantum degrees of freedom in one subset by taking the trace over it.

$$\rho_A = \text{Tr}_B \rho_{\text{total}}. \quad (1)$$

After this manipulation,  $\rho_A$  becomes a mixed state even if we start with pure state  $\rho_{\text{total}}$ . Then the entanglement entropy between regions  $A$  and  $B$  is defined as the von Neuman entropy of  $\rho_A$ ,

$$S_{EE} = -\text{Tr}_A \rho_A \log \rho_A. \quad (2)$$

One can in fact easily show that [1] if  $\rho_{\text{total}}$  is pure, then  $S_{EE} = -\text{Tr}_B \rho_B \log \rho_B$  is also true. This symmetry implies that if this quantity is well-defined then it should depend only on the boundary between  $A$  and  $B$ . This area law was explicitly confirmed through numerical computation in [1].

A refinement of entanglement entropy, as a one-parameter deformation, is given by the Rényi entropy.

$$S_{RE}(q) = \frac{\log \text{Tr}_A \rho_A^q}{1 - q}. \quad (3)$$

It immediately follows that

$$\lim_{q \rightarrow 1} S(q)_{RE} = S_{EE}. \quad (4)$$

Obviously the computation of the Rényi entropy will constitute a more robust check for a conjectured equality, for instance when one is to compare the result against calculation done in a very different setting, like the proposal of Ryu–Takayanagi formula (see e.g. [2] for a review) for holographic computation of entanglement entropy via AdS/CFT correspondence [3].

Although the computation of entanglement or the Rényi entropy may become very hard in general, for special cases it is possible to obtain an analytic answer. In this paper we choose to study free scalar field theory, and choose the sphere of radius  $R$  as the entangling surface between region  $A$  and  $B$ . The Rényi entropy for this particular example is given as follows [4–7],

$$S_{EE} = \alpha \left( \frac{R}{\epsilon} \right)^2 - \frac{(1+q)(1+q^2)}{360q^3} \log(R/\epsilon), \quad (5)$$

where  $\epsilon$  is UV cutoff, and the coefficient of area law  $\alpha$  is scheme-dependent and non-universal as it is usually the case with quadratic divergences in quantum field theory. The  $q$ -dependent function as the coefficient of log term is a physical result, which in more generality is given by Weyl anomaly coefficient [8].

We will numerically check the validity of the above formula for Rényi entropy, for a free scalar field theory. The motivation for this exercise is to attain experience and insight into the numerical computation of Rényi entropy, as a preparation of more challenging problems such as gauge field theory or interacting field theory. First of all as a general remark one expects the introduction of

E-mail address: [nkim@khu.ac.kr](mailto:nkim@khu.ac.kr).

$q$  should expediate the numerical computation since it replaces logarithm inside  $\text{Tr}$  of Eq. (2) with a power function. It will also help, as we increase  $q$ , that the summands in (3) will become smaller so we will have faster convergence and eventually smaller values of  $S_{EE}$ . We have confirmed these predictions and also obtained the numerical values. For  $q < 1$  the numerical calculation in average takes two to three times longer to finish than  $q > 1$  cases.

We note that there exist several papers which include numerical evaluation of entanglement and Rényi entropy. The logarithmic coefficient in entanglement entropy was first computed in [9]. Extension to different spacetime dimensions was studied in [10,11], and [12]. The case of entangling surface with cylindrical topology are studied in [13], and more recently in [14] for Rényi entropy.

## 2. Rényi entropy of a free scalar field on sphere

The discretization prescription of a free scalar field for spherical entangling surface was first worked out by Srednicki [1], and refined in subsequent works [9,10]. This section is largely a review of these earlier works and serves to setup the notation.

Our starting point is the Hamiltonian for a real, massless free scalar field in four dimensions.

$$H = \frac{1}{2} \int d^3x (\pi^2(\vec{x}) + (\nabla\phi(\vec{x}))^2). \quad (6)$$

We can expand using spherical harmonics and in terms of partial-wave Hamiltonians we have ( $x \equiv |\vec{x}|$ ).

$$H_{lm} = \frac{1}{2} \int dx \left\{ \pi_{lm}^2(x) + x^2 \left[ \frac{\partial}{\partial x} \left( \frac{\phi_{lm}(x)}{x} \right) \right]^2 + \frac{l(l+1)}{x^2} \phi_{lm}^2(x) \right\}. \quad (7)$$

We may now put this Hamiltonian on lattice (discretize coordinate  $x$ ) with size  $a$  and obtain a system of coupled harmonic oscillators (for each  $l, m$ )

$$H_{lm} = \frac{1}{2a} \sum_{i,j=1}^N (\delta_{ij} \pi_j^2 + \phi_i K_{ij} \phi_j), \quad (8)$$

where  $\phi_j \equiv \phi(x=ja)$ , etc. The mass matrix  $K$  can be computed easily and the result is

$$K_{11} = \frac{9}{4} + l(l+1), \quad (9)$$

$$K_{jj} = 2 + \frac{1}{j^2} \left( \frac{1}{2} + l(l+1) \right), \quad 2 \leq j \leq N, \quad (10)$$

$$K_{j,j+1} = K_{j+1,j} = -\frac{(j+1/2)^2}{j(j+1)}, \quad 1 \leq j \leq N-1. \quad (11)$$

Here  $N$  is the size of total space we introduce as an IR cut-off. The radius of the sphere in this prescription can be taken as  $R = (n+1/2)a$ .

For a coupled harmonics oscillators system it is straightforward to obtain the ground state density matrix, and tracing out the inside degrees of freedom when we divide the set of degrees of freedom into two. The computational prescription is as follows. The matrix  $K$  above is real and symmetric, and the eigenvalues are positive. One may thus find the “square root” of  $K$ , i.e.  $\Omega = \sqrt{K}$ . We then express it as

$$\Omega = \begin{pmatrix} A & B \\ B^T & C \end{pmatrix}, \quad (12)$$

where  $A$  is  $n \times n$  and  $C$  is  $(N-n) \times (N-n)$ . From  $\Omega$  we compute the following  $(N-n) \times (N-n)$  matrices step by step.

$$\beta = \frac{1}{2} B^T A^{-1} B, \quad \beta' = \frac{1}{\sqrt{C-\beta}} \beta \frac{1}{\sqrt{C-\beta}}. \quad (13)$$

Let us denote the eigenvalues of  $\beta'$  by  $\beta'_i$  ( $i = 1, 2, \dots, N-n$ ). Then all the eigenvalues of the reduced density matrix  $\rho_{\text{out}}$  are found to be

$$p_{i,k} = (1 - \xi_i) \xi_i^k, \quad i = 1, 2, \dots, (N-n), \quad k = 0, 1, 2, \dots \quad (14)$$

$$\xi_i = \frac{\beta'_i}{1 + \sqrt{1 - \beta'^2}}. \quad (15)$$

Now if we denote the eigenvalues of the reduced density matrix  $\rho_{\text{out}}$  by  $p_i$  (probability), they are given as

$$p_i = (1 - \xi_i) \xi_i^n, \quad \xi_i = \frac{\beta'_i}{1 + \sqrt{1 - \beta'^2}}. \quad (16)$$

If we substitute these eigenvalues into the definition of Rényi entropy Eq. (3), the Rényi entropy for each partial wave field  $\phi_{lm}$  is given as

$$S_{EE}(l) = \sum_{i=1}^{N-n} \frac{q(1 - \xi_i) - \log(1 - \xi_i^q)}{1 - q}. \quad (17)$$

Finally the entire Rényi entropy is

$$S_{EE} = \sum_{l=0}^{\infty} (2l+1) S_{EE}(l). \quad (18)$$

## 3. Implementation and the results

For each step of the evaluation we are given specific values of  $n, q, N, l$ . Using the matrix  $K$  and Eq. (17), one obtains a number  $S(n, q, N, l)$ . In reality what we need to calculate eventually is then

$$S_{RE}(n, q) \equiv \sum_{l=0}^{\infty} (2l+1) \lim_{N \rightarrow \infty} S(n, q, N, l). \quad (19)$$

One practical issue which was not mentioned in [9] is that some of the eigenvalues  $\beta'_i$  are negative. This boundary effect leads to small but non-vanishing imaginary part in the computation of entanglement entropy since it involves computing of  $\log \beta'_i$ . One can introduce a small cutoff and ignore the eigenvalues whose absolute value is smaller than the cutoff, making entanglement entropy real. For the Rényi entropy we are interested here there will not be imaginary part, but we will still use small cutoff but the cutoff  $10^{-9}/(2l+1)$  which will accelerate the computation.

Taking large  $N$  limit can be done by fitting the large  $N$  behavior of  $S(n, q, N, l)$  to asymptotic behavior  $S(n, q, N, l) \sim a_l + b_l/N^{2l+2}$ . This behavior was empirically discovered in [9], which we also confirmed in our results. Although this scaling does not precisely hold for large  $l$ , the function even more quickly converges to the limiting value  $S(n, q, \infty, l)$  for large  $l$  and the error can be ignored.

We should also approximate the sum over  $l$ . For this purpose we first compute and do summation of  $(2l+1)S(n, q, \infty, l)$  up to the point  $l = l_c$  where it becomes smaller than a pre-set value, which we chose to be  $10^{-4}$ . From there we evaluate  $S$  for ten different values of  $l$ , equally spaced from  $l_c$  to  $2l_c$ . Then these data points are fit against simple power dependence  $A/l^B$  and then the rest of the summation can be approximated using Euler–McLaurin formula.

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