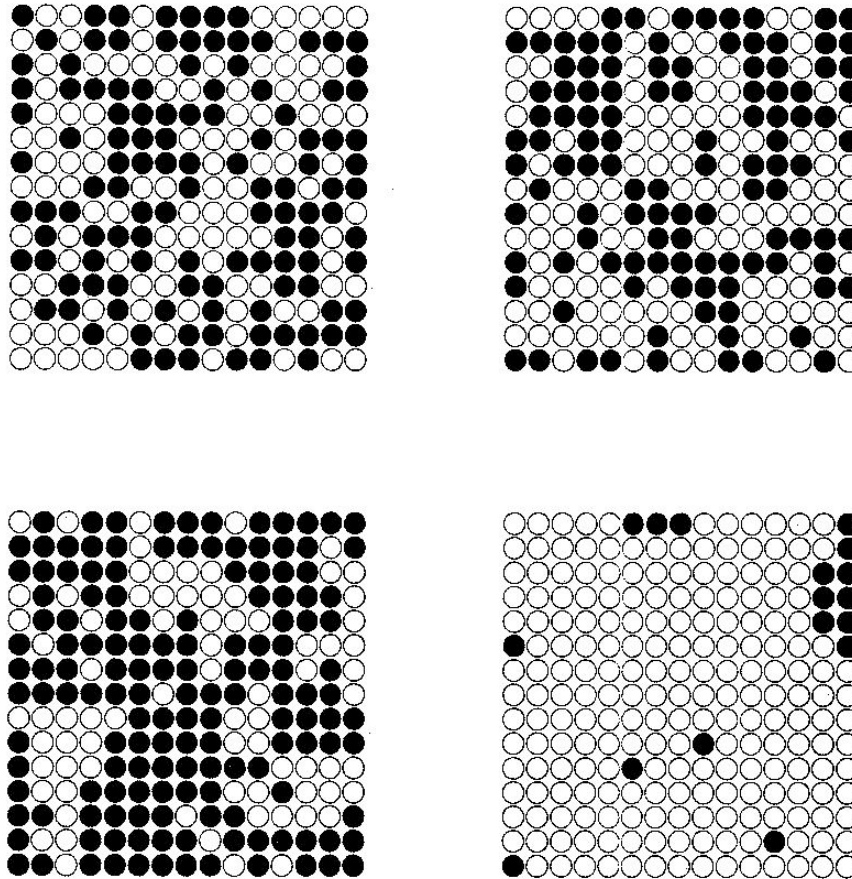


Typical quantum states at finite temperature

- How should one think about “typical quantum states” at finite temperature?
 - Density Matrices versus pure states
 - Why eigenstates are not “typical”
 - Measuring the heat bath to get a pure state
- Ancilla/Purification methods for finite T (DMRG)
- Typical States: properties and examples
- Bypassing ancilla for more efficient finite T calcs
- Real time evolution and entropy growth

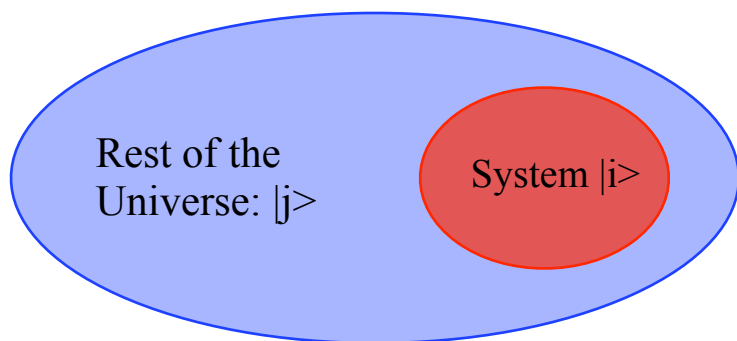
Typical states for the Ising model



- Ising model: classical state = eigenstate = typical state
- Heisenberg model: classical state has high energy, not typical of low T . At $T=0$, typical state should be ground state

What is a typical state at finite T?

- Pure states versus mixed states



$$|\psi\rangle = \sum_{ij} \psi_{ij} |i\rangle |j\rangle$$

$$\rho_{ii'} = \sum_j \psi_{ij}^* \psi_{i'j}$$

$$\langle A \rangle = \sum_{\alpha} w_{\alpha} \langle \alpha | A | \alpha \rangle$$

- Mixed state: think of a set of states $|\alpha\rangle$ with probability w_{α} , or just use ρ .
- Key principle of statistical mechanics: $\rho = e^{-\beta H}$

How does $\rho = e^{-\beta H}$ arise?

- Purely by quantum entanglement with a heat bath
 - Under idealized assumptions, recent work has shown $e^{-\beta H}$ arises naturally (see, e.g., P. Reimann, PRL 101, 190403 (2008))
 - Infinite size heat bath
 - Infinitesimal interaction for infinite time
 - **No decoherence**

- An ensemble of pure states $|i\rangle$, probs $P(i)$

$$\rho = \sum_i P(i) |i\rangle \langle i|$$

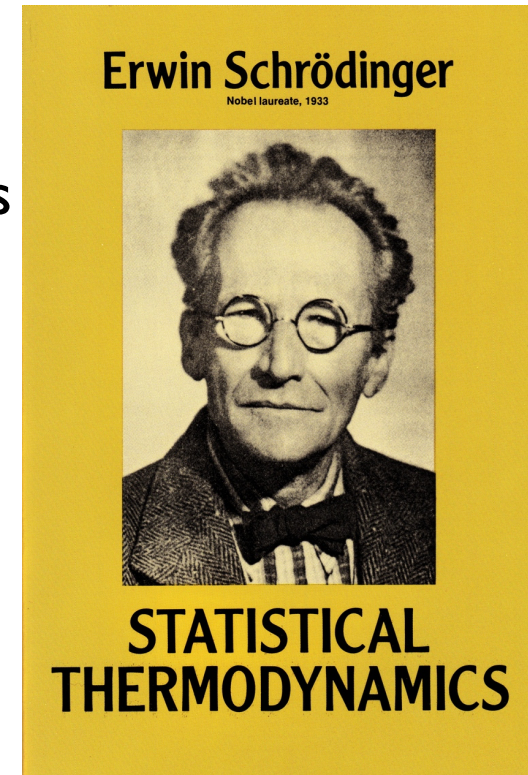


- Just because you can write this and get the right ρ doesn't mean the $|i\rangle$ are typical!

- An ensemble of slightly mixed states $\rho = \sum_i \rho_i$

Energy eigenstates as typical states

- Is an eigenstate of H a typical finite T state?
 - Schrodinger: “...the attitude is altogether wrong.”
 - “this assumption is irreconcilable with the very foundations of quantum mechanics”
 - “We yet decided to adopt it ... very convenient ... same results ...”
 - Modern textbooks: skip the warnings, sweep it under the rug
- Why is it so wrong?
 - No mechanism in thermalization to go to a definite eigenstate (heat bath or “ergodic” time evolution)
 - Level spacing is exponentially small, would take exponentially long to get to one eigenstate ($\exp(-10^{23})...$)
 - Exponentially small spacings mean even tiny perturbations (e.g. coupling to vacuum E&M fields) completely change states-- Exact highly excited eigenstates physically meaningless



(1946, 1952)

measurement and Measurement

- measurement, theoretical or numerical: calculate $\langle \psi | S_z | \psi \rangle$
 - Nothing happens to $|\psi\rangle$
- Physical Measurement:
$$|\psi\rangle \rightarrow \begin{cases} P(\uparrow)^{-\frac{1}{2}} |\uparrow\rangle \langle \uparrow | \psi \rangle & \text{prob } P(\uparrow) \\ P(\downarrow)^{-\frac{1}{2}} |\downarrow\rangle \langle \downarrow | \psi \rangle & \text{prob } P(\downarrow) \end{cases} \quad P(\uparrow) = \langle S_z \rangle + \frac{1}{2}$$
 - wavefunction projected into measured state,
- Decoherence: think of continual slight Measurement of each spin (mostly local)
 - Rapidly destroys non-local entanglement
 - Stronger at higher T
 - Nearly unavoidable
 - Classical states most robust against decoherence

Preparation of a pure typical state

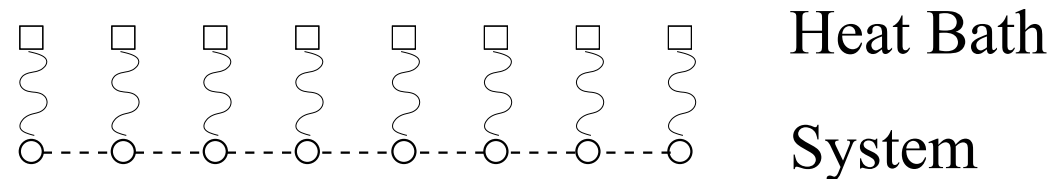
- Couple system to a heat bath, wait ...
- Gradually eliminate coupling. Even with no coupling, system still entangled with heat bath
- Induce strong decoherence/measurement on heat bath, putting heat bath and system into pure states
- I will show: equilibrium props of system not damaged by Measurement on heat bath
- Local Measurement induces maximally classical typical states
- The states are robust against decoherence, intuitive, and computational convenient!

Perfect Heat Bath for current finite T DMRG

Ancilla and finite temperature (Purification approach)

DMRG gets its efficiency because the basis is specialized for the state. Infinite temperature seems infinitely hard from this point of view.

Ancilla are artificial auxiliary sites paired with the real sites.



They can make a perfect heat bath (Suzuki, ..., [Verstraete and Cirac](#)). Let the state of each site-ancilla pair be a perfectly entangled state

$$|E_i\rangle = \sum_s |s\rangle |s\rangle_a$$

Then

$$|\psi\rangle = \prod_i |E_i\rangle$$

is a perfect representation of the $T = \infty$ ensemble, but requires a local DMRG basis of size $m = 1$!

Evolve in imaginary time to get $|\psi(t)\rangle = \exp(-\beta H/2)|\psi\rangle$, then any finite temperature

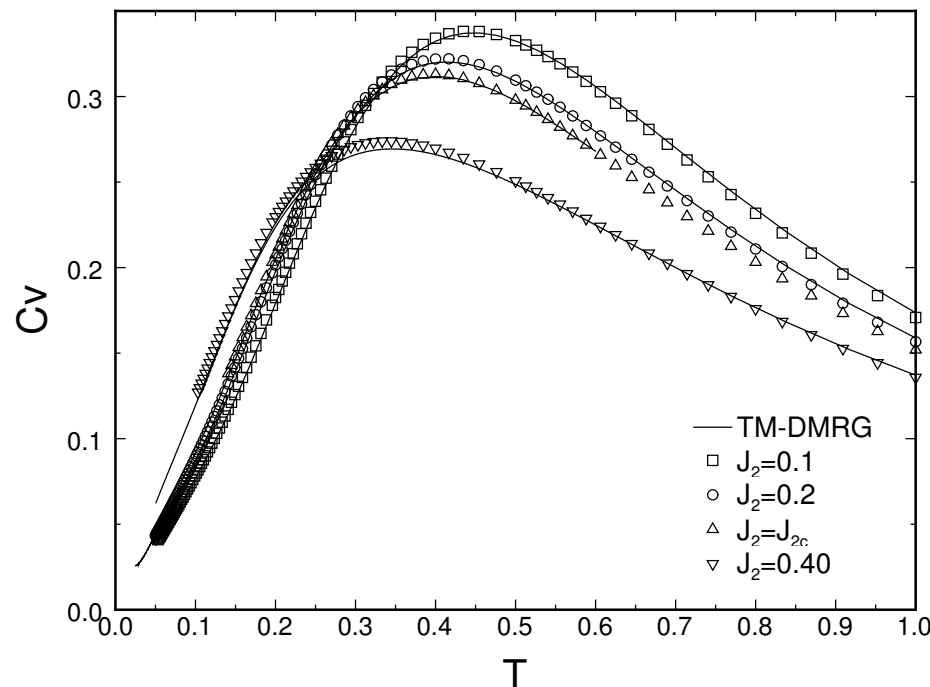
β observable can be obtained:

$$\langle A \rangle = \frac{\langle \psi(t) | A | \psi(t) \rangle}{\langle \psi(t) | \psi(t) \rangle}$$

The partition function, free energy, C_v , etc, as well as real-time finite temperature dynamics are easily obtained.

$J_1 - J_2$ model at finite temperature

Feiguin & White, PRB 72, 220401 (2005)



Difficulty at low T:

- 1) Long time evolution to $1/T$
- 2) At $T=0$, two copies of g.s, interspersed. Entanglement entropy doubled, $m \rightarrow m^2$

Typical states from perfect heat bath

$$|\psi(\beta = 0)\rangle = \sum_{i_1} \dots \sum_{i_N} |i_1\rangle_A |i_1\rangle_B \dots |i_N\rangle_A |i_N\rangle_B$$

$$|\psi(\beta)\rangle = \exp(-\beta H/2) |\psi(0)\rangle \quad \text{Tr}_B |\psi(\beta)\rangle \langle \psi(\beta)| = \exp(-\beta H)$$

- **Now Measure entire state i of B (same $P(i)$ as for A)**

$$P(i) = \langle i | \exp(-\beta H) | i \rangle$$

- **After Measurement,**

$$|i\rangle_B \langle i|_B \psi(\beta)\rangle = |i\rangle_B \exp(-\beta H/2) |i\rangle_A$$

- **Conclusion: Typical state is**

$$|\phi(i)\rangle = P(i)^{-1/2} \exp(-\beta H/2) |i\rangle$$

- **Local spin config i chosen by** $P(i) = \langle i | \exp(-\beta H) | i \rangle$

First Recipe for generating typical states

- Do heat bath/ancilla DMRG to get $|\psi(\beta)\rangle$
- Perform a Measurement of all ancilla to get spin configuration i (Monte Carlo through QM Measurement)
- Resulting state of system is typical state

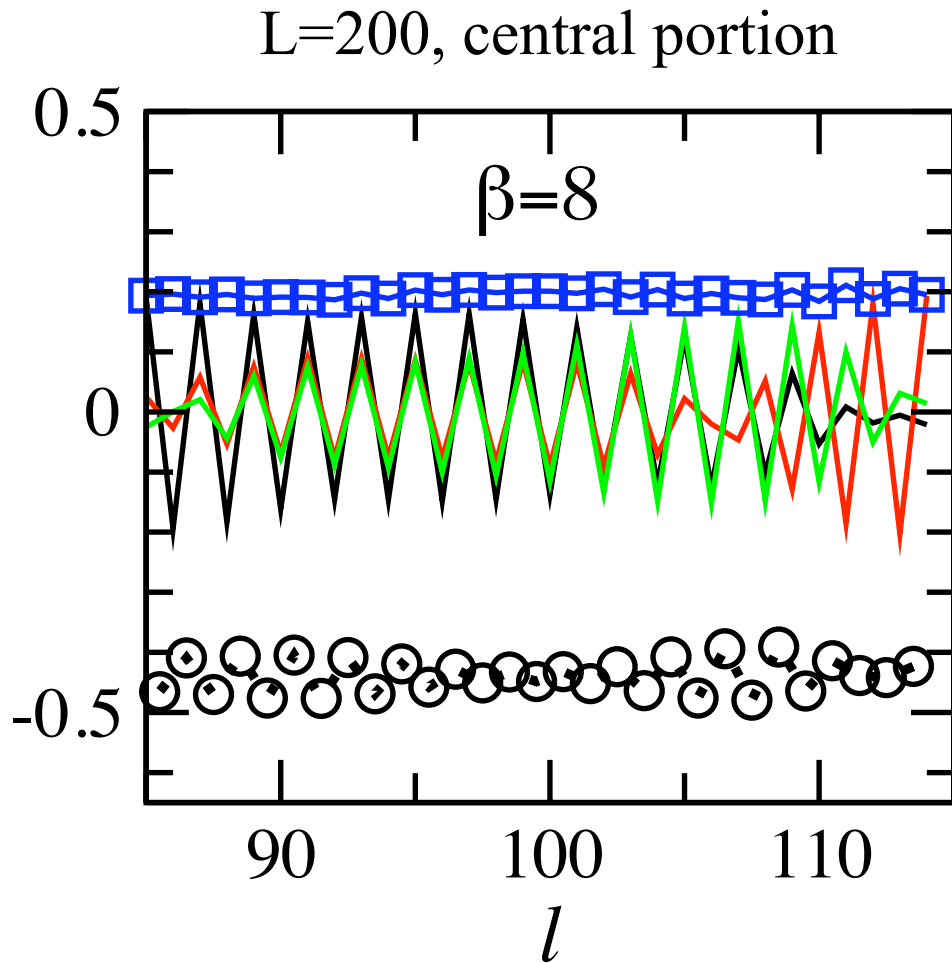
$$|\phi(i)\rangle = P(i)^{-1/2} \exp(-\beta H/2) |i\rangle$$

with $P(i) = \langle i | \exp(-\beta H) | i \rangle$

- Repeat Measurement to get as many typical states as desired with little effort
- Correct density matrix, ensemble averages

$$\langle O \rangle_\phi = \sum_i P(i) \langle \phi(i) | O | \phi(i) \rangle = \text{Tr}\{e^{-\beta H} O\}$$

Typical States for Heisenberg Chains



Orientation for each Measurement on a site chosen at random

$$(\langle \vec{S}_x \rangle^2 + \langle \vec{S}_y \rangle^2 + \langle \vec{S}_z \rangle^2)^{1/2} \equiv \tilde{S}$$

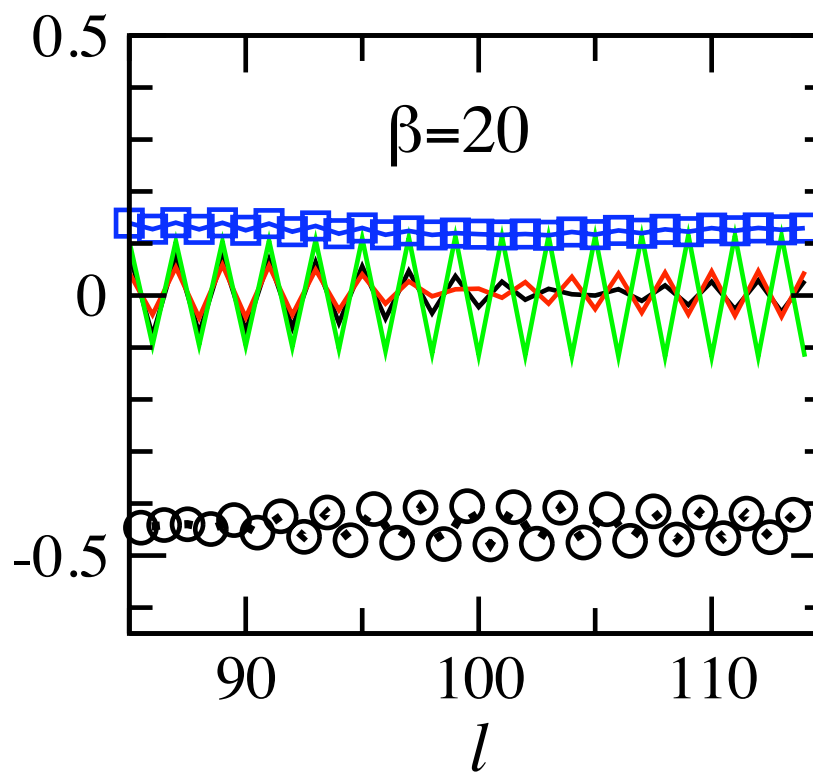
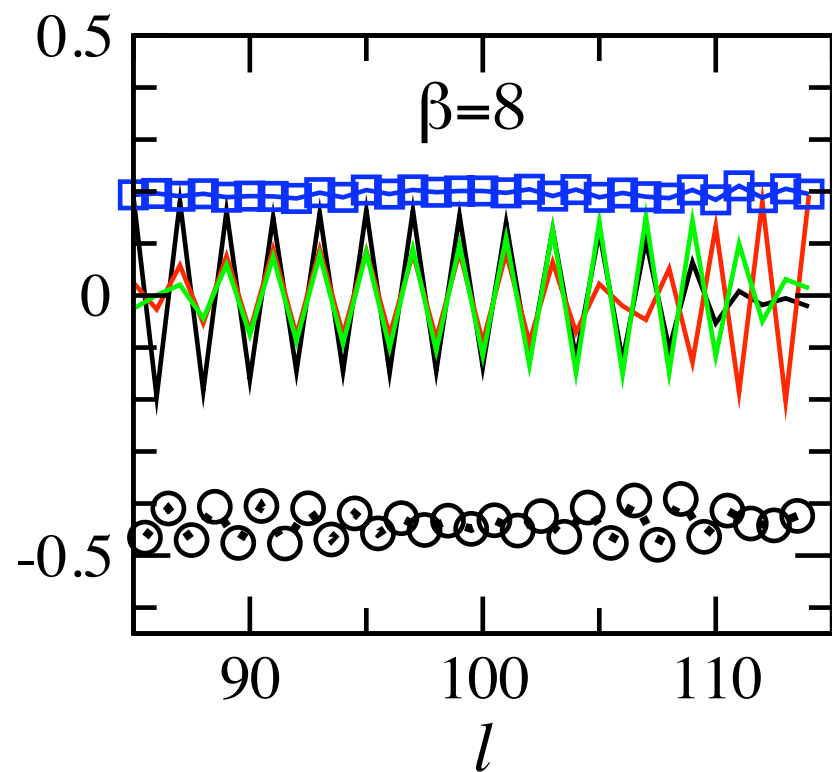
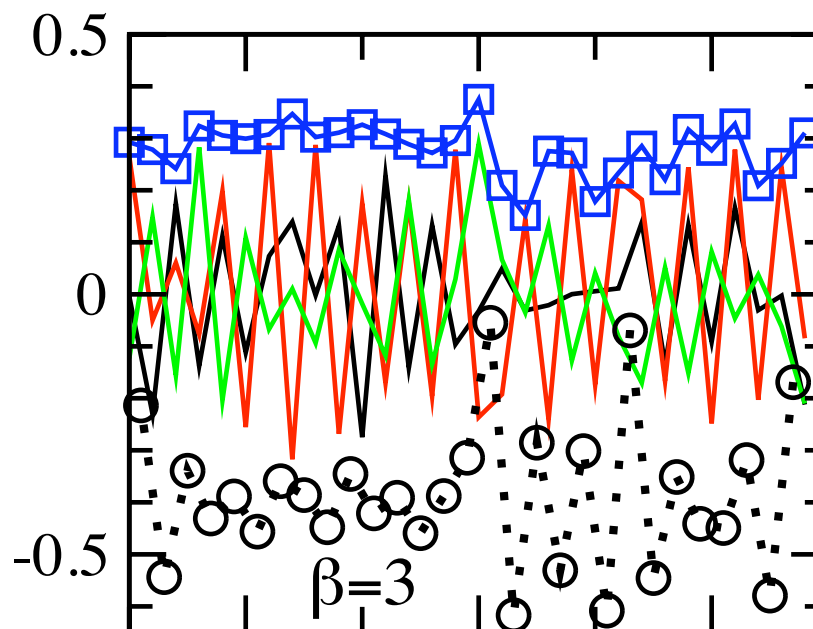
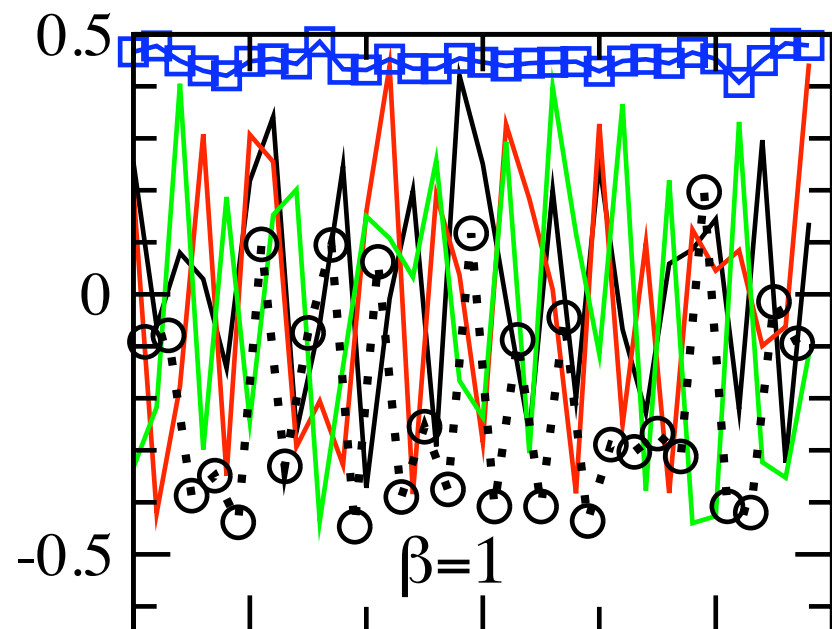
$$\langle \vec{S}_x \rangle, \langle \vec{S}_y \rangle, \langle \vec{S}_z \rangle$$

$$\langle \vec{S} \cdot \vec{S} \rangle \quad \text{on each bond}$$

For an unentangled spin in any state, \tilde{S} is 1/2. It provides a good measure of how classical a spin is.

The primary origin of the finite correlation length appears to be twisting of the order parameter--dimerization is slight.

Typical States for Heisenberg Chains



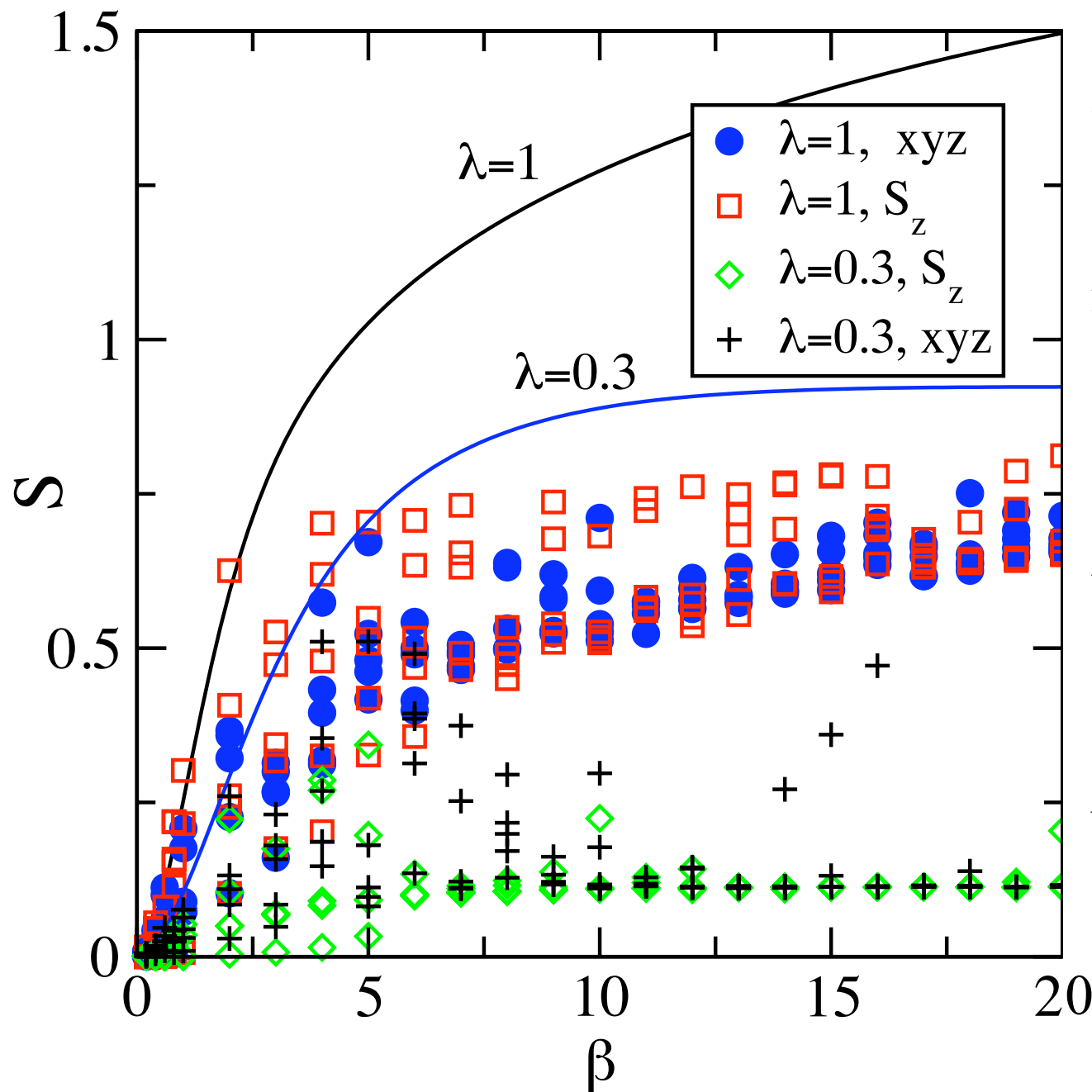
Second Recipe for generating typical states

- No heat bath/ancilla
- Generate a purely random classical spin configuration i
- * Evolve $|i\rangle$ in imaginary time to $\beta/2$
- Measure all the spins using any set of local operators to get a new spin configuration $|i\rangle$
- Go to *
- After an equilibration period, just before Measurement you have a typical state
- Advantages: no ancilla to evolve; no doubling of the entropy at low temperatures
- Equilibration and correlation time seems to be very short, fluctuations small, but still need MC averaging

Entanglement entropy, XXZ chains midpoint

$$H = \sum_{\ell} S_{\ell}^z S_{\ell+1}^z + \lambda(S_{\ell}^x S_{\ell+1}^x + S_{\ell}^y S_{\ell+1}^y)$$

L=200



Solid lines: heat bath/ancilla method

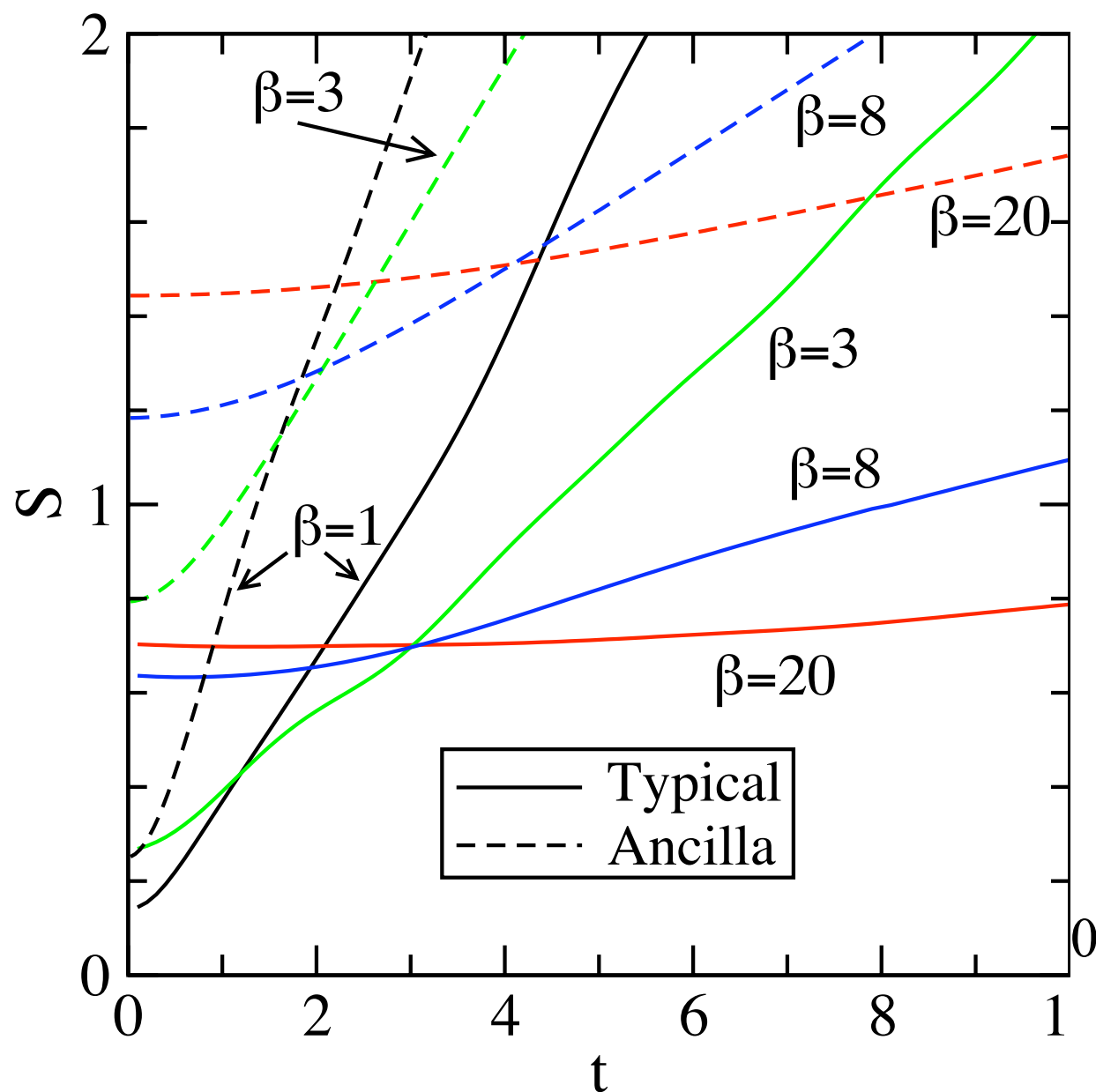
xyz: Measurements at random angles

Sz: Measurements in z dir

Heisenberg: xyz slightly better

Near-Ising: Sz preferred

Real time evolution, growth of entanglement



$L=40$ Heisenberg

Entanglement entropy
measured in center

Systems rapidly evolve away
from the classical regime to
highly entangled states

Entanglement grows much
faster at higher temperatures,
as seen earlier in ancilla
method

Decoherence would drive
them back towards classical
regime

Physical Consequences

- Maybe None:
 - No cloning theorem means the only way we can find out the wavefunction of a system is if we can create the same state repeatedly by identical preparation
 - Thermal states are inherently unrepeatable
 - Experimental predictions give standard stat mech
- Theoretical and computational consequences
 - Hopefully new insight into system properties
 - Easier approach to finite T in hard systems, e.g. 2D