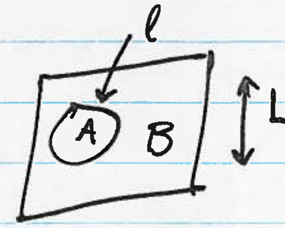
Roger Melko 01/09/14

Benasque 2014

(Entanglement) Entropy in (Q)MC



Renyi $\quad S_n(A) = \frac{1}{1-n} \log\left(\mathrm{Tr}\, \rho_A^n\right)$

$$S_1 = -\mathrm{Tr}\left(\rho_A \log \rho_A\right)$$

$$S_2 = -\log\left(\mathrm{Tr}\, \rho_A^2\right) \quad \text{etc...}$$

Properties
- $S_n(A) = 0$ if A & B are unentangled
- $S_n(A) = S_n(B)$ at $(T=0)$
- $S_n \geq S_m$ when $n < m$

2D Condensed Matter / Quantum Many-Body systems:

- $S_n \simeq A \frac{\ell}{\delta} + \dots$ "area law" (gapped, short-range corr.)

  $\simeq A \frac{\ell^{d-1}}{\delta^{d-1}} + \dots$ in other dimensions d

- $S_n = a\ell - \gamma$ gapped topological phase (e.g $\gamma = \log(2)$ in Z_2 spin liquid)

- $S_n = a\ell + b\log(\ell)$ continuous symmetry breaking

- $S_n = c\, l \log(l)$ Fermi surface Wolf Gioev Klich
- $S_n = a l + c_n \Gamma(l/L, \cdots)$ quantum critical points.

e.g. $c_n \Gamma = c_n^{(\theta)} \log(l)$ for a corner

↑ new universal quantity!

Purpose of measuring entanglement entropy in Monte Carlo

- characterize quantum phases
- locate QCP and determine universality class
- evaluate quantities relevant for monotonicity theorems (ie. c-theorems) : new inputs on constraints in phase diagrams
- confirm forms of Γ calculated in AdS/CFT for larger d (Myers, Casini, Huerta)
- evaluate validity of tensor network ansatz

Generally Renyi entropies are non-local quantities that give us a new perspective on correlations in condensed Matter / Quantum Many Body systems!

Challenge: Need a calculation of ρ_A (?)

The Replica Trick in Monte Carlo

Motivate the replica trick, starting with a random classical variable X: if the probability of some outcome $X=i$ is p_i

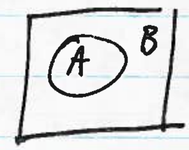
then $$S_n(X) = \frac{1}{1-n}\log\left(\sum_{i\in X} p_i^n\right)$$

(e.g. $n \to 1$ gives Shannon entropy).

Now imagine dividing your system into two subsystems A & B. One may ask:

- what is our uncertainty in the state of A, given knowledge of the state of B?

(2-point correlation functions incompletely quantify this knowledge, for example).



p_{i_A} : probability of a state i_A occurring in region A

p_{i_B} : probability of a state i_B occurring in region B.

if the total Boltzman probability of a state:

$$p_{i_A i_B} = e^{-\beta E(i_A, i_B)}/Z$$

$$Z = \sum_{i_A i_B} e^{-\beta E(i_A, i_B)}$$

Obtain the probability of a certain state in A:

$$p_{i_A} = \frac{\sum_{i_B} e^{-\beta E(i_A, i_B)}}{Z}$$

Then we can define the Renyi entropy of the bipartition; using $S_n(A) = \frac{1}{1-n} \log\left(\sum_{i_A} p_{i_A}^n\right)$

Consider the 2^{nd} Renyi entropy: then

$$p_{i_A}^2 = \frac{\sum_{i_B} e^{-\beta E(i_A, i_B)}}{Z} \; \frac{\sum_{j_B} e^{-\beta E(i_A, j_B)}}{Z}$$

$$= \frac{1}{Z^2} \sum_{i_B} \sum_{j_B} e^{-\beta\left(E(i_A, i_B) + E(i_A, j_B)\right)}$$

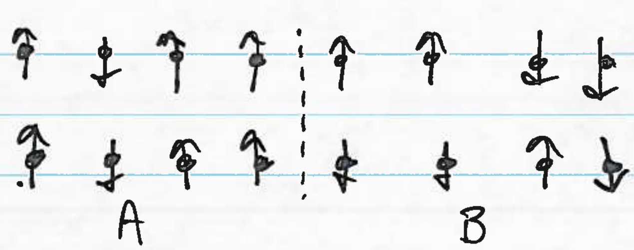
then $$S_2(A) = -\log\left[Z^{-2} \sum_{i_A} \sum_{i_B} \sum_{j_B} e^{-\beta\left(E(i_A i_B) + E(i_A j_B)\right)}\right]$$

$$= -\log Z[A,2,T] + 2 \log Z$$

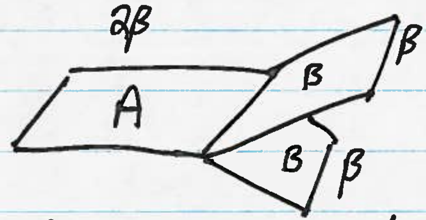
Turns into a calculation of log of the partition function (a "free energy").

Monte Carlo: draw (importance) samples from a probability distribution, by generating configurations.

$Z[A,2,T]$: special "replicated" simulation cell



valid configuration

"Book" picture 

I.e. • single copy of region A at 2β
• two "independent" copies of region B at β

A Similar picture occurs for S_3, S_4, S_5, etc...

$\boxed{\text{Only } \underline{\text{integer}} \text{ Renyi indices possible for } \underline{\text{MC}}.}$

How to calculate free energies?

• Thermodynamic integration:

$$S_2(A) = -S_A(\beta=0) + \int_0^{\beta} \langle E \rangle_A \, d\beta + 2 S_0(\beta=0) - 2\int_0^{\beta} \langle E \rangle_0 \, d\beta$$

• Direct calculation of ratio $\dfrac{Z[A,n,T]}{Z^n}$

"acceptance ratio" method (Bennett 1976)(Roscilde 2012)

– perform a move between $Z^2 \rightarrow Z[A,2,T]$

$$\frac{Z[A,n,T]}{Z^2} = \left\langle \frac{N_A}{N_{A=\emptyset}} \right\rangle_{MC}$$

N = # monte carlo steps in the ensemble with a given region A, or $A=\emptyset$.

What good is a classical $S_n(A)$ entropy?

- Groundstate: will detect degeneracies, disorder, etc.
- Finite-T: extensiveness depends on geometry of A.

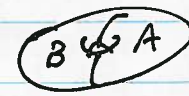
Interesting quantity: Mutual Information

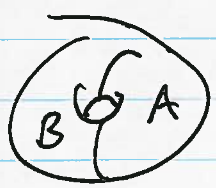
$$I_n(A;B) = S_n(A) + S_n(B) - S_n(A \cup B)$$

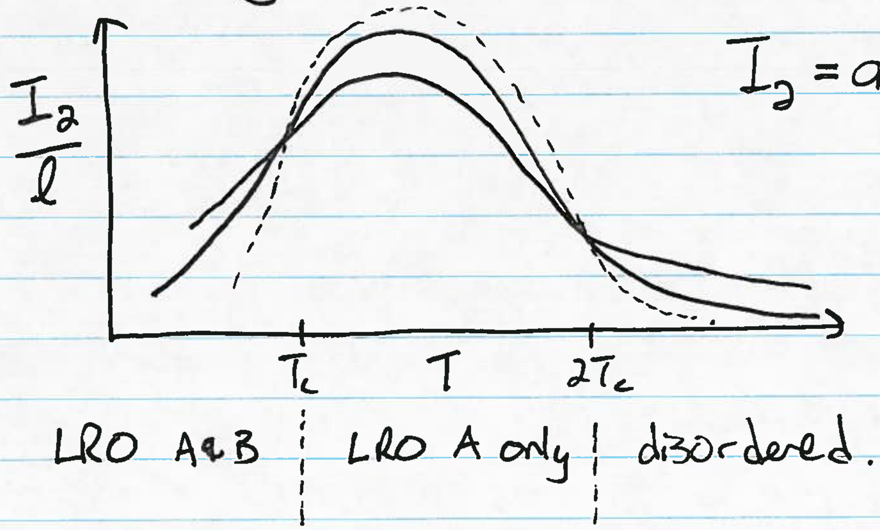
The information that <u>full knowledge</u> of B gives about A.

- Bounds correlation functions in some precise way (Wolf, Verstraete, Hastings, Cirac, 2008 PRL)

<u>Example</u>: 2D Ising model ($\ell = 2L$)







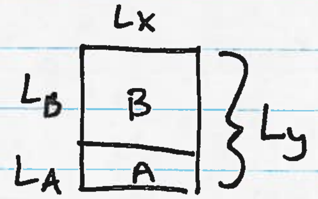
$I_2 = a(t)\,\ell + c(t) + d\,\frac{1}{\ell}$

↑ changes sign through T_c, $2T_c$

More generally, $c(t)$ depends on the aspect ratio of region A:

e.g. $C_n(T=T_c) = \frac{c}{2} \frac{1}{n-1} f\left(\frac{L_A}{L_x}, \frac{L_B}{L_x}, \frac{L_y}{L_x}\right)$

central charge of associated 1+1 CFT !



some Dedekind η functions

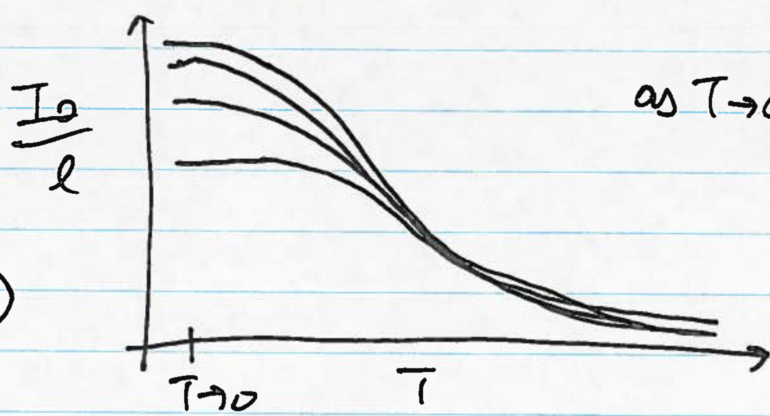
(see Stephan, Inglis, Fendley, RGM PRL 2014)

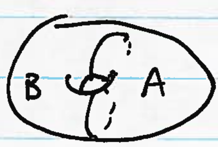
So not only can the critical point position T_c be identified, so can its universality class. No order parameters needed... !

Also interesting:

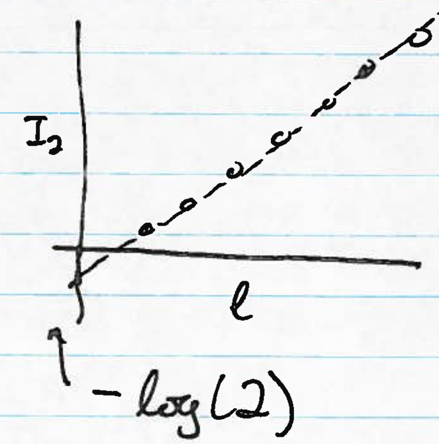
- Z_2 topological gauge theories ($\frac{1}{2}$ toric code)

$H = -\sum_p \prod_{i \in p} \sigma_i^z$ (Massive degeneracy)





as $T \to 0$



expect $I_2(A;B) = a\ell - 2\gamma$

$\gamma = \frac{1}{2}\log(2)$ for classical toric code!

→ what does LRE really mean?

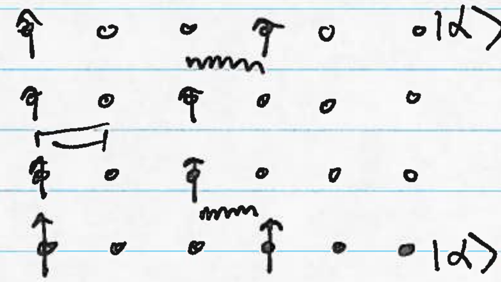
Finite-Temperature Quantum Monte Carlo

Back to the full Quantum definition of the Renyi entanglement entropy: consider $S_2(A) = -\log(\mathrm{Tr}\,\rho_A^2)$

QMC samples a $d+1$ dimensional configuration space:
- Stochastic Series Expansion (Sandvik)
- (continuous) world-line
- Path Integral: itinerant particles in the continuum

e.g.) SSE

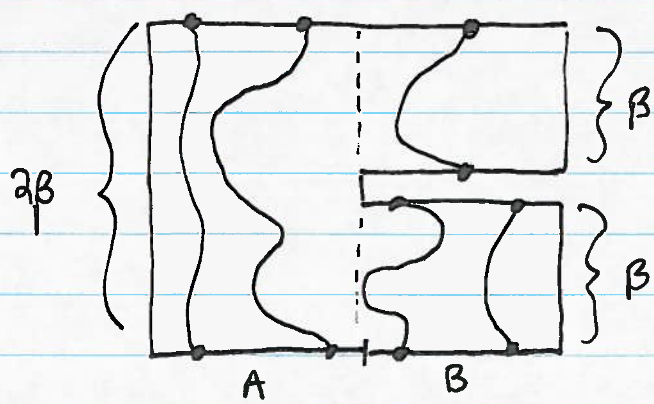
$$Z = \mathrm{Tr}\, e^{-\beta \hat{H}}$$
$$= \sum_\alpha \langle \alpha | e^{-\beta \hat{H}} | \alpha \rangle$$
$$= \sum_\alpha \sum_n \frac{(-\beta)^n}{n!} \langle \alpha | \hat{H}^n | \alpha \rangle$$



$n=3$

Measuring the Renyi entropy in QMC is a straightforward extension of this replica-trick to $d+1$ world-line picture.

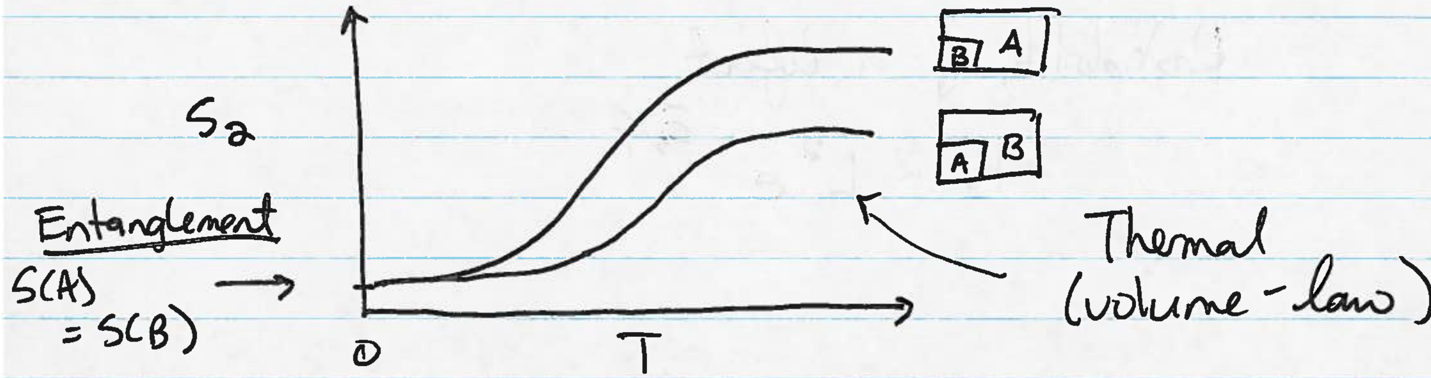
$Z[A,2,T]$



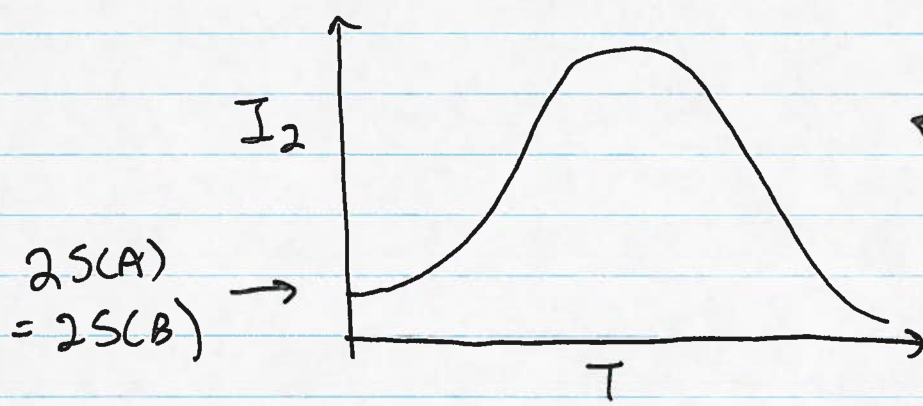
" n-sheeted Riemann surface "

Then $\mathrm{Tr}\,\rho_A^2 = \dfrac{Z[A,2,T]}{Z^2}$ ie. two simulations of different partition functions.

The entropy can be constructed by convention estimators (Thermodynamic Integration, Wang–Landau) or "acceptance ratio" methods.

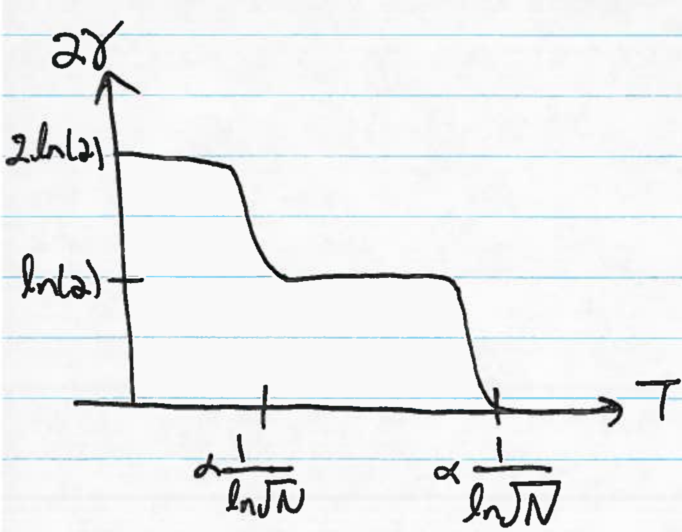


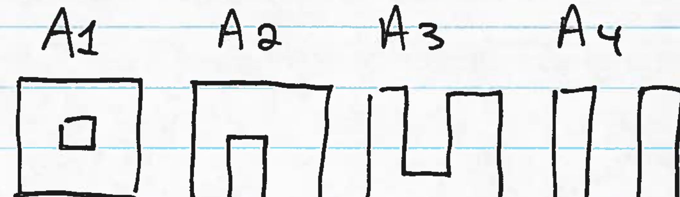
Can also construct a Mutual Information



← will also pick up T_c, $2T_c$ like the classical case (e.g. anisotropic XXZ)

e.g: Thermal onset of topological entanglement entropy in 2D Z_2 Quantum spin liquid.





$$-S_2(A_1) + S_2(A_2) + S_2(A_3) - S_2(A_4)$$

$$= 2\gamma \quad (\text{at } T \to 0$$

<u>independent</u> of n)

(Warning: KP with S_2 ...)

T=0 QMC

Many different methods exist to project out / sample the groundstate only:

- Valence Bond & Projector QMC (Sandvik)
- Variation Monte Carlo (Zhang Grover Vishwanath)
- PIGS (itinerant Bosons / continuum)

example: Projector QMC : $(-H)^m |\alpha\rangle \to c_0 |E_0|^m |\psi_0\rangle$

then $Z = \langle \alpha | (-H)^m (-H)^m | \alpha \rangle \to \langle \psi_0 | \psi_0 \rangle$

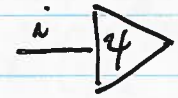
resbles SSE very closely (except importantly imaginary time periodicity)...

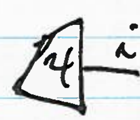
e.g $Z = \sum_{\{\alpha\}} \sum_{S_m} \prod_{j=1}^{2m} \langle \alpha_\ell | H_{t_j, a_j} | \alpha_r \rangle$

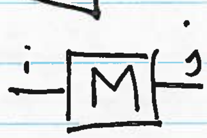
In this case we can conceptually write the replica-trick as the expectation value of an operator :

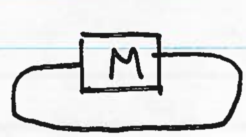
$$\langle O \rangle = \frac{1}{Z} \langle \psi_0' | O | \psi_0' \rangle$$

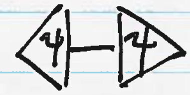
Use Tensor Diagram Notation ("Penrose" notation)

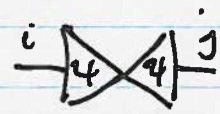
e.g.) $|\psi\rangle$ (vector)  index i

$\langle \psi |$ 

$\hat{M}$ matrix 

$\mathrm{Tr}(\hat{M})$ 

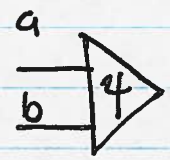
Inner product $\langle\psi|\psi\rangle$ is 

Tensor product $|\psi\rangle\langle\psi|$ is 

$= \rho$

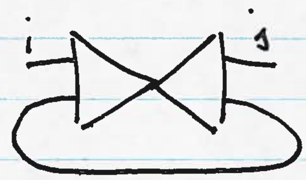
ie. the density matrix of the system.

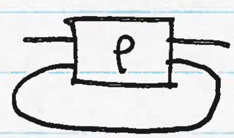
To write the entanglement entropy, we need a bipartition



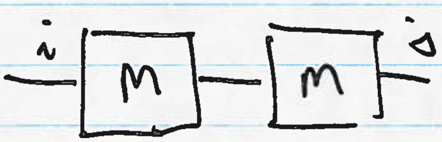
$= \sum_i \sum_j c_{ij} |a_i\rangle |b_i\rangle$ Schmidt decomposition

Then the reduced density matrix is a partial trace over only the states in region B

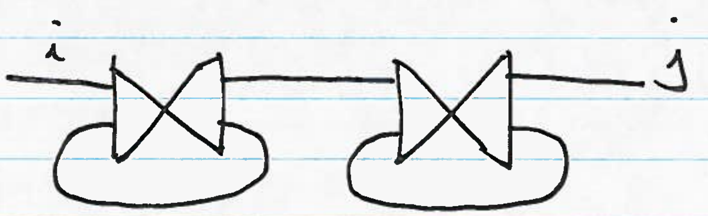
$\rho_A =$ 

$=$ 

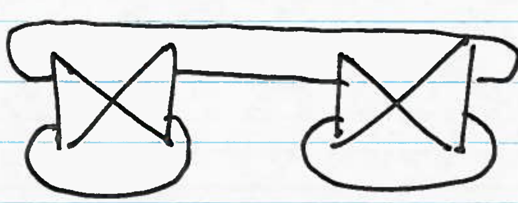
To calculate $S_2(A)$ we need ρ_A^2: matrix multiply



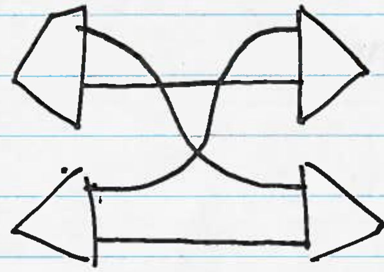
$= M^i_k M^k_j = M^2$ <u>or</u>



$= \rho_A^2$

and thus  $= \mathrm{Tr}_A \, \rho_A^2$

This is topologically equivalent to writing

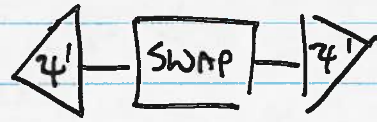


$= \langle \psi' | SWAP_A | \psi' \rangle$

↑ replicated wavefunction ↑

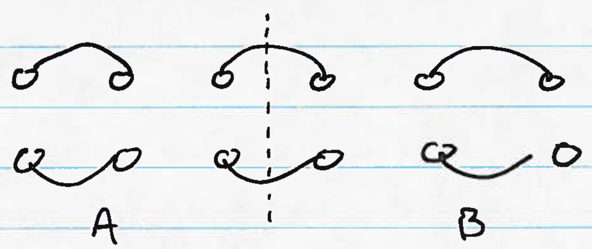
$\psi' = \psi \otimes \psi$

ie. the "replica trik" is equivalent to measuring the expectation value of a $SWAP_A$ "operator" which exchanges indices for <u>A</u> between replicas:

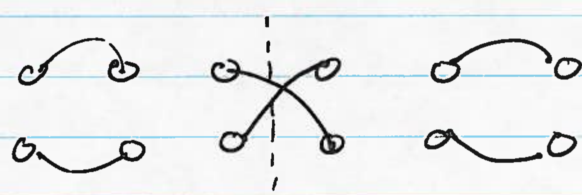


$= \langle \psi' | O | \psi' \rangle$

e.g.) Valence-Bond QMC



$|\psi'\rangle$ replicated wavefunction



$SWAP_A |\psi'\rangle$

and $S_2 = -\log\left(\langle \psi' | SWAP_A | \psi' \rangle\right) = -\log \langle SWAP_A \rangle$

This is the crucial idea - in practice large variances occur when A is large:

<u>Ratio</u> tricks: $S_2(A_n) = -\log\left(\frac{\langle SWAP_{A_n}\rangle}{\langle SWAP_{A_{n-1}}\rangle}\right) - \ln\left(\frac{\langle SWAP_{A_{n-1}}\rangle}{\langle SWAP_{A_{n-2}}\rangle}\right) \ldots$