Monte Carlo sampling with Tensor Network States

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DMRG achieved one of the major step in simulating of strongly correlated systems

DMRG: variational method within the class of MPS

DMRG can be generalized to deal with 2D systems: A family of variational ansatze has been proposed including PEPS, MERA and iPEPS

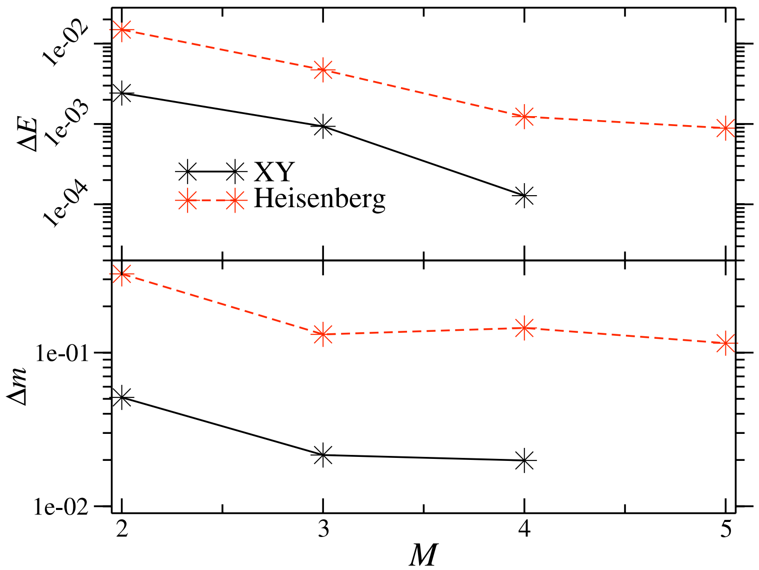


Figure 6. Convergence of relative errors $\Delta x = |x(\text{iPEPS}) - x(\text{QMC})|/|x(\text{QMC})|$ with bond dimension M. Monte Carlo results from [40, 41] are taken as exact. For the definition of the magnetization, refer to the text.

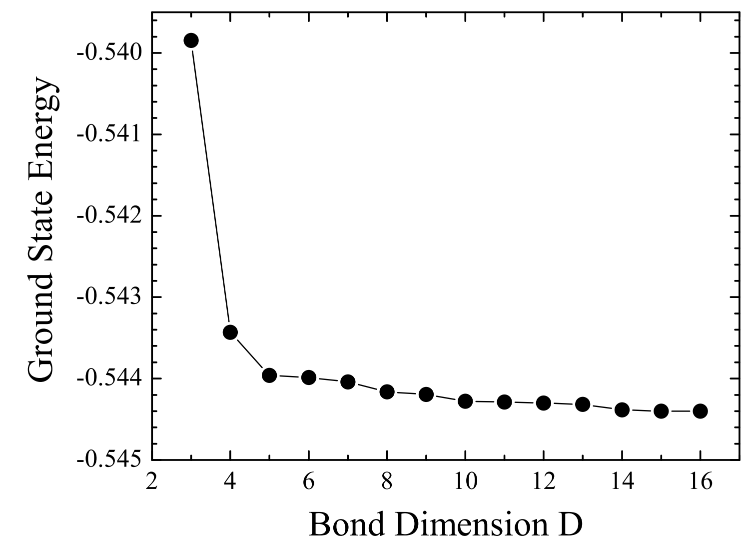
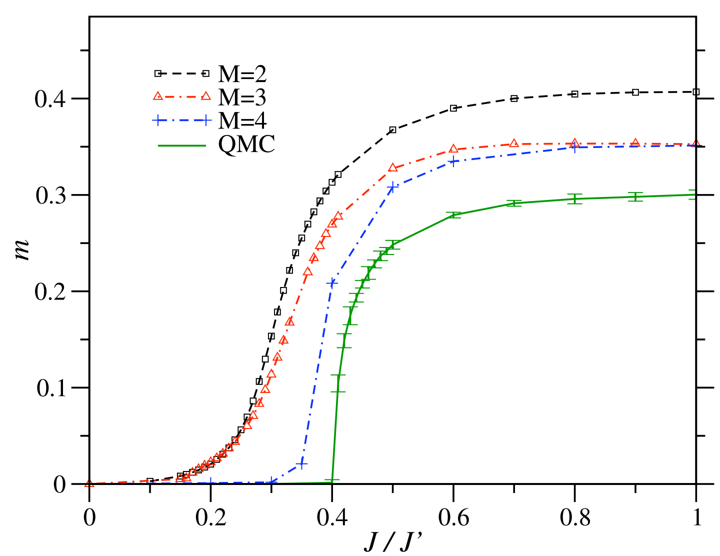
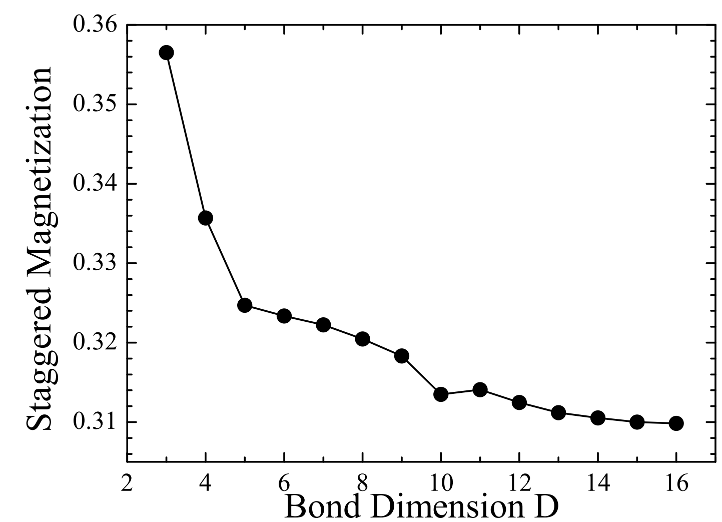


FIG. 20. (color online) The ground state energy of the Heisenberg model on a honeycomb lattice as a function of the bond dimension D obtained by the SRG with $D_{cut} = 130$.



$$M = 0.35(\text{iPEPS})$$
$$M = 0.307(\text{SSE})$$
$$\Delta M = 0.043$$

Figure 9. Staggered magnetization of the dimerized Heisenberg model as a function of the coupling ratio. $J/J' = 1$ corresponds to the isotropic Heisenberg model, while $J/J' = 0$ corresponds to isolated dimers on every second horizontal bond.



$$M = 0.3098(\text{SRG})$$
$$M = 0.2681(\text{MC})$$
$$\Delta M = 0.0417$$

FIG. 21. (color online) The staggered magnetization as a function of D for the Heisenberg model on a honeycomb lattice.

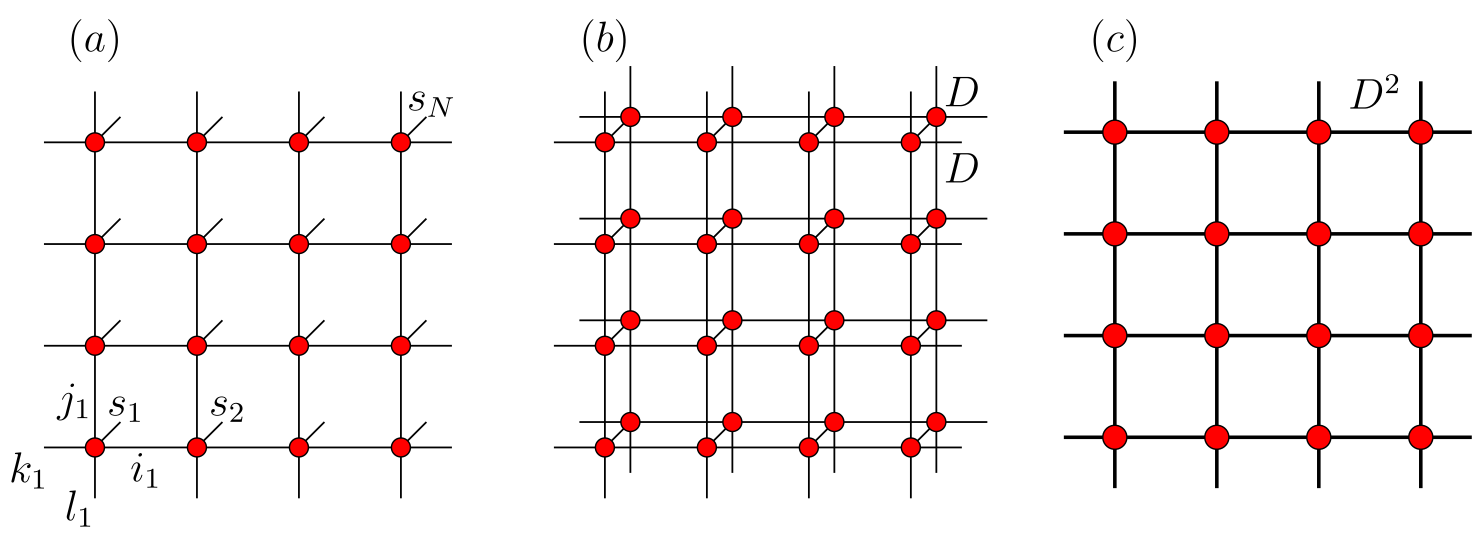
B. Bauer, et al., J. Stat. Mech. 2009 P09006

H.H. Zhao et al. Phys. Rev. B 81, 174411 (2010)

Method of PEPS ansatz often comes with very large complexity scaling with D

- PEPS with variational minimization of the ground state energy ~ D^{12}
- iPEPS with time evolution ~ $\chi^3 D^4$
- TERG contraction of square lattice ~ χ^6
- TERG contraction of honeycomb lattice ~ χ^5

χ is the Schmidt coefficients kept (also referred as D_{cut})



a square root speed up is obtained by using importance sampling over physical indices, which is first shown for MPS and string bond state.

A.W. Sandvik et al., Phys. Rev. Lett. 99, 220602 (2007).
N. Schuch et al., Phys. Rev. Lett. 100, 040501 (2008).

- We use poorman's update (the simple update) introduced by Xiang et al. to obtain the tensor describing the ground state of AF Heisenberg model on square lattice.

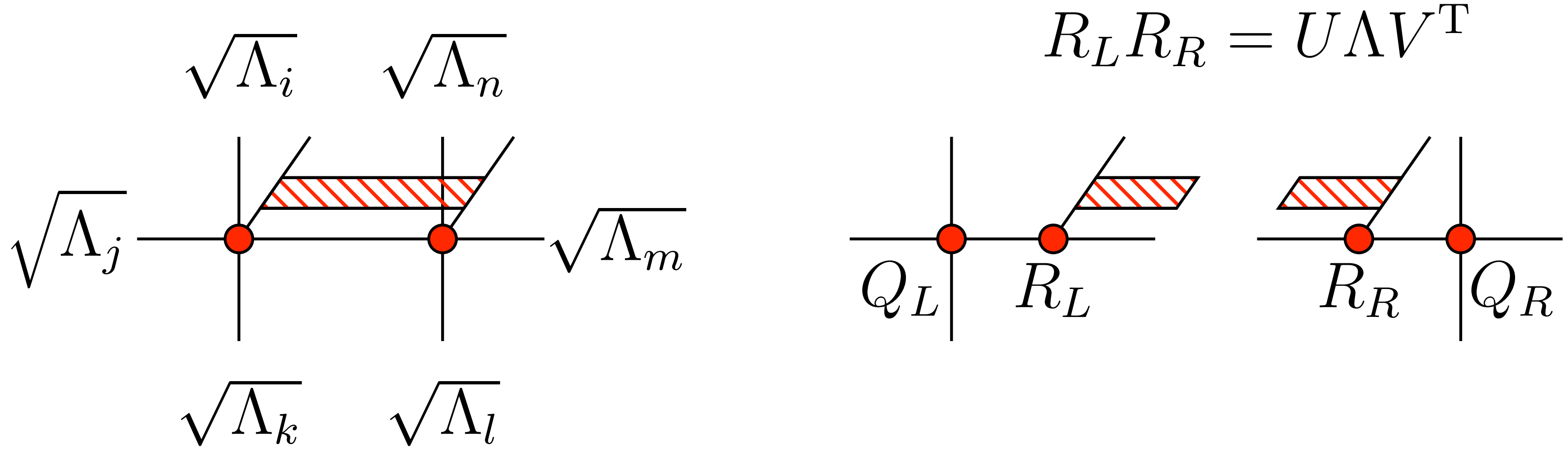
  H.-C. Jiang et al., Phys. Rev. Lett. 101090603 (2008)

- We use importance sampling QMC method to evaluate finite size energy and staggered magnetization for square lattices with periodic boundary condition. Especially, we choose TERG method to approximately contract a tensor network.

  Z.-C. Gu et al., Phys. Rev. B 78, 205116 (2008)

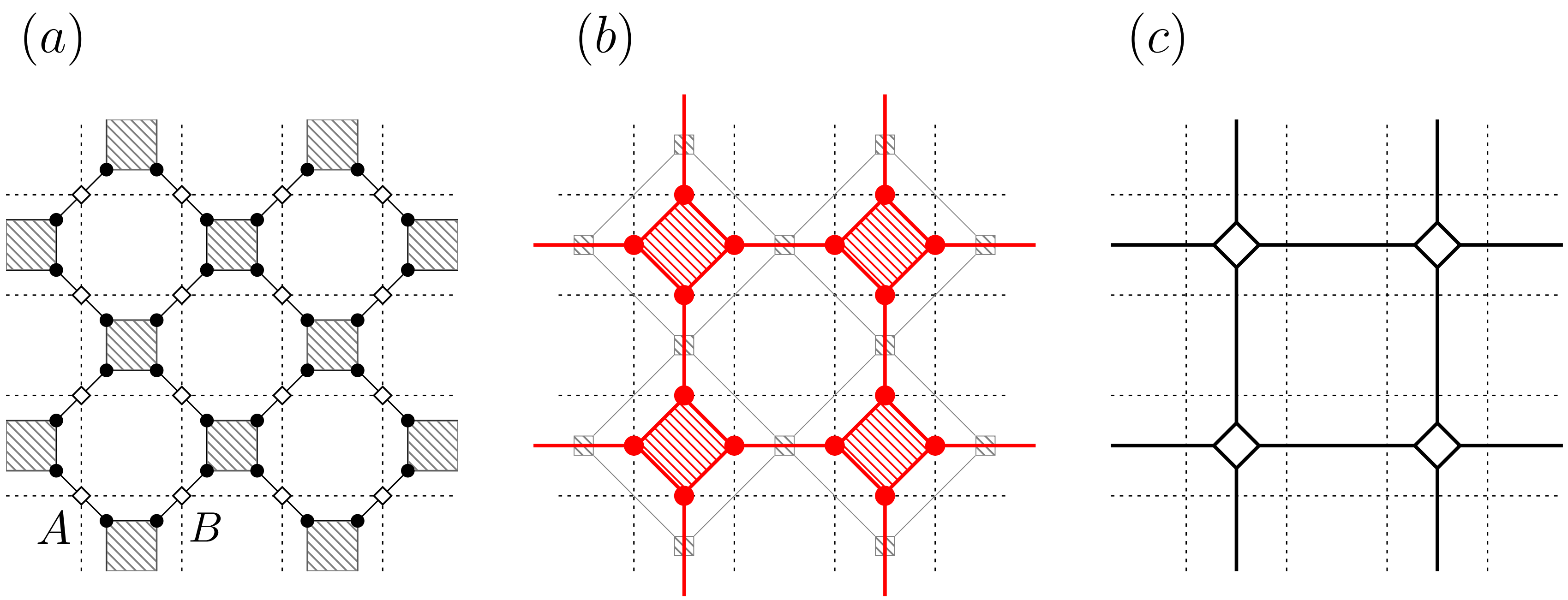
The poorman's update

$$R_L R_R = U\Lambda V^{\mathrm{T}}$$



this trick basically reduces the cost from D^9 to D^5

TERG algorithm



$$T^{\mathrm{B}}_{ijkl} = \sum_{\alpha} S^1_{ij\alpha} {S^3}_{kl\alpha},$$

$$T^{\mathrm{A}}_{jkli} = \sum_{\alpha} S^2_{jk\alpha} {S^4}_{li\alpha},$$

$$T'_{\alpha\beta\gamma\delta} = \sum_{ijkl} S^2_{jk\alpha} S^3_{kl\beta} S^4_{li\gamma} S^1_{ij\delta}.$$

$$T^{\mathrm{B}}_{ijkl} = \sum_{\alpha=1}^{D^2} U_{ij\alpha} \Lambda_\alpha V_{kl\alpha},$$

$$S^1 = \bar{U}\sqrt{\bar{\Lambda}} \quad S^3 = \bar{V}\sqrt{\bar{\Lambda}}$$

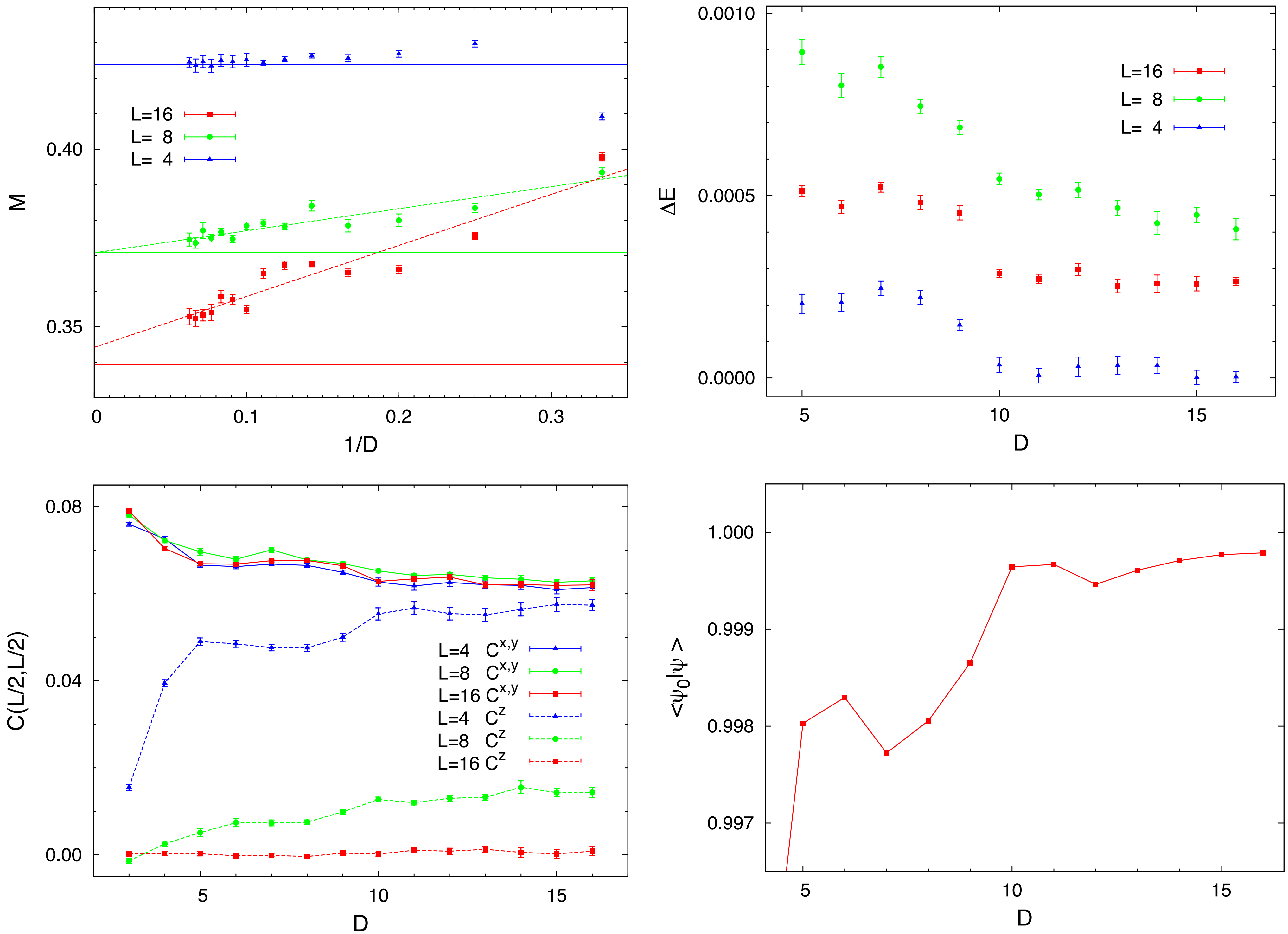
QM sampling

$$\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\sum_\sigma W^2(\sigma)\sum_{\sigma'}\frac{\langle\sigma|H|\sigma'\rangle W(\sigma')}{W(\sigma)}}{\sum_\sigma W^2(\sigma)}$$

$$W(\sigma) = \mathrm{tTr}\{T^{s_1}T^{s_2}\cdots T^{s_N}\}, \quad |\sigma\rangle \equiv |s_1, s_2, \cdots, s_N\rangle$$

$$P = \min\left[1, \frac{W^2(\sigma')}{W^2(\sigma)}\right], \quad \frac{W(\sigma')}{W(\sigma)} = \frac{g'}{g}\prod_{qp}\frac{f'^{q,p}}{f^{q,p}}$$

$$g \equiv \mathrm{tTr}\{T^{1,nr}T^{2,nr}T^{3,nr}T^{4,nr}\}, \quad f^{q,p} \equiv \max\{|T^{q,p}_{ijkl}|\}$$



$$C^{\alpha}(L/2, L/2) = \frac{1}{L^2} \sum_i S^{\alpha}(i_x, i_y) S^{\alpha}(i_x + \frac{L}{2}, i_y + \frac{L}{2}), \quad M^2 = \sum_{\alpha} C_{\alpha}(L/2, L/2).$$

The finite size magnetization errors are 0.003(2) and 0.013(2) at D=16 for a system of size L=8,16 respectively. Finite D extrapolation provides exact finite size magnetization for L=8, and reduces the magnetization error to 0.005(3) for L=16.