Quantum Information Theory and Strongly Correlated Quantum Systems

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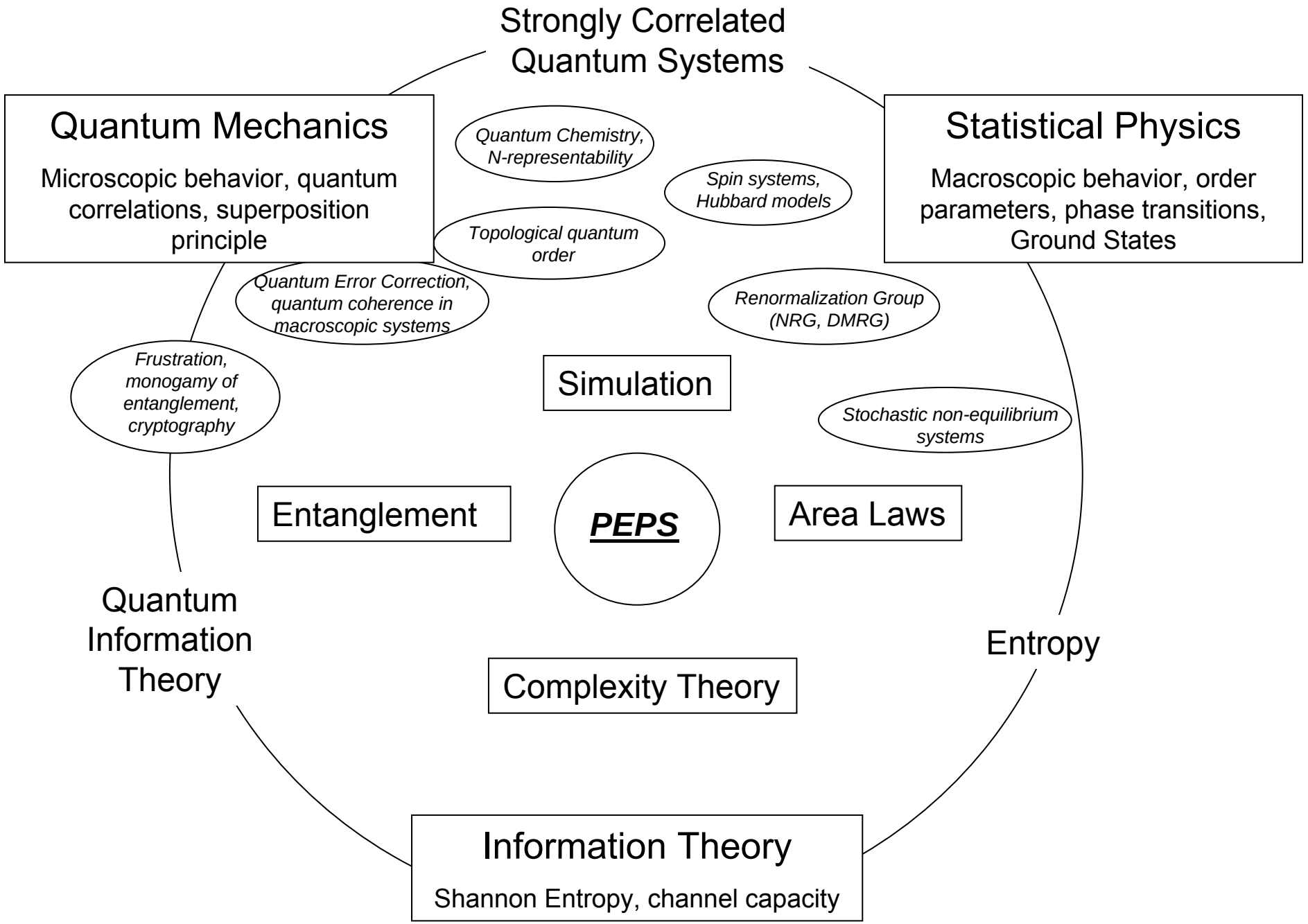
Overview

- Lecture 1: entanglement, frustration and quantum spin systems
- Lecture 2: from real-space renormalization group methods to variational wavefunctions
- Lecture 3: quantum computing with and computational complexity of simulating quantum many-body systems


Strongly Correlated Quantum Systems
Quantum Mechanics
Microscopic behavior, quantum correlations, superposition principle
Statistical Physics
Macroscopic behavior, order parameters, phase transitions, Ground States
Quantum Chemistry, N-representability
Spin systems, Hubbard models
Topological quantum order
Quantum Error Correction, quantum coherence in macroscopic systems
Renormalization Group (NRG, DMRG)
Frustration, monogamy of entanglement, cryptography
Simulation
Stochastic non-equilibrium systems
Entanglement
PEPS
Area Laws
Quantum Information Theory
Entropy
Complexity Theory
Information Theory
Shannon Entropy, channel capacity

Connecting entanglement theory with strongly correlated quantum systems

- Strongly correlated quantum systems are at forefront of current experimental research
  - Cfr. Realization of Mott insulator versus superfluid phase transition in optical lattices (Bloch et al.)
  - Building of universal quantum simulators using e.g. ion traps
  - No good theoretical understanding yet: main bottleneck is simulation of quantum Hamiltonians

- Quantum spin systems form perfect playground for investigating strongly correlated quantum systems:
  - Heisenberg model was put forward by Dirac and Heisenberg already in the ’20s as candidate Hamiltonian describing magnetism
  - Fermi-Hubbard model is believed to be minimal model exhibiting features of high Tc superconductivity (reduces to Heisenberg in some limit)
  - However, still many open questions!

- Quantum spin models arise naturally in the study of quantum error correcting codes
  - Q.E.C led Kitaev to introducing quantum spin model exhibiting new exotic phases of matter (topological quantum order)
  - Intriguing connection between ideas in quantum information and condensed matter (e.g. cluster states and valence bond states, …)

- What are the questions we would like to see answered?
  - Ground state properties, energy spectrum, correlation length, criticality, connection between those and entanglement
  - Are such systems useful, i.e. do they exhibit the right kind of entanglement and allow for the right kind of control, for building e.g. quantum repeaters, quantum memory or quantum computers?
  - Finite-T: what kind of quantum properties survive at finite T?
  - Connection between amount of entanglement present in system and simulatability on a classical computer?
  - Computational complexity of finding ground states?
  - Dynamics: how much entanglement can be created by local Hamiltonian evolution?

- We already have partial answers to those questions:
  - connection between spectrum and correlation length
  - criticality in 1-D is accompanied by diverging block entropy.
    Not such a signature in 2-D (PEPS)
  - Entanglement length in spin systems versus quantum repeaters
  - Cluster state quantum computation of Raussendorf and Briegel (cfr. PEPS)
  - Kitaev: using Toric Code states as fault-tolerant quantum memory in 4-D
  - Finite T: strict area law for mutual information
  - MPS/PEPS parameterize manifold of ground states of local Hamiltonians
  - Kitaev: finding ground states of disordered local Hamiltonians is QMA-complete (also: famous N-representability problem)
  - Dynamics: Lieb-Robinson bounds

Entanglement

Complementary viewpoints on entanglement:

- Quantum information theory: it is a resource that allows for revolutionary information theoretic tasks
- Quantum many-body physics: entanglement gives rise to exotic phases of matter
- Numerical simulation of strongly correlated quantum systems: enemy nr. 1!

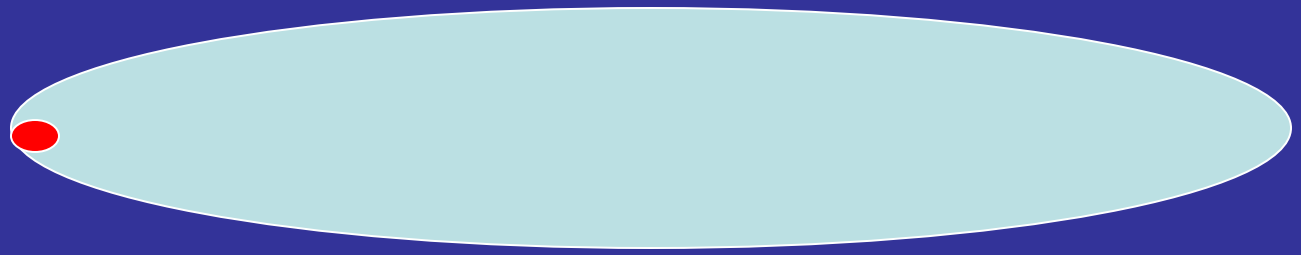
Of course these viewpoints are mutually compatible:

- Complexity of simulation vs. power of quantum computation
- Topological quantum order vs. quantum error correction

Key question: what kind of superpositions appear in nature?

Many-body Hilbert space is a convenient illusion

- Size of Hilbert space of system of N particles / modes / … scales exponentially with N.
  - What is the fraction of states that are physical, i.e. can be created as low-energy states of local Hamiltonians or by a quantum computer in poly time? Exponentially small !!!
  - Ground states (and low-energy states …) have very special properties
    - Amount of entanglement is very small: can be formalized using so-called area laws
    - Ground states have extremal local correlations: all (quasi-)long range correlations are a consequence of the fact that those local correlations must be made compatible with translational invariance

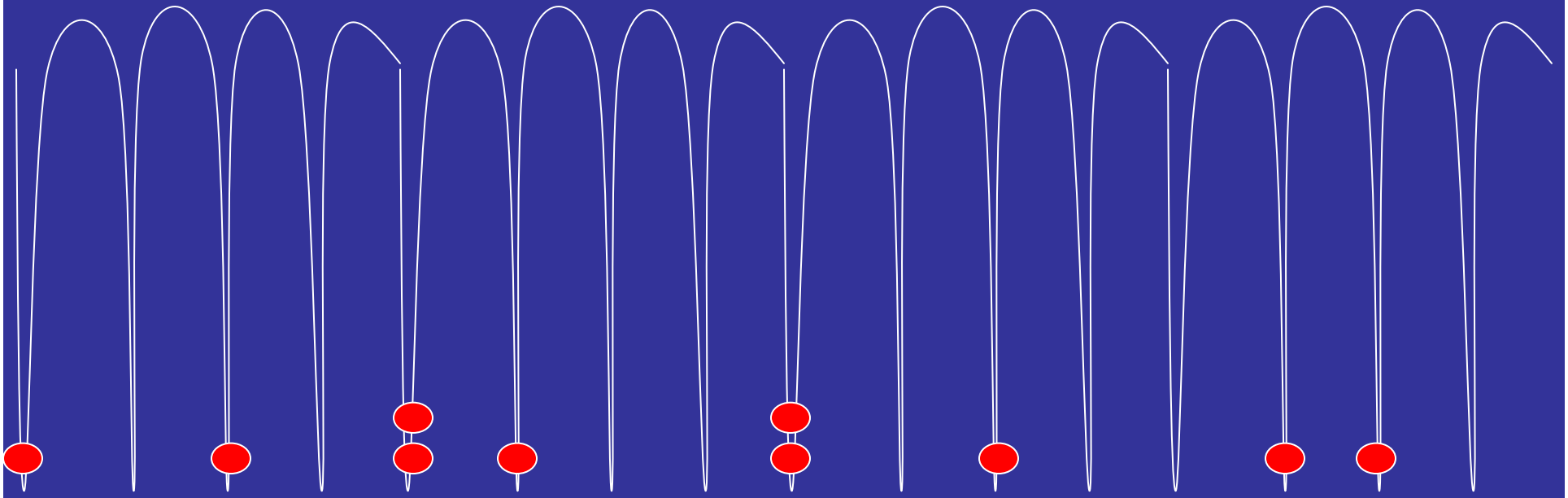


$$(cN)^{N^d \log \frac{N^d}{\varepsilon}} \quad \text{vs} \quad \varepsilon^{-D^N}$$

  - If we want to simulate a many-body system, we should be *smarter*

- Can we identify the corner in Hilbert space that corresponds to ground states of local many-body quantum Hamiltonians?
  - If so: this would lead to a systematic way of coming up with variational ansatze
    - Cfr. some of the biggest breakthroughs in condensed matter physics involved guessing the right wave function (BCS, Laughlin, …)
  - What is the structure of entanglement in those systems?

Strongly correlated many-body quantum systems



- Electrons in deep potential wells give rise to an effective Hubbard model

$$H_{Hubbard} = \sum_{<ij>,s} t_{ij} a^{*}_{i,s} a_{j,s} + \sum_{ijss'} U_{ij} n_{i,s} n_{j,s'}$$

- Big open question: phase diagram of 2-D Hubbard model as a function of the filling factor and of the on-site interaction
- Quantum spin systems: limit of strong onsite U at half-filling: Heisenberg model

$$H_{Heis} = \sum_{<ij>} X_i X_j + Y_i Y_j + Z_i Z_j$$

Quantum spin systems

- Provide perfect playground for investigating nature of entanglement in strongly correlated quantum systems
  - Most pronounced quantum effects arise at low temperature as large quantum fluctuations exist (ground states)
  - We assume some geometry and local interactions (cfr. Causality) such as Heisenberg model

- Ground states of local spin Hamiltonians are very special:

$$H = \sum_{\langle i,j \rangle} S_x^i S_x^j + S_y^i S_y^j + \Delta S_z^i S_z^j$$

  - Translational invariance implies that energy is completely determined by n.n. reduced density operator ρ of 2 spins:

$$E = N.\mathrm{Tr}\left(\rho\, H_{ij}\right)$$

  - Finding ground state energy is equivalent to maximizing E over all possible ρ arising from states with the right symmetry (Quantum Marginal Problem)
  - The extreme points of the convex set {ρ} therefore correspond to ground states: ground states are completely determined by their reduced density operators!

Translational invariant spin chains

$$H = \sum_{\langle i,j \rangle} S_x^i S_x^j + S_y^i S_y^j + \Delta S_z^i S_z^j$$

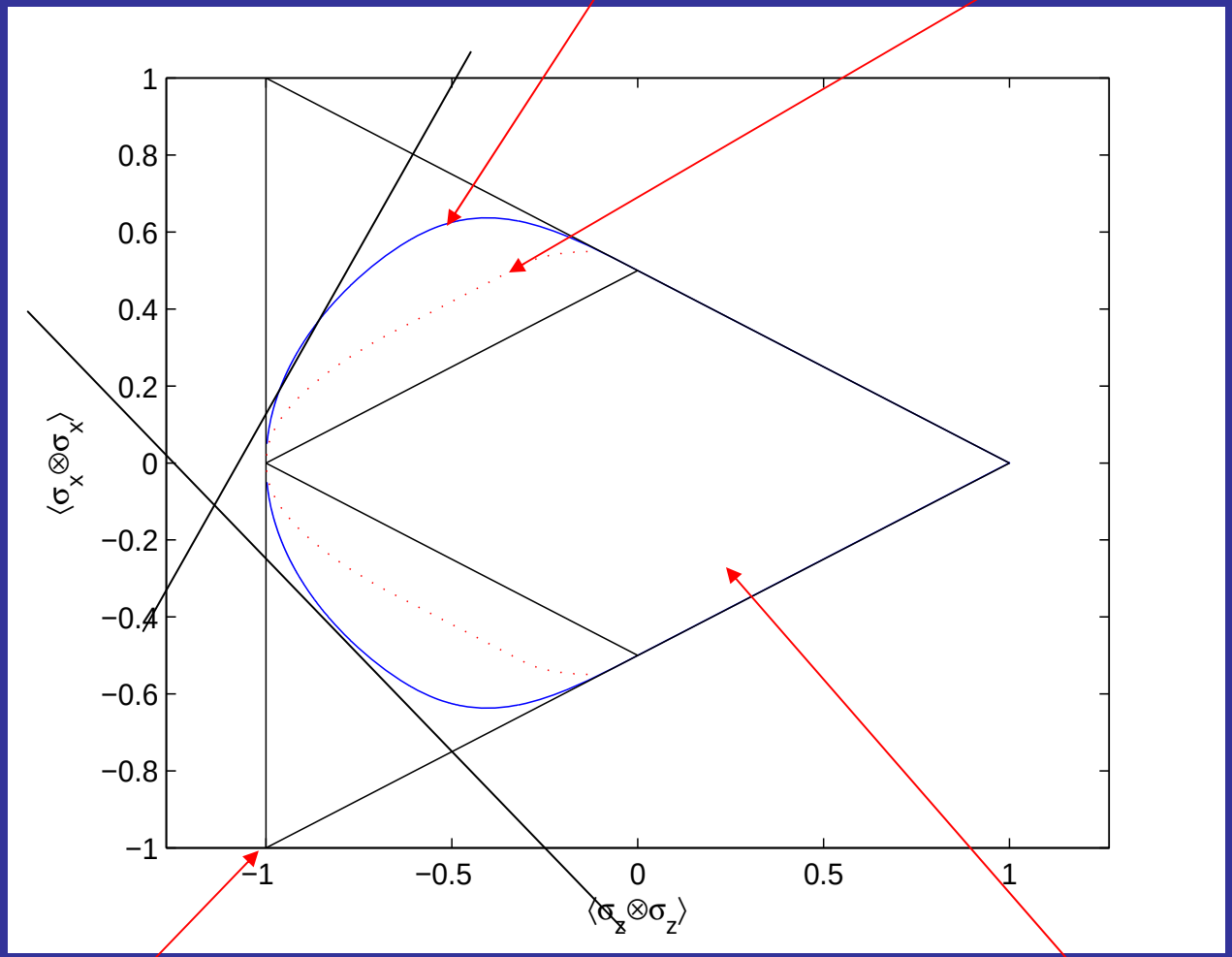
Symmetries enforce that the RDM of n.n. for the ground state is of the form:

$$\rho = \frac{1}{4}\left(\mathbb{1} \otimes \mathbb{1} + x(\sigma_x \otimes \sigma_x + \sigma_y \otimes \sigma_y) + z\sigma_z \otimes \sigma_z\right)$$

Positivity conditions: $-1 \leq z \leq 1 - 2|x|$

If we know the energy as a function of Delta, then we know the shape of the convex set for the translational invariant case:

$$2x + z\Delta + E(\Delta) = 0$$


1-D spin chain
2-D lattice
1
0.8
0.6
0.4
0.2
0
−0.2
−0.4
−0.6
−0.8
−1
−1
−0.5
0
0.5
1
⟨σx⊗σx⟩
⟨σz⊗σz⟩
singlet
Separable/ mean field states

- Difficulty in characterizing this convex set is due to monogamy / frustration properties of entanglement: a singlet cannot be shared !

  – The higher the dimension, the smaller the entanglement :

	Singlet	1-D	Hexagonal	square	Cubic
Energy/bond (Corr. Energie)	-3 (2)	-1.77 (.77)	-1.45 (.45)	-1.34 (.34)	-1.19 (.19)

M. Dowling et al., Phys. Rev. A 70, 062113 (2004).

  – In infinite dimensions: only separable states are compatible with the permutation symmetry; mean field theory becomes exact (cfr. De Finetti: Werner ‘88)

$$\rho = \sum_i p_i \, \rho_i \otimes \rho_i$$

Entanglement: basics

- Given a state of 2 spin ½'s (qubits):

$$|\Psi\rangle = a|0\rangle|0\rangle + b|0\rangle|1\rangle + c|1\rangle|0\rangle + d|1\rangle|1\rangle$$
$$|a|^2 + |b|^2 + |c|^2 + |d|^2 = 1$$

- Is this state a product state (separable)?
  - i.e.: can we write this state as a product

$$|\Psi\rangle = \left(\alpha|0\rangle + \beta|1\rangle\right) \otimes \left(\gamma|0\rangle + |1\rangle\right) \quad ?$$

  - Schmidt decomposition / singular value decomposition

$$X = \begin{bmatrix} a & b \\ c & d \end{bmatrix} = U\Sigma V^* = \sigma_1 |u_1\rangle\langle v_1| + \sigma_2 |u_2\rangle\langle v_2|$$

    - Separable iff second Schmidt coefficient is zero; entangled otherwise

Entanglement in a system of 2 qubits

- How to quantify entanglement?

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle|0\rangle + |1\rangle|1\rangle\right) \quad \Rightarrow \quad \mathrm{A} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$|\Psi\rangle = \frac{1}{2}\left(|0\rangle|0\rangle + |0\rangle|1\rangle + |1\rangle|0\rangle + |1\rangle|1\rangle\right) \Rightarrow \quad \mathrm{A} = \frac{1}{2}\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} = |a\rangle\langle a| \quad ; \quad |\mathrm{a}\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

- Entropy of entanglement: entropy of probability distribution obtained by squaring the Schmidt coefficients

$$p_i = |\sigma_i|^2 \qquad ; \qquad S = -\sum_i p_i \log_2 p_i$$

  - This is equivalent to the von-Neumann entropy of the reduced density operator
  - Has a very clear operational meaning: cfr. Talks of Kempe

- To check seperability: calculate rank of matrix A
  - Concurrence: C=2*det(A)
  - 1 to 1 relation between concurrence and entanglement entropy

Entanglement

- What about mixed states?
  - Entanglement of distillation: how useful is a state for doing quantum information processing?
    - Basic idea: given many copies, how can I extract perfect singlets by doing local operations assisted by classical communication (LOCC)
    - Drawback: we still don't know how to calculate this
  - Entanglement of formation: how many perfect singlets do I need to construct a mixed state starting from singlets and LOCC

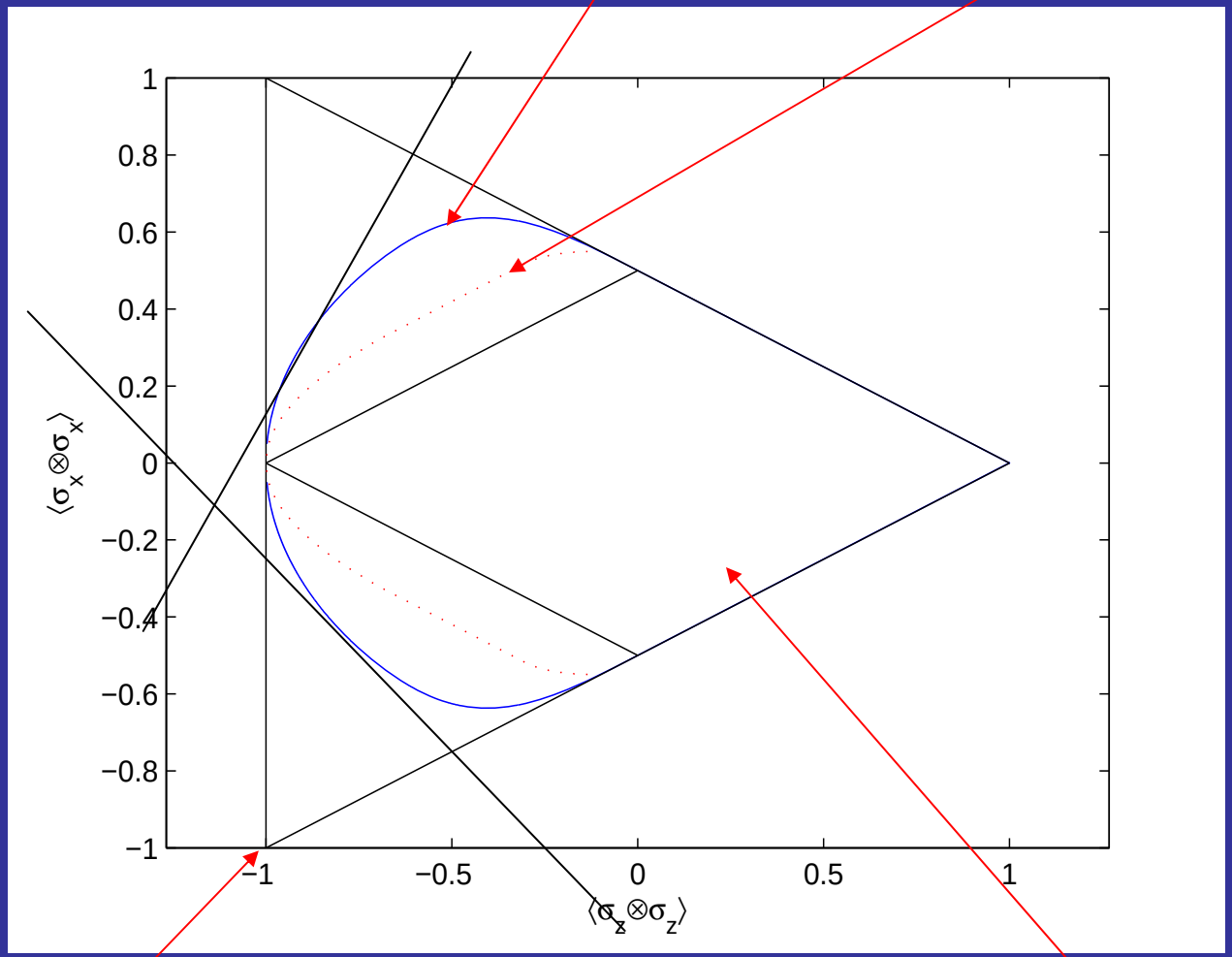
$$E_f(\rho) = \min_{\{p_i, |\psi_i\rangle\}} \sum_i p_i S(|\psi_i\rangle)$$

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$$

    - Is zero (separable) iff a state can be written as a convex sum of product states:

$$\rho = \sum_i p_i \ \rho_i \otimes \sigma_i$$

    - In case of 2 qubits: can be exactly calculated in form of concurrence (Wootters '98)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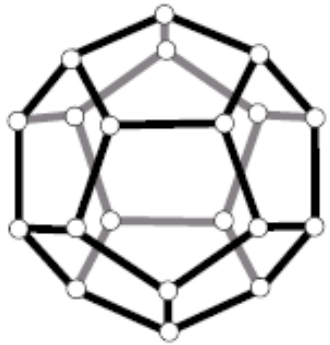
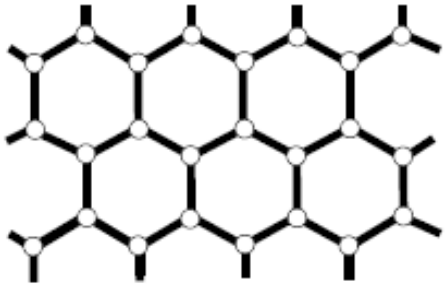
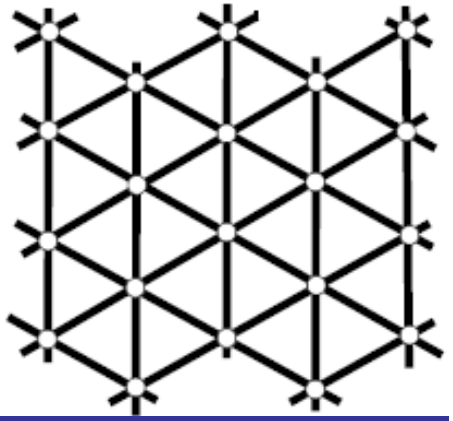
Gaussian states: calculation of maximal entanglement of formation of n.n. density matrices arising from a states with a given symmetry can be done exactly: extremal cases are ground states of quadratic Hamiltonians

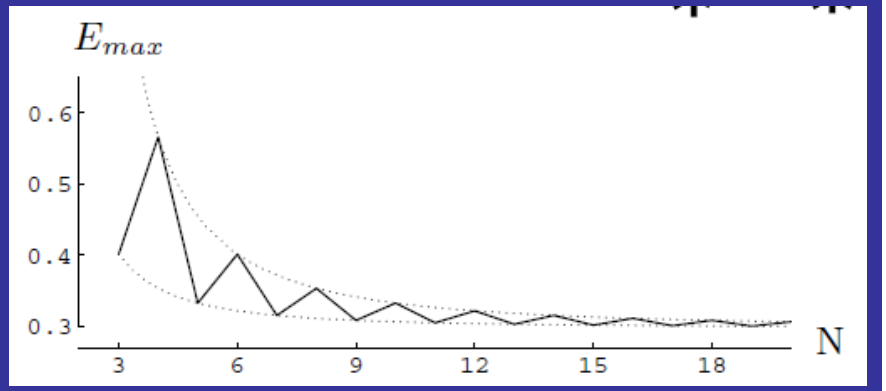
lattice	E_{max}	N_a
hexagonal (2d)	10.61	3
square (2d)	6.31	4
trigonal (2d)	2.69	6
cubic (3d)	2.62	6







platonic solid	E_{max}	N_a	N	E_0
tetrahedron	19.74	3	4	$\frac{1}{\sqrt{2}}$
cube	19.74	3	8	$\frac{1}{\sqrt{2}}$
dodecahedron	11.12	3	20	$\frac{1}{30}\left(12+5\sqrt{2}+2\sqrt{5}\right)$
octahedron	10.75	4	6	$\frac{1}{6}(3+\sqrt{3})$
icosahedron	5.37	5	12	$\frac{1}{\sqrt{5}}+\frac{1}{\sqrt{6}}$

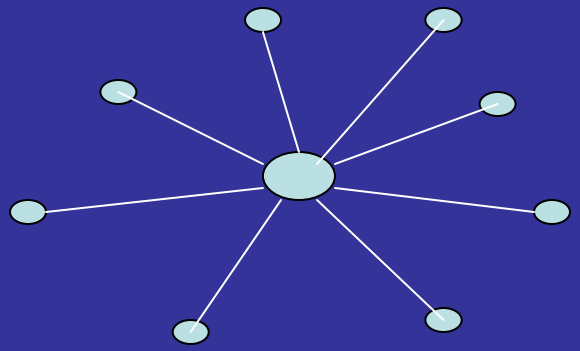


Finite size corrections: Ring of N particles

M. Wolf, FV, I. CiracPhys. Rev. Lett. 92, 087903 (2004)

Monogamy relations for states without symmetry constraints: Coffman-Kundu-Wootters inequality

- Given a N-qubit (spin ½) state, the sum of the concurrences (entanglement measure depending on 2-particle RDM) of one particle with all the rest is bounded by 1 minus its magnetization:



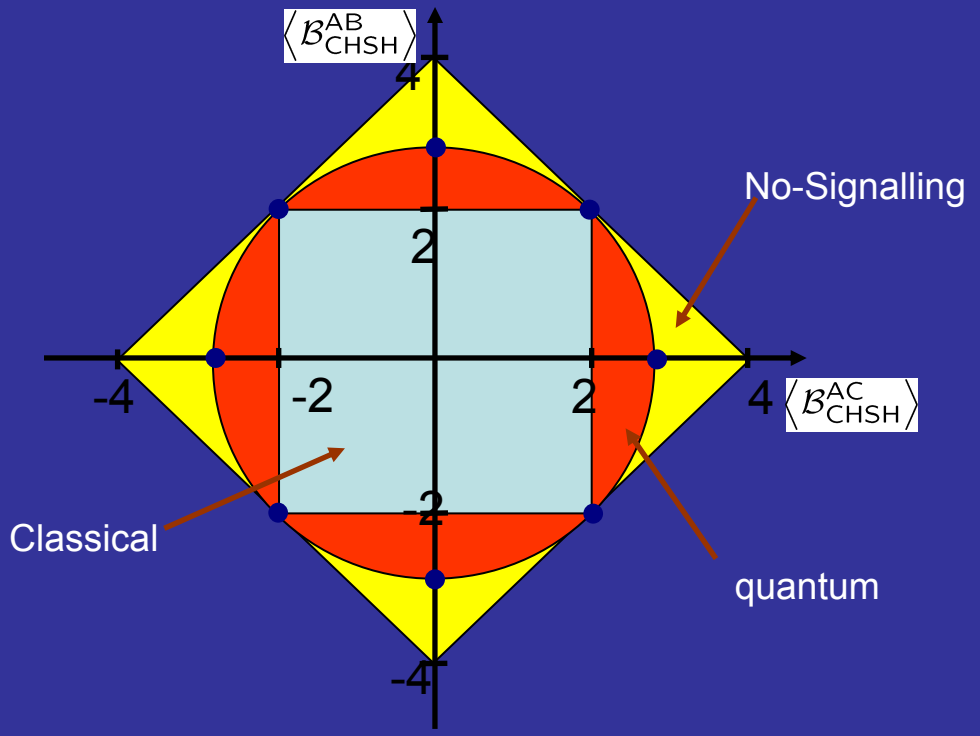
$$\sum_{i>1} C_{1i}^2 \leq 1 - \left\langle S_{\vec{n}}^1 \right\rangle^2$$

$$\langle C \rangle \leq \sqrt{\frac{1 - \left\langle S_{\vec{n}}^1 \right\rangle^2}{N}}$$

  - Is a nontrivial condition on the elements of the 2-particle reduced density operator -> what about analogue for fermions?

Monogamy of Bell correlations

- Monogamy of CHSH-Bell correlations is key ingredient of quantum cryptography



$$\beta(\rho) = \max_{-I \le A_i, B_i \le I} \langle A_1 \otimes (B_1 + B_2) + A_2 \otimes (B_1 - B_2) \rangle_\rho$$

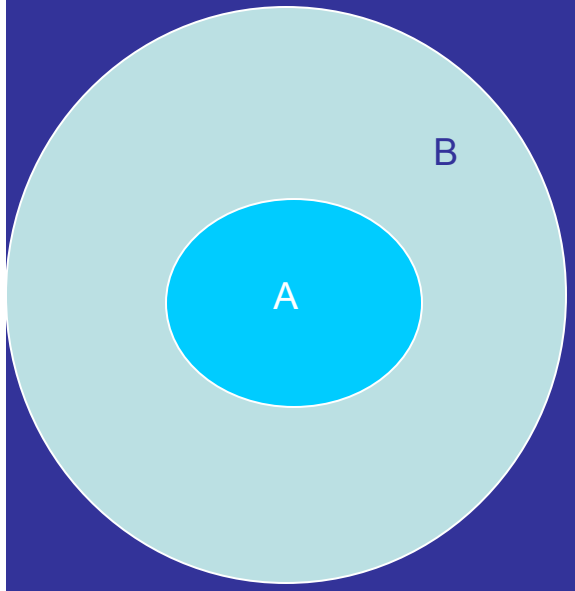
$$classical : \left| \langle \mathrm{B}^{AB}_{CHSH} \rangle \right| \le 2 \quad \text{and} \quad \left| \langle \mathrm{B}^{AC}_{CHSH} \rangle \right| \le 2$$

$$quantum : \langle \mathrm{B}^{AB}_{CHSH} \rangle^2 + \langle \mathrm{B}^{AC}_{CHSH} \rangle^2 \le 8$$

What makes ground states special?

- As we have seen yesterday: they have extremal local correlations compatible with some symmetry (e.g. translational invariance)
- We do not want to parameterize them with exponentially many parameters (size of Hilbert space)
- How to proceed?
    - Are there other properties that make ground states etc. special?
        - Area laws
        - Decay of correlations

Entanglement, correlations, area laws



Quantifying the amount of correlations between A and B: mutual information

$$I_{AB} = S(\rho_A) + S(\rho_B) - S(\rho_{AB})$$

All thermal states exhibit an exact area law (as contrasted to volume law)

$$\rho_{AB} \approx \exp(-\beta H)$$

$$F(\rho_A \otimes \rho_B) = Tr(H\rho_A \otimes \rho_B) - \beta S(\rho_A \otimes \rho_B) \geq Tr(H\rho_{AB}) - \beta S(\rho_{AB})$$

$$\Rightarrow I_{AB} \leq \frac{1}{\beta} Tr(H[\rho_A \otimes \rho_B - \rho_{AB}]) = \frac{1}{\beta} Tr(H_{AB}[\rho_A \otimes \rho_B - \rho_{AB}])$$

Cirac, Hastings, FV, Wolf

Similar results for ground states (critical systems might get logarithmic corrections)

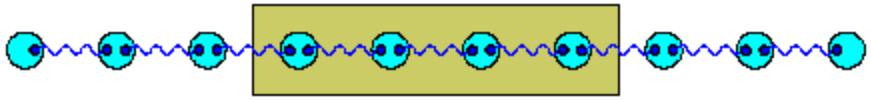
This is very ungeneric: entanglement is *localized* around the boundary

This knowledge is being exploited to come up with variational classes of states and associated simulation methods that capture the physics needed for describing such systems:

* Matrix Product States, Projected Entangled Pair States, MERA

Area laws

- Main picture: in case of ground states, entanglement is concentrated arou the boundary

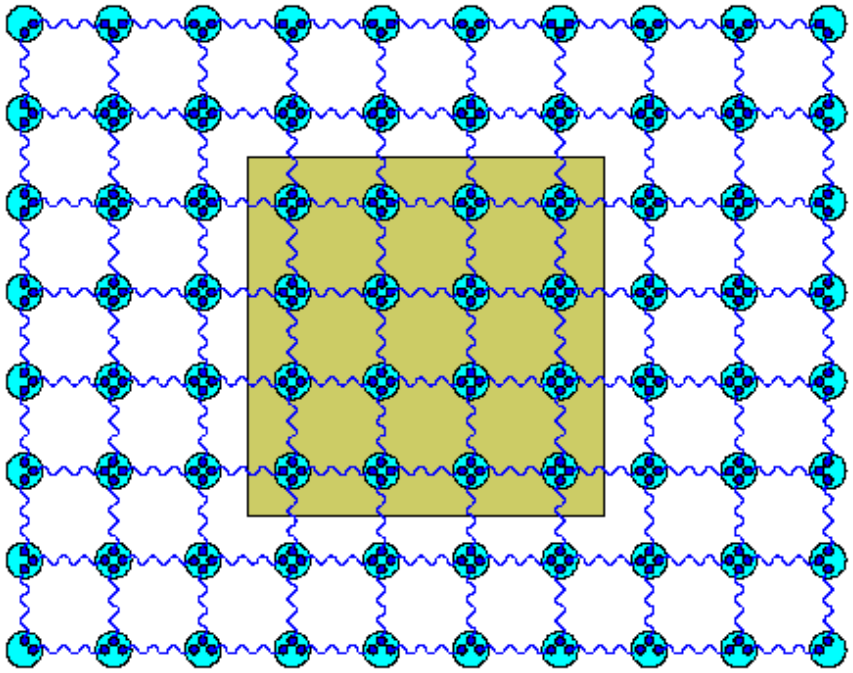


$$\text{Gapped}: \quad S(\rho_{1,2,\cdots,L}) \approx \frac{c+\bar{c}}{6}\ln(\xi)+\ldots$$

$$\text{Critical}: \quad S_\alpha(\rho_{1,2,\cdots,L}) \approx \frac{c+\bar{c}}{12}\left(1+\frac{1}{\alpha}\right)\ln(L)+\ldots$$

Kitaev, Vidal, Cardy, Korepin, …

- Rigorous proof for area law for any 1-D gapped spin system ! Hastings '0



$$\text{Gapped} \quad S(\rho_{1,2,\cdots,L^2}) \approx a.\mathrm{L}+\cdots$$

Critical

$$\text{Free fermions} \quad S(\rho_{1,2,\cdots,L^2}) \approx a.L\ln L+\ldots$$ Wolf, Klich

$$\text{Critical spin:} \quad S(\rho_{1,2,\cdots,L^2}) \approx a.L+\ldots$$ quant-ph/0601075

Topological entropy: detects topological quantum order locally!

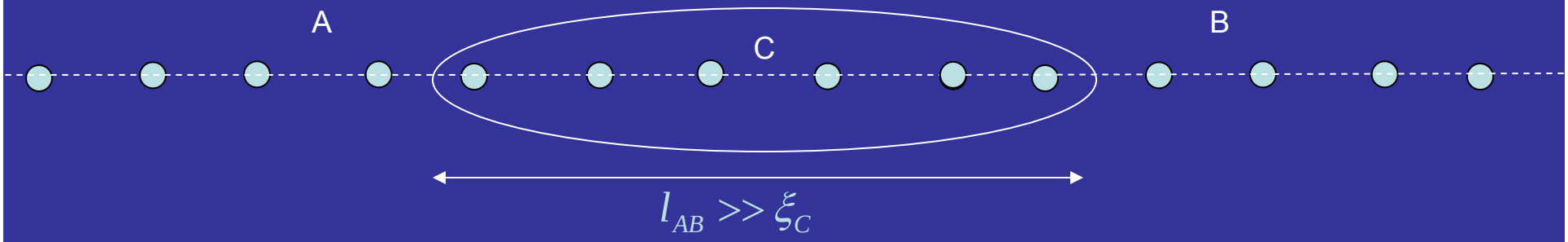
$$S(\rho_{ABC})-S(\rho_{AB})-S(\rho_{AC})-S(\rho_{BC})+S(\rho_A)+S(\rho_B)+S(\rho_C)$$

Kitaev, Preskill, Levin, Wen

Ground states of spin Systems

- Ground states of gapped local Hamiltonians have a finite correlation length:

$$\langle O_A O_B \rangle - \langle O_A \rangle \langle O_B \rangle \approx \exp\left(-\frac{l_{AB}}{\xi_C} \right)$$



- Let's analyze this statement from the point of view of quantum information theory, assuming that

$$\rho_{AB} \approx \rho_A \otimes \rho_B$$

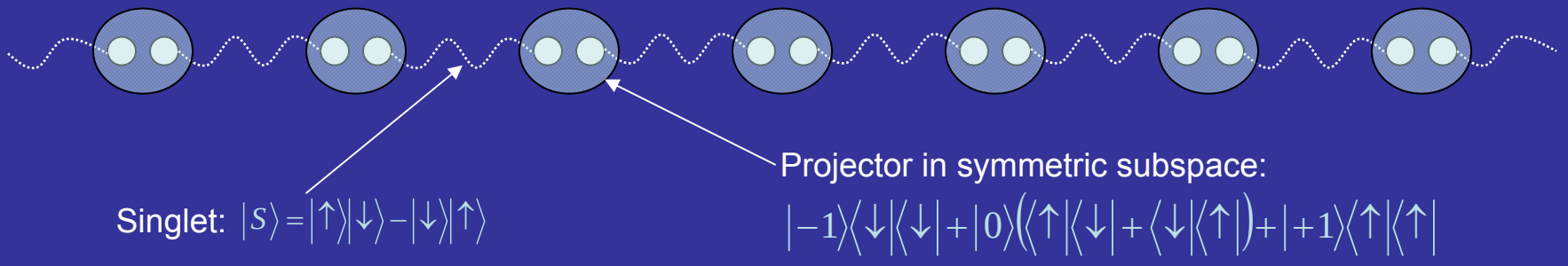
  - There is a separable purification of ρ_{AB} , so there exists a unitary in region C that disentangles the two parts
  - Blocking the spins in blocks of log(ξ_C) spins, then we can write the state as:

$$|\psi_{ABC}\rangle = \sum_{\alpha,\beta,i_l,i_r} U_{\alpha\beta}^{i_l i_r} |l_\alpha\rangle |i_l\rangle |i_r\rangle |r_\beta\rangle$$

  - Doing this recursively yields a matrix product state: $|\psi_{i_1 i_2 \ldots i_N}\rangle = \sum A^{i_1} A^{i_2} \ldots A^{i_N} |i_1\rangle |i_2\rangle \ldots |i_N\rangle$

Matrix Product States / Valence Bond States

$$H_{AKLT} = \sum_i \vec{S}_i . \vec{S}_{i+1} + \frac{1}{3} \sum_i \left(\vec{S}_i . \vec{S}_{i+1} \right)^2$$



I. Affleck, T. Kennedy, E.H. Lieb, H. Tasaki, Commun. Math. Phys. 115, 477 (1988)

- Translational invariant by construction
- Extremal local correlations
- Original motivation: quantum repeater (exploiting topological features)

Matrix Product States (MPS)

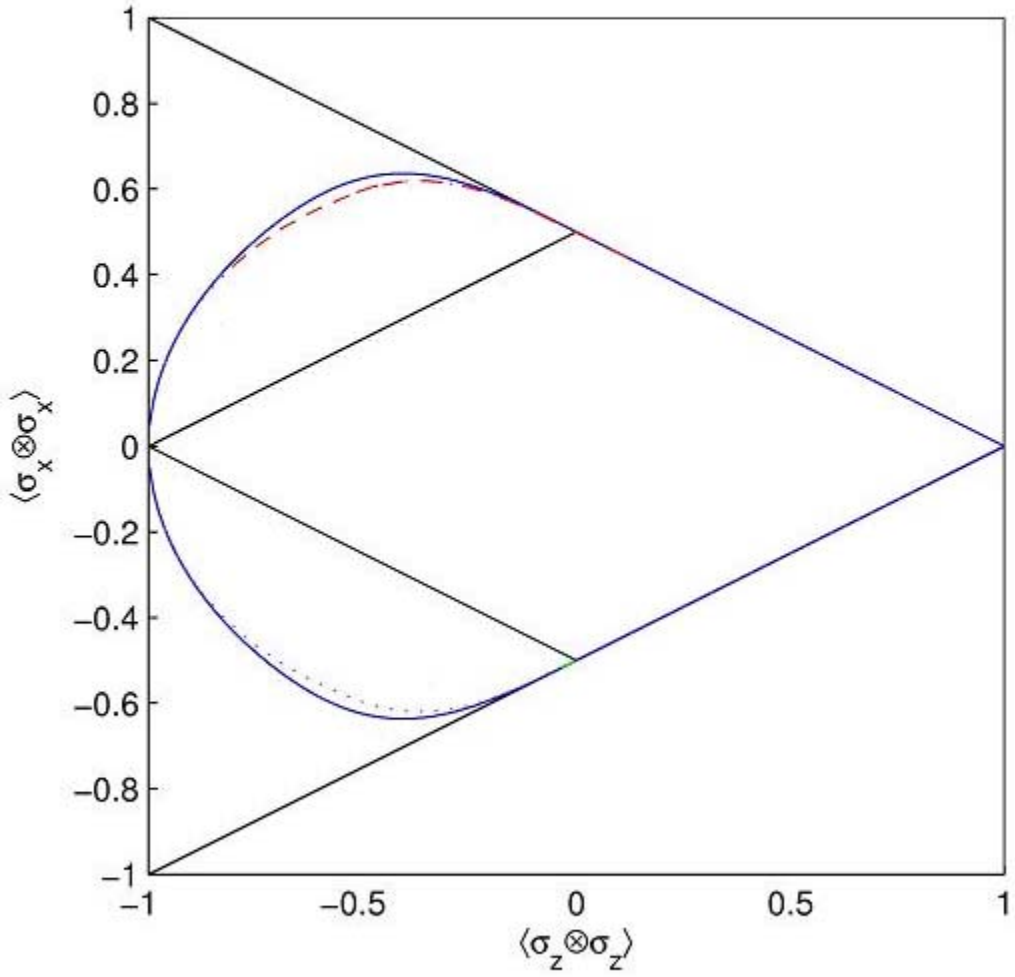
$$|I\rangle = \sum_{i=1}^{D} |i\rangle|i\rangle$$

$$\text{Map P} : H^D \otimes H^D \rightarrow H^d$$

State is defined on a d^N dimensional Hilbert space

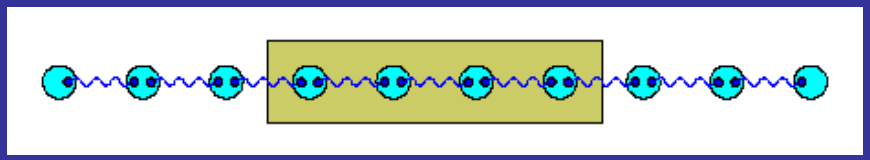
- Generalizations of AKLT-states (Finitely correlated states, Fannes, Nachtergaele, Werner '92)
- Gives a LOCAL description of a multipartite state
- Translational invariant by construction
- Guaranteed to be ground states of gapped local quantum Hamiltonians
- The number of parameters scales linearly in N (# spins)
- The set of all MPS is complete: *Every* state can be represented as a MPS as long as D is taken large enough
- The point is: if we consider the set of MPS with fixed D, their reduced density operators already approximate the ones obtained by all translational invariant ones very well (and hence also all possible ground states)
- MPS have bounded Schmidt rank D
- Correlations can be calculated efficiently: contraction of D^2x D^2 matrices
- Numerical renormalization group method of Wilson and Density matrix renormalization group method of S. White can be reformulated and improved upon as variational methods within class of MPS

Convex set of reduced density operators of ground states of XXZ-chains approximated with MPS of D=1,2



Matrix Product States

- If an area law applies, then a state can efficiently be parameterized by a so-called matrix product state (MPS) / valence bond state / finitely correlated state
  - MPS: most general state in 1-D that obeys a strict area law by construction: rank of reduced density operators is cst (D^2)



  - We want to bound the cost of approximating state that obeys area law with a MPS for given precision as a function of number of spins:

$$\left\| \left|\psi_{ex}^{N}\right\rangle - \left|\psi_{D}^{N}\right\rangle \right\| \leq \varepsilon \qquad\qquad D_N \leq \frac{cst}{\varepsilon} N^{f(c)}$$

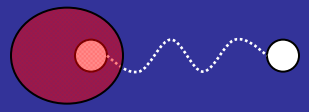
    - Breaking of exponential wall: polynomial vs. exponential complexity

- Complete identification of manifold of ground states of gapped quantum spin systems
  - DMRG, MPS-based algorithms: variational methods within this class of states!

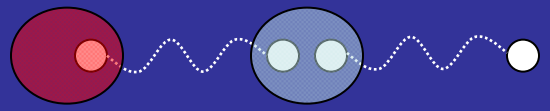
Wilson's numerical renormalization group

- Consider Kondo-impurity-like problem with Hamiltonian

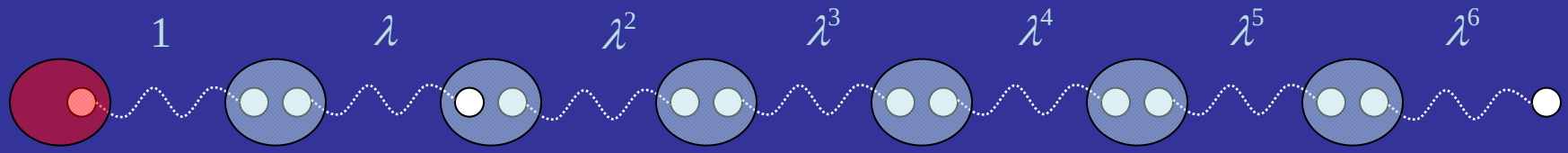
$$\mathrm{H} = \sum_{k=0}^{N} \lambda^k \left(\sigma_x^k \otimes \sigma_x^{k+1} + \sigma_y^k \otimes \sigma_y^{k+1} \right)$$



$$\left| \psi_\alpha^{[2]} \right\rangle = \sum_{i_1, i_2} A_{i_1 \alpha}^{i_2} \left| i_1 \right\rangle \left| i_2 \right\rangle$$



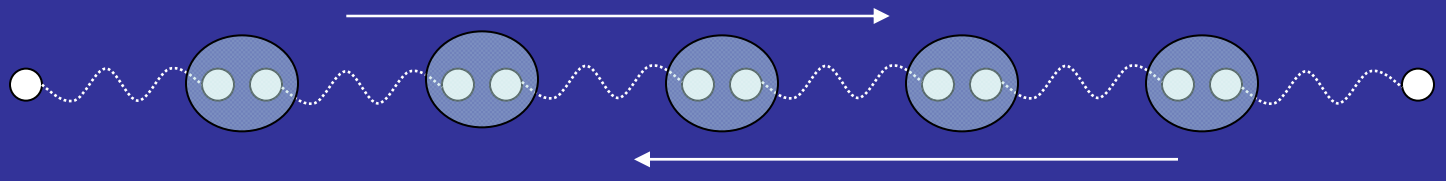
$$\left| \psi_\beta^{[3]} \right\rangle = \sum_{\alpha, i_3} A_{\alpha\beta}^{i_3} \left| \psi_\alpha^{[2]} \right\rangle \left| i_3 \right\rangle$$



$$\left| \psi_\tau^{[N]} \right\rangle = \sum_{\substack{i_1, i_2, \ldots \\ \alpha, \beta, \ldots}} A_{i_1 \alpha}^{i_2} A_{\alpha\beta}^{i_3} A_{\beta\gamma}^{i_4} \ldots A_{\sigma\tau}^{i_N} \left| i_1 \right\rangle \left| i_2 \right\rangle \ldots \left| i_N \right\rangle = \sum_{i_1, i_2, \ldots} A^{i_2} A^{i_3} A^{i_4} \ldots A^{i_N} \left| i_1 \right\rangle \left| i_2 \right\rangle \ldots \left| i_N \right\rangle$$

- NRG method creates an effective Hamiltonian which is the original Hamiltonian projected in a basis of matrix product states (MPS)
- Success of NRG follows from the fact that those MPS parameterize well the low-energy sector of the Hilbert space
- Main new ingredient from DMRG: sweep!

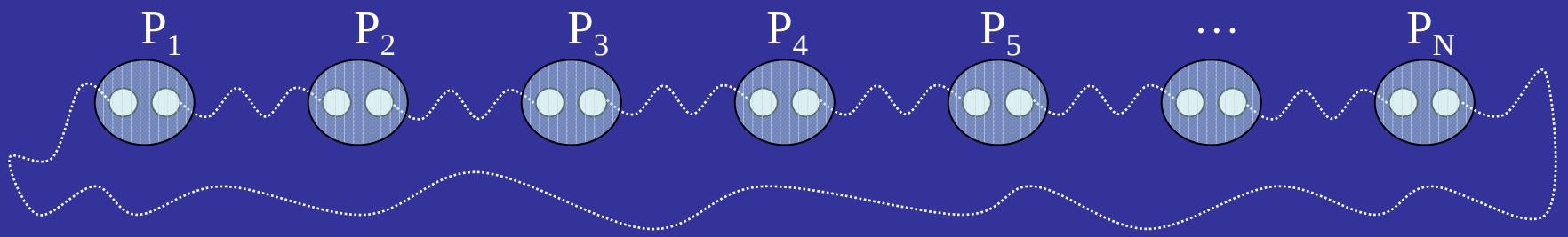
S. White's DMRG method

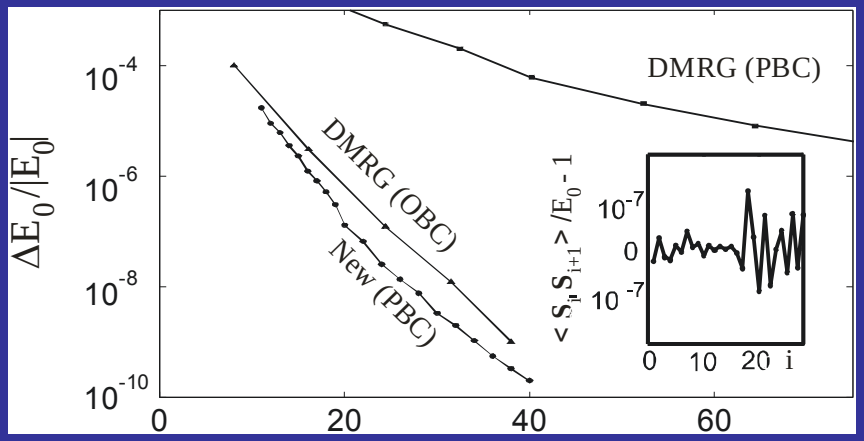


$$|\psi_j\rangle = \sum_{\alpha,\beta,i} [A_j^i]_{\alpha,\beta} |\alpha\rangle_j |i\rangle_j |\beta\rangle_j$$

$$H_{eff}^{new} = f(A_{j\pm1}^i, H_{eff}^{old}, H)$$

- Extending DMRG to periodic boundary conditions:





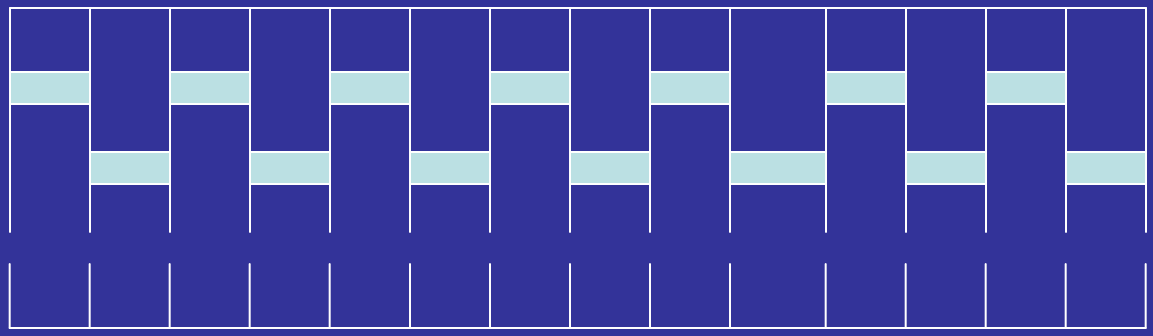
Variational dimensional reduction of MPS

- Given a D-dimensional $|\psi_D\rangle$ MPS parameterized by the DxD matrices A^i, find $|\chi_{D'}\rangle$ parameterized by D'xD'matrices B^i (D'< D) such as to minimize

$$\left\| |\psi\rangle - |\chi\rangle \right\|^2 = \mathrm{Tr}\left[\left(\sum_i B_1^i \otimes B_1^i \right) \left(\sum_i B_2^i \otimes B_2^i \right) \cdots \left(\sum_i B_N^i \otimes B_N^i \right) \right]$$
$$- 2\mathrm{Tr}\left[\left(\sum_i B_1^i \otimes A_1^i \right) \left(\sum_i B_2^i \otimes A_2^i \right) \cdots \left(\sum_i B_N^i \otimes A_N^i \right) \right] + cst$$

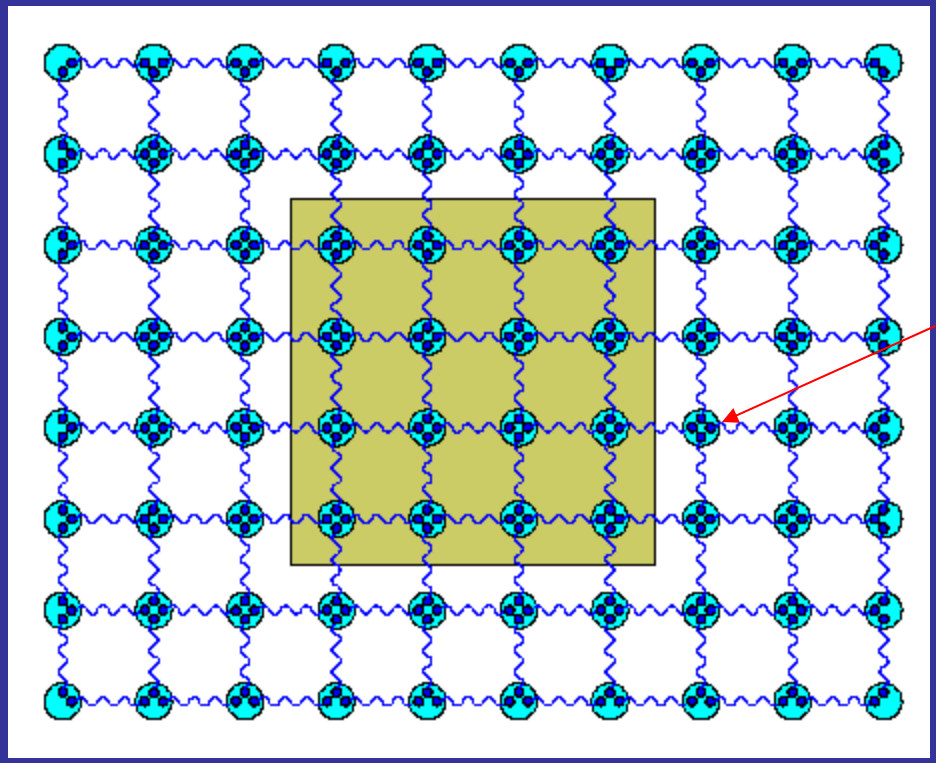
  - Can be minimized variationally by iteratively solving linear systems of equations

- This can be used to describe both real and imaginary time-evolution



Generalizations of MPS to higher dimensions

- The MPS/AKLT picture can be generalized to any geometry : Projected Entangled Pair States (PEPS)

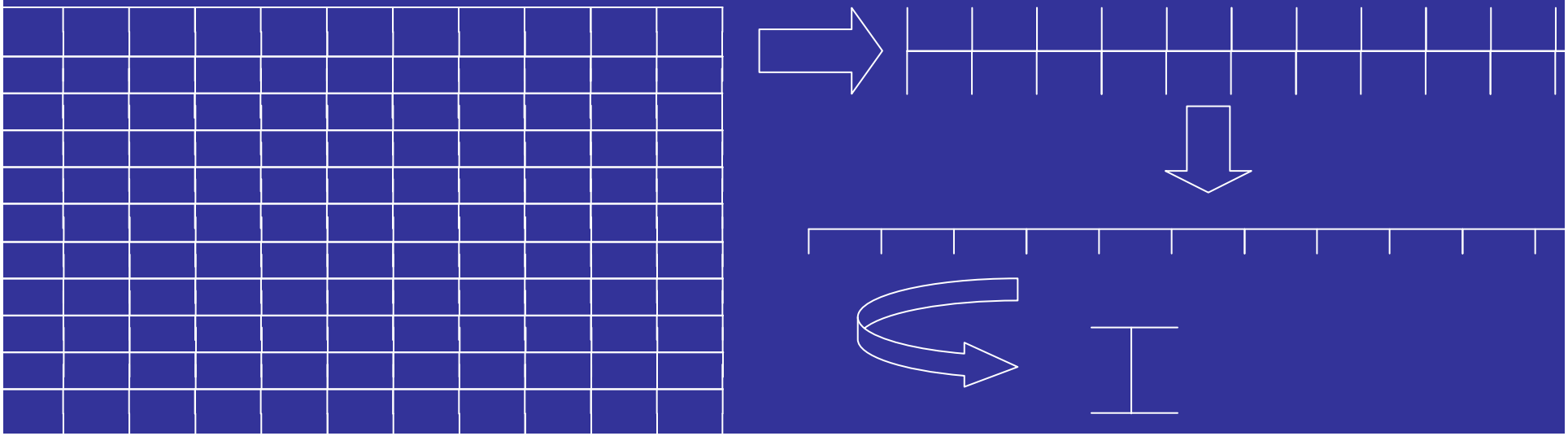


- Properties: Area Law automatically fulfilled; local properties can be approximated very well ; guaranteed to be ground states of local Hamiltonians; again, every state can be written as a PEPS

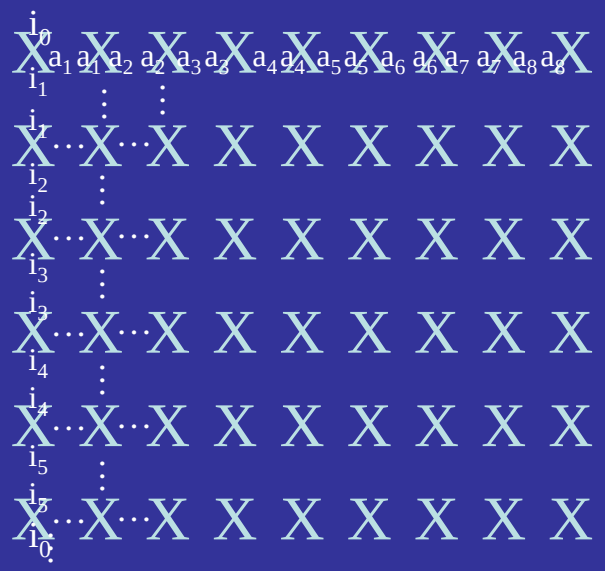
- A variational approach based on those states provides a solution to the problem of the numerical renormalization group approach where the number of degrees of freedom of a block grows exponentially with the size of the block

Holographic principle: dimensional reduction

- Crucial property of MPS/PEPS: dimensional reduction
  - Start from quantum system in 2 dimensions (2+1)
  - The PEPS ansatz maps the quantum Hamiltonian to a state corresponding to a partition function in 2 dimensions (2+0)
  - The properties of such a state are described by a (1+1) dimensional theory (eigenvectors of transfer matrices)
  - Those eigenvectors are well described by MPS
  - Properties of MPS are trivial to calculate: reduction to a partition function of a 1-D system (1+0)



- How to calculate correlation functions?
  - Instead of contracting matrices, we have to contract tensors:



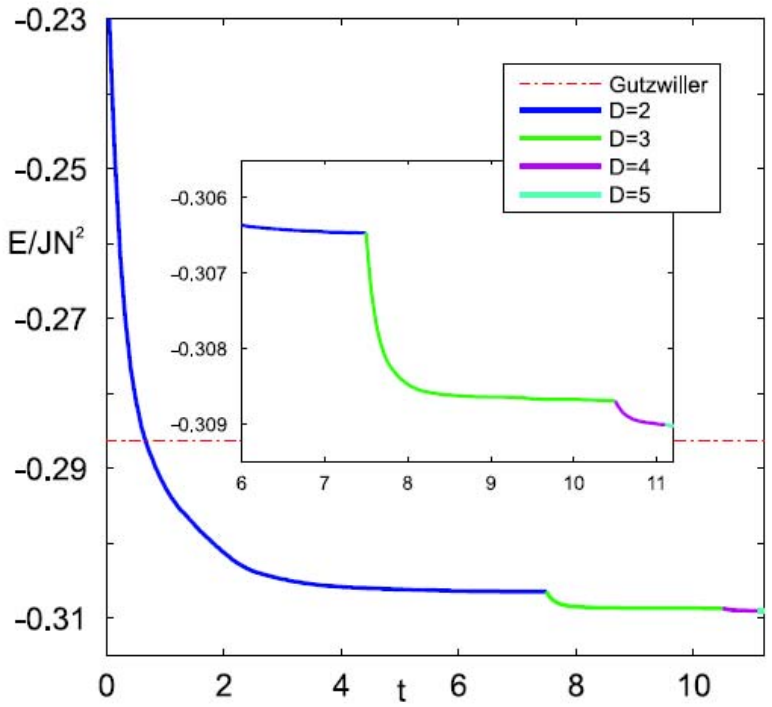


FIG. 4: Energy as a function of time for the imaginary time–evolution of the system of hard–core bosons on a 11×11–lattice. The evolutions are performed sequentially with PEPS of virtual dimension $D = 2$, $D = 3$, $D = 4$ and $D = 5$. For comparison, the energy of the optimal Gutzwiller ansatz is included.

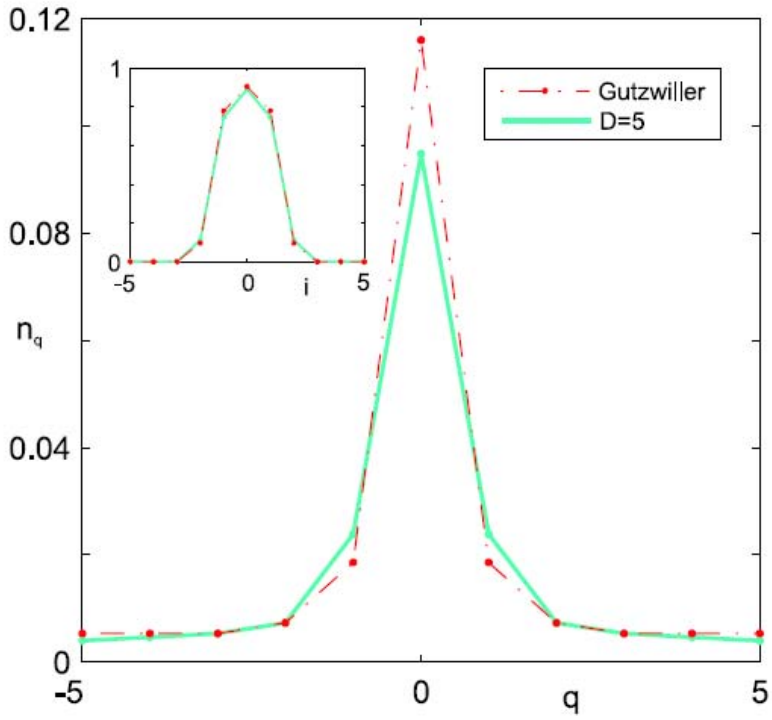


FIG. 5: (Quasi)–momentum distribution of the particles in the ground state of a 11×11–lattice. Plotted are results of the variational calculations with PEPS of dimension $D = 5$ and with the Gutzwiller ansatz. From the inset, the density of the particles can be gathered.

V. Murg, FV, I. Cirac

Examples of PEPS

- Cluster states of Briegel and Raussendorf are PEPS with D=2: allow for universal quantum computation with local measurements only. We can also construct other states that are universal using PEPS
- PEPS with topological quantum order:
  - Toric code states of A. Kitaev (D=2): fault-tolerant quantum memory
  - Resonating valence bond states (D=3)

- PEPS with D=2 can be critical: power law decay of correlations
  - Many examples can be constructed by considering coherent versions of classical statistical models:

$$|\Psi\rangle \propto \sum_{\sigma_1\sigma_2\cdots\sigma_N} \exp\left[-\frac{\beta}{2}\sum_{\langle i,j\rangle}\sigma_i\sigma_j\right]|\sigma_1\rangle|\sigma_2\rangle\cdots|\sigma_N\rangle$$

  - Resolves open question about scaling of entanglement in critical 2-D quantum spin systems: no logarithmic corrections
  - PEPS construction shows that for every classical temperature-driven phase transition there exists a quantum spin model in the same dimension exhibiting a zero-T quantum phase transition with same features

- PEPS provide perfect playground for considering open questions like existence of deconfined criticality: all PEPS are ground states

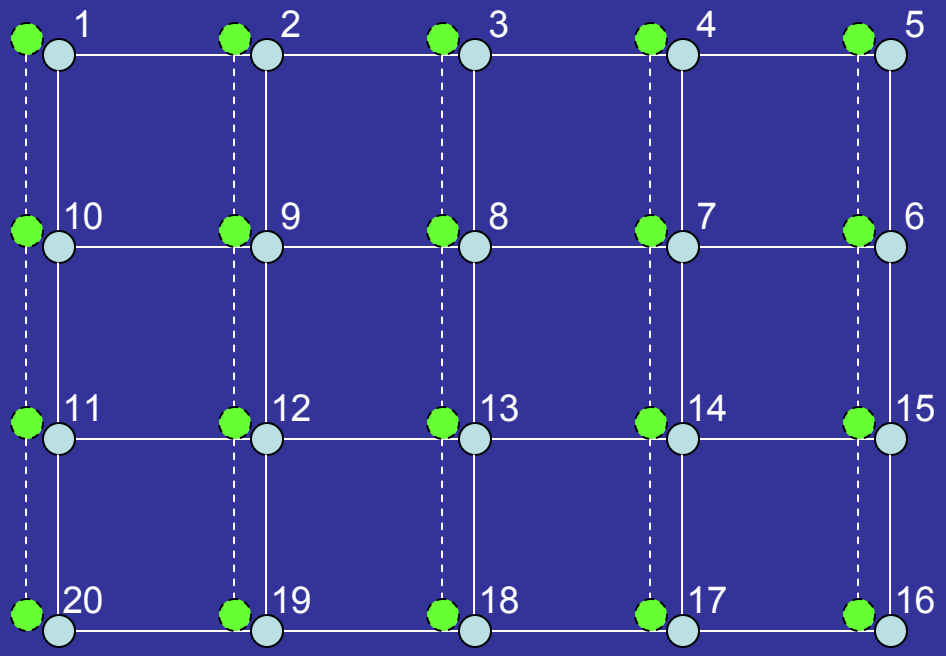
Interludum: fermionic systems vs. spin systems

- Fundamental question: are fermions fundamentally different from bosons/spins or can local fermionic Hamiltonians be understood as effective Hamiltonians describing low energy sector of specific local spin systems?
- Hilbert space associated to fermions is Fock space, which is obtained via second quantization:

$$|\Psi\rangle = \sum_{i_1 i_2 \ldots} c_{i_1 i_2 \ldots} \left(a_1^*\right)^{i_1} \left(a_2^*\right)^{i_2} \ldots |\Omega\rangle$$

- What we want to approximate is $c_{i_1 i_2 \ldots}$
- Effective Hamiltonian for this tensor is obtained by doing the Jordan-Wigner transformation on the original one (note the ordering of the fermions in second quantization)
- Consider hopping terms in 2-D: J-W induces long-range correlations
- Solution: use auxiliary Majorana fermions to turn this Hamiltonian into a local Hamiltonian of spins (cfr. Kitaev)

- Similar approach taken by X.G. Wen to show how fermions and actually all fundamental particles can be understood as emerging from some much simpler bosonic model



FV, Cirac '06

Vertical hopping terms become nonlocal by JW-transformation:

$$a_1^\dagger a_{10} + a_{10}^\dagger a_1 \xrightarrow{JW} \sigma_1^x \left(\bigotimes_{k=2}^{9} \sigma_k^z \right) \sigma_{10}^x + \sigma_1^y \left(\bigotimes_{k=2}^{9} \sigma_k^z \right) \sigma_{10}^y$$

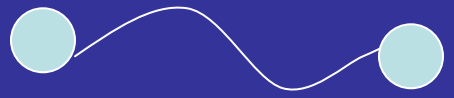
Solution: add ancillary chains of free fermions b_i constructed as follows: define Majorana fermions $c_i = b_i + b_i^\dagger$, $d_i = i(b_i - b_i^\dagger)$ and free Hamiltonian

$$H_{anc} = -\sum_{\langle k,l \rangle} i c_k d_l$$

As all terms $ic_k d_l$ are constants of motion (i.e. +1) and commute with each other, we can change the original vertical hopping terms $a_1^\dagger a_{10} + a_{10}^\dagger a_1 \longrightarrow \left(a_1^\dagger a_{10} + a_{10}^\dagger a_1 \right) ic_1 d_{10}$ without changing the physics of the Hamiltonian. Renumbering everything makes everything local after the JW

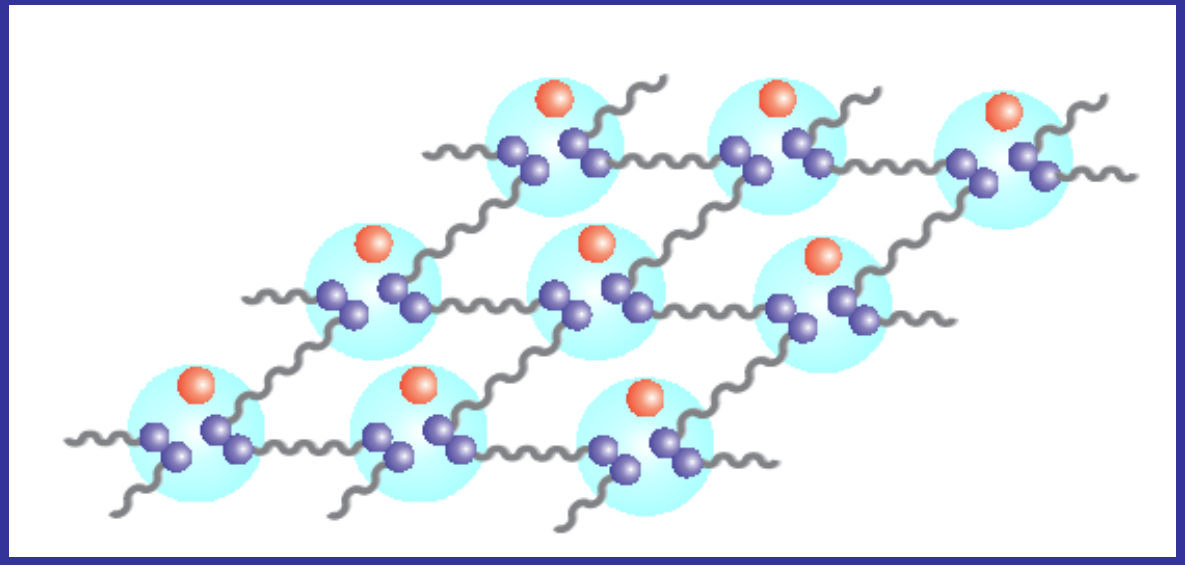
Fermionic PEPS

- How to build ansatz states for fermionic systems?
  - Instead of taking maximally entangled spins as building blocks, take Cooper pair type maximally entangled fermions



$$\left(I + a^* b^*\right)\left|\Omega\right\rangle$$

  - As a projector, take any parity-preserving map (i.e. a linear map that e.g. maps 1 fermion to 1 and 2 to 0 or 2).
    - Must be so because of locality reasons!



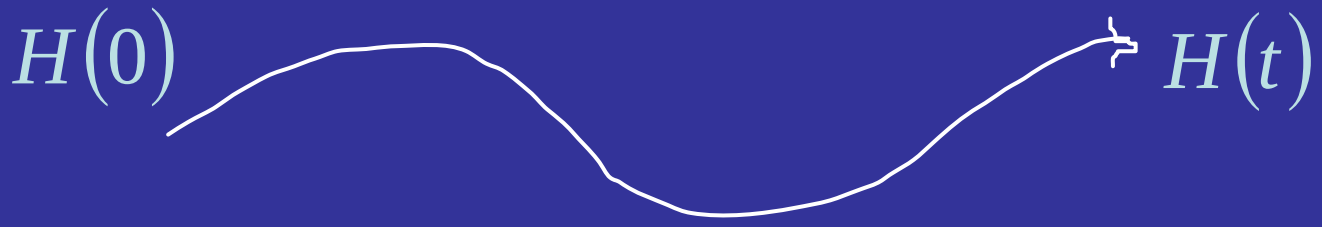
arXiv:0904.4667

Connection to real-space renormalization group transformations?

- We have already seen that DMRG of White is a variational variant of NRG of Wilson; what about other real-space RG methods?
- Connection is via quantum circuits
  - Cfr: physical Hilbert space is tiny submanifold of whole Hilbert space
  - can be parameterized by quantum circuits!

Quantum simulators for finding ground states: adiabatic time evolution

Farhi et al.'00



- Adiabatically following the ground state of a Hamiltonian; adiabatic condition:

$$T >> \min_s \frac{\Gamma(s)}{\Delta(s)^2} \qquad \Gamma(s) = \left\langle \left(\frac{dH}{ds} \right)^2 \right\rangle - \left\langle \frac{dH}{ds} \right\rangle^2$$

- That means: we can prepare ground state in phases different from the one we start from on a QC if no level crosssing and/or gap scales polynomial in system size

- This suggests that a very good way of representing ground states can be found using a quantum circuit!

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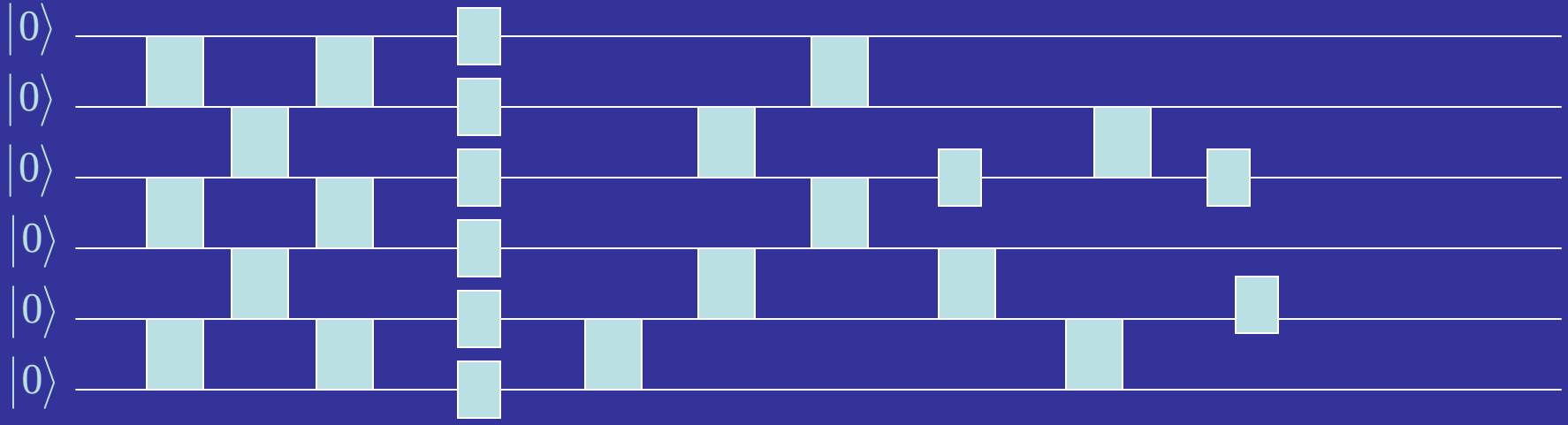
Quantum Circuits

- Quantum circuit is a representation of every possible Hamiltonian evolution



- What kind of quantum circuits are needed to prepare ground states of general Hamiltonians?
  - Find inspiration in field of renormalization group methods and perturbation theory

Renormalization group methods as quantum circuits

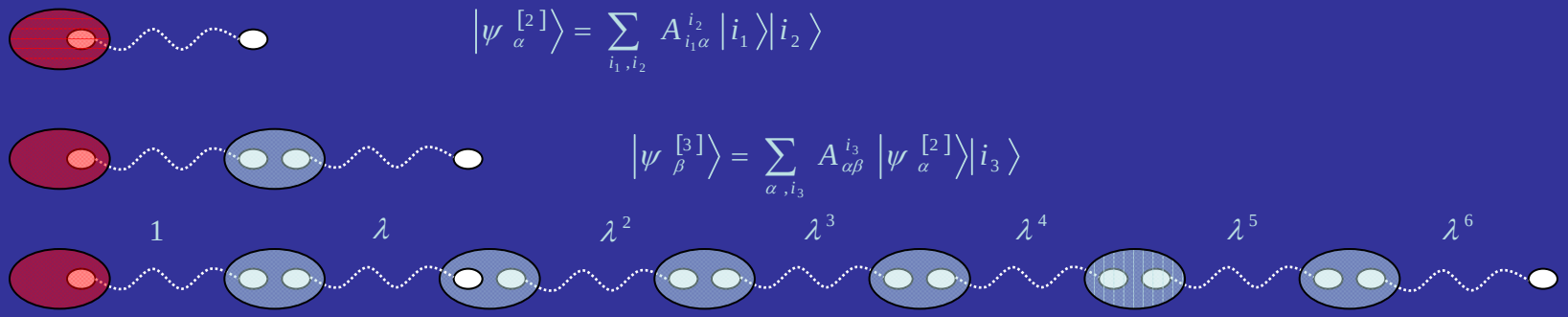
- General theme:
  - All successful RG-methods can be understood as the construction of simple quantum circuits to parameterize low-energy manifold
  - Those quantum circuits can be simulated efficiently in a classical way

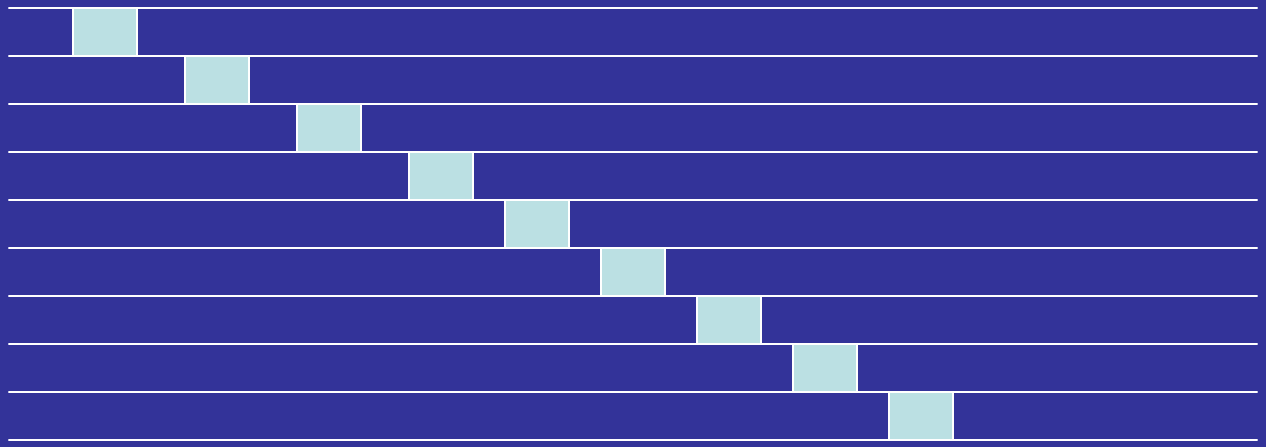
- For strongly correlated quantum spin systems, we can go beyond that as first implicitly done by S. White: take these classes of states seriously, and do variational calculations within those classes of states

    - Case of 1D MPS / Finitely correlated states: DMRG
      - Extensions to 2D: PEPS
    - Case of DMF: MERA

RG-methods as quantum circuits

- Numerical renormalization group:





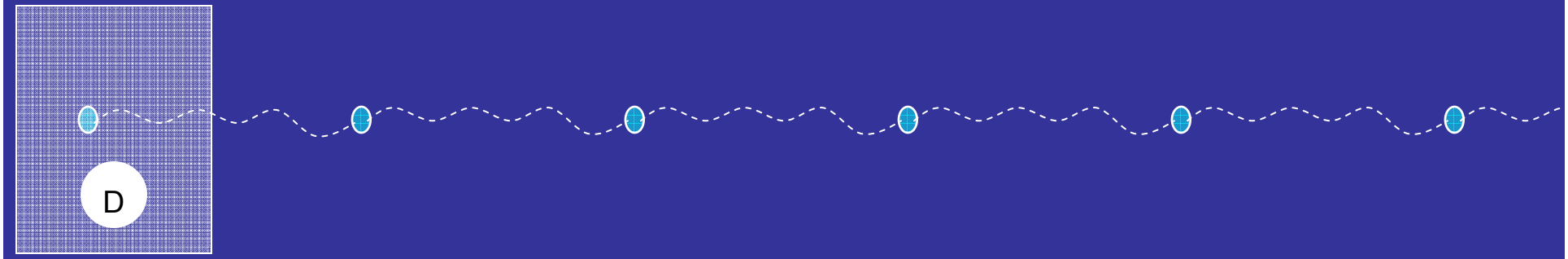
Class of states generated like this:

Matrix Product States

Virtue: possible to calculate any tensor product expectation value efficiently -> quantum circuit that can be simulated efficiently on a classical computer

RG quantum circuit in the lab

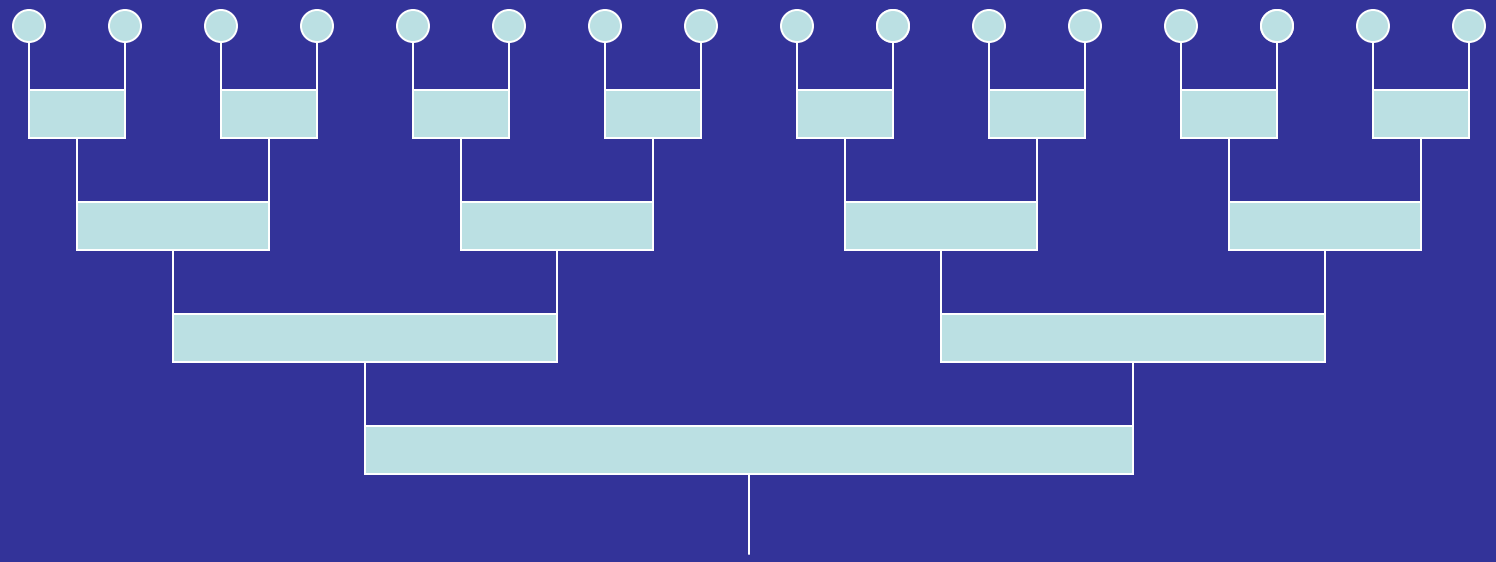
- Class of D-dim. MPS gives a complete characterization of all N-particle states that can be created by sequential generation through coupling to a D-level ancillary system (Markov chain)
  - Photonic qubits generated by a cavity QED source
  - Quantum dot coupled to a microcavity
  - Interaction of ions with phonons in ion trap



- 1-to-1 correspondence between maps P and unitaries occurring in “cavity”
  - Constructive: MPS-structure automatically yields description of how to generate states
- Example for D=2: GHZ-, cluster-, W- states

C. Schoen, E. Solano, F. Verstraete, J. I. Cirac, M. M. Wolf ‘05

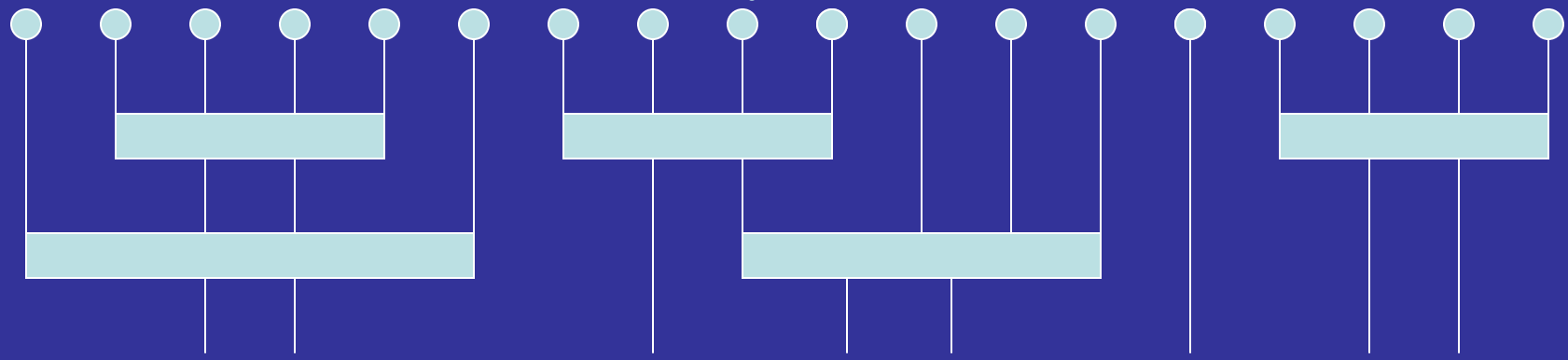
Coarse-graining real-space RG methods



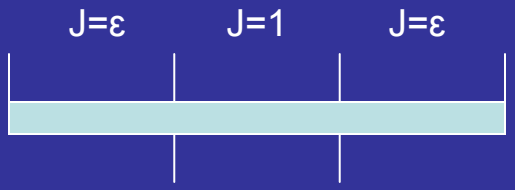
- Properties: block entanglement entropy can grow logarithmically with system size over some cuts
- explicit breaking of translational invariance
- Cannot be readily extended to 2D (entropy too small)
- One can do DMRG on such states in exactly the way you do it on MPS

- Other RG schemes: Ma-Dasgupta-Fisher renormalization group
  - Random Heisenberg model

$$H = \sum_{<ij>} J_{ij} \vec{S}_i . \vec{S}_j$$

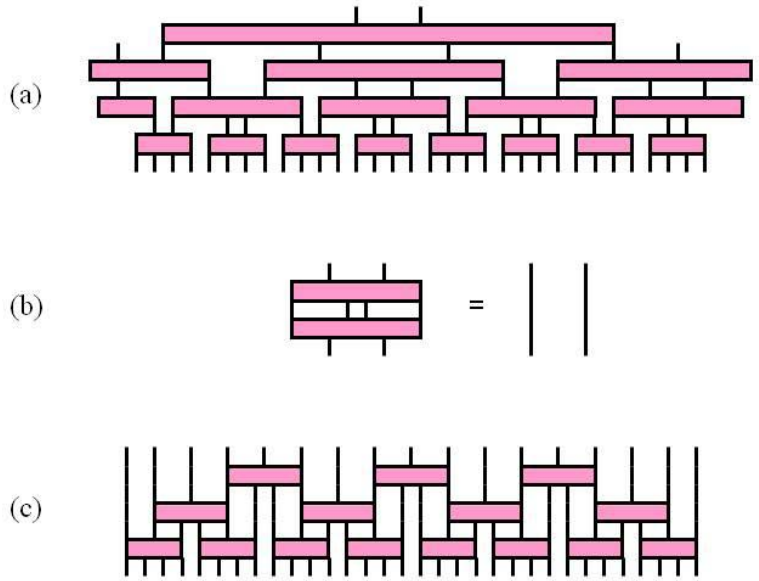


  - Second order perturbation theory:



$$\begin{bmatrix} -\varepsilon^2 AB^{-1}A^* & O(\varepsilon^3) \\ O(\varepsilon^3) & Q \end{bmatrix} = \begin{bmatrix} I & \varepsilon X \\ -\varepsilon X^* & I \end{bmatrix} \begin{bmatrix} 0 & \varepsilon A \\ \varepsilon A^* & B \end{bmatrix} \begin{bmatrix} I & -\varepsilon X \\ \varepsilon X^* & I \end{bmatrix}$$

  - This is a smarter way of blocking as it preserves locality (mapping of e.g. 4 spins to 2 but in such a way that locality is preserved)

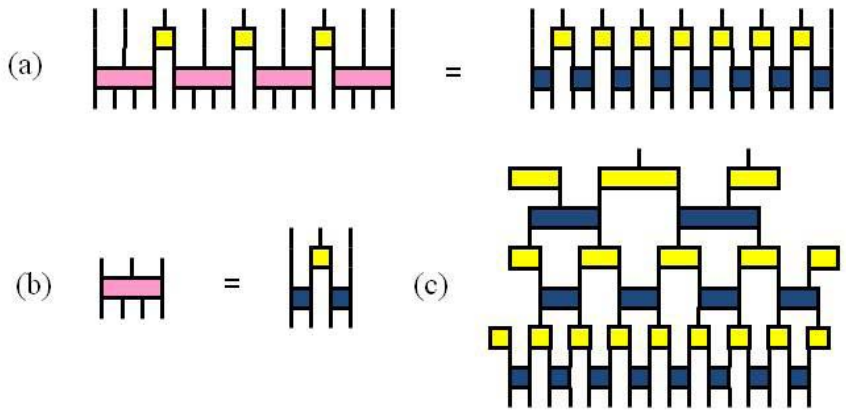


States obtained in Ma-Dasgupta-Fisher RG:

- can violate area laws in 1D
- can be extended to 2D
- critical exponents can be obtained by looking at fixed points of rescaling transformations

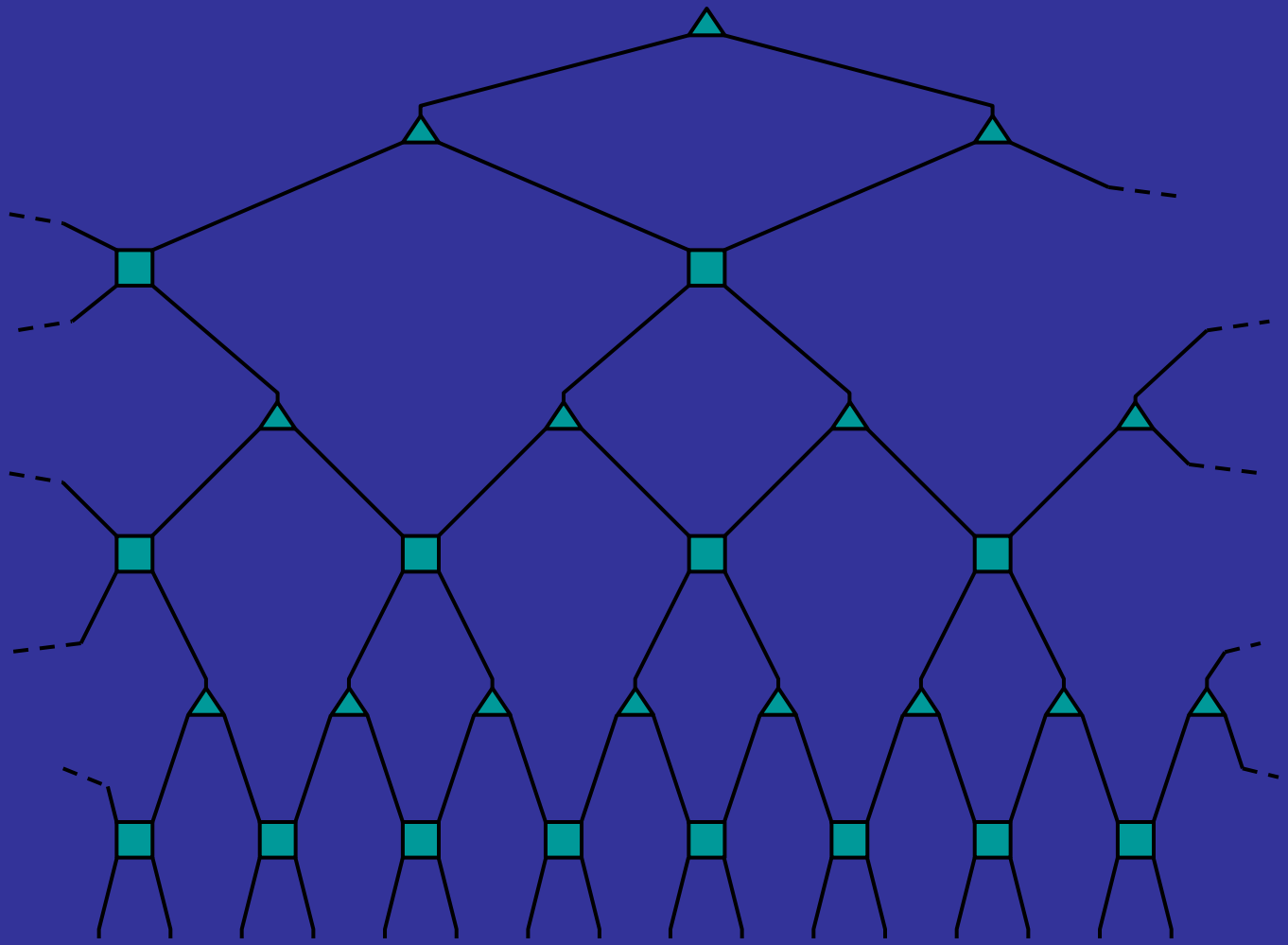
Multiscale Entanglement Renormalization Ansatz (MERA) of Vidal can be reinterpreted as a formalization of this class of Ma-Dasgupta-Fisher states

Lesson teached to us by Steven White: take a RG method, look at the structure of the underlying states, and do a variational calculation over this class of states



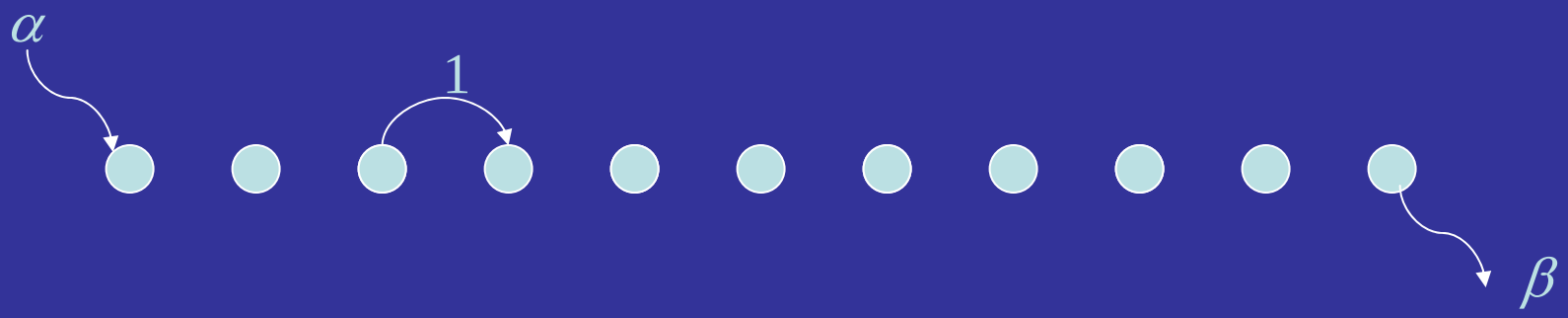
MERA: coarse-graining of lattice

Vidal '06

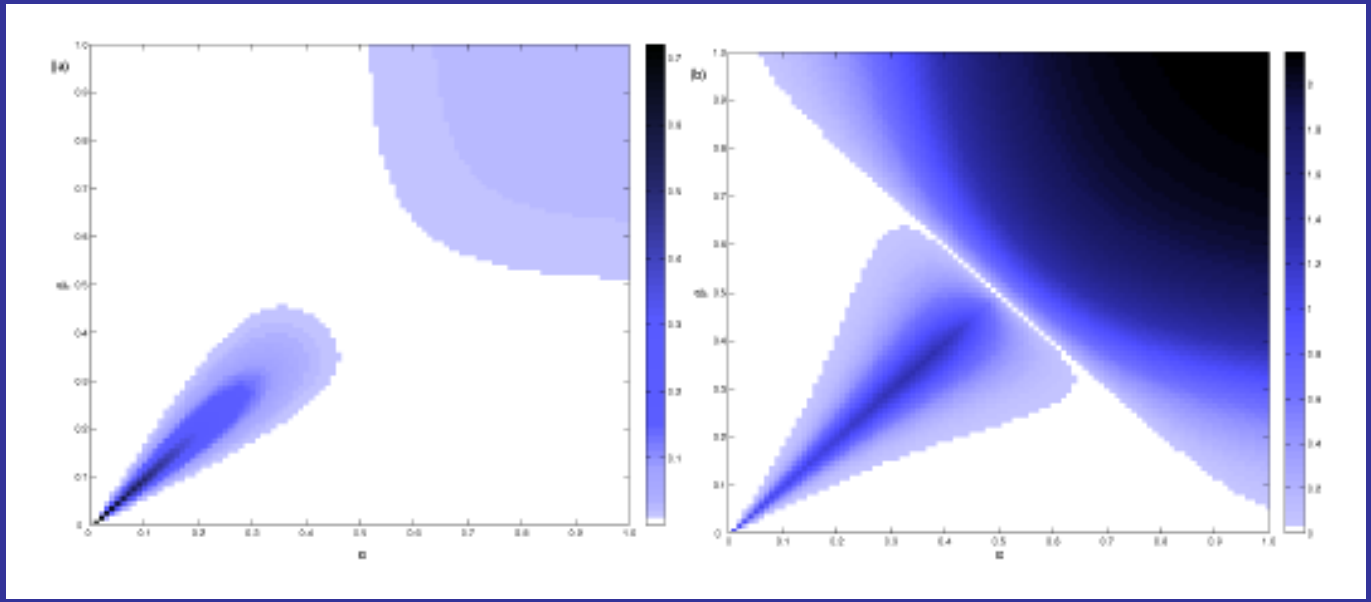


- What about scale-invariant states for fermions: OK Corboz, Evenbly, FV, Vidal '09
- PS: all MERA states obey strict area law in dimensions>1

What happens for non-equilibrium systems?



- Quantum circuits with CP-maps instead of unitaries
- Can again be very well described by MPS; figure of merit is the so-called common information or the entanglement of purification



Mutual information and entropy cost / entanglement of purification as a function of α, β

Quantum circuits for diagonalizing Hamiltonians

- One can in principle go further and try to diagonalize a complete Hamiltonian using a quantum circuit (cfr. Original approach of Wilson and Ma-Dasgupta-Fisher)
  - Possible if all low-energy states are “special”

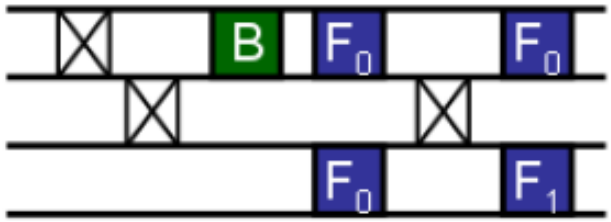
$$UHU^{*} = H_{coarse-grained}$$

  - Should in principle be possible for all cases where the low-energy sector can be described by a system of quasi-particles
    - Simple example: XY or Ising model in transverse field in 1-D:

$$H_{eff} = UH_{XY}U^{*} = \sum_{i} \omega_i \, \sigma_i^z$$

Example: Ising and XY-model in transverse field

$$\mathcal{H}_{XY} = \sum_{i=1}^{n} \left(\frac{1+\gamma}{2} \sigma_i^x \sigma_{i+1}^x + \frac{1-\gamma}{2} \sigma_i^y \sigma_{i+1}^y \right) + \lambda \sum_{i=1}^{n} \sigma_i^z$$

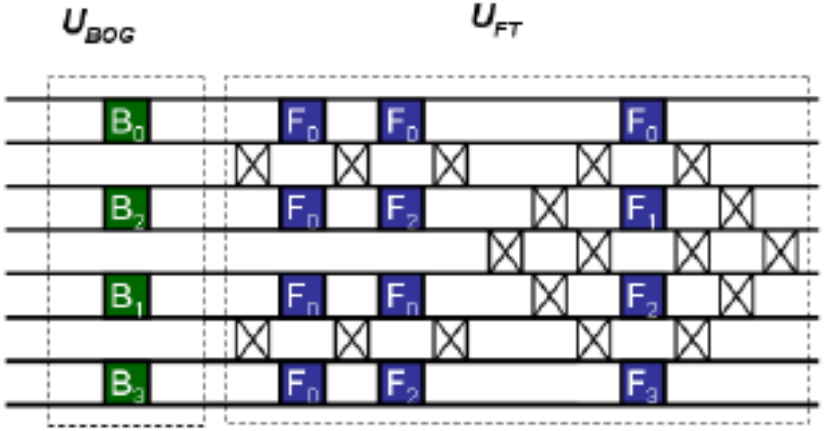


$$U_{SWAP} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

$$B_k = \begin{pmatrix} \cos\theta_k & 0 & 0 & i\sin\theta_k \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ i\sin\theta_k & 0 & 0 & \cos\theta_k \end{pmatrix}$$

$$F_k = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{\alpha(k)}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} & -\frac{\alpha(k)}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & -\alpha(k) \end{pmatrix}$$

$$\alpha(k) = \exp(i2\pi k/n)$$



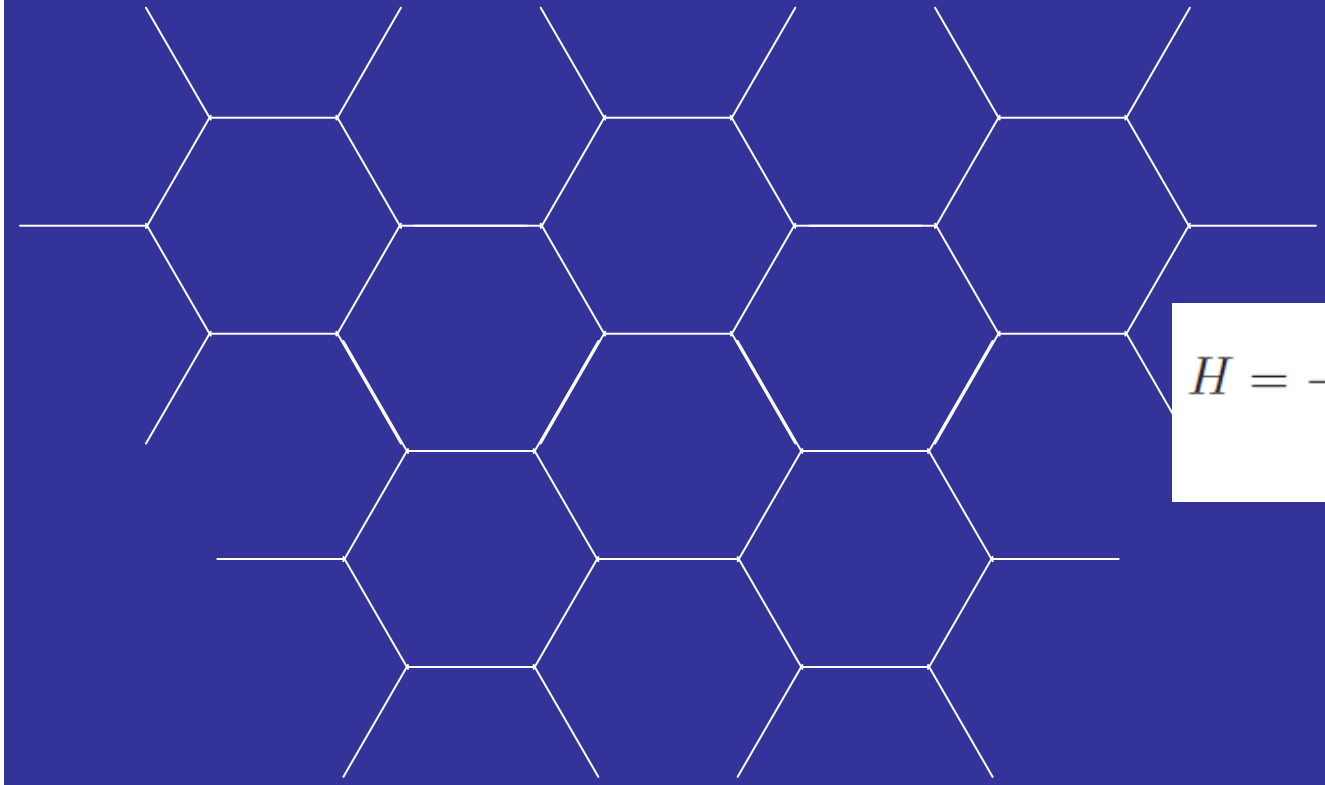
$$H_{eff} = UH_{XY}U^* = \sum_i \omega_i \sigma_i^z$$

- Clearly, full simulaton can be done of any time evolution, thermal states can be prepared, …if this quantum circuit has been determined

Cirac, Latorre, FV ‘08

Real space RG transformation on the toric code Hamiltonian

- Consider Kitaev's toric code Hamiltonian on a hexagonal (honeycomb) lattice with 3-body vertex terms and 6-body plaquette terms



$$H = -J \sum_{\text{plaq}} Z^{\otimes 6} - J \sum_{\text{vertex}} X^{\otimes 3}$$

- Is this Hamiltonian a fixed point of some real-space RG transformation? Certainly OK for ground state which has zero-correlation length

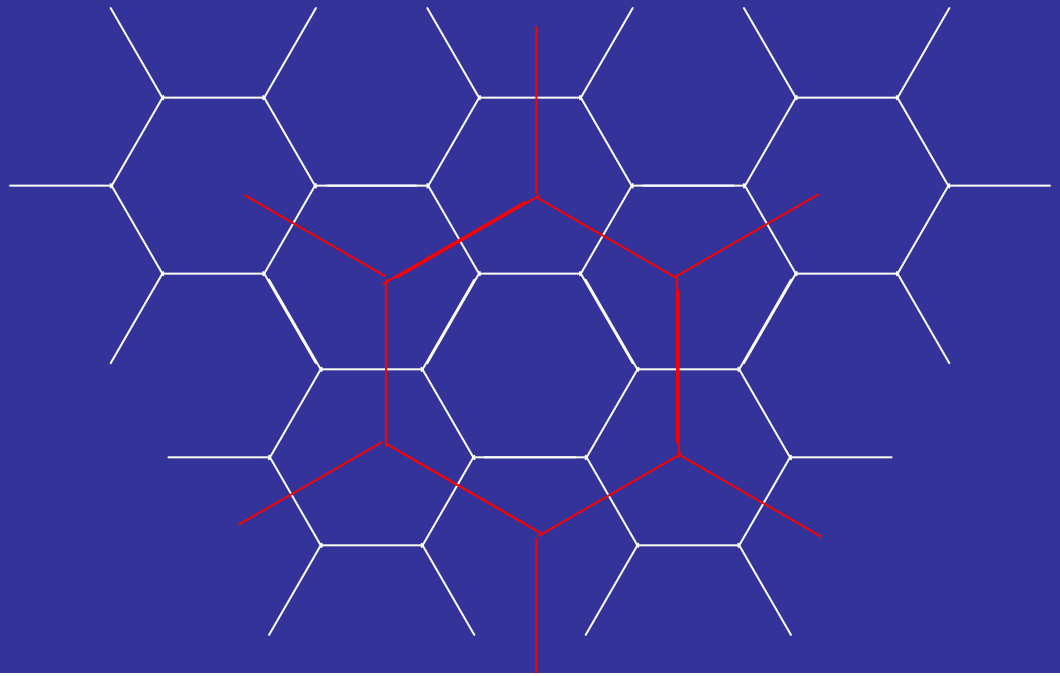
- Any Hamiltonian that only consists of frustration-free commuting terms is probably fixed point of some RG

- Possible formalism for defining real-space RG on Hamiltonians of quantum lattice systems:
  - Apply unitary transformations on local blocks such that quantum degrees of freedom are turned into classical degrees of freedom

$$UH_kU^* \approx \lambda\, Z \otimes \mathrm{I} + \lambda'\, Z \otimes \mathrm{H}' + \lambda''\, \mathrm{I} \otimes \mathrm{H}''$$

$$H_{k+1} \approx \lambda'\, \mathrm{H}' + \lambda''\, \mathrm{H}''$$

  - This can be done exactly on the toric code Hamiltonian: coarse-graining a 12-qubit cluster to a 6-qubit one:



- There are now 2 obvious approaches that one can take
  1. Study the RG flow when adding a magnetic field
  2. Study the RG flow at finite T

- Finite-T flow: do the unitary transformation, trace out the *classical* degrees of freedom, and calculate new effective temperature.
  - For low T:

$$\beta_{\text{eff}} = \beta - \frac{3}{4}\log 2$$

  - As expected, you flow away from the zero-T fixed point and there is no finite-T phase transition that can be detected
  - Situation in 3D and 4D should be different: the disentangling couples excitations with each other, which can lead to a decrease of T during the RG flow

Can we characterize all the possible fixed point Hamiltonians of such RG transformations ?

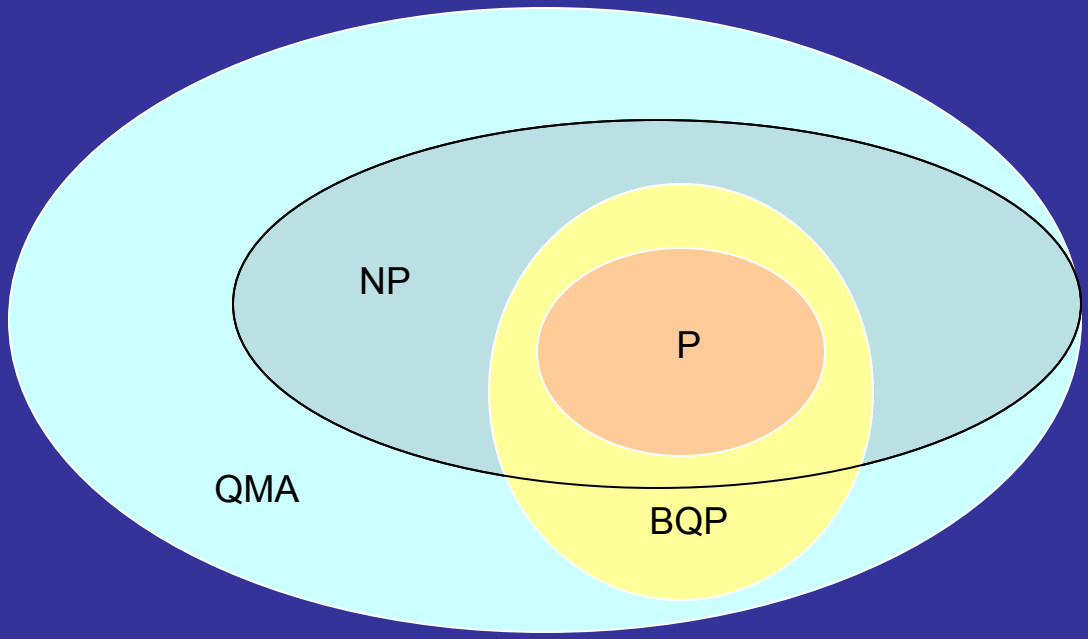
Quantum many-body systems and computational complexity

- Open question: what is the difficulty of finding ground states of many-body quantum systems?
  - Finding approximate solutions of many-body Hamiltonians has been the central problem in quantum mechanics since 75 years

    "The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble. It therefore becomes desirable that approximate practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation." (Dirac, 1929)

- Obvious that a brute force approach scales exponentially in the number of particles; we have seen that in principle you can do better (breaking of exponential wall), but can we proof this?

Computational complexity of finding ground states



- P: class of problems that can be solved efficiently using classical computer
- BQP: class of problems that can be solved efficiently using quantum computer
- NP: class of problems whose solution can be checked efficiently using classical computer
- QMA: class of problems whose solution can be checked efficiently using quantum computer

Complexity of simulation many body systems

- Quantum computing puts us in a unique position to quantify the complexity of simulating quantum systems
  - Contrasting quantum to classical is crucial to get a deeper understanding of the power of quantum information processing
  - There are very successful algorithms out to simulate strongly correlated quantum systems in quantum chemistry and condensed matter physics: it is relevant to identify their limitations
  - Interesting fundamental questions on the nature of entanglement in physical systems
    - Identifying manifold of all low-energy states of all local quantum spin Hamiltonians

Density Functional Theory

$$H\Psi = [T + V + U]\,\Psi = \left[\sum_{i}^{N} -\frac{\hbar^2}{2m}\nabla_i^2 + \sum_{i}^{N} V(\vec{r}_i) + \sum_{i<j} U(\vec{r}_i, \vec{r}_j)\right]\Psi = E\Psi$$

- Hohenberg-Kohn: ground state energy is completely determined by the local single electron density n(r)

$$n(\vec{r}) = N \int \mathrm{d}^3 r_2 \int \mathrm{d}^3 r_3 \cdots \int \mathrm{d}^3 r_N \Psi^*(\vec{r}, \vec{r}_2, \ldots, \vec{r}_N)\Psi(\vec{r}, \vec{r}_2, \ldots, \vec{r}_N).$$

  - T and U are universal for all systems, and V is a simple function of n(r); so if we fix n(r), we can for once and for all solve

$$\psi \equiv \arg\min_{n(\Psi)=n(r)} \left\langle \Psi \middle| T + U \middle| \Psi \right\rangle = F(n(r))$$

    and then minimize F(n(r))+T(n(r)) as a function of n(r)
  - Similar treatment when spins and magnetic fields are included
  - This effectively reduces an N-body problem to a 1-body problem

- Assume that we have an efficient (P) description of the function F(n(r)); what power would it give us, i.e. what would that imply in terms of computational complexity?
  - QMA (quantum NP) collapses to P !

    this is exactly quantum many-body versus quantum 1-body
  - Proof uses perturbation gadgets and essentially maps Schrodinger equation to Hubbard model to 2-D local Hamiltonians which is known to be QMA-complete

Complexity of finding ground state energy of quantum spin Hamiltonians

- 2-D classical spin glass: NP-complete (Barahona '82)

$$H = \sum_{\langle i,j \rangle} J_{ij} Z_i Z_j + \sum_i B_i Z_i$$

- General 2-local quantum spin Hamiltonian: QMA-complete (Kitaev, Kempe, Regev '03)

$$H = \sum_{ij} A_i^{\alpha} \otimes B_j^{\alpha}$$

- General 2-local quantum Hamiltonian with n.n. interactions on a 2-D lattice: QMA-complete (Oliveira, Terhal '05)

- General n.n. interactions on a line with 12-level systems: QMA-complete (Gottesman, Aharonov, Kempe '07)

N-representability

$$H = \sum_{ij} A_{ij} a_i^* a_j + \sum_{ijkl} B_{iklm} a_i^* a_k^* a_l a_m$$

- Central problem in quantum chemistry: characterize the convex set of 2-body reduced density operators
  - Reduces to checking consistency of a set of correlations: is there a global state compatible with set of 2-body correlations

$$\left\langle a_i^* a_k^* a_l a_m \right\rangle$$

  - Difficulty stems from frustration / monogamy of entanglement (cfr.also de-Finetti theorem, mean-field theory (Werner '88)).

- By using mapping $\sigma_i^x \leftrightarrow a_i^\dagger b_i + b_i^\dagger a_i,\ \sigma_i^y \leftrightarrow i\left(b_i^\dagger a_i - a_i^\dagger b_i\right),\ \sigma_i^z \leftrightarrow \mathbb{1} - 2b_i^\dagger b_i.$ and a Turing reduction, checking consistency can be shown to be equivalent to QMA-complete problem of Kitaev

Liu, Christandl, FV

- But nature does itself not find those ground states: all we have to do it so be as smart as nature!
  - Hardness in finding ground states is just the worst-case scenario, and even then simulation must not outperform nature!
  - Note that there is no contradiction in hardness results and proofs of easy way of parameterizing all possible solutions in terms of MPS/PEPS/MERA
  - In practice: we think that quantum lattice Hamiltonians (spins and fermions) can be simulated using classical computers at polynomial cost

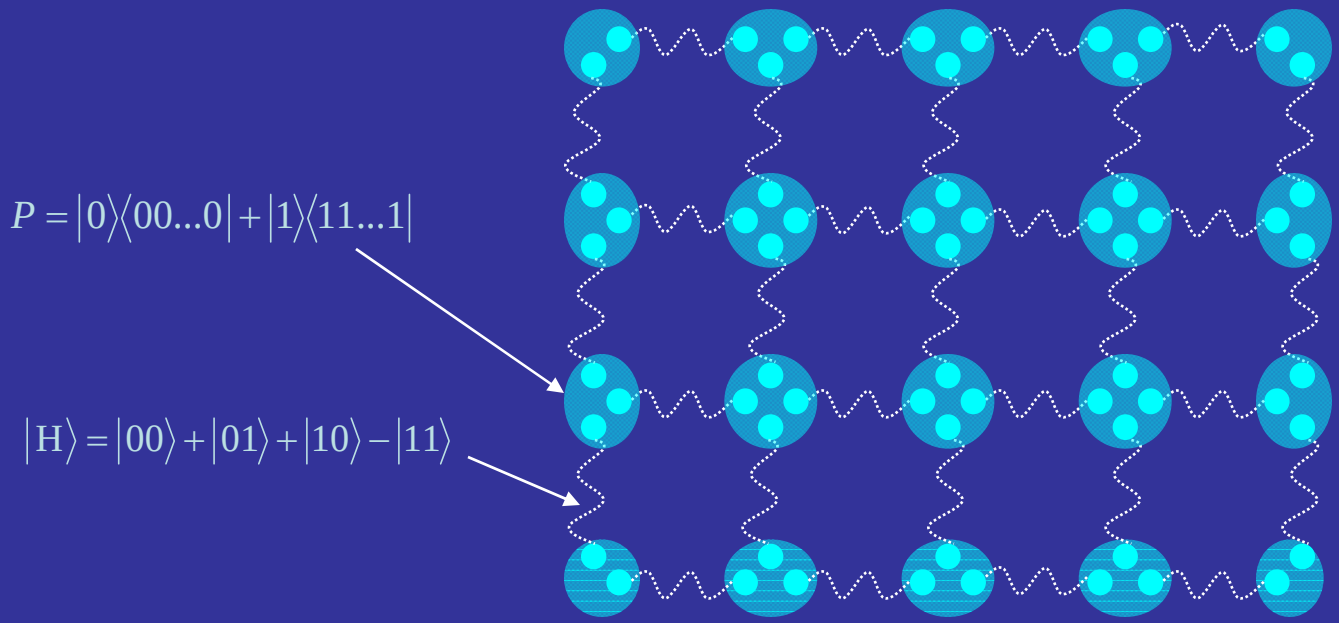
Using ground states of quantum Hamiltonians to do quantum computation

- As there are so many quantum correlations in ground states, can we exploit them to do quantum computation?
- Or differently: can we exploit a cooling mechanism as used in nature to do quantum computation for us?

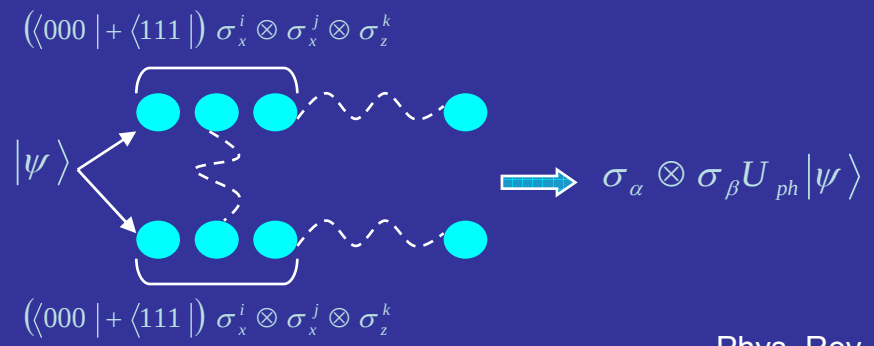
- Both answers can be answered affirmatively:
  - Cluster state quantum computation of Briegel
  - Dissipation based quantum computation

Multipartite entanglement and quantum computation

- Measurement based quantum computation with PEPS: cluster state quantum computation of Raussendorf and Briegel; the *virtual* qubits represent the logical qubits



= Postselected teleportation-based computation



Phys. Rev. A 70, 060302R (2004)

FV, Wolf, Cirac, Nat.Phys. '09

Dissipation based quantum computation

- What is the minimal level of control needed to do universal quantum computation?
  - To what extent can we relax the DiVincenzo criteria?
  - Can we use dissipation as a good thing instead of fighting it?

- Enough to engineer time-independent couplings of system with a Markovian reservoir, wait poly time until system relaxes, and read out result of your quantum computation in the steady state

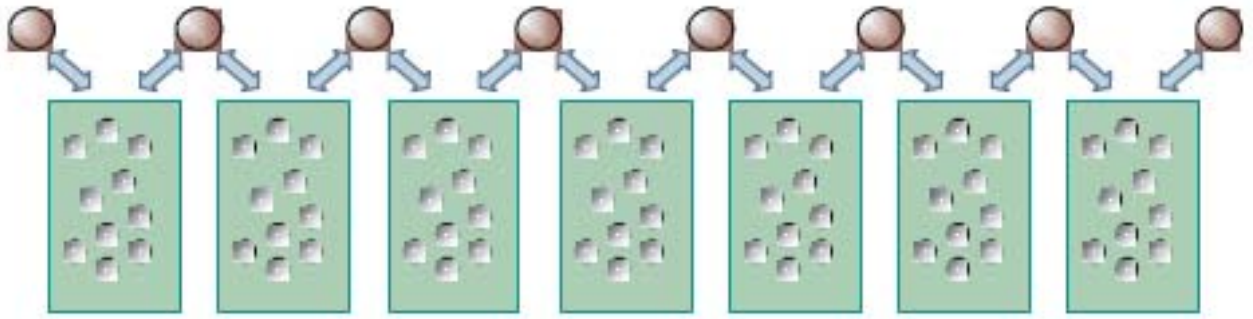


Figure 1: Schematic representation of the setup. We consider a collection of N quantum particles, locally coupled to a set of environments. The couplings are engineered in such a way that the system reaches the desired state in the long–time limit

What about simulating quantum systems using dissipative processes ?

- Q analogue of Markov-chain algorithms:

$$\frac{d}{dt}\rho = \sum_i L_i \rho L_i^* - \frac{1}{2}\left(\sum_i L_i^* L_i \rho + \sum_i \rho L_i^* L_i \right)$$

- This is particularly well suited for finding ground states of frustration-free quantum Hamiltonians:

$$H = \sum_t P_t \quad ; \quad P_t \geq 0 \quad ; \quad P_t \left| \chi_0 \right\rangle = 0$$

  - The ground state is a fixed point of the Liouvillian if $\forall i: \quad L_i \left| \psi_0 \right\rangle = 0$

    - Natural choice: $L_i = U_i P_i$ (U e.g. random unitary)

- Such frustration free Hamiltonians pop up everywhere:
  - 2-SAT, 3-SAT, quantum 2-SAT, …
  - MPS/PEPS are guaranteed to be ground states of frustration free Hamiltonians
    - Kitaev/Hastings: every ground state of a gapped local Hamiltonian is also the ground state of a local frustration free Hamiltonian
  - Kitaev Hamiltonian used in construction of QMA-complete quantum Hamiltonian:

$$H = H_0 + \sum_{t=0}^{T-1} H_t + H_f$$

$$H_0 = \left(\sum_{k=anc} |1\rangle_k \langle 1| \right) \otimes |0\rangle\langle 0| \qquad ; \qquad \mathrm{H_f} = |1\rangle_{res}\langle 1| \otimes |T\rangle\langle \mathrm{T}|$$

$$H_t = U_t \otimes |t+1\rangle\langle t| + U_t^{-1} \otimes |t\rangle\langle t+1|$$

    - Frustration-free if we leave out Hf and include proper initialization conditions-> Hamiltonian used in universal adiabatic quantum computation!

Dissipative quantum computation

- What is the computational power of a purely dissipative quantum systems with local Lindblad operators and no coherent evolution?

$$\frac{d}{dt}\rho = \sum_i L_i \rho L_i^* - \frac{1}{2}\left(\sum_i L_i^* L_i \rho + \sum_i \rho L_i^* L_i \right)$$

  - BQP-complete: as powerful as a quantum computer!
  - Proof:

$$\begin{aligned} L_i &= |0\rangle_i\langle 1| \otimes |0\rangle_t\langle 0| \\ L_t &= U_t \otimes |t+1\rangle\langle t| + U_t^\dagger \otimes |t\rangle\langle t+1|, \end{aligned}$$

$$\rho_0 = \frac{1}{T+1}\sum_t |\psi_t\rangle\langle\psi_t| \otimes |t\rangle\langle t|.$$

  - Gap of Liouvillian independent of actual quantum computation done: $\Delta = \pi^2/(2T+3)^2$
  - Defies some of DiVincenzo criteria for QC: no initialization, no unitaries, …
  - Robustness issues, fault tolerance, comparison with adiabatic QC?

- Gap of the Liouvillian quantifies complexity of simulating system on a quantum computer: P vs. NP
  - Gap of Hamiltonian: does not tell anything about computational complexity: Ising spin glasses have gap 1, but gap in Liouvillian should be exponentially small (has this been proven?)

Dissipatively driven quantum phase transitions

- Can a quantum phase transition be driven by dissipation?
- One can easily construct families of frustration free Hamiltonians that exhibit quantum phase transitions: "**Rokhsar-Kivelson"** Hamiltonians
  - Take any classical spin system exhibiting finite-T phase transition (e.g. Ising model)

$$Z = \sum_{s_1 s_2 \ldots} \exp\left(-\beta \sum_{\langle k,l \rangle} H(s_k, s_l) \right)$$

  - Define the quantum state which is coherent version of partition function:

$$|\Psi\rangle = \frac{1}{\sqrt{Z}} \sum_{s_1 s_2 \ldots} \exp\left(-\frac{\beta}{2} \sum_{\langle k,l \rangle} H(s_k, s_l) \right) |s_1\rangle |s_2\rangle |s_3\rangle \ldots$$

    - Has exactly the same correlation functions as classical one
    - Is ground state of local frustration-free Hamiltonian which depends on parameter beta : PEPS!
    - Obviously exhibits a quantum phase transition if parameter beta is varied

- Hence: zero-temperatuere quantum phase transitions can be driven by dissipative processes

Conclusion

- Formalism of quantum information theory provides new perspectives on strongly correlated quantum systems
  - MPS/PEPS picture describes low-energy sector of local Hamiltonians, and opens a whole new toolbox of numerical renormalization group methods that allows to go where nobody has gone before
    - Similar ideas can be used in context of lattice gauge theories, quantum chemistry, …
  - Frustration and monogamy properties of entanglement (cryptography), quantum error correction, and the complexity of simulating quantum systems are basic notions in the fields of quantum information and statistical physics
  - Synergy of quantum information and the theory of strongly correlated quantum systems opens up many new themes for both fields and could lead to a much more transparent description of the whole body of many-body quantum physics