Workshop on QIS and QMP, Dec 20, 2009

Plaquette Renormalized Tensor Network States: Application to Frustrated Systems

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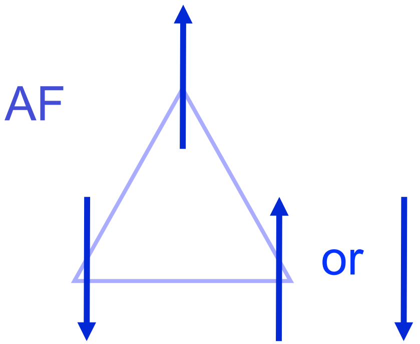
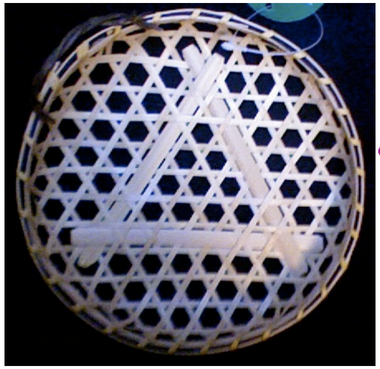
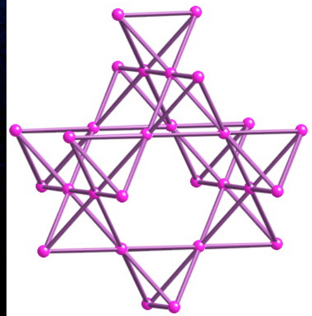
Frustration





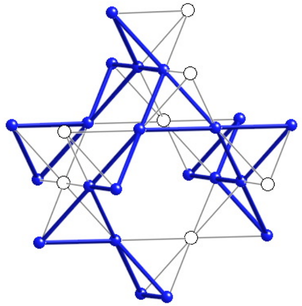
Kagome

$ZnCu_3(OH)_6Cl_2$



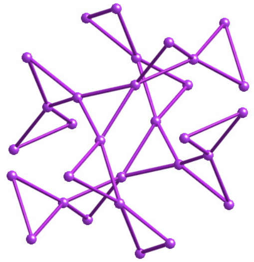
Pyrochlore

$Tb_2Ti_2O_7$



Hyperkagome

$Na_4Ir_3O_8$



Garnet

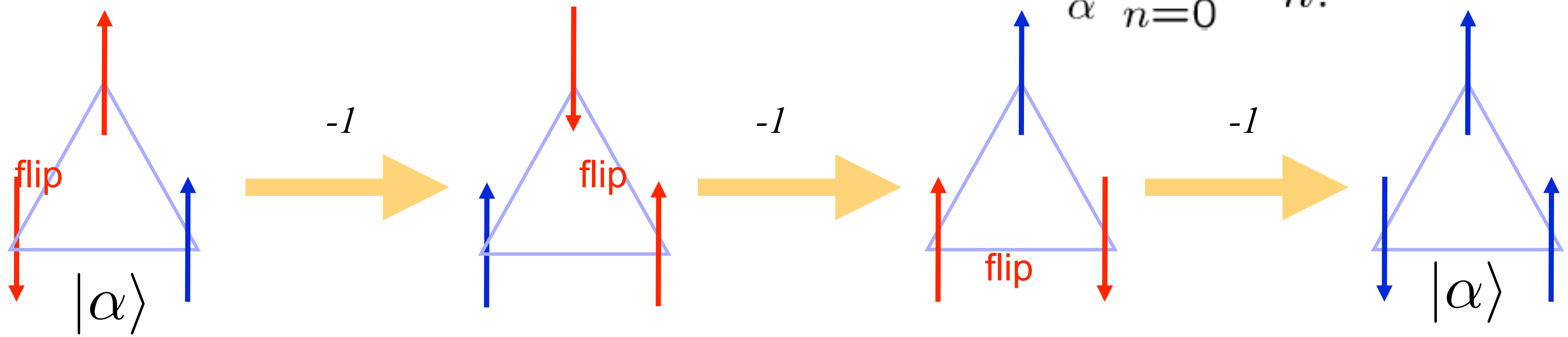
$Gd_3Ga_5O_{12}$

- Large number of degenerate classical ground states
- Emergence of novel spin-disordered ground states due to quantum fluctuations
- Hard to study numerically: size limitation in Exact Diagonalization, sign problem in QMC (also fermion), dimension limit for DMRG (d=1)

Negative Sign Problem

$$H = \sum_{\langle ij \rangle} H_{ij} = \sum_{\langle ij \rangle} (S_i^+ S_j^- + S_i^- S_j^+)$$

$$Z = Tr\left[e^{-\beta \mathcal{H}}\right] = \sum_{\alpha} \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \langle \alpha | \mathcal{H}^n | \alpha \rangle$$



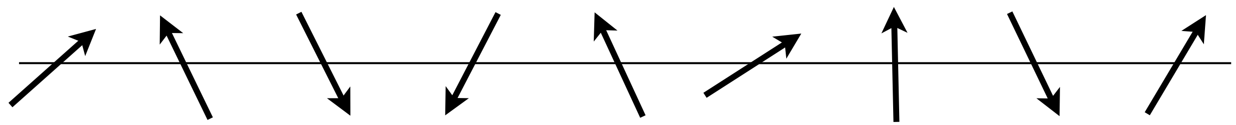
$$p(c) = (-1)^3 \langle \alpha | H_{12} H_{23} H_{31} | \alpha \rangle < 0$$

$$\langle A \rangle_{p(c)} = \frac{\langle A s \rangle_{|p(c)|}}{\langle s \rangle_{|p(c)|}}$$

- Negative matrix elements
- Fluctuations in signs:ensemble average diverges at low temperature

Simulation of Quantum Systems

- Is it possible to classically simulate faithfully a quantum system?



- To represent a quantum state:

$$|\psi\rangle = \sum_{i_1, i_2, \ldots, i_n = 1}^{d} c_{i_1 i_2 \ldots i_n} |i_1 i_2 \ldots i_n\rangle$$

classical representation requires d^n complex coefficients which grows exponentially with n

- Ground states of quantum many-body systems are usually entangled.

Entanglement

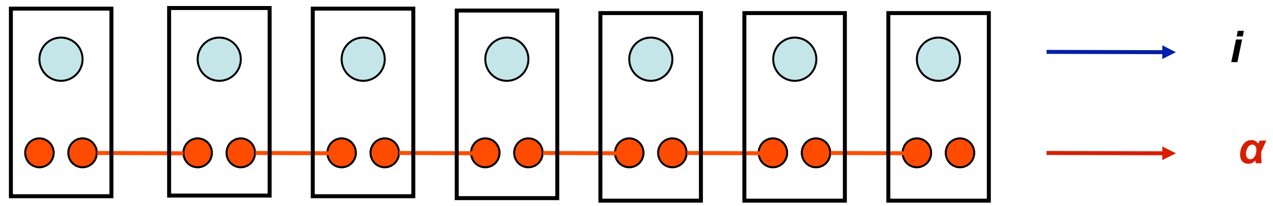
Complementary viewpoints on entanglement:

- Quantum information theory: a crucial resource to process and send information in novel ways
- Quantum many-body physics: entanglement gives rise to exotic phases of matter
- Numerical simulation of strongly correlated quantum systems: source of difficulties !!

What kind of superpositions appear in nature?

symmetries, local interactions, little entanglement

Entanglement: Matrix Product State



$A^{[1]i_1}_{\alpha_1\alpha_2}$ $A^{[2]i_2}_{\alpha_2\alpha_3}$ $A^{[3]i_3}_{\alpha_3\alpha_4}$ $A^{[4]i_4}_{\alpha_4\alpha_5}$ $A^{[5]i_5}_{\alpha_5\alpha_6}$ $A^{[6]i_6}_{\alpha_6\alpha_7}$ $A^{[7]i_7}_{\alpha_7\alpha_8}$

- Between each nearest-neighbor lattice site, we introduce a D-dimensional maximally entangled state: $|\phi >= \frac{1}{\sqrt{D}} \sum_{\alpha=1}^{D} |\alpha\alpha >$
- At each lattice site there are two ends to these maximally entangled states
- Operator A: project D^2 to d (AKLT GS: $D=2, d=3$)

$$|\psi\rangle = \sum_{i_1,\ldots,i_N=1}^{d} A_1(i_1)A_2(i_2)\cdots A_N(i_N)|i_1, i_2, \ldots, i_N\rangle$$

- We reexpress the 2^N coefficients of in terms of about $2D^2N$ parameters (linear in N)
- Key ingredient behind the success of DMRG

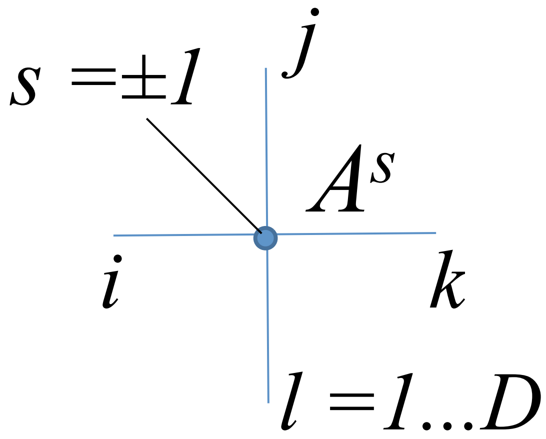
S. Ostlund and S. Rommer, Phys. Rev. Lett. 75, 3537(1995)
Afflect, Kennedy, Lieb, Tasaki, Commun Math Phys 115 (1988)

Tensor product states

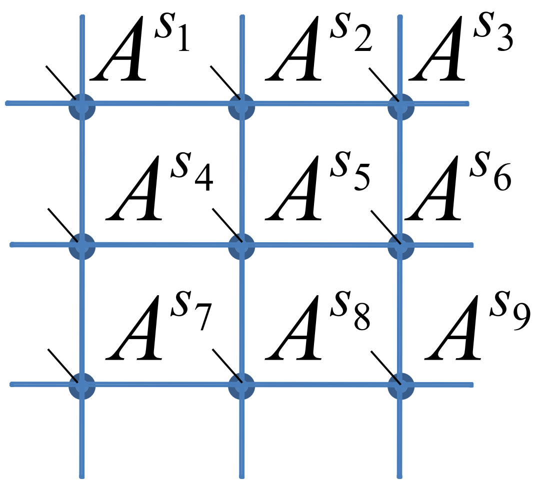
- Extension similar ideas to higher dimension:

  tensor product states, projected entangled paired state (PEPS)

$$|\psi\rangle = \sum_{\{s\}} \mathrm{tTr}\{A(s_1)A(s_2)\cdots A(s_N)\}|s_1, s_2, \ldots, s_N\rangle$$



A_{ijkl}: rank-4 tensor



F. Verstraete and J. I. Cirac, arXiv:cond-mat/0407066

Variational wave function

- Use tensor product state as trial wave function

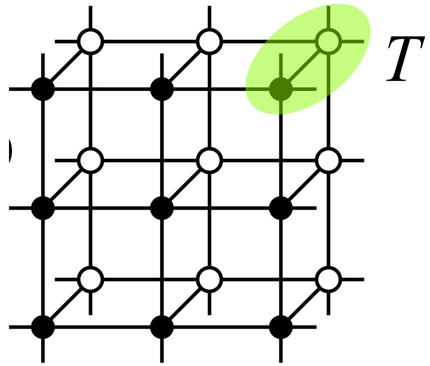
$$E = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} \geq E_0$$

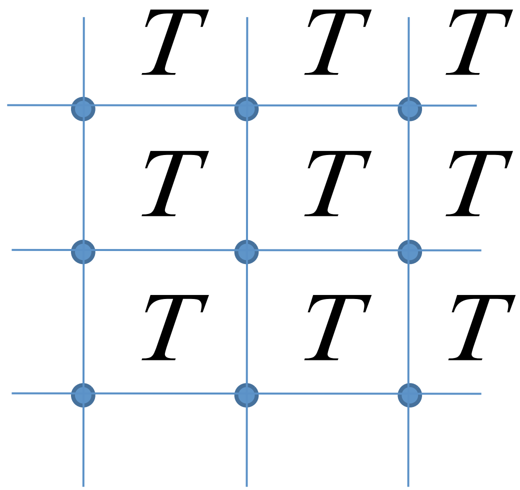
$$\begin{aligned} H &= \sum_i H_i \\ H_i &= \hat{O}_i^0 + \hat{O}_i^1 \hat{O}_j^2 + \dots \end{aligned}$$

$$\begin{aligned} \langle \psi | \psi \rangle &= \sum_{s_1, s_2, \dots} \sum_{i,j,k,l,\dots} A^{s_1 *}_{i',j',k',l'} A^{s_1}_{i,j,k,l} A^{s_2 *}_{k',m',n',o'} A^{s_1}_{k,m,n,o} \cdots \\ &= \mathrm{tTr} \left[T \otimes T \otimes T \otimes \dots \right] \end{aligned}$$

- Double tensor

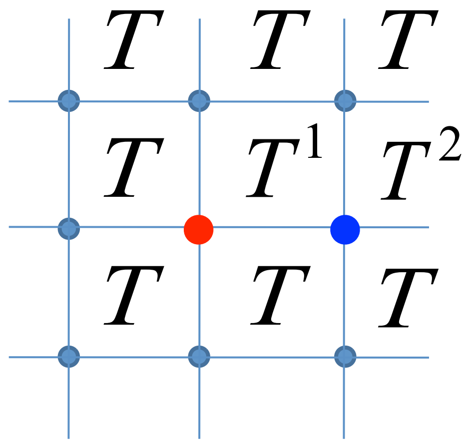
$$T = \sum_{s,s'} A^{s'*} \otimes A^{s}$$





Variational Energy

$$
\begin{aligned}
H &= \sum_i H_i \\
H_i &= \hat{O}_i^0 + \hat{O}_i^1 \hat{O}_j^2 + \ldots \\
\langle\psi|H|\psi\rangle &= \mathrm{tTr}\left[T_i^0 \otimes T \otimes T \otimes \ldots\right] \\
&\quad + \mathrm{tTr}\left[\boxed{T_i^1} \otimes \boxed{T_j^2} \otimes T \otimes \ldots\right] + \ldots
\end{aligned}
$$

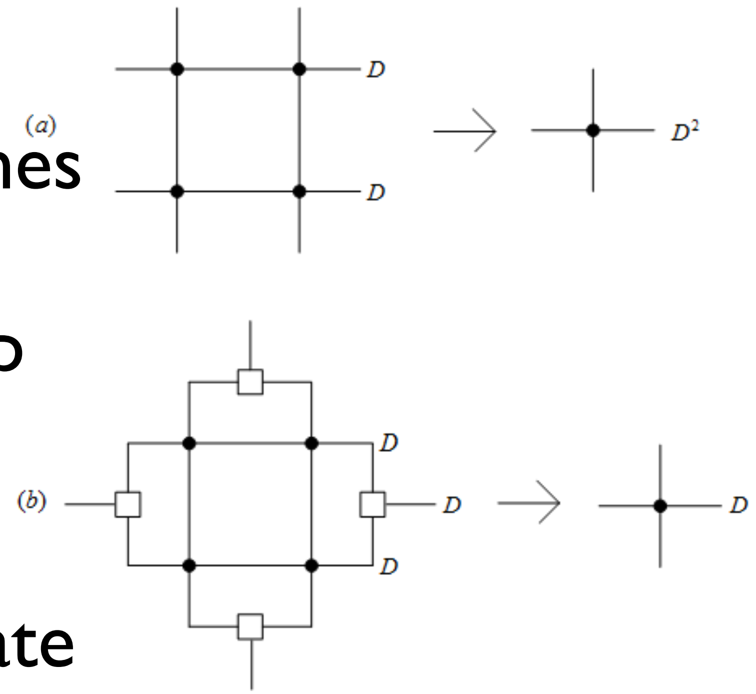


$$T^a = \sum_{s,s'} A^{s'*} \otimes A^s \langle s'|\hat{O}^a|s\rangle$$

- Computationally intensive: D^{N_bond}
- Direct computation of contraction is impossible: approximation (RG schemes)

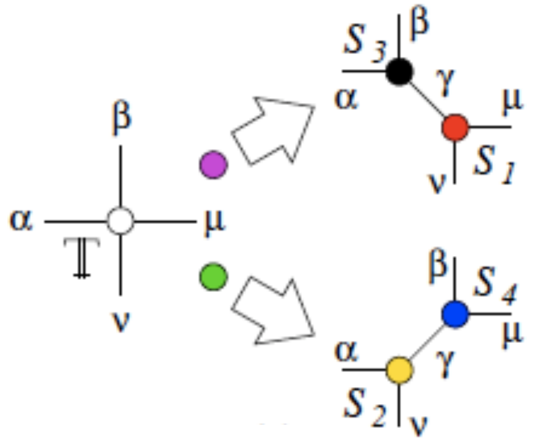
Tensor Contraction

- Contracting the internal indices, the four-leg tensor can be viewed as a single tensor.
- External link dimension becomes D^2 after one contraction; exponential growth as we keep contracting D^4,D^8......
- Computationally intensive; Impossible to store intermediate results.
- Need some RG scheme.



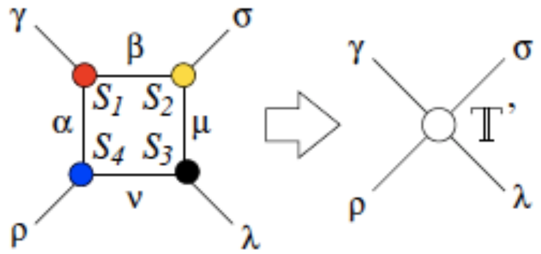
Tensor entanglement renormalization

- Singular Value Decomposition: rank-3 tensors S



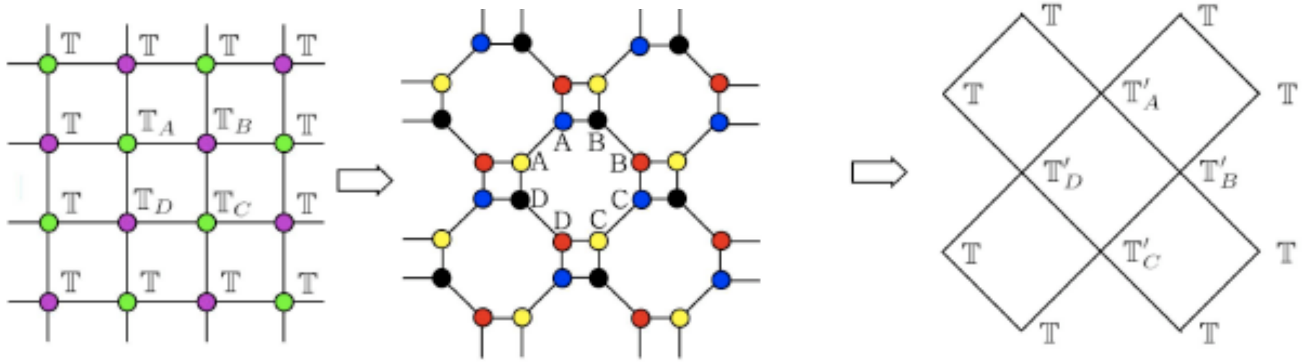
$$T_{\alpha\beta\mu\nu} \approx \sum_{\gamma'=1}^{D_{\rm cut}} S^{1}_{\mu\nu\gamma'} S^{3}_{\alpha\beta\gamma'}$$

$$T_{\alpha\beta\mu\nu} \approx \sum_{\gamma'=1}^{D_{\rm cut}} S^{2}_{\alpha\nu\gamma'} S^{4}_{\mu\beta\gamma'}$$



$$T'_{\gamma\sigma\lambda\rho} \approx \sum_{\alpha\beta\mu\nu} S^{1}_{\beta\alpha\gamma} S^{2}_{\mu\beta\sigma} S^{3}_{\nu\mu\gamma} S^{4}_{\alpha\nu\rho}$$

- Introduce cut-off for the bond-contraction

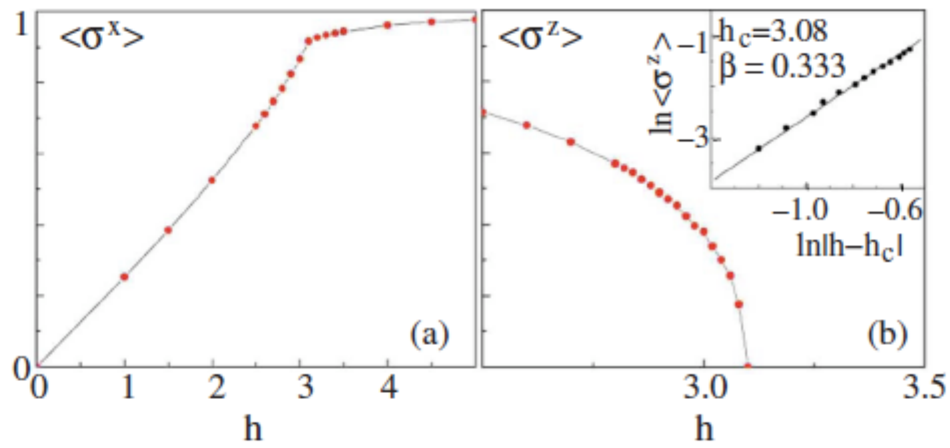


H. C. Jiang, Z. Y. Weng, and T. Xiang, Phys. Rev. Lett. 101, 090603 (2008)
Gu, Levin, Wen, Phys. Rev. B, 78, 205116 (2008)

Tranverse ising model

$$H = -\sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z - h \sum_i \sigma_i^x$$

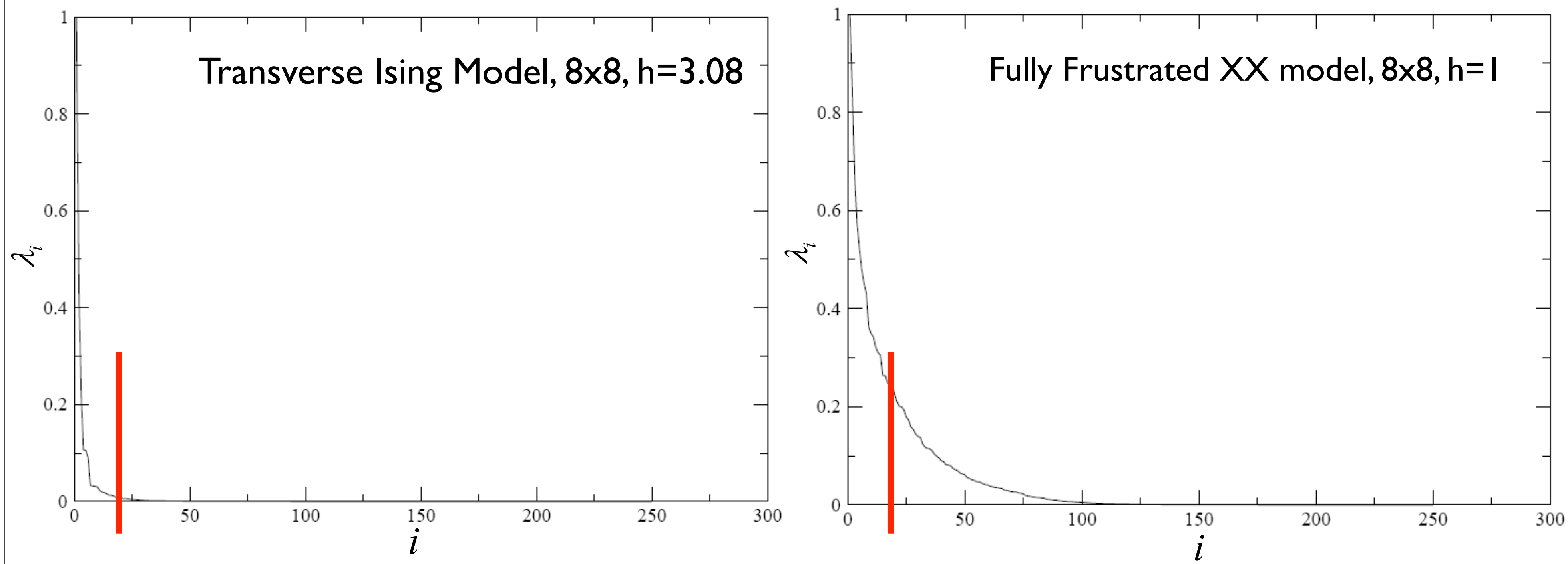
- D=2, D_{cut}=18, non-MF results is obtained
- Method is not variational
  - Locally optimized
  - SVD truncation
- Translational invariance explicitly broken



Gu, Levin, Wen, Phys. Rev. B, 78, 205116 (2008)

Distribution of Singular Values

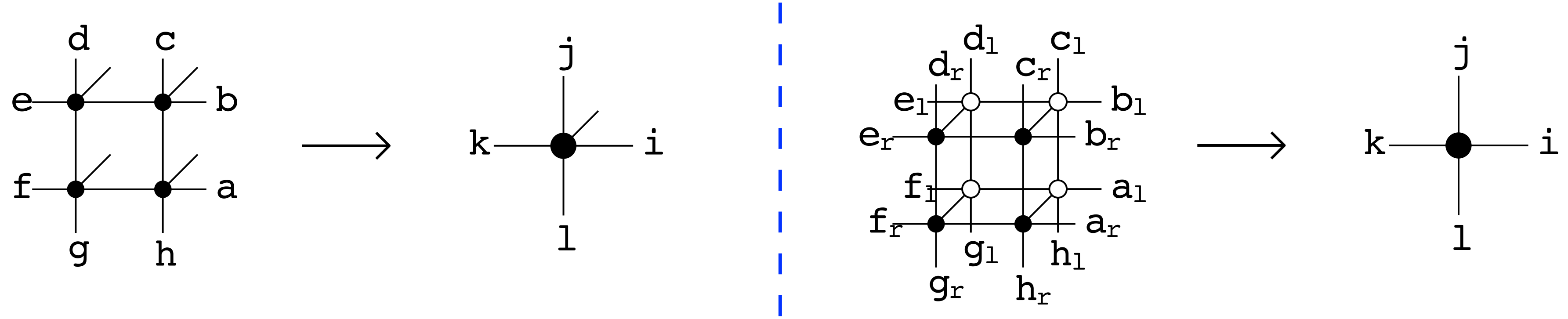
$$T_{\alpha\beta\mu\nu} = M_{\alpha\beta,\mu\nu} = \sum_{\gamma} U_{\alpha\beta,\gamma} \lambda_{\gamma} V^{T}_{\gamma,\mu\nu} \quad \lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \cdots$$



Frustrated Systems Remain Difficult

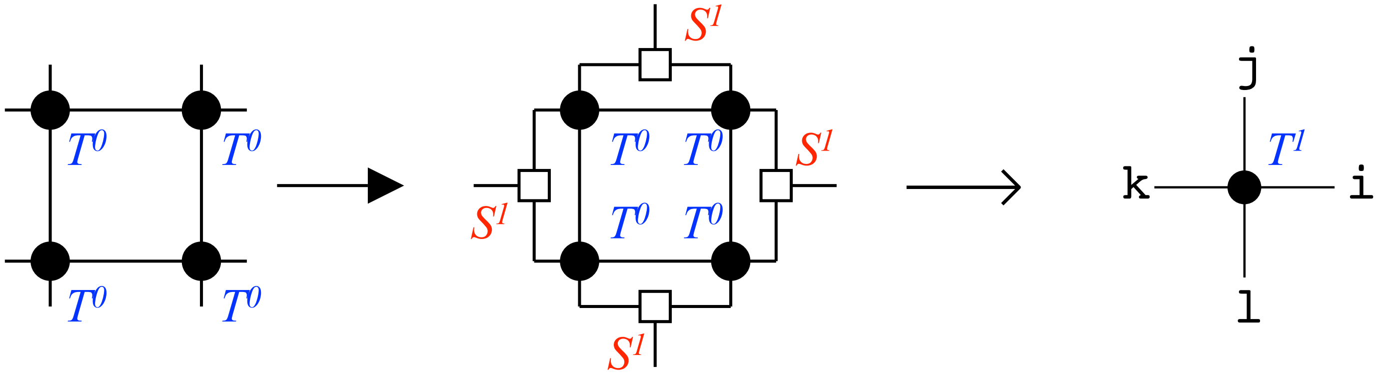
Plaquette-Renormalization

8-index tensor: D^8 4-index tensor: D_{cut}^4 | 8-index dbl-tensor: D^{16} 4-index dbl-tensor: D_{cut}^8



$a,b,\ldots g,h=1\ldots D$ $i,j,k,l=1\ldots D_{cut}$ $a,b,\ldots g,h=1\ldots D$ $i,j,k,l=1\ldots D_{cut}^2$

Renormalization of an 8-index plaquette tensor using auxiliary 3-index tensors S.



Department of Physics
National Taiwan University

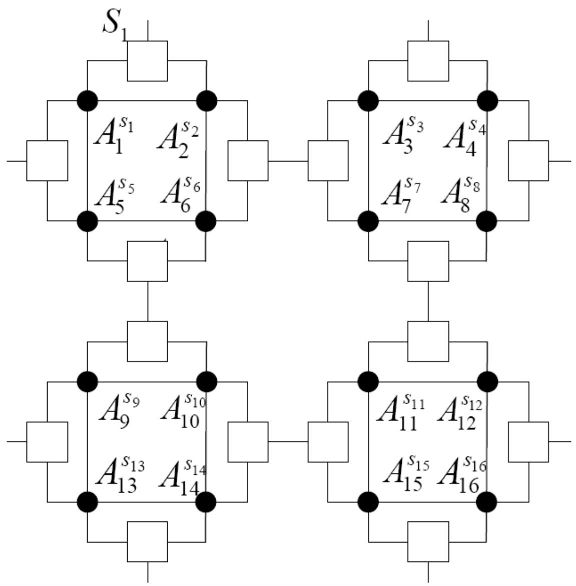
Wang, Kao, Sandvik, arXiv:0901.0214

Plaquette renormalized trial wave function

$$|\psi\rangle = \sum_{\{s\},i,j,k,l,\ldots} (A_1^{s_1})_{i,j,k,l}(A_2^{s_2})_{k,m,n,o}(S_1)_{m,j,p}(S_2)_{q,p,r}\cdots|s_1 s_2 \cdots s_N\rangle$$

$$= \sum_{\{s\}} tTr(A_1^{s_1} \otimes A_2^{s_2} \otimes S_1 \otimes S_2 \otimes \cdots \otimes A_N^{s_N})|s_1 s_2 \cdots s_N\rangle$$

- We treat the elements in the A and S tensors as variational parameters, and minimize the total energy.
- Principal axis method: derivative-free, but computationally expensive.



Expectation values

$$H = \sum_i \hat{O}_i^0 + \sum_{\langle i,j \rangle} \hat{O}_i^1 \hat{O}_j^2 + \sum_{\langle\langle i,j \rangle\rangle} \hat{O}_i^1 \hat{O}_j^2 + \cdots$$

Normalization factor:

$$\langle \psi | \psi \rangle = tTr\left[T_1 \otimes T_2 \otimes R_1 \otimes \cdots \otimes T_N\right]$$

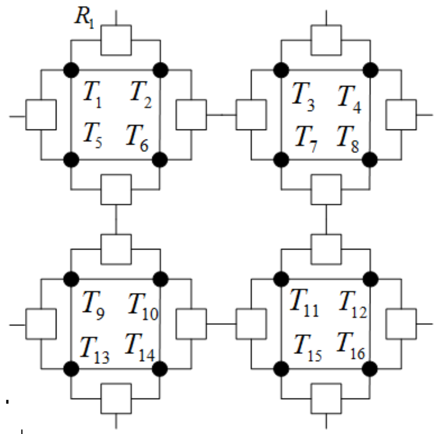
Two - body interaction:

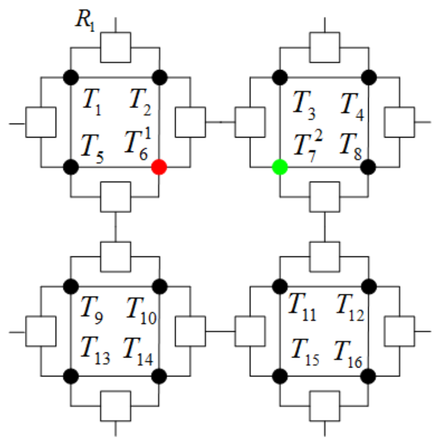
$$\left\langle \psi \middle| \hat{O}_i^1 \hat{O}_j^2 \middle| \psi \right\rangle = tTr\left[T_1 \otimes T_2 \otimes R_1 \otimes \cdots \otimes T_i^1 \otimes T_j^2 \otimes \cdots \otimes T_N\right]$$

$$T_j = \sum_{s_j} A_j^{s_j\,*} \otimes A_j^{s_j}$$

$$T_j^a = \sum_{s'_j, s_j} A_j^{s'_j\,*} \otimes A_j^{s_j} \langle s'_j | \hat{O}_j^a | s_j \rangle$$

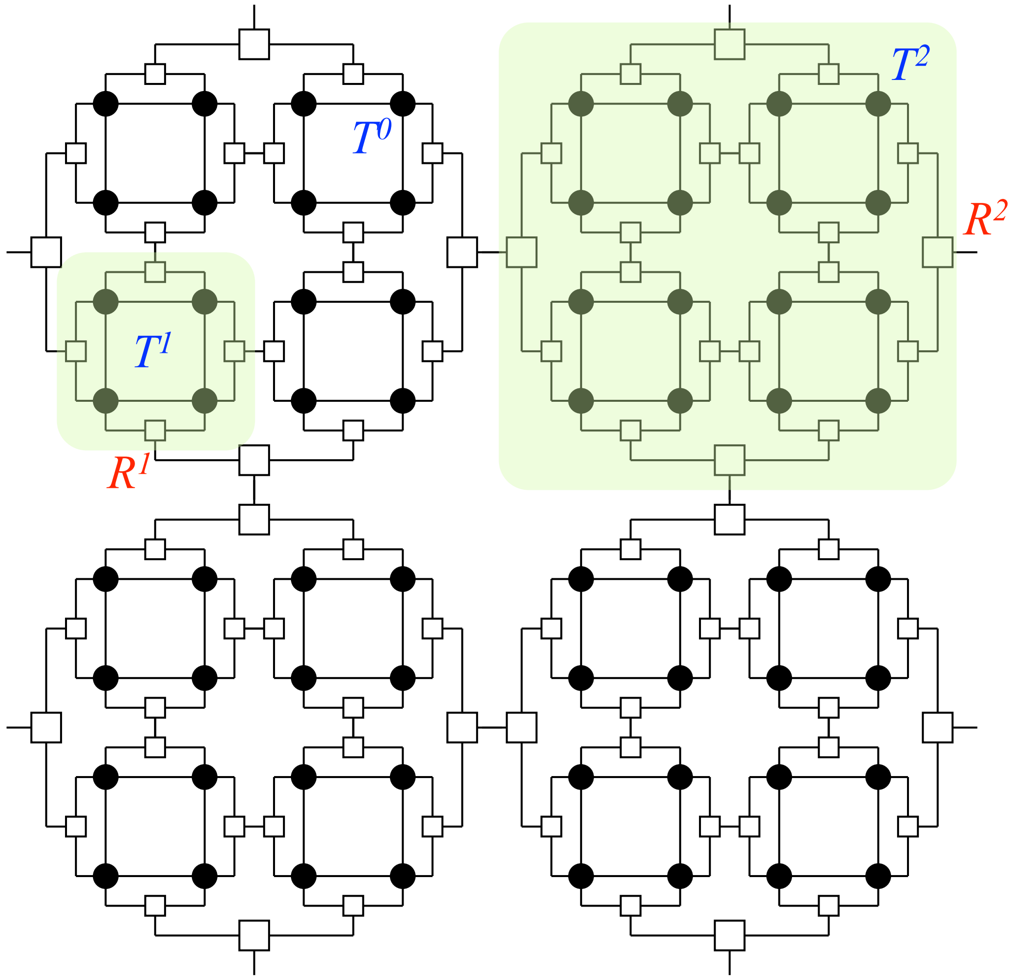
$$R_i = S_i^* \otimes S_i$$





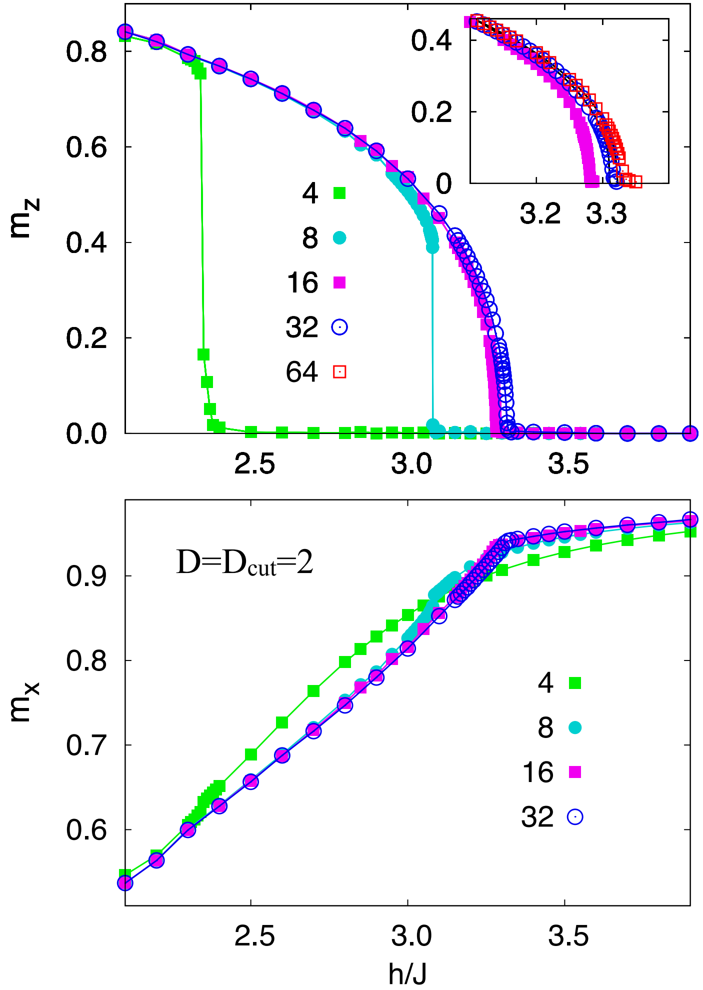
Plaquette-Renormalization of TNS

- Effective reduced tensor network for a 8x8 lattice
- Summing over all unequivalent bonds and sites
- Method is variational
- Optimize T and R globally
- Size scaling: $L^2 \mathrm{Log}(L)$



Wang, Kao, Sandvik, arXiv:0901.0214

Transverse Ising Model

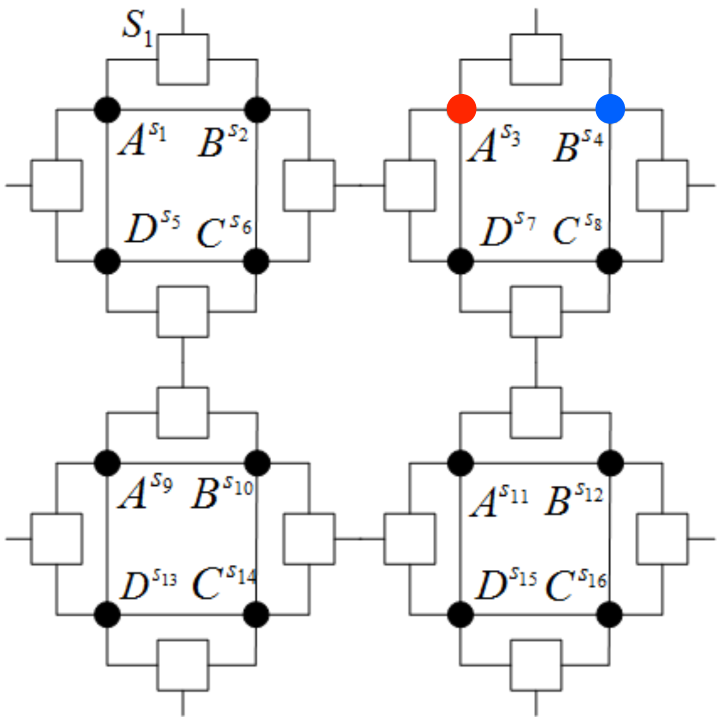


- Assume translational invariance: all initial T's are the same.
- Globally optimized T and R.
- h_c=3.33 (3.04,QMC)
- m_z~ $(h-h_c)^\beta$, β~0.40
- h~h_c, β~0.50 mean-field like. (Sanvik's talk).

L	h	D	E_{var}/N	E/N	Δ_E
4	3.0	2	−3.1978372	-3.2155081(exact)	5.4955×10^{-3}
8	3.0	2	−3.1717845	−3.19750(QMC)	8.0437×10^{-3}

Wang, Kao, Sandvik, arXiv:0901.0214

Transverse Ising Model



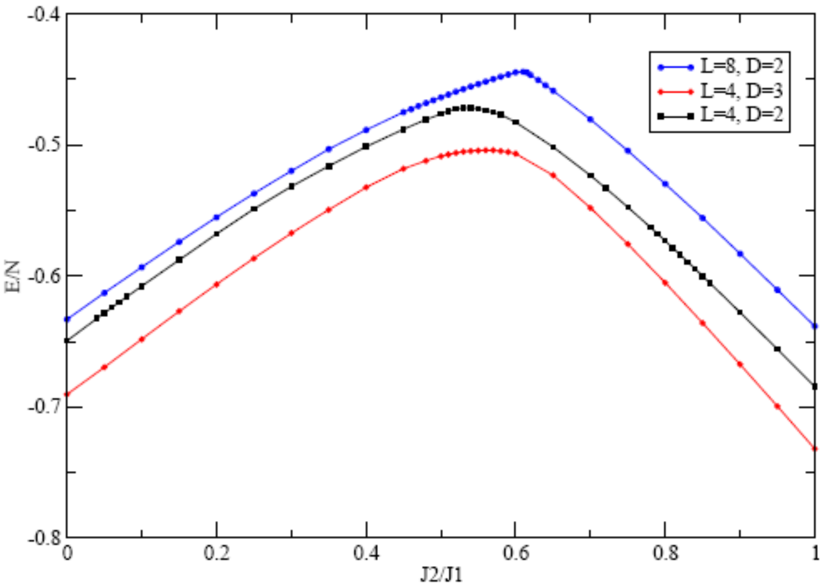
- Spins at different lattice sites inside the plaquette have different environments.
- We use different tensors inside a plaquette.

L	h	D	E_{var}/N	E/N	Δ_E
4	3.0	2	−3.1978372	-3.2155081(exact)	5.4955×10^{-3}
8	3.0	2	−3.1717845	−3.19750(QMC)	8.0437×10^{-3}

L	h	D	E_{var}/N	E/N	Δ_E
4	3.0	2	−3.2044358	-3.2155081(exact)	3.4434×10^{-3}
4	3.0	3	−3.2152333	-3.2155081(exact)	8.546×10^{-5}

L	h	D	E_{var}/N	E/N	Δ_E
8	3.0	2	−3.17712	−3.19750(QMC)	6.3737×10^{-3}
8	3.044	2	−3.21404	−3.23627(QMC)	6.869×10^{-3}

J1-J2 Heisenberg Model



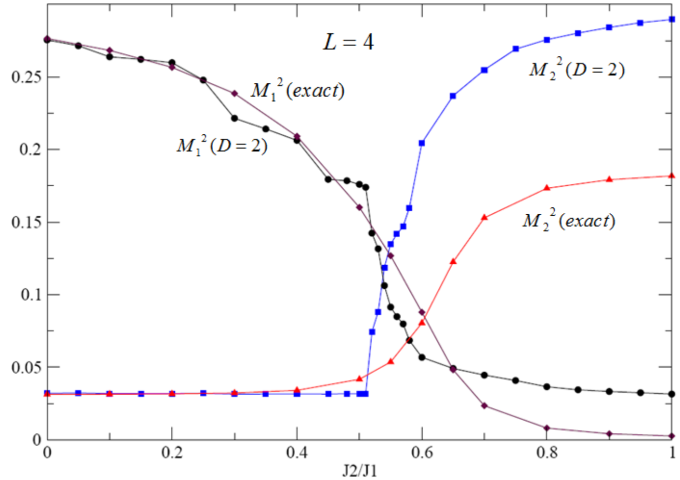
$$H = J_1 \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle ij \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

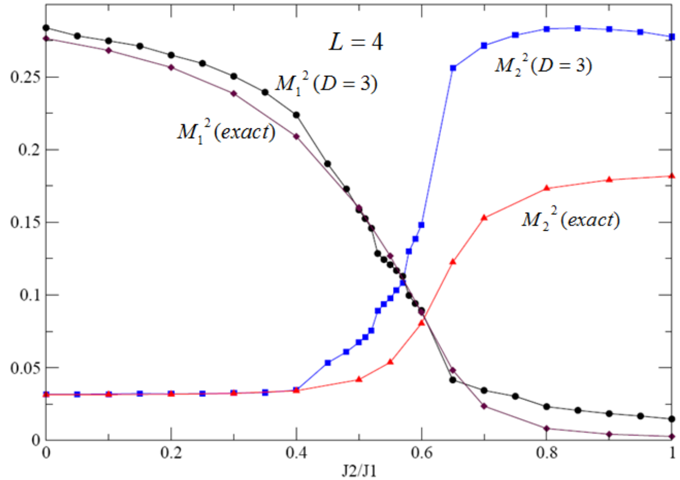
$$M^2 = \langle (\frac{1}{N} \sum_j f(j) \vec{S}_j)^2 \rangle$$

$$f(j) = \exp[i\vec{Q} \cdot \vec{R}_j], \vec{R}_j = (x_j, y_j)$$

$$M_1^2 \text{ at } \vec{Q} = (\pi, \pi)$$

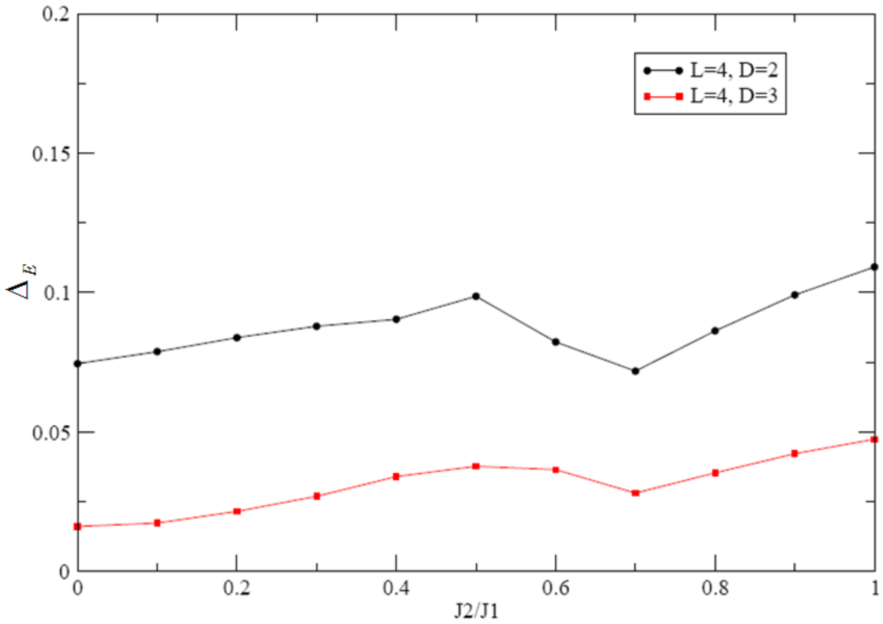
$$M_2^2 \text{ at } \vec{Q} = (\pi, 0) \text{ or } \vec{Q} = (0, \pi)$$





H. J. Schulz, T.A. Ziman and D. Poilblanc, J. Phys. I 6 (1996) 675-703

Error in energy



- Improvement in accuracy as D increase.
- D also sets a length scale.

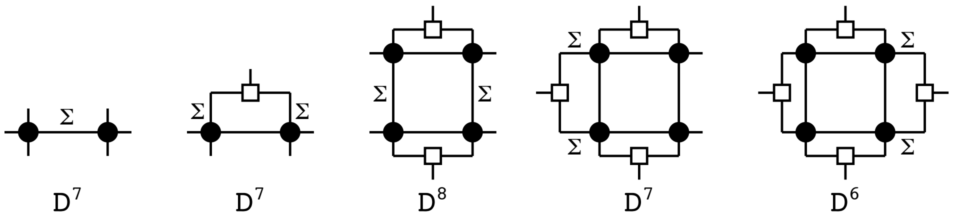
- J_2=0

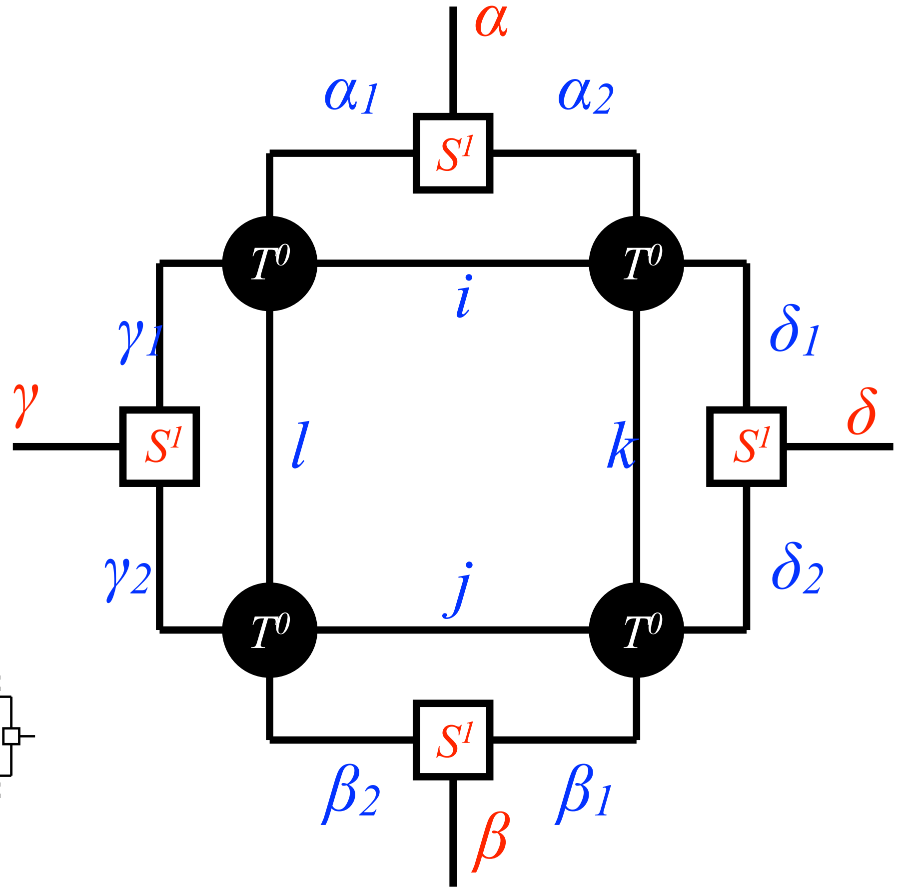
L	D	E_{var}/N	E/N	Δ_E
4	2	-0.649491	-0.701781(exact)	7.451×10^{-2}
8	2	-0.633135	-0.673487(QMC)	5.991×10^{-2}
16	2	-0.630080	-0.669976(QMC)	5.954×10^{-2}

A. W. Sandvik, Phys. Rev. B 56, 11678 (1997)

Building block: plaquette

- 12 internal sums. Maximum computational effort: D^8.
- Each free index and summation contributes D.





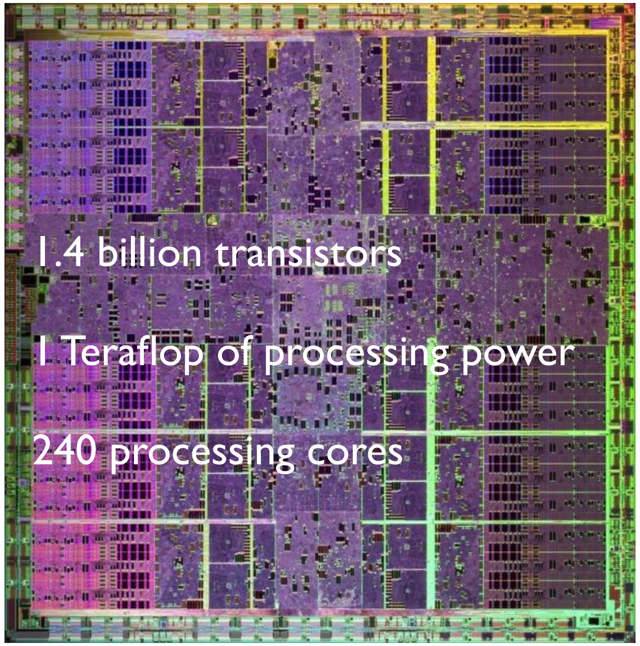
$$T^{(1),\alpha\beta}_{\gamma\delta} = \sum_{\alpha_1,\alpha_2,\ldots,\delta_1,\delta_2,ijkl} S^{(1),\alpha}_{\alpha_1\alpha_2} S^{(1),\beta}_{\beta_1\beta_2} S^{(1),\gamma}_{\gamma_1\gamma_2} S^{(1),\delta}_{\delta_1\delta_2} T^{(0),\alpha_1 l}_{\gamma_2 i} T^{(0),\alpha_2 j}_{i\delta_1} T^{(0),j\beta_1}_{k\delta_2} T^{(0),l\beta_2}_{\gamma_1 k}$$

Computational Costs

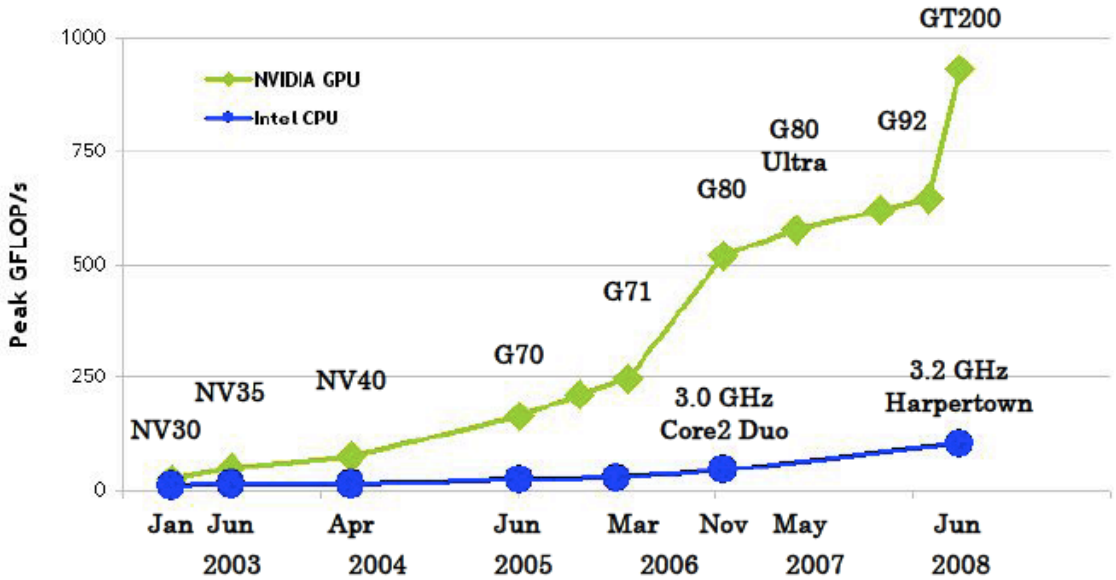
- Globally optimized T and R.
- Contraction calculation is highly parallelizable.
- IBM Blue Gene/L at BU. D=2, takes weeks to optimize.
- Bottleneck: plaquette internal contractions.
- Take advantage of GPU (Graphic Processing Unit).

GPU supercomputing

- The GPU is specialized for compute-intensive, massively data parallel computation



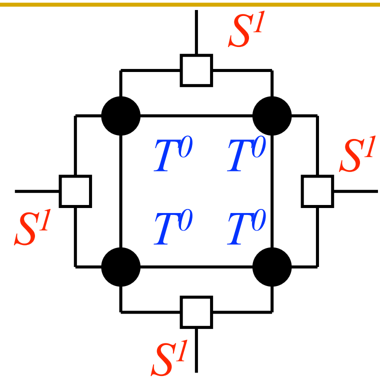
nVidia Tesla 10-Series Processor



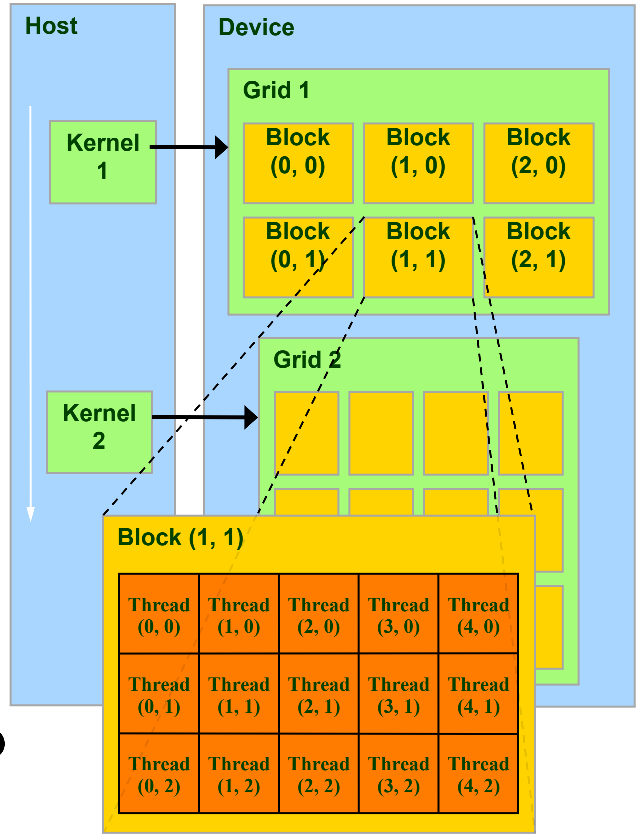
GT200 = GeForce GTX 280	G71 = GeForce 7900 GTX	NV35 = GeForce FX 5950 Ultra
G92 = GeForce 9800 GTX	G70 = GeForce 7800 GTX	NV30 = GeForce FX 5800
G80 = GeForce 8800 GTX	NV40 = GeForce 6800 Ultra	

NTU CQSE GPU cluster
16x Tesla S1070=64 Teraflops

GPU kernel Strategy



- Inputs: T (D^4), S (D^3) (unchanged during contraction)
  - Load into texture memory (optimized for 2D read)
- Output: T' (D^4)
- Thread block geometry up to 3D (t_x,t_y,t_z), grid of blocks geometry up to 2D (b_x,b_y).
  - Reshape T into a D^2xD^2 matrix, S into a DxD^2 matrix.
  - Use D^2xD^2 thread blocks, each block has DxD threads. Each block computes an element of T'. Use block indices (b_x,b_y) to represent external indices.



NVIDIA

Benchmark: One plaquette contraction

- CPU code: Intel Core 2 Duo E4700 2.6GHz
  - D=6, 2.1 GFLOPS
  - D=8, 3.4 GFLOPS
- GPU, Single Precision code (unoptimized):
  - D=6, 24.9 GFLOPS (GTX8800), 49.7GFLOPS (GTX280)
  - D=8, 92.2 GFLOPS (GTX280)
- 10x to 30x speedup. A factor of at least 8 performance hit for DP.
- GPU code requires optimization
  - Bank conflict in shared memory R/W
  - Low stream multiprocessor occupancy
  - Current scheme D bound by shared memory size
  - Global memory bandwidth hiding

Conclusion

- Tensor network states are promising candidates to understand frustrated quantum spin systems.
- In plaquette renormalized tensor network representation, no approximations are made when contracting the effective renormalized tensor network.
- Non-MFT results even with the smallest possible non-trivial tensors and truncation (D = 2)
- Larger internal bond dimension D is necessary to get the right physics.
- GPU can potentially speed up the computationally intensive part of the calculation.
- Use Monte Carlo sampling in the future.