Real-space renormalization group methods

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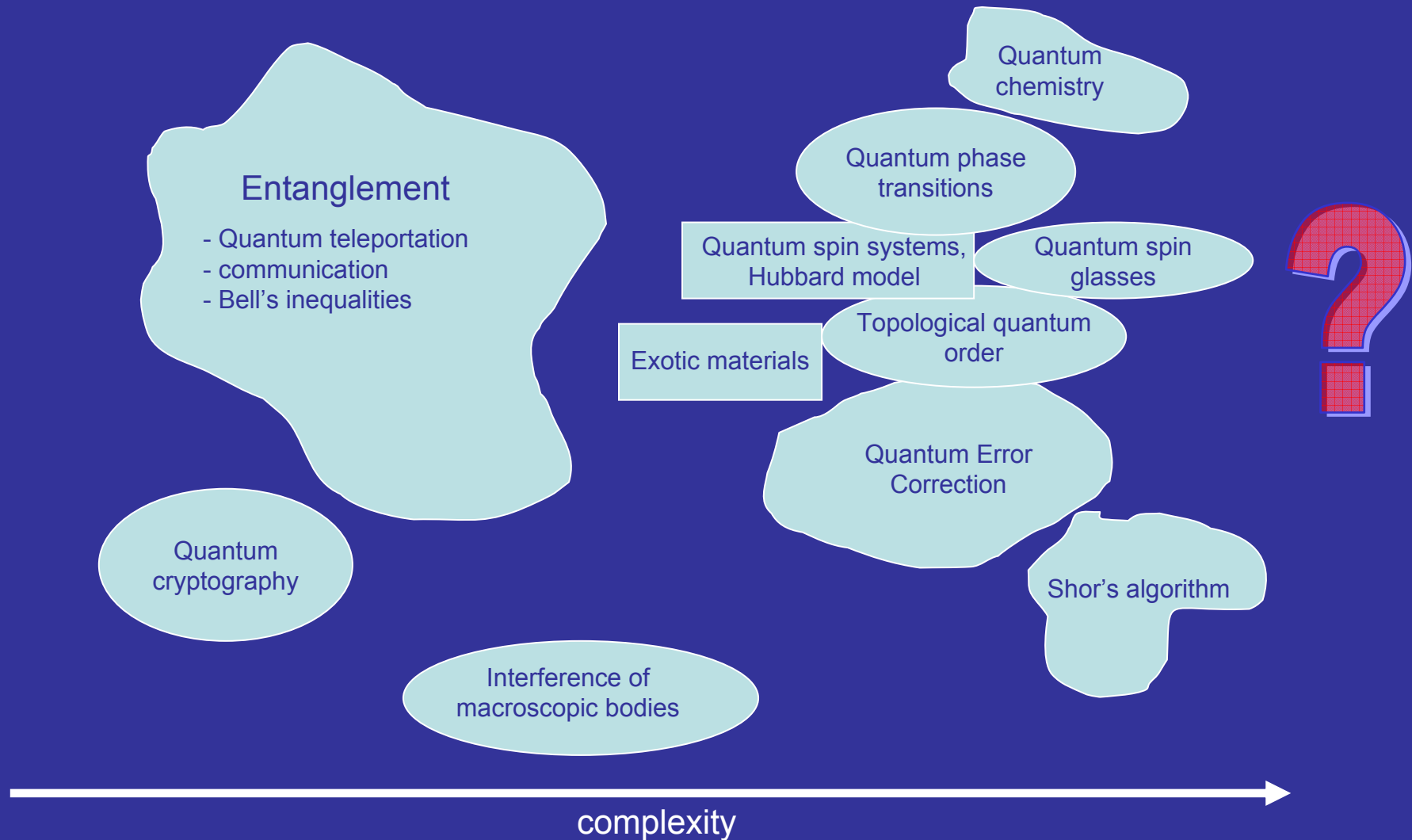
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Overview

- 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

Quantum chemistry

Quantum phase transitions

Entanglement

- Quantum teleportation
- communication
- Bell's inequalities

Quantum spin systems, Hubbard model

Quantum spin glasses

Exotic materials

Topological quantum order

?

Quantum Error Correction

Quantum cryptography

Shor's algorithm

Interference of macroscopic bodies

complexity

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

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

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

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

- How much does this cover in Hilbert space?

How big is the physical Hilbert space?

- Consider Trotter expansion for time-dependent Hamiltonians:

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

- Solovay-Kitaev: given a standard universal gate set on N spins (cN gates), then any 2-body unitary can be approximated with $\log(1/\varepsilon)$ 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

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

- 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)

$$H(0) \qquad\qquad H(t)$$
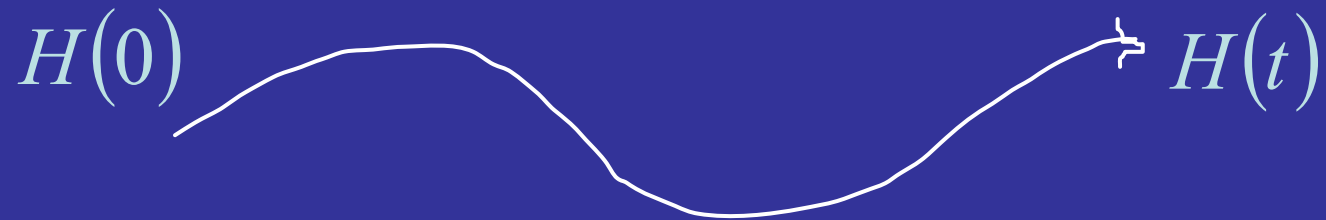
- Are there more features that make ground states very special?

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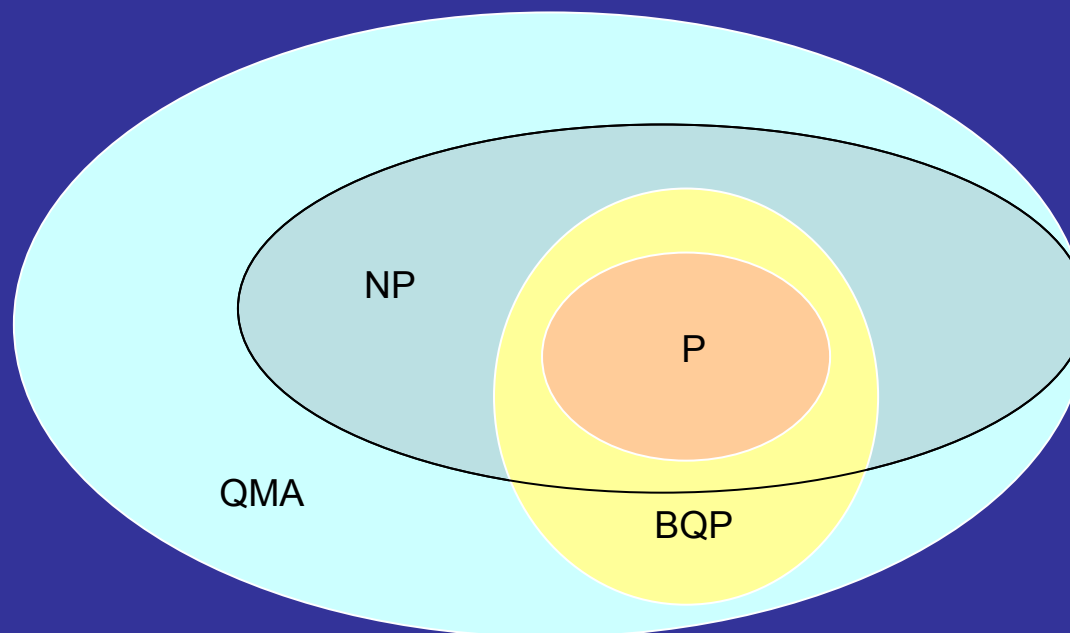
- P: class of problems that can be solved efficiently using classical computer
- BQP: class of problems that can be solved efficiently using quantum computer
- NP: class of problems whose solution can be checked efficiently using classical computer
- QMA: class of problems whose solution can be checked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

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

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)
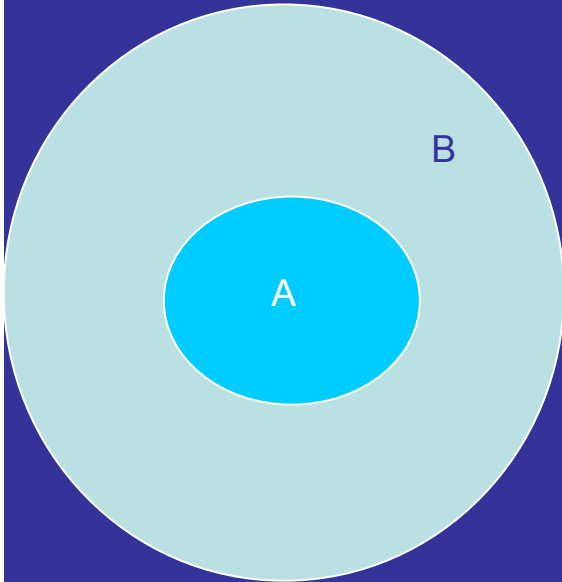
Area laws

- Main picture: in case of ground states, entanglement is concentrated around the boundary
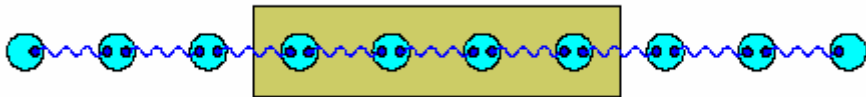
Gapped: $S(\rho_{1,2,\cdots,L}) \approx \dfrac{c+\bar{c}}{6}\ln(\xi)+...$

Critical: $S(\rho_{1,2,\cdots,L}) \approx \dfrac{c+\bar{c}}{6}\ln(L)+...$

Kitaev, Vidal, Cardy, Korepin, …
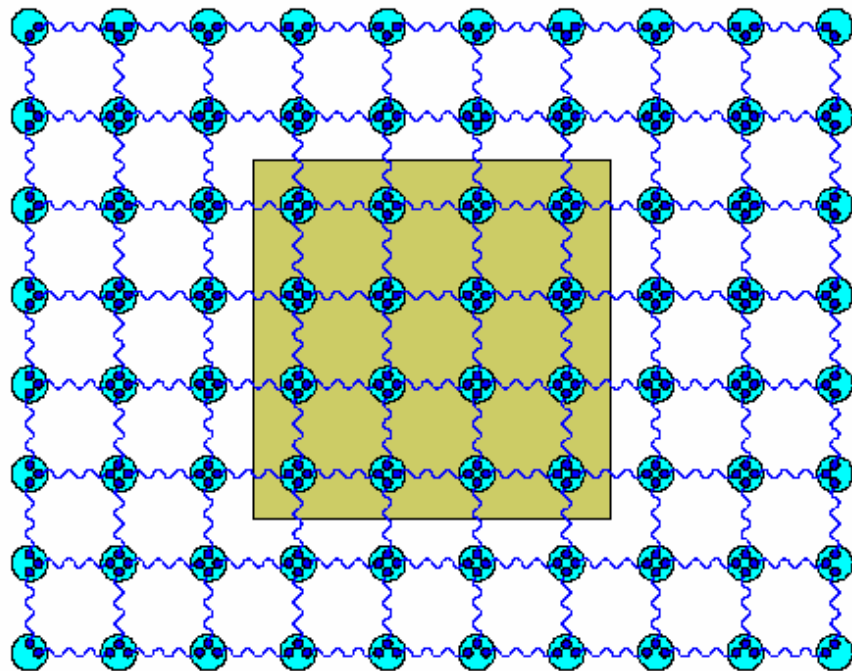
Gapped $S(\rho_{1,2,\cdots,L^2}) \approx a.L+\cdots$

Critical

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

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

  – MPS: most general state in 1-D that obeys a strict area law by construction: rank of reduced density operators is cst (D^2)
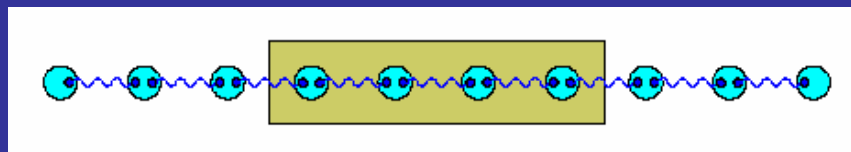
  – We want to bound the cost of approximating state that obeys area law with a MPS for given precision as a function of number of spins:

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

  - 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

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

$$\text{Map } P : H^D \otimes H^D \rightarrow H^d$$
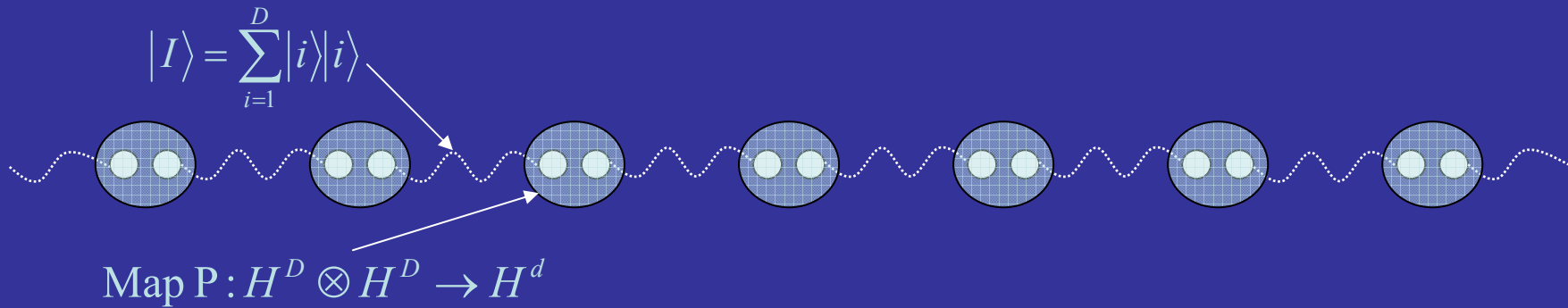
- 2-D analogue: PEPS / TPS
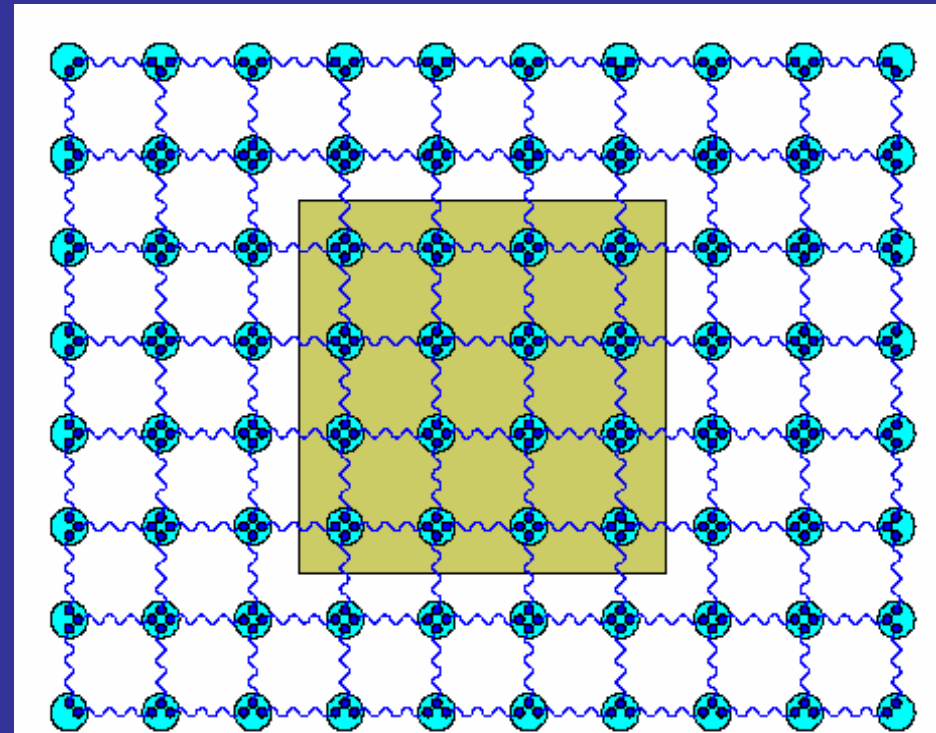
Properties of MPS/PEPS

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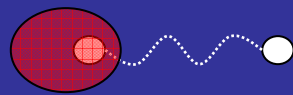
$$\left| \psi_\alpha^{[2]} \right\rangle = \sum_{i_1,i_2} A_{i_1\alpha}^{i_2} \left| i_1 \right\rangle \left| i_2 \right\rangle$$

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

$$1 \qquad \lambda \qquad \lambda^2 \qquad \lambda^3 \qquad \lambda^4 \qquad \lambda^5 \qquad \lambda^6$$
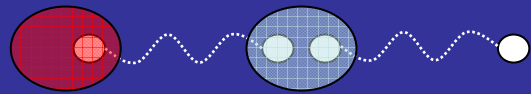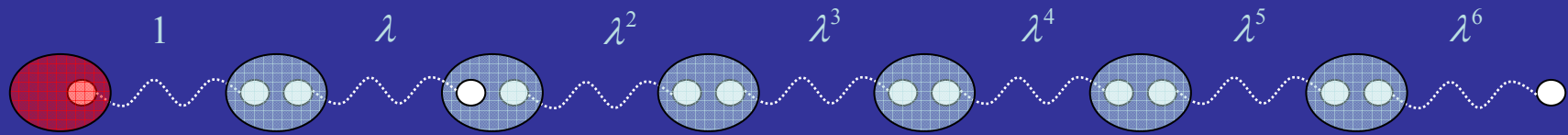
$$\left| \psi_\tau^{[N]} \right\rangle = \sum_{\substack{i_1,i_2,... \\ \alpha,\beta,...}} A_{i_1\alpha}^{i_2} A_{\alpha\beta}^{i_3} A_{\beta\gamma}^{i_4} ... A_{\sigma\tau}^{i_N} \left| i_1 \right\rangle \left| i_2 \right\rangle ... \left| i_N \right\rangle = \sum_{i_1,i_2,...} A^{i_2} A^{i_3} A^{i_4} ... A^{i_N} \left| i_1 \right\rangle \left| i_2 \right\rangle ... \left| i_N \right\rangle$$

- Other way of looking at NRG:
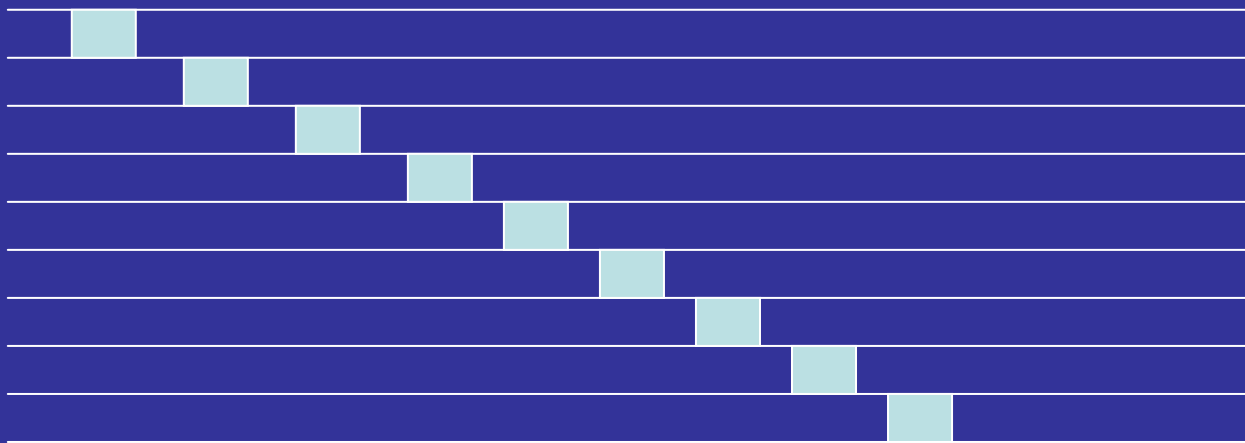
Construction of a quantum circuit that diagonalizes the low energy spectrum of the Hamiltonian

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

J=ε   J=1   J=ε
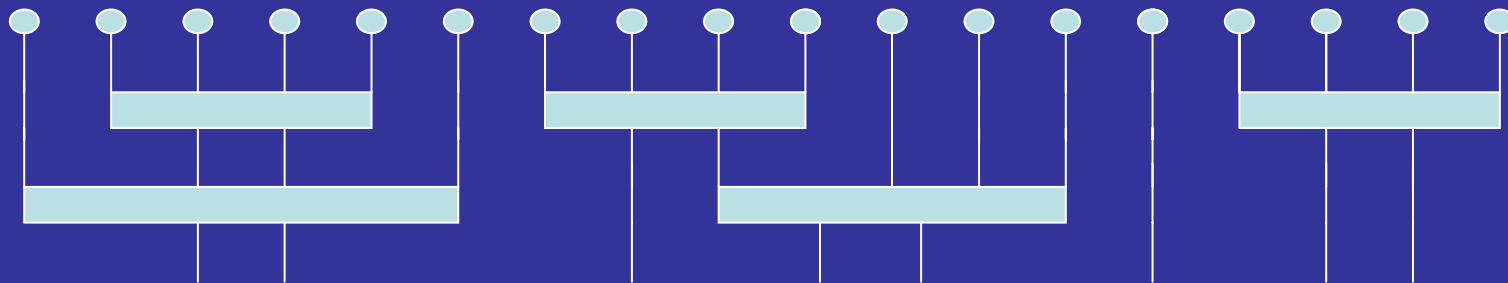
  – Second order perturbation theory:

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

$$J' = \frac{\varepsilon^2}{J}$$
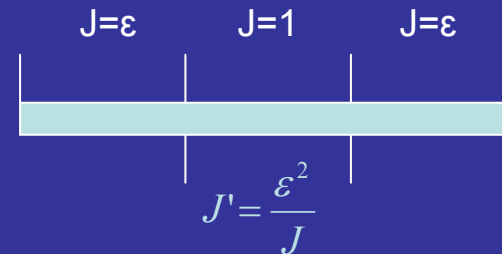
- Perturbation theory gives rise to quantum circuits that can be simulated efficiently on a classical computer
- Make it variational: allows to use it on TI systems, …: MERA (Vidal)

- More real-space RG methods: CORE
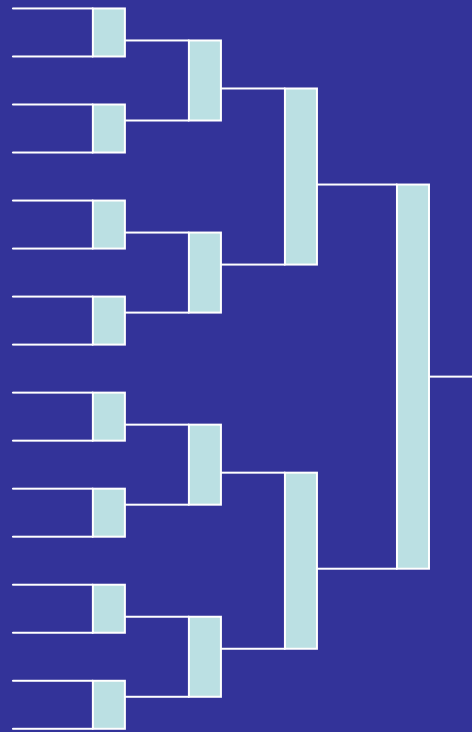
Basic idea: same as NRG, but block different parts in parallel

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
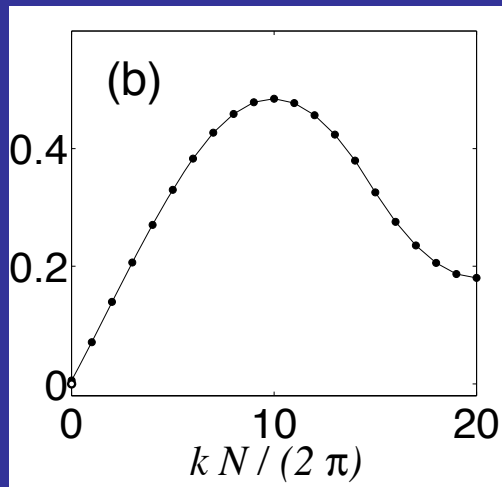
Dispersion relation in bilinear-biquadratic spin 1 chain
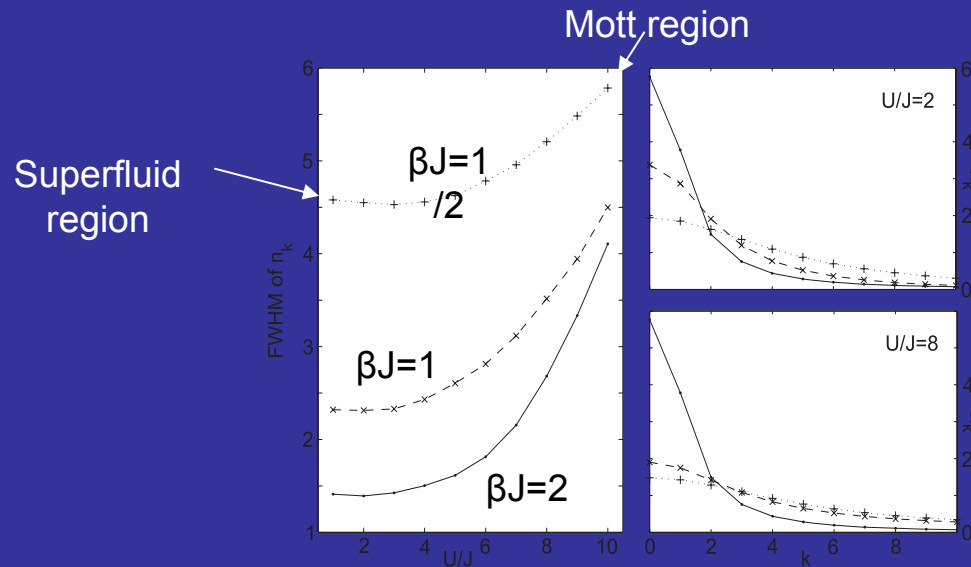
Mott-superfluid transition of bosons in 1-D optical lattices at finite T
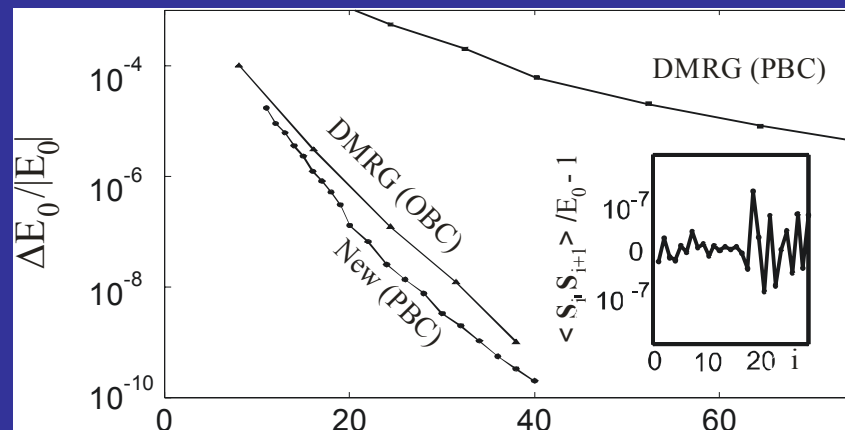
Simulating Heisenberg spin ½ with PBC: MPS vs. DMRG

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
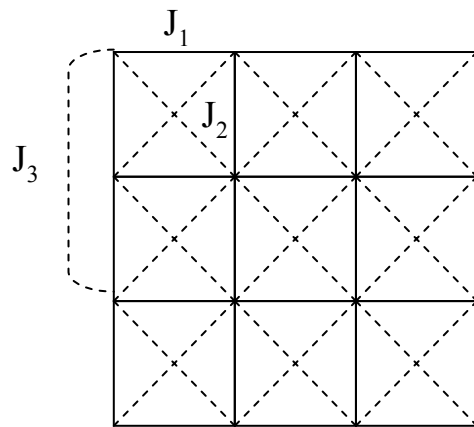
$$H = J_1 \sum_{<ij>} s_i \ s_j + J_2 \sum_{<<ij>>} s_i \ s_j + J_3 \sum_{<<<ij>>>} s_i \ s_j$$
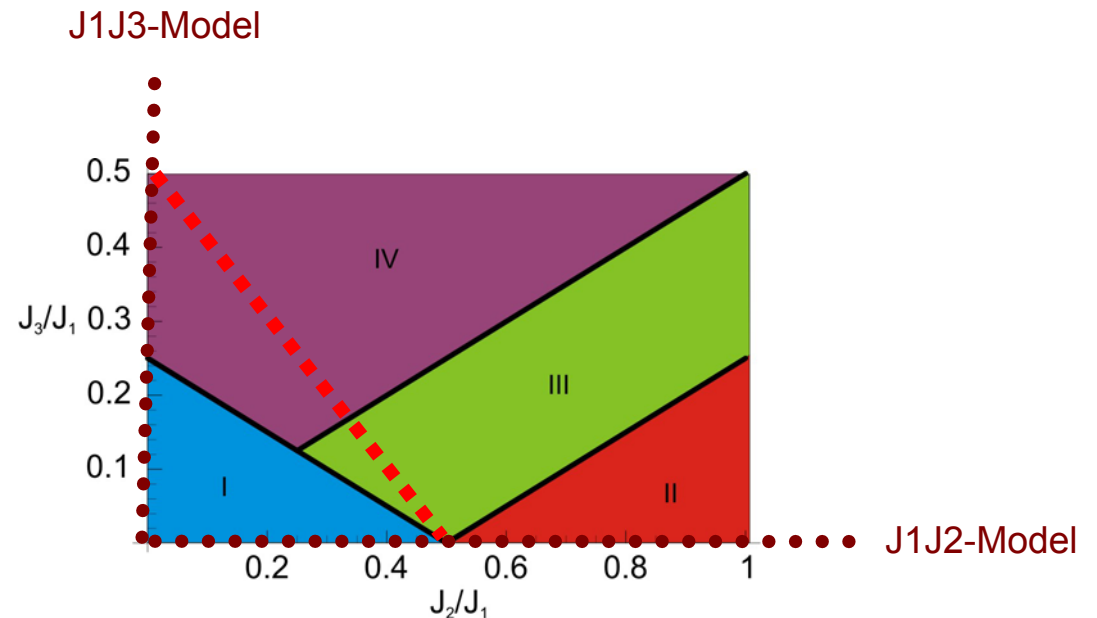
Structure Factor

$$S(\boldsymbol{Q}) = \frac{1}{N} \sum_{kl} e^{i\boldsymbol{Q}\ (r_k - r_l)} < \boldsymbol{s}_k\ \boldsymbol{s}_l >$$
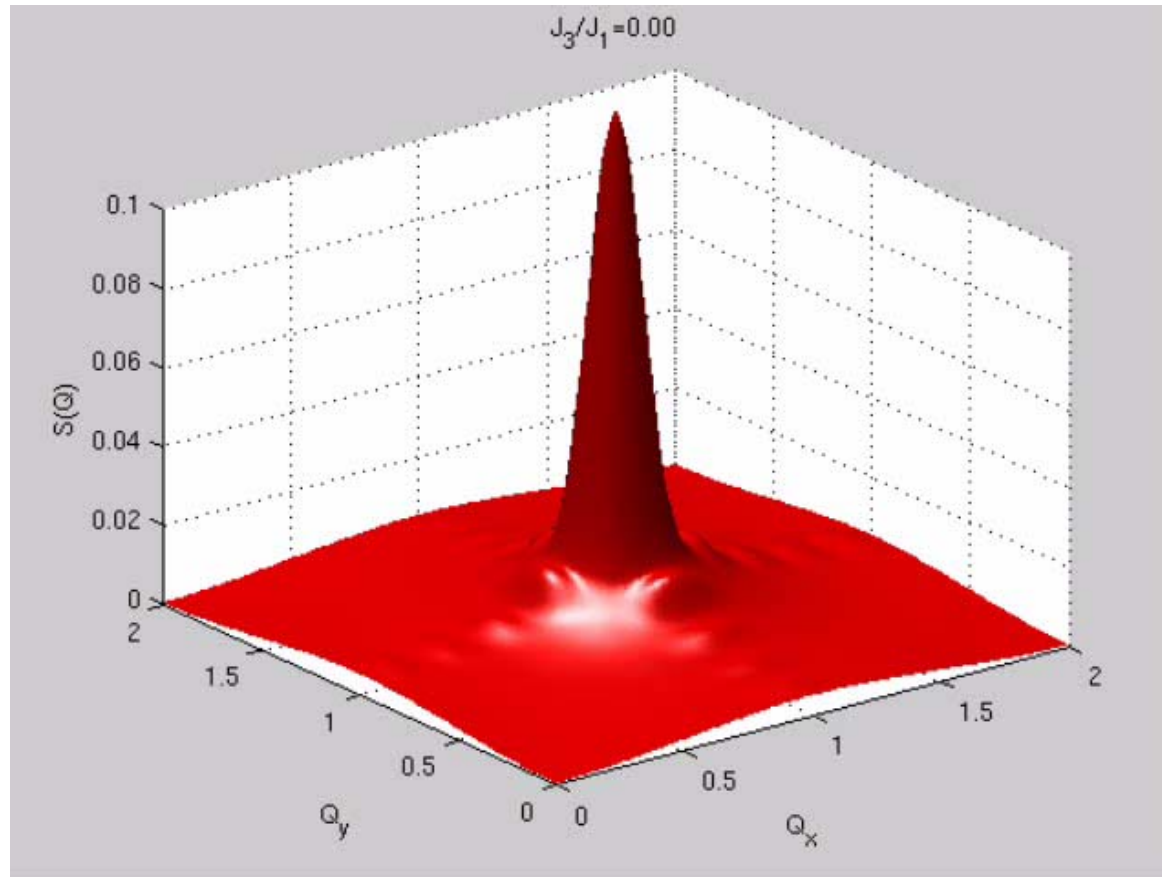
$10x10,\ D=3$

Structure Factor

$J_3 / J_1 = 0$

$J_3 / J_1 = 0.5$
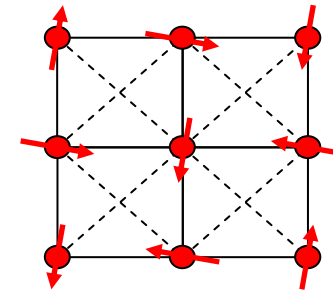
$J_3 / J_1 = 1$

Néel Order:

$\boldsymbol{Q} = (\pi, \pi)$
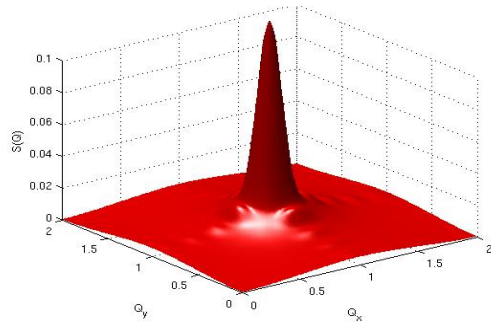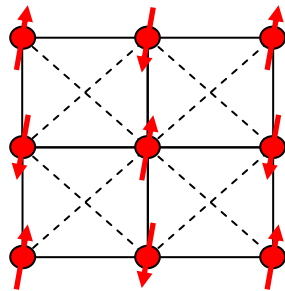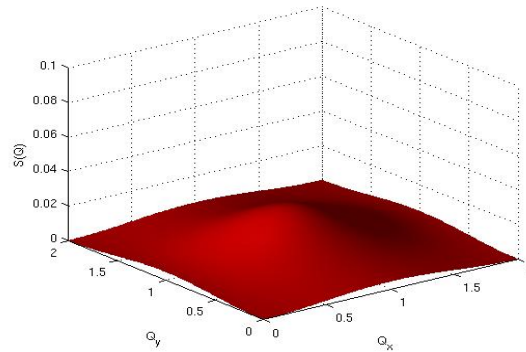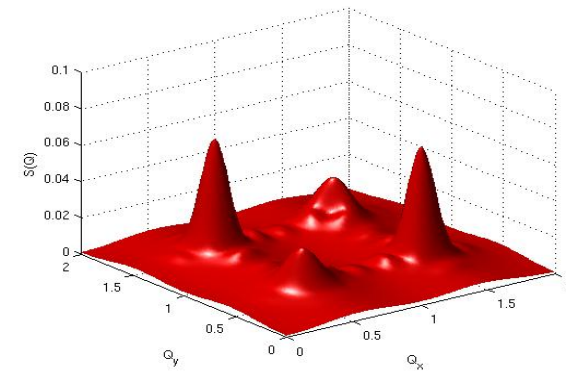
No long range order!

Néel Order on
four Sublattices:
$\boldsymbol{Q} = (\pi/2, \pi/2)$
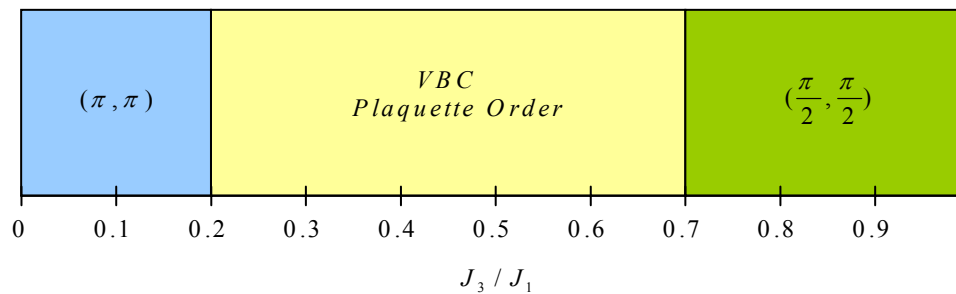
Structure Factor

$$J_2 / J_1 = 0 \qquad\qquad J_2 / J_1 = 0.6 \qquad\qquad J_2 / J_1 = 1$$
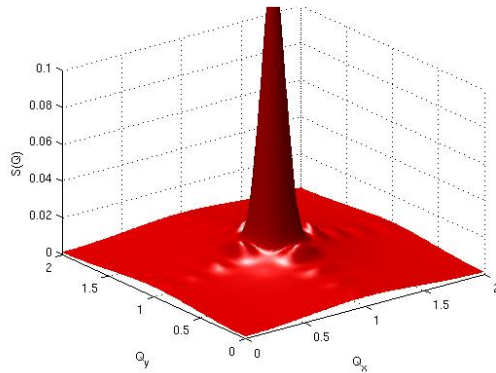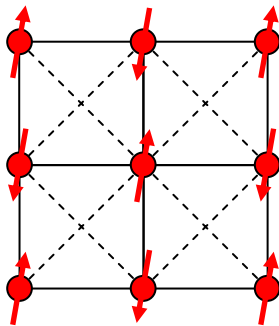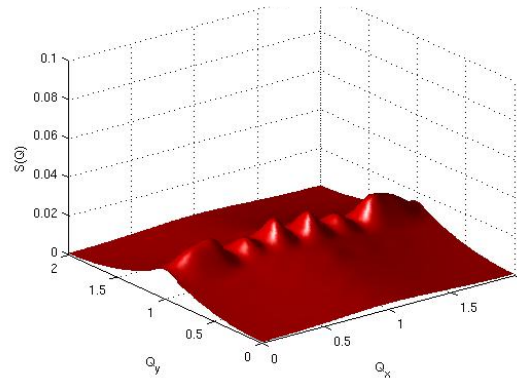
Néel Order: No long range order!   Columnar Order:
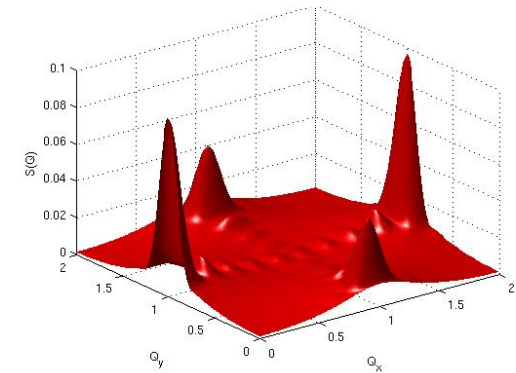
$$\boldsymbol{Q} = (\pi, \pi) \qquad\qquad\qquad\qquad\qquad \boldsymbol{Q} = (\pi, 0),\ (0, \pi)$$
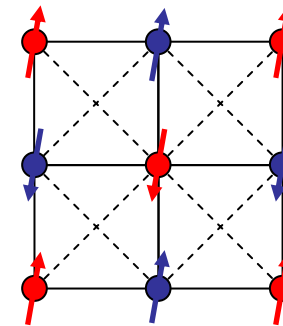
Conclusion

- 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