Entanglement spectrum calculation using quantum Monte Carlo by Dr. Zheng yan

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The idea first came from PDE, i.e. can one hear the shape of a drum. Am. Math. Mon. 73, 1 (1966) It is natural to generalize the idea to the free energy. Nucl. Phys. B 300, 377, 1988

$$F = f_{\mathrm{B}}|A| + f_{\mathrm{S}}L - \frac{1}{6}c\chi \ln L + \mathcal{O}(1). \tag{1}$$

where $1/6$ is the conformal anomaly number, and χ is the Euler characteristic. Finally we arrive the idea of the relation boundary and entanglement entropy: We have

$$S = F_A + F_B - F_{A\cup B}, \tag{2}$$

and we find

$$S = f_{\mathrm{S}}L_{A\cap B} - \frac{1}{6}c \tag{3}$$

the last term being the topological entanglement entropy.

Now we discuss how to calculate entanglement entropy. The explicit definition of von Nuemann entanglement entropy

$$S_A = -\operatorname{tr}_A \rho_A \ln \rho_A, \quad \rho_A = \operatorname{tr}_B \rho_B, \tag{4}$$

but it is hard to calculate. We usually calculate the generalized

$$S_A^{(n)} = \frac{1}{1-n}\operatorname{tr}_A \rho_A \ln \rho_A^n, \tag{5}$$

and the usual entanglement entropy is the $n \to 1$ limit.

$$S_A^{(n)} = \frac{1}{1-n}\ln \frac{Z_A^{(n)}}{Z_\emptyset^{(n)}}, \tag{6}$$

where $Z_A^{(n)}$ is the partition function of all possible field configuration obtained by gluing n configuration of A together, and $Z_\emptyset^{(n)}$ is simply multiplication of n partition functions of A.

Naive Monte Carlo calculation of (6) suffers from small probabilities. A trick to work around this is Phys. Rev. Lett. 124, 110602, 2020, Entanglement Entropy from Nonequilibrium work. We have

$$S_A^{(n)} = \frac{1}{1-n}\int_0^1 \mathrm{d}\lambda \, \frac{\partial \ln Z_A^{(n)}(\lambda)}{\partial \lambda}, \tag{7}$$

where

$$Z_A^{(n)}(\lambda) = \sum_{B\subseteq A} \lambda^{N_B}(1-\lambda)^{N_A - N_B} Z_B^{(n)}, \quad Z_A^{(n)}(0) = Z_\emptyset^{(n)}, \quad Z_A^{(n)}(1) = Z_A^{(n)}. \tag{8}$$

$$\frac{\partial \ln Z_A^{(n)}(\lambda)}{\partial \lambda} = \tag{9}$$

A straight forward approach is to run a Monte Carlo process for each λ separately, but note that nonequilibrium statistic mechanics tells us regardless of whether the system has reached equilibrium, we can slowly change λ during *one* Monte Carlo simulation, and therefore efficiently calculate (7).