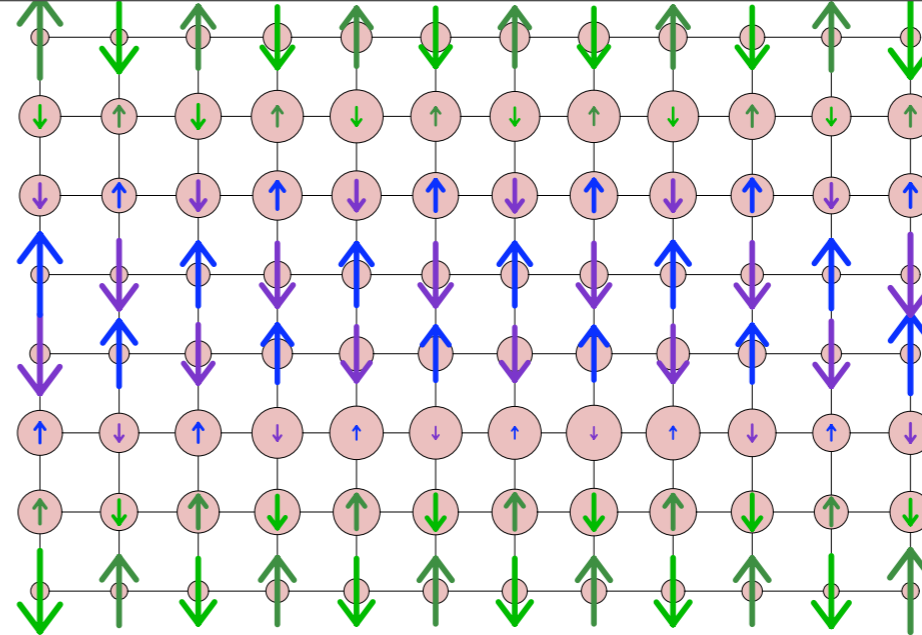


DMRG results you've seen:



White &
Scalapino

What some of you have noticed: (a) in 1D, excellent dynamics [e.g. Pereira, White, Affleck, key advance in real-time evolution by Vidal (QI)]
(b) In 1D, finite temperature (two methods: transfer matrix DMRG; direct calculation of thermodynamic density matrix (QI))

What you haven't seen: DMRG on 2D clusters with dynamics or finite temperature (computational efficiency)

Rest of talk: can we do finite temperature for 2D clusters? YES

Key question (old): What is a typical wavefunction of a quantum system at finite T?

--Much more efficient algorithm for finite T DMRG

--Highly intuitive (“semiclassical”) results in an exact framework

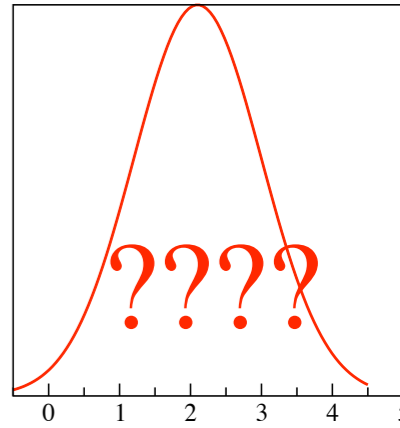
Minimally entangled typical thermal states

Physics Viewpoint: <http://physics.aps.org/articles/v2/39> (May 11) & PRL

- “Typical quantum states” at finite temperature
 - What are typical states?
 - Why energy eigenstates are a poor choice
- METTS: typical wavefunctions which are as classical as possible
- Examples for Heisenberg spin systems
 - 1D
 - 2 leg ladders
 - Square lattice
 - Kagome lattice

“Typical”

- Example of usefulness of typical versus averages: average number of kids per family in US: 2.1 ± 0.9
- Generically: want $|x\rangle$ with $P(x)$, choose $|x\rangle$ at random
 - If $|x\rangle$ not chosen from whole space (e.g. only people in phone book) want no “atypical”, “biased” characteristics
 - Expect statistics to duplicate whole space
- Typical wavefunctions $|\phi(i)\rangle$ at finite T (pure, not mixed):
 - Expect usual, correct statistical mechanics from unweighted averages over typical states



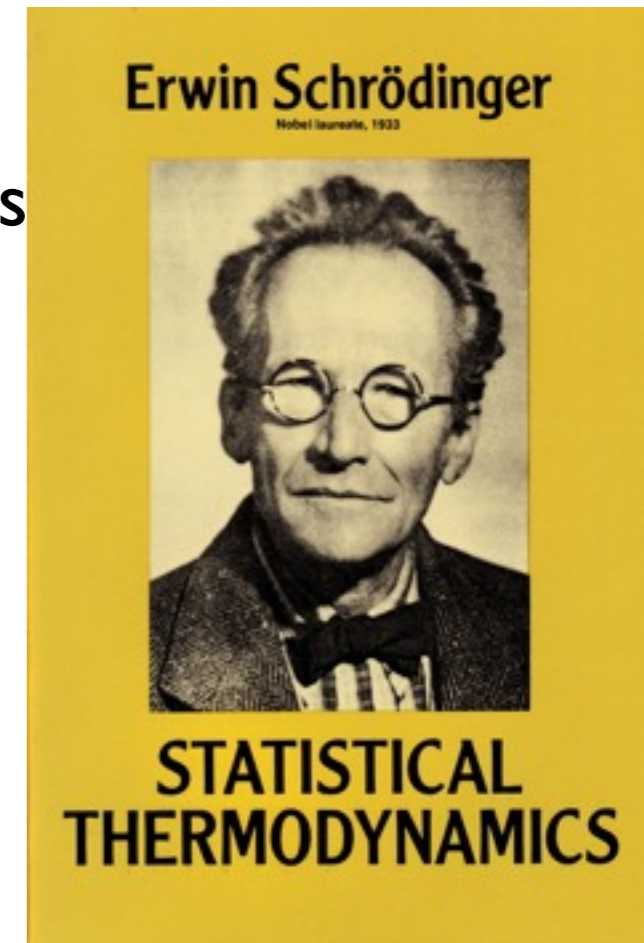
$$\langle A \rangle_{SM} = \sum_i P(i) \langle \phi(i) | A | \phi(i) \rangle$$

- This holds if $\sum_i P(i) |\phi(i)\rangle \langle \phi(i)| = e^{-\beta H}$
- At $T=0$, the typical wavefunction should be the ground state!
- Introductory SM textbook answer: energy eigenstates are typical!

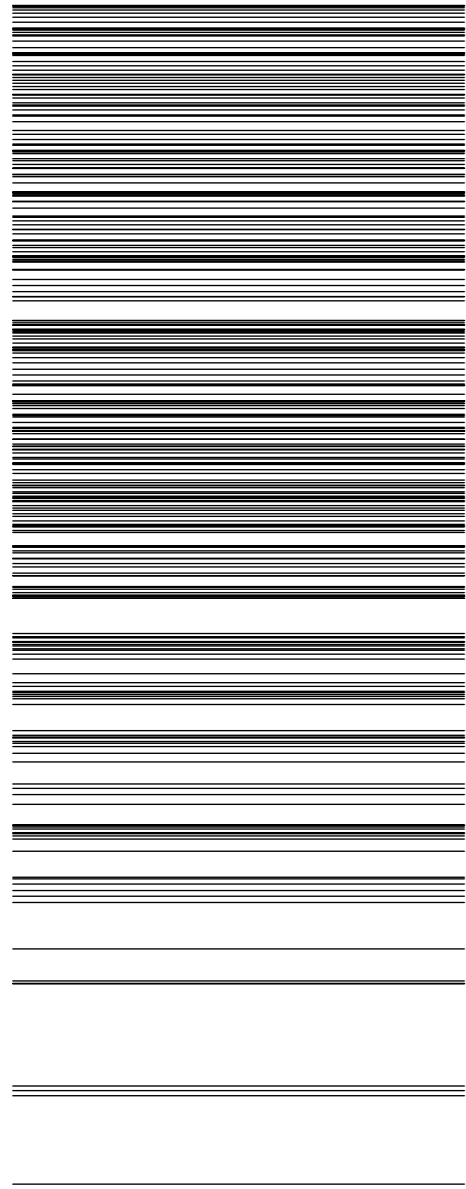
$(0,0,0,0,0,1,0,0,0,\dots)$ versus $(0.3742,-0.43838,0.04172,-0.14499-0.2377i,\dots)$

Energy eigenstates as typical states

- Is an eigenstate of H a typical finite T state?
 - Schrödinger: “...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 subtle questions under the rug
- Why is it so wrong? (eigenstates = senators)
 - 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

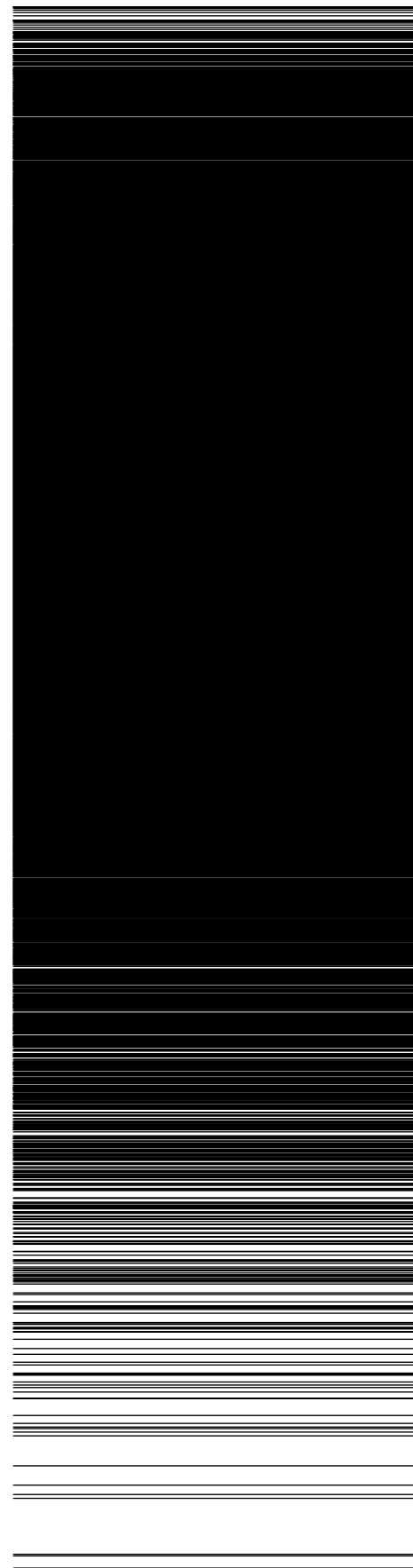


(1946, 1952)



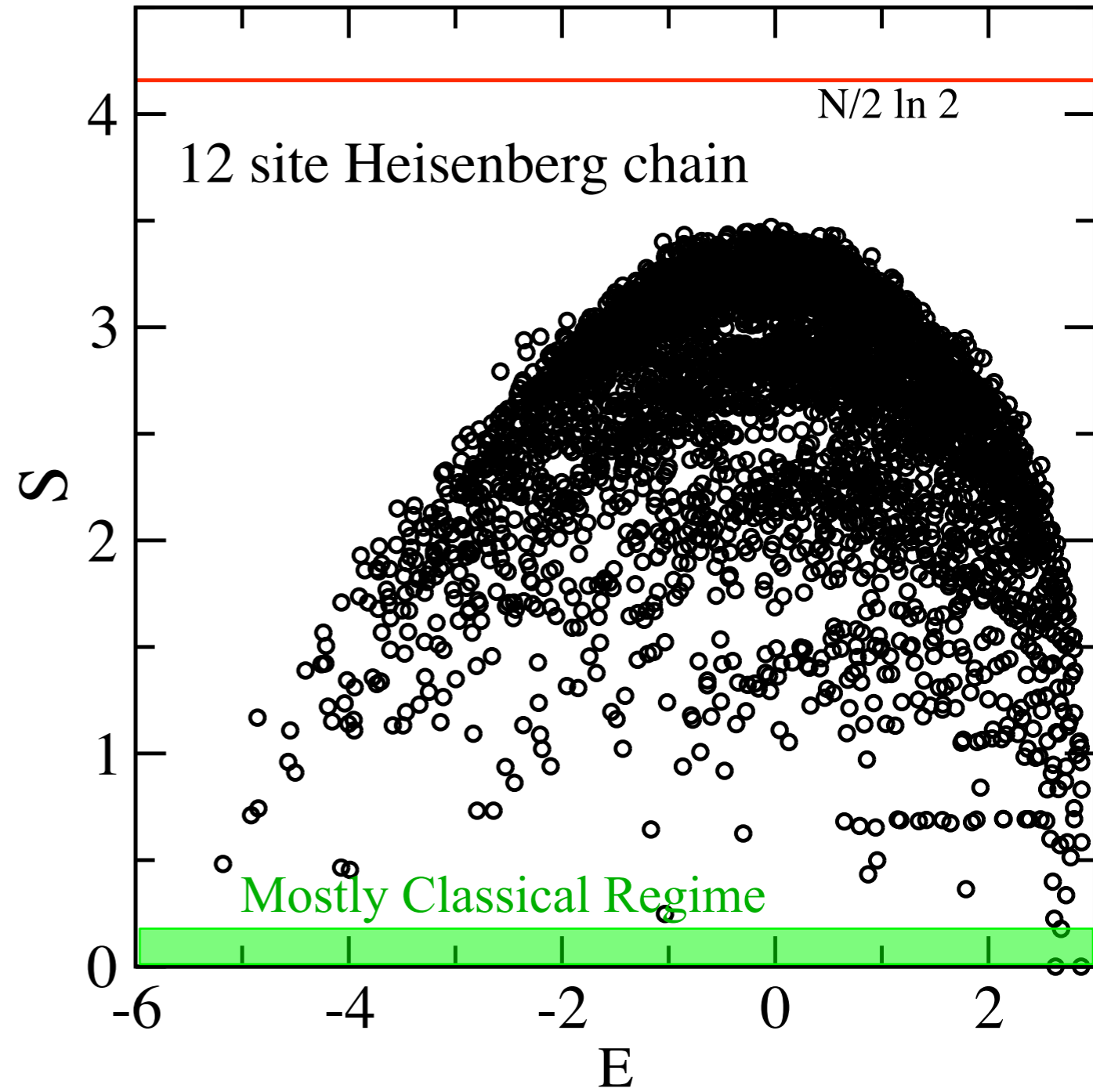
N=8

Energy levels of $S=1/2$
Heisenberg chains



N=12

Bulk eigenstates are “super-entangled”



Von Neumann Entanglement
entropy S for every eigenstate
(system divided in center)

What is the key problem?

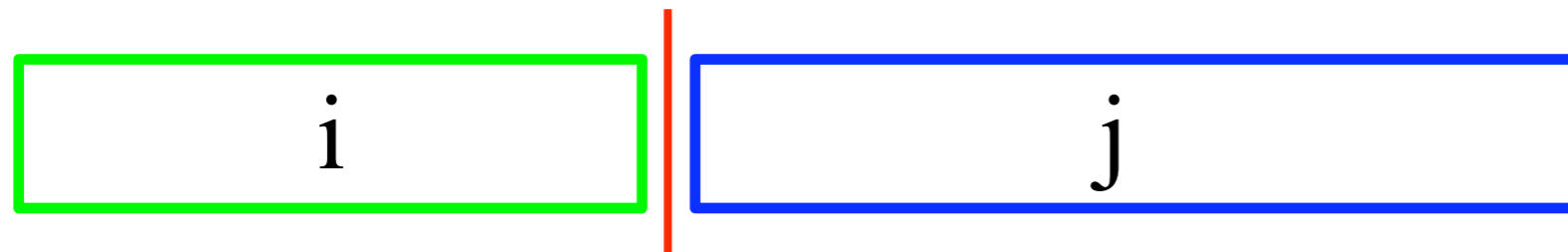
- Ask an experimentalist: systems at high temperature show smaller quantum effects than at low T
- The eigenstate formalism describes high T in terms of much more entangled states--is there another representation that is more classical at high T??
- Yes: Density matrix formalism $\rho = e^{-\beta H}$
 - Trotter/QMC: short world lines for small β
 - DMRG applied directly to ρ : $\rho \approx 1$ for small β
 - But: sign problem, computational inefficiency
- Yes: METTS
 - Wavefunction based
 - Minimal entanglement at high T
 - Very intuitive
 - Much more efficient computationally

Von Neuman entanglement entropy

Ordinary entropy: $S \sim \ln(\text{number of accessible states})$

$S_{\text{VN}} = S_{\text{VN}}(\psi, \text{bipartition}) \sim \ln(\text{number of states required to represent quantum fluctuations across the cut})$

Even ground state has finite S_{VN}



$S \sim$ entanglement
across the cut

- Purely classical states: $S_{\text{VN}} = 0$ for every partition--classical product state $|\uparrow\downarrow\uparrow\downarrow\uparrow\uparrow\downarrow\downarrow\uparrow\downarrow\rangle$
- If S_{VN} is fairly small, DMRG works
 - Throw away low probability states
 - “Low entanglement approximation”

Definition of METTS

- A typical state is one selected from an ensemble $\{|\phi(i)\rangle\}$ with probability $P(i)$

- To reproduce Stat Mech, require $\sum_i P(i) |\phi(i)\rangle \langle \phi(i)| = e^{-\beta H}$

- To rewrite ρ in terms of some set of “typical” states:

- Insert 1: $\rho = e^{-\beta H/2} 1 e^{-\beta H/2}$

- For any orthonormal set $\{|i\rangle\}$: $\rho = e^{-\beta H/2} \sum_i |i\rangle \langle i| e^{-\beta H/2}$

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

$$P(i) \equiv \langle i | \exp(-\beta H) | i \rangle = \text{Tr}\{\rho |i\rangle \langle i|\}$$

$$\text{Then } \sum_i P(i) |\phi(i)\rangle \langle \phi(i)| = \sum_i \frac{P(i)}{P(i)} e^{-\beta H/2} |i\rangle \langle i| e^{-\beta H/2} = e^{-\beta H}$$

- So far very general: could take $|i\rangle =$ eigenstates (bad choice)
- To construct minimally entangled typical thermal states: choose $\{|i\rangle\}$ to be a complete set of classical product states, e.g. $|\uparrow\downarrow\uparrow\uparrow\downarrow\downarrow\rangle$
- The “seed” $|i\rangle$ is completely unentangled, so we expect $|\phi(i)\rangle$ to be minimally entangled

Nice properties of METTS

- Reproduces exact standard Statistical Mechanics
- As classical as possible: high T , completely classical; $T=0$, ground state
- Breaks symmetries: no unphysical superpositions of order params
- The METTS of two widely separated subsystems has no entanglement between them
- Provides nice intuition
- Very easy and fast to compute (DMRG, ED, etc): seed $|i\rangle$ based on previous METTS via quantum measurement

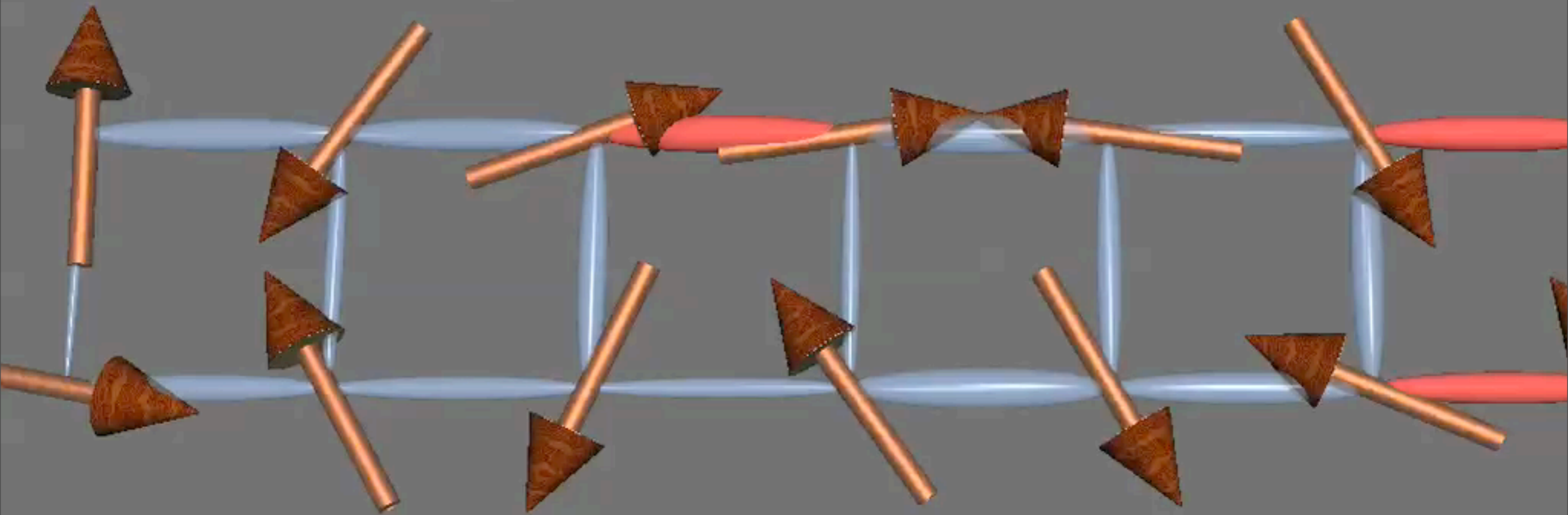
Imaginary time evolution to get a METTS

Arrow represents $\langle \phi(i) | \vec{S} | \phi(i) \rangle$
Bond represents $\langle \phi(i) | S \cdot S | \phi(i) \rangle$

An unentangled spin has length 1/2.
Entanglement reduces length.

Imaginary time evolution to get a METTS

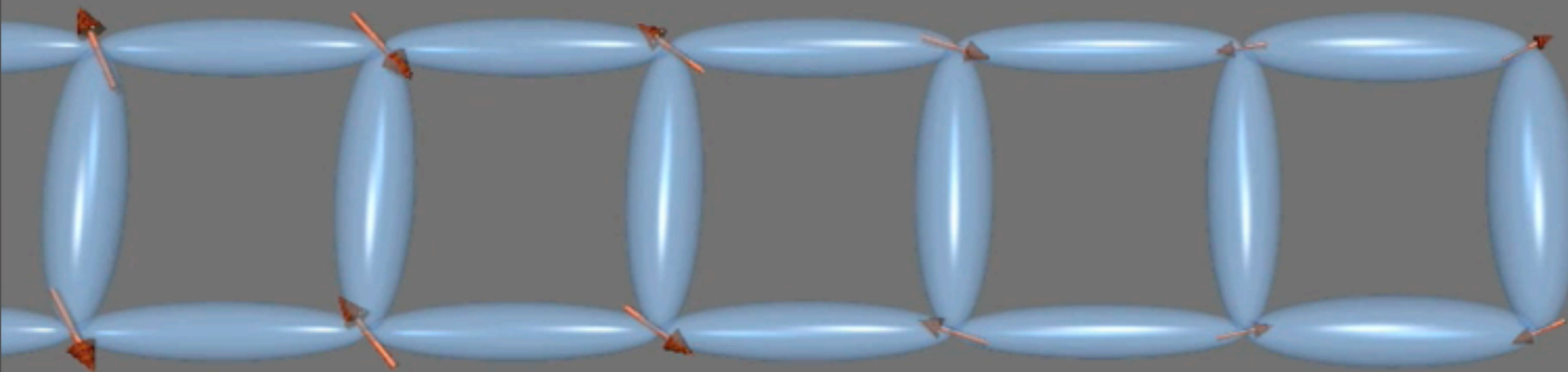
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An unentangled spin has length 1/2.
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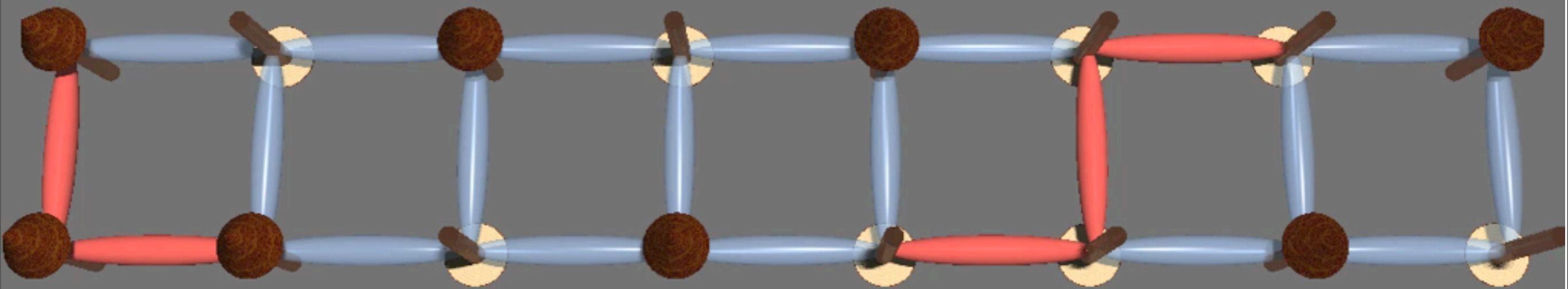
Quantum Measurement to get new seed $|i\rangle$

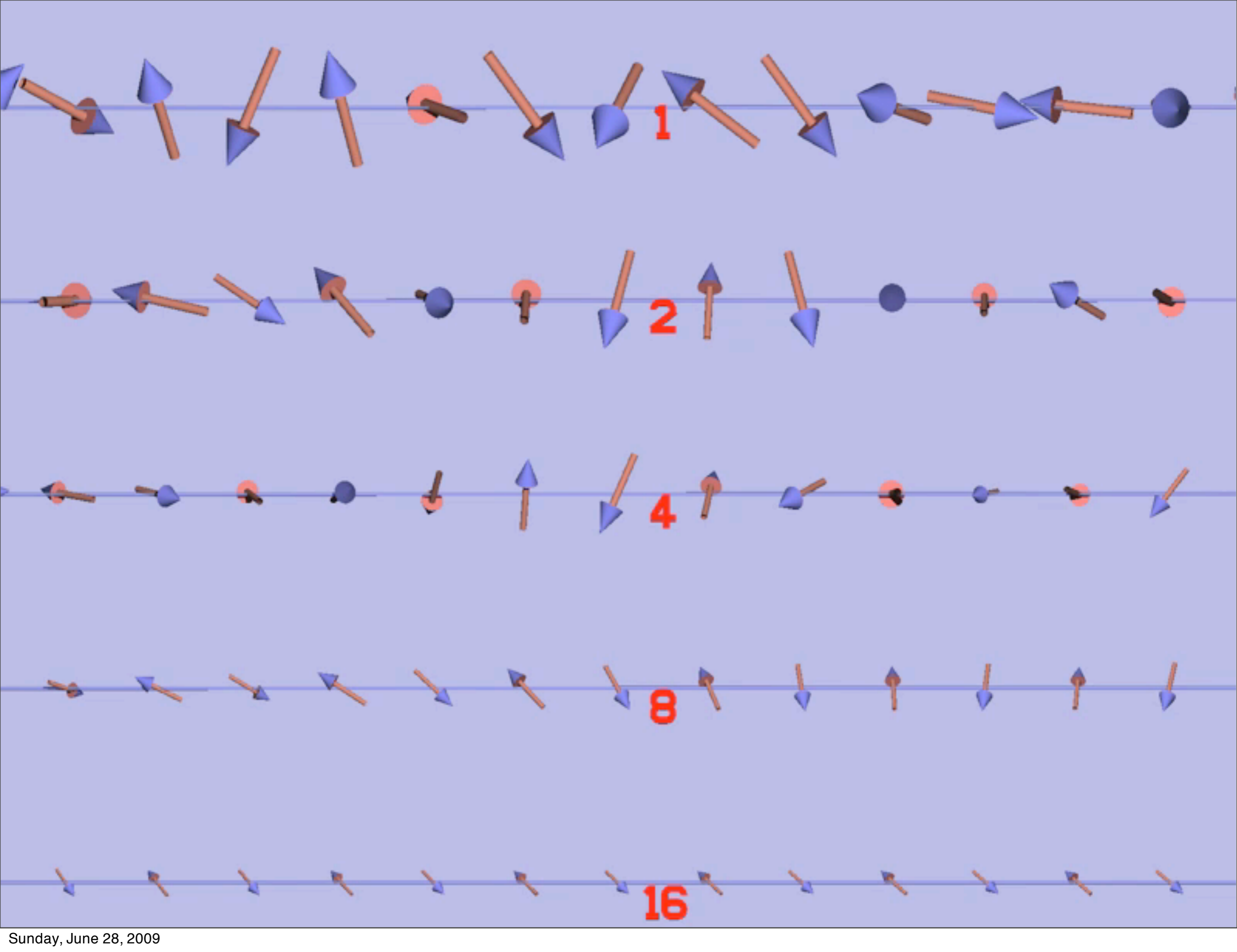
Quantum Measurement to get new seed $|i\rangle$



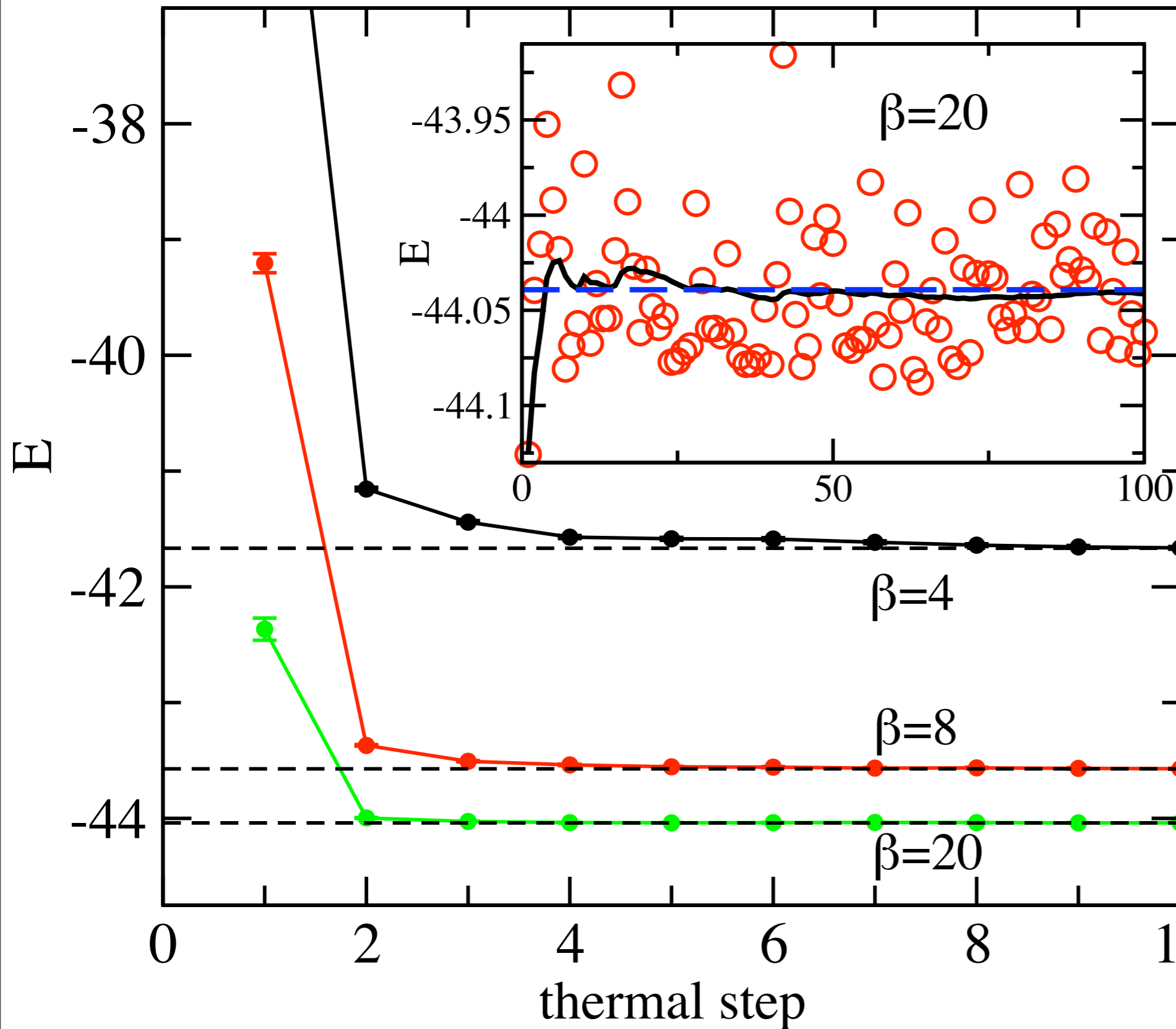
Complete METTS Algorithm $\beta=5$

Complete METTS Algorithm $\beta=5$





How many METTS do you need?



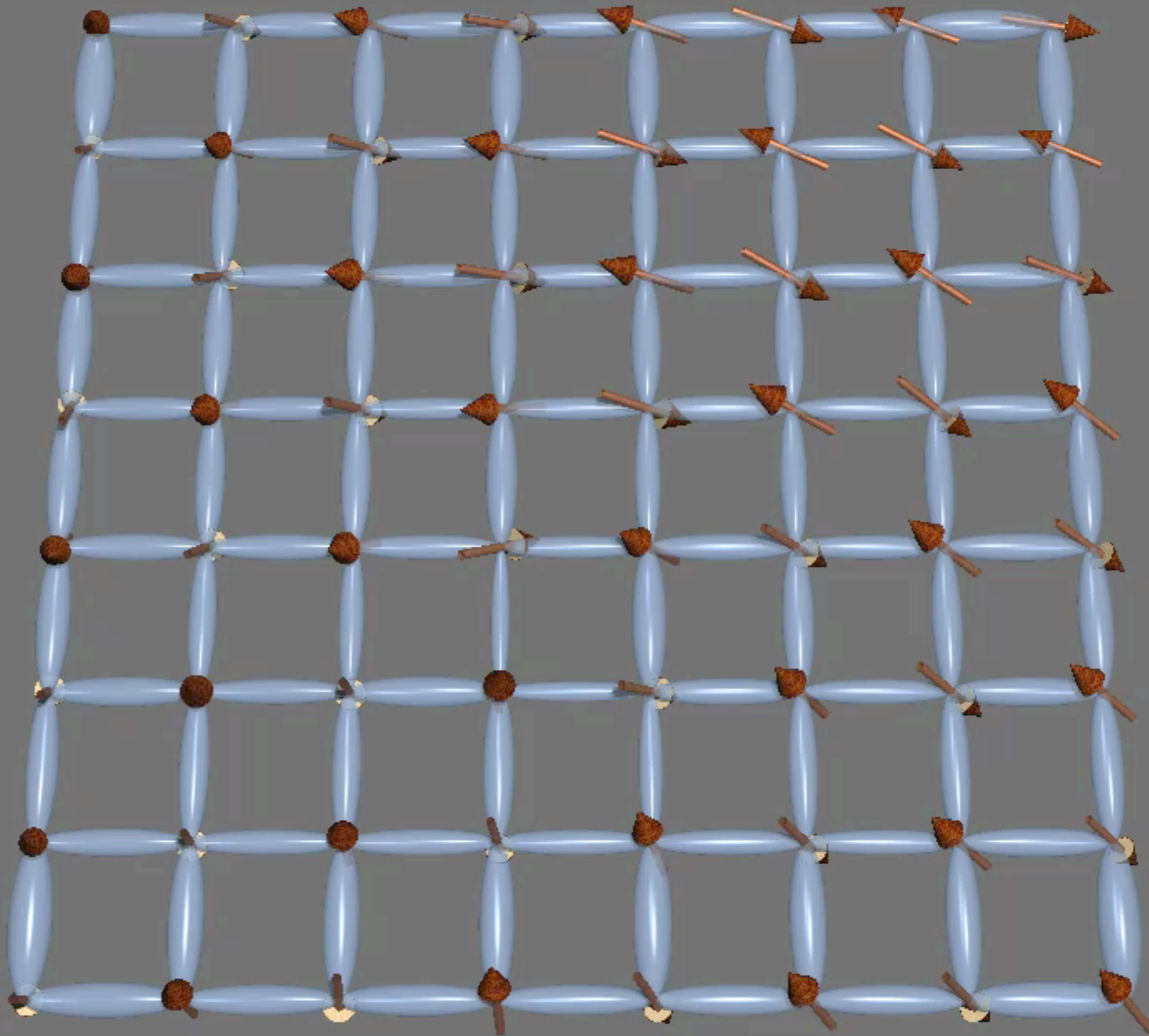
What are the fluctuations in E over different METTS?

What is the sampling autocorrelation time?

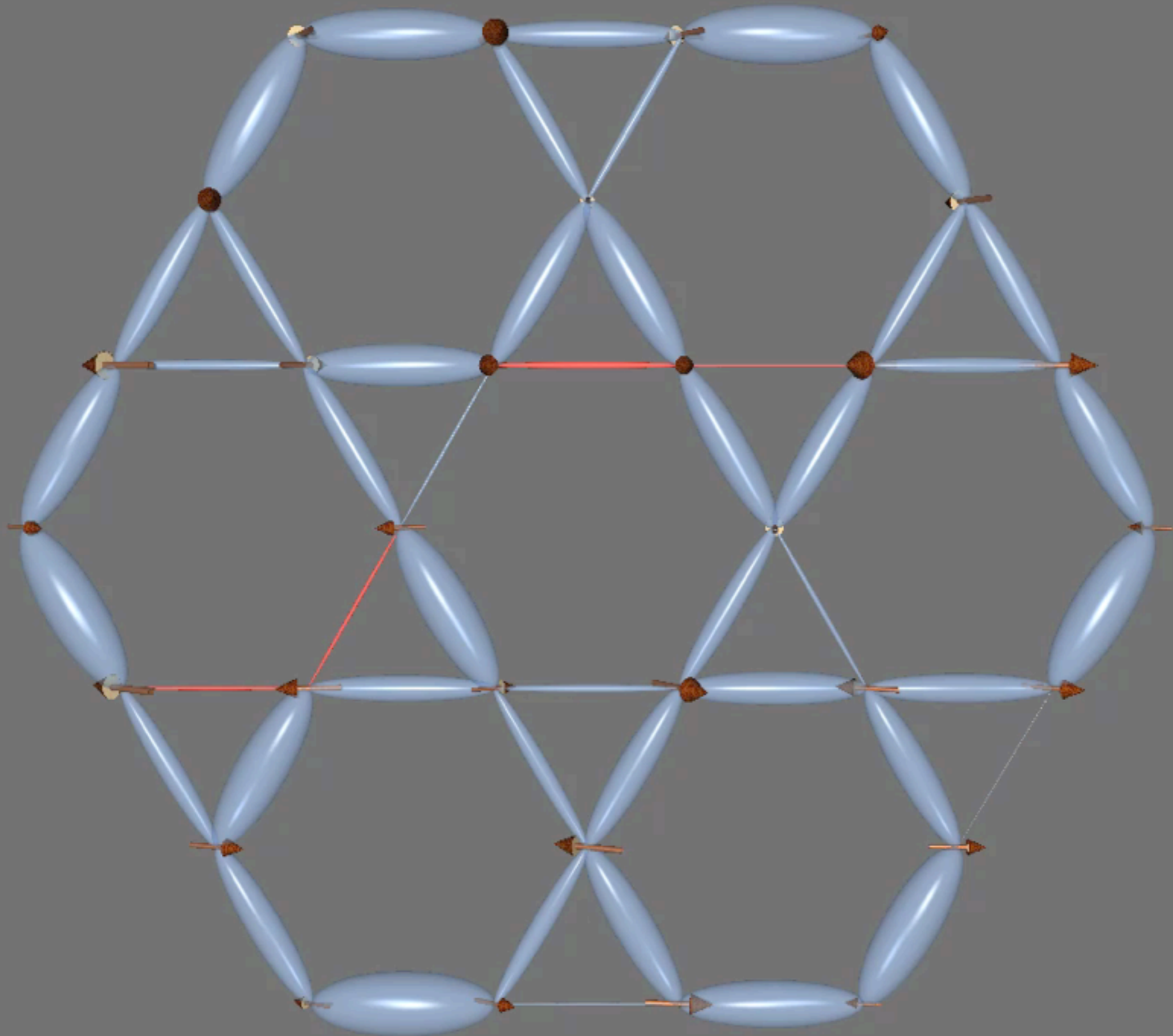
Efficiency of METTS for thermal properties

- Alternative finite T approaches
 - Quantum Monte Carlo: sign problem for frustration and fermions
 - Transfer matrix DMRG: not (yet) capable of 2D clusters, ...
 - Purification of density matrix (heat bath/ancilla) approach
 - Doesn't need averaging over states, but...
 - Entanglement twice that of METTS
- DMRG uses matrix product state with $m \times m$ matrices, $m \sim \exp(a S)$
 - DMRG calculation time $\sim N m^3$
 - Finite T heat-bath: $\sim N \beta m^6$,
 - METTS: $\sim N \beta m^3$ (# METTS sampled = 10-100)
 - Ratio $\sim m^3/100$; if $m \sim 1000$, METTS faster by $\sim 10^7$

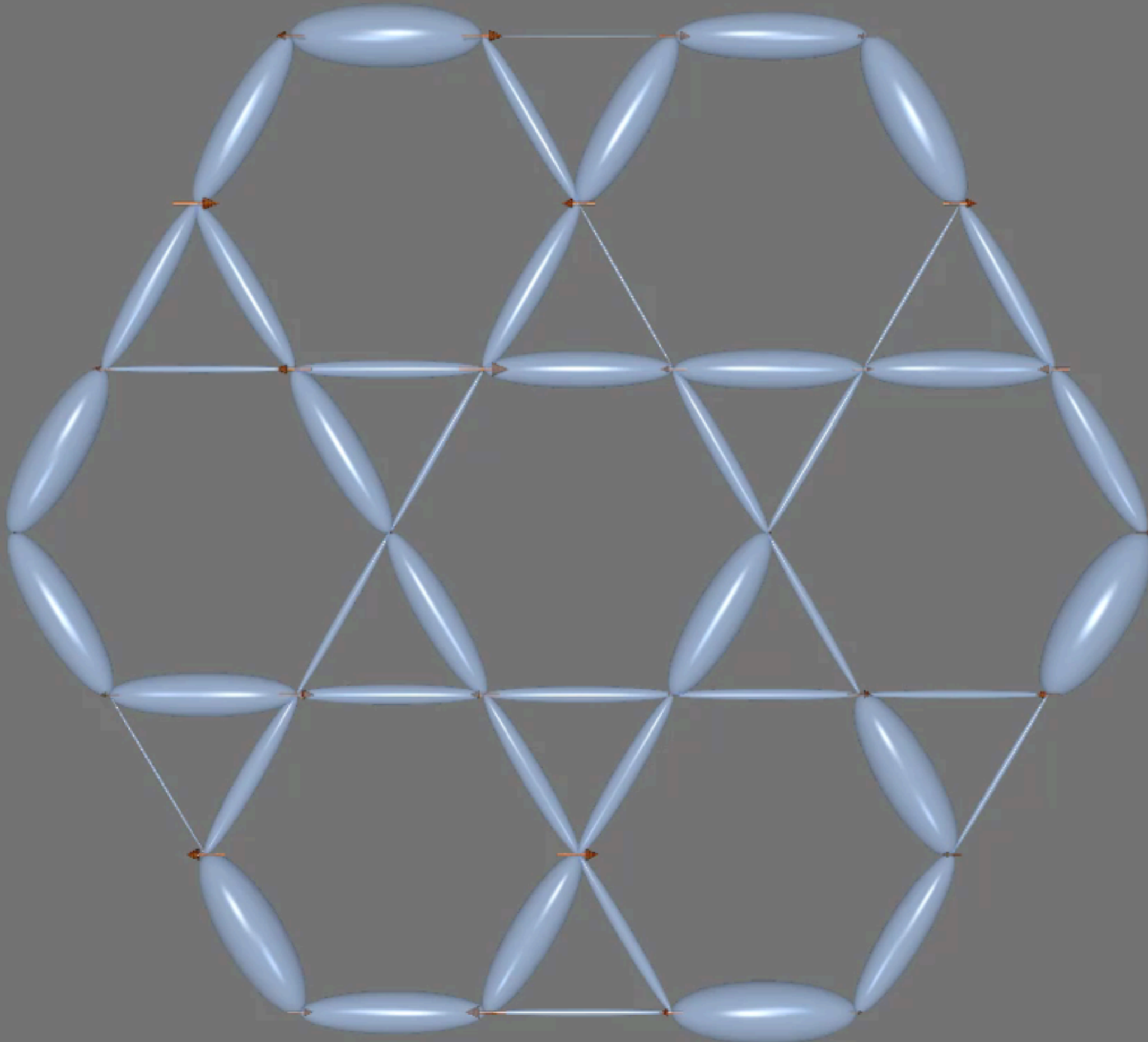
METTS for 2D Heisenberg, $\beta=4$



METTS for Kagome Heisenberg, $\beta=10$



METTS for Kagome Heisenberg, $\beta=20$



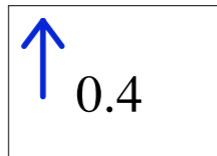
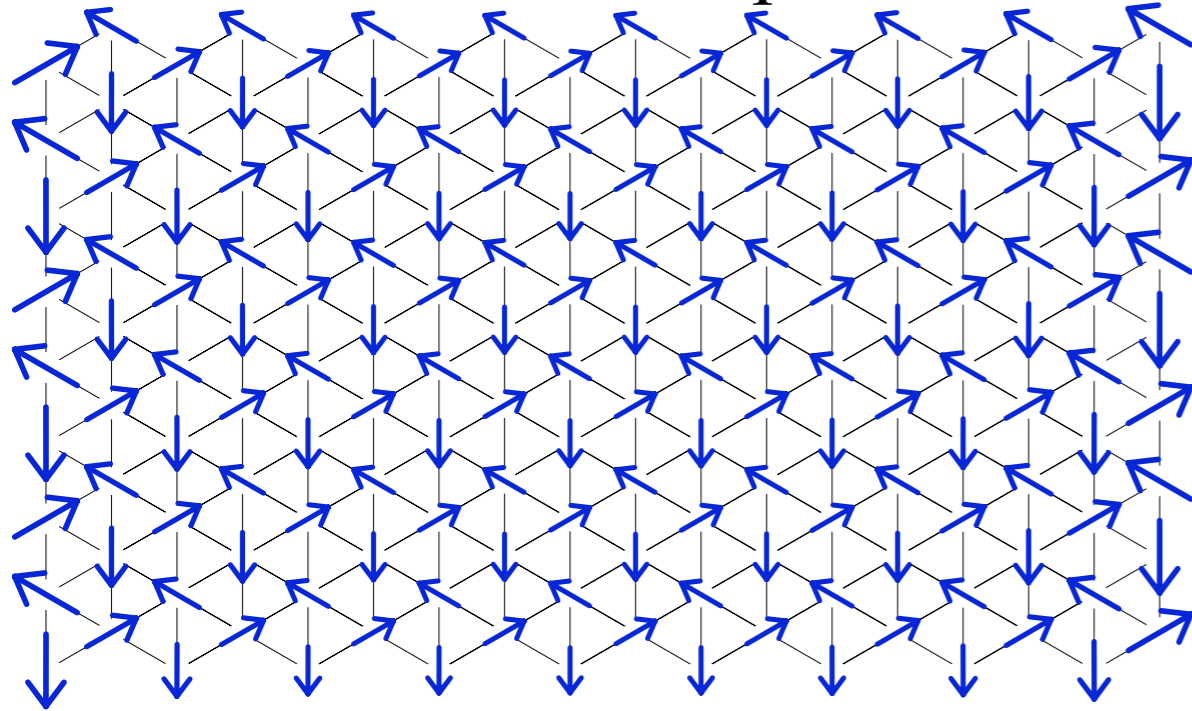
Consequences

- Experimental:
 - 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:
 - Hopefully new insight into system properties
 - Easier approach to finite T in hard systems, e.g. 2D
 - Maybe 100-1000 times as much CPU time as for ground state

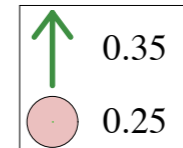
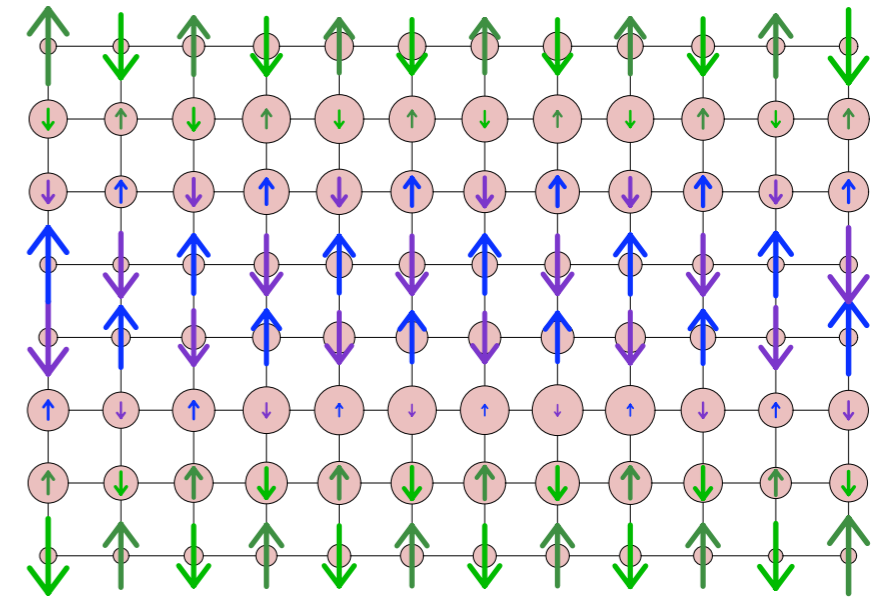
Summary

- METTS provide a new answer to an old question:
 - What is a typical quantum wavefunction at finite T ?
- They provide very intuitive understanding of the fluctuating properties of the system
- They are much more efficient within DMRG than previous methods
- To paraphrase the bible:
 - “Give unto Schrödinger that which is Schrödinger’s; give unto Boltzmann that which is Boltzmann’s”
 - (Classical part via an ensemble; quantum part in the wavefunction)

Two examples of state-of-the-art ground state DMRG



White & Chernyshev



12 x 8 system, Vertical PBC's
 $J_x/t = 0.55, J_y/t = 0.45, \mu = 1.165, \text{doping} = 0.1579$

White & Scalapino

Triangular system: sign problem, 2D, but no competing phases: quantitative determination of order parameter

t-J model: good ground state for specified cluster, but: competing forms of order, sensitive to small terms (t'), other small terms may be missing... simply improving algorithm by factor of 10 or 100 may not help much...

Real time evolution, growth of entanglement

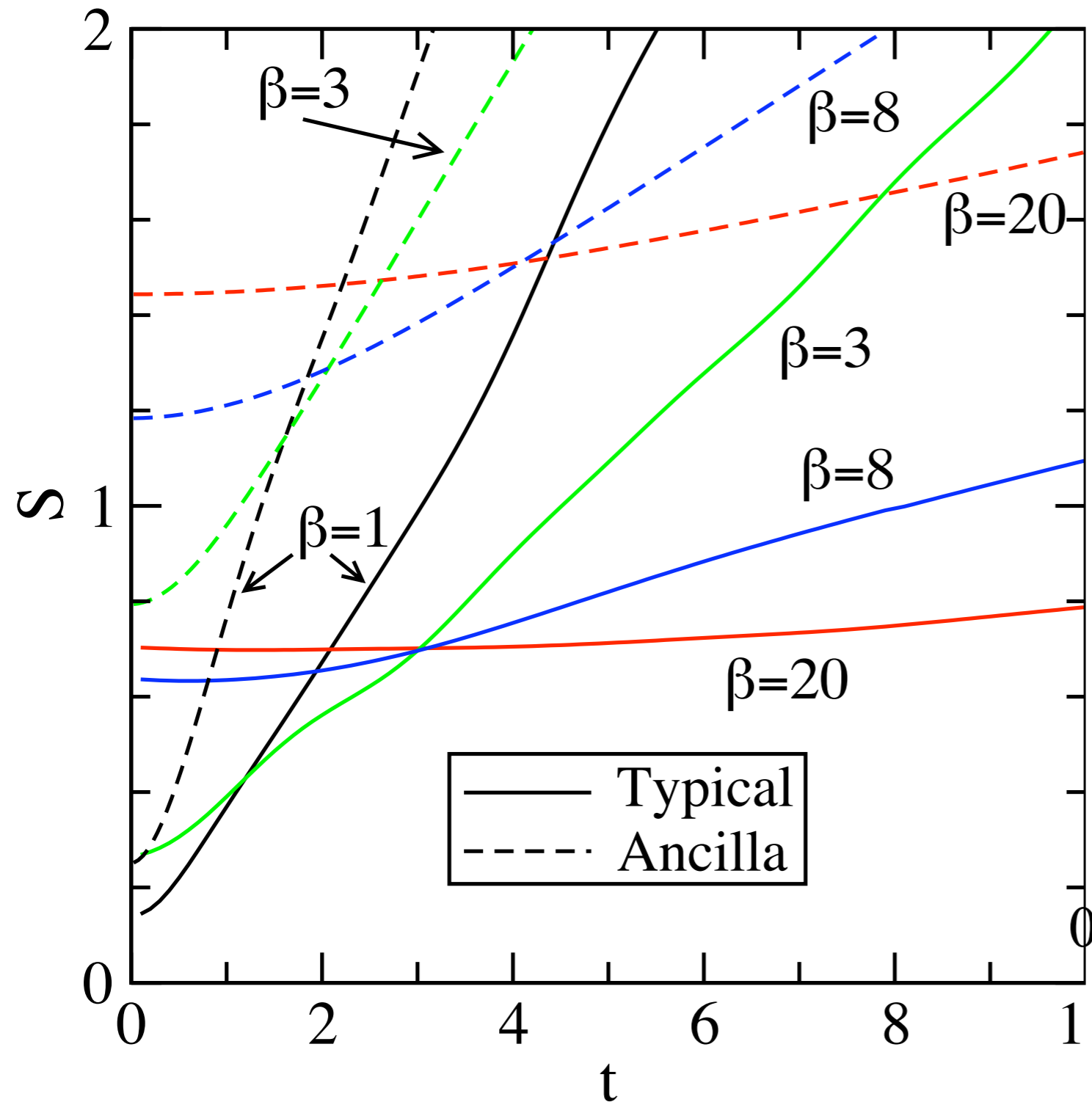
N=40 1D Heisenberg model

Entanglement entropy measured in center

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

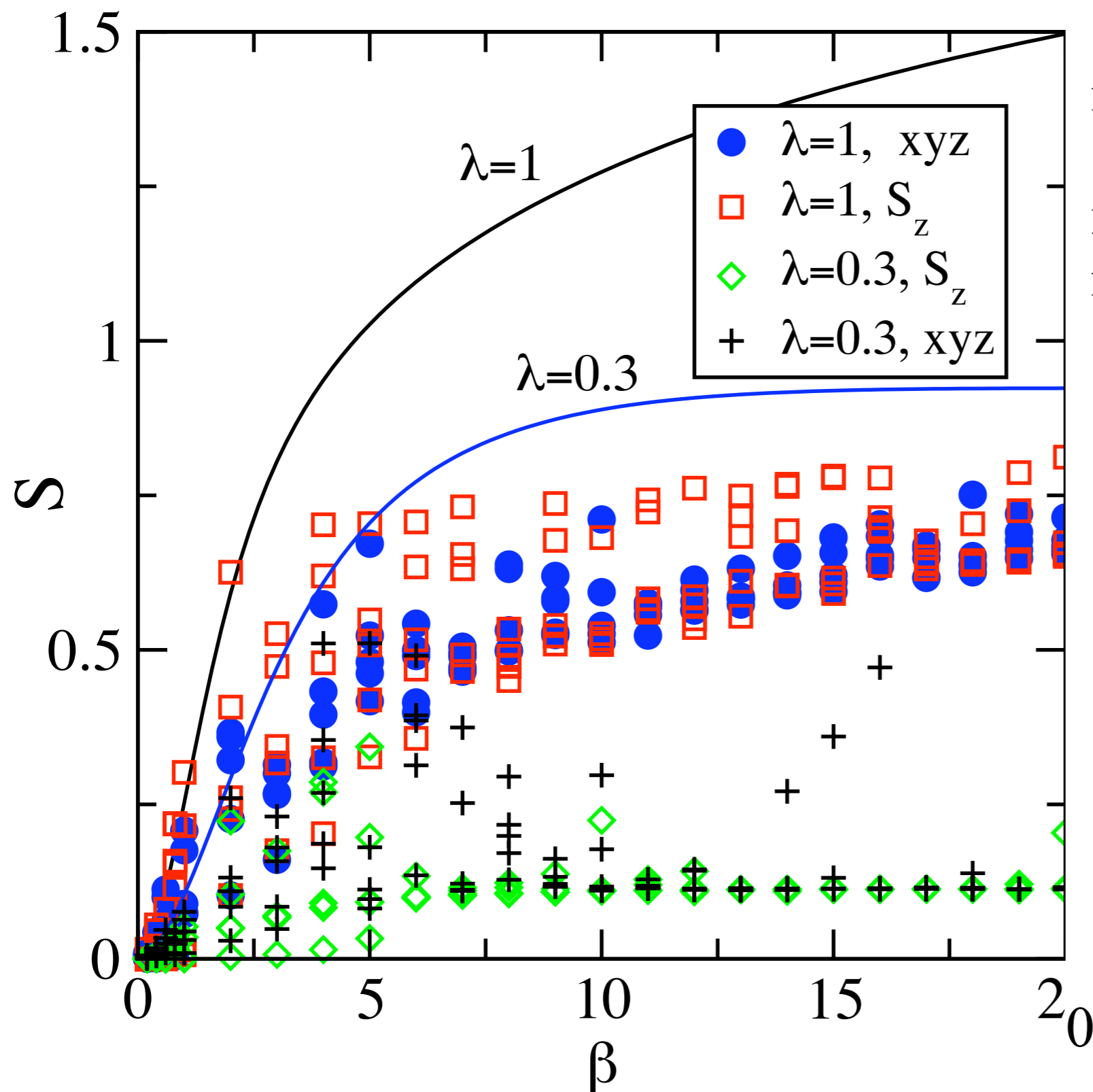
Entanglement grows much faster at higher temperatures, as seen earlier in ancilla method

Decoherence would tend to counteract the entanglement growth in a real system



Entanglement entropy, XXZ chains (midpoint)

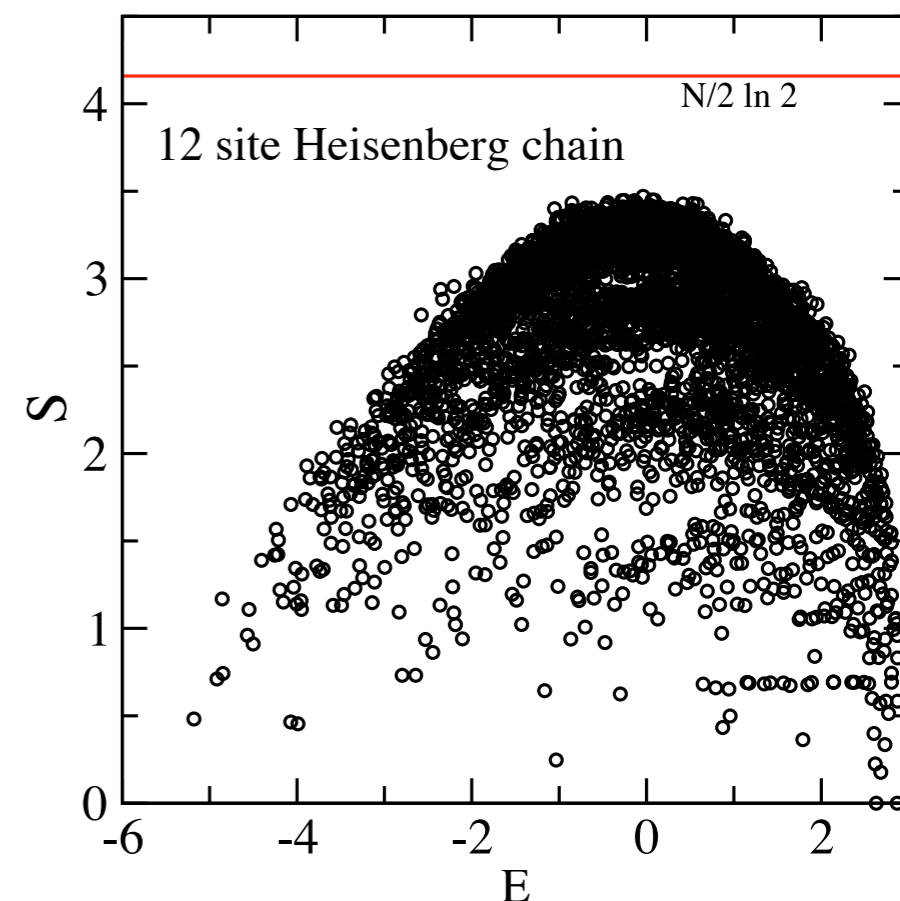
$$H = \sum_{\ell} S_{\ell}^z S_{\ell+1}^z + \lambda(S_{\ell}^x S_{\ell+1}^x + S_{\ell}^y S_{\ell+1}^y) \quad L=200$$



Solid lines: heat bath/ancilla method

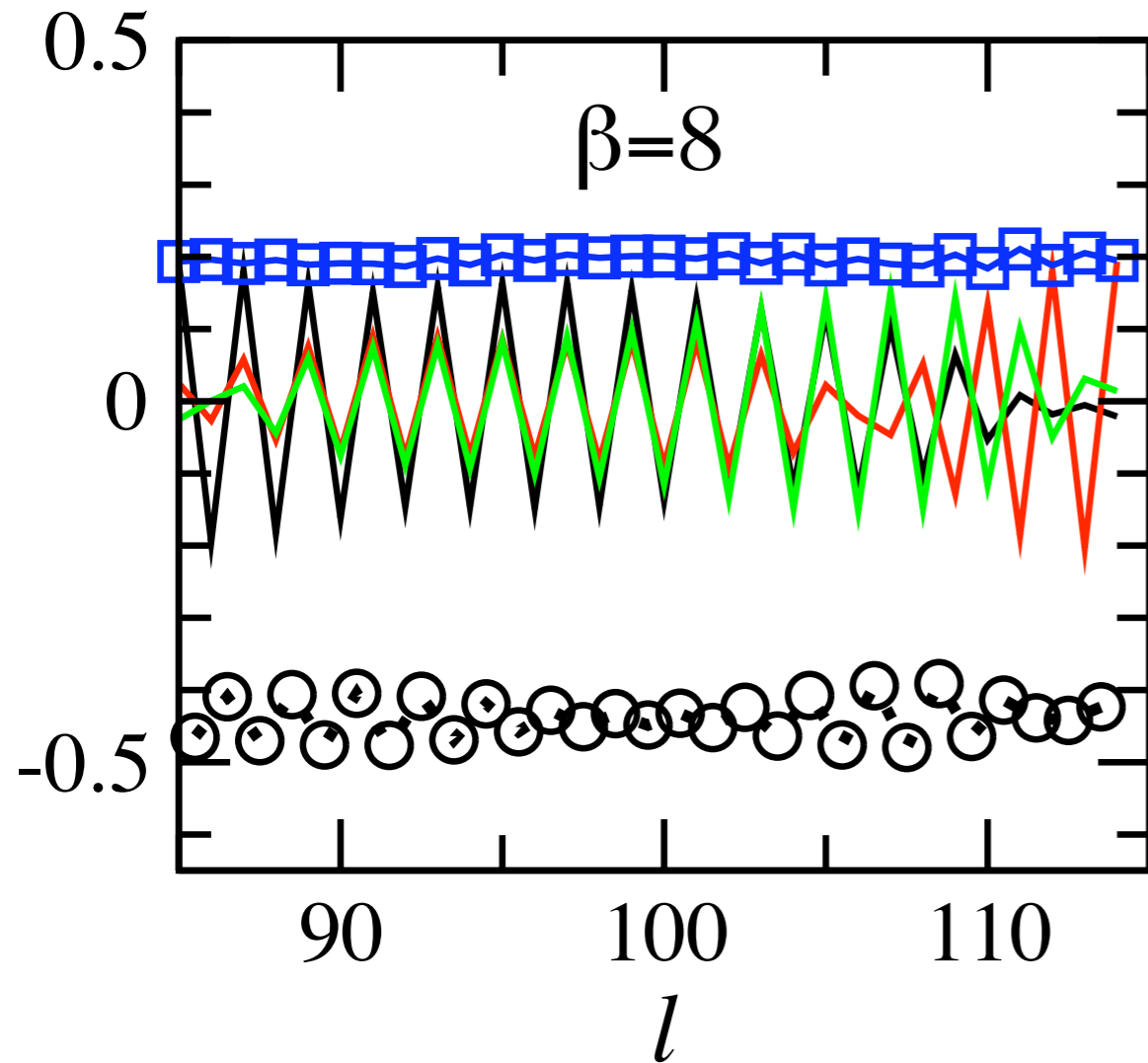
xyz: Measurements at random angles

Sz: Measurements in z dir



Typical States for Heisenberg Chains

L=200, central portion



Orientation for each Measurement on a site chosen at random

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

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

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

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

