KITP Program: Frustrated Magnetism and Quantum Spin Liquids: From Theory and Models to Experiments (Aug 13 - Nov 9, 2012)

Spin Liquid Ground State of the Spin-1/2 Square J_1-J_2 Antiferromagnetic Heisenberg Model

Hong-Chen Jiang

KITP, University of California, Santa Barbara

H. C. Jiang, H. Yao, and L. Balents: PRB **86**, 024424 (2012) (arXiv:1112.2241)

Collaborators: **Hong Yao** (Tsinghua) **Leon Balents** (KITP, UCSB)

Sep. 11, 2012, KITP, UCSB

Outline

- Introduction and Motivation
- Previous study of S=1/2 AFM square J_1-J_2 model
- DMRG study of the S=1/2 AFM square J_1-J_2 model
  1) Vanishing of magnetic order
  2) Finite spin excitation gap
  3) Vanishing of Valence-Bond-Solid order
  4) Finite topological entanglement entropy
  5) Phase diagram
- Further evidences for spin liquid and comments
- Summary and conclusion

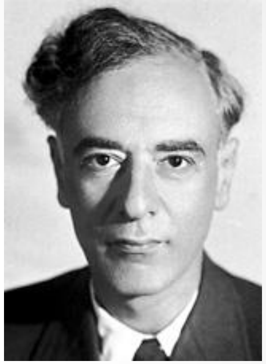
Introduction: Conventional Landau Paradigm

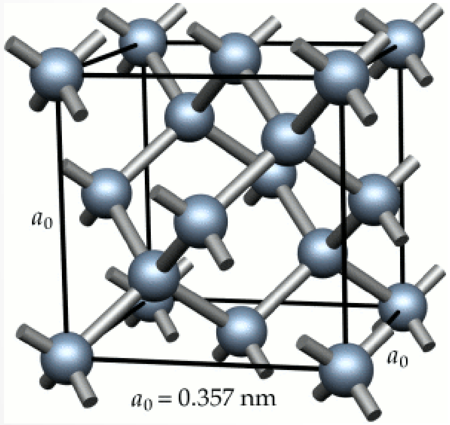
- Conventional states of matter:

Broken symmetry principle (by Landau)

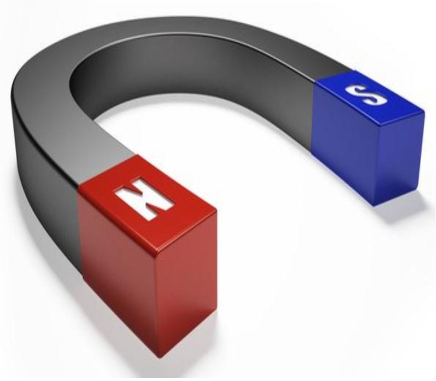
- Local order parameters

- Ginzburg-Landau description

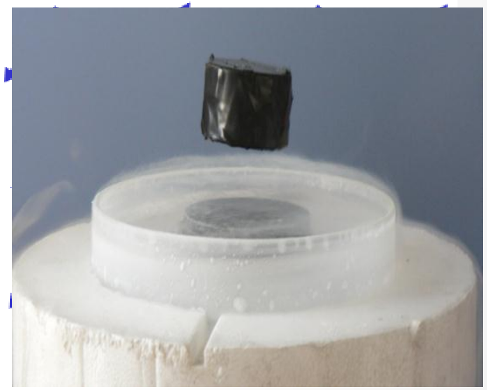




Crystal



Magnet



Superconductor

Exotic states of "matter“ beyond Landau Paradigm

- Fractional quantum Hall states (Laughlin, 1983):

  Quasi-particles carry fractional charge

- Topological insulators and superconductors (Kane & Mele (2005), and many others) Stable gapless edge or surface modes

- Quantum spin liquids (Anderson, 1973)

  For example, topological quantum spin liquid

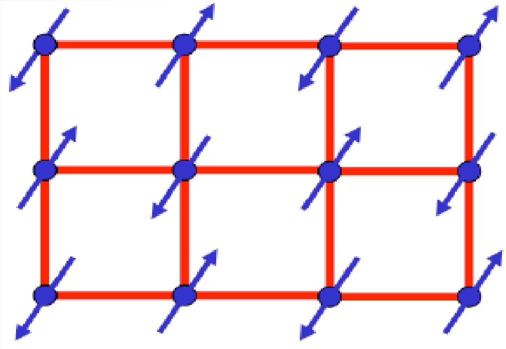
- One new principle for exotic phases:

  Topological order and long-range entanglement for gapped states

  (Wen, 1989; Wen & Niu, 1990; Levin & Wen, 2006; Preskill & Kitaev, 2006)

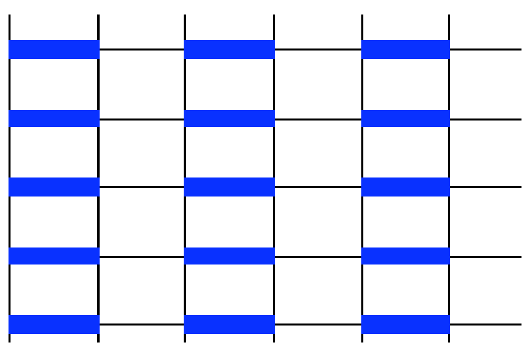
Conventional orders of magnets

- ✓ Magnetic Long Range Order



Antiferromagnetic order

- ✓ Non-Magnetic Long Range Order

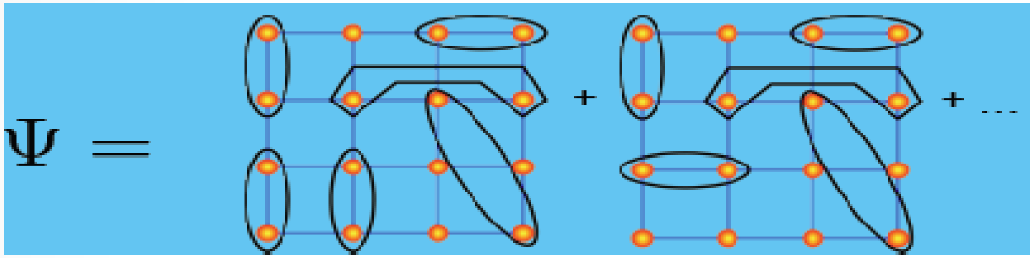


Valence Bond Solid order

Quantum Spin Liquids in 2D

- The first 2D spin liquid wave function: resonating valence bond (RVB)

  (Anderson 1973)



Anderson

- No magnetic order, no translational symmetry breaking

- **What is the definition of quantum spin liquids (QSL)?**

○ Intuitive definition:

A magnet has no broken symmetries even at zero temperature

(Leon Balents, Nature 2010)

○ Definition from adiabatic principle:

An insulator which cannot be adiabatically connected to a band insulator.

Quantum Spin Liquids in 2D

Three classes of quantum spin liquids

1) Topological Quantum Spin Liquids: spinon fully gapped

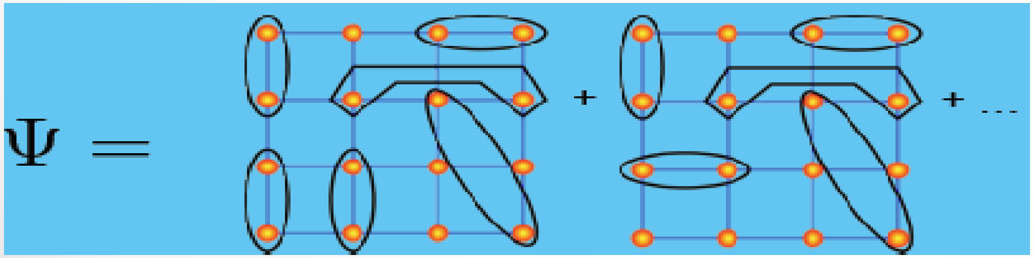
2) Algebraic Spin Liquids: spinon gapless at discrete momentum points

3) "Quantum Spin Metals": spinon Fermi surface

What is topological quantum spin liquid

1) Mott insulators with no broken symmetries
2) Gapped excitations with fractional statistics:
   Abelian and non-Abelian
3) Ground state degeneracies on a torus, or cylinder
4) Finite topological entanglement entropy

(Anderson 1973)

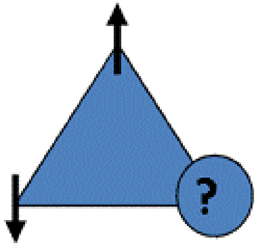


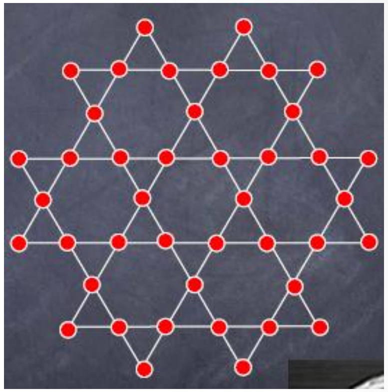
Short-range RVB

Where to look for spin liquids: Guidance

- Geometric frustrations:

  e.g. AF magnets on the Kagome lattice ?





- Multi-spin interactions, e.g., ring exchange (Fisher, Motrunich et al)

  - Strong charge fluctuation near a Mott transition: weak Mott insulators.

    e.g. Organic materials

- Strong spin-orbital coupling (Kitaev, et al)

  - Coupling to orbital degree of freedom could help destroy spin ordering.

    e.g. Kitaev model.

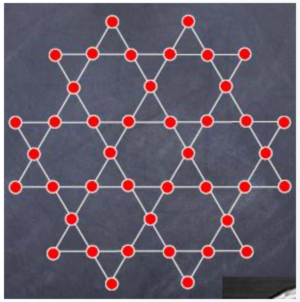
Theoretical and numerical search for spin liquids

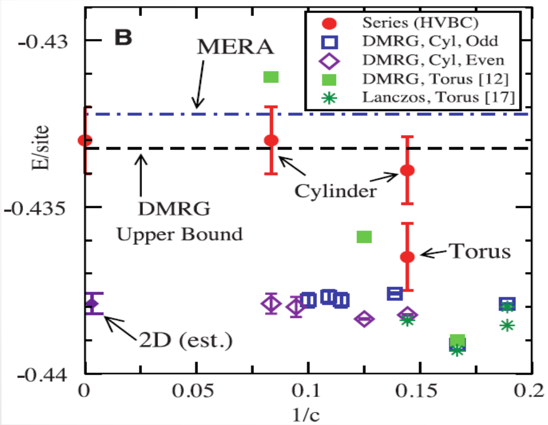
- Examples of Exactly solvable models with spin liquid GS:
  - Quantum dimer model and generalizations

    (Rokhsar and Kivelson, 1988; Moessner and Sondhi, 2001; Yao and Kivelson, 2011)
  - Toric code model (Kitaev, 2003)
  - Honeycomb Kitaev model and generalizations

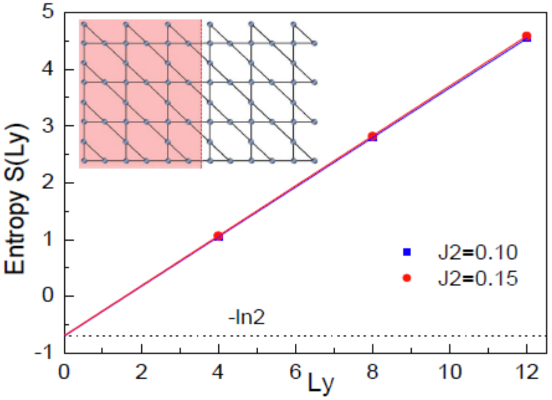
    (Kitaev, 2006; Yao et. al., 2007; V. Chua et. al.,, 2011, H.C.Jiang et. al., 2011)

- DMRG study of Kagome anti-ferromagnet:
  - Topological quantum spin liquid ground state.





S. Yan et al., Science 2011



H. C. Jiang et al, arXiv:1205.4289

H.C. Jiang et al, PRL 2008
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S. Depenbrock et al, PRL 2012

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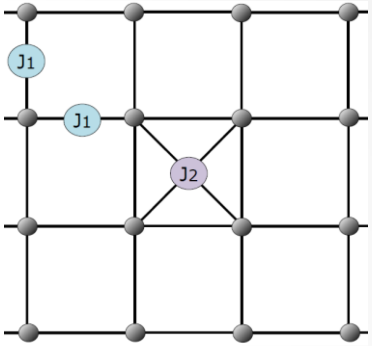
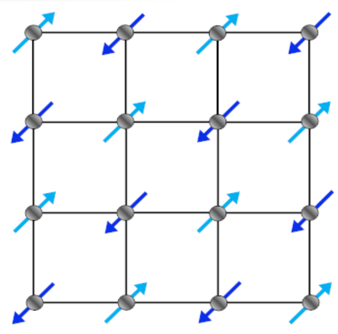
Spin-1/2 AF Heisenberg J_1-J_2 Model

$$H = J_1 \sum_{<ij>} S_i \cdot S_j + J_2 \sum_{<<ij>>} S_i \cdot S_j$$

- ➢ Strong Frustrations J2/J1 ~ 1/2
- ➢ Relevance to Cuprate, Fe-based superconductor





Neel AFM: k=(π,π)

0

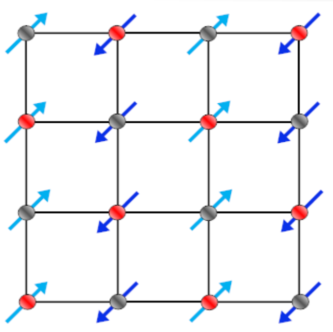
1st

∞

$J_2/J_1=0.5$

J_2/J_1

Phase transition in classical level



Stripe AFM: k=(0,π)

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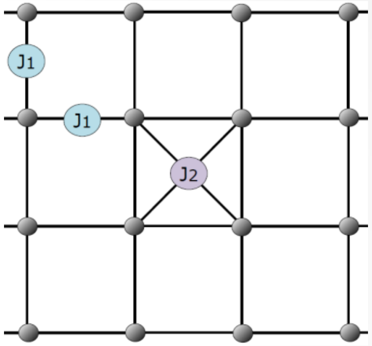

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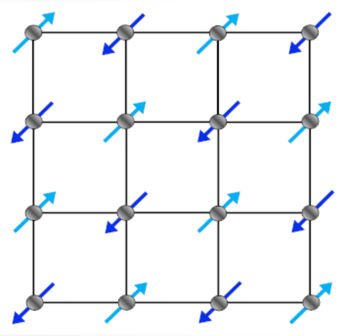


Neel AFM: k=(π,π)

0

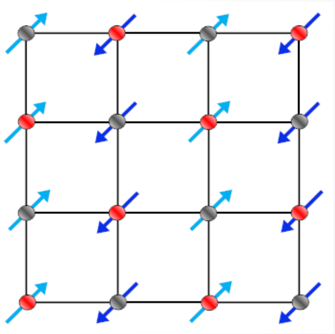
∞

$J_2/J_1<0.5$

$J_2/J_1>0.5$

J_2/J_1

Phase transition in quantum level



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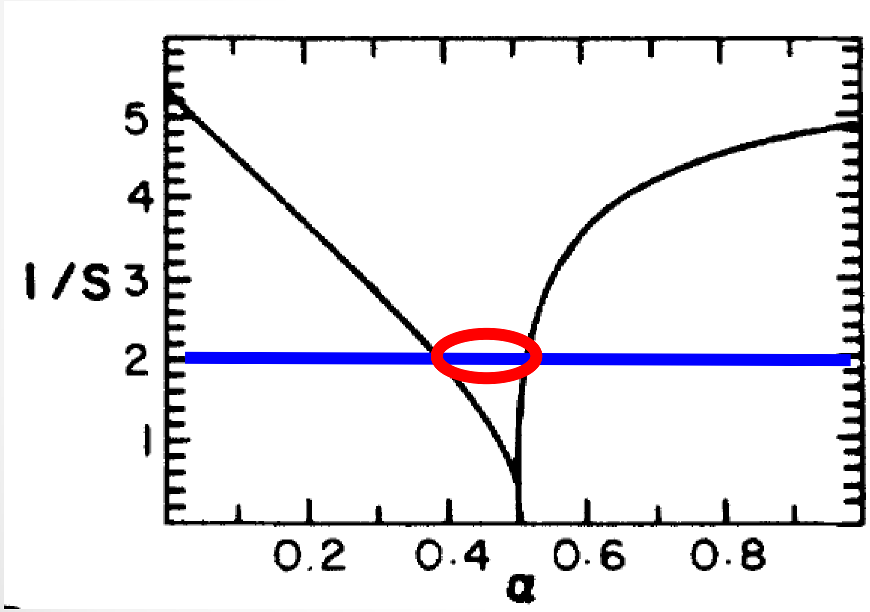
Earlier Studies of S=1/2 Square J1-J2 Model

Spin-wave calculation

- Likely Spin Liquid at [0.38, 0.51]

P. Chandra, and B. Doucot, PRB 1988



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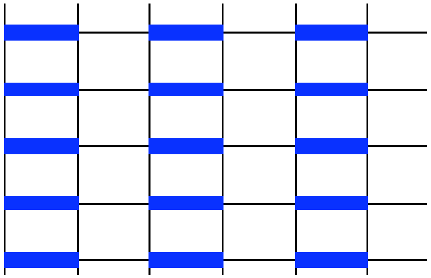
- ➢ Valence bond crystal (Dimer order)

N. Read, and S. Sachdev, PRL 1989

Series expansion

- ➢ Columnar Dimer order [0.34,0.61]

M. P. Gelfand, R. R. P. Singh, D. A. Huse, PRB 1989



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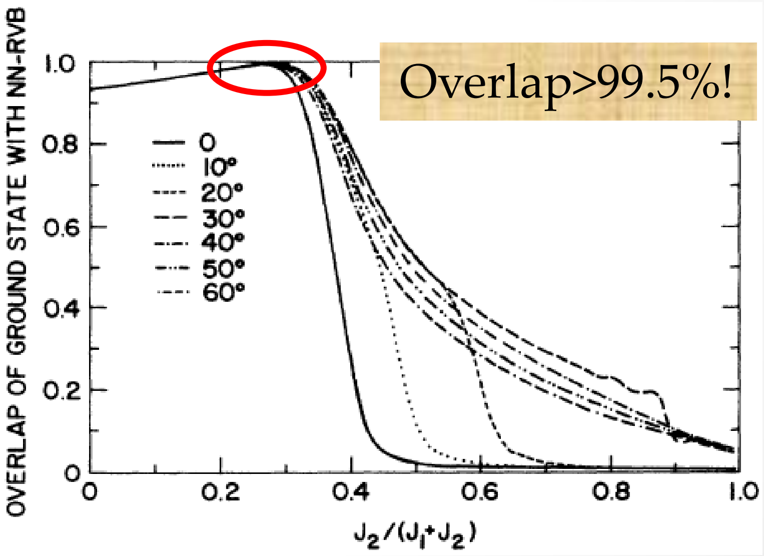
F. Figueirido, S. Kivelson, et al., PRB 1989



Overlap>99.5%!

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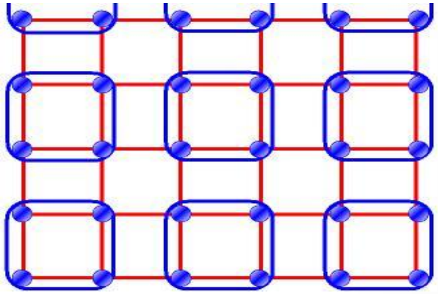

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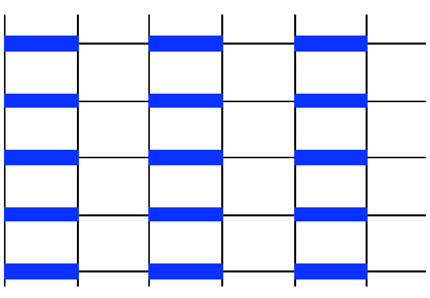

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ED on larger cluster N=20,32,36,40

- Gapped quantum paramagnetic phase

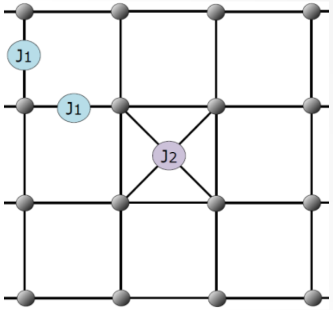
J. Richter, J. Schulenburg, PRB 2010

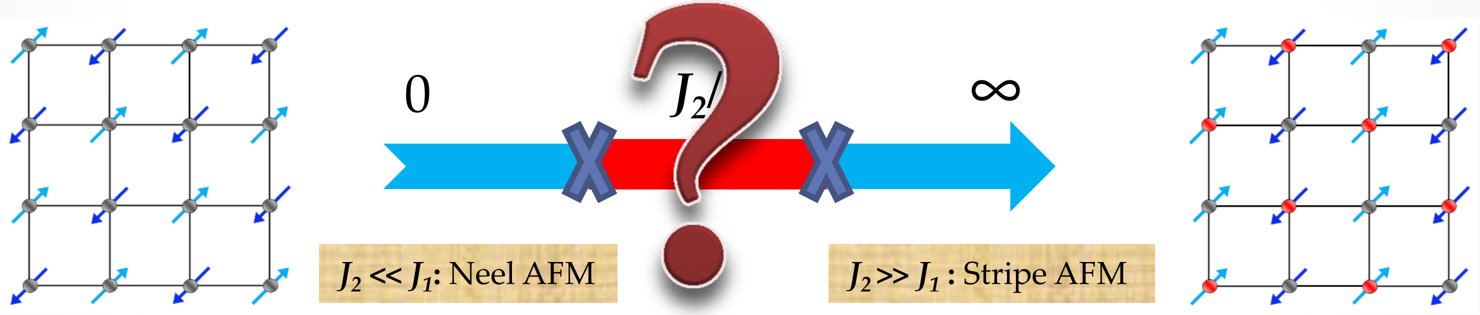
2D Quantum Spin Liquid State

- **S=1/2 Square AFM J_1-J_2 model:**

$$H = J_1 \sum_{<ij>} S_i \cdot S_j + J_2 \sum_{<<ij>>} S_i \cdot S_j$$

Relevance to Cuprate, Fe-based superconductor





$J_2 << J_1$: Neel AFM

$J_2 >> J_1$: Stripe AFM

Nature of the intermediate phase?

Spin liquid ground state (Spin-wave calculation, ED with N=4x4)

Dimer or plaquette order state (Large-N, Series expansion, PEPS, and so on)

P. Chandra, and B. Doucot, PRB 1988, F. Figueirido, S. Kivelson, et al., PRB 1989, N. Read, and S. Sachdev, PRL 1989

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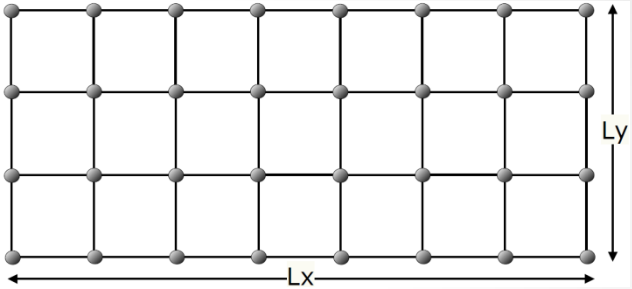
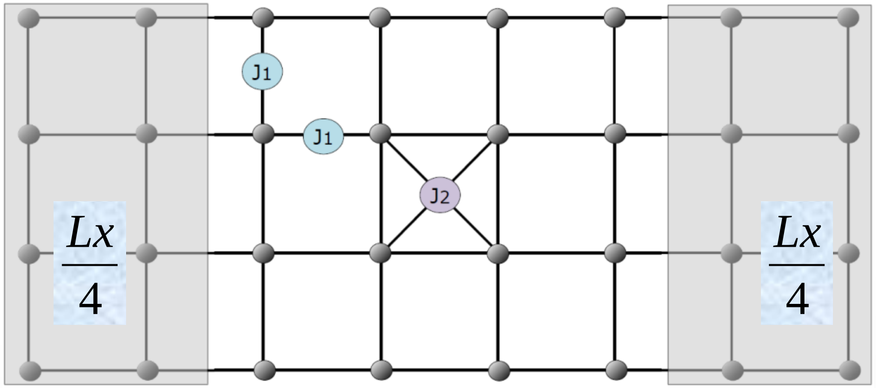


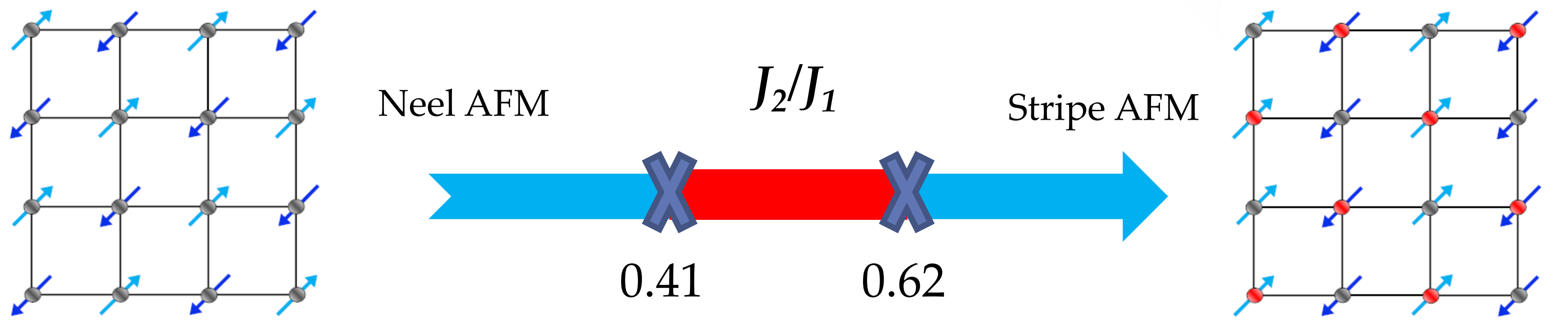
- Cylinder boundary condition, up to **Ly=14**
- **Fixed ratio Lx/Ly=2**, with minimum finite-size effect *White et al., PRL (2007)*
- Measurement restricted to central-half of the system

$\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$



$$\frac{L_x}{2} \times L_y = L_y \times L_y$$

DMRG Study of S=1/2 Square J1-J2 Model



Neel AFM

J_2/J_1

Stripe AFM

0.41

0.62

k=(pi,pi)

Non-magnetic phase

k=(0,pi)/(pi,0)

- Static structure factor

$$M_s(\mathbf{k}) = \frac{1}{L^2}\sum_{ij} e^{i\mathbf{k}\cdot(\mathbf{r}_i-\mathbf{r}_j)}\langle \mathbf{S}_i\cdot\mathbf{S}_j\rangle$$

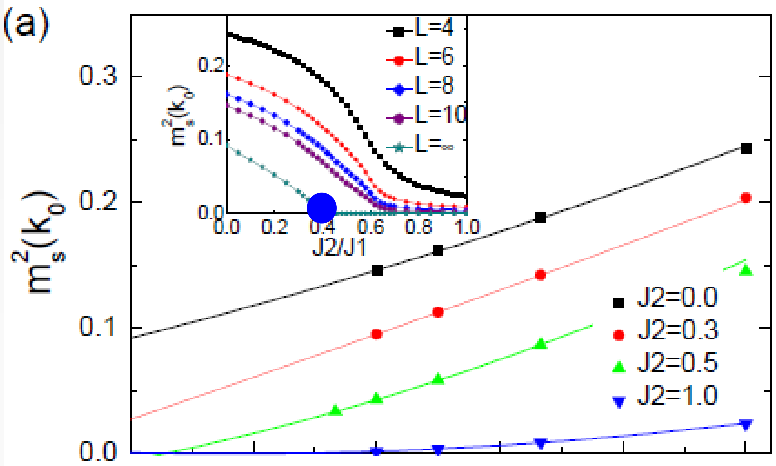
- Staggered magnetization

$$m_s^2(\mathbf{k}) = \frac{1}{L^2}M_s(\mathbf{k})$$

- Fitting function

$$\boxed{m_s^2(k,L) = m_s^2(k,\infty) + \frac{a}{L} + \frac{b}{L^2}}$$

Vanishing Magnetic Order Parameter



1/L

Neel AFM order

- Non-zero for J2<0.41
- At J2=0, $m_s(k_0,\infty)=0.304$
- Close to QMC result $m_s=0.307$

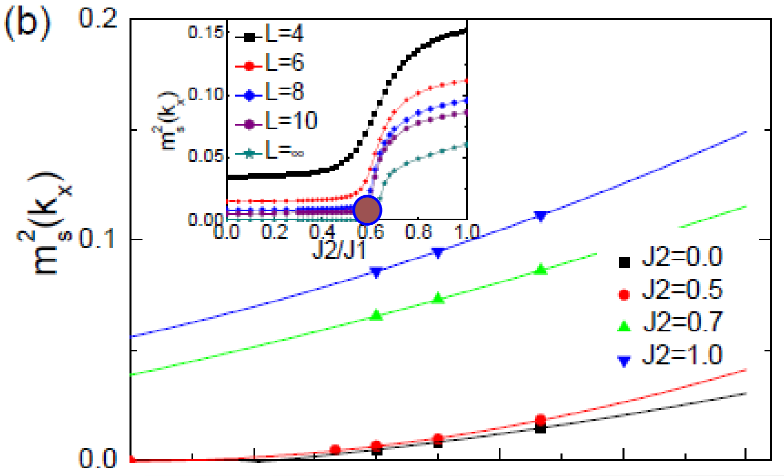
A. W. Sandvik, PRB, 1997

Stripe AFM order

- Non-zero for J2>0.62

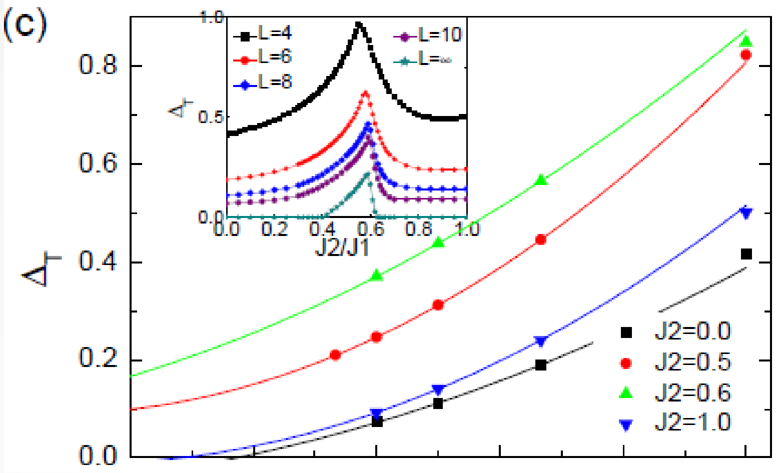
Intermediate phase at **0.41<J2<0.62**,

Both Neel and stripe AFM order vanish



1/L

Finite Spin Singlet and Triplet Gap



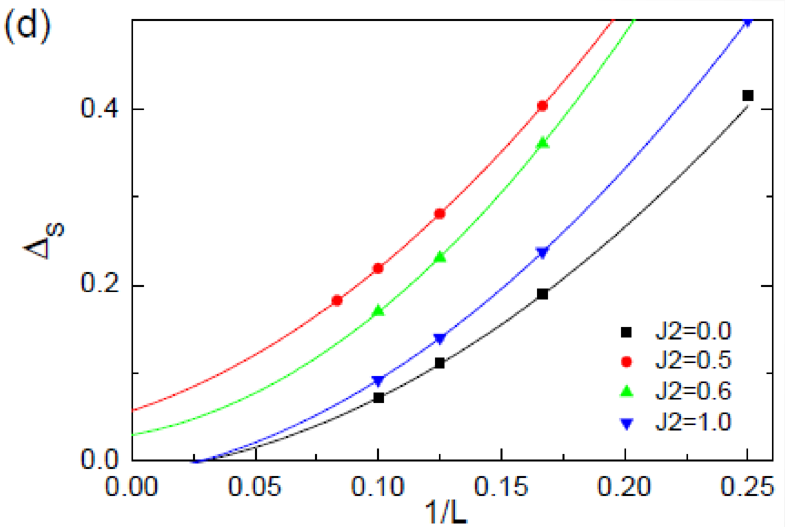
1/L

Spin triplet gap

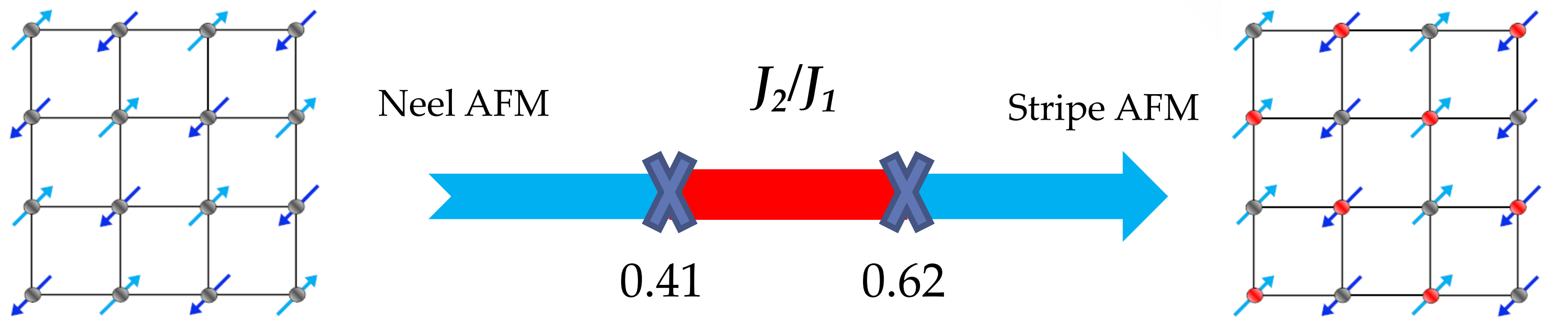
- Zero for magnetic order phase
- Non-zero in the intermediate phase
- At J2=0.5, $\Delta_T \approx 0.1$

Spin singlet gap

- Zero for magnetic ordered phase
- Non-zero in the intermediate phase
- At J2=0.5, $\Delta_S \approx 0.05$



Phase diagram of S=1/2 Square J1-J2 Model



Neel AFM

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k=(pi,pi)

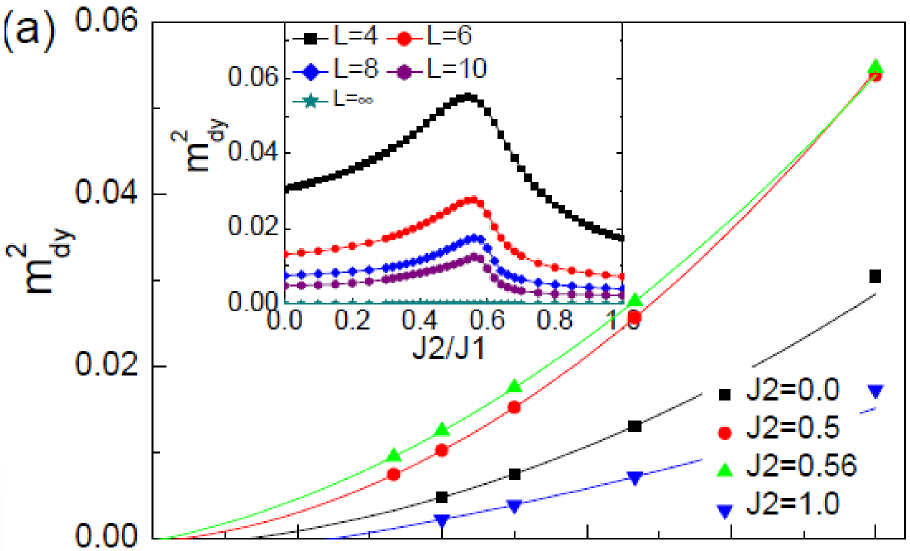
Non-magnetic phase

k=(0,pi)/(pi,0)

So how about the VBS order?

Vanishing Dimer VBS Order

- Dimer operator on bond(i, i+α) (α=x/y) $D_i^\alpha \equiv \mathbf{S}_i \cdot \mathbf{S}_{i+\alpha}$
- Dimer structure factor $M_d^{\alpha\beta}(\mathbf{k}) = \frac{1}{L^2}\sum_{ij} e^{i\mathbf{k}\cdot(\mathbf{r}_i-\mathbf{r}_j)}\left(\langle D_i^\alpha D_j^\beta\rangle - \langle D_i^\alpha\rangle\langle D_j^\beta\rangle\right)$
- Dimer order parameter $m_{d,a}^2 = \frac{1}{L^2} M_d^{aa}(\mathbf{k}_a)$



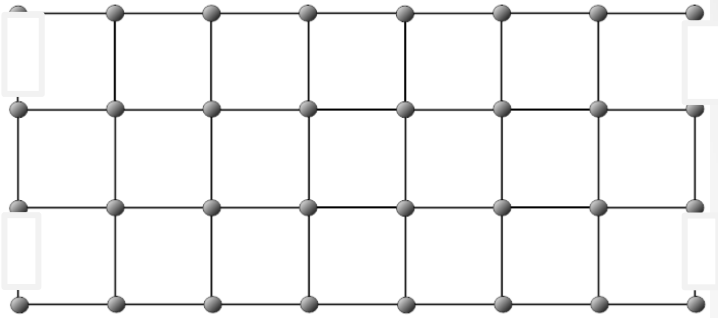
✓ Dimer order parameter vanishes in all $0<=J_2<=1$

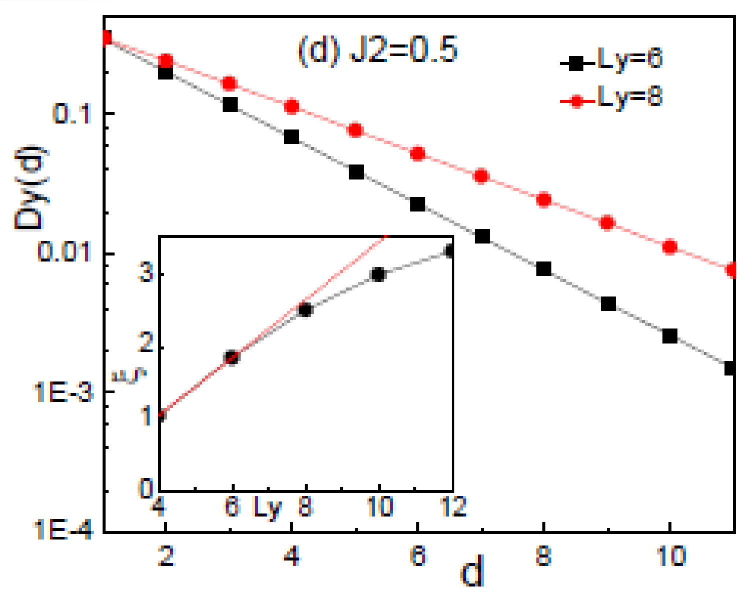
✓ Similarly, dimer order along x-direction also vanishes in the same region.

Pinning field does not induce dimer VBS order

- For Ly=even, e.g. Ly=4, 6, 8…

Pinning field at the boundary will not induce dimerization in the bulk





VBS correlation length ξ_{VBS} **increases slower than linearly in Ly**, and saturates to a small and finite value ξ_{VBS}**~4-5** in the Ly=∞, clearly **opposite** with the VBS ordered ground state, but consistent with the disordered spin liquid ground state

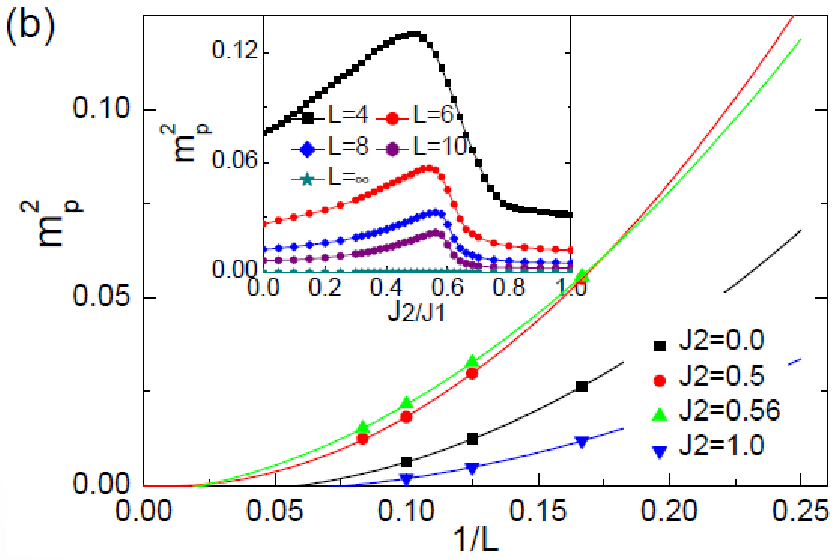
Vanishing Plaquette VBS Order

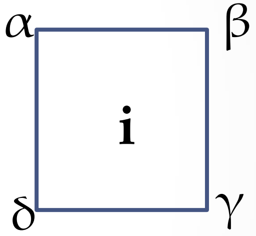
- Plaquette operator in plaquette i

$$
\begin{aligned}
P_i &= \frac{1}{2}(\Pi_i + \Pi_i^{-1}) = 2[(\mathbf{S}_\alpha \cdot \mathbf{S}_\beta)(\mathbf{S}_\gamma \cdot \mathbf{S}_\delta \\
&+ (\mathbf{S}_\alpha \cdot \mathbf{S}_\delta)(\mathbf{S}_\beta \cdot \mathbf{S}_\gamma) - (\mathbf{S}_\alpha \cdot \mathbf{S}_\gamma)(\mathbf{S}_\beta \cdot \mathbf{S}_\delta)] \\
&+ \frac{1}{2}[\mathbf{S}_\alpha \cdot \mathbf{S}_\beta + \mathbf{S}_\gamma \cdot \mathbf{S}_\delta + \mathbf{S}_\alpha \cdot \mathbf{S}_\delta \\
&+ \mathbf{S}_\beta \cdot \mathbf{S}_\gamma + \mathbf{S}_\alpha \cdot \mathbf{S}_\gamma + \mathbf{S}_\beta \cdot \mathbf{S}_\delta + \frac{1}{4}].
\end{aligned}
$$

- Plaquette structure factor

$$
M_p(\mathbf{k}) = \frac{1}{L^2} \sum_{ij} e^{i\mathbf{k}\cdot(\mathbf{r}_i - \mathbf{r}_j)} (\langle P_i P_j \rangle - \langle P_i \rangle \langle P_j \rangle)
$$

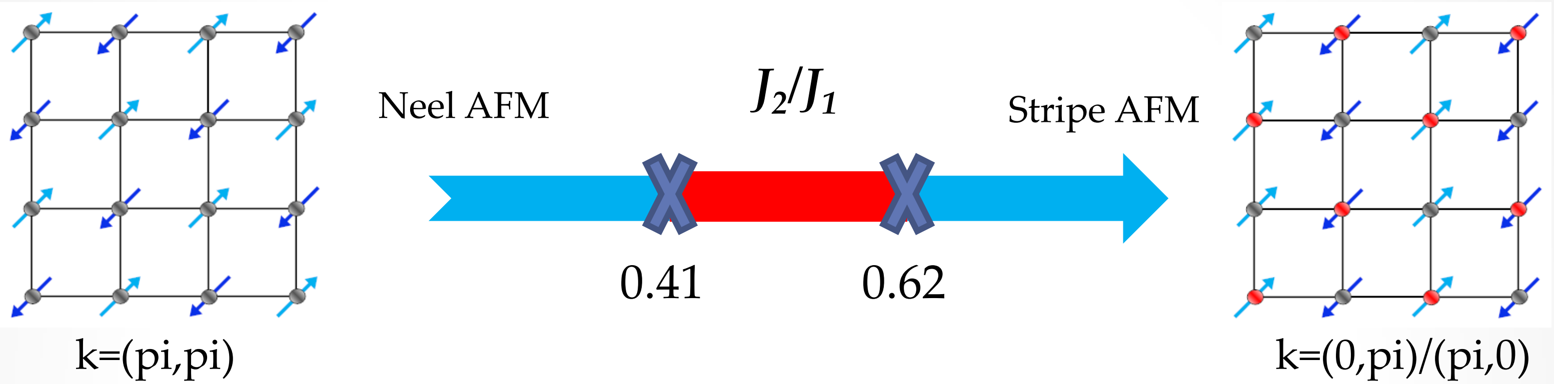




✓ Plaquette VBS order parameter vanishes in all 0<=J_2<=1,

➔ There is no plaquette VBS order in the intermediate phase

Phase diagram of Square J_1-J_2 Heisenberg Model



Intermediate phase

1) No magnetic order
2) Spin excitations are fully gapped
3) No dimer VBS order
4) No plaquette VBS order

➔Most likely: Topological quantum spin liquid

Outline

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- Previous study of S=1/2 AFM square J_1-J_2 model
- DMRG study of the S=1/2 AFM square J_1-J_2 model
    1) Vanishing of magnetic order
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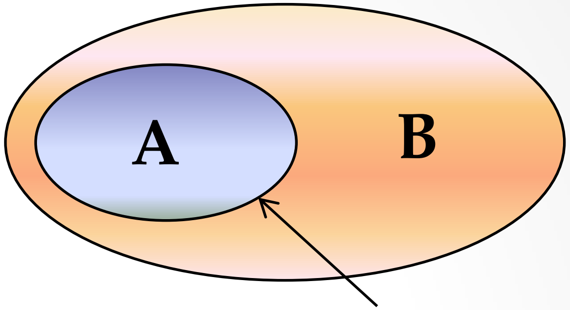
    3) Vanishing of Valence-Bond-Solid order
    4) Finite topological entanglement entropy
    5) Phase diagram
- Further evidences for spin liquid and comments
- Summary and conclusion

Entanglement Entropy: Area Law and Correction

Von Neumann Entanglement Entropy

$$S_1(\rho_A) = -\mathrm{Tr}(\rho_A \ln \rho_A)$$

$$\rho_A = \mathrm{Tr}_B |\psi\rangle\langle\psi|$$



Smooth boundary ***L***

- Gapped phase

$$S(A) = \underbrace{aL}_{\text{Boundary law term}} - \underbrace{\gamma}_{\text{Universal constant term, topological entanglement entropy}}$$

Kitaev and Preskill Phys. Rev. Lett. 96, 110404 (2006)

Levin and Wen, Phys. Rev. Lett. 96, 110405 (2006)

(1) For topological trivial phase, e.g., VBS ordered state, γ=0;

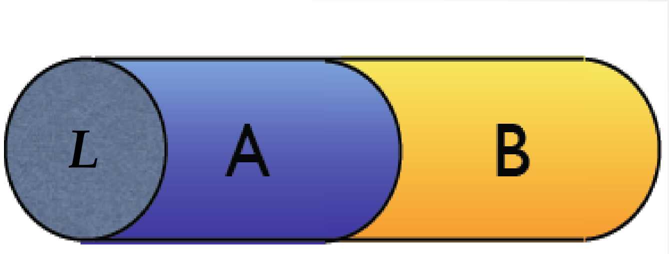
(2) For topological ordered phase, e.g., topological spin liquid state, γ=ln(D), with D the total quantum dimension.

Entanglement Entropy: Cylinder construction

Von Neumann Entanglement Entropy

$$S_1(\rho_A) = -\mathrm{Tr}(\rho_A \ln \rho_A)$$

$$\rho_A = \mathrm{Tr}_B|\psi\rangle\langle\psi|$$



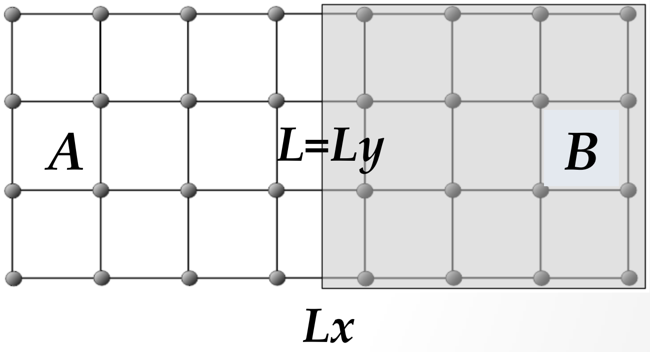
- Gapped phase

$$S(A) = aL - \gamma$$

In the long-cylinder limit (Lx=∞), **cylinder geometry with vertical cut** guarantees us to get the minimal entangled state, i.e., maximal topological entanglement entropy. Therefore,

(1) For topological ordered phase, $\gamma=\ln(D)$

(2) For topological trivial phase, $\gamma=0$

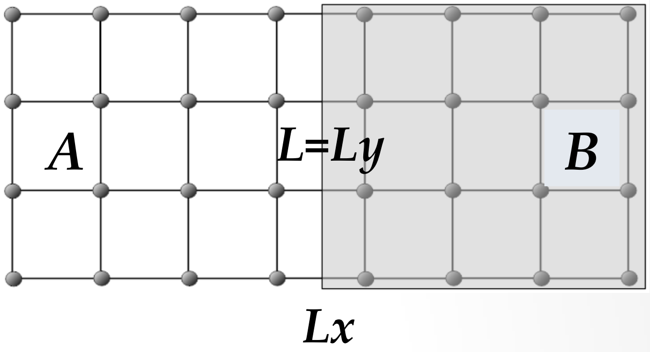


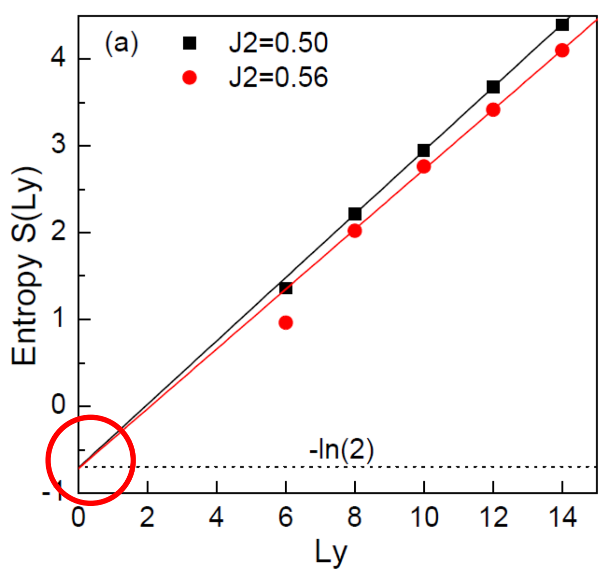
H. C. Jiang, Z. Wang, L. Balents, arXiv:1205.4289

Finite Topological Entanglement Entropy

Von Neumann Entanglement Entropy

$$S(Ly) = aLy - \gamma$$



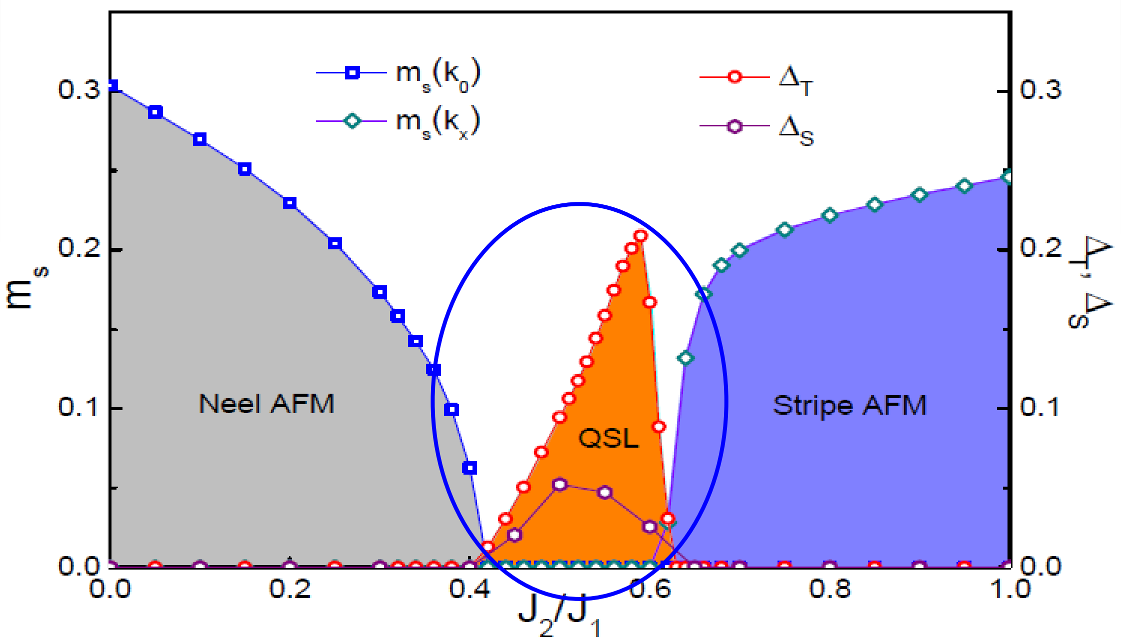


(1) J2=0.50, γ =0.70(2)

(2) J2=0.56, γ =0.72(4)

- For intermediate phase, **γ =0.70±0.02, very close to ln(2)=0.693**, showing that such a phase is a **topological quantum spin liquid**

Phase diagram of Square J_1-J_2 Heisenberg Model



Z_2 topological quantum spin liquid ground state at $0.41<J_2/J_1 < 0.62$

1) No magnetic order
2) Spin excitations are fully gapped
3) No dimer and plaquette VBS order
4) Finite topological entanglement entropy γ **=ln(2)**

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Questions raised by Sandvik in PRB **85**, 134407 (2012) (arXiv:1202.3118)
Could a weak VBS look like a SL on the modest size cylinder?
Addressed on J-Q_2 model

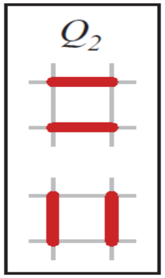
S=1/2 Square J-Q model

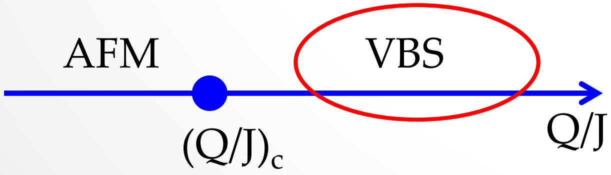
$$\boxed{H = H_J + H_{Q_n}}$$

$$H_J = -J \sum_{\langle i,j \rangle} C(i,j)$$

$$H_{Q_n} = -Q_n \sum_a \prod_{b=1}^{n} C(i[a,b], j[a,b])$$

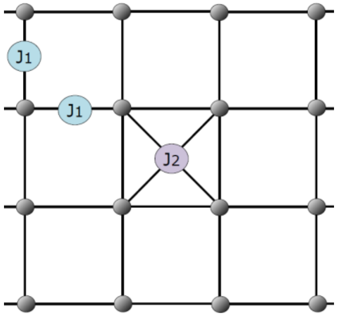
$$C(i,j) = \frac{1}{4} - \mathbf{S}_i \cdot \mathbf{S}_j$$

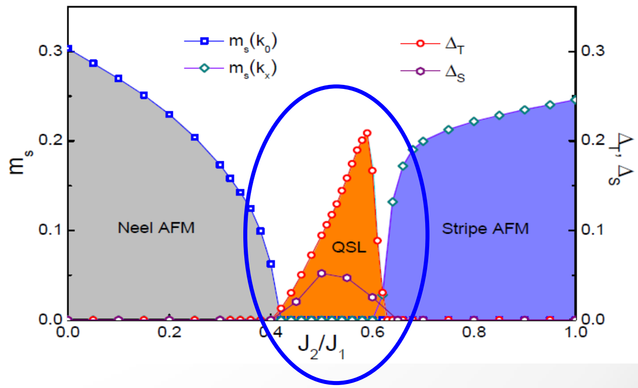




S=1/2 Square J_1-J_2 model

$$H = J_1 \sum_{<ij>} S_i \cdot S_j + J_2 \sum_{<<ij>>} S_i \cdot S_j$$



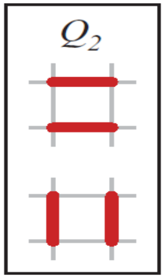


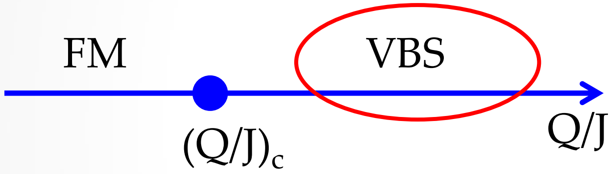
1. Difference of models

S=1/2 Square J-Q model

$$H = H_J + H_{Q_n}$$

$$H_{Q_n} = -Q_n \sum_{a} \prod_{b=1}^{n} C(i[a,b], j[a,b])$$

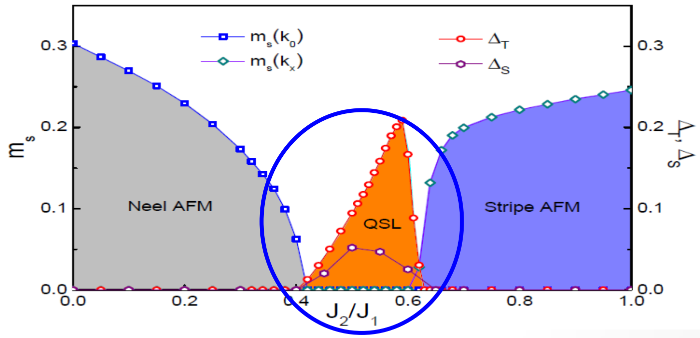




Multispin interactions involve interactions between dimers, and naturally favor VBS states. Mean-field calculation indeed give us VBS states for the Q model. Thus, it is natural and intuitive to expect a VBS phase in the J-Q model when Q term becomes important.

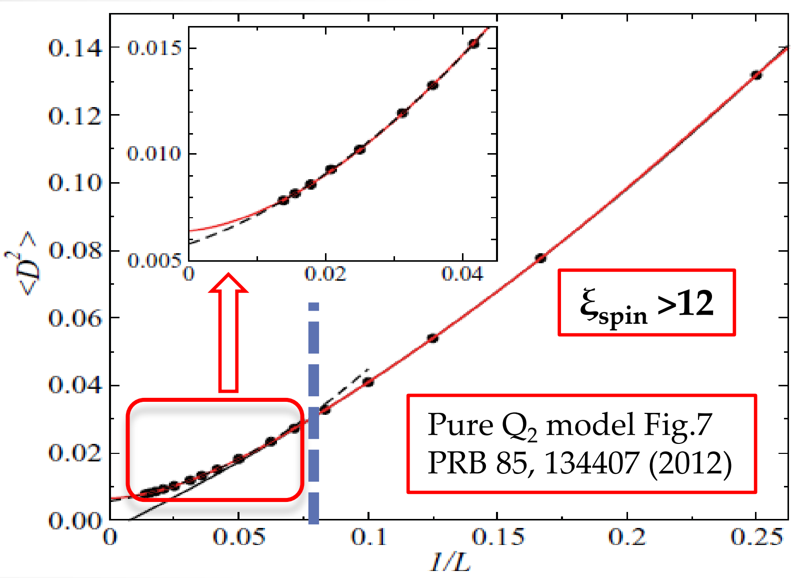
S=1/2 Square J_1-J_2 model

$$H = J_1 \sum_{<ij>} S_i \cdot S_j + J_2 \sum_{<<ij>>} S_i \cdot S_j$$



No multispin interactions, no interaction between dimers. Therefore, there is no a priori reason to expect VBS order in the Square J_1-J_2 model.

2. Finite-size scaling behavior of VBS order parameter



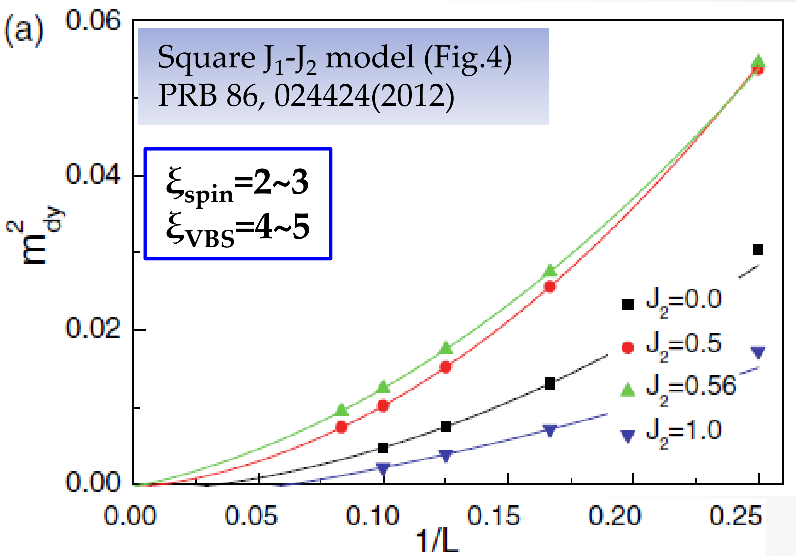
ξ_{spin} >12

Pure Q_2 model Fig.7
PRB 85, 134407 (2012)

(1) Spin correlation length is pretty big, i.e., ξ_{spin} **>12.** *(Melko, HFM 2012 Canada)*

(2) Conclusion only based on L=4-12 is not reliable, because $L<\xi_{spin}$. (Black line)

(3) Reliable finite-size scaling should at least have $L>\xi_{spin}$, i.e., ratio $L/\xi_{spin}>1$. (Red line, See inset)



Square J_1-J_2 model (Fig.4)
PRB 86, 024424(2012)

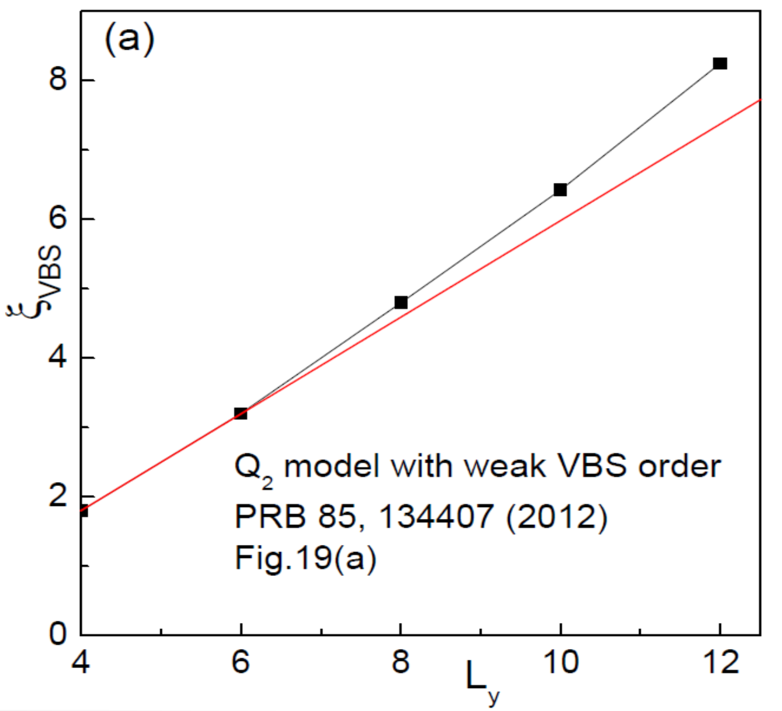
ξ_{spin}=2~3
ξ_{VBS}=4~5

(1) Spin correlation length is pretty small i.e., ξ_{spin} **=2~3**.

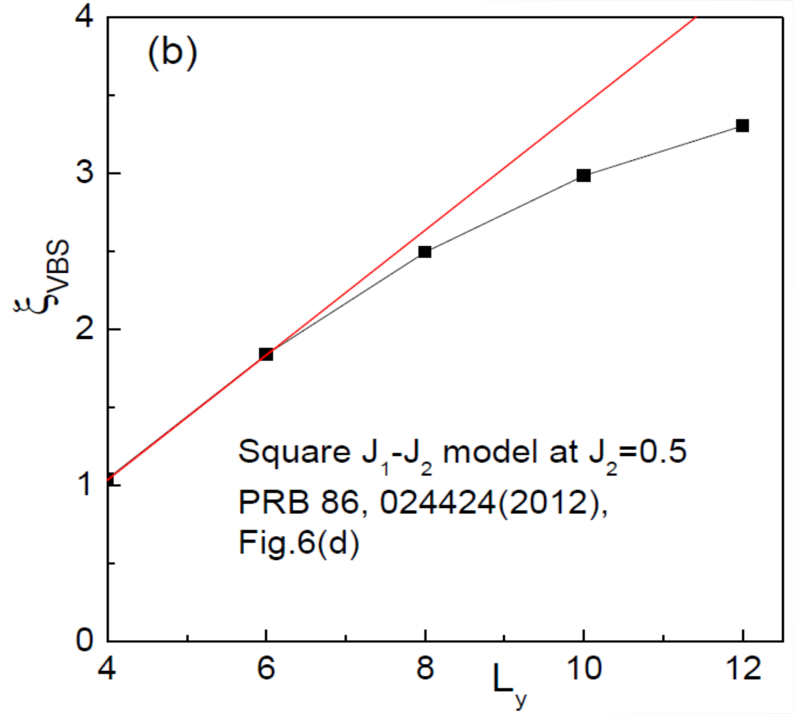
(2) VBS correlation length is also pretty small, i.e., ξ_{VBS} **=4~5**.

(3) Finite-size scaling with Ly=6-14 is reliable, showing no VBS order

3. Finite-size scaling behavior of VBS correlation length



VBS correlation length **ξ_{VBS} increases faster than linearly in Ly**, and diverses when Ly=∞, **consistent** with the VBS ordered ground state.



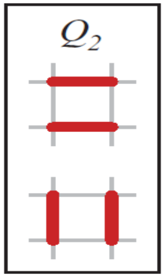
VBS correlation length **ξ_{VBS} increases slower than linearly in Ly**, and saturates to a small and finite value **ξ_{VBS}~4~5** when Ly=∞, consistent with the topological spin liquid ground state

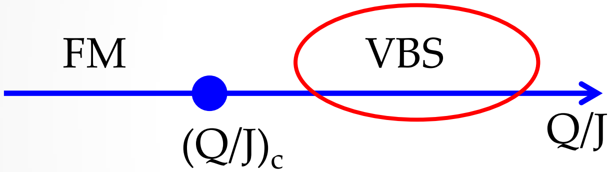
4. Topological entanglement entropy γ

S=1/2 Square J-Q model

$$\boxed{H = H_J + H_{Q_n}}$$

$$H_{Q_n} = -Q_n \sum_a \prod_{b=1}^{n} C(i[a,b], j[a,b])$$

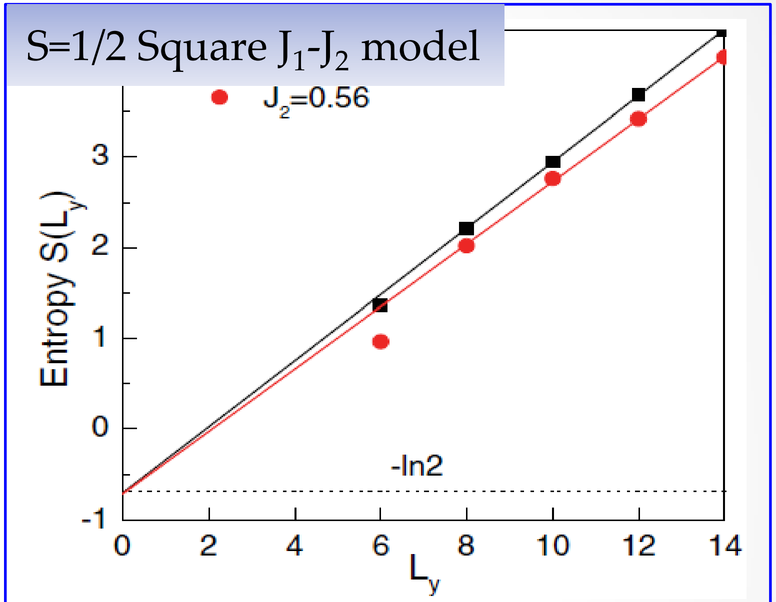




(1) Spin correlation length is pretty big, i.e., ξ_{spin} **>12**. *(Melko, HFM 2012,Canada)*

(2) Entanglement entropy S(Ly) using fitting function S(Ly)=a*Ly-γ, gives **γ=0** in the VBS phase. *(Melko HFM 2012 Canada)*

S=1/2 Square J_1-J_2 model



(1) Correlation length are pretty small, i.e., **ξ_{spin} =2~3, and ξ_{VBS} =4~5.**

(2) Entanglement entropy S(Ly) using fitting function S(Ly)=a*Ly-γ, gives **γ=0.70(2) for J_2=0.5**

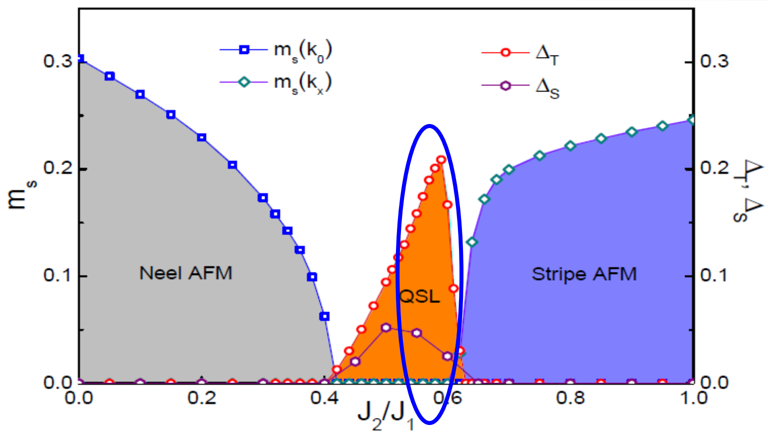
5. Other issues and Conclusions for Square J_1-J_2 model

1. There are some other issues, like “Even-Odd effects”, “Boundary effect” and phase transition are also dramatically different between the J-Q model, and the Square J_1-J_2 model. *Jiang, Yao, and Balents, PRB, 2012; Yao, and Kivelson, PRL 2012; Moon, and Xu, arXiv: 1204.5486*

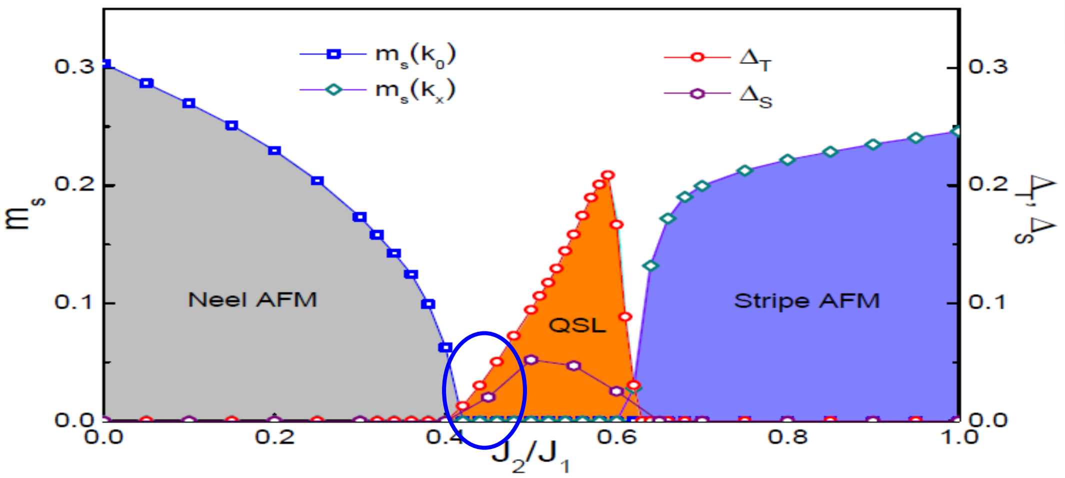
2. A parallel work based on tensor-network study, also comes to the similar conclusion with our DMRG study, and support the topological spin liquid state. *Wang, Gu, Verstraete, and Wen, arXiv:1112.3331*

Conclusion for the intermediate phase:

We have presented compelling evidence for a topological quantum spin liquid state of the 2D square J_1-J_2 model of the intermediate phase, but not a (even weak) VBS state.



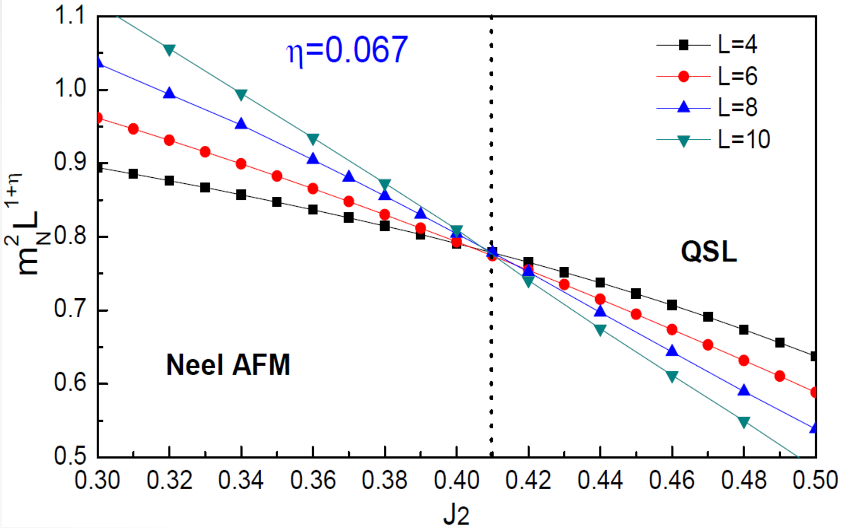
6. How about the region close to the phase boundary?



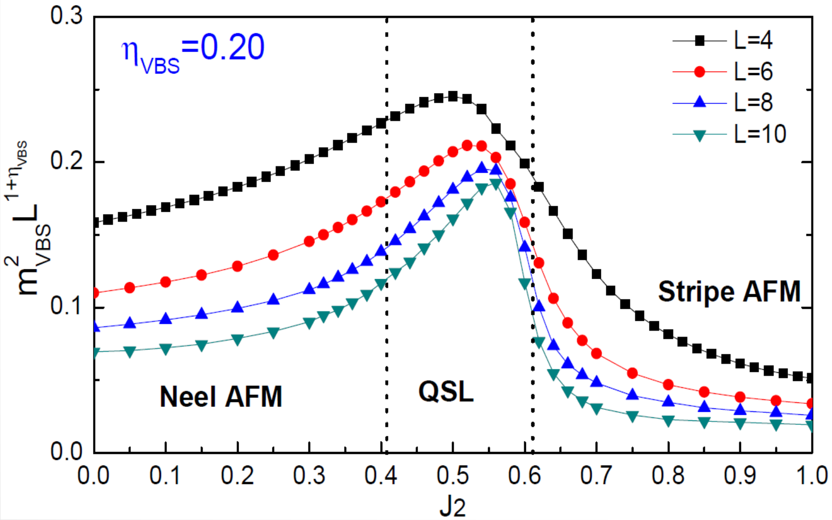
"How about the parameter region close to the Neel-to-QSL phase boundary? Is it possible to have a (weak) VBS order phase there?"

Question raised by Senthil

6. How about the region close to the phase boundary?

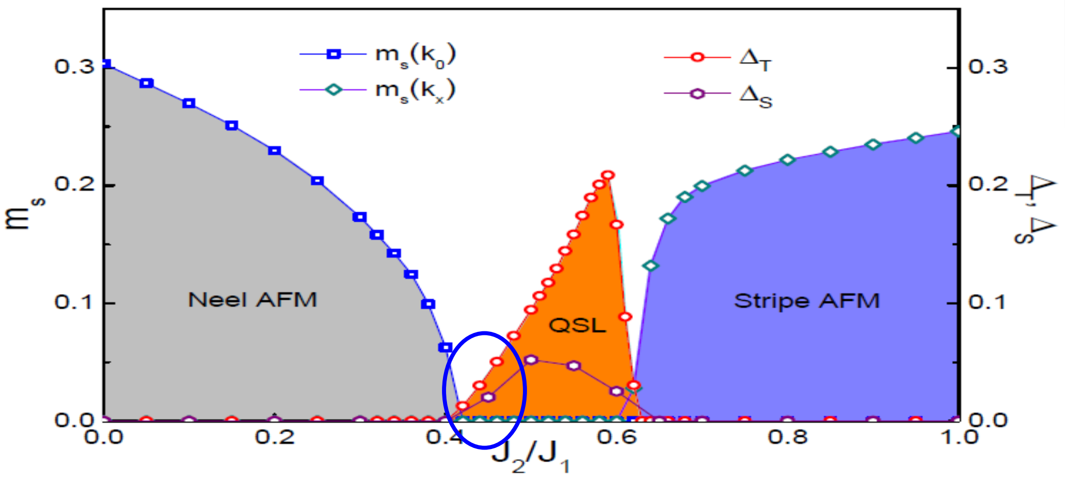


1. Neel order parameter square $m_N^2L^{1+\eta}$ crosses at J_2/J_1~0.41 point, with critical exponent **η~0.067**, much smaller than that of the J-Q model, which is **η=0.35**.



2. Dimer VBS parameter square $m_{VBS}^2L^{1+\eta_{VBS}}$ **does not** cross over the whole J2/J1 parameter region, if we take the critical exponent η_{VBS}=0.20(2) of the J-Q model

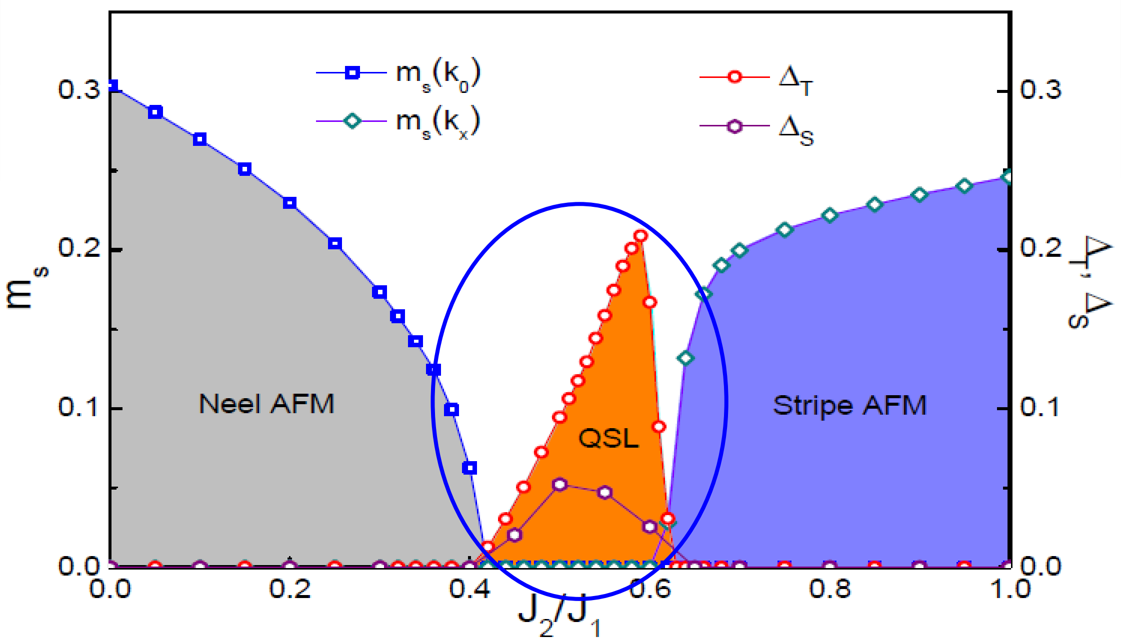
6. How about the region close to the phase boundary?



"How about the parameter region close to the Neel-to-QSL phase boundary? Is it possible to have a (weak) VBS order phase there?"

Answer is No, i.e., no such a region.

Summary and Conclusion



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