Computation of quantum entanglement in quantum magnetism via Monte Carlo simulations

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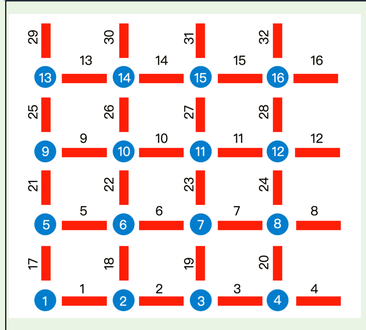
Abstract

This research is about the entanglement entropy, a smoking gun for quantum critical phenomena. The QMC algorithm, stochastic series expansion (SSE) is used to probe the Rényi entropy of the Heisenberg model by constructing the so-called 'Qiu-Ku' manifold. Two different calculation schemes are presented. One is to monitor the transition between two ensembles, an independent one and a 'glued' one. Another is a non-equilibrium measurement in which the entanglement region grows gradually. It is shown that both result obtain satisfactory results and the non-equilibrium measurement cures the large systematic error when the entangled region is large.

Stochastic Series Expansion



$$H = J\sum_{<i,j>}\left[S_i^xS_j^x + S_i^yS_j^y + S_i^zS_j^z\right] - JN_bC$$

$$= -J\sum_{b=1}^{N_b}\{(C - S_{i(b)}^zS_{j(b)}^z) - \frac{1}{2}(S_{i(b)}^+S_{j(b)}^- + S_{i(b)}^-S_{j(b)}^+)\}$$

$$= -J\sum_{b=1}^{N_b}\{H_{1,b} - H_{2,b}\}$$

$$H_{1,b} = C - S_{i(b)}^zS_{j(b)}^z \qquad H_{2,b} = \frac{1}{2}(S_{i(b)}^+S_{j(b)}^- + S_{i(b)}^-S_{j(b)}^+)$$

H_1 is the diagonal operator and H_2 is the off-diagonal operator. The partition function is Taylor expanded. It is nothing but the summation of weights in the enlarged configuration space $\{\sigma, n\}$,

$$Z = Tr\{e^{-\beta\hat{H}}\} = \sum_\alpha\sum_{n=0}^{\infty}\frac{(-\beta)^n}{n!}\langle\alpha|\hat{H}^n|\alpha\rangle$$

$$W(\sigma,n) = \frac{(-\beta)^n}{n!}\langle\alpha|\hat{H}^n|\alpha\rangle$$

$$= \frac{(-\beta)^n}{n!}\sum_{S_n}^{(2N_b)^n}(-1)^n\cdot(-1)^{number\ of\ H_{2,b}}\cdot\langle\alpha|\prod_{p=n}^{1}H_{a(p),b(p)}|\alpha\rangle$$

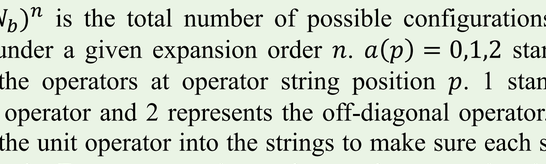
$$= \frac{(\beta)^n}{n!}\sum_{S_n}^{(2N_b)^n}(-1)^{number\ of\ H_{2,b}}\cdot\langle\alpha|\prod_{p=n}^{1}H_{a(p),b(p)}|\alpha\rangle$$

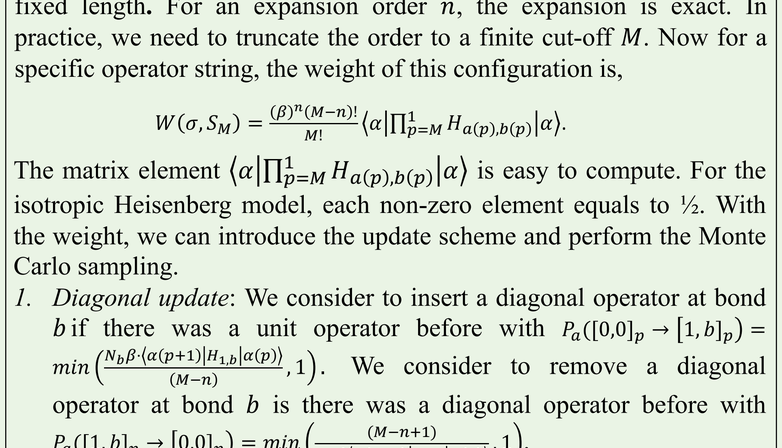
Here $(2N_b)^n$ is the total number of possible configurations (operator strings) under a given expansion order n. $a(p) = 0,1,2$ stands for the type of the operators at operator string position p. 1 stands for the diagonal operator and 2 represents the off-diagonal operator. We insert $H_0 = \mathbf{1}$, the unit operator into the strings to make sure each string has a fixed length**.** For an expansion order n, the expansion is exact. In practice, we need to truncate the order to a finite cut-off M. Now for a specific operator string, the weight of this configuration is,

$$W(\sigma,S_M) = \frac{(\beta)^n(M-n)!}{M!}\langle\alpha|\prod_{p=M}^{1}H_{a(p),b(p)}|\alpha\rangle.$$

The matrix element $\langle\alpha|\prod_{p=M}^{1}H_{a(p),b(p)}|\alpha\rangle$ is easy to compute. For the isotropic Heisenberg model, each non-zero element equals to ½. With the weight, we can introduce the update scheme and perform the Monte Carlo sampling.

1. *Diagonal update*: We consider to insert a diagonal operator at bond b if there was a unit operator before with $P_a([0,0]_p \to [1,b]_p) = min\left(\frac{N_b\beta\cdot\langle\alpha(p+1)|H_{1,b}|\alpha(p)\rangle}{(M-n)},1\right)$. We consider to remove a diagonal operator at bond b is there was a diagonal operator before with $P_a([1,b]_p \to [0,0]_p) = min\left(\frac{(M-n+1)}{N_b\beta\langle\alpha(p+1)|H_{1,b}|\alpha(p)\rangle},1\right)$.
2. *Loop update*: Construct closed loops. When encountering an operator, it switches or goes straight with some probabilities. If a loop switches at an operator, the type of the operator changes. All the spins visited by the loop are flipped.



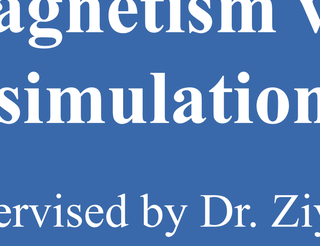


Computing the Rényi Entropy

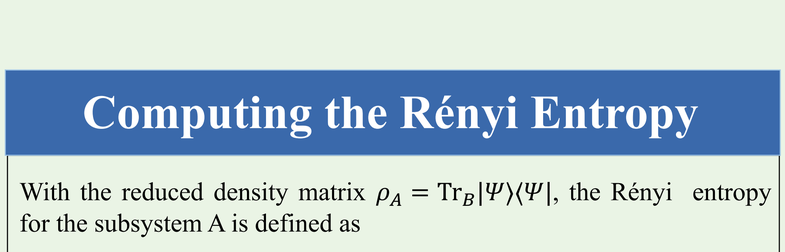
With the reduced density matrix $\rho_A = \mathrm{Tr}_B|\Psi\rangle\langle\Psi|$, the Rényi entropy for the subsystem A is defined as

$$S_A^{(\alpha)} = -\frac{\ln[\mathrm{Tr}(\rho_A^\alpha)]}{1-\alpha}$$

where α is the order of the Rényi entropy.



The starting point to write the Rényi entropy as ratio of two partition functions, $S^\alpha = \frac{\ln R_A^{(\alpha)}}{1-\alpha}, R_A^{(\alpha)} = \frac{Z_A^{(\alpha)}}{Z^\alpha}$. Here $Z^\alpha = [\mathrm{Tr}(e^{-\beta H})]^\alpha$ is the ordinary partition function for α replicas of the system, while $Z_A^{(\alpha)}$ is a modified partition function for replicas which are 'glued' together in the



With this topology, we can estimate $R_A^{(\alpha)}$ by $\frac{P_{\emptyset\to A}}{P_{A\to\emptyset}}$ and thus,

$$S^\alpha = \frac{1}{1-\alpha}\ln\left(\frac{P_{\emptyset\to A}}{P_{A\to\emptyset}}\right)$$

(a) $P_{\emptyset\to A}$ is determined by performing all the simulations in the independent ensemble and monitor whether the configurations meet the periodic criterion for the glued ensemble, $|n_A\rangle = |m_A\rangle$. Thus,

$$P_{\emptyset\to A} = \langle\frac{N_{meet\ glued\ criterion}}{N_{tot}}\rangle_{MC}$$

(b) $P_{A\to\emptyset}$ is determined by performing all the simulations in the glued ensemble and counting the number of configurations which satisfy periodic condition in the independent ensemble, $|n_A\rangle = |n'_A\rangle$ and $|m_A\rangle = |m'_A\rangle$ simultaneously. Similarly, $P_{A\to\emptyset}$ is estimated by

$$P_{A\to\emptyset} = \langle\frac{N_{meet\ independent\ criterion}}{N_{tot}}\rangle_{MC}\ .$$

Non-equilibrium Measurement

We parametrize the partition function $Z_A^{(\alpha)}$ with a parameter $\lambda \in [0,1]$, such that $Z_A^{(\alpha)}(\lambda=0) = Z_{A=\emptyset}^{(\alpha)}$ and $Z_A^{(\alpha)}(\lambda=1) = Z_A^{(\alpha)}$. This is done by defining

$$Z_A^{(n)}(\lambda) = \textstyle\sum_{D\subseteq A}\lambda^{N_D}(1-\lambda)^{N_A-N_D}Z_D^{(n)}$$

D represents all the possible subsets of A including the empty set $\emptyset$ and A itself. Let $g_A(\lambda,N_D) = \lambda^{N_D}(1-\lambda)^{N_A-N_D}$ and the Rényi entropy is estimated by computing the work along the non-equilibrium path in which λ is adjusted smoothly from 0 to 1:

$$W_A^{(n)} = -\frac{1}{\beta}\int_{t_i}^{t_f}dt\,\frac{d\lambda}{dt}\frac{\partial\ln g_A(\lambda(t),N_D(t))}{\partial\lambda}$$

By the *Jarzynski's equality*, which tells that the Rényi entropy can be computed as

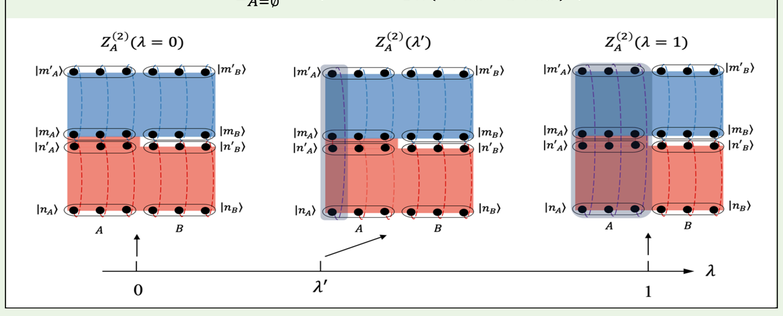
$$S_A^{(n)} = \frac{1}{1-n}\ln(\langle e^{-\beta W_A^{(n)}}\rangle)$$

Now the task is to compute and add all the increments $\partial\ln g_A(\lambda(t),N_D(t))$ along the interval $\lambda \in [0,1]$. One can compute that the increment equals to

$$\Delta\ln g_A(\lambda,N_B) = (N_A - N_B(t_m))\ln\left(\frac{1-\lambda(t_{m+1})}{1-\lambda(t_m)}\right) + N_D(t_m)\ln\left(\frac{\lambda(t_{m+1})}{\lambda(t_m)}\right).$$

Therefore, we can write the estimator for the Rényi entropy concisely as:

$$\frac{Z_A^{(\alpha)}}{Z_{A=\emptyset}^{(\alpha)}} = \left\langle\prod_{p=M}^{1}\frac{g_A(\lambda(t_{m+1}),N_B(t_m))}{g_A(\lambda(t_m),N_B(t_m))}\right\rangle.$$



Results

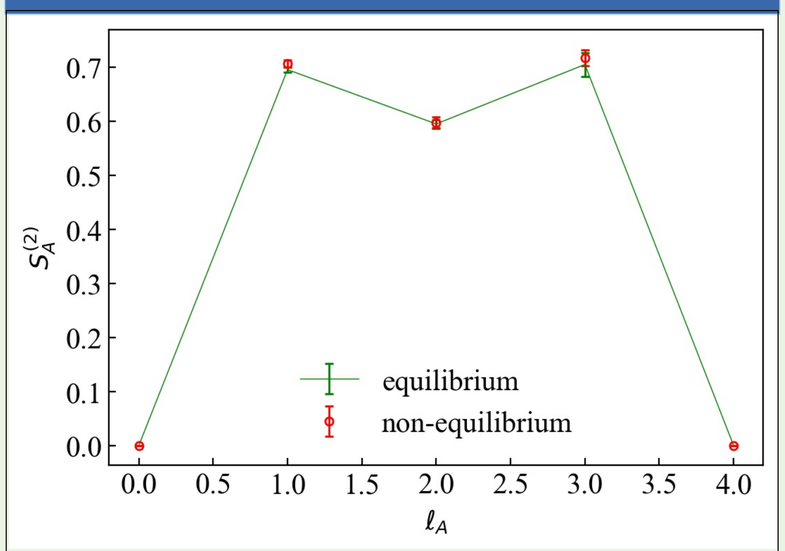


Figure 1: 2nd order Rényi entropy for 1-d Heisenberg chain of $l_x = 4$

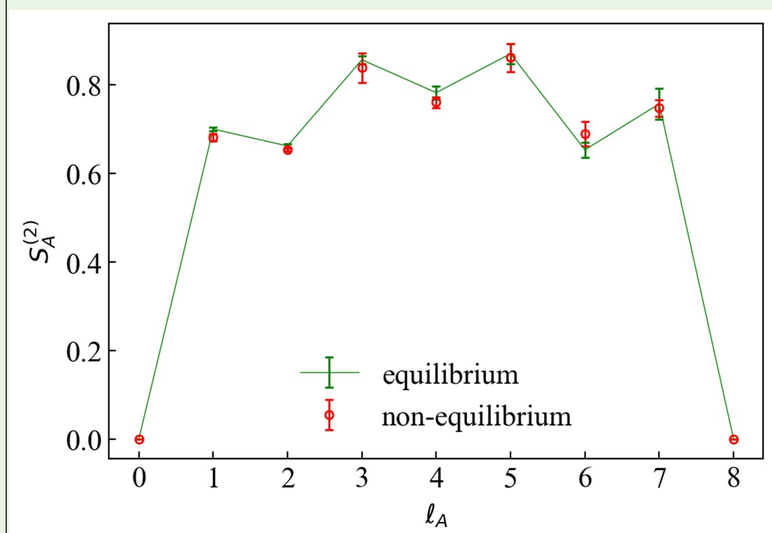


Figure 2: 2nd order Rényi entropy for 1-d Heisenberg chain of $l_x = 8$

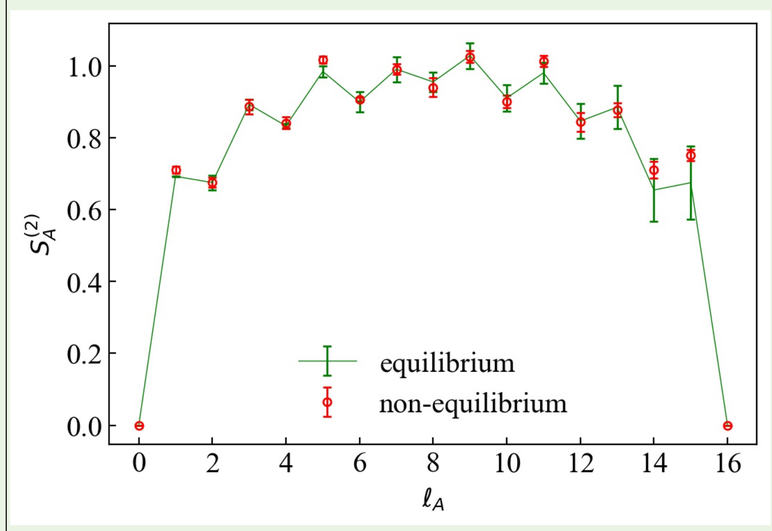


Figure 3: 2nd order Rényi entropy for 1-d Heisenberg chain of $l_x = 16$

Conclusion

To conclude, in this research we have developed two algorithms to compute the Rényi entropy via SSE, one involves the ratio of the transition probabilities between two ensembles with different trace topologies and another involves a non-equilibrium measurement. From the Fig. 1, 2, 3, both algorithms can compute the 2nd order Rényi entropy for the 1-d Heisenberg chain accurately. The zigzag and symmetric behavior of the Rényi entropy is clearly revealed via QMC simulations. Comparing two algorithms, the equilibrium one is more efficient in computing small systems. However, large systematic errors occurs when the entangled region becomes large, e.g., $l_A = 14, 15$. Non-equilibrium methods cure this problem with the compensation of the computing time.

Reference List

1. Calabrese, P., & Cardy, J. (2004). Entanglement entropy and quantum field theory. *Journal of Statistical Mechanics: Theory and Experiment*, *2004*(06). https://doi.org/10.1088/1742-5468/2004/06/p06002
2. Humeniuk, S., & Roscilde, T. (2012). Quantum Monte Carlo calculation of entanglement Rényi entropies for generic quantum systems. *Physical Review B*, *86*(23). https://doi.org/10.1103/physrevb.86.235116
3. Luitz, D. J., Plat, X., Laflorencie, N., & Alet, F. (2014). Improving entanglement and thermodynamic Rényi entropy measurements in quantum Monte Carlo. *Physical Review B*, *90*(12). https://doi.org/10.1103/physrevb.90.125105
4. D'Emidio, J. (2020). Entanglement entropy from nonequilibrium work. *Physical Review Letters*, *124*(11). https://doi.org/10.1103/physrevlett.124.110602