NDNS: from DMRG to TNF
Kyoto, Japan 10/29/2010

Plaquette Renormalized Tensor Network States: Application to Frustrated Systems

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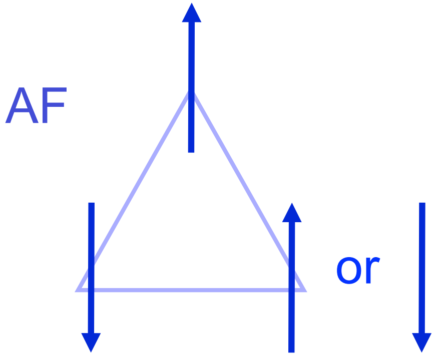
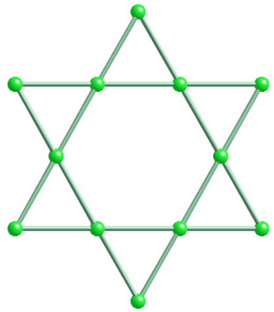
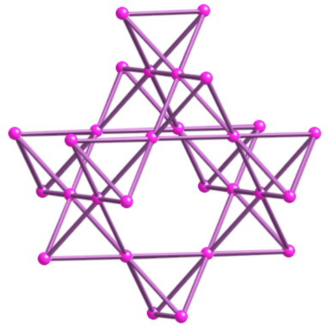
Frustration





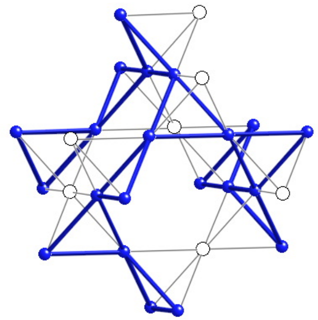
Kagome

$ZnCu_3(OH)_6Cl_2$



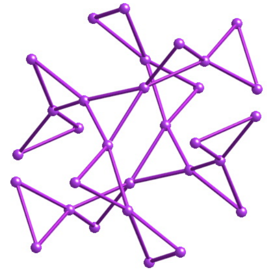
Pyrochlore

$Tb_2Ti_2O_7$



Hyperkagome

$Na_4Ir_3O_8$



Garnet

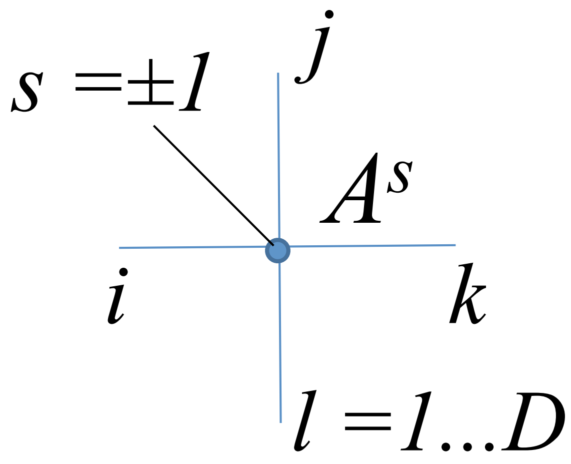
$Gd_3Ga_5O_{12}$

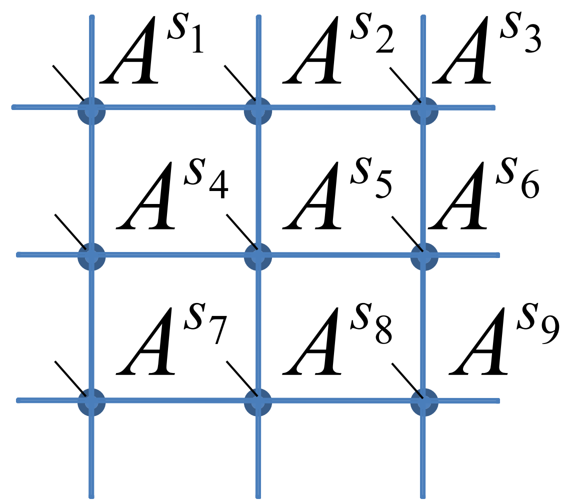
- Large number of degenerate classical ground states
- Emergence of novel spin-disordered ground states due to quantum fluctuations
- Hard to study numerically: size limitation in Exact Diagonalization, sign problem in QMC (also fermion), dimension limit for DMRG

Tensor product states

- Tensor product states, projected entangled paired state (PEPS)

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



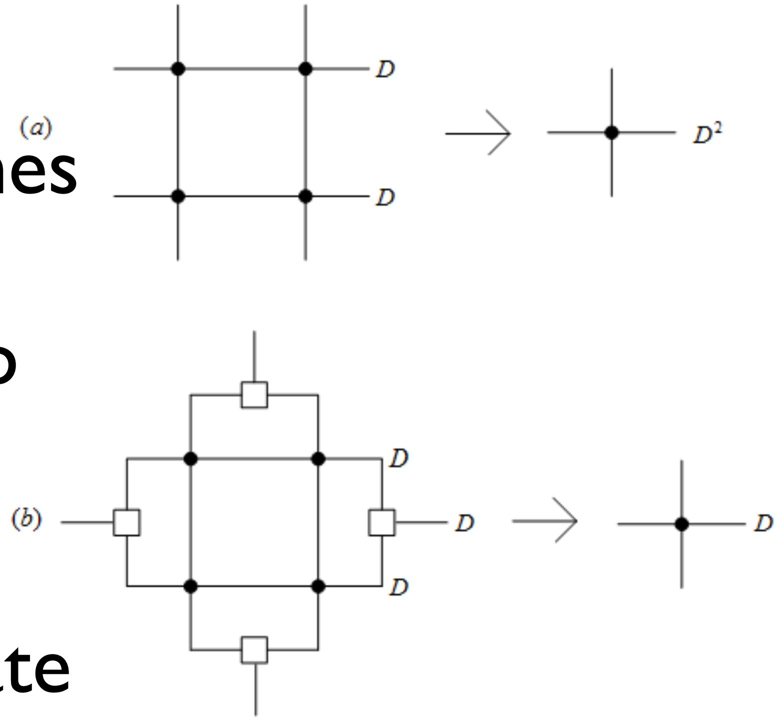


A_{ijkl}: rank-4 tensor

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

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.

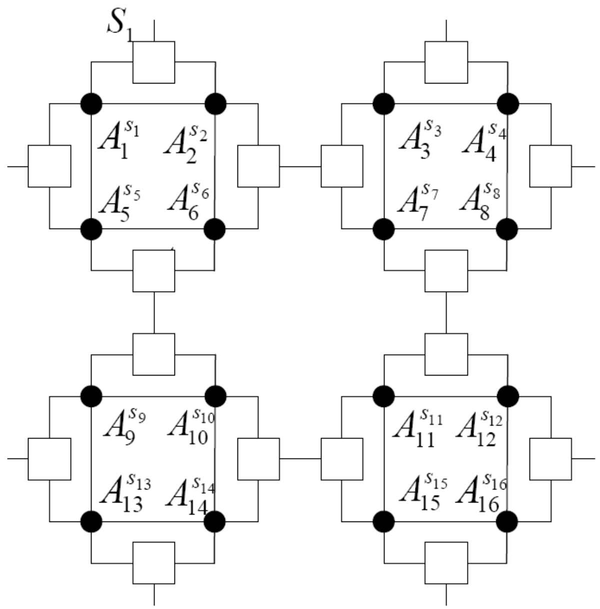


Plaquette renormalized trial wavefunction

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

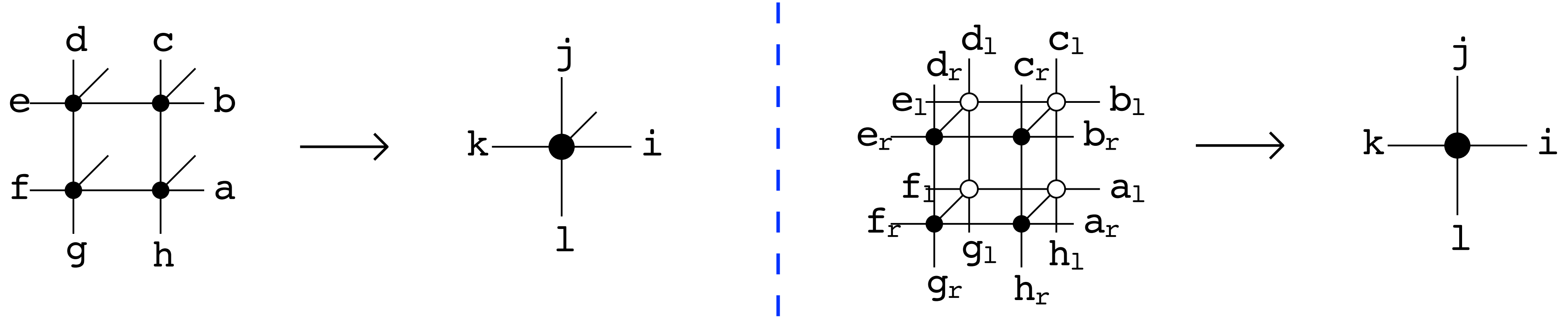
$$= \sum_{\{s\}} tTr(A_1^{s_1} \otimes A_2^{s_2} \otimes S_1 \otimes S_2 \otimes \cdots \otimes A_N^{s_N}) |s_1 s_2 \cdots s_N\rangle$$

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



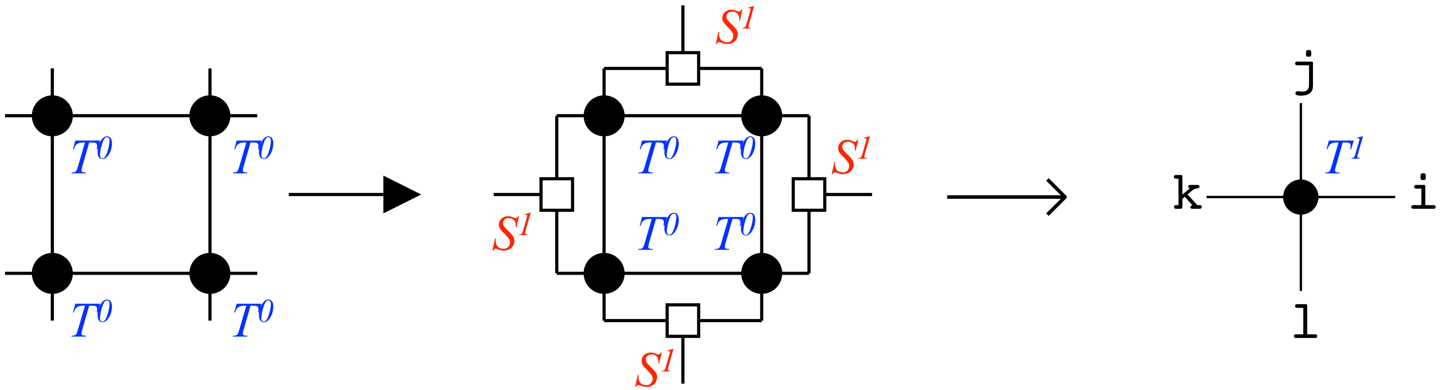
Plaquette-Renormalization

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



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

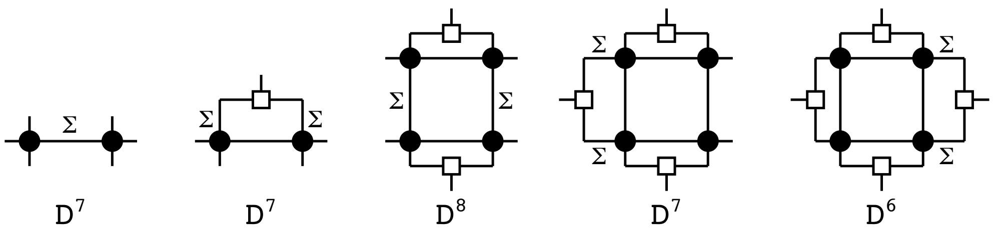
Renormalization of an 8-index plaquette tensor using auxiliary 3-index tensors S.

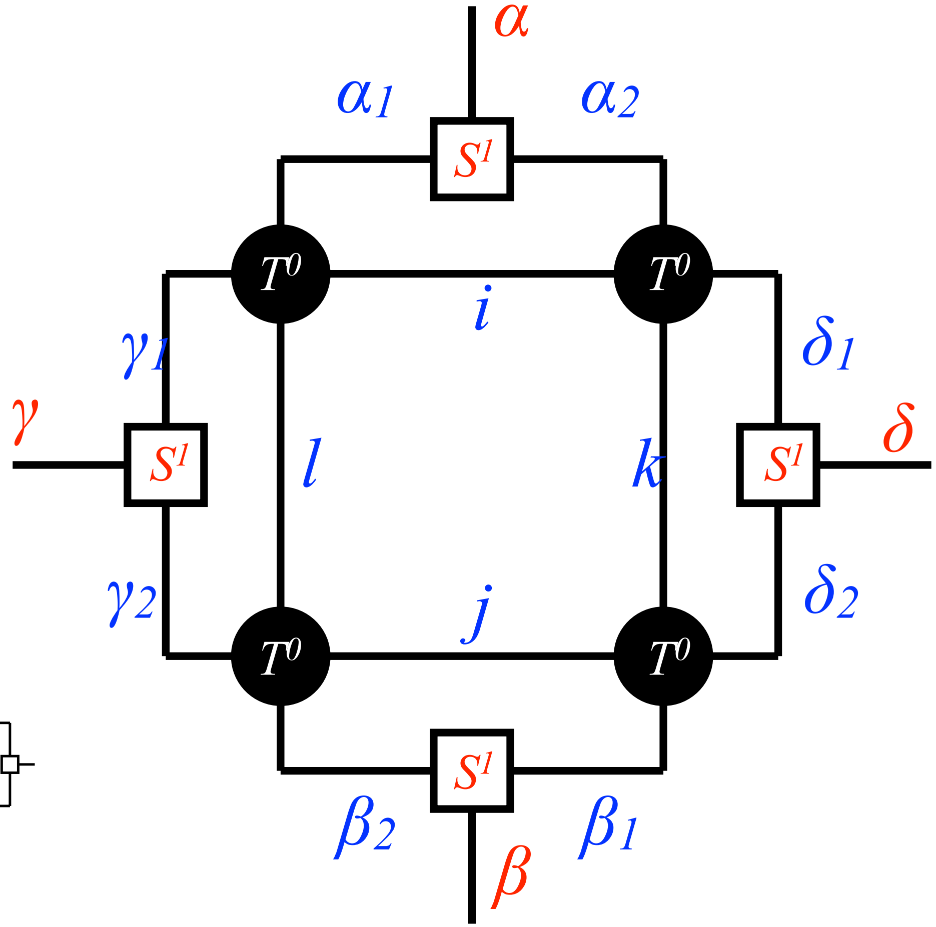


Wang, Kao, Sandvik, arXiv:0901.0214

Building block: plaquette

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

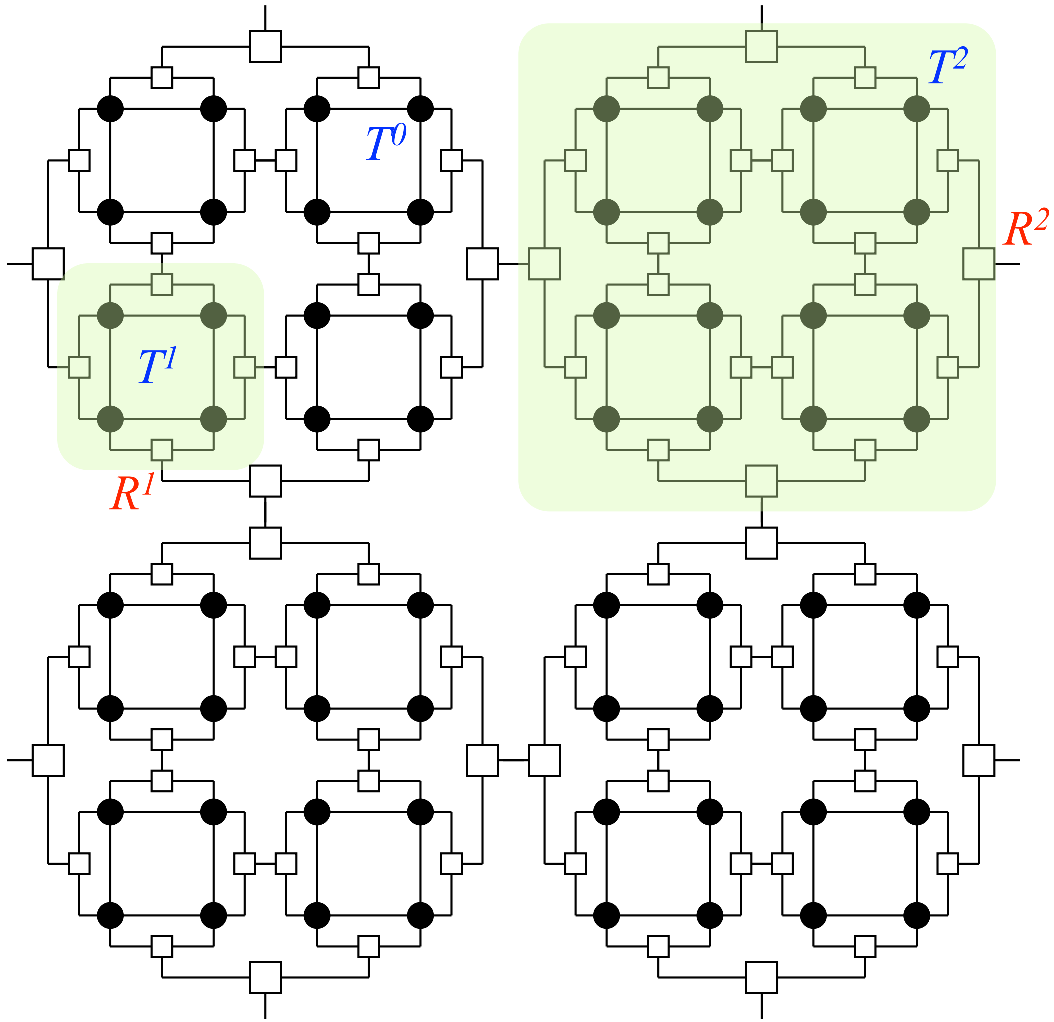




$$T^{(1),\alpha\beta}_{\gamma\delta} = \sum_{\alpha_1,\alpha_2,\dots,\delta_1,\delta_2,ijkl} S^{(1),\alpha}_{\alpha_1\alpha_2} S^{(1),\beta}_{\beta_1\beta_2} S^{(1),\gamma}_{\gamma_1\gamma_2} S^{(1),\delta}_{\delta_1\delta_2} T^{(0),\alpha_1 l}_{\gamma_2 i} T^{(0),\alpha_2 j}_{i\delta_1} T^{(0),j\beta_1}_{k\delta_2}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

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: $L^2 Log(L)$



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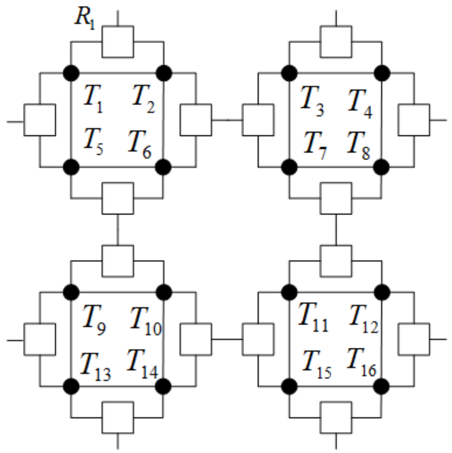
Wang, Kao, Sandvik, arXiv:0901.0214

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:

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



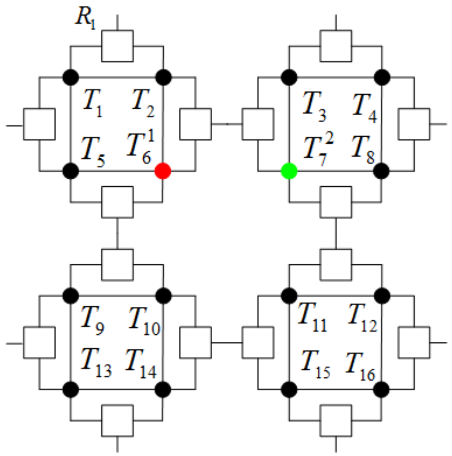
Two - body interaction:

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

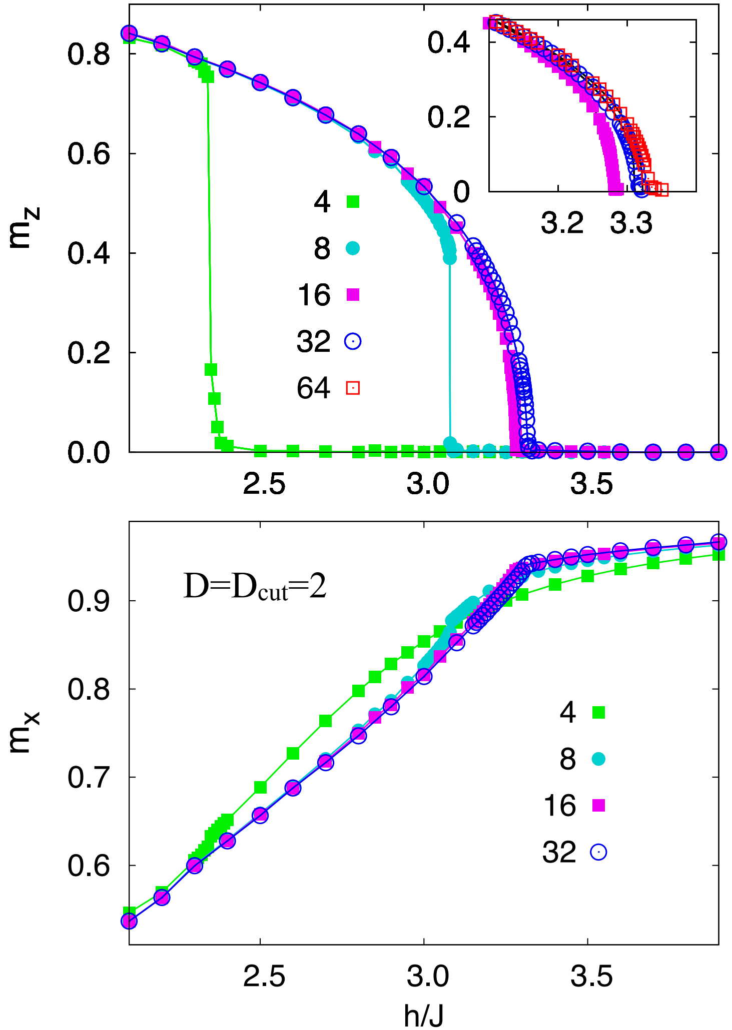
$$T_j = \sum_{s_j} A_j^{s_j *} \otimes A_j^{s_j}$$

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

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



Transverse Ising Model

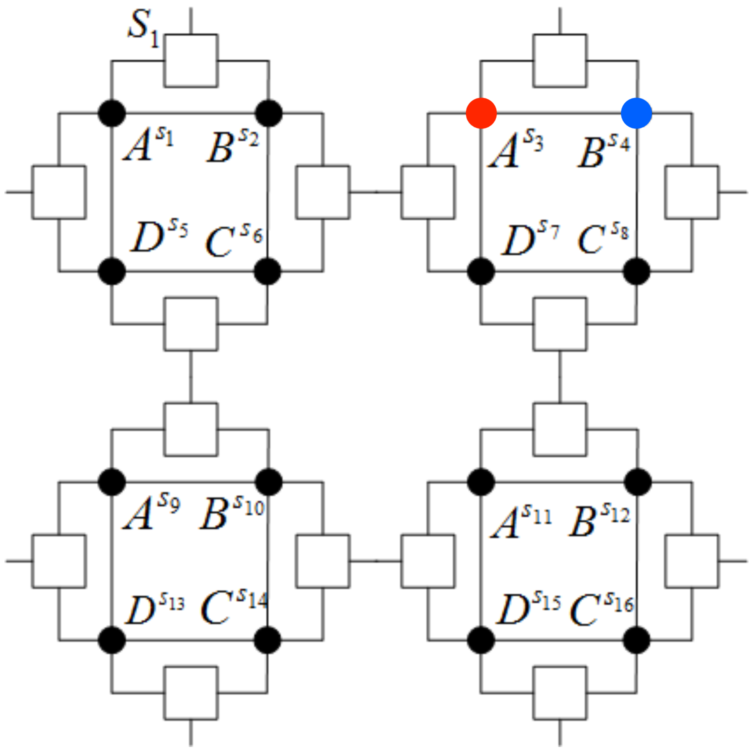


- Assume translational invariance: all initial T's are the same.
- Globally optimized T and R.
- h_c=3.33 (3.04,QMC)
- $m_z \sim (h-h_c)^\beta$, $\beta \sim 0.40$
- $h \sim h_c$, $\beta \sim 0.50$ mean-field like.

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. Wang, Y.-J. Kao, A. W. 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.

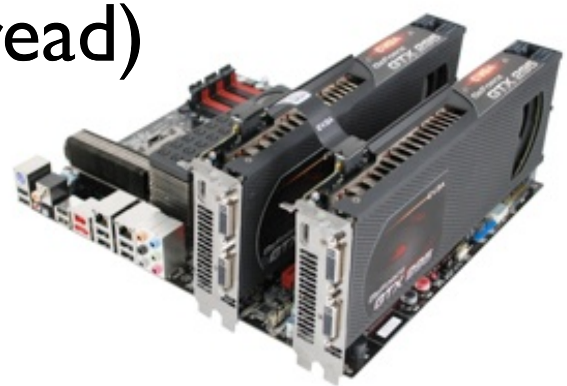
L	h	D	E_{var}/N	E/N	Δ_E
4	3.0	2	−3.1978372	-3.2155081(exact)	5.4955×10^{-3}
8	3.0	2	−3.1717845	−3.19750(QMC)	8.0437×10^{-3}

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}

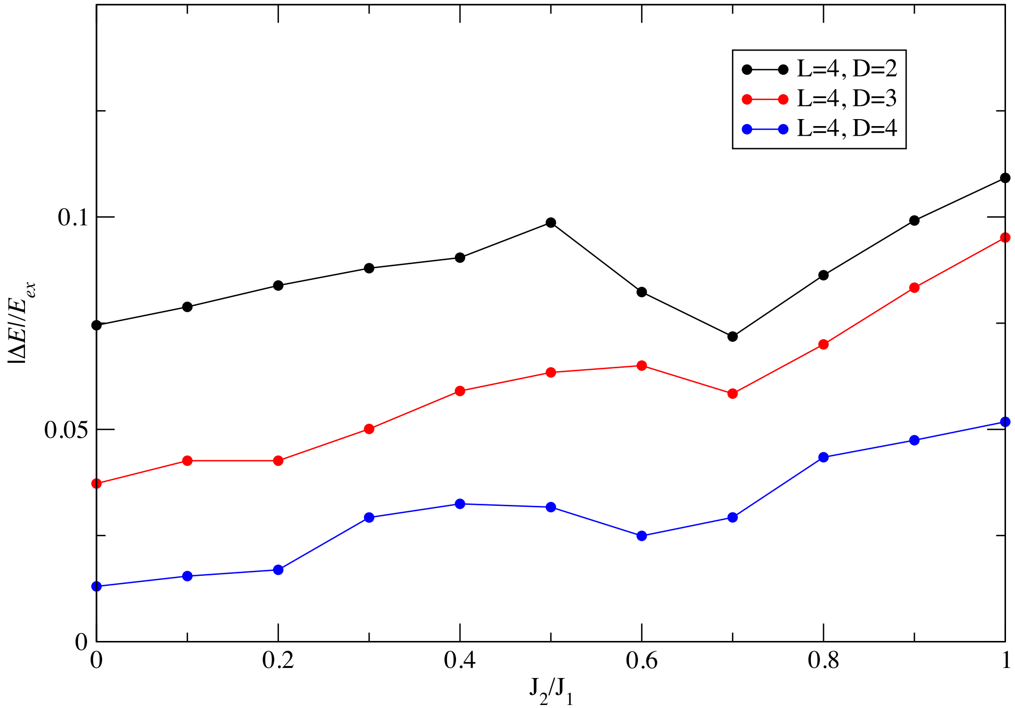
Computational Costs

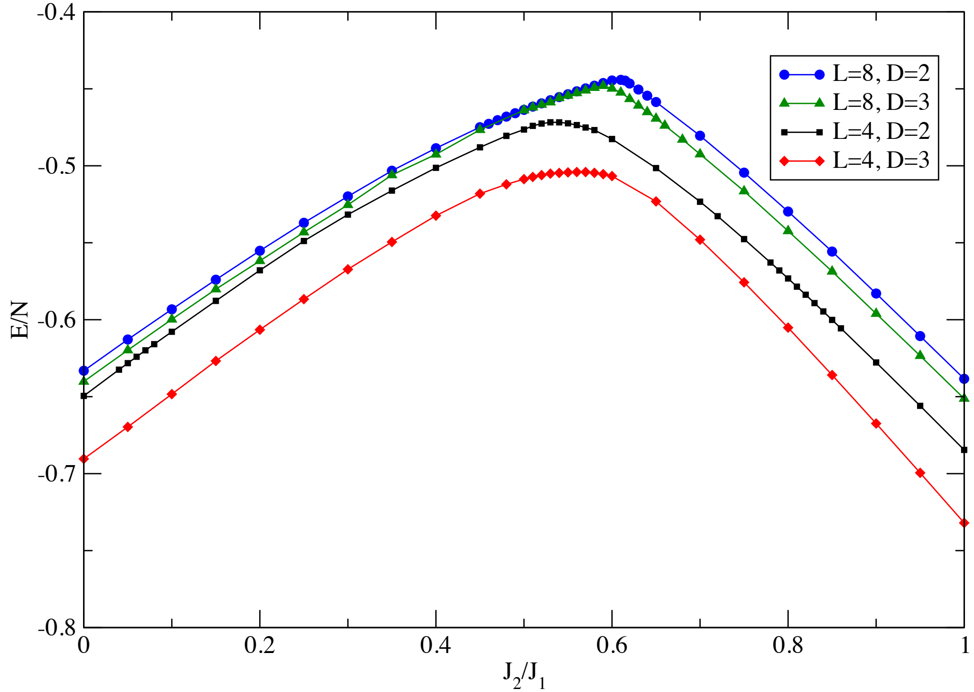
- Globally optimized T and R.
- Contraction calculation is highly parallelizable.
- IBM Blue Gene/L at BU. D=2, takes weeks to optimize.
- Bottleneck: plaquette contractions.
- Take advantage of GPU (Graphic Processing Unit)
- SIMT (Single-instruction, multiple-thread) device.



J_1-J_2 Model

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





- Need large size and large D to see the real physics.
- Currently L=8, D=3 is very time consuming on CPU.

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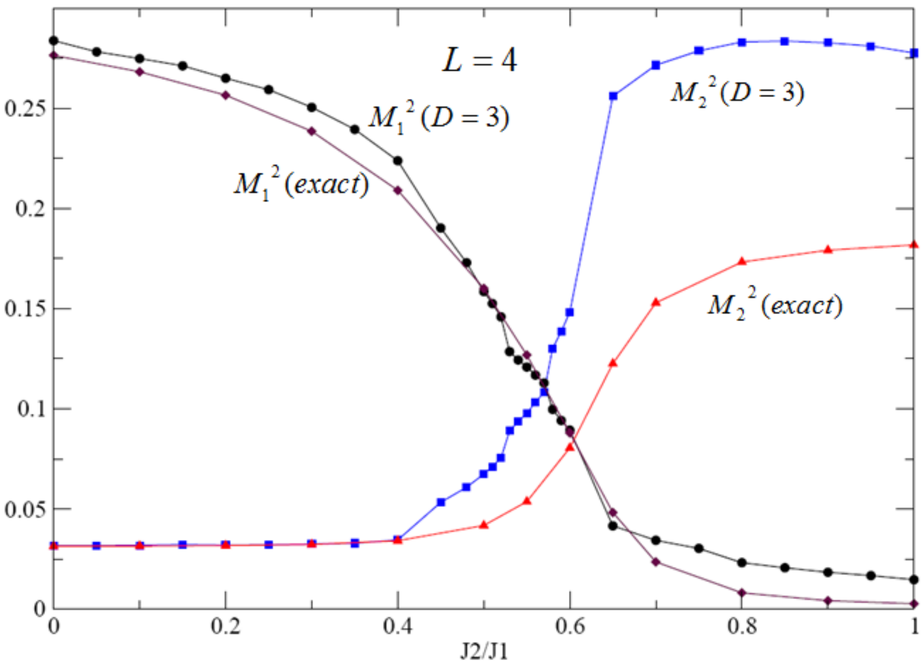
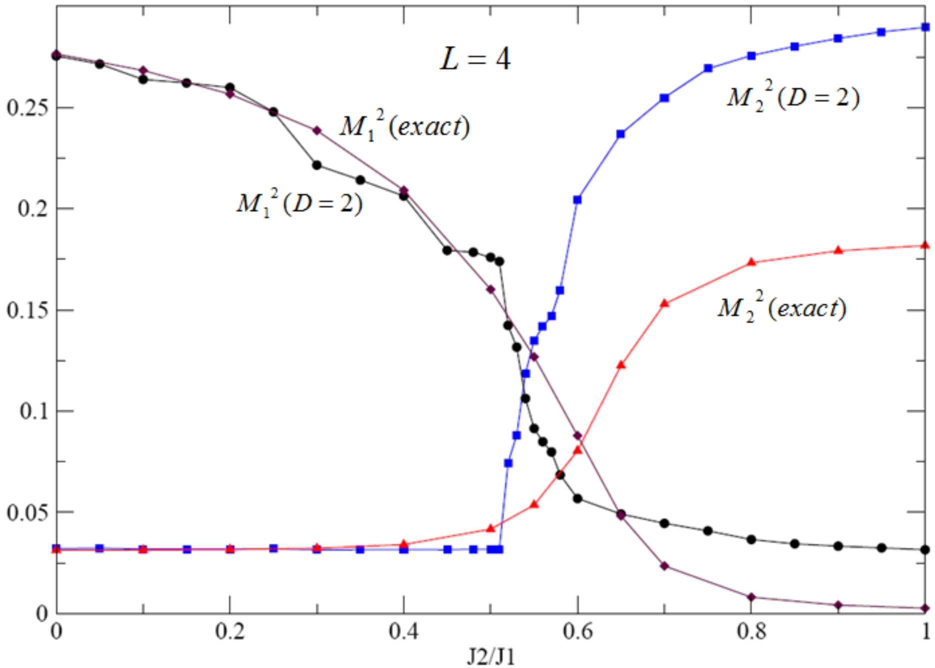
H. J. Schulz, T. A. Ziman and D. Poilblanc, J. Phys. I 6 (1996) 675-703
A. W. Sandvik, Phys. Rev. B 56, 11678 (1997)

J1-J2 Model

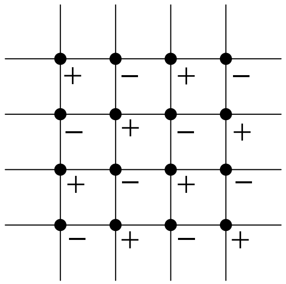




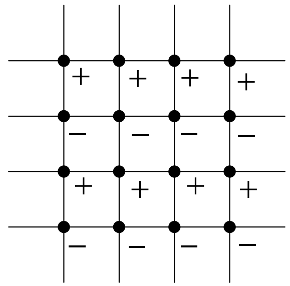
- Order parameters

$$M^2(q_x, q_y) = \left\langle \left(\frac{1}{N} \sum_j e^{i(q_x j_x + q_y j_y)} S_j \right)^2 \right\rangle$$

$M_1 = M(\pi,\pi)$



$M_2 = M(0,\pi)$



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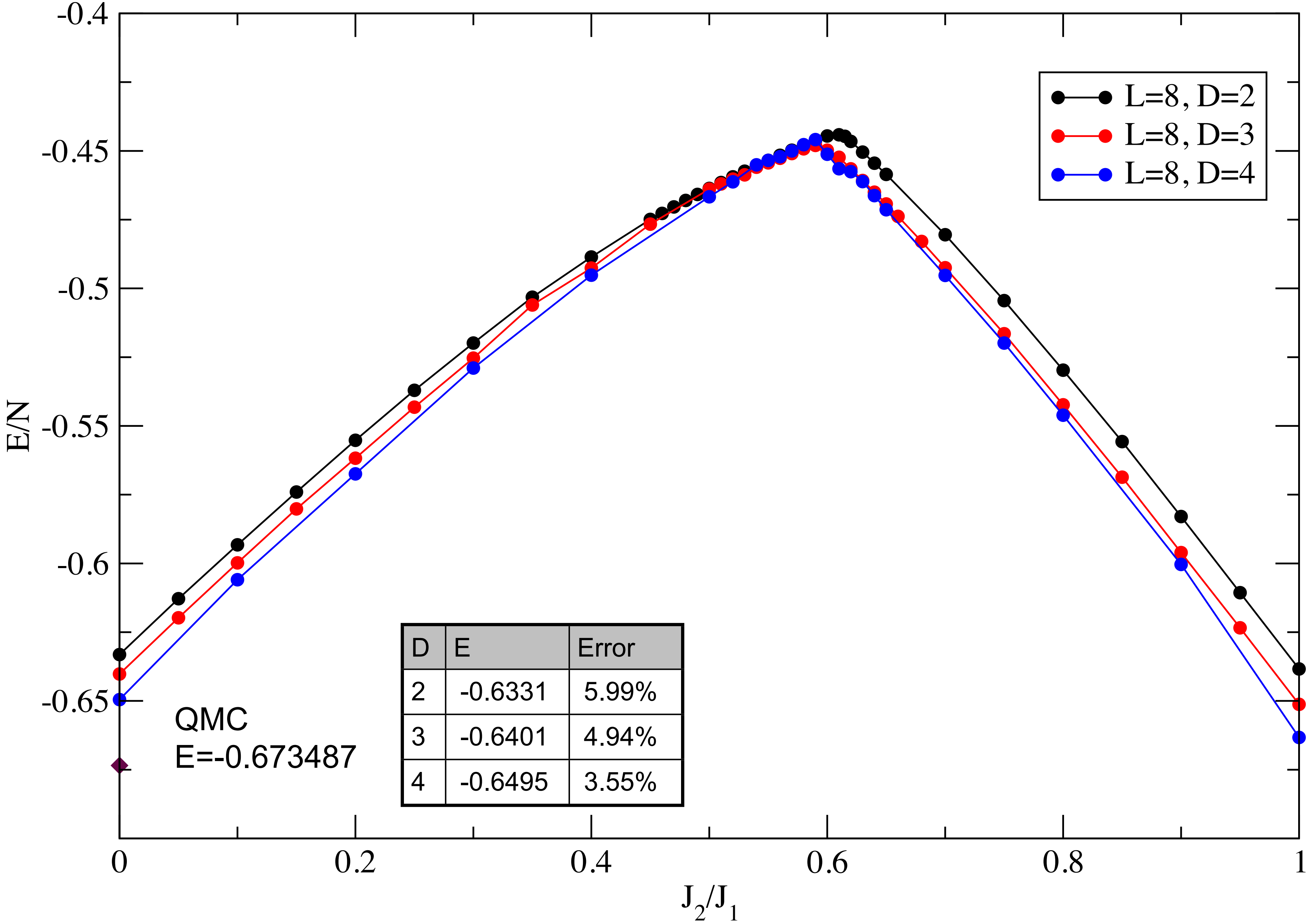
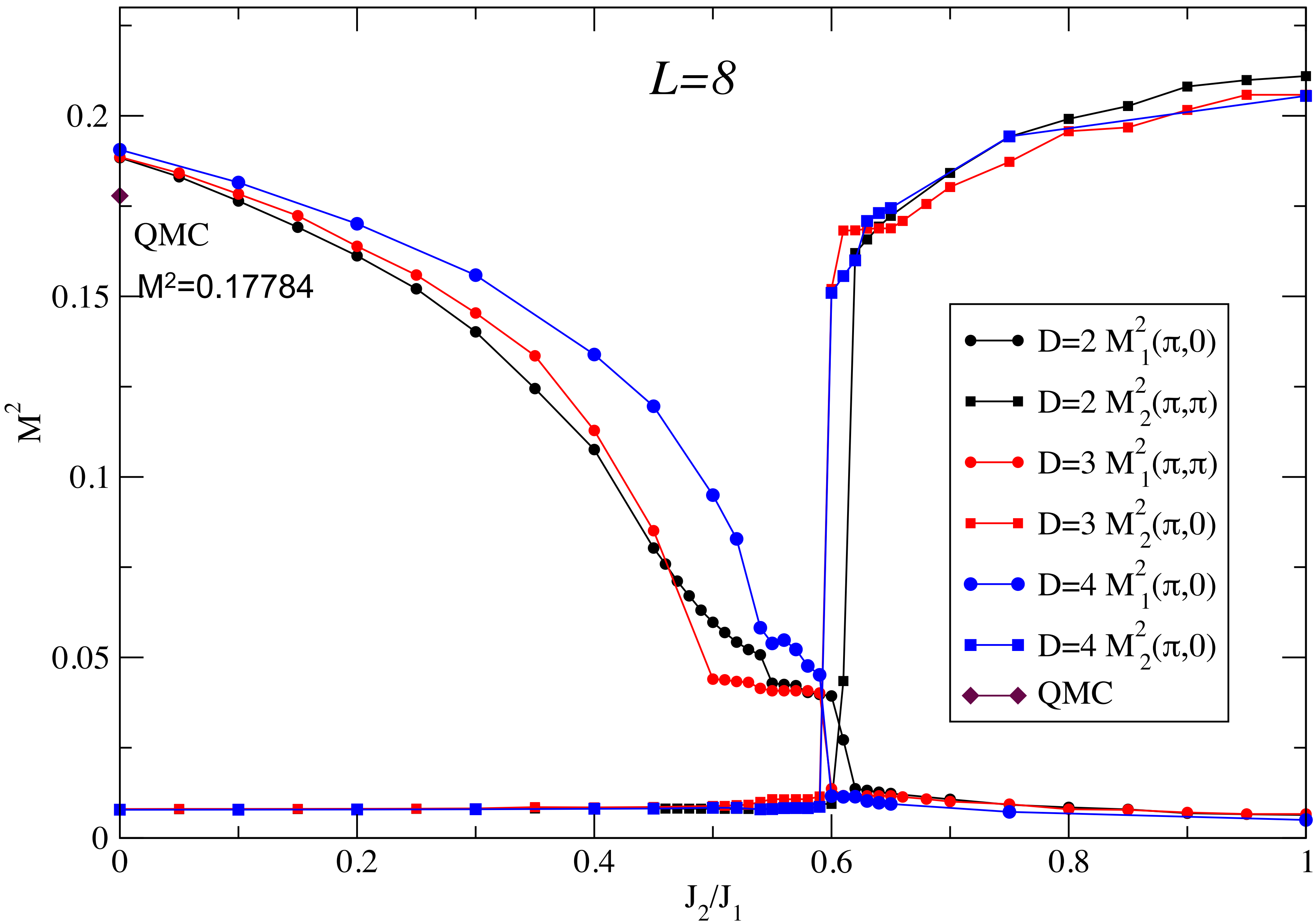


D	E	Error
2	-0.6331	5.99%
3	-0.6401	4.94%
4	-0.6495	3.55%



L=8
QMC
M²=0.17784
D=2 M²₁(π,0)
D=2 M²₂(π,π)
D=3 M²₁(π,π)
D=3 M²₂(π,0)
D=4 M²₁(π,0)
D=4 M²₂(π,0)
QMC
M²
J₂/J₁
0
0.05
0.1
0.15
0.2
0
0.2
0.4
0.6
0.8
1

Summary and Outlook

- 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 ($D = 2$) in 2d transverse Ising model.
- GPU can potentially speed up the computationally intensive part of the calculation.
- GS for $J_2/J_1 \sim 0.6$? VBS order?