Equivalence of Ensembles in Quantum Statistical Mechanics

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based on joint work with

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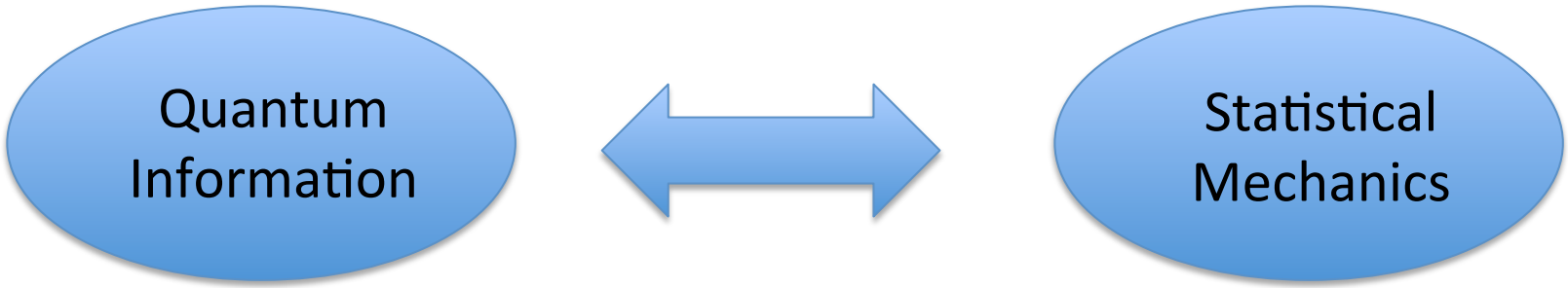
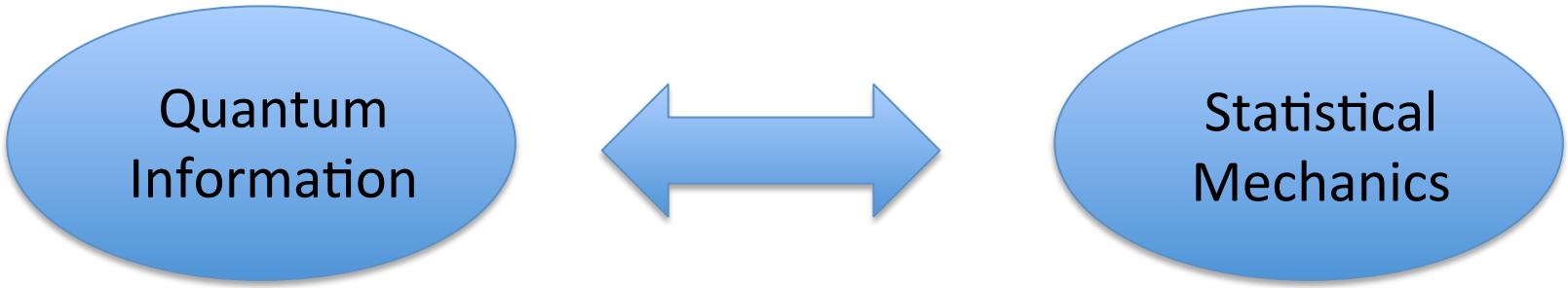
Quantum Information vs Quantum Statistical Mechanics



Ex.

- Microcanonical typicality vs measure concentration
- Thermodynamics as a resource theory
- Area laws and tensor networks for thermal states
- Generic thermalization vs quantum pseudo-randomness
- ....

Quantum Information vs Quantum Statistical Mechanics



Ex.

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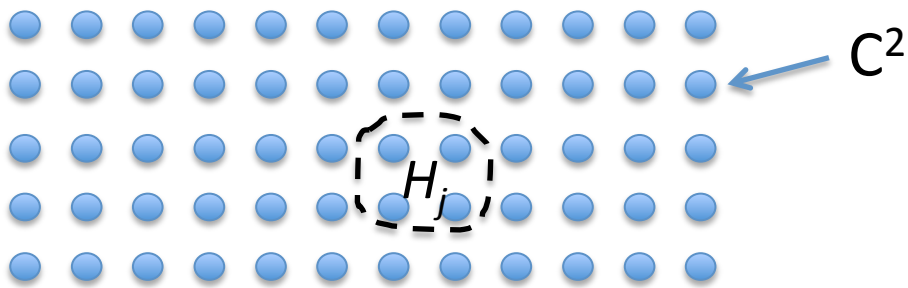
This talk: Equivalence of microcanonical and canonical ensembles for non-critical systems (using ideas from quantum information theory)

Microcanonical and Canonical Ensembles

Given a Hamiltonian of *n* particles :

$$H = \sum_j H_j = \sum_k E_k |E_k\rangle\langle E_k|$$



Microcanonical and Canonical Ensembles

Given a Hamiltonian of *n* particles :

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Microcanonical:

$$\langle X \rangle_{mc,e} := \mathrm{tr}(\tau_e X)$$

$$\tau_{e,\delta} := \frac{1}{|M_{e,\delta}|} \sum_{k \in M_{e,\delta}} |E_k\rangle\langle E_k|$$

$$M_{e,\delta} = \{k : |E_k - en| \leq \delta\sqrt{n}\}$$

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Canonical:

$$\langle X \rangle_{c,\beta} := \mathrm{tr}(\rho_\beta X)$$

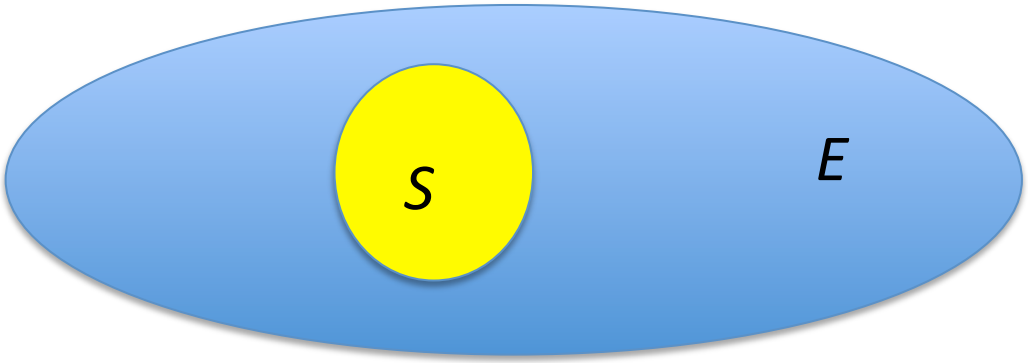
$$\rho_\beta := e^{-\beta H}/Z$$

Microcanonical and Canonical Ensembles

When should we use each?

Micro: System in isolation
Macro: System in equilibrium with a heat bath at temperature $1/\beta$

Can derive **macro** from **micro** by considering the *system* and *bath* in the microcanonical ensemble and looking at the reduced state of the system. Justified whenever the interactions of system and bath are very weak.

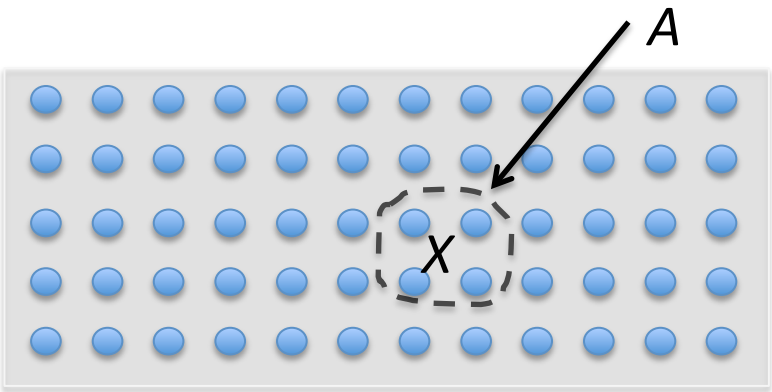


Microcanonical and Canonical Ensembles

When should we use each?

Micro: System in isolation
Macro: System in equilibrium with a heat bath at temperature 1/β

What if we are only interested in expectation values of local observables?



Is the system an environment for itself?

i.e. For every β, is $\langle X \rangle_{mc,e(\beta)} \approx \langle X \rangle_{c,\beta}$ for e(β) = tr(H ρ_β) ?

Previous Results

- Equivalence when *A* interacts weakly with A^c

$$H = H_A + H_{A^c} + \lambda H_I$$

(…, Goldstein, Lebowitz, Tumulka, Zanghi '06; Riera, Gogolin, Eisert '12)

Previous Results

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$$H = H_A + H_{A^c} + \lambda H_I$$

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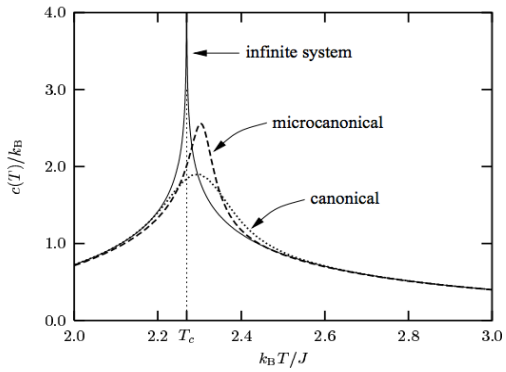
- Non-equivalence for critical systems
  (e.g. 2D Ising model log(n) sized region)

(Desermo '04)



- Equivalence for local observables in infinite lattices in the "unique phase region" (i.e. only one KMS state).

(requires translation invariance and gives no bounds on the size of *A*)

(…, Lima '72; Muller, Adlam, Masanes, Wiebe '13)

Equivalence of Ensembles for non-critical systems

Gibbs 1902: For the average square of the anomalies of the energy, we find an expression which vanishes in comparison to the square of the average energy, when the number of degrees of freedom is indefinitely increased. An ensemble of systems in which the number of degrees of freedom is of the same order of magnitude as the number of molecules in the bodies with which we experiment, if distributed canonically, would therefore appear to human observation as an ensemble of systems in which all have the same energy.

$$c(T) = \mathrm{var}(E) = O(n)$$

Fluctuations of energy of order $O(n^{1/2})$ only!

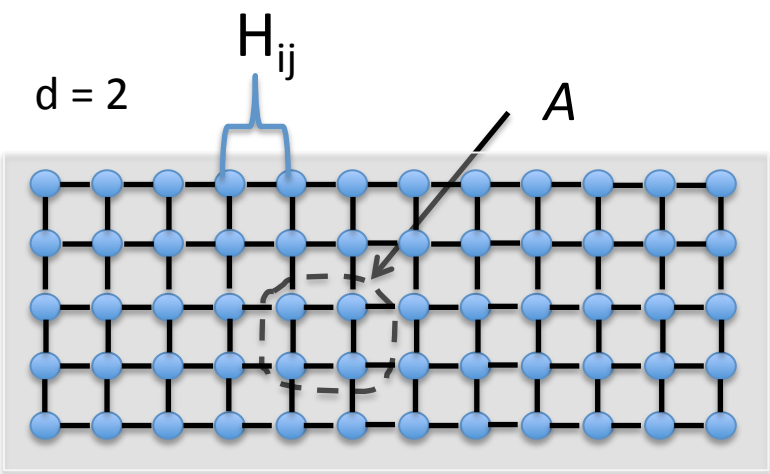
To simplistic, microcanonical and canonical states are almost orthogonal for large systems

Equivalence of Ensembles for non-critical systems

thm Let H be a Hamiltonian of n particles on a d-dimensional lattice. Let β be such that ρ_β has a correlation length ξ.

Then for most regions A of size at most $\left(\frac{n}{\log(n)}\right)^{1/d} \varepsilon^{2/d} \frac{1}{1+\xi}$

$$\left\| \mathrm{tr}_{A^c}\left(\tau_{e(\beta)}\right) - \mathrm{tr}_{A^c}\left(\rho_\beta\right) \right\|_1 \leq \varepsilon$$



Correlation length ξ: For all X, Z

$$\mathrm{cov}(X,Z)_{\rho_\beta} \leq 2^{-\mathrm{dist}(X,Z)/\xi}$$

$$\mathrm{cov}(X,Z)_{\rho_\beta} := \langle XZ \rangle_{\rho_\beta} - \langle X \rangle_{\rho_\beta} \langle Z \rangle_{\rho_\beta}$$

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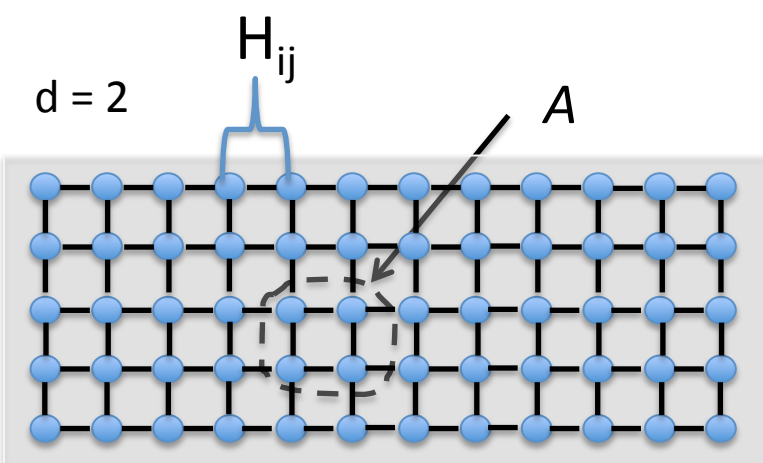


Obs1: Equivalent to

$$\langle X \rangle_{mc,e(\beta)} \approx \langle X \rangle_{c,\beta}$$

for all observables X in A

Obs2: For every H, ρ_β has finite ξ for β sufficiently small (Kliesch et al '13)

Obs3: All 1D H have finite ξ (Araki '69)

Strengthening of Theorem

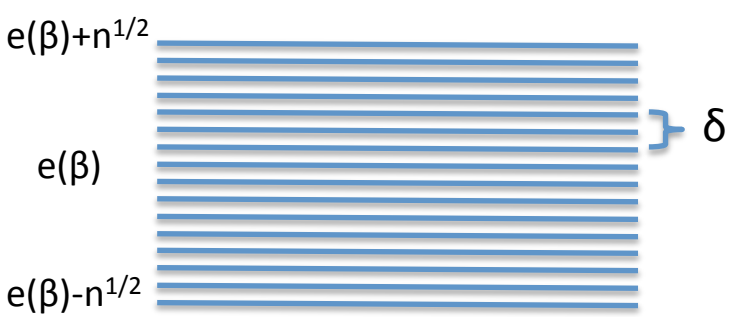
thm Let H be a Hamiltonian of n particles on a d-dimensional lattice. Let β be such that ρ_β has a correlation length ξ.

Let $m := \left(\frac{n}{\log(n)}\right)^{1/d^2} \left(\frac{1}{\xi}\right)^{1/d} \varepsilon^{2/d}, \quad \delta \geq \Omega\left(\frac{1}{\sqrt{n}}\right)$

and $e(\beta) - \sqrt{n} \leq \tilde{e} \leq e(\beta) + \sqrt{n}\,.$

Then for most regions A of size at most m^d

$$\left\| \mathrm{tr}\left(\tau_{\tilde{e},\delta}\right) - \mathrm{tr}\left(\rho_\beta\right) \right\|_1 \leq \varepsilon$$



Eigenstate Thermalization Hypothesis (Srednicki '94):

Same is true for δ = 0

False in general (e.g. many-body localization)

Why is it interesting?

- Works for non-translational invariant states
- It's based on finite correlation length (simpler than unique KMS state)
- It gives explicit finite size bounds
- Shows equivalence works even when energy spread is of order O(polylog(n))
- Covers more than microcanonical stat. Any state of concentrated energy and high entropy looks thermal locally.

Further Implications

(Popescu, Short, Winter '05; Goldstein, Lebowitz, Timulka, Zanghi '06, …)

Let H be a Hamiltonian and S_e the subspace of states with energy $(en-\delta n^{1/2}, en+\delta n^{1/2})$. Then for almost every state $|\psi\rangle$ in S_e, and region *A* sufficiently small,

$$\mathrm{tr}_{A^c}(|\psi\rangle\langle\psi|) \approx \mathrm{tr}_{A^c}(\tau_e)$$

Consequence: If $\rho_{\beta(e)}$ has finite correlation length,

$$\mathrm{tr}_{A^c}(|\psi\rangle\langle\psi|) \approx \mathrm{tr}_{A^c}(\tau_e) \approx \mathrm{tr}_{A^c}(\rho_{\beta(e)})$$

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(Kliesch, Gogolin, Kastoryano, Riera, Eisert '14) If $\rho_{\beta(e)}$ has finite correlation length,

$$\mathrm{tr}_{A^c}\left(\rho_{\beta(e)}\right) \approx \mathrm{tr}_{A^c}\left(\frac{e^{-\beta H_{A+\partial(A)}}}{Z_{A+\partial(A)}}\right)$$

Proof Structure

Part 1: Show that for every $|\tilde{e} - e(\beta)| \leq \sqrt{n}$: $\tau_{\tilde{e},\delta} \leq c \frac{e^{\beta\delta\sqrt{n}}}{\delta} \rho_\beta$

Use version of Berry-Esseen thm for energy measurement on Gibbs state with finite ξ (generalizing (Cramer '11, Mahler et al '03) from product states to states with finite ξ)

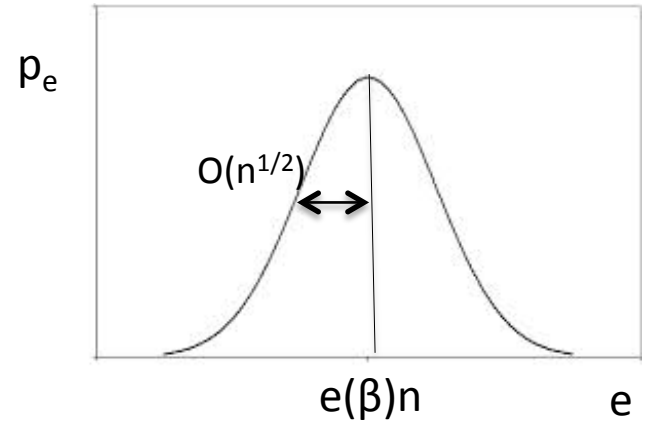
Part 2: Equation above implies $S(\tau_{\tilde{e},\delta} || \rho_\beta) \leq \log\left(c \frac{e^{\beta\delta\sqrt{n}}}{\delta}\right)$

Use basic properties of entropy/relative entropy (data processing, subadditivity, Pinsker's inequality, …) to obtain the result of the thm

Berry-Essen for States with Finite Correlation Length

Let $\rho_{e,\delta} := \frac{1}{Z_{e,\delta}} \sum_{k \in M_{e,\delta}} e^{-\beta E_k} |E_k\rangle\langle E_k|$

and $\rho_\beta = \sum_e p_e \rho_{e,\delta}$



Then for $|en - e(\beta)n| \leq n^{1/2}$, $p_e \geq \Omega(\delta)$

and so $\rho_{e,\delta} \leq O(1/\delta)\rho_\beta$

Since $\tau_{e,\delta} \leq e^{\beta\delta\sqrt{n}} \rho_{e,\delta}$, $\tau_{e,\delta} \leq O\left(\frac{e^{\beta\delta\sqrt{n}}}{\delta}\right)\rho_\beta$

By monotonicity of the log:

$$\boxed{S(\tau_{e,\delta}||\rho_\beta) \leq \log\left(\frac{e^{\beta\delta\sqrt{n}}}{\delta}\right)}$$

Entropy and Relative Entropy

Entropy: $S(\rho) := -\mathrm{tr}(\rho \log(\rho))$

Subaditivity: $S(\rho_{AB}) \leq S(\rho_A) + S(\rho_B)$

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Subaditivity: $S(\rho_{AB}) \leq S(\rho_A) + S(\rho_B)$

Relative Entropy: $S(\rho||\sigma) := \mathrm{tr}(\rho(\log \rho - \log \sigma))$

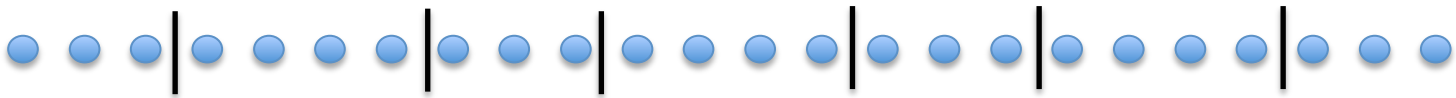
S(ρ || σ) measures the *distinguishability* of ρ and σ

Positivity: $S(\rho||\sigma) \geq 0$

Data Processing Inequality: $S(\rho_{AB}||\sigma_{AB}) \geq S(\rho_A||\sigma_A)$

Pinsker Ineq: $S(\rho||\sigma) \leq \varepsilon \implies \|\rho - \sigma\|_1 \leq O(\varepsilon^{1/2})$

Part 2: Proof I



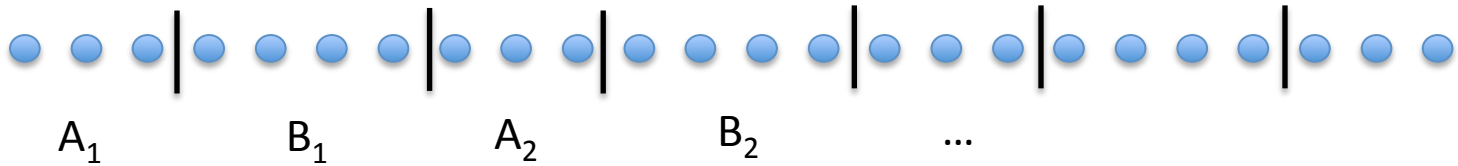
A_1 B_1 A_2 B_2 …

size(A_i) = $n\varepsilon^2/\log(n)$, size(B_i) = $10\xi n\varepsilon^2/\log(n)$

Let $\delta = 1/n^{1/2}$.

$$S(\tau_{\tilde{e},\delta}||\rho_\beta) \leq \log\left(c\frac{e^{\beta\delta\sqrt{n}}}{\delta}\right) \leq 2\log(n)$$

Part 2: Proof II



size(A_i) = $n\varepsilon^2/\log(n)$, size(B_i) = $10\xi n\varepsilon^2/\log(n)$

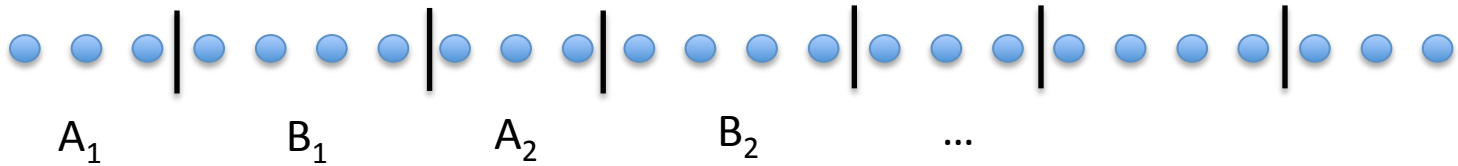
$$\tau_{e',\delta} = \tau_{A_1 B_1 A_2 B_2 \ldots A_m B_m} \qquad \rho_\beta = \rho_{A_1 B_1 A_2 B_2 \ldots A_m B_m}$$

$$S(\tau_{A_1 A_2 \ldots A_m} || \rho_{A_1 A_2 \ldots A_m}) \leq S(\tau_{A_1 B_1 \ldots A_m B_m} || \rho_{A_1 B_1 \ldots A_m B_m}) \leq 2\log(n)$$

data processing

previous slide

Part 2: Proof II



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data processing

previous slide

Claim 1: Correlation length ξ implies:

$$\|\rho_{A_1 \ldots A_m} - \rho_{A_1} \otimes \ldots \otimes \rho_{A_m}\|_1 \leq O\left(\frac{n}{m}\right) e^{-n/\log(n)}$$

Claim 2:

$$S(\tau_{A_1 \ldots A_m} || \rho_{A_1} \otimes \ldots \otimes \rho_{A_m}) \leq 3\log(n)$$

Part 2: Proof II

A_1

$$\tau_{e',\delta} = \tau_{A}$$

$$S(\tau_{A_1 A_2 \ldots A_m} ||$$

dat

Claim 1: Correla

$$\|\rho_{A_1 \ldots A_m} - \ldots \otimes \rho_{A_m}\|_1 \leq O\left(\frac{n}{m}\right) e^{-n/\log(n)}$$

$$\tau_{A_1 \ldots A_m} \leq 2n\rho_{A_1} \otimes \ldots \rho_{A_m} + X_n$$

$$\|X_n\|_1 \leq cnO\left(\frac{n}{m}\right) e^{-n\log(n)} =: \nu$$

By (Datta, Renner '08)

$$\tilde{\tau}_{A_1 \ldots A_m} \leq 2n\rho_{A_1} \otimes \ldots \otimes \rho_{A_m}$$

$$\|\tilde{\tau}_{A_1 \ldots A_m} - \tau_{A_1 \ldots A_m}\|_1 \leq 2\sqrt{\nu}$$

Claim 2:

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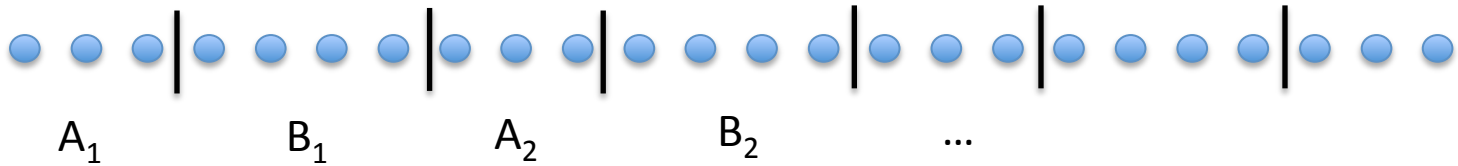
Part 2: Proof III



size(A_i) = $n\varepsilon^2/\log(n)$, size(B_i) = $10\xi n\varepsilon^2/\log(n)$

To finish

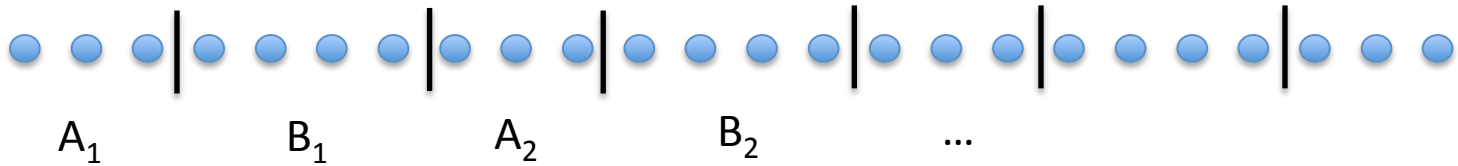
$$\sum_{i=1}^{m} S(\tau_{A_i}||\rho_{A_i}) \leq S(\tau_{A_1\ldots A_m}||\rho_{A_1}\otimes\ldots\otimes\rho_{A_m}) \leq 3\log(n)$$

subadditivity entropy

previous slide

$$\begin{aligned}\sum_{i=1}^{m} S(\tau_{A_i}||\rho_{A_i}) &= -\sum_{i=1}^{m} S(\rho_{A_i}) - \sum_{i=1}^{m}\log(\tau_{A_i}\log\rho_{A_i}) \\ &\leq -S(\tau_{A_1\ldots A_m}) - \log(\tau_{A_1\ldots A_m}\log(\rho_{A_1}\otimes\ldots\otimes\rho_{A_m}))\end{aligned}$$

Part 2: Proof III



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To finish

$$\sum_{i=1}^{m} S(\tau_{A_i}||\rho_{A_i}) \leq S(\tau_{A_1\ldots A_m}||\rho_{A_1}\otimes\ldots\otimes\rho_{A_m}) \leq 3\log(n)$$

subadditivity entropy

previous slide

Since m = log(n)/(1 + 10ξ): $\mathbb{E}_i S(\tau_{A_i}||\rho_{A_i}) \leq \dfrac{3\log(n)}{m} \leq O(\varepsilon^2)$

By Pinsker's inequality: $\boxed{\mathbb{E}_i \|\tau_{A_i} - \rho_{A_i}\|_1 \leq O(\varepsilon)}$

Conclusions

Quantum Information theory provides new tools for studying thermalization/equilibration and poses new questions about them.

The talk gave an example:
Info-theoretical proof of equivalence of ensembles for non-critical systems.

Open Questions:
How small can δ be?

What can we say about critical systems for regions smaller than log(n)?

Thanks!