Real-space renormalization group methods

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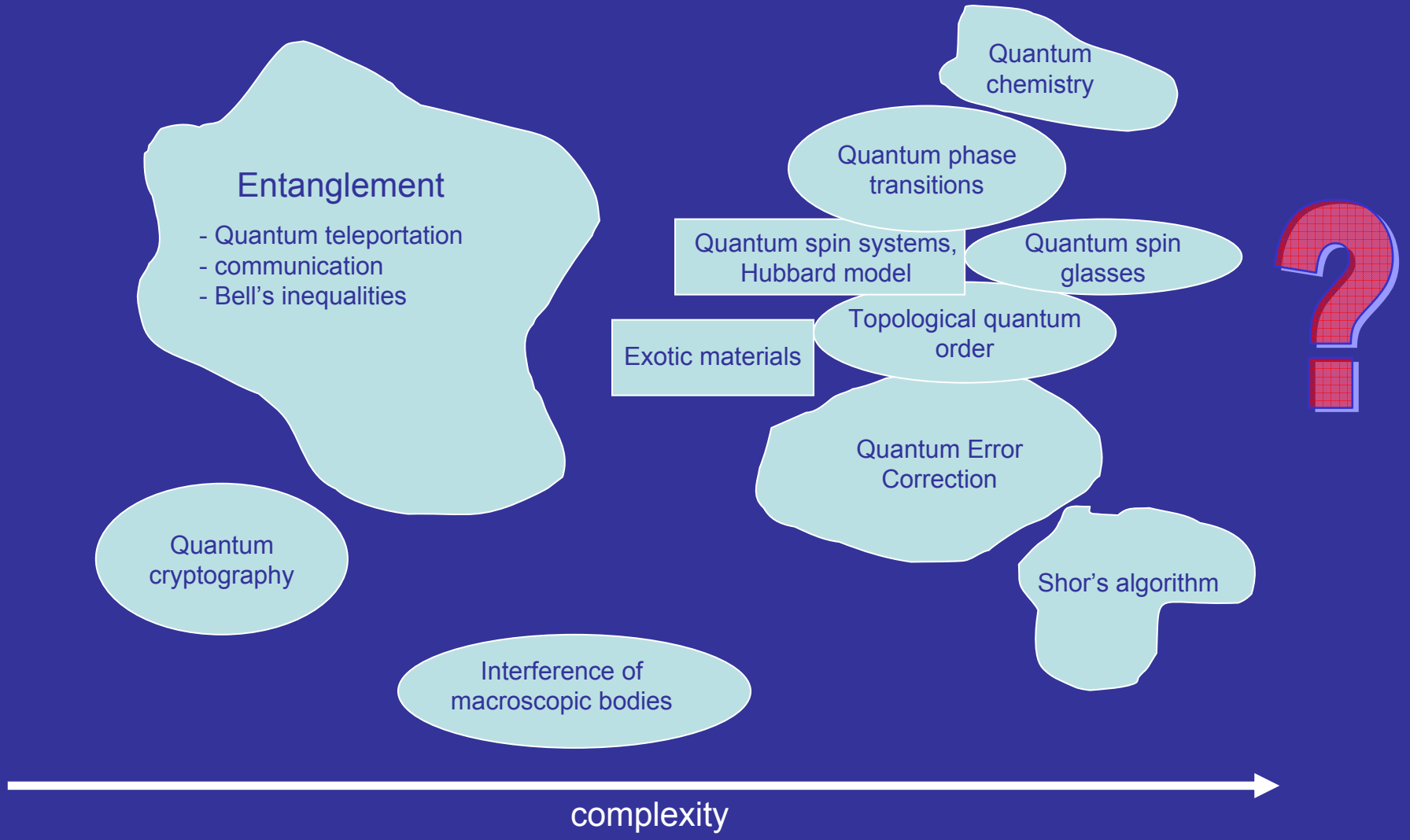
Overview

- Quantum information theory and many-body quantum systems
  - Entanglement, area laws
  - Parameterization of low-energy manifold of states
- Real-space and numerical RG methods

Quantum information science as an approach for studying complex quantum many-body systems



Entanglement

- From the point of view of
  - Quantum information theory: resource that allows for quantum computation, quantum communication
  - Condensed matter theory: allows for quantum phase transitions, topological quantum order
  - Computational physics: nightmare because of exponentially large Hilbert space, sign problem
- What can entanglement theory contribute to condensed matter physics?
  - Provides a simple and transparent formalism to describe many-body correlations
  - Identification of relevant/physical manifold of states
  - Natural connections between topological quantum order and quantum error correction
  - Yields formalism to make quantitative statements about complexity of thermalizing
  - Motivation for many experiments in optical lattices and cold atoms comes from quantum information theory

Physical States for quantum spin systems

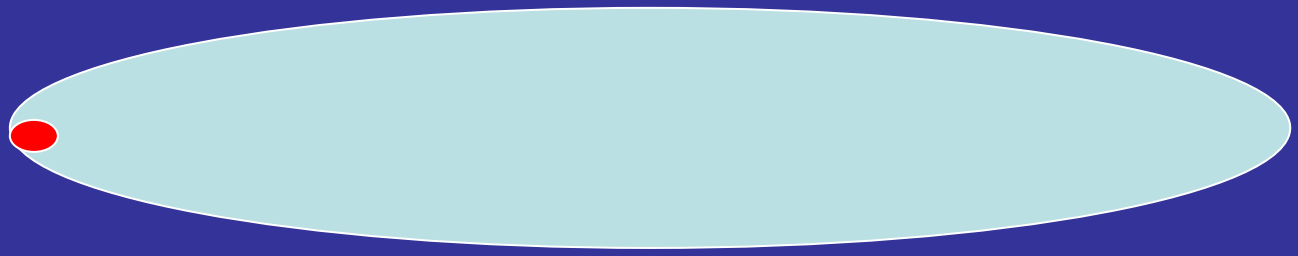
- Attempt of a definition: physical states are the ones that can be created by evolution of a a fiducial state (e.g. vacuum, ferromagnetic state, …) with a time-dependent quantum Hamiltonian containing only bounded 2-body terms over a time that scales at most polynomial in the number of particles/spins

$$H(t) = \sum_{\alpha\beta ij} J_{ij}^{\alpha\beta}(t)\sigma_i^{\alpha} \otimes \sigma_j^{\beta}$$

$$\left|\psi(t)\right\rangle = \hat{T}\exp\left[-i\int_0^t H(\tau)d\tau\right]\left|\Omega\right\rangle$$

Basic assumption: there is some symmetry between time and space: time over which systems can evolve does not scale exponentially in number of particles

  - How much does this cover in Hilbert space?



How big is the physical Hilbert space?

- Consider Trotter expansion for time-dependent Hamiltonians:

$$\hat{T}\exp\left(-i\int_0^{\varepsilon} dt'\, H_A(t') + H_B(t')\right) = \hat{T}\exp\left(-i\int_0^{\varepsilon} dt'\, H_A(t')\right)\hat{T}\exp\left(-i\int_0^{\varepsilon} dt'\, H_B(t')\right) + O\left(\varepsilon^2\right)$$

- Solovay-Kitaev: given a standard universal gate set on N spins (cN gates), then any 2-body unitary can be approximated with log(1/ε) standard gates such that $\| U\text{-}U_\varepsilon \| < \varepsilon$
- Given any quantum circuit acting on pairs and of polynomial depth N^d, this can be reproduced up to error ε by using $N^d \log(N^d/\varepsilon)$ standard gates. The total number of states that can hence be created using that many gates scales as

$$(\mathrm{cN})^{N^d \log \frac{N^d}{\varepsilon}}$$

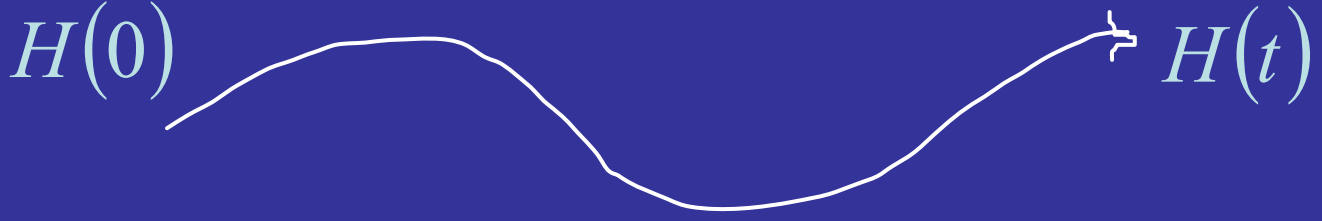
- Consider however the D^N dimensional hypersphere; the number of points that are ε-far from each other scales doubly exponential in N:

$$\varepsilon^{-D^N}$$

- Conclusion: Hilbert space is a convenient illusion

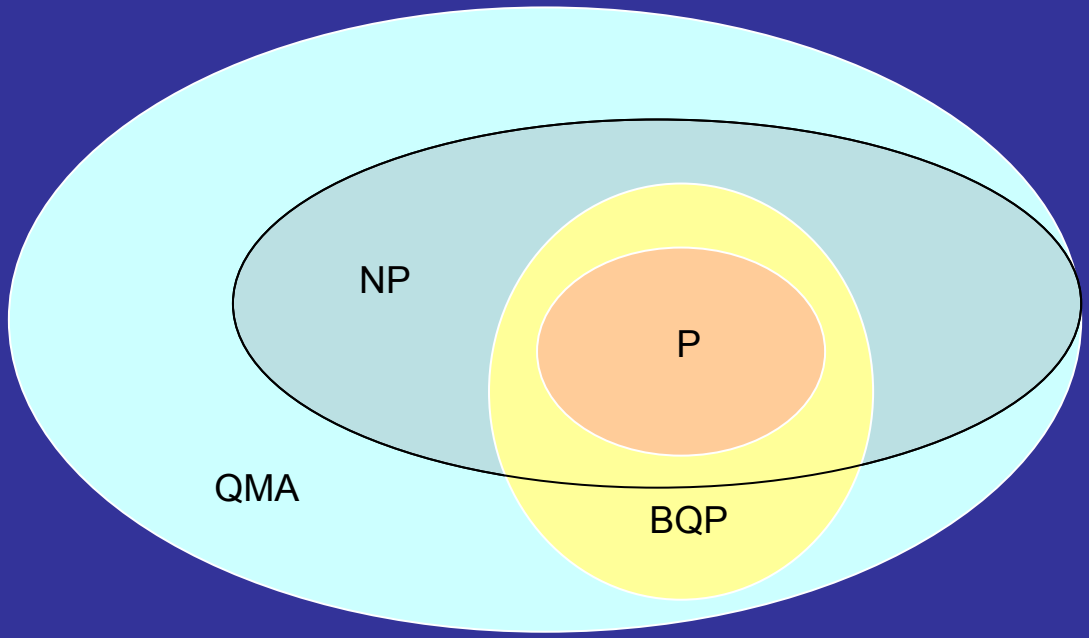
What about ground states of local spin Hamiltonians?

- Ground states can efficiently be simulated on a quantum computer using adiabatic time evolution (assuming gaps are not exponentially small)



- Are there more features that make ground states very special?
  - They have extremal local correlations compatible with symmetries (monogamy properties of entanglement!)
  - They exhibit relatively a small amount of entanglement: area laws

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

- Kitaev: finding ground state of local (i.e. few-body) quantum Hamiltonian is QMA-complete

- Oliveira and Terhal (’04): general nearest neighbour Hamiltonian of spin ½ on a square lattice: finding ground state is QMA-complete
  - Also: Aharonov, Gottesman, Kempe ‘07: 12-level system on a line

- More physical models:
  - Hubbard model with local varying magnetic field: QMA-complete

$$H_{\mathrm{Hubbard}} = -t \sum_{<i,j>,s} a^{\dagger}_{i,s} a_{j,s} + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow} - \sum_{i} \vec{B}_i \cdot \vec{\sigma}_i$$

Schuch, FV ‘08

  - Heisenberg model with local varying magnetic field: QMA-complete

  - Consequences for density functional theory:
    - if an efficient description exists for the universal functional, then QMA=P !

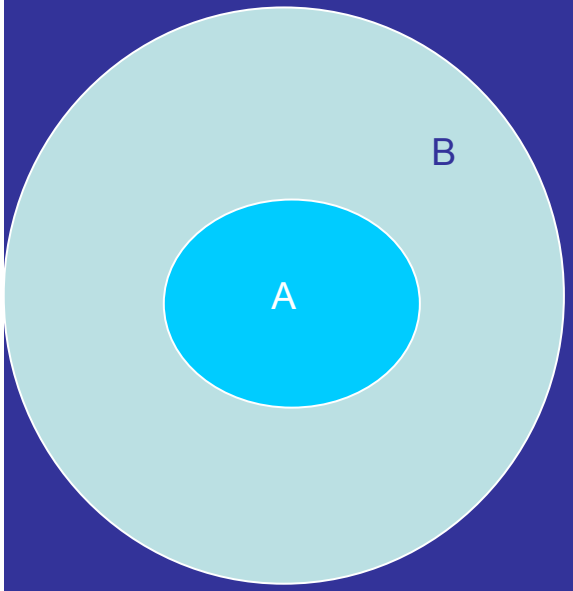
Schuch, FV ‘08

  - N-representability problem in quantum chemistry: QMA-complete

Liu, Christandl, FV ’07

- However: nature does not find the ground state itself in case of QMA, so we should not worry too much!

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)

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

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

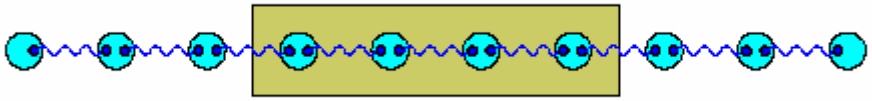
$$\Rightarrow I_{AB} \leq \beta\, Tr(H[\rho_A \otimes \rho_B - \rho_{AB}]) = \beta\, Tr(H_{AB}[\rho_A \otimes \rho_B - \rho_{AB}])$$

Cirac, Hastings, FV, Wolf '08

- All correlations are *localized* around the boundary, which is a big constraint
- What happens at zero temperature?
  - Classical: nothing
  - Quantum: gapped systems still seem to obey area law, critical systems might get a logarithmic correction (still exponentially smaller than what we get for random states)

Area laws

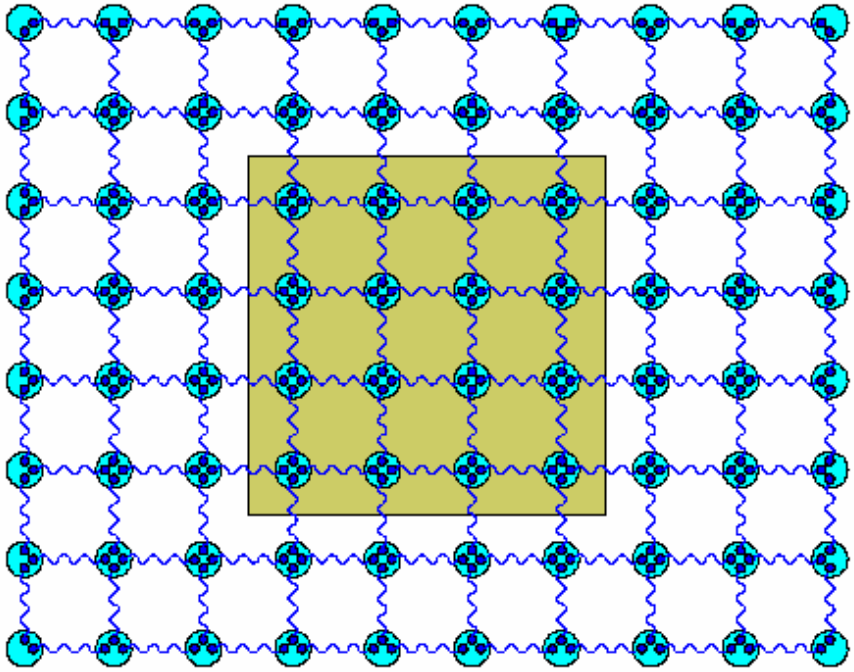
- Main picture: in case of ground states, entanglement is concentrated around the boundary



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

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

Kitaev, Vidal, Cardy, Korepin, …



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

Critical

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

Wolf, Klich

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

FV, Wolf

Topological entropy: detects topological quantum order locally!

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

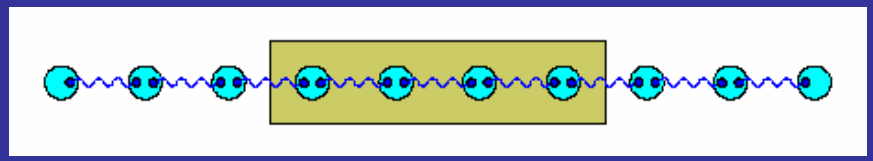
Kitaev, Preskill, Levin, Wen

Area laws for 1-D systems

- 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

  Cirac, FV '06

  - 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:

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

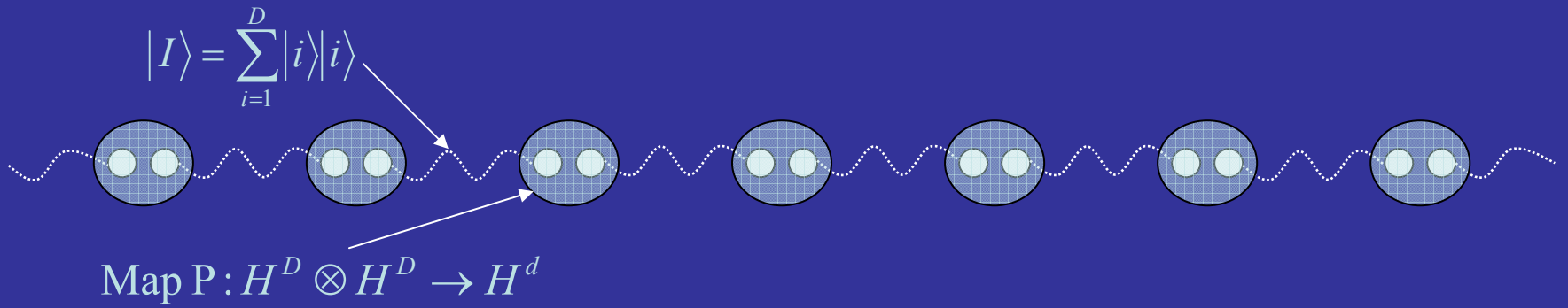
    - Breaking of exponential wall: polynomial vs. exponential complexity

- M. Hastings '07: every ground state of a gapped quantum spin Hamiltonian in 1-D obeys an area law

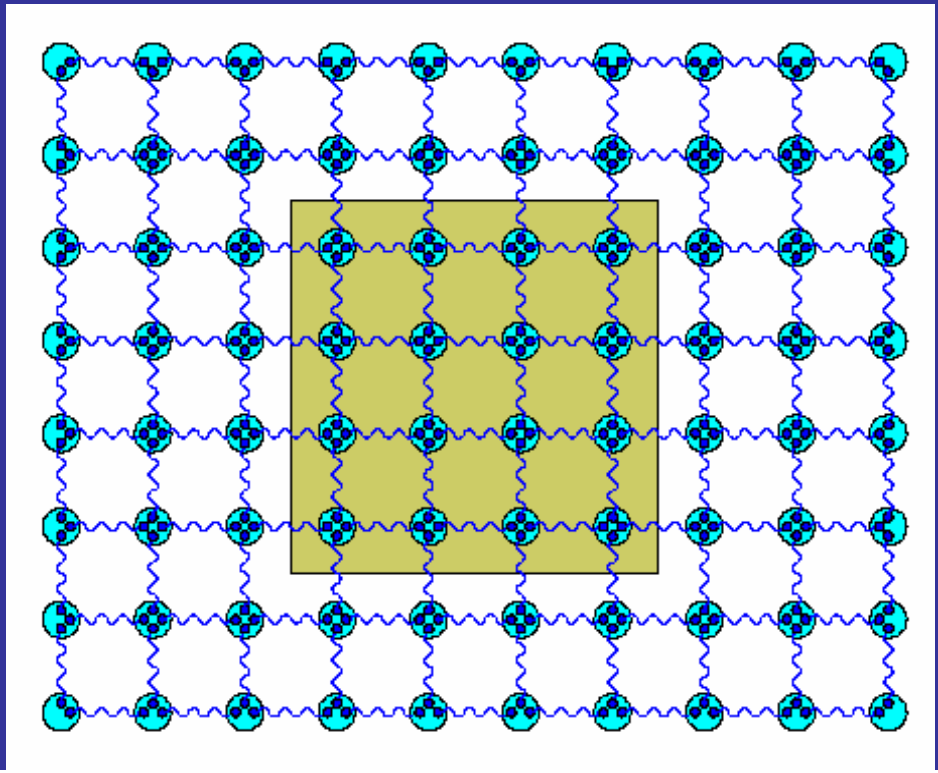
    - Identification of the relevant manifold

Matrix product states et al.

- Class of MPS: VBS-picture



- 2-D analogue: PEPS / TPS

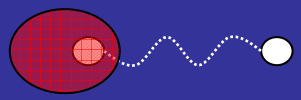


Properties of MPS/PEPS

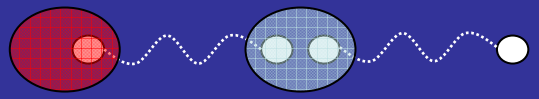
- Ground states of local frustration-free quantum Hamiltonians
  - Possible to prove uniqueness (injectivity)
- Obey area law by construction
- Can be made translational invariant
- correlation functions can be calculated efficiently
- Levin-Wen models exhibiting topological quantum order: very simple parameterization in terms of PEPS
- Symmetries:
  - String order parameter for unique GS implies a global symmetry in the system
  - Continuous symmetries impose strong conditions on form of matrices because virtual degrees of freedom must form irreducible representation of group if GS is unique: Lieb-Schultz-Mattis in any dimension for MPS/PEPS
- Holographic principle: mapping of quantum system to classical system of same dimension

Connection to real-space RG methods

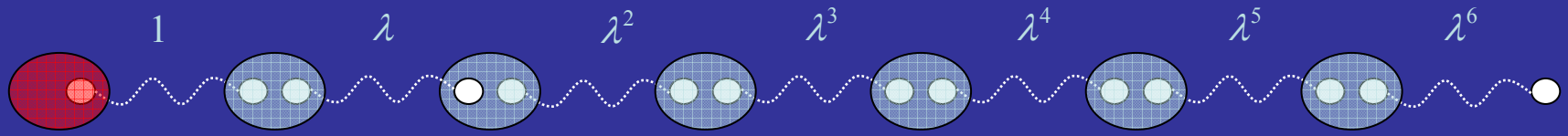
- MPS were already used by Wilson in analyzing Kondo problem



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

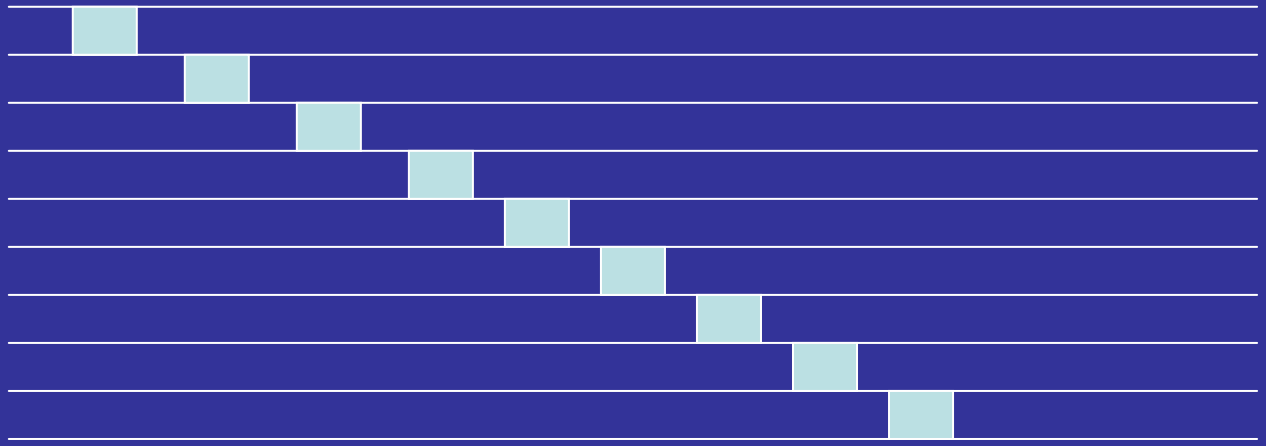


$$\left|\psi_{\beta}^{[3]}\right\rangle = \sum_{\alpha,i_3} A_{\alpha\beta}^{i_3} \left|\psi_{\alpha}^{[2]}\right\rangle \left|i_3\right\rangle$$



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

- Other way of looking at NRG:



Construction of a quantum circuit that diagonalizes the low energy spectrum of the Hamiltonian

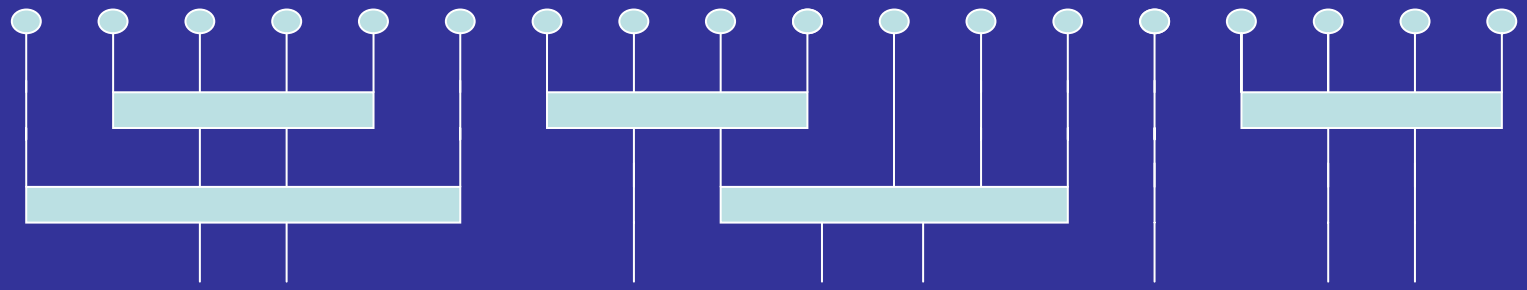
DMRG as variational MPS

- Obviously, class of MPS is an interesting class of states as they allow to simulate Kondo impurity
  - Original problems when applied to translational invariant systems: no separation of energies
  - what happens if we use that class to do variational calculations? DMRG! (S. White ’92)

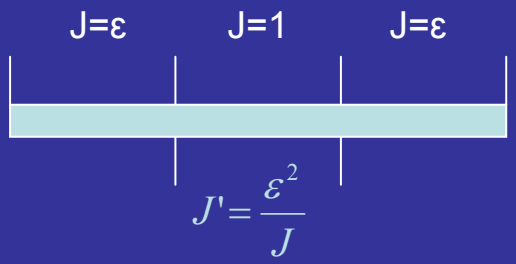
- Reformulation of DMRG in terms of MPS has allowed for many generalizations:
  - MPS with periodic boundary conditions
  - Real-time evolution
  - Simulation of thermal states
  - Random systems
  - Dispersion relations
  - …

- What about other real-space RG methods; what classes of states do they generate?

- Ma-Dasgupta-Fisher RG for random spin systems: $H = \sum_{<ij>} J_{ij} \vec{S}_i . \vec{S}_j$



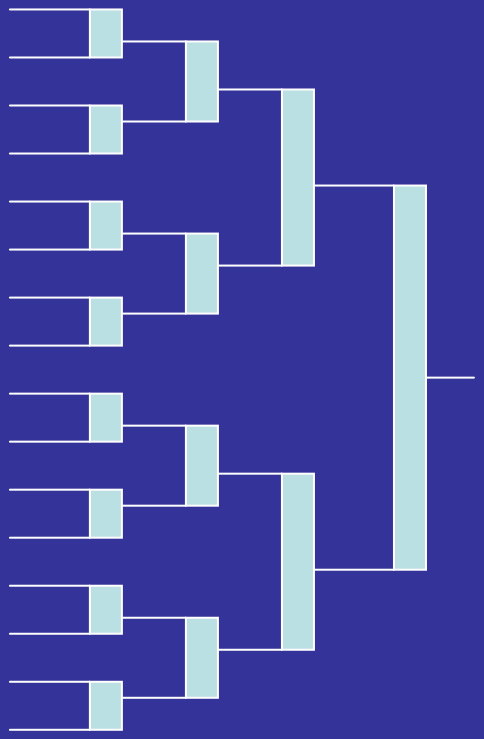
  - Second order perturbation theory:



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

  - Perturbation theory gives rise to quantum circuits that can be simulated efficiently on a classical computer
  - Make it variational: allows to use it on TI systems, …: MERA (Vidal)

- More real-space RG methods: CORE



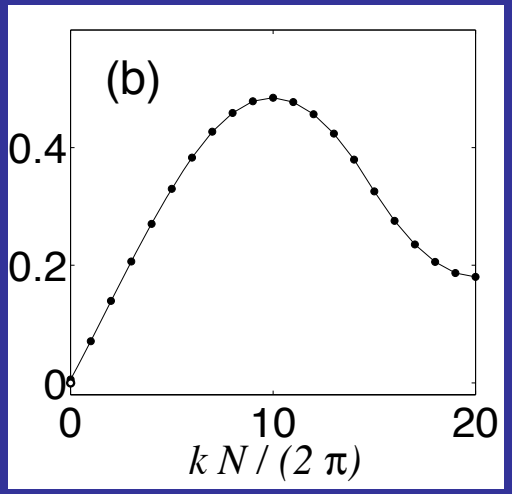
Basic idea: same as NRG, but block different parts in parallel

Class of states obtained like that: tree states (still efficiently simulatable on a classical computer)

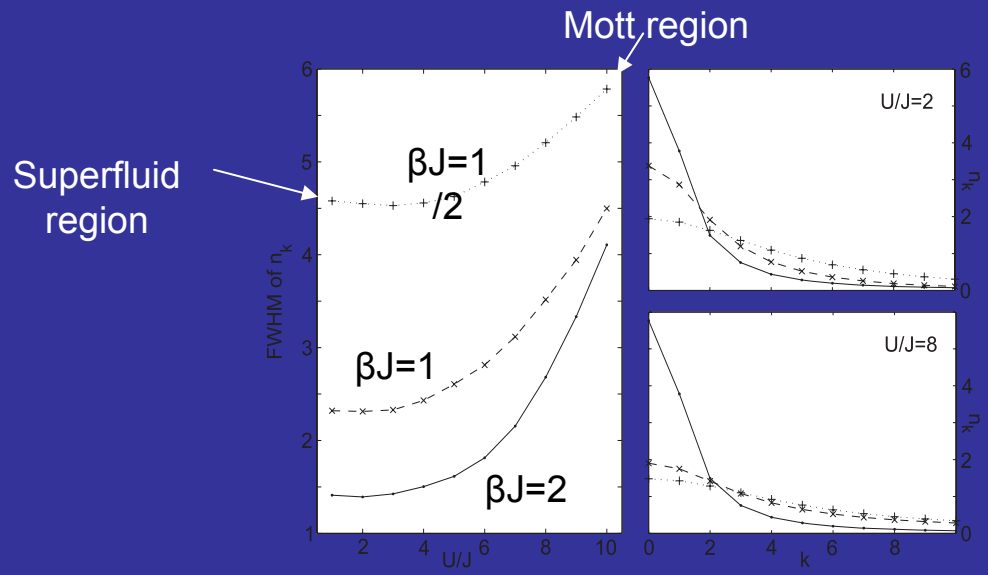
Clear how to generalize to 2D, 3D, …

- Any more RG methods that can be made variational?

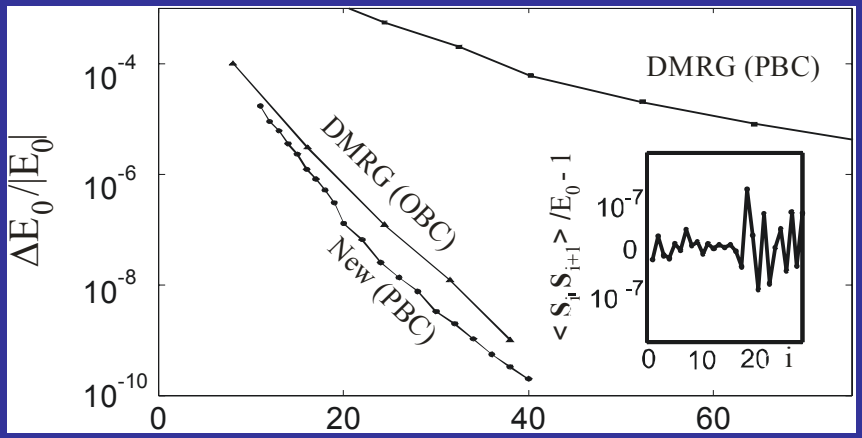
Some numerics with MPS



Dispersion relation in bilinear-biquadratic spin 1 chain



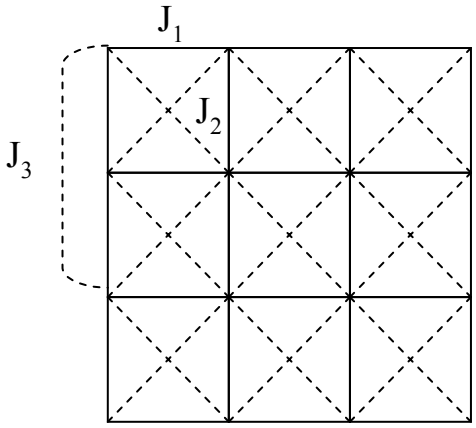
Mott-superfluid transition of bosons in 1-D optical lattices at finite T



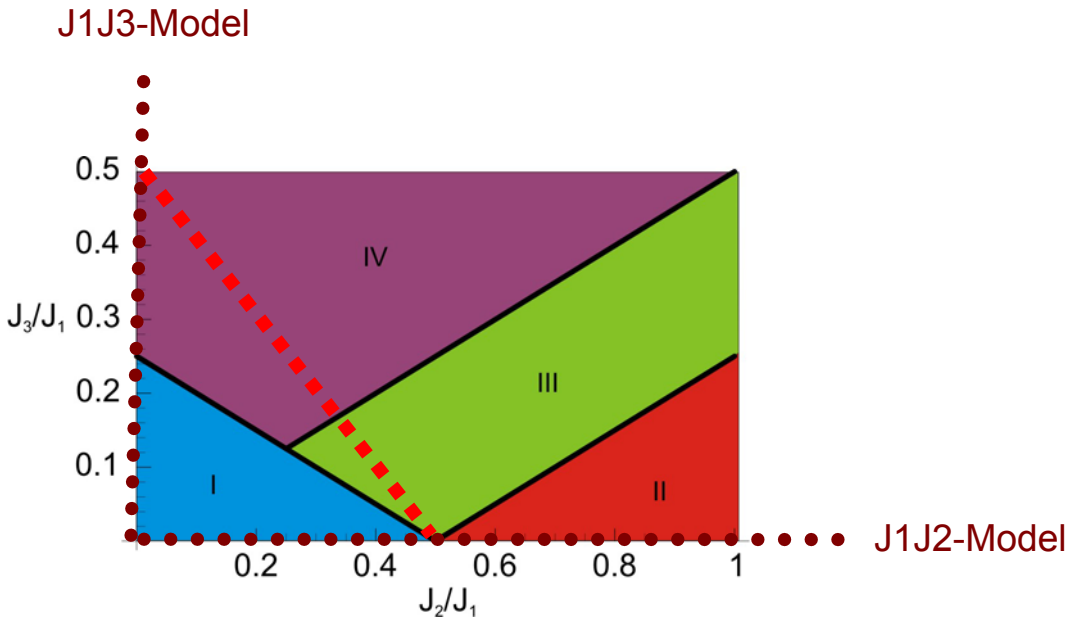
Simulating Heisenberg spin ½ with PBC: MPS vs. DMRG

PEPS simulations: J1-J2-J3 Heisenberg model

- Frustrated quantum spin model that has been predicted to exhibit exotic plaquette, columnar, … order parameters but cannot be simulated using quantum Monte Carlo due to frustration

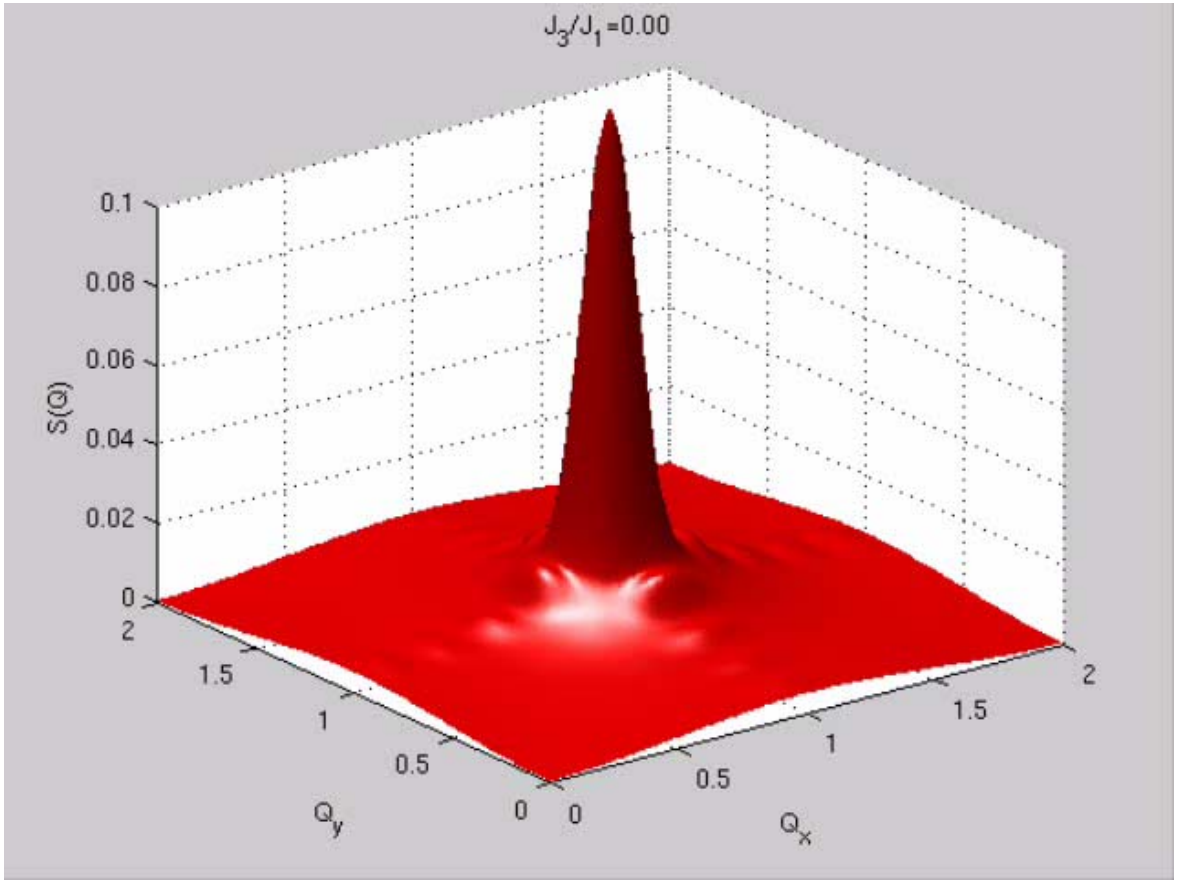


$$H = J_1 \sum_{\langle ij \rangle} \boldsymbol{s}_i \cdot \boldsymbol{s}_j + J_2 \sum_{\langle\langle ij \rangle\rangle} \boldsymbol{s}_i \cdot \boldsymbol{s}_j + J_3 \sum_{\langle\langle\langle ij \rangle\rangle\rangle} \boldsymbol{s}_i \cdot \boldsymbol{s}_j$$



Structure Factor

$$S(\boldsymbol{Q}) = \frac{1}{N}\sum_{kl} e^{i\boldsymbol{Q}\cdot(\boldsymbol{r}_k - \boldsymbol{r}_l)} < \boldsymbol{s}_k \cdot \boldsymbol{s}_l >$$

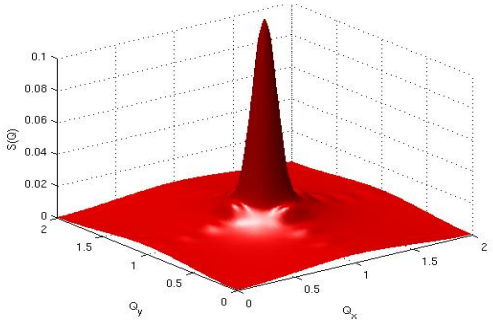


$10x10,\ D=3$

Long Range Order

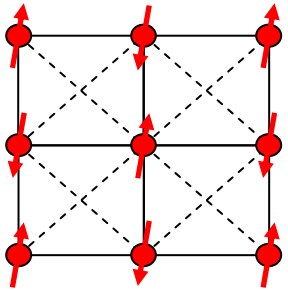
Structure Factor

$J_3 / J_1 = 0$

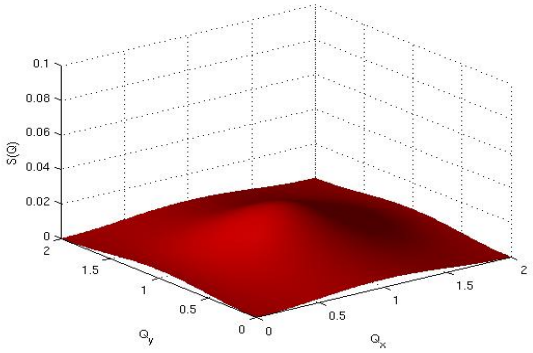


Néel Order:

$\boldsymbol{Q} = (\pi, \pi)$

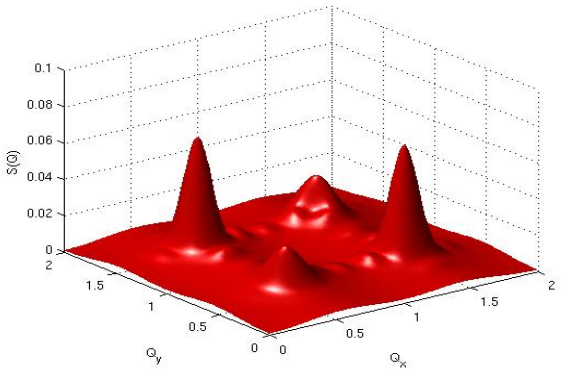


$J_3 / J_1 = 0.5$



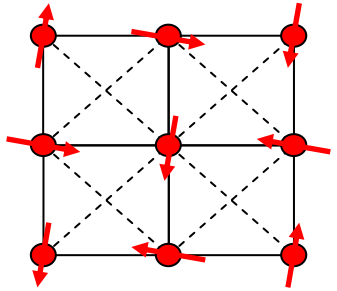
No long range order!

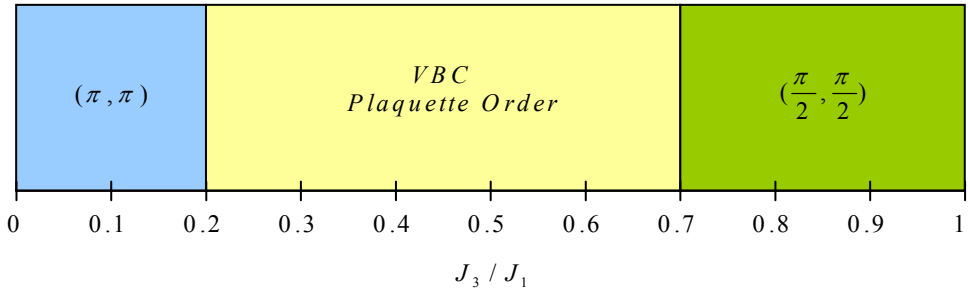
$J_3 / J_1 = 1$



Néel Order on four Sublattices:

$\boldsymbol{Q} = (\pi / 2, \pi / 2)$

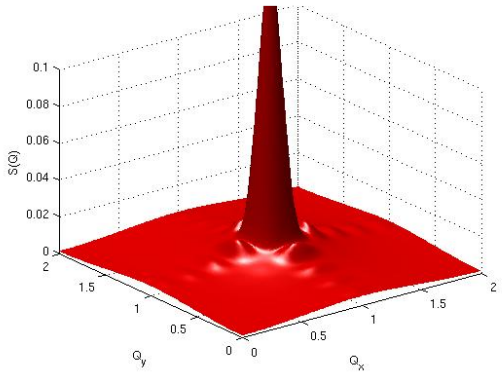




Long Range Order

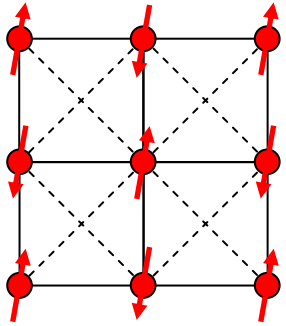
Structure Factor

$J_2/J_1 = 0$

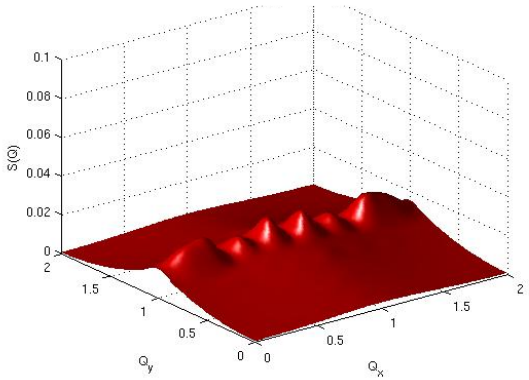


Néel Order:

$\boldsymbol{Q} = (\pi, \pi)$

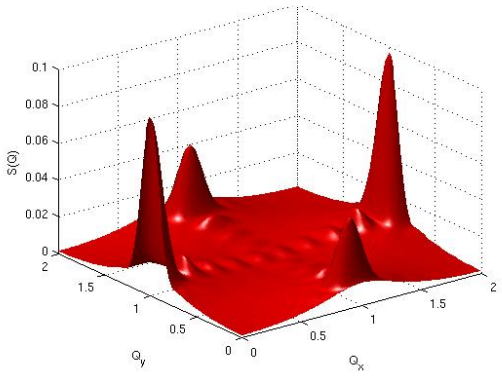


$J_2/J_1 = 0.6$



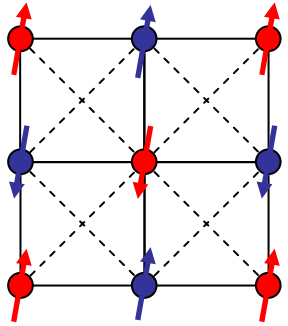
No long range order!

$J_2/J_1 = 1$



Columnar Order:

$\boldsymbol{Q} = (\pi, 0),\ (0, \pi)$



Conclusion

- Theory of quantum entanglement provides new tools to understand structure of wavefunctions arising in strongly correlated quantum many-body systems
- Identification of manifold of relevant physical states
- Real-space RG methods can be rephrased and improved upon as variaional methods
- Long-term workshop on “entanglement and correlations in many-body quantum systems” next year in Erwin Schrodinger Institute for Mathematical physics in Vienna (Aug. 15-Oct. 15 2009)
- Postdoc+PhD positions