An alternative method for extracting the von Neumann entropy from Renyi entropies

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Bibliography

Based on

- Eric D'Hoker, Xi Dong, and Chih-Hung Wu, "An alternative method for extracting the von Neumann entropy from Renyi entropies", arXiv:2008.10076

Building on earlier work

- P. Calabrese, J. Cardy and E. Tonni, "Entanglement entropy of two disjoint intervals in conformal field theory", J. Stat. Mech **0911** (2009) P11001, arXiv:0905.2069.
- P. Calabrese, J. Cardy and E. Tonni, "Entanglement entropy of two disjoint intervals in conformal field theory II", J. Stat. Mech **1011** (2011) P01021, arXiv:1011.5482.

Introduction

- **von Neumann entropy for a thermal density matrix**
  - reduces to the thermal entropy
  - evaluated in terms of the partition function
  - in QFT given by standard functional integral

- **von Neumann entropy for density matrix of a subsystem**
  - provides a measure for the entanglement of subsystems
  - no direct evaluation in QFT (unless modular Hamiltonian is known)
  - replica trick in terms of Renyi entropies + "analytic continuation"

- **Here, the goal is to develop a more systematic method**
  - for extracting von Neumann from Renyi entropies
  - without invoking the replica trick
  - applications to simple
    - $\star$ analytical calculations
    - $\star$ numerical calculations

The density matrix

- **The density matrix ρ in a Hilbert space $\mathcal{H}$**
  - self-adjoint $\rho^\dagger = \rho$
  - positive $\rho \geq 0$
  - normalized $\mathrm{Tr}_{\mathcal{H}}(\rho) = 1$
  - may be diagonalized in an orthonormal basis $|n\rangle$ of $\mathcal{H}$

$$\rho = \sum_\alpha p_\alpha \, |\alpha\rangle\langle\alpha| \qquad\qquad \langle\alpha'|\alpha\rangle = \delta_{\alpha\alpha'} \qquad\qquad 0 \leq p_\alpha \leq 1$$

- **For a subsystem $\mathcal{H}_A \subset \mathcal{H}$ such that $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$**
  - A pure state $|\Psi\rangle \in \mathcal{H}$ generally reduces to an entangled state of $\mathcal{H}_A$ with reduced density matrix $\rho = \rho_A = \mathrm{Tr}_{\mathcal{H}_B}(|\Psi\rangle\langle|\Psi|)$ for $\langle\Psi|\Psi\rangle = 1$

- **The Schmidt number gives a rough measure of entanglement**
  - Schmidt number $=$ rank(ρ)
  - $\star$ rank$(\rho) = 1$ iff ρ corresponds to a pure state
  - $\star$ rank$(\rho) > 1$ corresponds to an entangled state

The von Neumann and Renyi entropies

- **von Neumann entropy is defined by**

$$S(\rho) = -\mathrm{Tr}(\rho \ln \rho) = -\sum_\alpha p_\alpha \ln p_\alpha$$

  - $S(\rho) \geq 0$ for all ρ, and $S(\rho) = 0$ iff ρ corresponds to a pure state
  - $S(\rho)$ provides a refined measure of entanglement

- **For a thermal distribution, reduces to thermodynamic entropy**
  - which may be evaluated in terms of the partition function Z

$$\rho = \frac{e^{-\beta H}}{Z} \qquad Z = \mathrm{Tr}(e^{-\beta H}) \qquad S(\rho) = \ln Z - \beta \frac{\partial \ln Z}{\partial \beta}$$

  - and more generally when a modular Hamiltonian is known

- **Renyi entropies are defined for integer $n = 2, 3, \cdots$ by**

$$S_n(\rho) = \frac{1}{1-n} \ln \Big(\mathrm{Tr}(\rho^n) \Big)$$

  - do give some measure of entanglement
  - but do not reduce to thermodynamic entropy
  - do not obey additivity and sub-additivity properties

Density matrix in 2-d CFT

- **Consider a unitary 2-d CFT**

  – free boson $\phi(\tau, x)$ with Hamiltonian H and Lagrangian L
  – Matrix element of $e^{-\beta H}$ between two field eigenstates is

$$\langle \phi_2 | e^{-\beta H} | \phi_1 \rangle = \int_{\mathcal{B}} \mathcal{D}\phi \, \exp \left\{ - \int_0^\beta d\tau L \right\}$$

  – with boundary conditions

$$\mathcal{B} \begin{cases} \phi(0, x) = \phi_1(x) \\ \phi(\beta, x) = \phi_2(x) \end{cases}$$

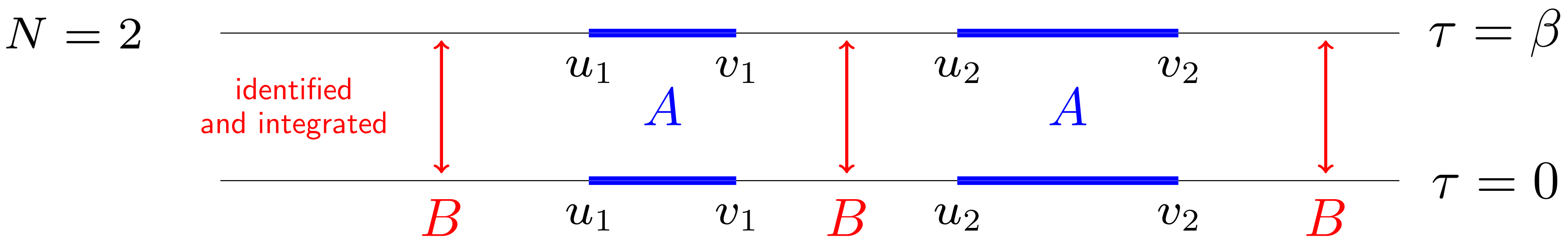
  – The partition function is given by

$$Z = \int \mathcal{D}\phi_1 \, \langle \phi_1 | e^{-\beta H} | \phi_1 \rangle$$

Disjoint intervals in 2-d CFT

- **For a subsystem A consisting of N disjoint intervals**

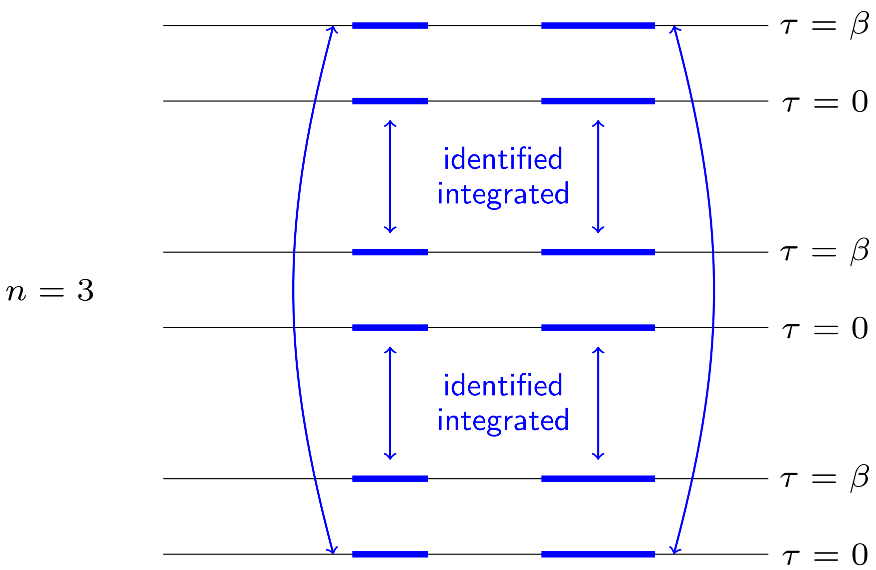
$$A = [u_1, v_1] \cup [u_1, v_2] \cup \cdots \cup [u_N, v_N] \qquad\qquad B = \mathbb{R} \setminus A$$



  - the reduced density matrix ρ is obtained by
    - ⋆ specifying functions at $\tau = 0, \beta$ with support on A
    - ⋆ integrating (tracing) over the functions with support on B

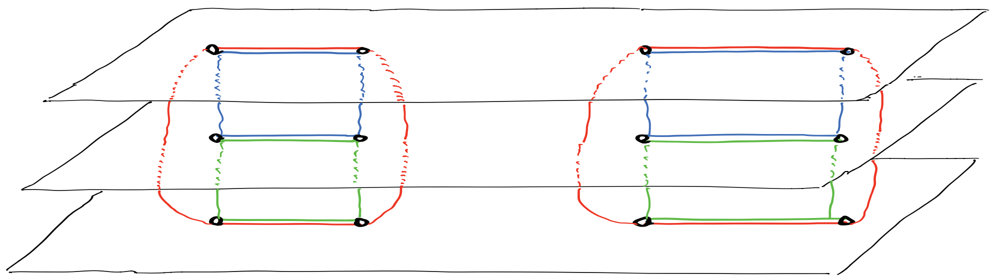
Disjoint intervals in 2-d CFT cont'd

- **From the reduced density matrix ρ**
  - unknown how to access $\ln \rho$ or $\mathrm{Tr}(\rho \ln \rho)$ directly;
  - but we can obtain $\mathrm{Tr}(\rho^n)$ for $n \in \mathbb{N}$ by sewing n copies of ρ



Riemann surface picture of disjoint intervals

– 2-dim picture is a Riemann surface with N branch cuts of order n
– produced in the CFT by twist field operators at branch points
– giving a Riemann surface of genus $(n-1) \times (N-1)$
– for $n = 3$ and $N = 2$



Renyi entropies for disjoint intervals in 2-d CFT

- **Consider a 2-dim. unitary CFT with central charge c**

  ⋆ one interval $A = [x_1, x_2]$ and UV cutoff ε

$$\mathrm{Tr}(\rho^n) = e^{\left(\frac{1}{n}-n\right)y} \qquad\qquad y = \frac{c}{6} \ln \frac{|x_{12}|}{\varepsilon}$$

  ⋆ two intervals $A = [x_1, x_2] \cup [x_3, x_4]$

$$\mathrm{Tr}(\rho^n) = e^{\left(\frac{1}{n}-n\right)y} \mathcal{F}_n(x) \qquad\qquad y = \frac{c}{6} \ln \frac{|x_{12}x_{34}|}{\varepsilon^2}$$

  – where $\mathcal{F}_n$ is given by

$$\mathcal{F}_n(x) = 1 + \mathcal{N} \left(\frac{x}{4n^2}\right)^{\alpha} \sum_{\ell=1}^{n-1} \frac{\ell}{\left(\sin \frac{\pi \ell}{n}\right)^{2\alpha}} + \cdots \qquad\qquad x = \frac{x_{12}x_{34}}{x_{13}x_{24}}$$

  – $\alpha/2$ is the lowest operator dimension in the CFT (greater than zero)

  – $\mathcal{N}$ is the multiplicity of the lowest dimensional operator

  – the $\cdots$ stand for higher order terms in powers of x

  – gives the leading order in x for well-separated intervals

  (Calabrese, Cardy, Tonni 2009-2010)

von Neumann entropy from Renyi entropies

- **IF Renyi entropies were known for real $n=\nu$ near $\nu=1$ then**
  - von Neumann entropy could be obtained as a limit

$$S(\rho) = -\mathrm{Tr}(\rho \ln \rho) = \lim_{\nu \to 1} S_\nu(\rho) = \lim_{\nu \to 1} \frac{\ln \mathrm{Tr}(\rho^\nu)}{1-\nu}$$

  - the *replica trick* relies on "analytically continuing" in n to $\nu \in \mathbb{C}$
  - Does such an analytic continuation exist ?
  - if it exists, is it unique ?

- **Carlson's theorem** addresses the last question

A function $f(\nu)$ that is holomorphic in ν for $\mathrm{Re}(\nu) \geq 1$, vanishes for positive integer ν, is bounded by $|f(\nu)| < C\, e^{\lambda|\nu|}$ for $\mathrm{Re}(\nu) \geq 1$ with constants $C, \lambda > 0$, and satisfies this bound with $\lambda < \pi$ on $\mathrm{Re}(\nu) = 1$, must vanish identically for all ν.

  - the function $\sin \pi\nu$ vanishes for all integer ν but violates the bound !

von Neumann entropy from Renyi entropies cont'd

- **Replica trick: does the analytic continuation exist ?**
  - and if it exists, how to obtain it ?

- **Trivial for the one-interval case** since $S_n(\rho)$ is analytic in n

$$S_n(\rho) = \frac{c}{6}\left(1+\frac{1}{n}\right)\ln\frac{L}{\varepsilon} \qquad \to \qquad S(\rho) = \frac{c}{3}\ln\frac{L}{\varepsilon}$$

- **Highly non-trivial for two or more intervals**
  - nonetheless, for two intervals, by guessing and trial and error
  - a viable analytic continuation was found

$$\mathcal{F}_n(x) = 1 - \mathcal{N}\left(\frac{x}{4}\right)^{\alpha}\frac{\sqrt{\pi}\,\Gamma(\alpha+1)}{4\,\Gamma(\alpha+\frac{3}{2})} + \cdots$$

(Calabrese, Cardy, Tonni 2010)

The alternative method (ED, Dong, Wu)

- **Assuming that all Renyi entropies are known for integer n**
  - hence we know $\mathrm{Tr}(\rho^n)$ for all $n \in \mathbb{N}$

- **Assemble $\mathrm{Tr}(\rho^n)$ in a generating function with parameter z**

$$G(z;\rho) = \sum_{n=1}^{\infty} \frac{z^n}{n} \Big(\mathrm{Tr}(\rho^{n+1}) - 1 \Big)$$

  - Series is absolutely convergent in the unit disc $|z| < 1$ and gives

$$G(z;\rho) = - \mathrm{Tr} \Big(\rho \, \ln \frac{1 - z\rho}{1 - z} \Big)$$

  - Discrete spectrum of p_α: branch cuts $[1, \infty]$, $[1/p_1, \infty]$, $[1/p_2, \infty]$, $\cdots$

- **Standard analytic continuation in z from unit disc to $\mathrm{Re}(z) < 0$**
  - always exists since there are no singularities for $\mathrm{Re}(z) < 0$
  - provides a formula for the von-Neumann entropy

$$S(\rho) = \lim_{z \to -\infty} G(z;\rho) = - \mathrm{Tr} \big(\rho \ln \rho \big)$$

Application to the one-interval case

- **This case was trivial by analytic continuation in n**
- **For the alternative method, introduce the generating function**

$$G(z;\rho) = \sum_{n=1}^{\infty} \frac{z^n}{n} \left[e^{y(1/(n+1)-n-1)} - 1 \right] \qquad\qquad y = \frac{c}{6} \ln \frac{L}{\varepsilon}$$

  - Expand in powers of $\frac{y}{n+1}$

$$G(z;\rho) = \ln(1-z) + e^{-y} \sum_{n=1}^{\infty} \frac{z^n e^{-ny}}{n} \sum_{j=0}^{\infty} \frac{y^j}{j!} \frac{1}{(n+1)^j}$$

  - Interchange order of summations

$$G(z;\rho) = \ln(1-z) + e^{-y} \sum_{j=0}^{\infty} \frac{y^j}{j!} F_j(ze^{-y})$$

  - $F_j(z)$ is given by a series that converges absolutely for $|z| < 1$

$$F_j(z) = \sum_{n=1}^{\infty} \frac{z^n}{n(n+1)^j}$$

Application to the one-interval case cont'd

- **The analytic continuation of $F_j(z)$**

partial fraction decomposition
$$\frac{1}{n(n+1)^j} = \frac{1}{n} - \sum_{s=1}^{j} \frac{1}{(n+1)^s}$$

– In terms of polylogarithms

$$F_j(z) = k + \mathrm{Li}_1(z) - \frac{1}{z}\sum_{s=1}^{j} \mathrm{Li}_s(z) \qquad \mathrm{Li}_s(z) = \sum_{n=1}^{\infty} \frac{z^n}{n^s}$$

– Asymptotics as $z \to -\infty$ is given by the Sommerfeld expansion

$$\mathrm{Li}_s(z) = -2\sum_{m=1}^{\infty} \frac{(1-2^{m-1})\zeta(2m)}{\Gamma(s-2m+1)} \big[\ln(-z)\big]^{s-2m} + \mathcal{O}(z^{-1})$$

– so that $F_j(z) = j - \ln(-z) + \mathcal{O}(z^{-1})$ and therefore

$$G(z;\rho) = \ln(1-z) + e^{-y}\sum_{j=0}^{\infty} \frac{y^j}{j!}\Big(j - \ln(-ze^{-y})\Big) + \mathcal{O}(z^{-1})$$

– and we recover the von Neumann entropy in the limit $z \to -\infty$

$$\lim_{z\to-\infty} G(z;\rho) = 2y = \frac{c}{3}\ln\frac{L}{\varepsilon}$$

Application to the two-interval case

- **The two-interval case presents a more challenging test**
  - recall the expression $\mathrm{Tr}(\rho^n) = e^{\left(\frac{1}{n}-n\right)y}\mathcal{F}_n(x)$ with

$$\mathcal{F}_n(x) = 1 + \mathcal{N}\left(\frac{x}{4n^2}\right)^{\alpha} \sum_{\ell=1}^{n-1} \frac{\ell}{(\sin\frac{\pi\ell}{n})^{2\alpha}} + \cdots$$

  - stripping off $\mathcal{N}(x/4)^\alpha$ we use the generating function

$$\tilde{G}(z;\rho) = \sum_{n=1}^{\infty} \frac{z^n}{n} e^{(1/(n+1)-n-1)y} \frac{1}{(n+1)^{2\alpha}} \sum_{\ell=1}^{n} \frac{\ell}{\left(\sin\frac{\pi\ell}{n+1}\right)^{2\alpha}}$$

  - expand in powers of $\frac{y}{n+1}$ as for the case of one interval

$$\tilde{G}(z;\rho) = e^{-y} \sum_{j=1}^{\infty} \frac{y^j}{j!} \sum_{n=1}^{\infty} \frac{z^n e^{-ny}}{n(n+1)^{2\alpha+j}} \sum_{\ell=1}^{n} \frac{\ell}{\left(\sin\frac{\pi\ell}{n+1}\right)^{2\alpha}}$$

  - Use the same expansion as was used by Calabrese, Cardy, Tonni 2010

$$\left(\frac{u}{\sin u}\right)^{2\alpha} = \sum_{k=0}^{\infty} p_k(\alpha) u^{2k}$$

    - ⋆ $p_k(\alpha)$ is a polynomial in α of degree k
    - ⋆ radius of convergence $|u| < \pi$

Application to the two-interval case cont'd

- **Substitution gives**

$$\tilde{G}(z;\rho) = \frac{e^{-y}}{\pi} \sum_{k=0}^{\infty} p_k(\alpha) \sum_{j=1}^{\infty} \frac{y^j}{j!} \sum_{n=1}^{\infty} \frac{z^n e^{-ny}}{n(n+1)^{2k+j}} \sum_{\ell=1}^{n} (\pi \ell)^{2k+1-2\alpha}$$

  – now use an integral representation

$$\sum_{\ell=1}^{n} (\pi\ell)^{2k+1-2\alpha} = \frac{1}{\Gamma(2\alpha-1)} \int_0^\infty \frac{dt}{t}\, t^{2\alpha-1} \left(\frac{\partial}{\partial t} \right)^{2k} \sum_{n=1}^{n} e^{-\pi \ell t}$$

  – to get the final integral representation for finite z

$$\tilde{G}(z;\rho) = \frac{1}{\pi} \sum_{k=0}^{\infty} \frac{p_k(\alpha)}{\Gamma(2\alpha-1)} \int_0^\infty \frac{dt}{t}\, t^{2\alpha-1} \left(\frac{\partial}{\partial t} \right)^{2k} \left(\frac{H_k(z,t)}{e^{\pi t}-1} \right)$$

$$H_k(z,t) = e^{-y} \sum_{j=1}^{\infty} \frac{y^j}{j!} \sum_{n=1}^{\infty} \frac{z^n e^{-ny}}{n(n+1)^{2k+j}} (1 - e^{-n\pi t})$$

  – partial fraction decomposition in n as for the 1-interval case
  – recasting in terms of F_j and polylogarithms
  – with the following limit

$$H_k(z,t) = -\pi t + \mathcal{O}(z^{-1})$$

Application to the two-interval case cont'd

- **Recovering the Calabrese Cardy Tonni result**

$$\lim_{z\to-\infty}\tilde{G}(z;\rho) = -\sum_{k=0}^{\infty}\frac{p_k(\alpha)}{\Gamma(2\alpha-1)}\int_0^{\infty}\frac{dt}{t}\,t^{2\alpha-1}\left(\frac{\partial}{\partial t}\right)^{2k}\left(\frac{t}{e^{\pi t}-1}\right)$$

  - The integral for each k is absolutely convergent for $\mathrm{Re}(\alpha) > \frac{1}{2}$

$$\lim_{z\to-\infty}\tilde{G}(z;\rho) = -\sum_{k=0}^{\infty}p_k(\alpha)\pi^{2k-2\alpha}(2\alpha-2k-1)\zeta(2\alpha-2k)$$

  - The series in k is only asymptotic and requires Borel resummation
  - Use the functional equation for ζ and the integral representation

$$\pi^{2k-2\alpha}(2\alpha-2k-1)\zeta(2\alpha-2k) = \frac{2}{\pi}(-)^{k+1}\sin(\pi\alpha)\int_0^{\infty}\frac{dt}{e^{\pi t}-1}\frac{\partial}{\partial t}t^{2k-2\alpha+1}$$

  - Now we can carry out the summation over k

$$\lim_{z\to-\infty}\tilde{G}(z;\rho) = \frac{\sin(\pi\alpha)}{\pi}\int_0^{\infty}\frac{dt}{(\mathrm{sh}\,t)^{2\alpha+2}} = -\frac{\sqrt{\pi}\,\Gamma(\alpha+1)}{4\Gamma(\alpha+\frac{3}{2})}$$

  - recovering the result of Calabrese, Cardy, Tonni 2010

Numerical calculations

- **Numerical calculations that require analytic continuation ?**
  - rational interpolation method

    (Agon, Headrick, Jafferis, Kasko 2013; De Nobili, Coser, Tonni 2015)

- **Our method provides a way around this**

$$G(z;\rho) = \sum_{n=1}^{\infty} \frac{z^n}{n} \Big(\mathrm{Tr}(\rho^{n+1}) - 1 \Big) = -\mathrm{Tr} \Big(\rho \ln \frac{1 - z\rho}{1-z} \Big)$$

  - The series is absolutely convergent for $|z| < 1$
  - Change variables $z \to w$ by Möbius transformation $z = \frac{w}{w-1}$

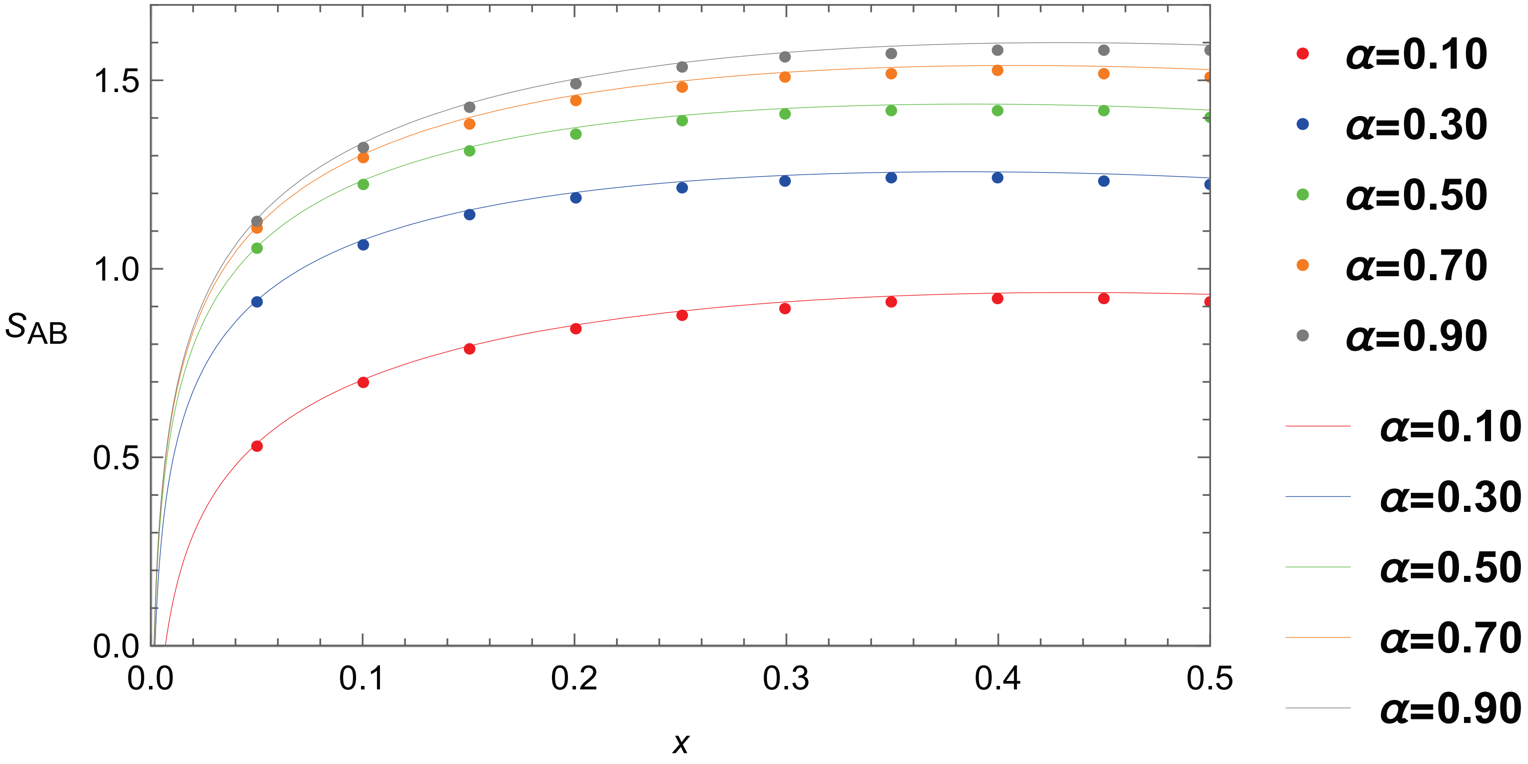
$$G(z;\rho) = -\mathrm{Tr} \Big(\rho \ln \big(1 - w(1-\rho) \big) \Big) = \sum_{n=1}^{\infty} \frac{w^n}{n} \mathrm{Tr} \Big(\rho (1-\rho)^n \Big)$$

  - The limit $z \to -\infty$ is mapped to the limit $w \to 1$
  - coefficients computed by binomial expansion from Renyi entropies

$$\mathrm{Tr} \Big(\rho (1-\rho)^n \Big) = \sum_{m=0}^{n} \binom{n}{m} (-)^m \mathrm{Tr}(\rho^{m+1})$$

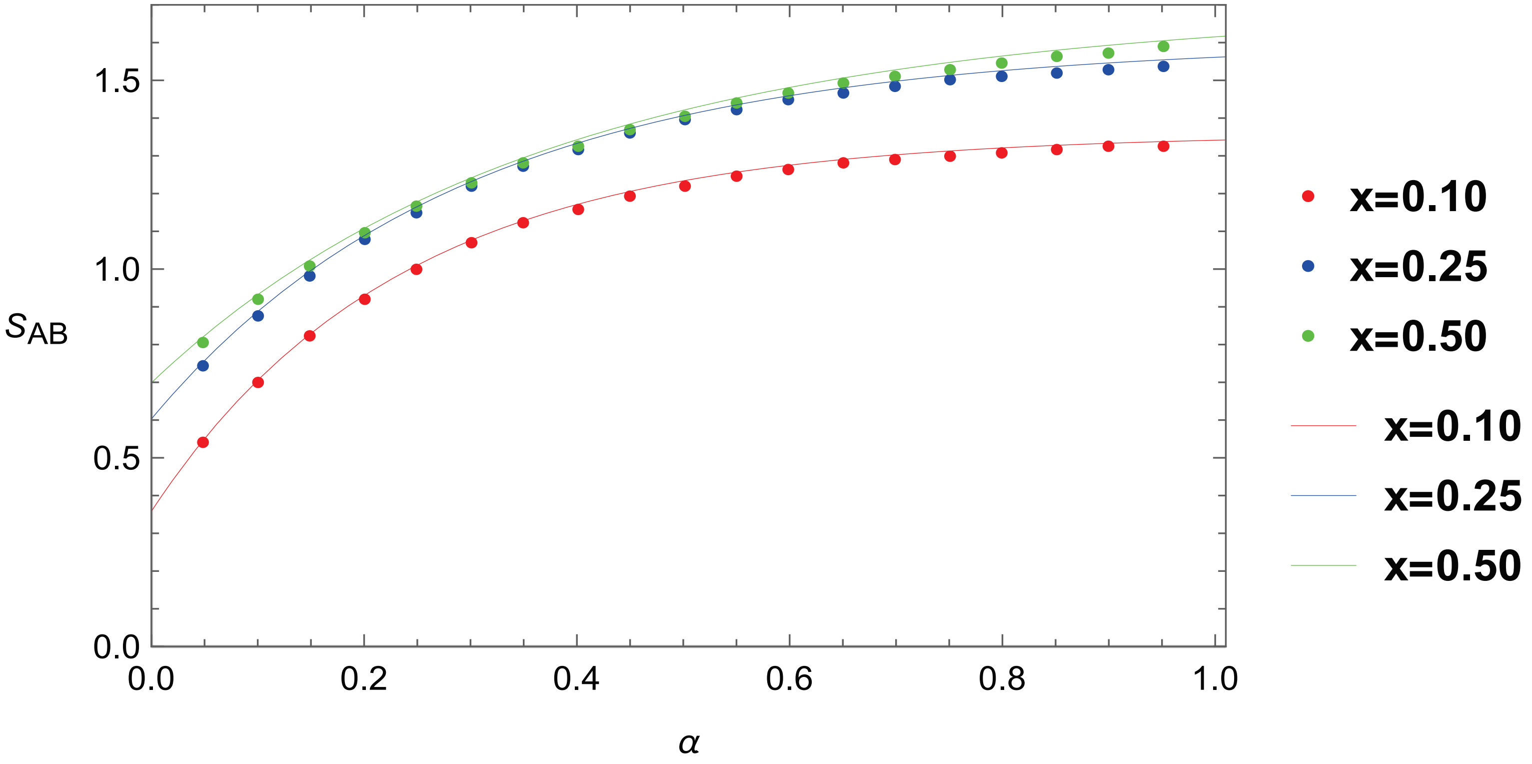
Numerical: two disjoint intervals

- **Numerical calculations for two intervals in the small x limit**
  - solid lines are exact result in this limit
  - dots are result of numerical calculations using above method



Numerical: two disjoint intervals cont'd

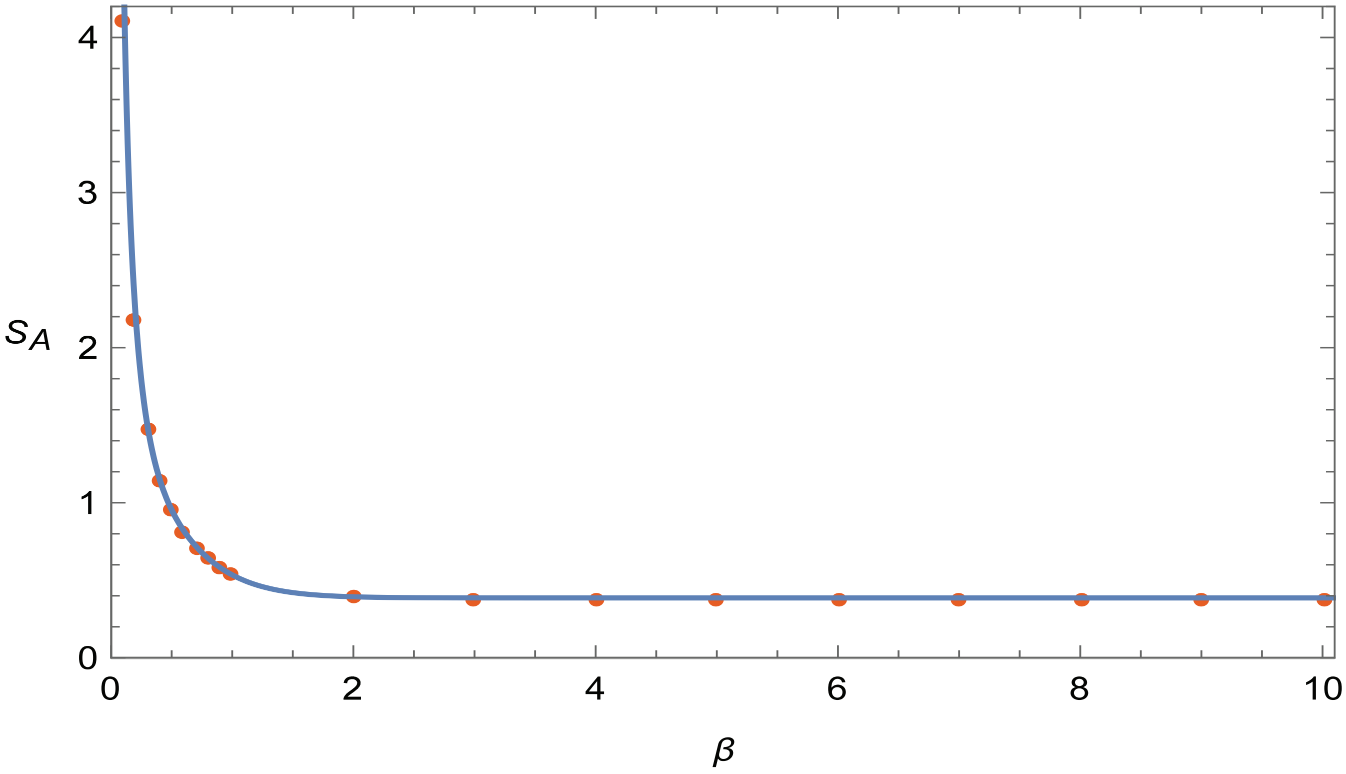
- **Numerical calculations for two intervals in the small x limit**
  - solid lines are exact result in this limit
  - dots are result of numerical calculations using above method



Numerical: one interval and finite temperature

- solid lines are exact result

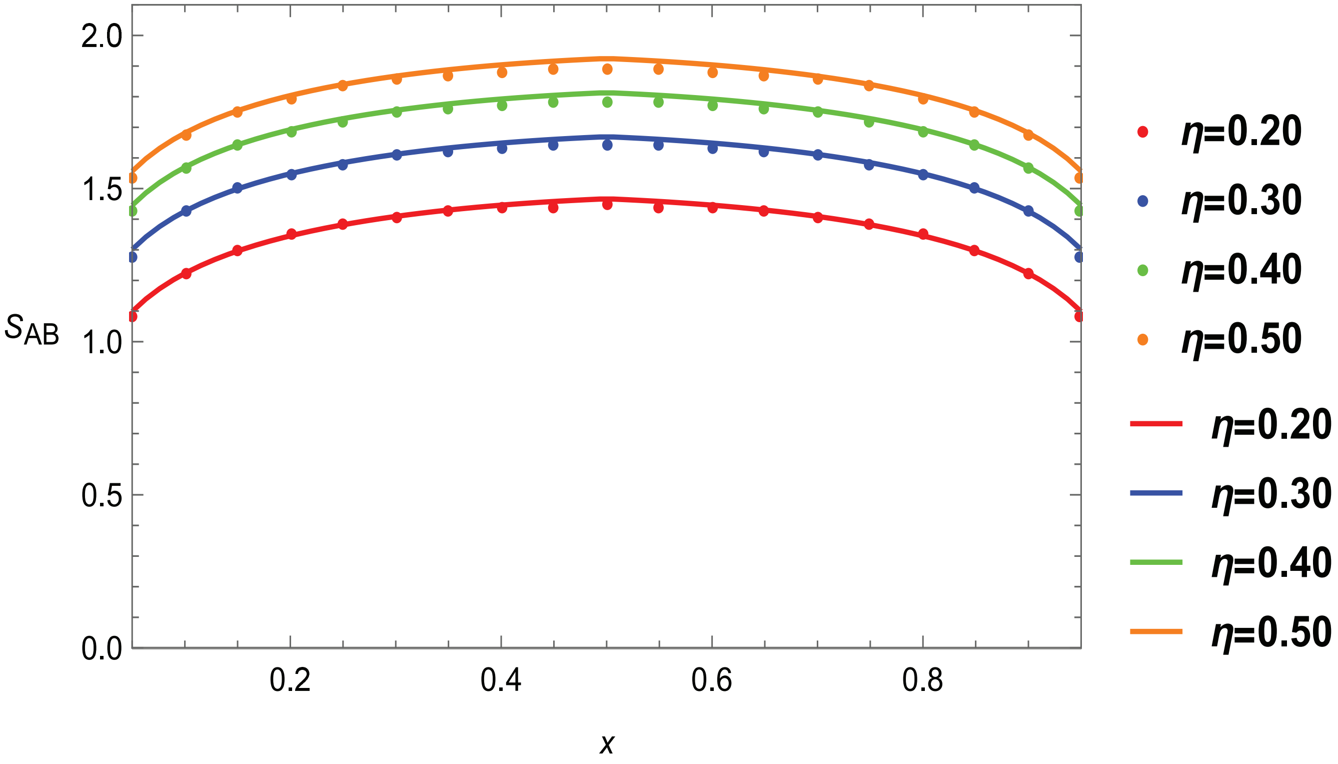
  (Azeyanagi, Nishioka, Takayanagi 2008; Blanco, Garbarz, Perez-Nadal 2019)
- dots are result of numerical calculations using our method



Numerical: decompactification limit

- solid lines are exact result

  (Calabrese, Cardy, Tonni 2010; Furukawa, Pasquier, Shiraishi 2008)
- dots are result of numerical calculations using our method



Challenges with the exact 2-interval solution

- **Exact Renyi entropies for the two-interval case in free boson CFT**
  - Recall $\mathrm{Tr}(\rho^n) = \exp\{y(\frac{1}{n} - n)\}\mathcal{F}_n(x,\eta)$
  - Exact solution derived by using twist operators (Calabese, Cardy, Tonni)

$$\mathcal{F}_n(x,\eta) = \frac{\Theta(0|\eta\Omega)\Theta(0|\Omega/\eta)}{|\Theta(0|\Omega)|^2}$$

  - where Θ is the Riemann theta constant of rank $n-1$

$$\Theta(0|\Omega) = \sum_{M\in\mathbb{Z}^{n-1}} e^{i\pi M^t\Omega M}$$

  - and Ω is an $(n-1)\times(n-1)$ matrix with elements

$$\Omega_{rs} = \frac{2i}{n}\sum_{k=1}^{n-1}\sin\left(\frac{\pi k}{n}\right)\cos\left(\frac{2\pi k}{n}(r-s)\right)\frac{{}_2F_1(y,1-y;1;1-\frac{k}{n})}{{}_2F_1(y,1-y;1;\frac{k}{n})}$$

  - $\eta \sim R^2$, with R the radius of the circle of the $c=1$ CFT

- **Alternative method gives a formula for the generating function**
  - but unknown how to simplify and analytically continue in z
  - numerical results available, but nothing to compare with.

Outlook

- **New method for extracting the von Neumann from Renyi entropy**
  - generating function out of series in z of Renyi entropies
  - always convergent for $|z| < 1$
  - always exists an analytic continuation in z to $z \to -\infty$
  - allows for numerical approximations

- **But we need better methods to simplify the generating functions**
  - even for the two-interval case in the small x limit

- **Numerical methods for precision calculation of Θ-functions**

  (Deconinck, Heil, Bobenko, Van Hoeij, Schmies 2004)

  (Frauendiener, Jaber, Klein 2017)

- **Generalization to orbifold constructions of $\mathrm{Tr}\left(\rho^{\frac{1}{N}}\right)$?**

  (Witten 2018)