

Title: A tensor product state approach to spin-1/2 square J1-J2 Heisenberg model: spin liquid vs. deconfined quantum criticality

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Abstract: The ground state phase diagram of spin-1/2 J1-J2 antiferromagnetic Heisenberg model on square lattice around the maximally frustrated regime ($J_2 \sim 0.5J_1$) has been debated for decades. I will discuss some progresses on this old problem based on recent numerical results from density matrix renormalization group(DMRG) and tensor product states algorithms.

A tensor product state approach to spin-1/2 square J1-J2 Heisenberg model: evidence for deconfined quantum criticality

Zheng-Cheng Gu

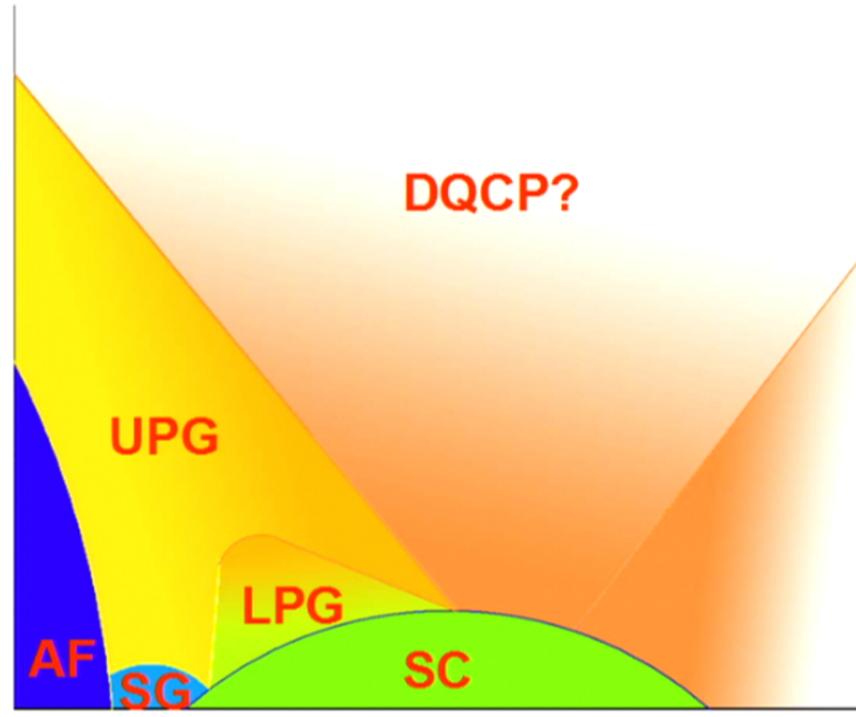
Perimeter Institute

Collaborator:

Dr. Ling Wang (Caltech)
Prof. Xiao-Gang Wen (MIT)
Prof. F. Verstraete (U. of Vienna)

Deconfined Quantum critical point (QCP) in cuprates?

Subir Sachdev, Science 288, 475, (2000)



DQCP in spin models

Theory: beyond Landau's paradigm

$$\mathcal{L}_z = \sum_{a=1}^N |(\partial_\mu - ia_\mu) z_a|^2 + s|z|^2 + u(|z|^2)^2 + \kappa (\epsilon_{\mu\nu\kappa} \partial_\nu a_\kappa)^2$$

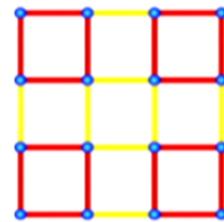
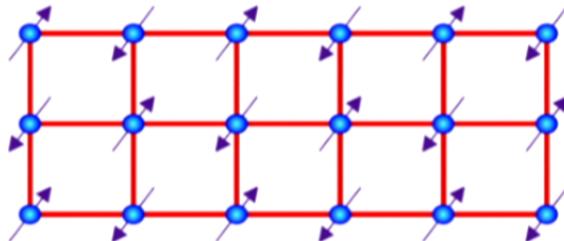
$$Q = \frac{1}{4\pi} \int d^2r \hat{n} \cdot \partial_x \hat{n} \times \partial_y \hat{n},$$

On square lattice, Q always changes by four, thus the instanton effect becomes dangerous irrelevant!

T. Senthil, Ashvin Vishwanath, Leon Balents, Subir Sachdev, M. P. A. Fisher, Science 303, 1490 (2004).

Numerical: J-Q model(simulated by using QMC)

$$H = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - Q \sum_{\langle i j k l \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4})(\mathbf{S}_k \cdot \mathbf{S}_l - \frac{1}{4})$$



Anders W. Sandvik, Phys.
Rev. Lett. 98, 227202 (2007)

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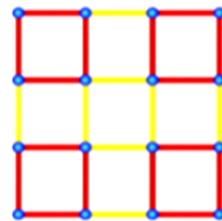
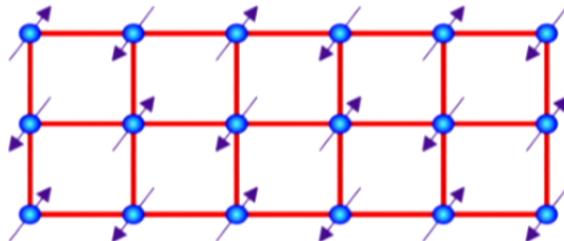
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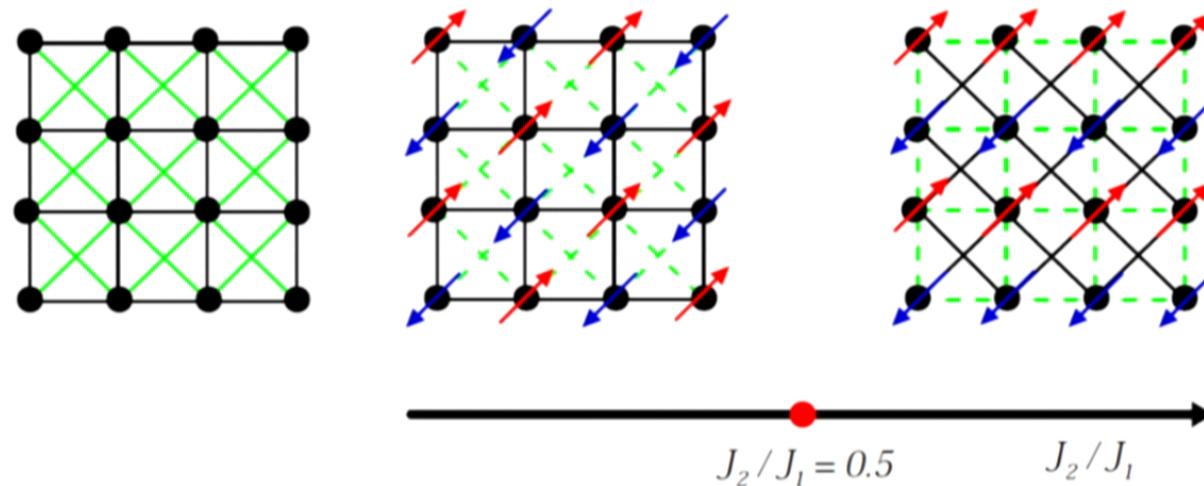
Anders W. Sandvik, Phys. Rev. Lett. 98, 227202 (2007)

Relevant spin model for cuprates

J1-J2 model:

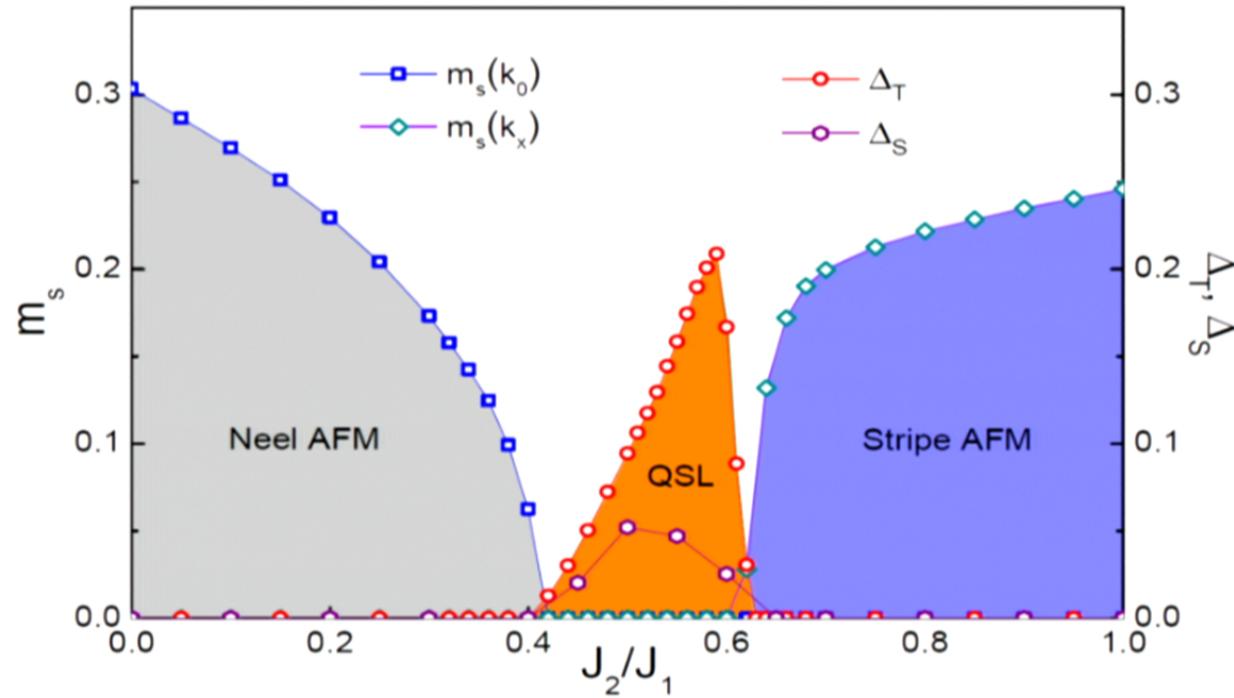
$$H = J_1 \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle ij \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

Landau Paradigm: a meanfield phase diagram



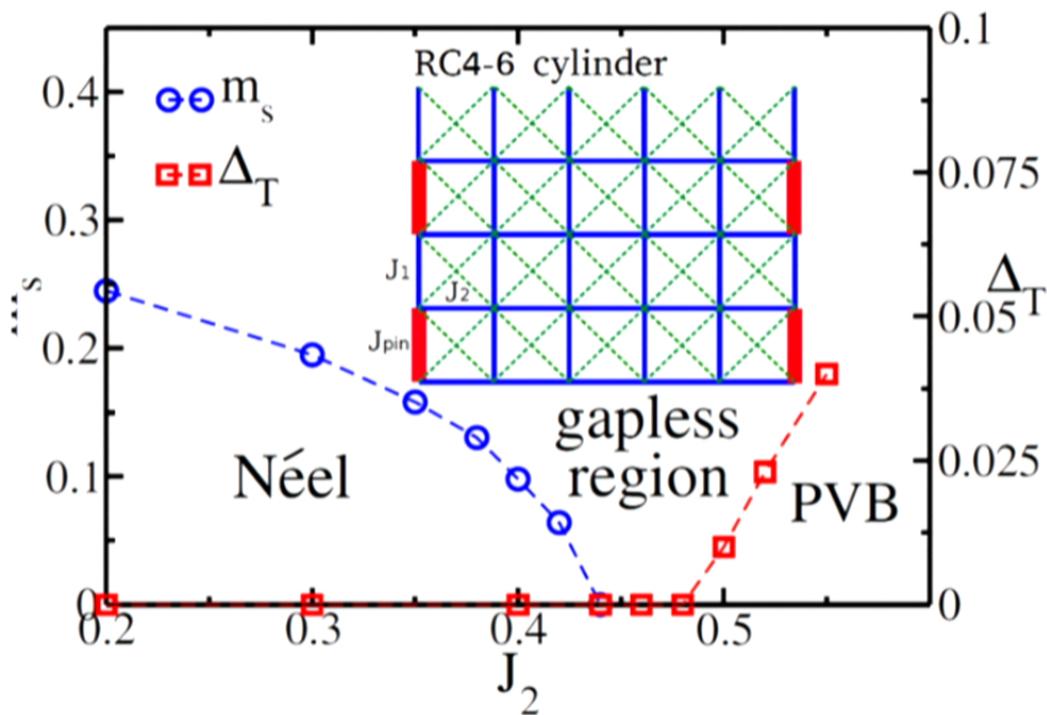
Recent progress

A recent work by using density matrix renormalization group(DMRG) algorithm claims a Z2 spin liquid



Hong-Chen Jiang, Hong Yao, Leon Balents, Phys. Rev. B 86, 024424 (2012)

Another work by using SU(2) symmetry DMRG algorithm suggests a different result



Shou-Shu Gong, Wei Zhu, D. N. Sheng, Olexei I. Motrunich, Matthew P. A. Fisher
Phys. Rev. Lett. 113. 027201 (2014)

Landau paradigm: meanfield approach

- The key concept is to find an ideal trial wave function, e.g., for a spin $\frac{1}{2}$ system:

$$|\Psi_{trial}\rangle = \otimes (u^\uparrow |\uparrow\rangle_i + u^\downarrow |\downarrow\rangle_i)$$

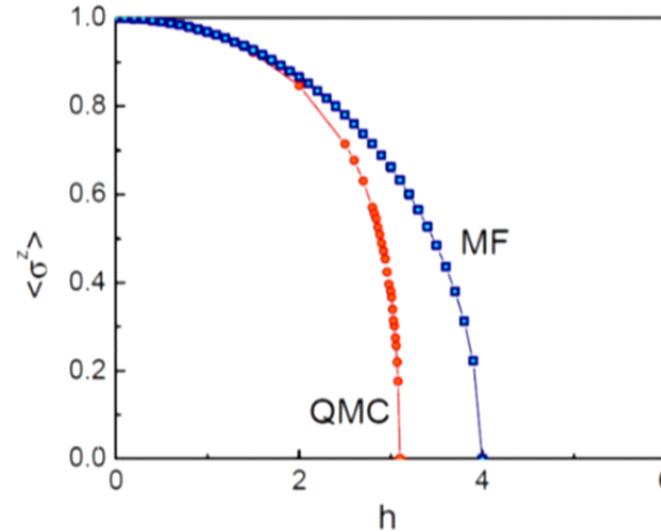
- After minimizing the energy, we can find various symmetry ordered phases.

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

$$h_{MF}^c = 4$$

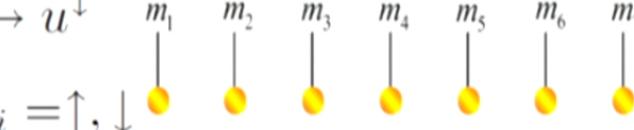
$$\beta_{MF}^c = 0.5$$

$$\langle \sigma_z \rangle \propto |h - h_c|^\beta$$



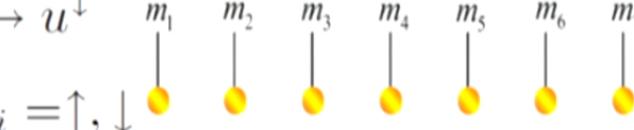
Tensor Product State approach

Mean-field states: $\uparrow \longrightarrow u^\uparrow$; $\downarrow \longrightarrow u^\downarrow$

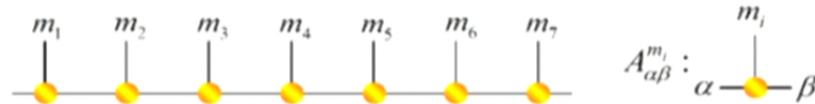
$$\Psi(\{m_i\}) = u^{m_1} u^{m_2} u^{m_3} u^{m_4} \cdots; \quad m_i = \uparrow, \downarrow$$


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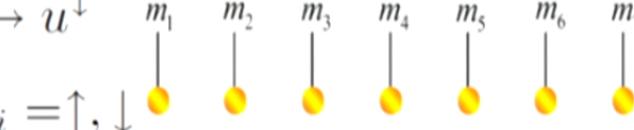
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MPS/DMRG(the most powerful method in 1D):

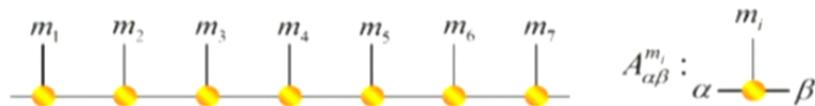
$$\Psi(\{m_i\}) = \text{Tr} [A^{m_1} A^{m_2} A^{m_3} A^{m_4} \dots]; \quad m_i = \uparrow, \downarrow \quad \uparrow \rightarrow A^\uparrow; \quad \downarrow \rightarrow A^\downarrow$$


Tensor Product State approach

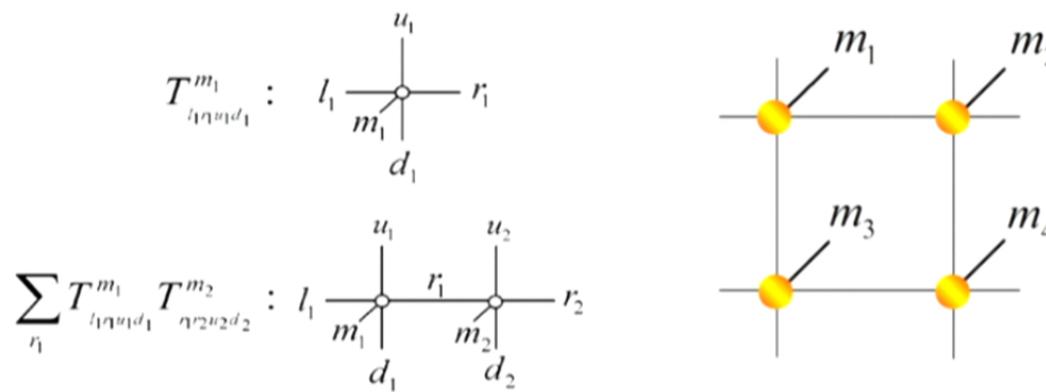
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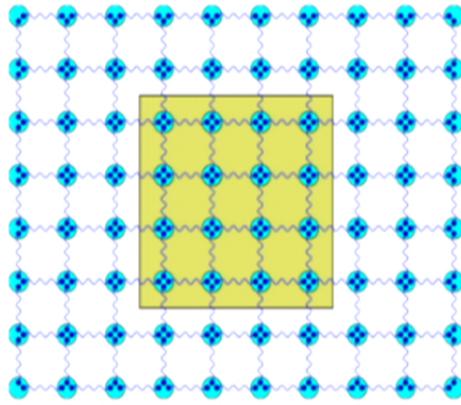
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TPS: $\uparrow \rightarrow T_{l r u d}^\uparrow; \quad \downarrow \rightarrow T_{l r u d}^\downarrow$ (F. Verstraete and J. I. First 2004)



Properties of TPS:



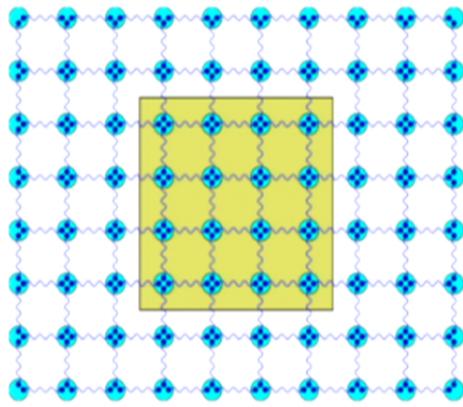
- Entanglement entropy satisfies area law

$$S(\rho_L) = \alpha L \quad (\text{F. Verstraete et al.})$$

$$|\Psi_0\rangle = \prod_{link} |I\rangle \quad |I\rangle = \sum_{l=1}^D |ll\rangle$$

$$|\Psi_{TPS}\rangle = \prod_i P_i |\Psi_0\rangle \quad P_i = T_{lrud}^{m_i} |m_i\rangle \langle lrud|$$

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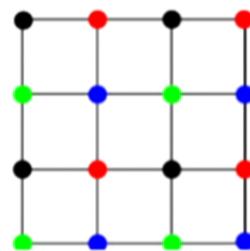
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- TPS faithfully represent non-chiral topologically ordered states
(Z.C. Gu, et al., PRB, 2008, O. Buerschaper, et al., PRB, 2008)

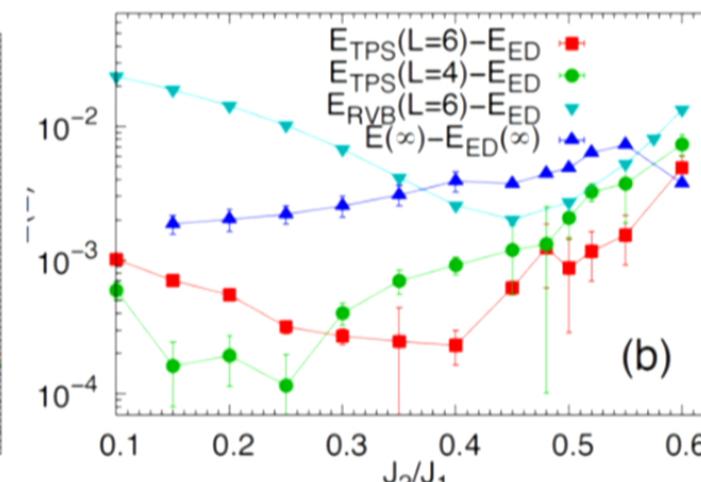
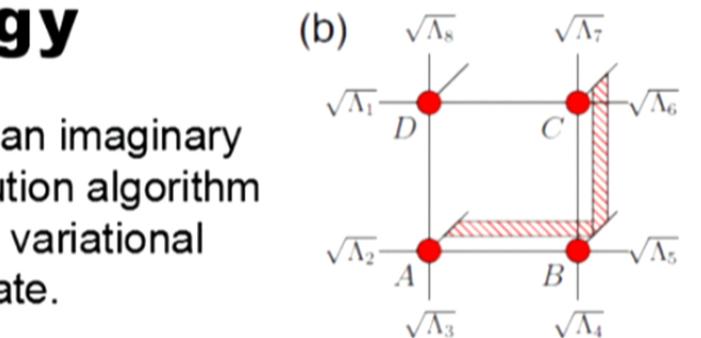
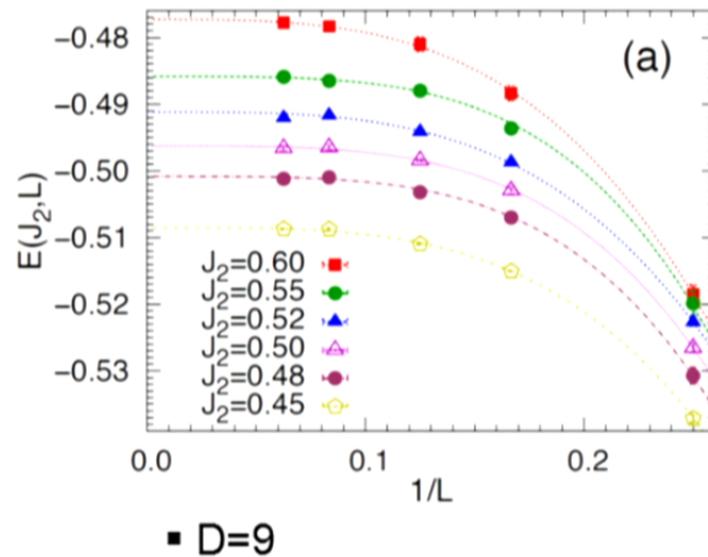
Ground state energy

- T_A
- T_B
- T_C
- T_D



- We use an imaginary time evolution algorithm to find the variational ground state.

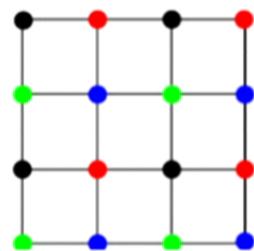
$$|\Psi_{GS}\rangle = \lim_{\tau \rightarrow \infty} e^{-\tau H} |\Psi_0\rangle = \lim_{N \rightarrow \infty} e^{-N\delta\tau H} |\Psi_0\rangle$$



The TPS energy is lower than the best VMC energy!

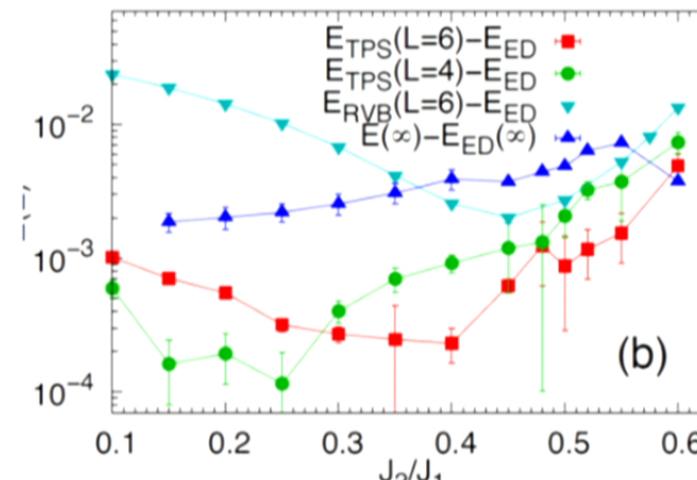
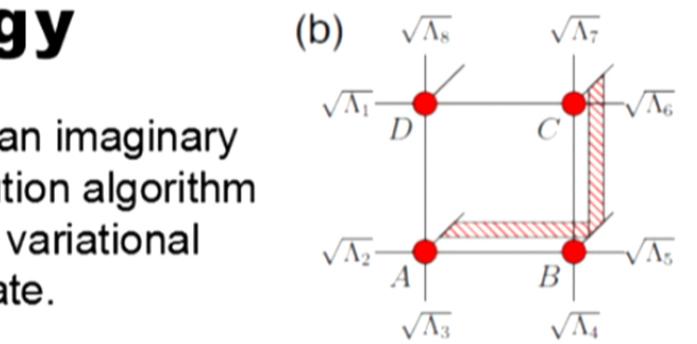
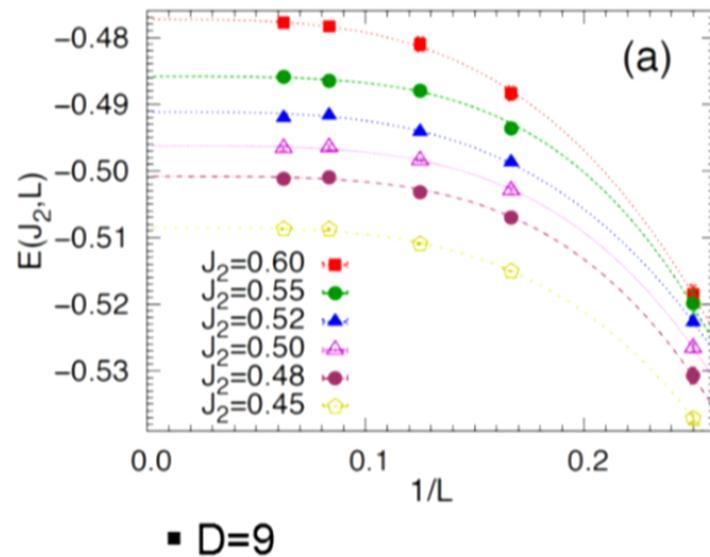
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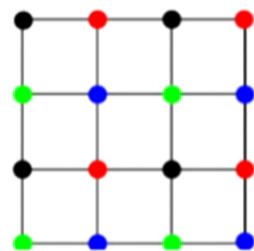
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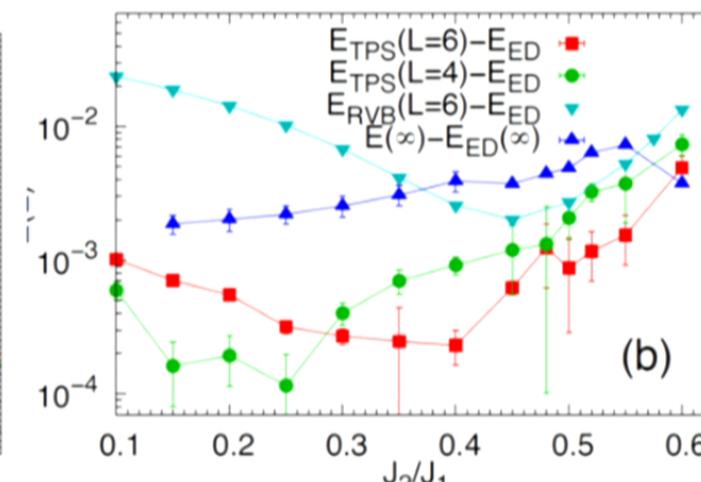
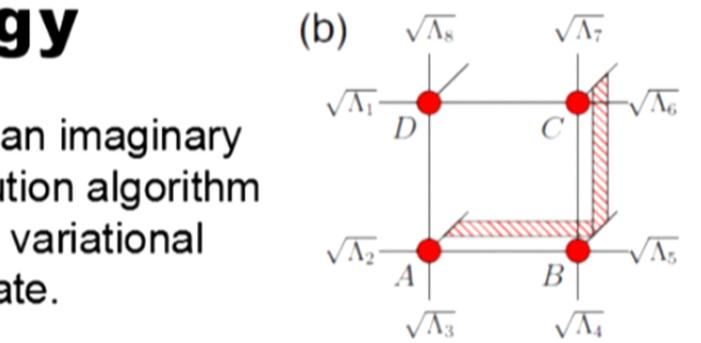
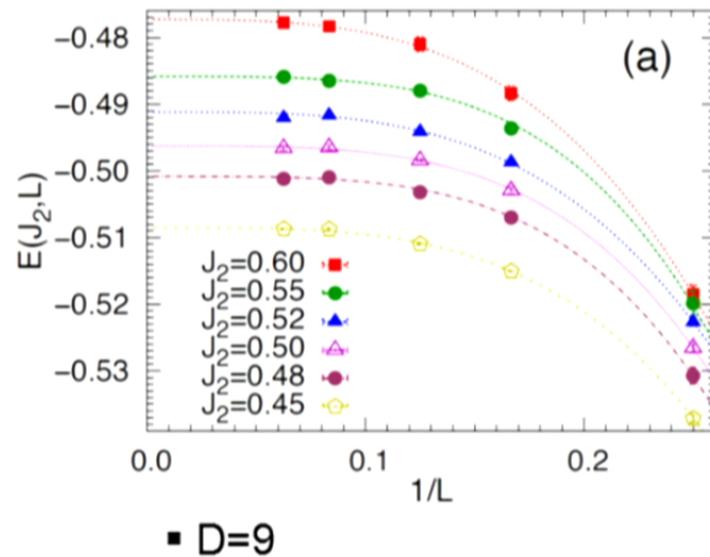
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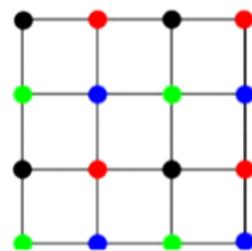
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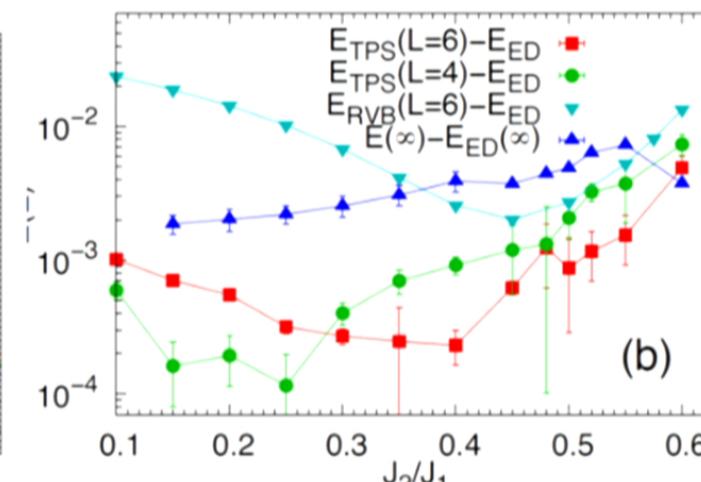
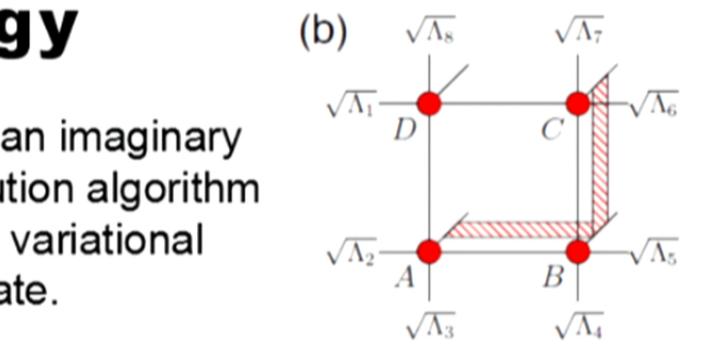
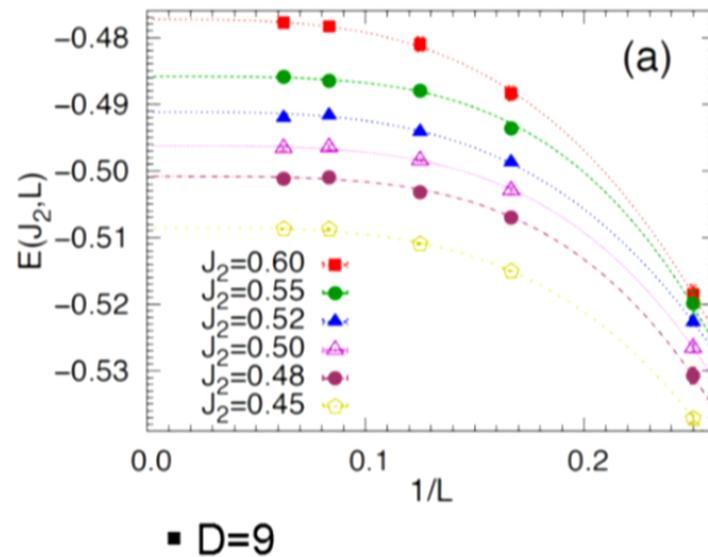
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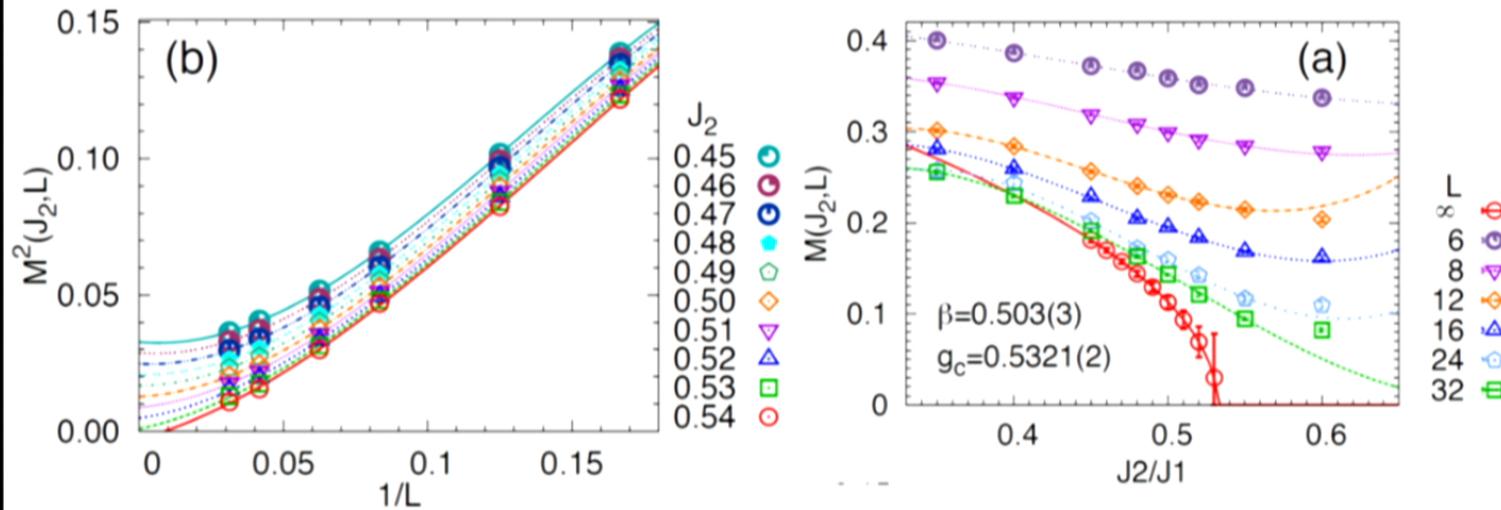
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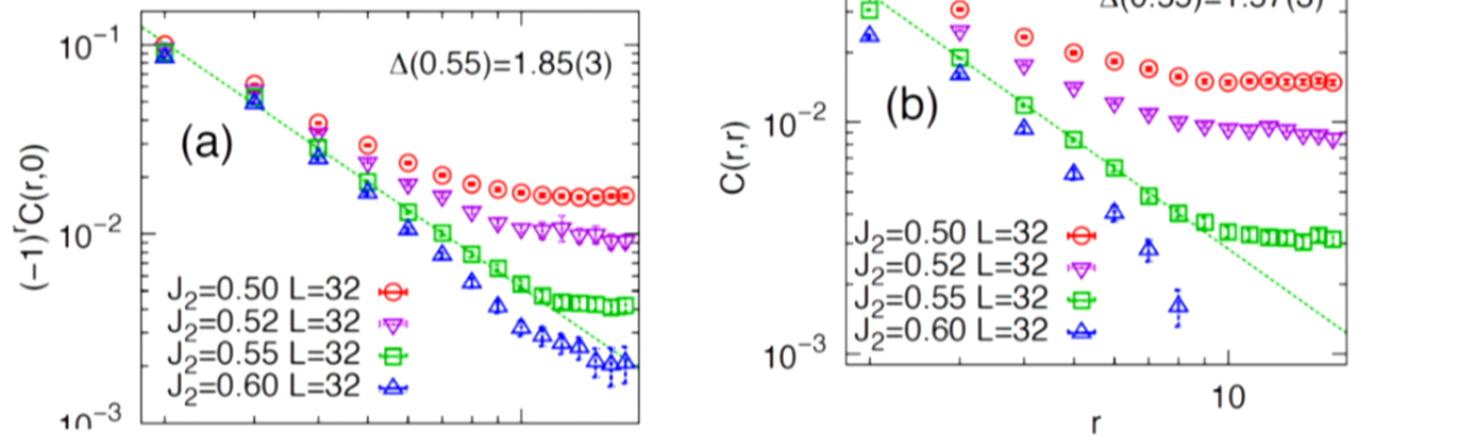


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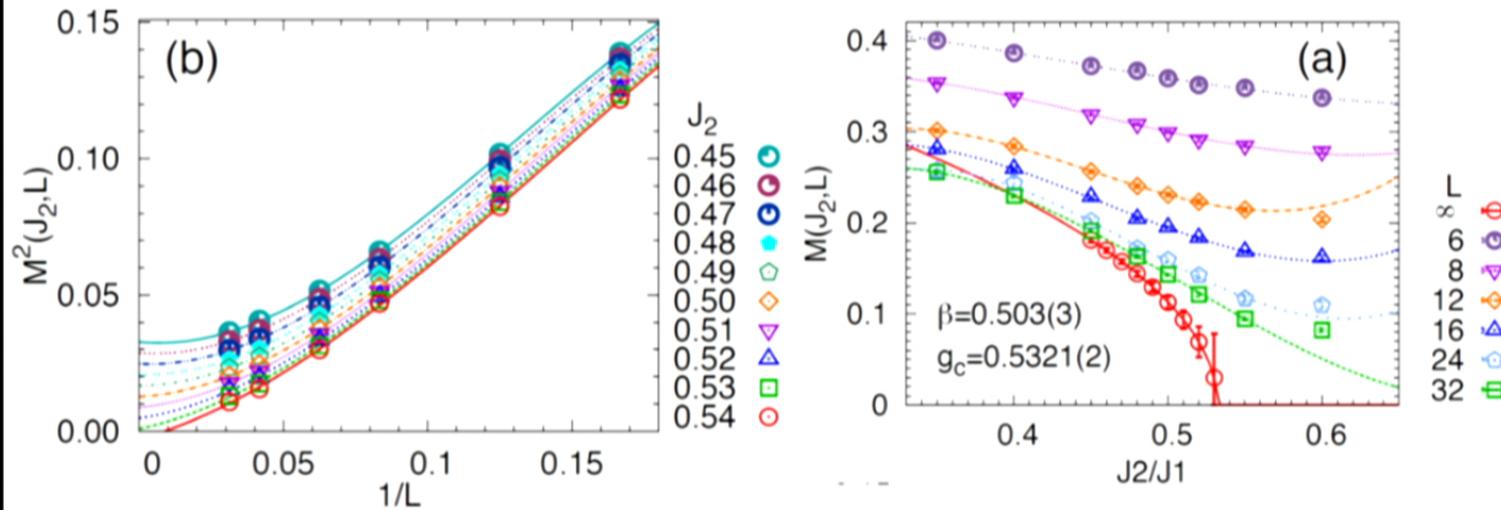
AF order parameter:



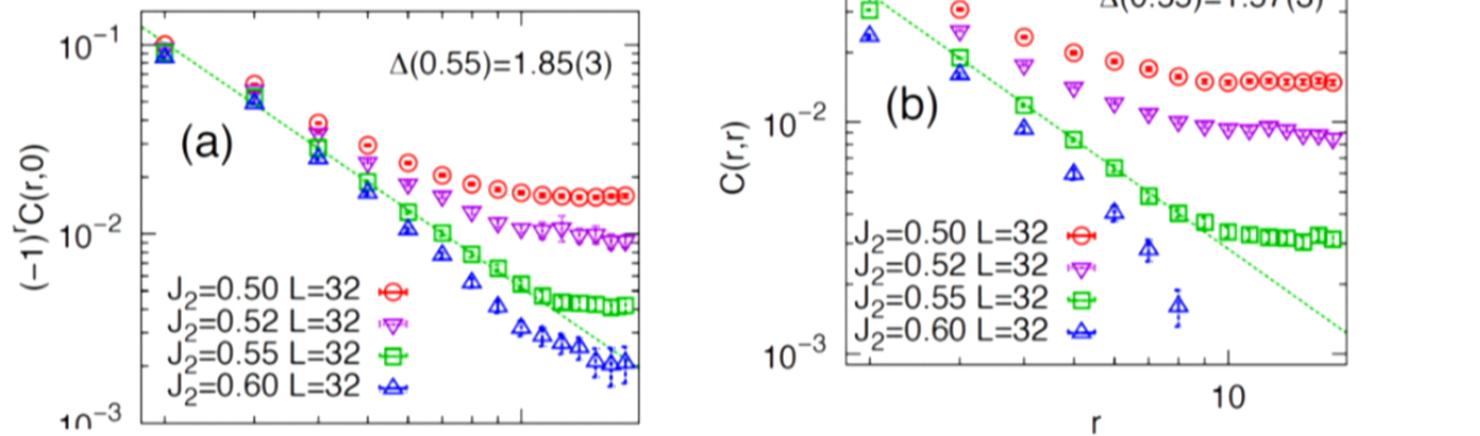
Spin-Spin Correlation:



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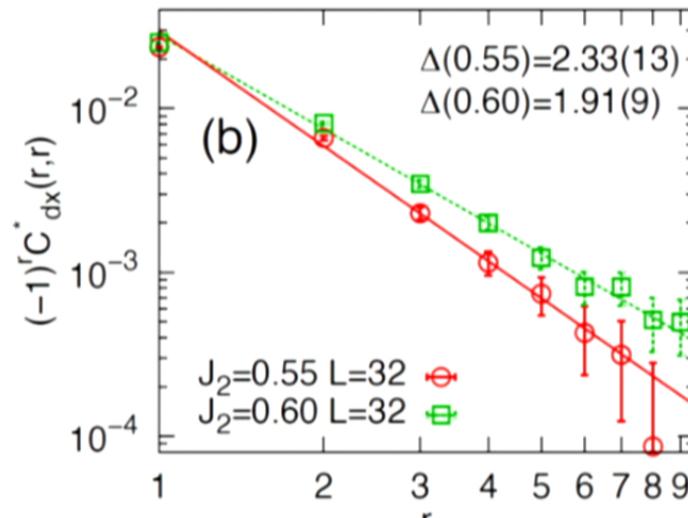
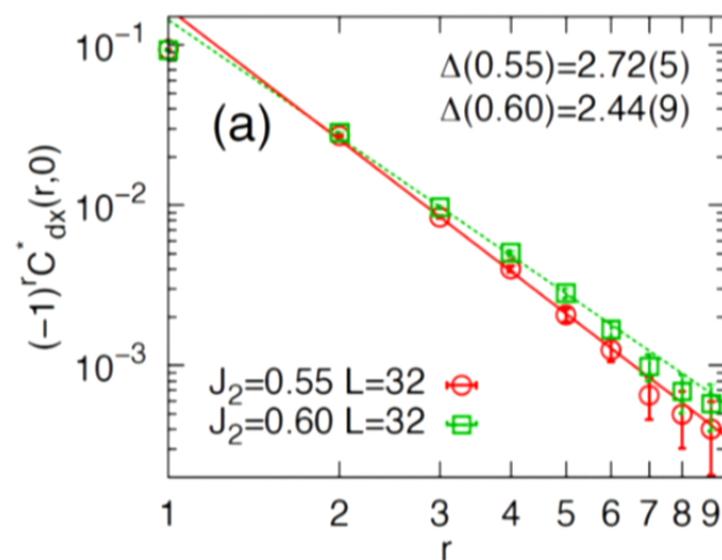
Dimer-Dimer Correlation:

$$C_{dx}^*(r, 0) = C_{dx}(r, 0) - C_{dx}(r - 1, 0), \quad D_x(x, y) = \mathbf{S}_{(x,y)} \cdot \mathbf{S}_{(x+1,y)},$$

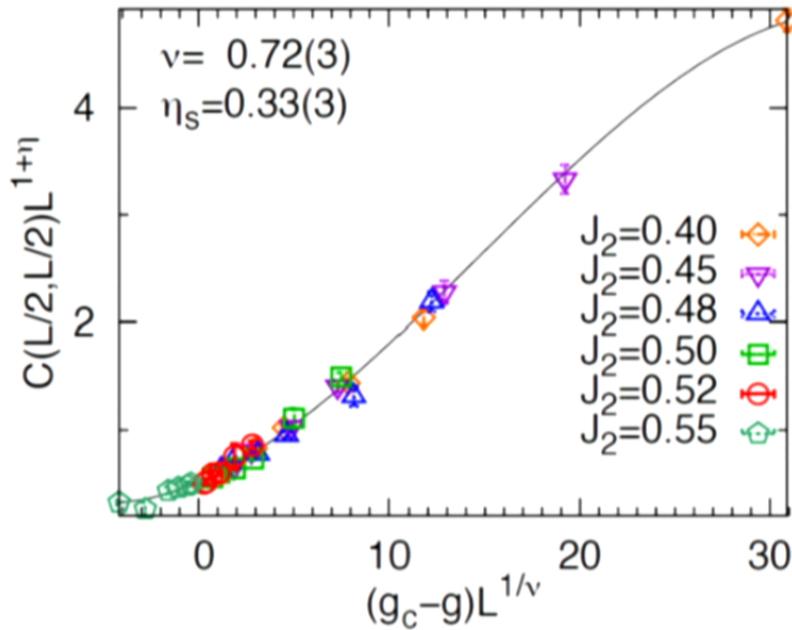
$$C_{dx}^*(r, r) = C_{dx}(r, r) - C_{dx}(r - 1, r). \quad D_y(x, y) = \mathbf{S}_{(x,y)} \cdot \mathbf{S}_{(x,y+1)}.$$

$$C_{dx}(r_x, r_y) = \frac{1}{N} \sum_{x,y} D_x(x, y) D_x(x + r_x, y + r_y),$$

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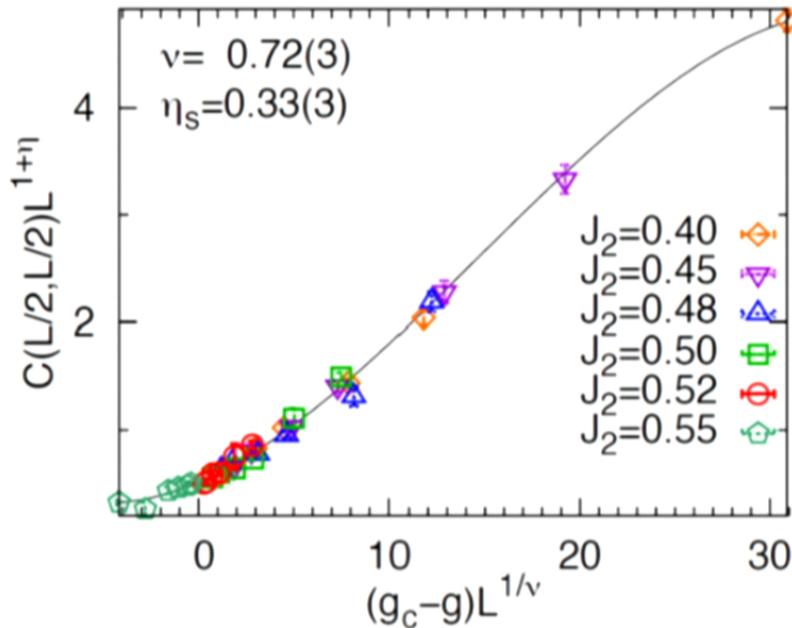
The universal scaling function



$$C(L/2, L/2) = L^{-1-\eta} f(L^{1/\nu}(g_c - g)/g_c),$$

The critical exponents are intrinsically close to the DQCP behavior observed in other systems, e.g., J-Q model

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U(1) spin liquid is unstable, a VBS order with exponentially small amplitude might develop at long wave length

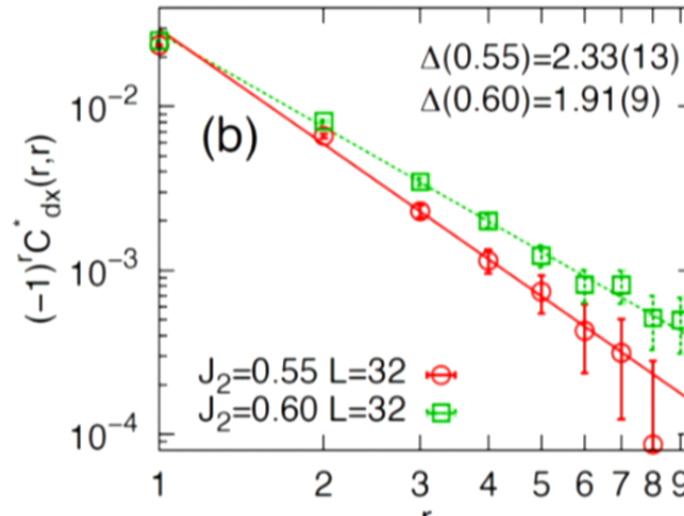
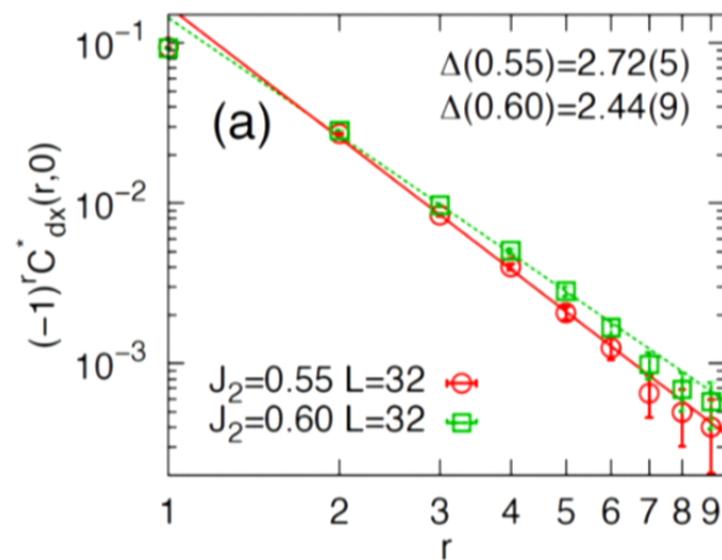
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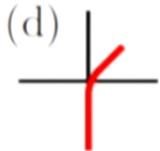
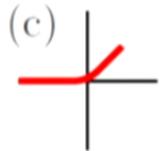
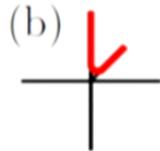
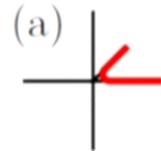
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Single parameter variational approach

A D=3 TPS description of short range RVB state

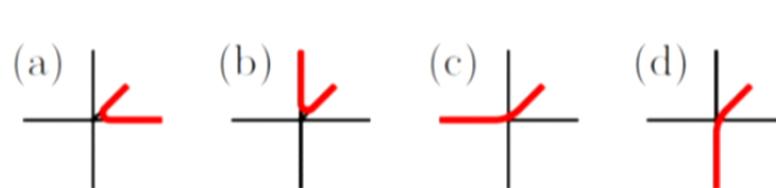


$$\mathcal{P}_1 = \sum_{k=1}^4 (|\uparrow\rangle\langle 0|_k + |\downarrow\rangle\langle 1|_k) \otimes \langle 222|_{/k}$$
$$|\mathcal{S}\rangle = |01\rangle - |10\rangle + |22\rangle$$

$$|\Psi\rangle_{\text{s-RVB}} = \prod_V \mathcal{P}_1 \prod_B |\mathcal{S}\rangle$$

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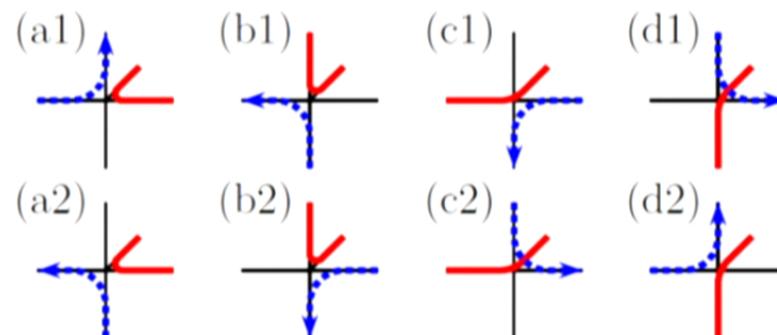


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Including longer range RVB

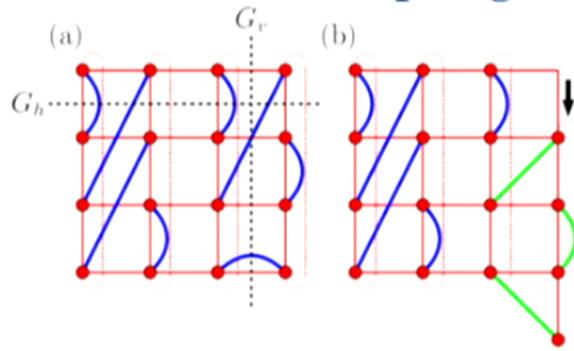
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$$\mathcal{P}_2 = \sum_{i \neq j \neq k \neq l} (|\uparrow\rangle\langle 0|_i + |\downarrow\rangle\langle 1|_i) \otimes \langle 2|_j \otimes \langle \epsilon|_{kl}$$

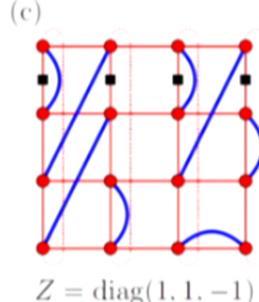


Topological sectors and variational energy

Similar to the short range RVB state, we can define four different topological sectors.



(c)

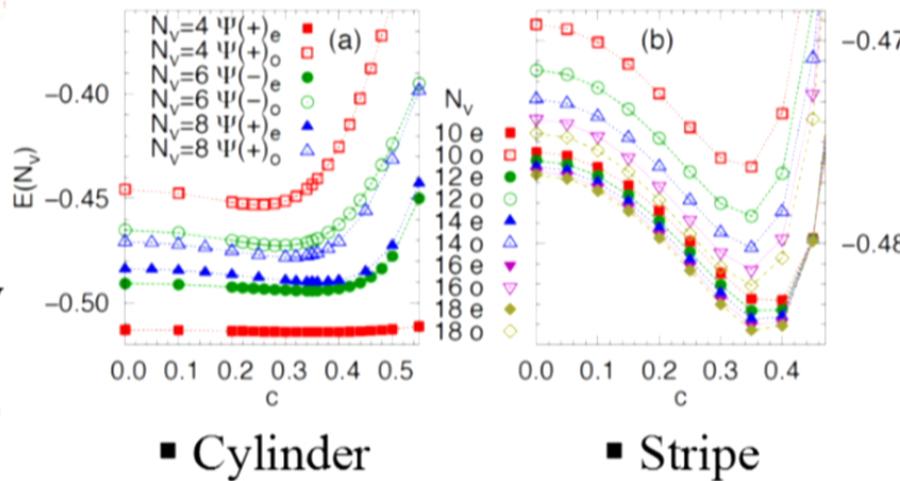


Vison sectors

$$|\Psi(\pm)\rangle \equiv |\Psi\rangle_{G_h=1} \pm |\Psi\rangle_{G_h=-1}$$

Best variational energy at $c=0.35$

- $E = -0.4862/\text{site}$ on cylinder/stripe geometry
- Comparing to $E = -0.494/\text{site}$ with $D=9$

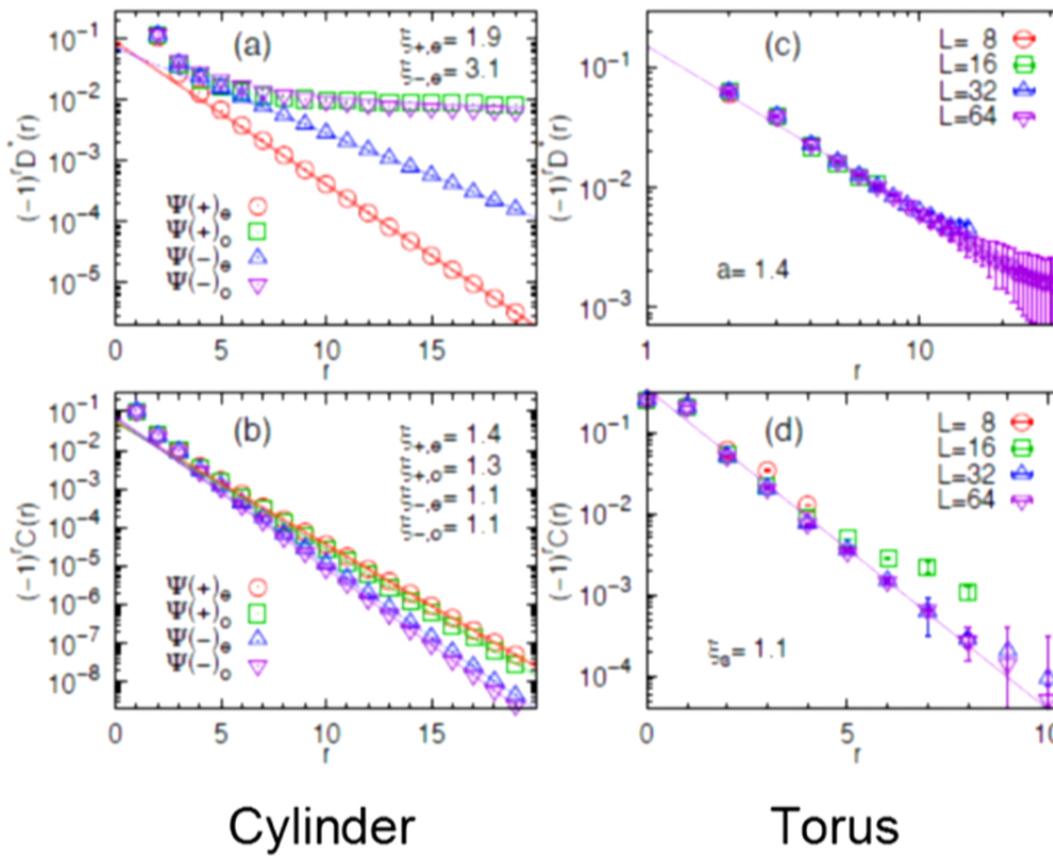


▪ Cylinder

▪ Stripe

Correlation functions

Dimer-dimer correlation shows different behaviors on cylinder and torus!(Challenges to DMRG)

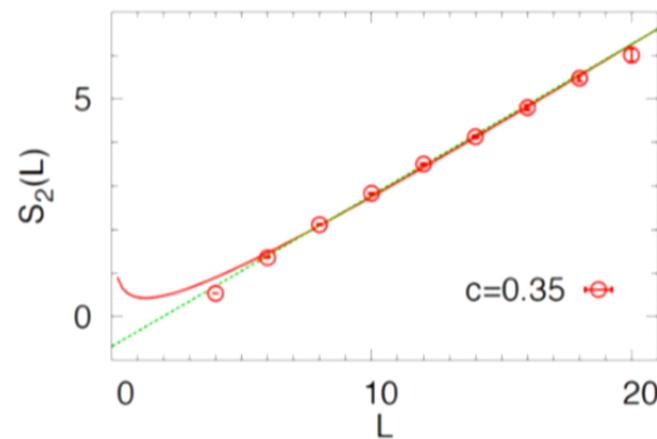


Cylinder

Torus

Entanglement entropy

Both dimer-dimer correlation and entanglement entropy indicate gapless spin liquid behaviors!



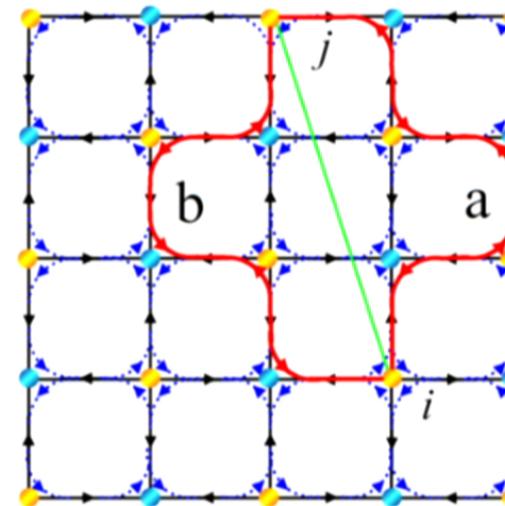
A linear fitting leads to a negative constant close to $\ln 2$

All these results can be understood as vanishing of same sublattice pairing in our variational ansatz, which describes a U(1) spin liquid

$$S_2(L) = a_1 L - \frac{1}{2} \ln L + b_1$$

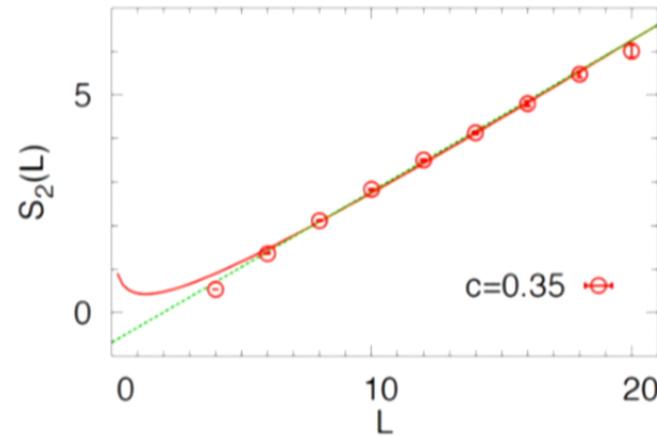
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$$b_2 = -0.68(1)$$



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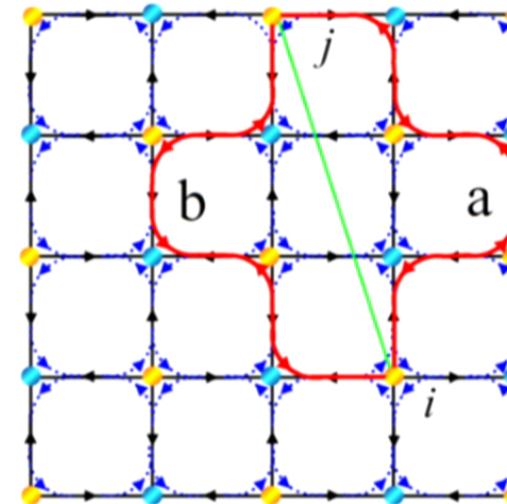
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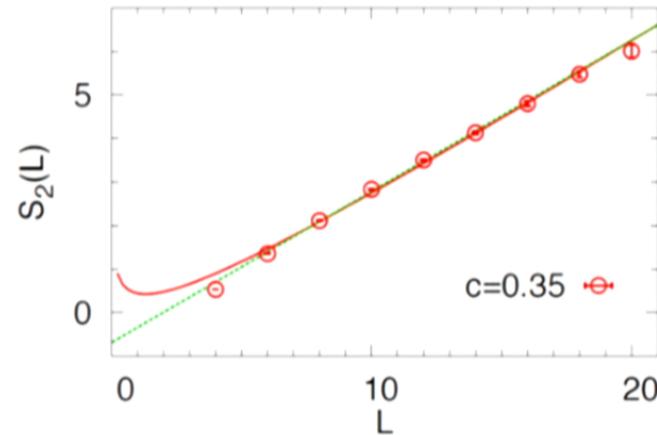
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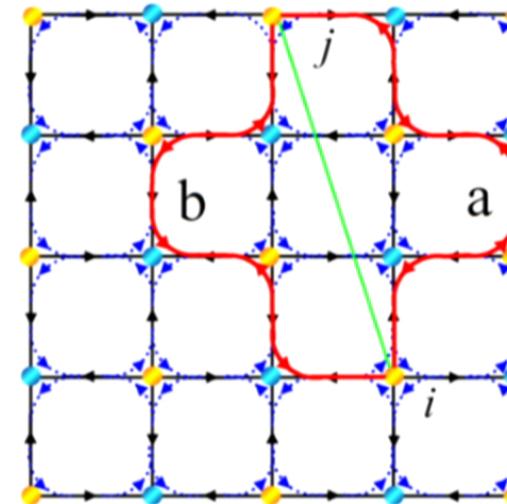
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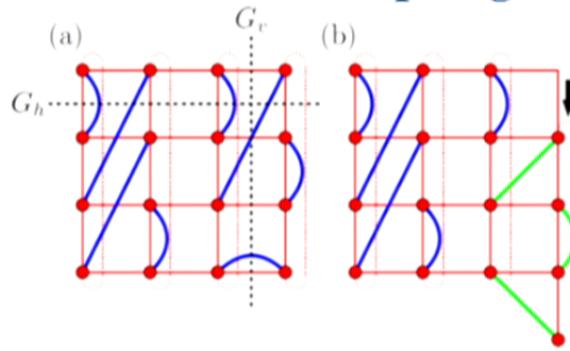
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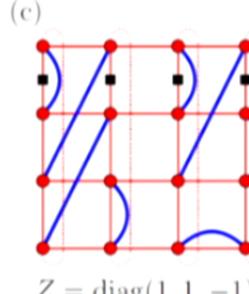


Topological sectors and variational energy

Similar to the short range RVB state, we can define four different topological sectors.



(c)

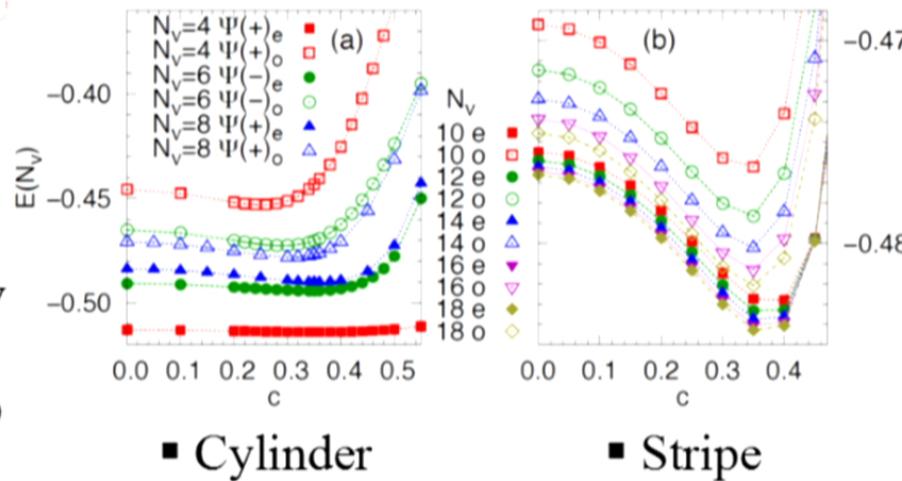


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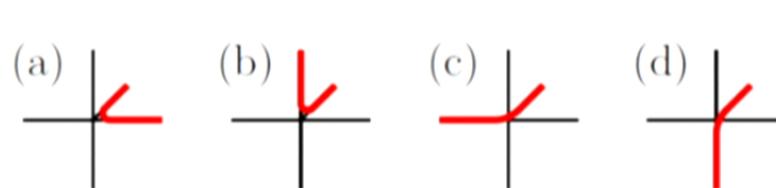


▪ Cylinder

▪ Stripe

Single parameter variational approach

A D=3 TPS description of short range RVB state



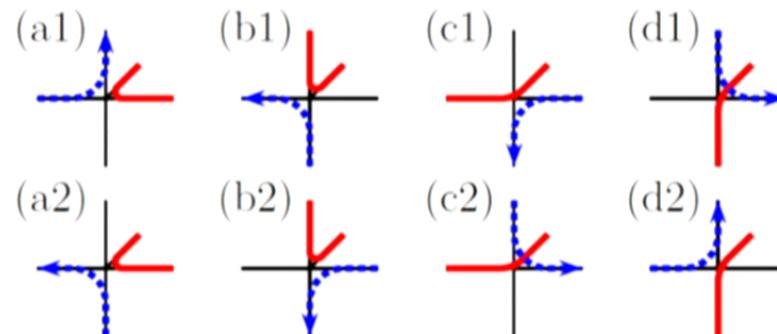
$$\mathcal{P}_1 = \sum_{k=1}^4 (|\uparrow\rangle\langle 0|_k + |\downarrow\rangle\langle 1|_k) \otimes \langle 222|_{/k}$$
$$|\mathcal{S}\rangle = |01\rangle - |10\rangle + |22\rangle$$

Including longer range RVB

$$|\Psi\rangle_{\text{s-RVB}} = \prod_V \mathcal{P}_1 \prod_B |\mathcal{S}\rangle$$

$$\mathcal{P}_2 = \sum_{i \neq j \neq k \neq l} (|\uparrow\rangle\langle 0|_i + |\downarrow\rangle\langle 1|_i) \otimes \langle 2|_j \otimes \langle \epsilon|_{kl}$$

A single-parameter
ansatz



$$\mathcal{D} = \mathcal{D}_1 + c\mathcal{D}_2$$

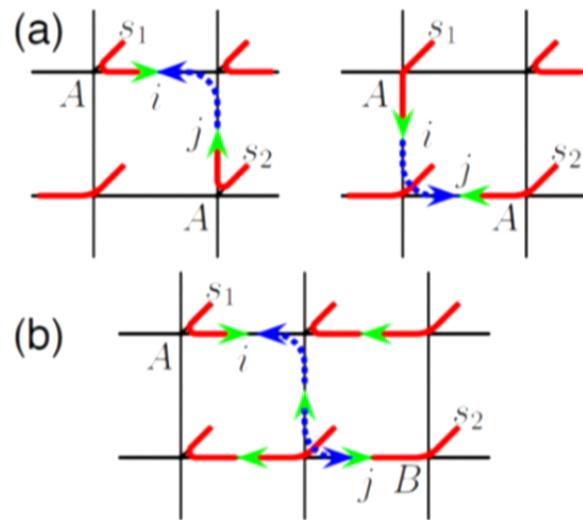
Discussions and future directions:

Other variational approach

- The best Schwinger VMC approach also predicts gapless U(1) spin liquid.
- The best Slave boson VMC approach predicts gapless Z2 spin liquid with a very small vison gap.
- In general, symmetric spin liquid must be gapless if it is close to AF state.

Properties of the variational state

Longer range RVB configurations can be generated through quantum teleportation



Longer range RVB decays exponentially

