







Total correlations of the diagonal ensemble herald the many-body localization transition

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The intriguing phenomenon of many-body localization (MBL) has attracted significant interest recently, but a complete characterization is still lacking. We introduce the total correlations, a concept from quantum information theory capturing multi-partite correlations, to the study of this phenomenon. We demonstrate that the total correlations of the diagonal ensemble provides a meaningful diagnostic tool to pin-down, probe, and better understand the MBL transition and ergodicity breaking in quantum systems. In particular we show that the total correlations has sub-linear dependence on the system size in delocalized, ergodic phases, whereas we find that it scales extensively in the localized phase developing a pronounced peak at the transition.

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The total correlations

■ Definition: Consider an *N*-partite system, then

$$T(
ho) \coloneqq \sum_{m=1}^{N} S(
ho_m) - S(
ho).$$

Where $S(\rho) := -\text{tr}(\rho \log_2 \rho)$ is the von Neumann entropy.

Intuition: Measures distinguishability from product state:

$$T(
ho) = \min_{\pi \text{ product state}} S(
ho \| \pi)$$

Where $S(\rho \| \sigma) := -\text{tr}(\rho \log_2 \sigma) - S(\rho) \ge \|\rho - \sigma\|_1^2/2$ is the relative entropy.

Ergodicity

- Starting point:
 - Ergodic Hypothesis: ergodic ⇔ systems explore phase space uniformly ⇒ infinite time average = microcanonical average Essentially impossible in QM hence ask for less:
- Definition (in words):

A pair of Hamiltonian and initial state is ergodic (as oppose to MBL) if it explores at least a constant fraction of the available Hilbert space.

Quantify: For a fixed initial state ρ and non-degenerate Hamiltonian H define the dephased or time-averaged state (diagonal ensemble)

$$\omega \coloneqq \sum_{n} |E_n\rangle\langle E_n|\, \rho\, |E_n\rangle\langle E_n| = \lim_{ au o \infty} \frac{1}{ au} \int_0^ au dt \, \mathrm{e}^{-itH} \, \rho \, \mathrm{e}^{itH},$$

with $|E_n\rangle$ eigenvectors of H.

A family of systems of increasing size N is ergodic if $\exists \lambda > 0$ such that for most product initial states from some subspace (i.e., fixed magnetization) of dimension d it holds (with high probability over the disorder average)

$$S(\omega) \ge \log_2(\lambda d)$$

Scaling of T with N

Non-ergodic: As $T(\omega)$ involves the sum $\sum_{m=1}^{N} S(\omega_m)$ of the N subsystem entropies:

$$T(\omega) \propto N$$

■ Ergodic: If a family of disordered systems is ergodic however, then $\exists \lambda > 0$ such that for most product initial states with high probability

$$T(\omega) \leq \sum_{m=1}^{N} S(\omega_m) - \log_2(\lambda d).$$

For a spin-1/2 chain the magentization zero subspace has $d = {N \choose N/2} = N! / \left(\frac{N}{2}!\right)^2 \ge \sqrt{8\pi} \, \mathrm{e}^{-2} \, 2^N / \sqrt{N}$ and $S(\omega_m) \le \log_2 2 = 1$, so that

$$T(\omega) \leq \log_2(N)/2 - \log_2(\lambda \sqrt{8\pi} e^{-2}).$$

Intuition: Transport in ergodic systems makes parts so mixed that their distinguishability from the closest product state only grows logarithmically.

Heisenberg spin-1/2 chain . . .

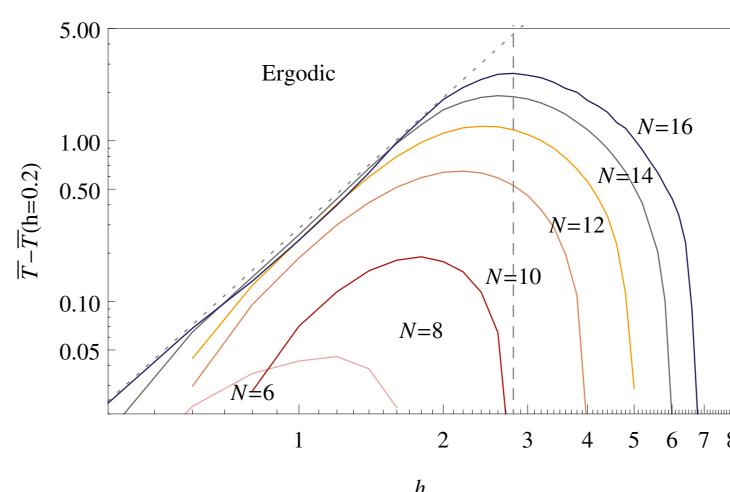
... of N sites with coupling constants J, J_{zz} and disorder strenght h:

$$H = \sum_{i=1}^{N} \left[J\left(\sigma_x^i \sigma_x^{i+1} + \sigma_y^i \sigma_y^{i+1}\right) + J_{zz} \sigma_z^i \sigma_z^{i+1} + h_i \sigma_z^i \right]$$

Where we set $J = J_{zz} = 1$ and take $h_i \in [-h, h]$ uniformly distributed. Then it has a MBL transition at $h = h_c \in [2, 4]$ [1].

Numerical results

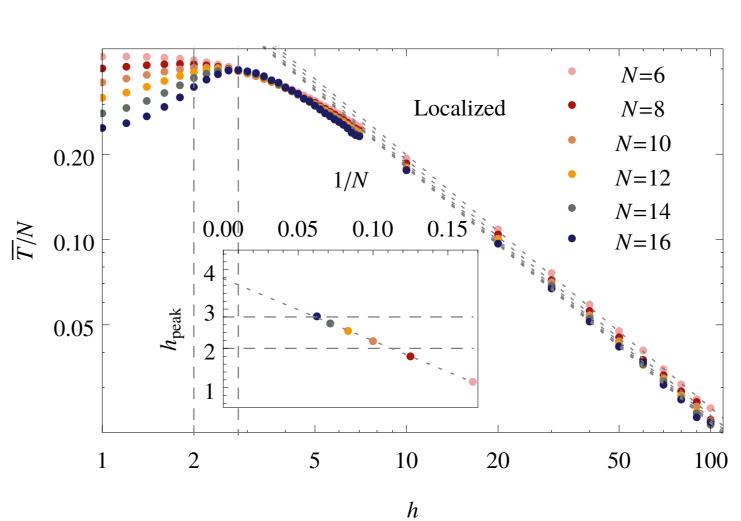
- Restrict to zero magnetization subspace
- **2** For product initial states compupte $T(\omega)$.
- lacksquare Average over all initial states and disorder $o \overline{T}(\omega)$.



non-ergodic $\propto N$ $\longrightarrow h = 4$ $h \approx 0$ contact contact

Figure 1: Initial increase for small *h* is power-law like with exponent 2.7(2). The deviation maks beginning of the MBL transition

Figure 3: For small *h* we see logarithmic growth, as expected in an ergodic system, and at large *h* linear growth.



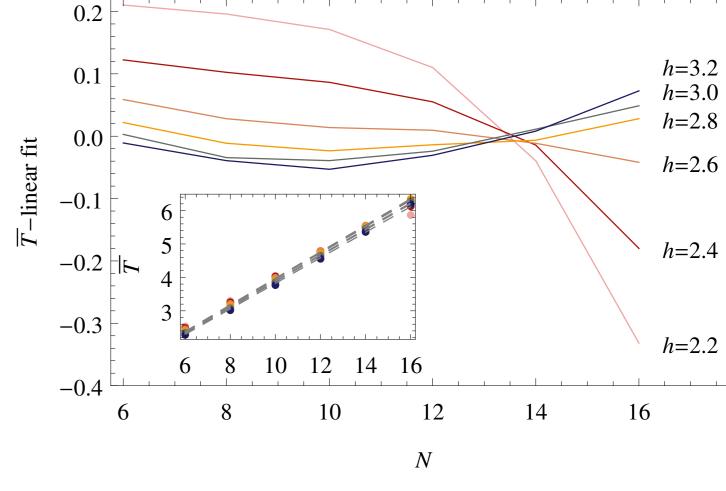


Figure 2: For high h, \overline{T} decays as a power-law with exponents of -0.9(1). Inset shows position of peaks in Figure 1.

Figure 4: Difference between \overline{T} and best possible linear fit for different values of h. Crossover from a nearly linear scaling to a sub-linear scaling happens at h=2.6(2) (robust against omitting data points and holds also for affine fits). The inset shows raw data.

Conclusions

region.

- Total correlations in the diagonal ensemble signal the MBL transition
- They expose how this transition involves reorganization of correlations
- Results suggests two step transition in line with [2, 3, 4]

