Emergent gapless quantum spin liquid from deconfined quantum critical point

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Wenyuan Liu, *etal*. arXiv:2009.01821 (2020)

Wenyuan Liu, *etal*., to appear (2021)

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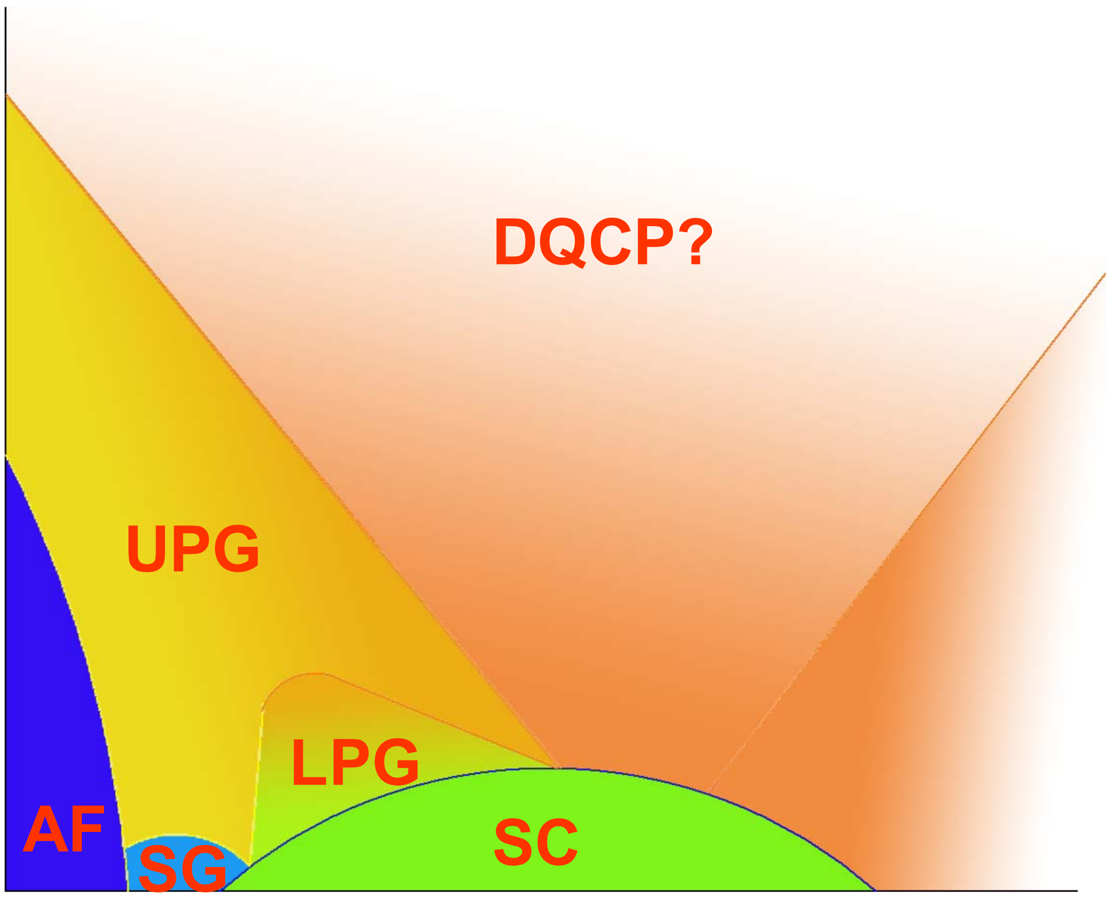
Potential deconfined Quantum critical point (QCP) in cuprates

Subir Sachdev, Science 288, 475, (2000)



DQCP in unfrustrated spin models

Theory: beyond Landau's paradigm

$$\mathcal{L}_{\mathrm{DQCP}} = \frac{1}{g}\sum_{a=1}^{2} |(\partial_\mu - i a_\mu) z_a|^2 + m^2 |z|^2 + u(|z|^2)^2 + \kappa(\epsilon_{\mu\nu\lambda}\partial_\nu a_\lambda)^2,$$

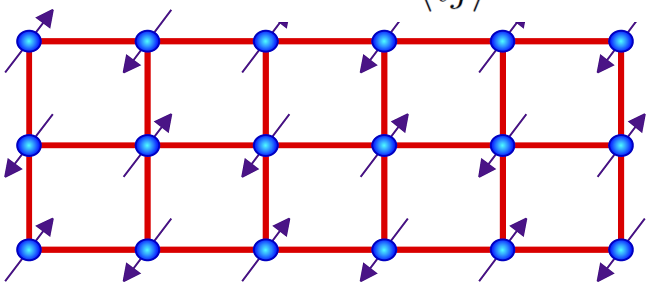
$$Q = \frac{1}{4\pi}\int d^2 r\, \hat{n}\cdot\partial_x \hat{n}\times\partial_y \hat{n},$$

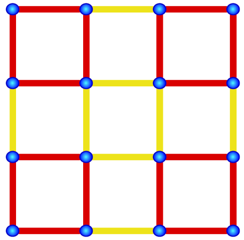
- On square lattice, Q always changes by four, thus the instanton effect becomes dangerous irrelevant!

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

Numerical: J-Q model

$$H = J\sum_{\langle ij\rangle} \mathbf{S}_i\cdot\mathbf{S}_j - Q\sum_{\langle ijkl\rangle}(\mathbf{S}_i\cdot\mathbf{S}_j - \tfrac{1}{4})(\mathbf{S}_k\cdot\mathbf{S}_l - \tfrac{1}{4})$$



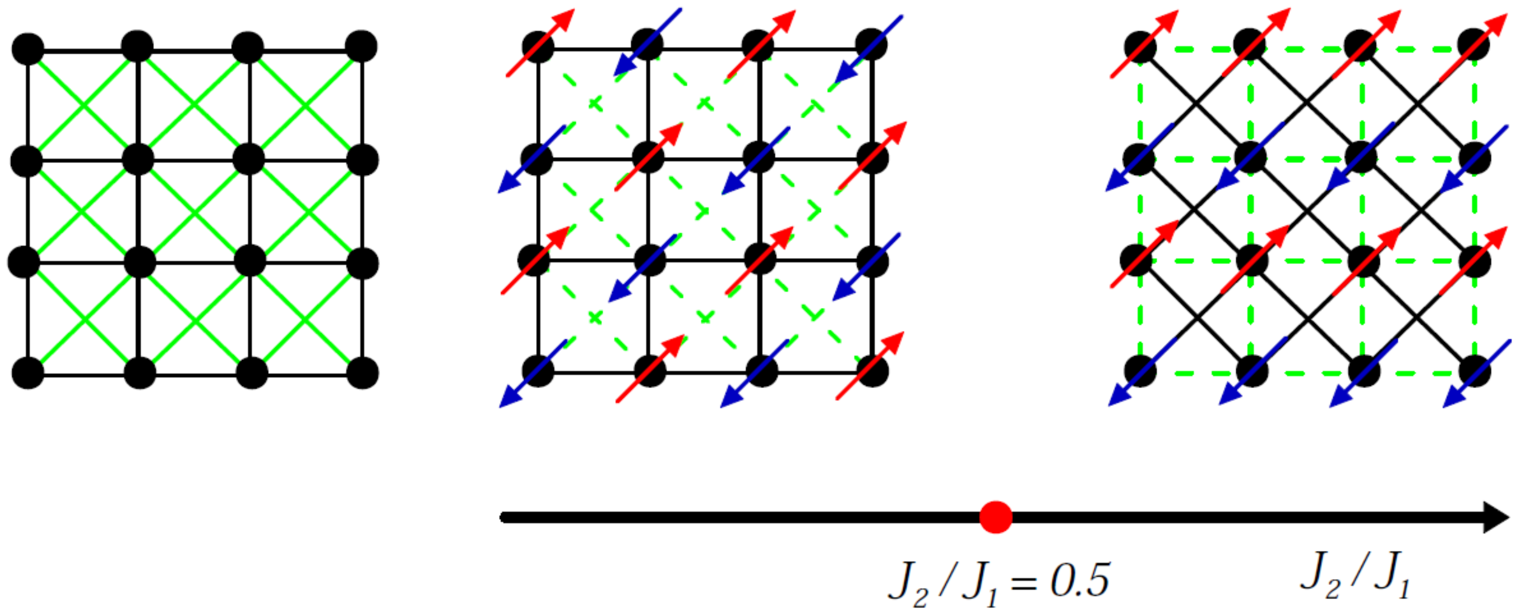


Anders W. Sandvik, Phys. Rev. Lett. 98, 227202 (2007)

- Direct (Landau forbidden) phase transition from anti-ferromagnetic(AFM) order to valence bond solid(VBS) order is observed.

DQCP vs. stable quantum spin liquid in frustrated magnets

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



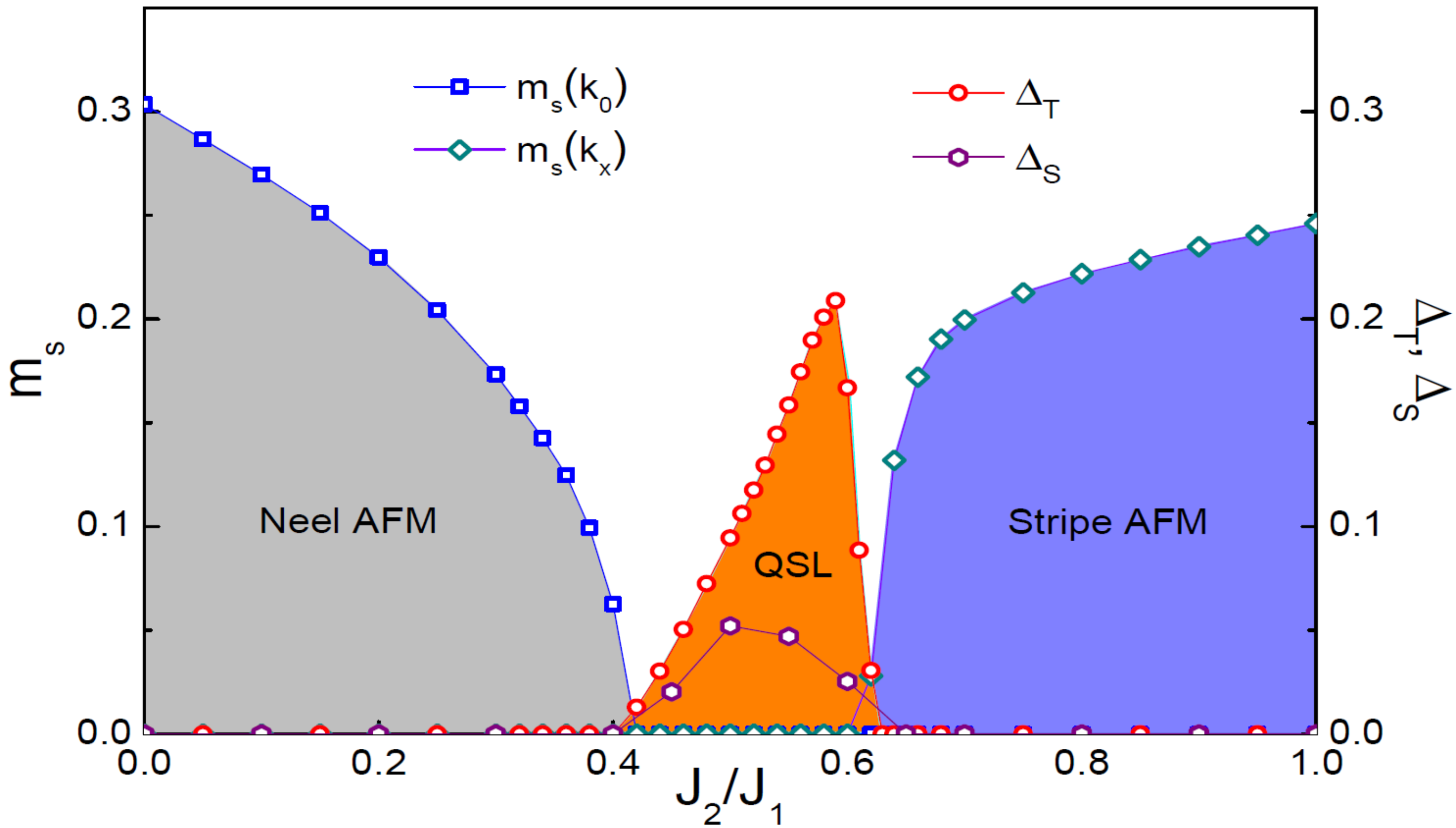
- Landau paradigm predicts a first order phase transition at J2/J1=0.5

- It has been believed that the Landau paradigm fails around J2/J1=0.5 due to quantum fluctuations, but DQCP or stable quantum spin liquid?

A puzzle for more than twenty years!

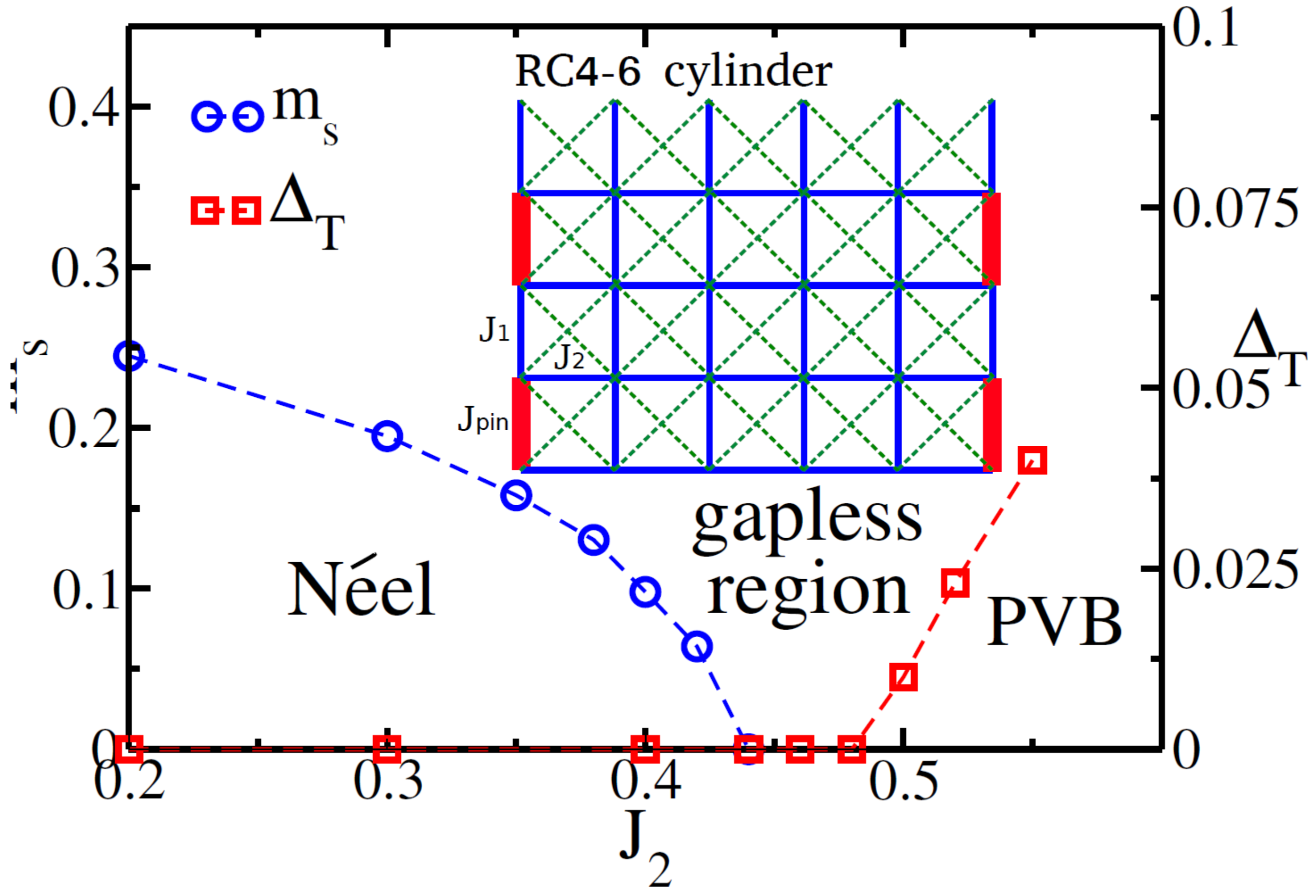
Recent numerical progress

Early density matrix renormalization group(DMRG) algorithm claims a gapped spin liquid



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

Recent work by using SU(2) symmetry DMRG algorithm suggests a different scenario!



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

Ling Wang and Anders W. Sandvik Phys. Rev. Lett. 121, 107202 (2018)

Limitation of DMRG: essentially a quasi 1D system

2D variational approach(biased):

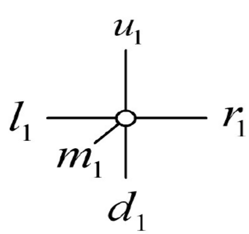
- The best Schwinger boson VMC approach predicts gapless U(1) spin liquid.(The so-called short range RVB state with exponential decay of spin-spin correlation.)

- The best Slave boson VMC approach predicts gapless Z_2 spin liquid with a very small vison gap.(Due to the presence of Dirac spinon, we should expect $1/r^4$ decay of spin-spin correlation.)

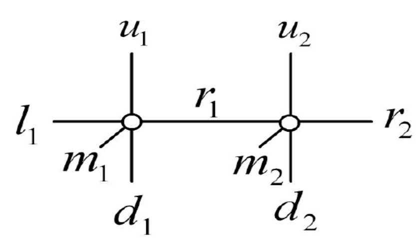
How to understand 2D system in an unbiased way?

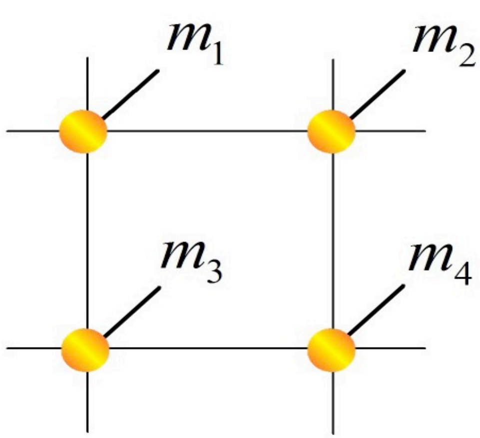
PEPS! $\uparrow \longrightarrow T^{\uparrow}_{lrud}; \quad \downarrow \longrightarrow T^{\downarrow}_{lrud}$ (F. Verstraete and J. I. First 2004)

$T^{m_1}_{l_1 r_1 u_1 d_1}$:



$\sum_{r_1} T^{m_1}_{l_1 r_1 u_1 d_1} T^{m_2}_{r_1 r_2 u_2 d_2}$:

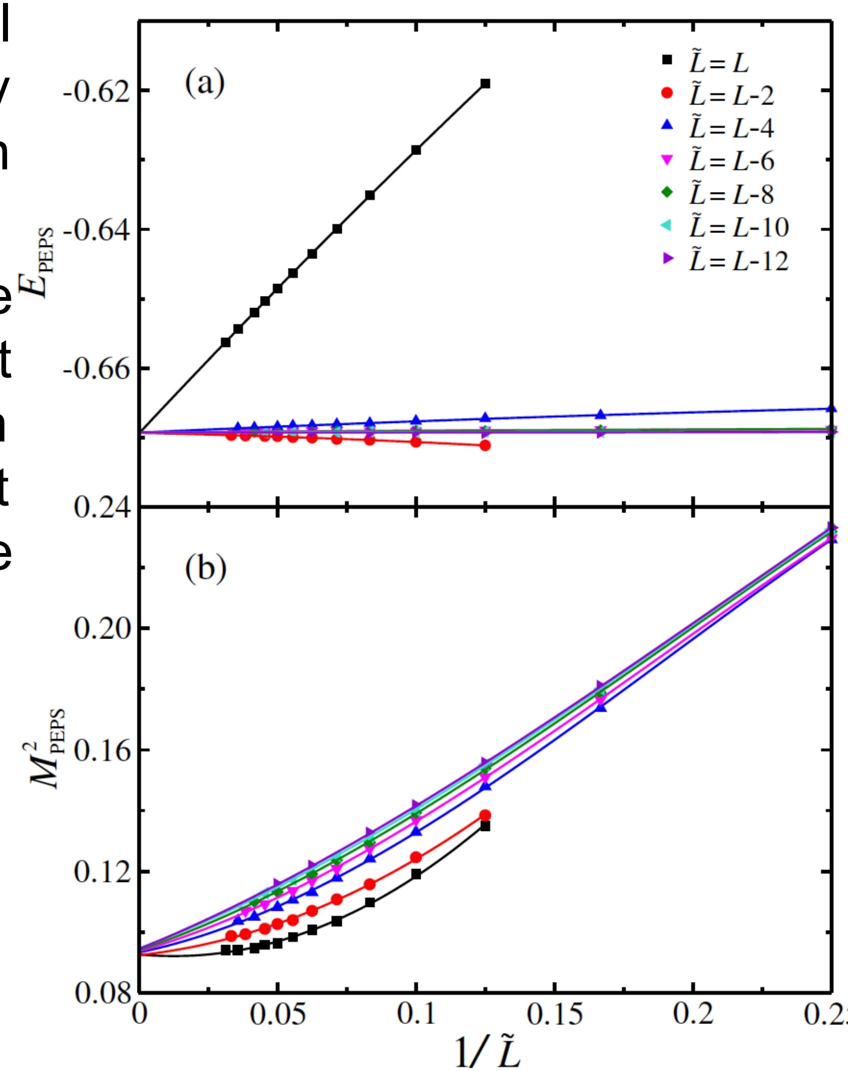




Benchmark results for J_2=0

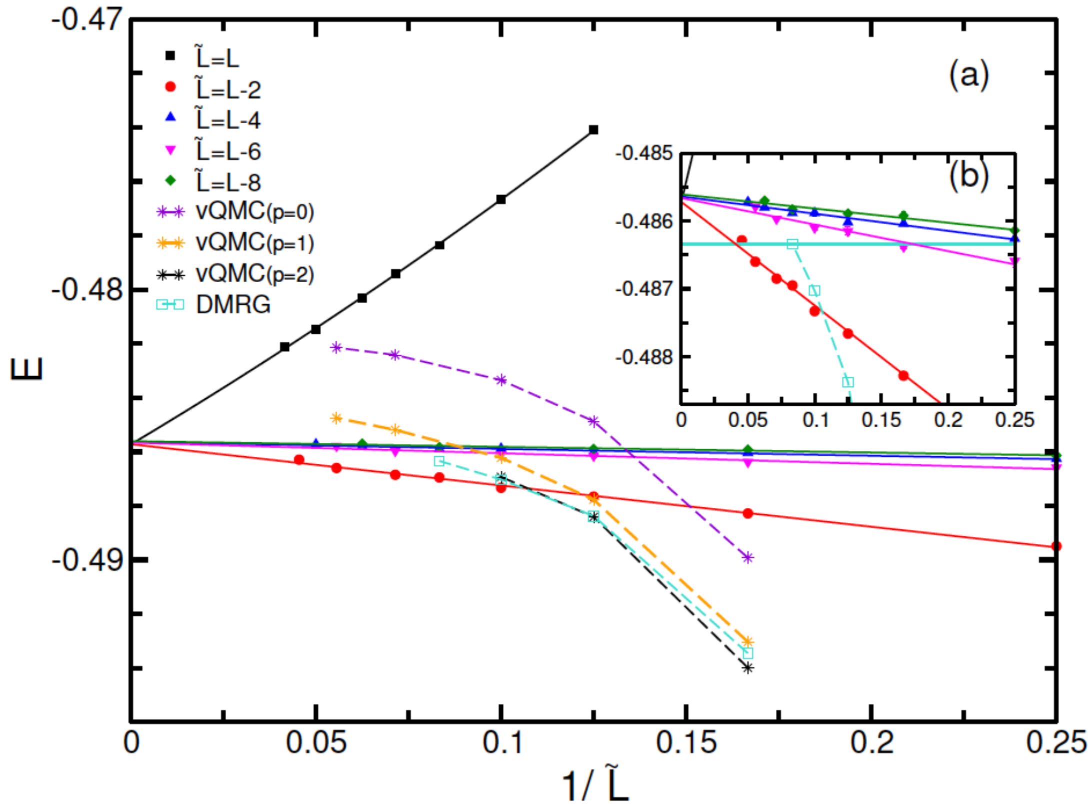
- With open boundary condition, all physical quantities can be efficiently simulated by MPS based method with Monte Carlo Sampling.
- we first use the simple update imaginary time evolution method to get a rough ground state for initialization then use stochastic gradient optimization method to obtain the ground state with D=8.

$\tilde{L}$	$E(\infty)$	$M^2(\infty)$	$M(\infty)$
L	-0.66940(2)	0.0924(11)	0.304
$L-2$	-0.66933(6)	0.0926(10)	0.304
$L-4$	-0.66929(5)	0.0944(06)	0.307
$L-6$	-0.66928(3)	0.0947(08)	0.308
$L-8$	-0.66926(6)	0.0940(13)	0.306
$L-10$	-0.66928(6)	0.0937(13)	0.306
$L-12$	-0.66927(8)	0.0933(12)	0.305
exact	-0.669437 [8]	0.09451 [9]	0.30743(1) [9]



- Ground state energy and magnetization actually agree with QMC for all sizes, for more details. (Wenyuan Liu, *etal.* arXiv:1908.09359)

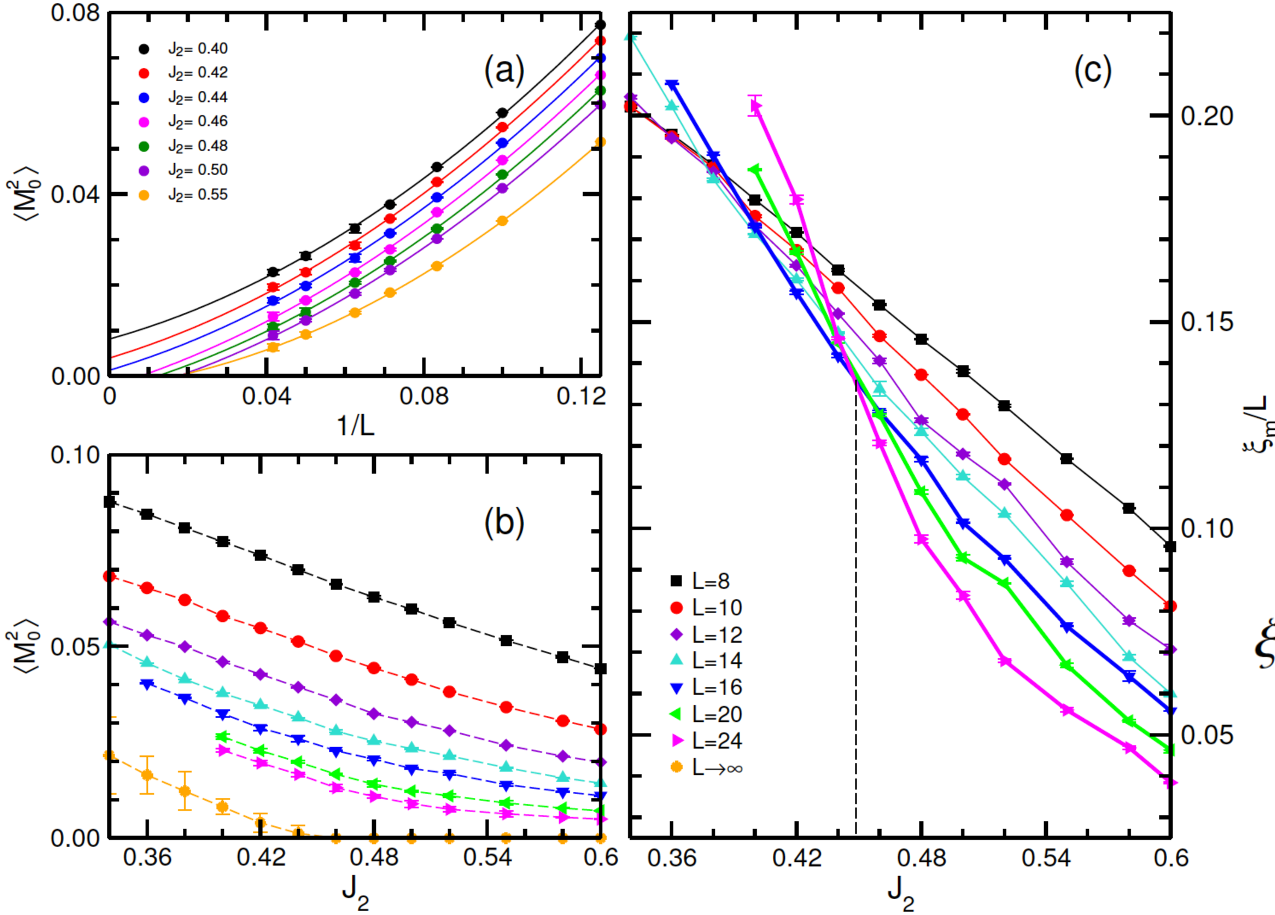
Ground state energy for J_2=0.55J_1



- We compute ground state energy with D=8 up to 24 by 24 and apply finite size scaling for different central bulk size.

- DMRG results are obtained for cylinder geometry with different circumference and vQMC results are obtained on periodic boundary condition(PBC).

AFM order parameter



$$\mathbf{M}_0 = \frac{1}{L^2}\sum_{\mathbf{i}}(-1)^{\mathbf{i}}\mathbf{S}_{\mathbf{i}}$$

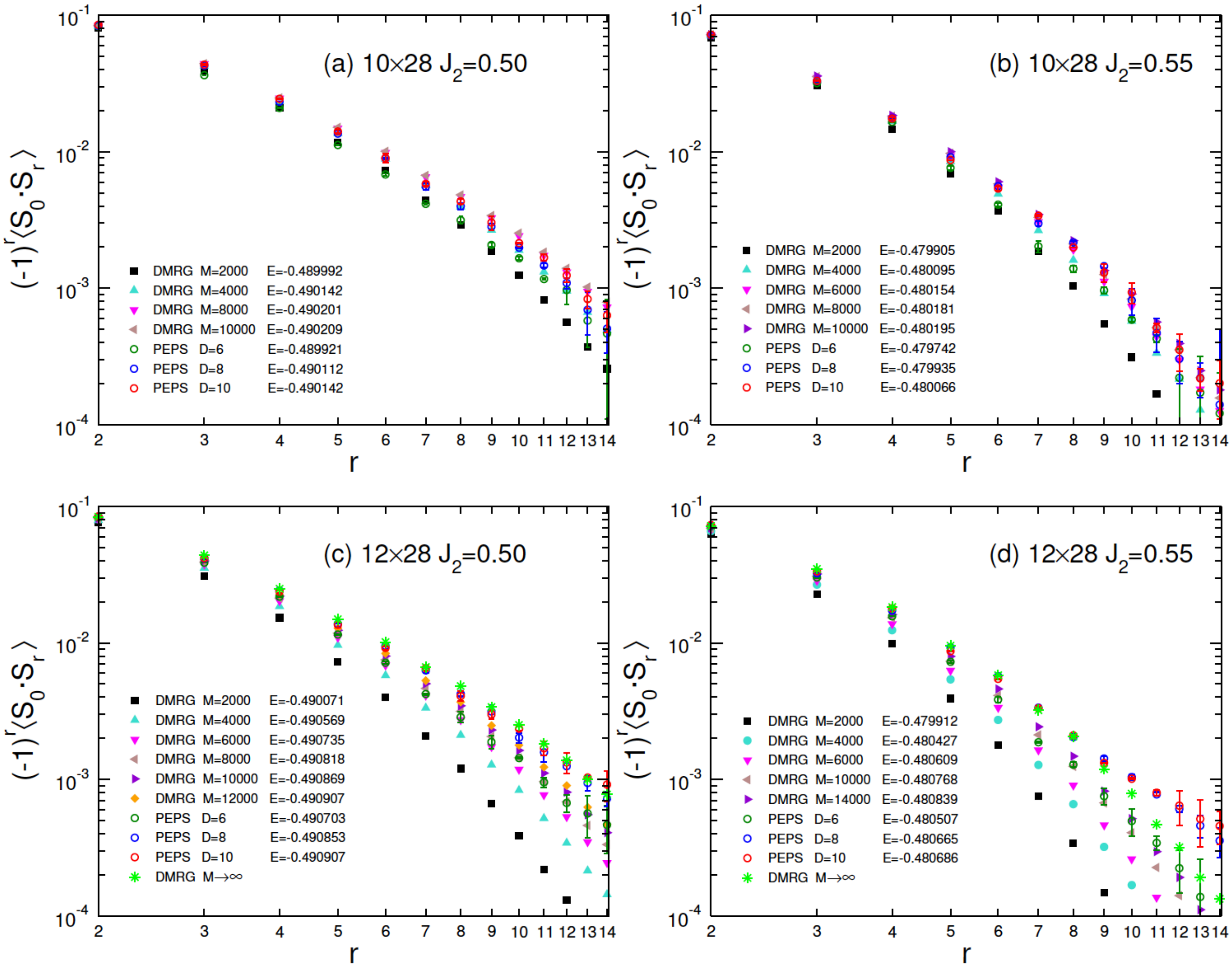
- Determine the transition point using correlation length.

$$\xi_m = \frac{L}{2\pi}\sqrt{\frac{m_s^2(\pi,\pi)}{m_s^2(\pi,\pi+2\pi/L)} - 1}$$

$$m_s^2(\mathbf{k}) = \frac{1}{L^4}\sum_{\mathbf{ij}}\langle\mathbf{S}_{\mathbf{i}}\cdot\mathbf{S}_{\mathbf{j}}\rangle e^{i\mathbf{k}\cdot(\mathbf{i}-\mathbf{j})}$$

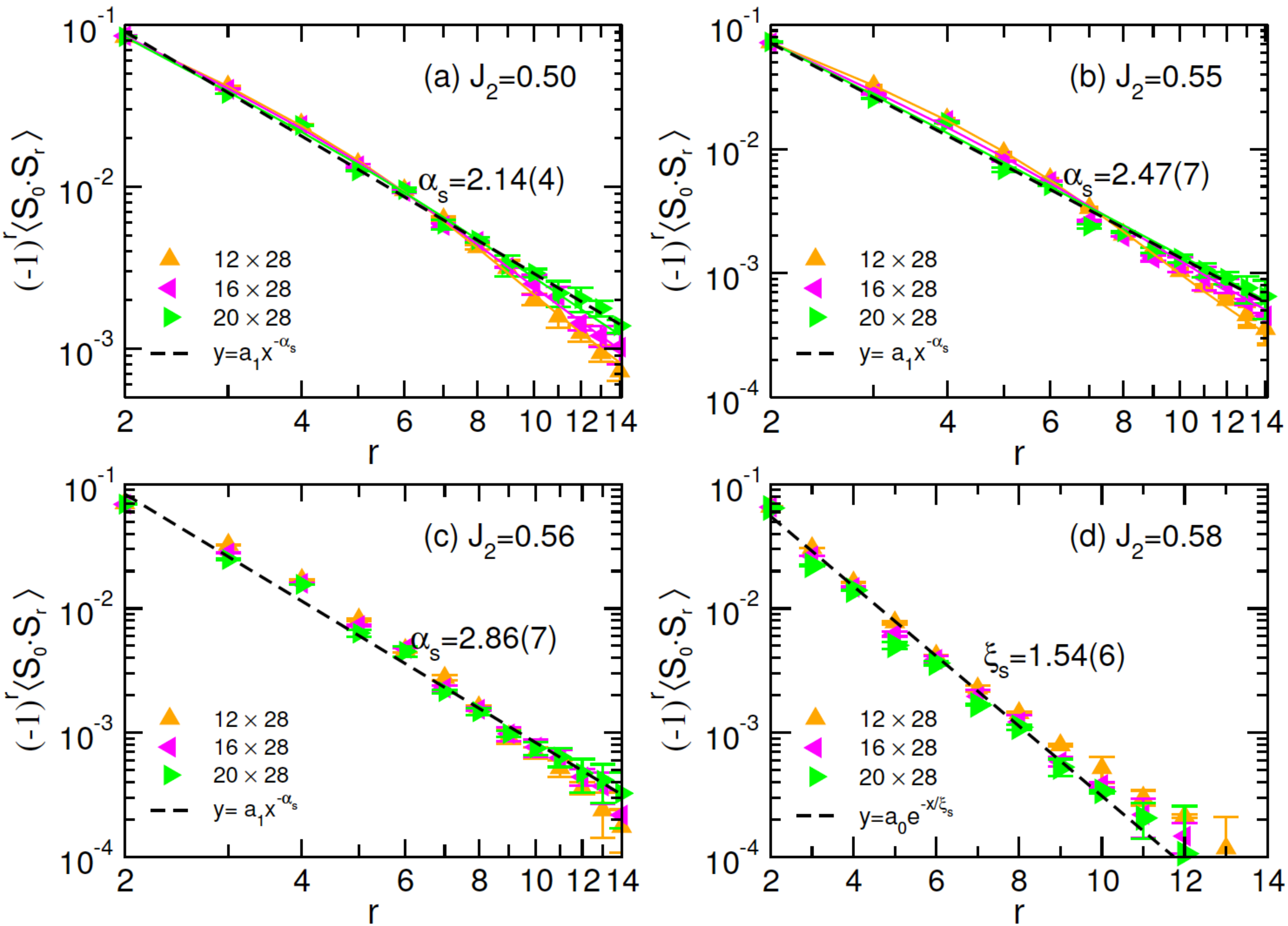
- The finite size scaling results of magnetization indicate the vanishing of AFM order around J_2=0.46J_1 Perfect agree with previous DMRG results!

A detailed benchmark of spin-spin correlation with DMRG:



- Spin-spin correlation along the central line well agree with DMRG!

spin-spin correlation for large system size(D=8):

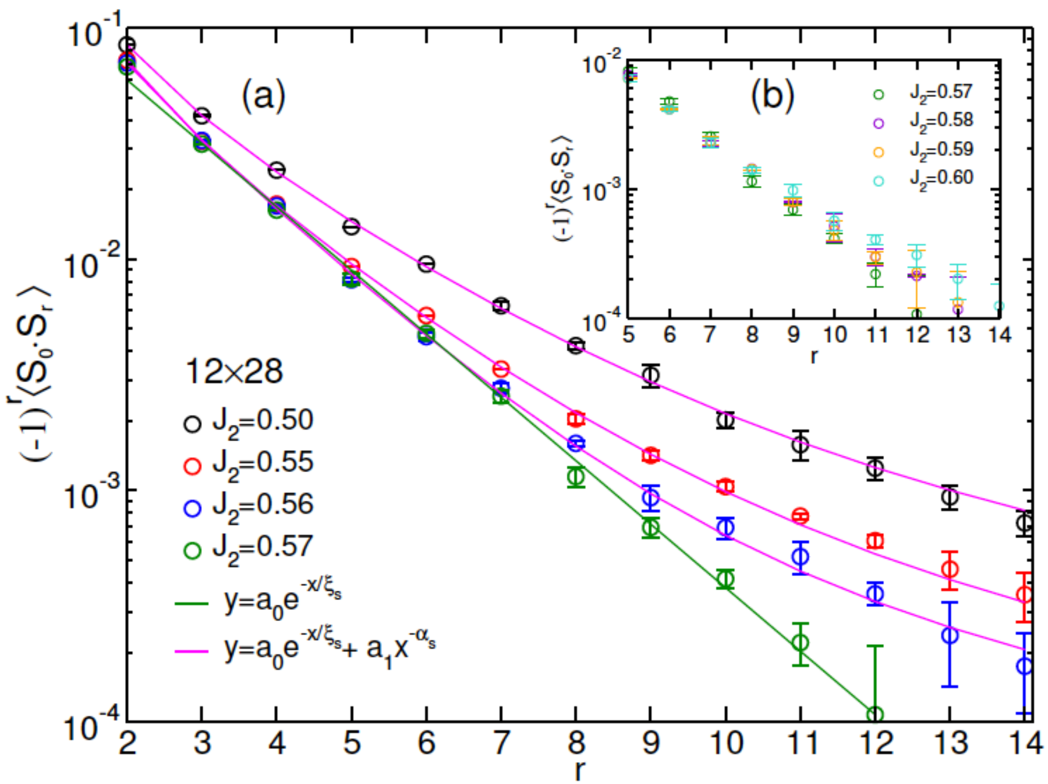


Two component fitting for spin-spin correlation:

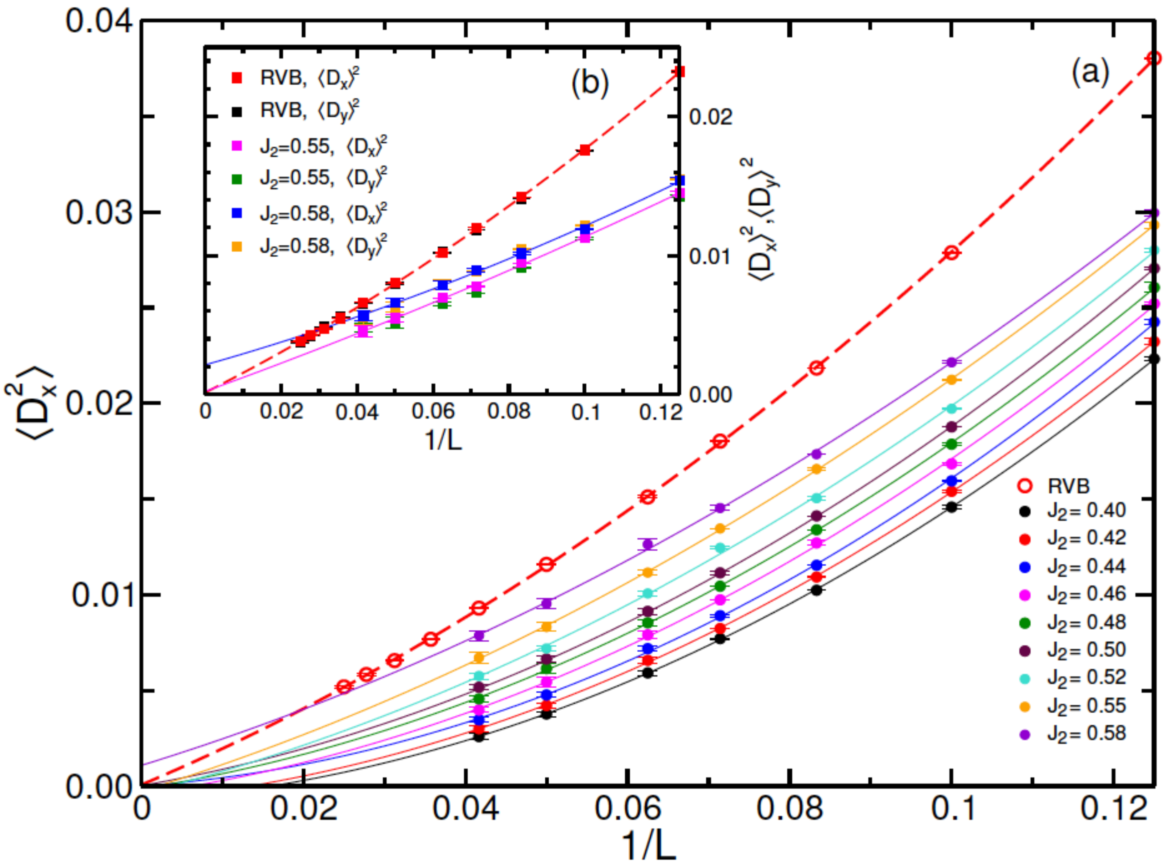
- The spin-spin correlation can be well fitted as: $y = a_0 e^{-x/\xi_s} + a_1 x^{-\alpha_s}$

J_2	L_y	a_0	a_1	ξ_s	α_s
0.50	12	0.095(9)	0.22(2)	1.99(9)	2.16(9)
0.50	16	0.064(13)	0.27(3)	2.07(28)	2.16(13)
0.50	20	0.032(18)	0.31(4)	2.29(98)	2.12(21)
0.55	12	0.107(6)	0.22(1)	1.69(6)	2.50(8)
0.55	16	0.043(29)	0.32(7)	1.74(73)	2.45(35)
0.55	20	0.004(4)	0.39(2)	1.89(87)	2.45(9)

- For J_2>0.57J_1, all spin-spin correlation correlations can be well fitted with exponential decay, suggest a VBS phase!



VBS order parameter



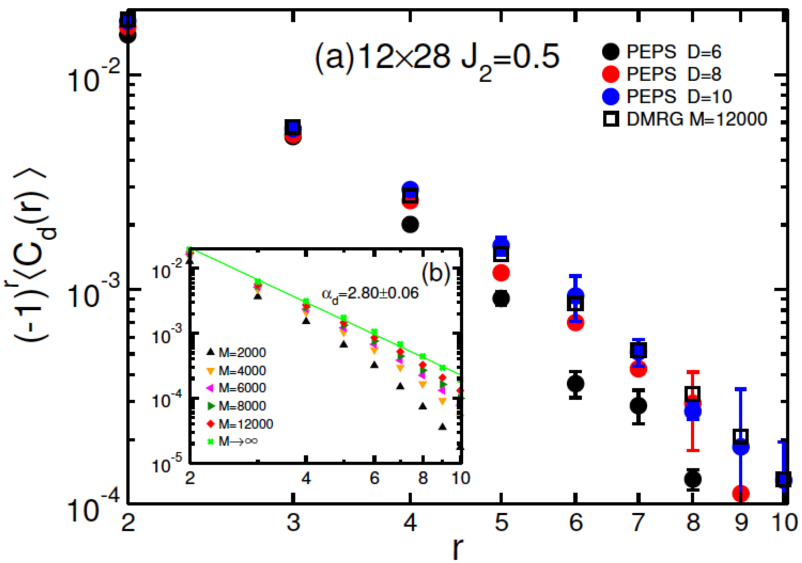
$$D_\alpha = \frac{1}{N_b} \sum_{\mathbf{i}} (-1)^{i_\alpha} B_{\mathbf{i}}^\alpha$$

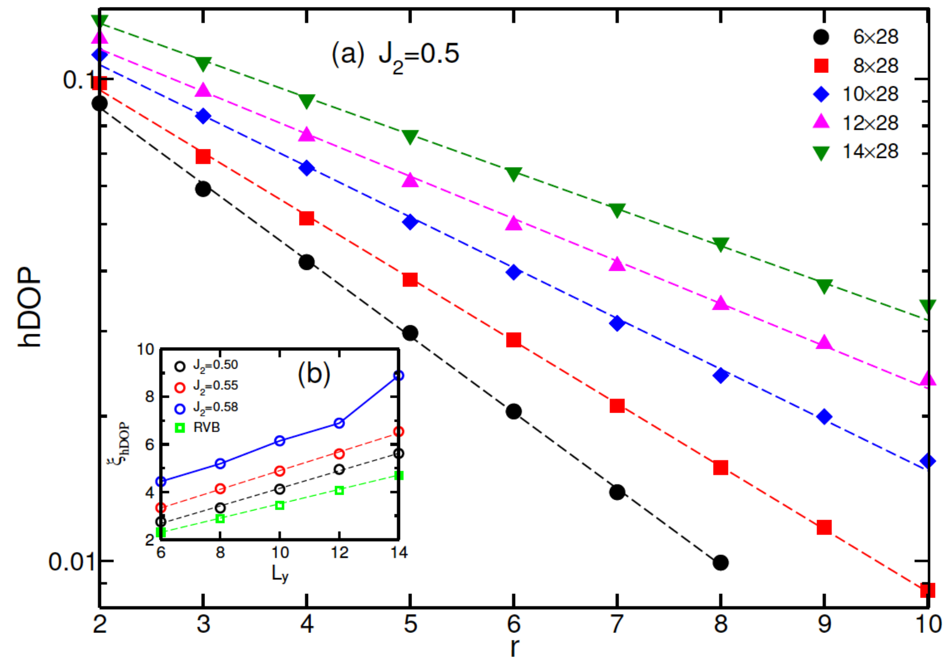
$$B_{\mathbf{i}}^\alpha = \mathbf{S}_{\mathbf{i}} \cdot \mathbf{S}_{\mathbf{i}+\mathbf{e}_\alpha}$$

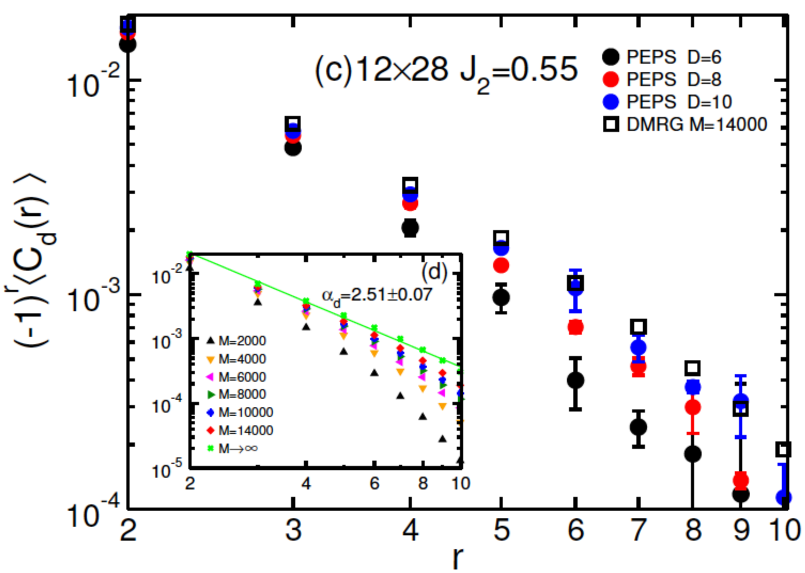
- The finite size scaling results of dimer order parameter indicate the arising of VBS order around J_2=0.57J_1

- The intermediate paramagnetic phase could be a potential gapless quantum spin liquid!

Dimer- dimer Correlation:



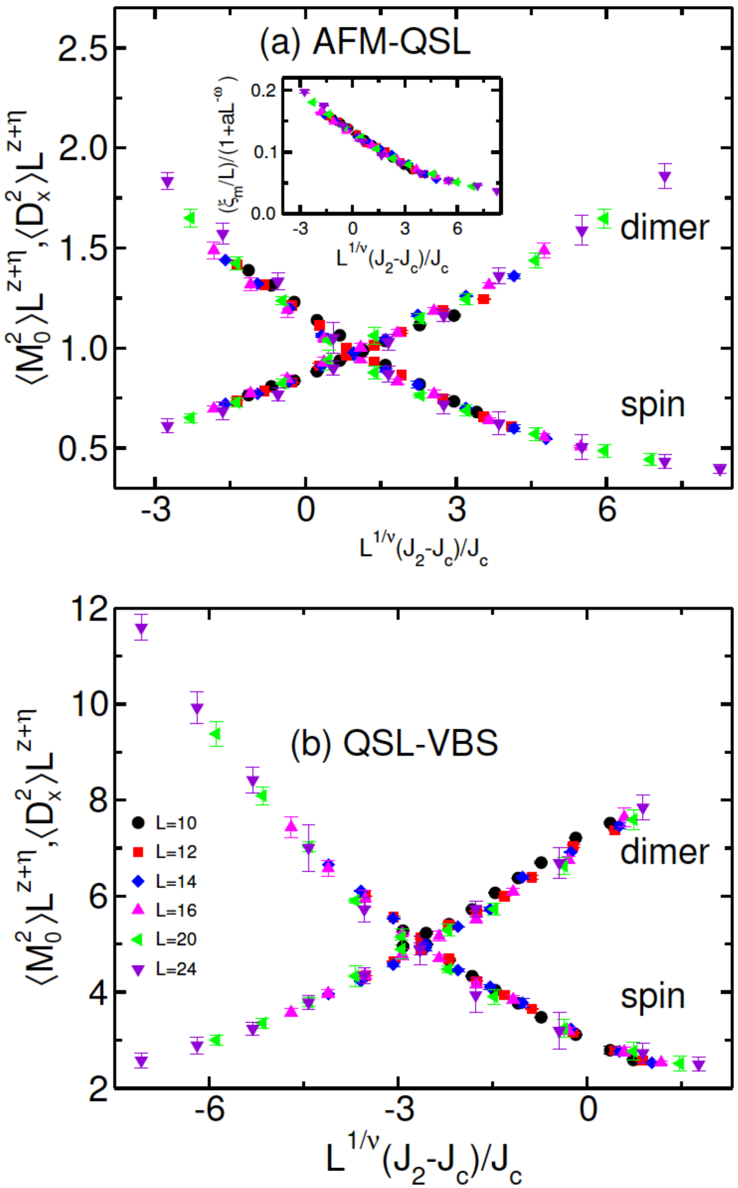




$$\Delta B(r) = |B_r^x - B_{r+e_x}^x|.$$

- On a strip, the decay length of horizon dimer order parameter(hDOP) is very similar to the (short-range) RVB state, which has very good ground state energy around J_2=0.5J_1 and could be a metal-stable state for J_1-J_2 model. (Y Qi, ZC Gu Physical Review B 89 (23), 235122 (2014))

The universal scaling function



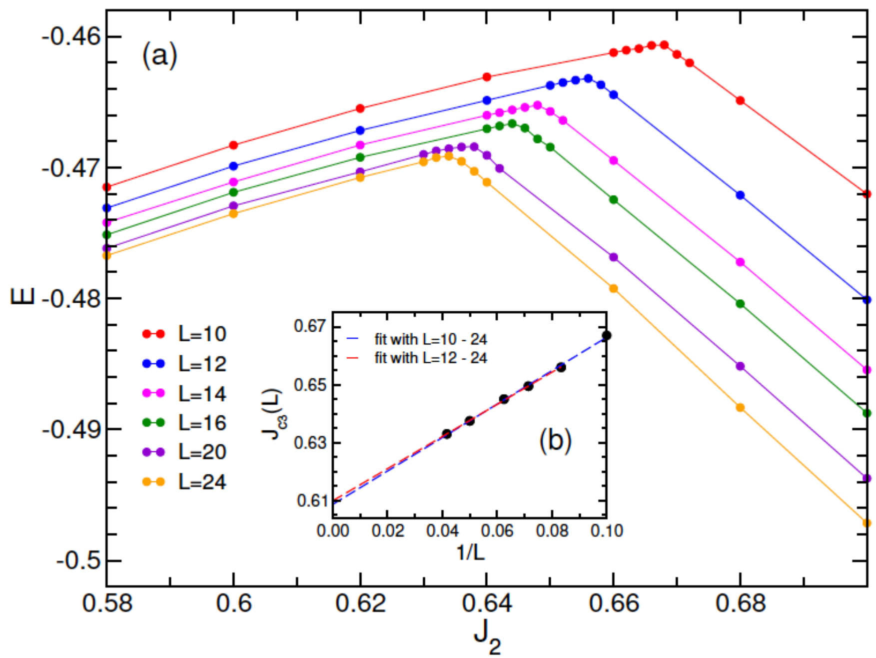
- By fitting a universal scaling function, we can determine the two phase transition points accurately.

$$\langle M_0^2\rangle = L^{z+\eta_s} F_s[L^{1/\nu}(J_2 - J_c)/J_c]$$
$$\langle D_x^2\rangle = L^{z+\eta_d} F_d[L^{1/\nu}(J_2 - J_c)/J_c]$$

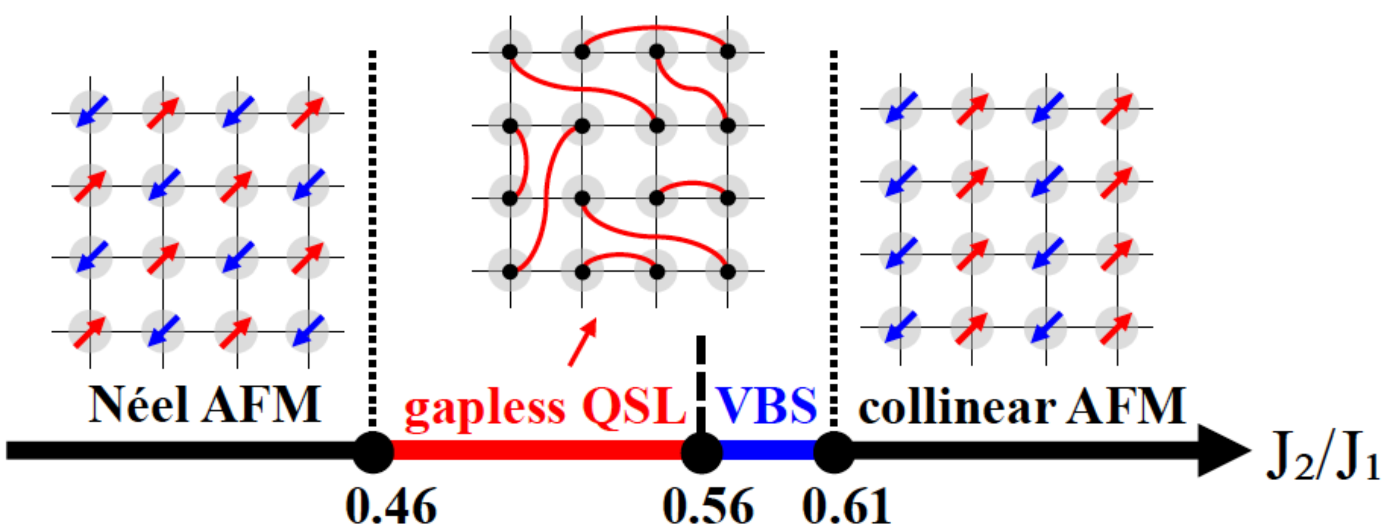
model	type	η_s	η_d	ν
J_1-J_2	AFM-QSL	0.38(3)	0.72(4)	0.99(6)
J_1-J_2	QSL-VBS	0.96(4)	0.26(3)	0.99(6)
J-Q_2(a)	AFM-VBS	0.26(3)	0.26(3)	0.78(3)
J-Q_2(b)	AFM-VBS	0.35(2)	0.20(2)	0.67(1)
J-Q_3	AFM-VBS	0.33(2)	0.20(2)	0.69(1)

- We find the same correlation length exponents at both transition points, indicating a stable intermediate paramagnetic phase(assume z=1).

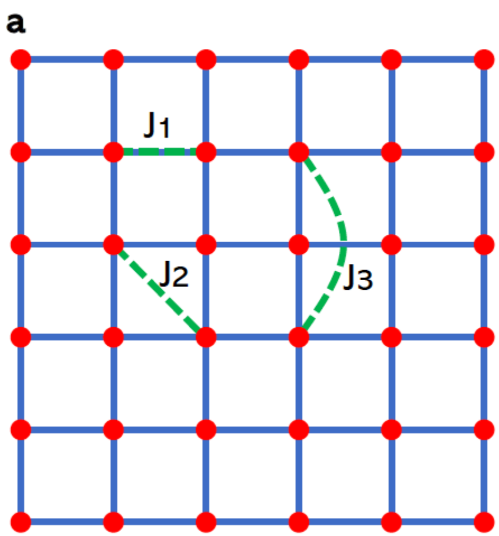
Global phase diagram

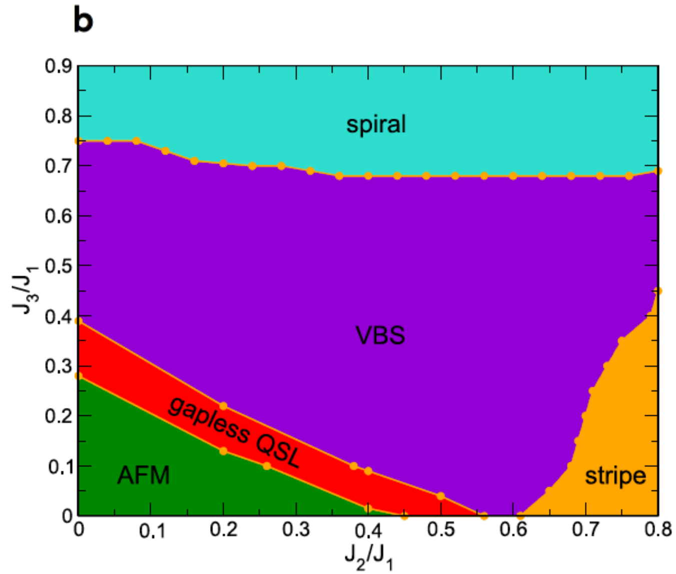


- Similar as previous study, a colinear AFM phase is expected at large J_2, through very careful finite size scaling, we find the transition is first order and the estimated transition point is around J_2=0.61J_1

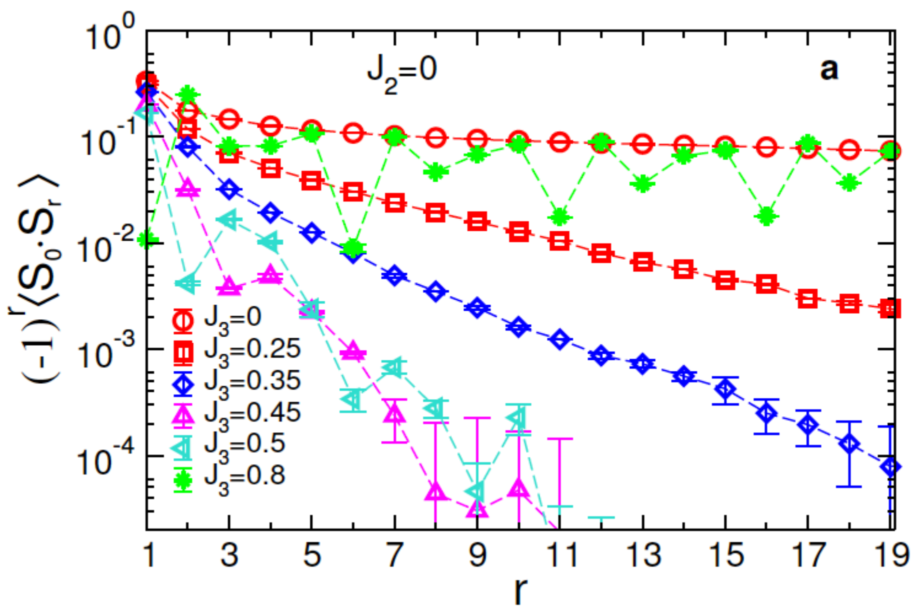


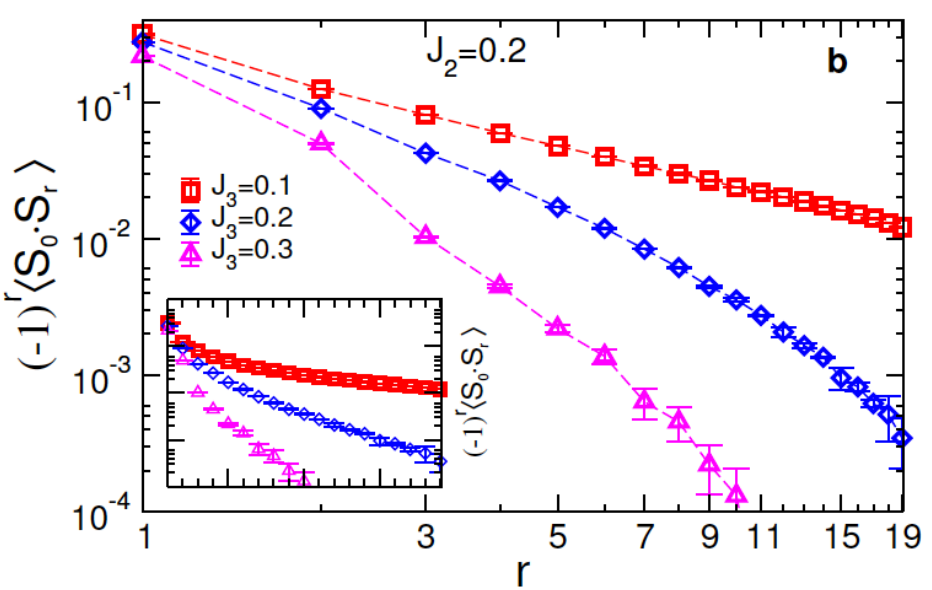
J_1-J_2-J_3 model



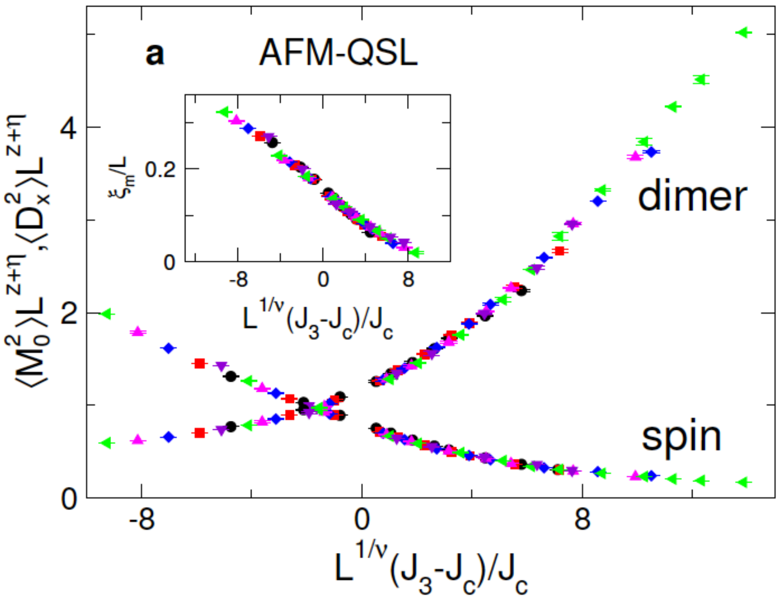


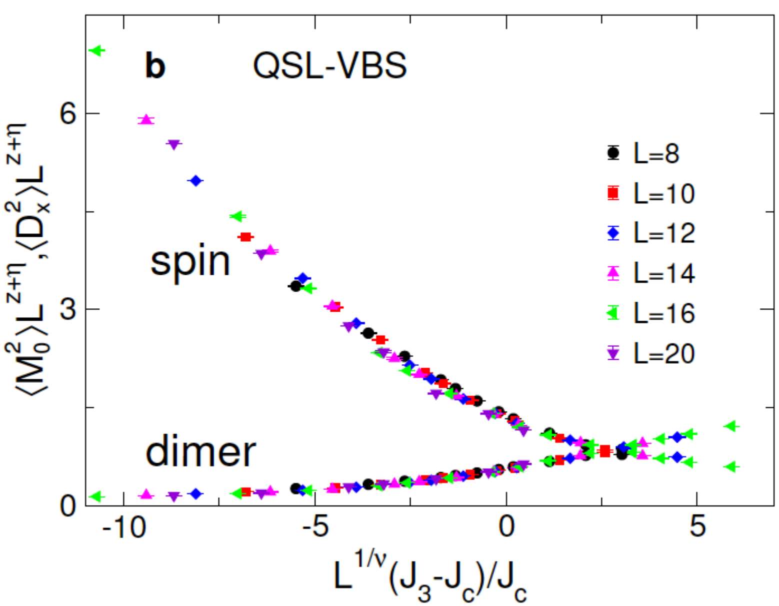
- The frustrated J_3 term will further stabilize the gapless spin liquid phase!





J_1-J_2-J_3 model





model	type	η_s	η_d	ν	J_c
$J_2 = 0$	AFM-QSL	0.22(6)	0.92(3)	1.04(5)	0.28
$J_2 = 0$	QSL-VBS	0.69(4)	0.39(5)	1.04(5)	0.39
$J_2 = 0.2$	AFM-QSL	0.21(5)	0.95(4)	1.01(7)	0.13
$J_2 = 0.2$	QSL-VBS	0.63(7)	0.45(4)	1.01(7)	0.24
$J_2 = 0.4$	AFM-QSL	0.31(3)	0.88(3)	0.99(5)	0.015
$J_2 = 0.4$	QSL-VBS	0.62(4)	0.51(3)	0.99(5)	0.09
$J_3 = 0.1$	AFM-QSL	0.21(2)	0.96(2)	1.01(2)	0.26
$J_3 = 0.1$	QSL-VBS	0.60(2)	0.58(3)	1.01(2)	0.38
J_1-J_2	AFM-QSL	0.38(3)	0.72(4)	0.99(6)	0.45
J_1-J_2	QSL-VBS	0.96(4)	0.26(3)	0.99(6)	0.56
J-Q_2(a)	AFM-VBS	0.26(3)	0.26(3)	0.78(3)	
J-Q_2(b)	AFM-VBS	0.35(2)	0.20(2)	0.67(1)	

- Along both critical lines, the correlation length exponents are intrinsically close to 1, which is quite different from DQCP.

The nature of gapless quantum spin liquid

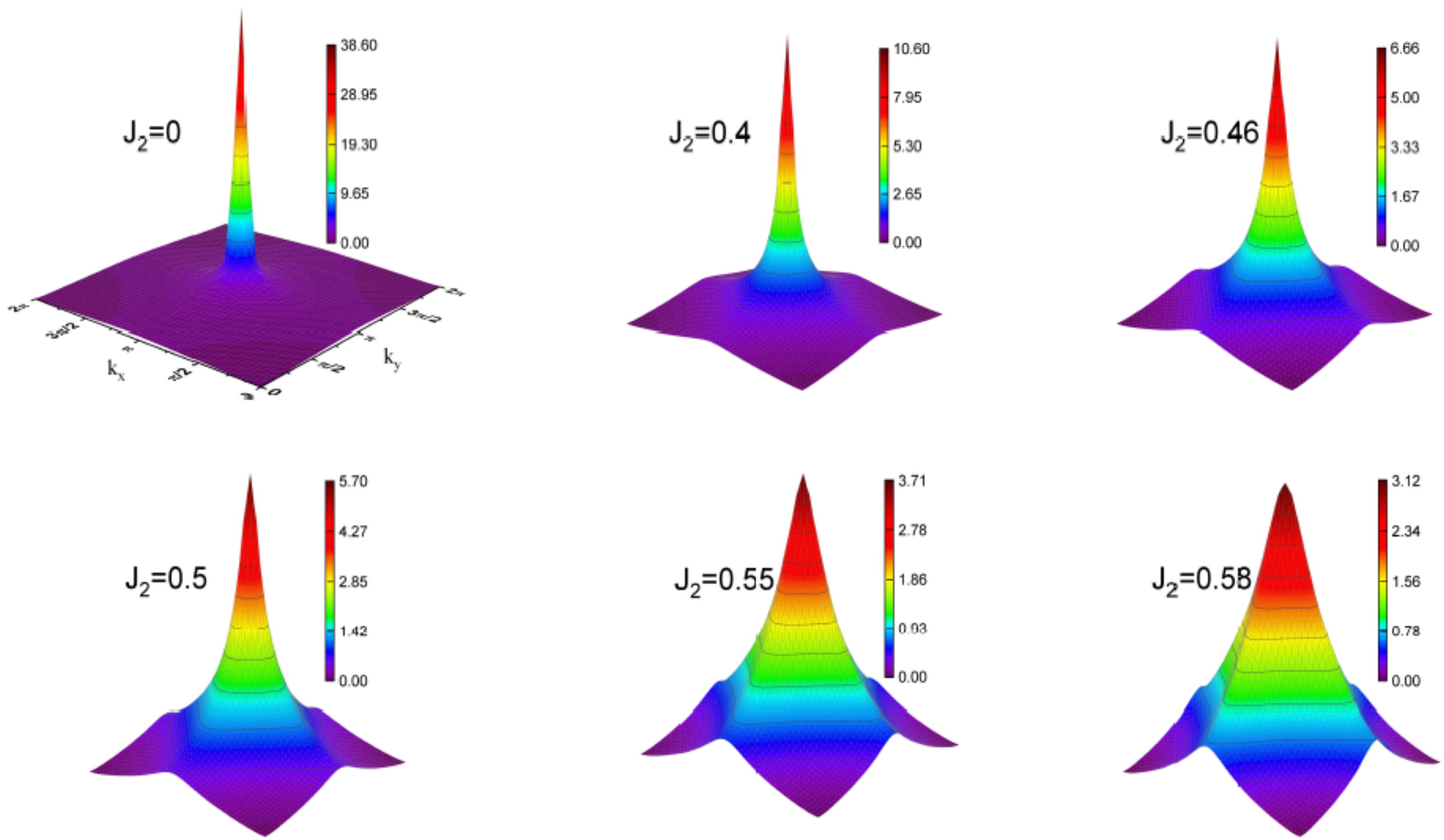
Adding a topological theta term(Hopf term) into the CP[1] model will lead to a gapless quantum spin liquid!

$$\mathcal{L}_\theta = \frac{\theta}{4\pi^2}\epsilon_{\mu\nu\lambda}a_\mu\partial_\nu a_\lambda \qquad \text{with } \theta = \pi$$

- We can rigorously proof:

$$\int D[z_a]D[z_a^*]D[a_\mu]\exp\left\{-\int d^3x\left[\sum_{a=1}^{2}|(\partial_\mu - a_\mu)z_a|^2 + m^2|z|^2 + \frac{i}{4\pi}\epsilon^{\mu\nu\lambda}a_\mu\partial_\nu a_\lambda\right]\right\}$$
$$= \text{constant}\cdot\int D[\psi_\alpha]D[\bar{\psi}_\alpha]\exp\left\{-\sum_{\alpha=1}^{4}\int d^3x\bar{\psi}_\alpha\gamma^\mu\partial_\mu\psi_\alpha\right\}$$

- With respecting to the lattice symmetry, the four Dirac spinon is expected to sit at $(\pm\pi/2, \pm\pi/2)$
- In the presence of Maxwell term, interaction among Dirac fermions can be generated



• Sub-peak is observed in spin structure factor, which might be contributed by Dirac spinons.

Discussions and future directions:

- By applying finite PEPS algorithm with MC-sampling and stochastic gradient optimization methods, we are able to study some frustrated magnets model.

- The gapless quantum spin liquid might emerge from the underlying DQCP with a topological theta term of the gauge field.

- Although finite PEPS algorithm with open boundary conditions is still suffer from the boundary problem, the results are reasonable after very careful finite size scaling.

- Finite PEPS algorithm with periodic boundary conditions are very desired, loop-TNR with MC-sampling is very promising! (S Yang, ZC Gu, XG Wen, PRL118 (11), 110504 (2017))

The doped J_1-J_2 model might be a d-wave superconductor!