Phase diagram of Heisenberg Model on Honeycomb lattice with J_1-J_2 interaction

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Sep. 27, 2012, KITP, USCB

Outline

- **Possible valence bond crystal (VBC) and magnetic ordered state on Honeycomb lattice.**

- **DMRG study of this model**

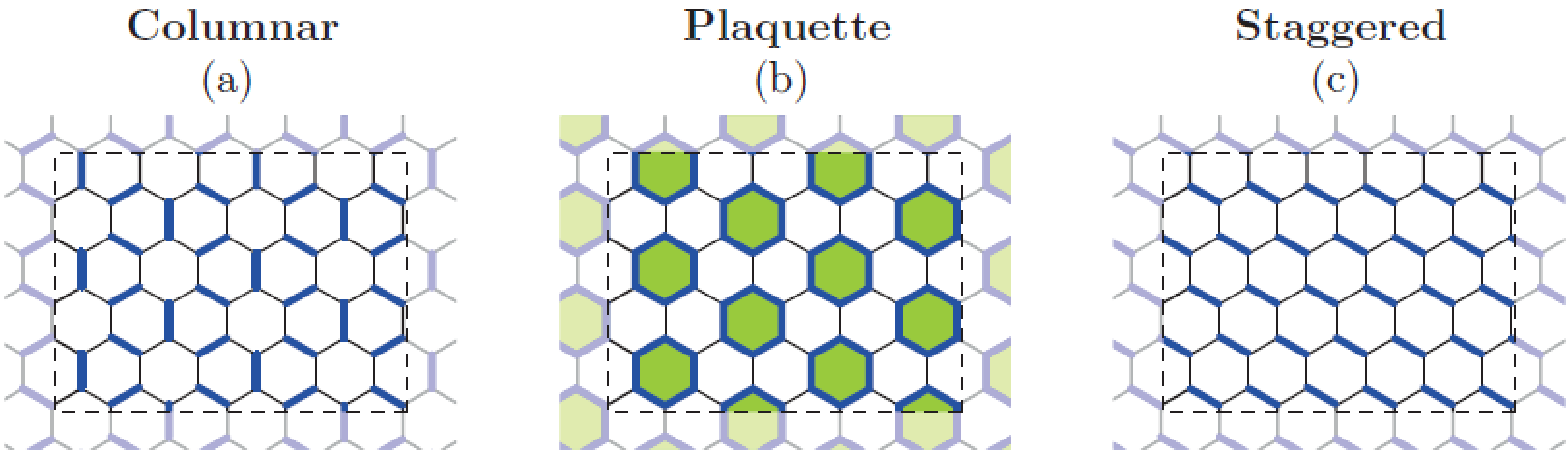
  (1) Pinning field to determine **Neel order** for $0<J_2<0.26$.

  (2) Use entanglement entropy to determine **staggered valence bond crystal (ladder phase)** for $J_2>0.36$.

  (3) Intermediate phase ($0.26<J_2<0.36$), **weak plaquette valence bond crystal (PVB)**, **instead of spin liquid**.

- **Conclusion**

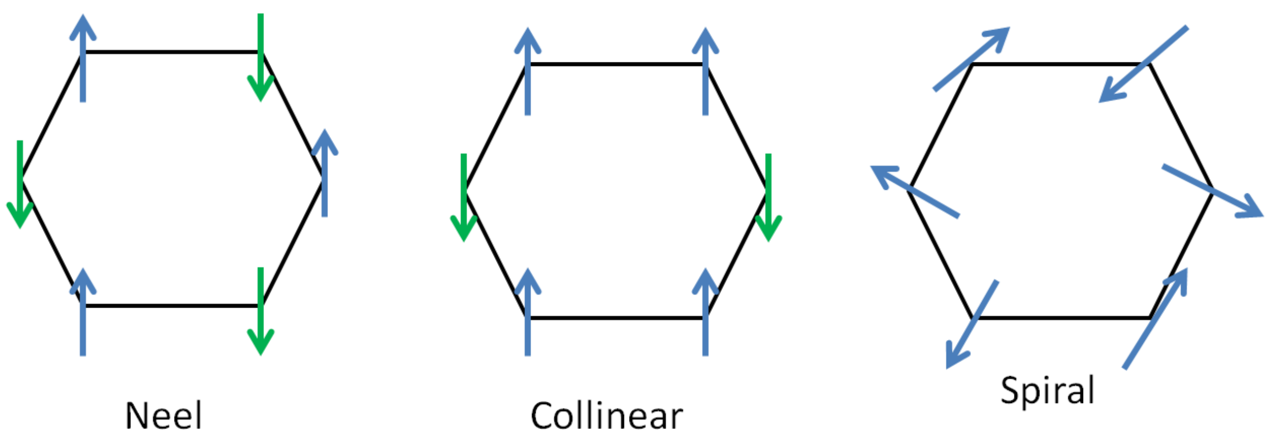
Three kinds of possible valence bond states on honeycomb lattice.



CVBC PVBC SVBC

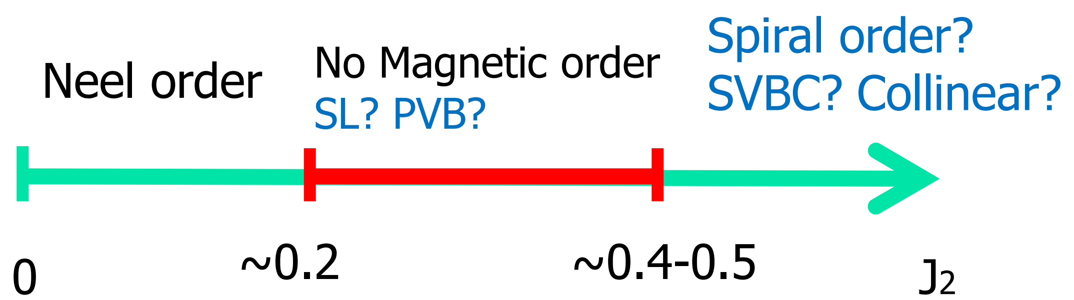
(A. F. Albuquerque, et al. PRB 2011)

Some possible magnetic ordered states on honeycomb lattice.



$$H = J_1 \sum_{<i,j>} S_i \cdot S_j + J_2 \sum_{<<i,j>>} S_i \cdot S_j$$

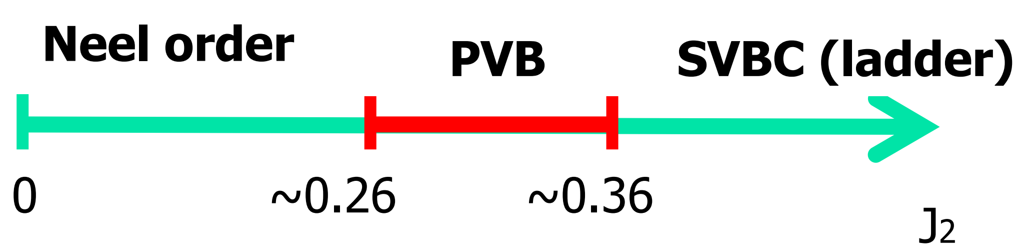
Previous studies



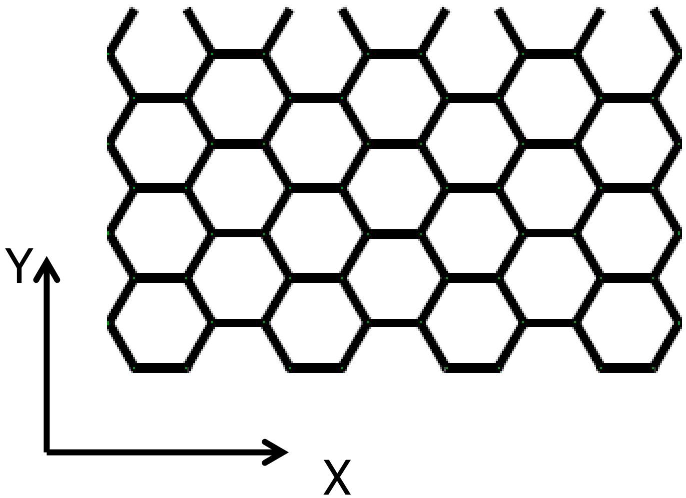
Spin liquid (SL) by VMC.
(B. K. Clark, *et al.* PRL 2011)
(F. Mezzacapo, *et al.* PRB 2012)

PVB order by exact diagonalization etc.
(H. Mosadeq, *et al*, JPC 2011)
(A. F. Albuquerque, et al. PRB 2011)
(P. H. Y. Li, *et al.* JPC 2012)

Our results

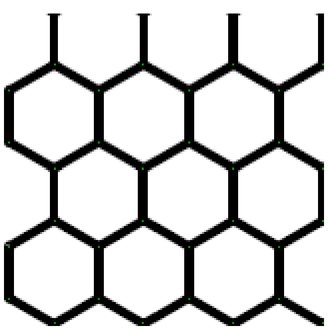


Cylinder geometries.



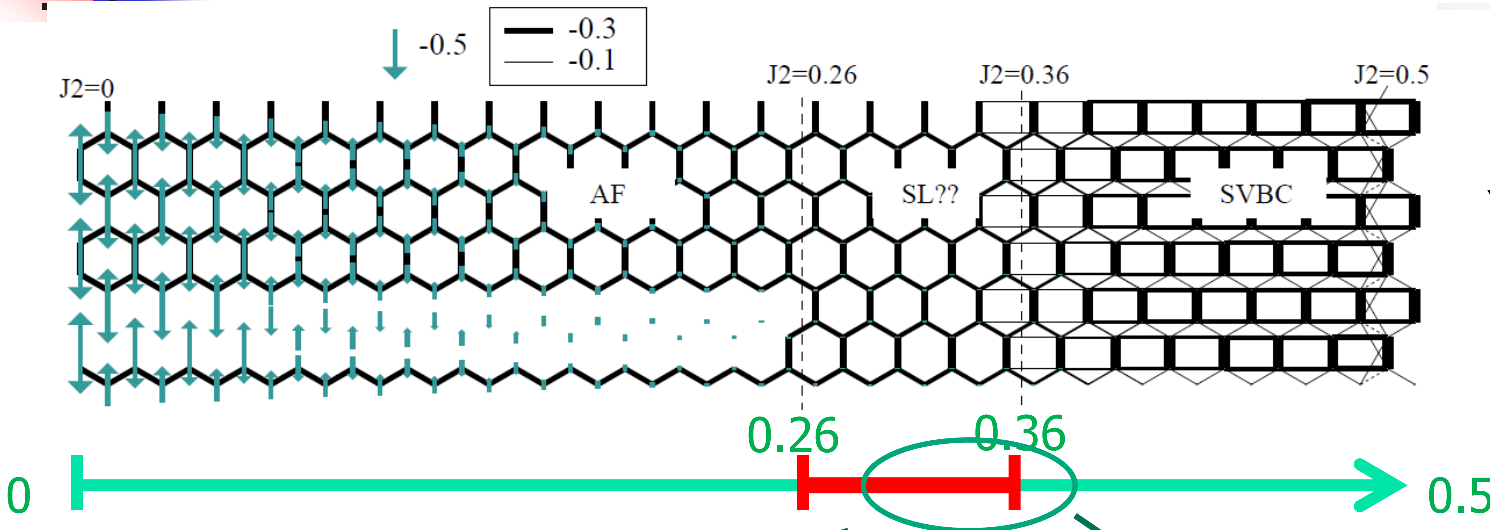
XC cylinder, XCM-N.
M is # of sites along the zigzag chain, eg XC8-0.
N is # of columns with a shifted periodic connection.

The reason for considering these geometries is because NOT every geometry can accommodate PVB order.



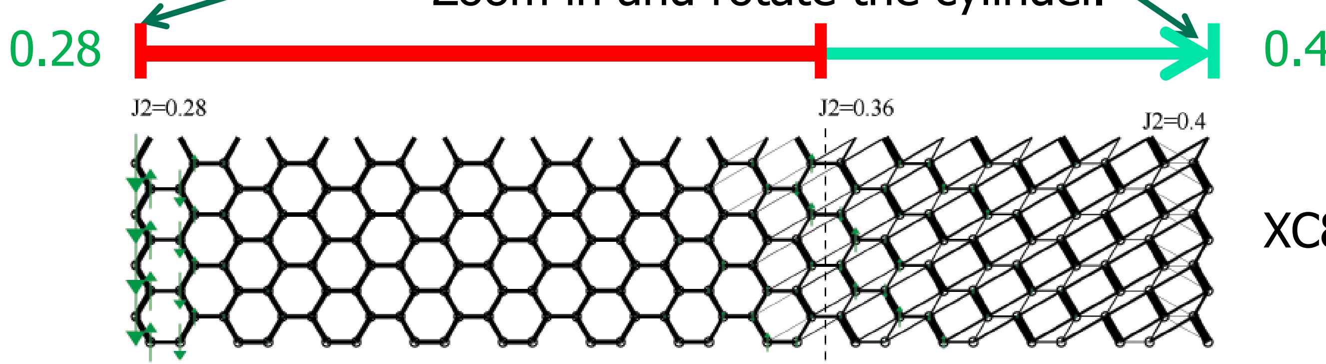
YC cylinder, YCM-N.
M is # of sites along the vertical direction, eg YC4-0.

Determine all the possible phases on honeycomb lattice YC6-0 and XC8-0 cylinder



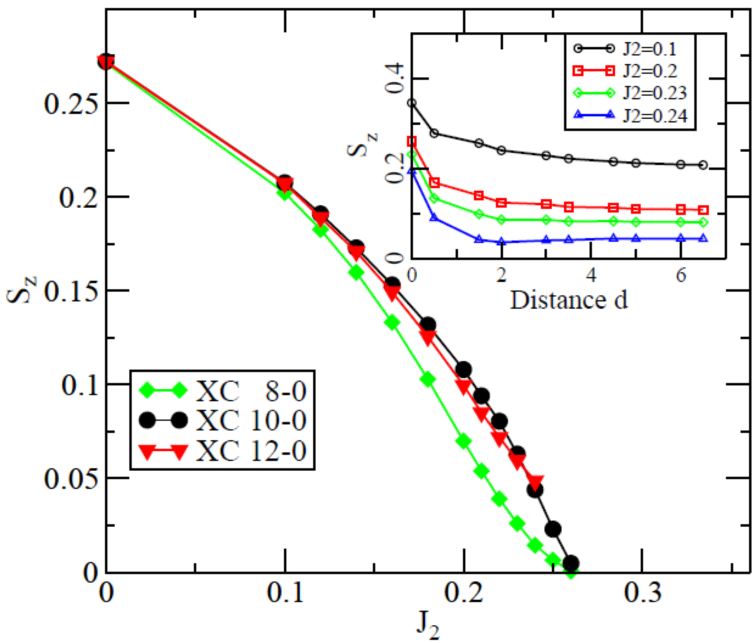
YC6-0

Zoom in and rotate the cylinder.

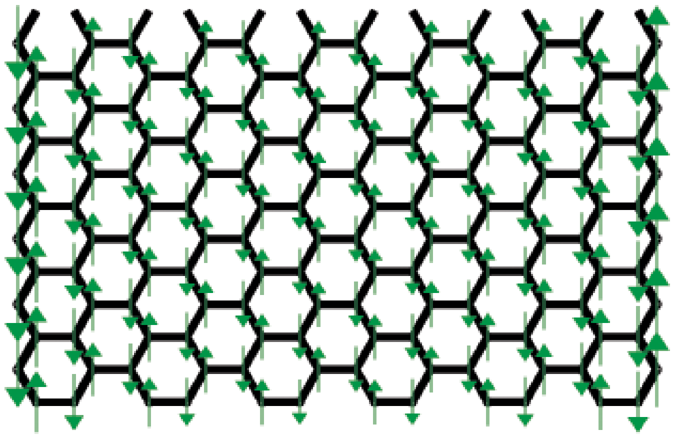


XC8-0

Determine magnetic order with pinning field on the ends.



(1) Apply pinning field on both ends to favor Neel order.
(2) Aspect ratio=1.73, close to 2 have smaller finite size effect.
(White and Chernyshev PRL, 2007)

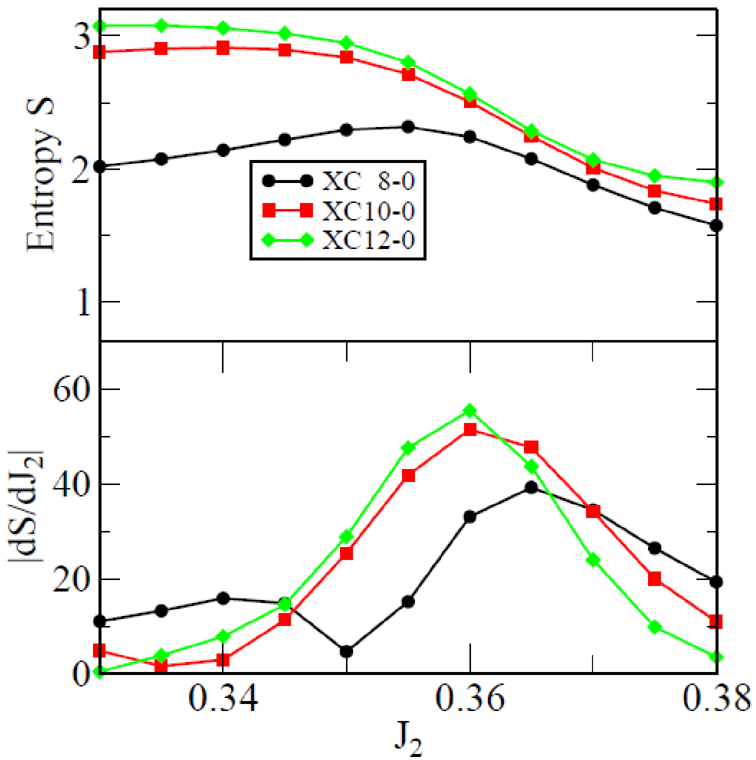


J2=0.1

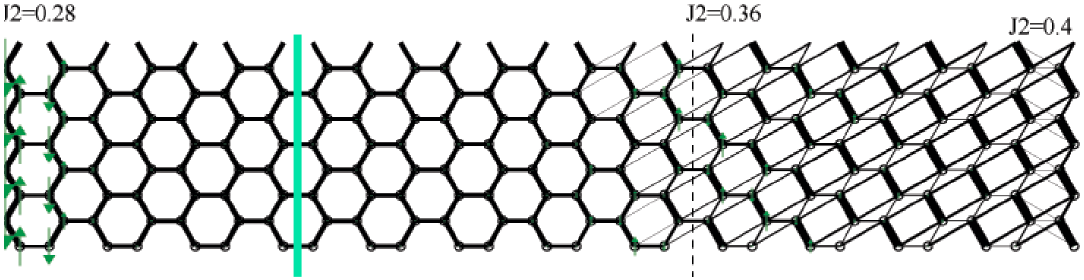
$J_2=0$, $<S_z>=0.272$. Magnetization close to series expansion 0.266(9) (J. Oitmaa, *et al.* PRB, 1992) and QMC value 0.2677 (E.V. Castro, *et al.* PRB, 2006).

Determine the SVBC phase transition point using entanglement entropy.

$$S_{von} = -Tr[\rho_A log \rho_A] = -\sum_i \rho_i log(\rho_i)$$



Measure the entanglement entropy of long cylinder with J2 variation, since each column has the same J2 value.



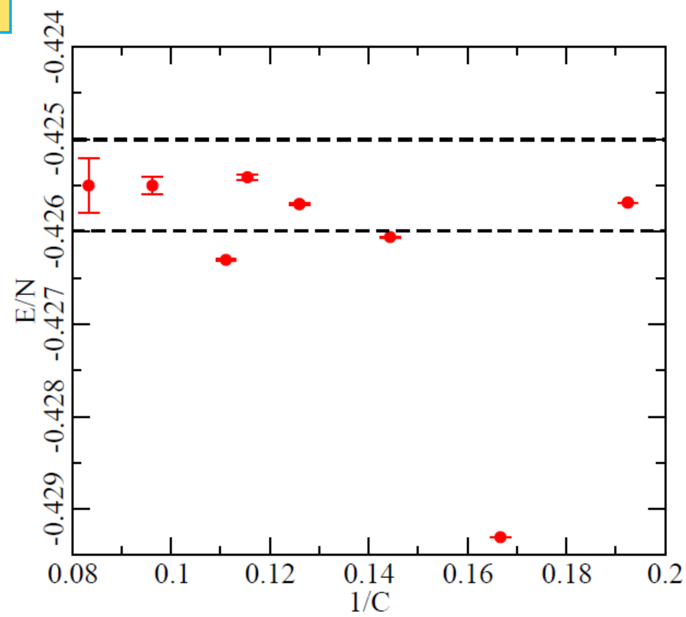
Use discontinuity in entanglement entropy or its derivative to determine the phase transition. (O. Legeza, *et al.* PRL, 2006)

$J_2>0.36$, J_1 bond form staggered VBC. J_2 bond gets stronger, connect them to form ladder phase.

Focus on the intermediate phase with J_2=0.3

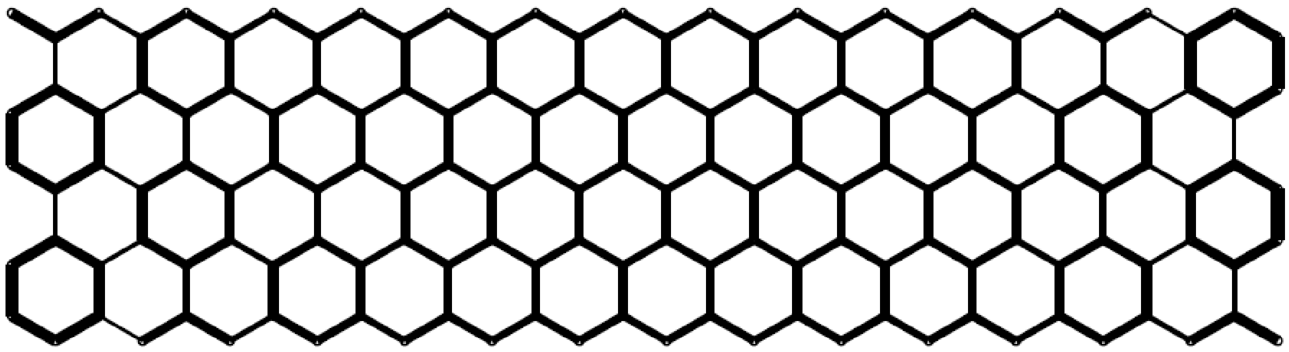
Ground state energy per site.

	c^2	E/N
XC6-0/YC3-3	27	-0.425684
YC4-0	36	-0.429305
XC8-0	48	-0.426057
XC9-1/YC5-3	63	-0.42570(1)
XC10-0	75	-0.42541(3)
YC6-0	81	-0.42630(1)
XC12-0	108	-0.4255(1)
YC7-3	117	-0.4255(2)
YC8-0	144	-0.4255(3)



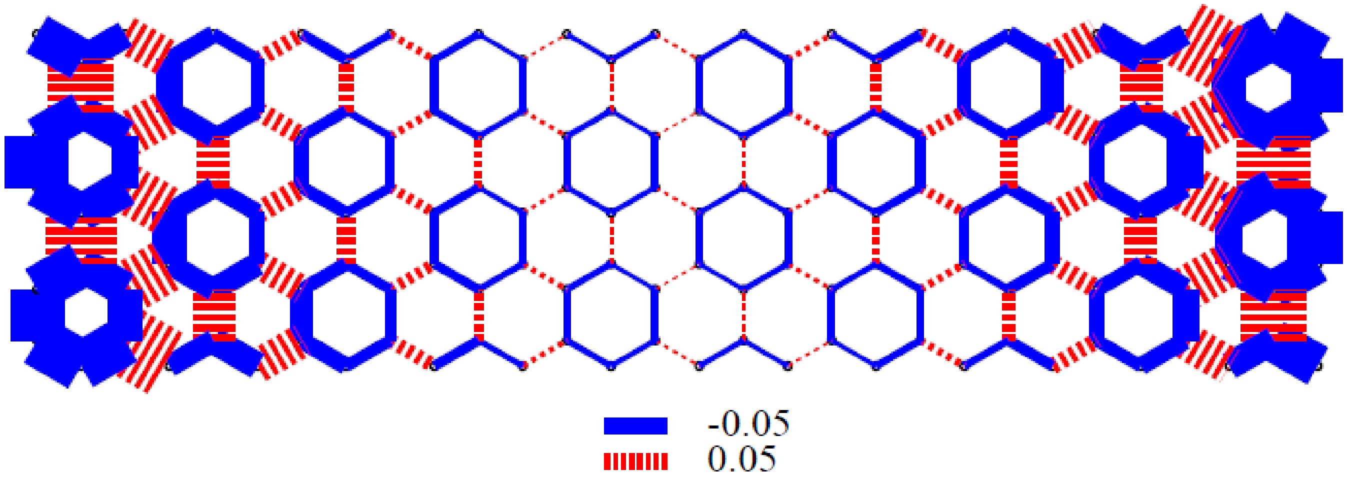
We estimate E=-0.4255(5).
Lower than VMC estimate
-0.4169, (B. K. Clark, *et al.* PRL 2011)
-0.4210, (F. Mezzacapo, *et al.* PRB 2012)

PVB versus SL on XC and YC cylinders for $J_2=0.3$



YC5-3

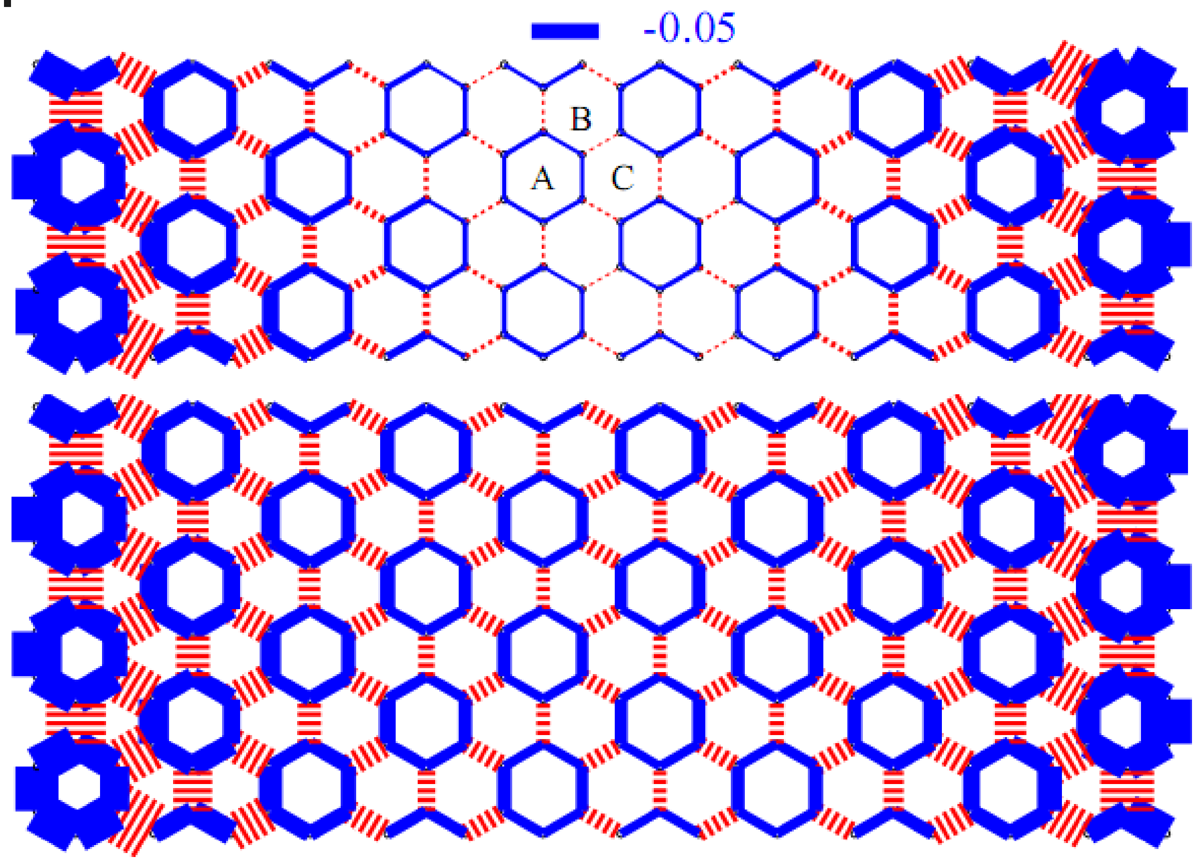
Before subtracting average, looks like SL.

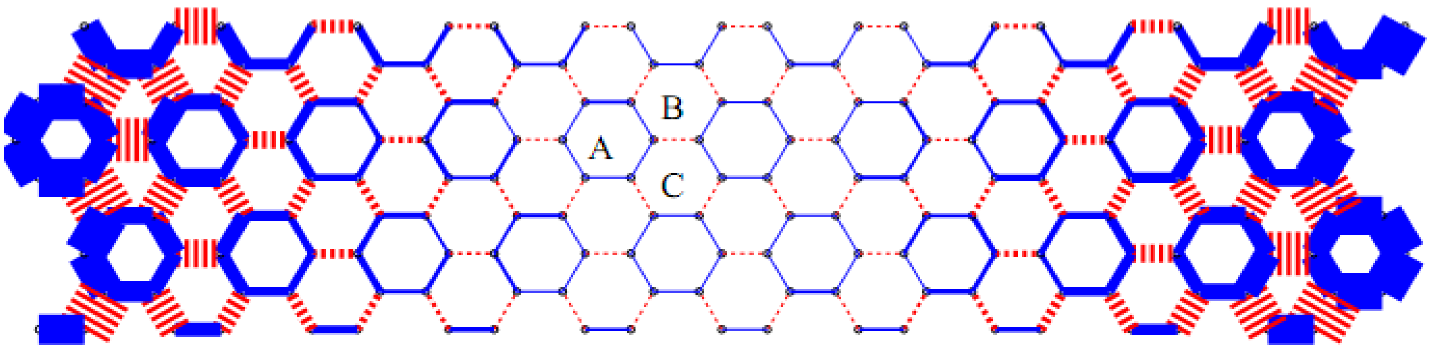


YC5-3

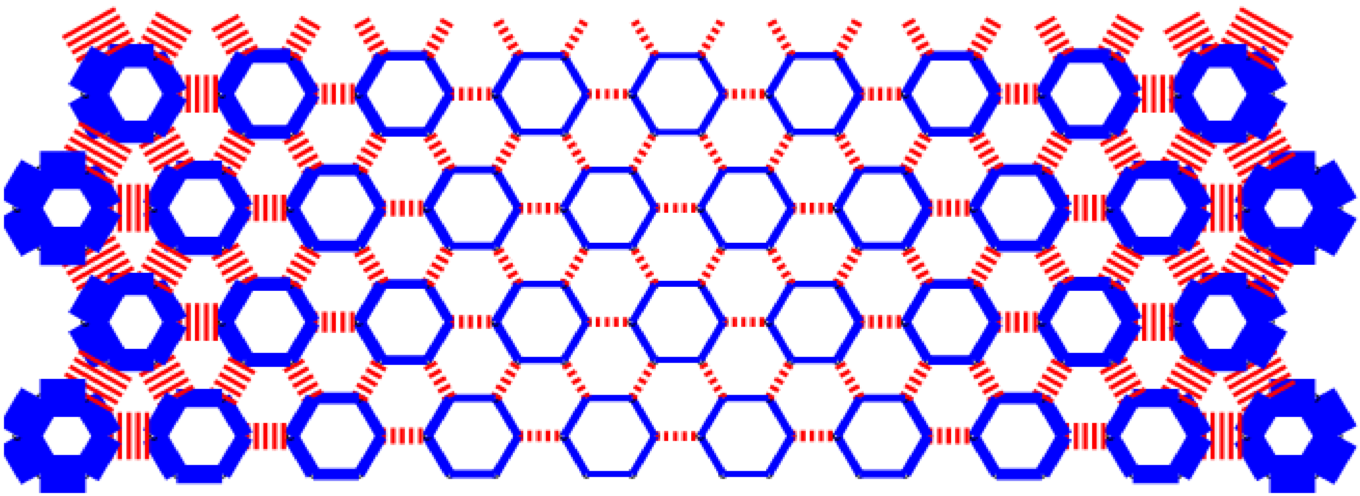
after subtracting average -0.32, PVB order appears. Not SL!

XC6-0, XC9-1, XC12-0 and YC5-3, YC7-3, YCN-0 cylinders can accommodate PVB order with proper length and edge.





XC9-1

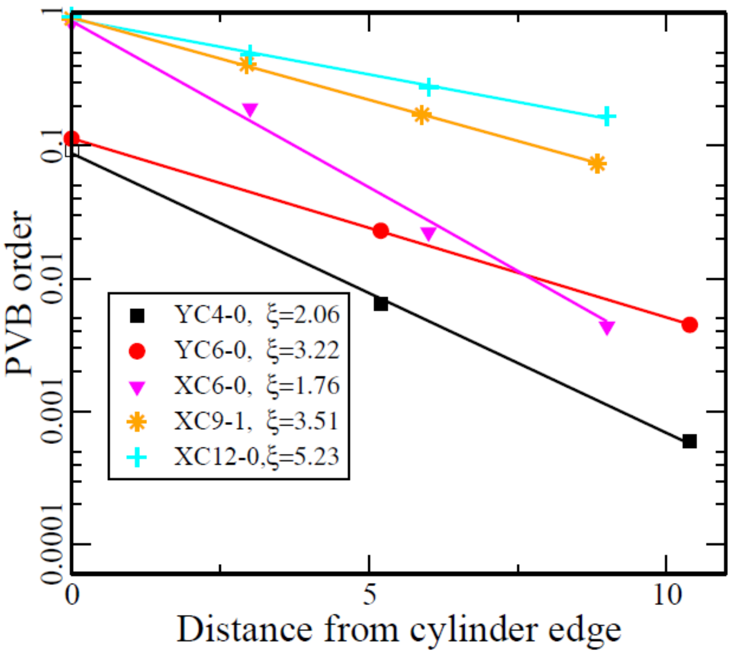


XC12-0

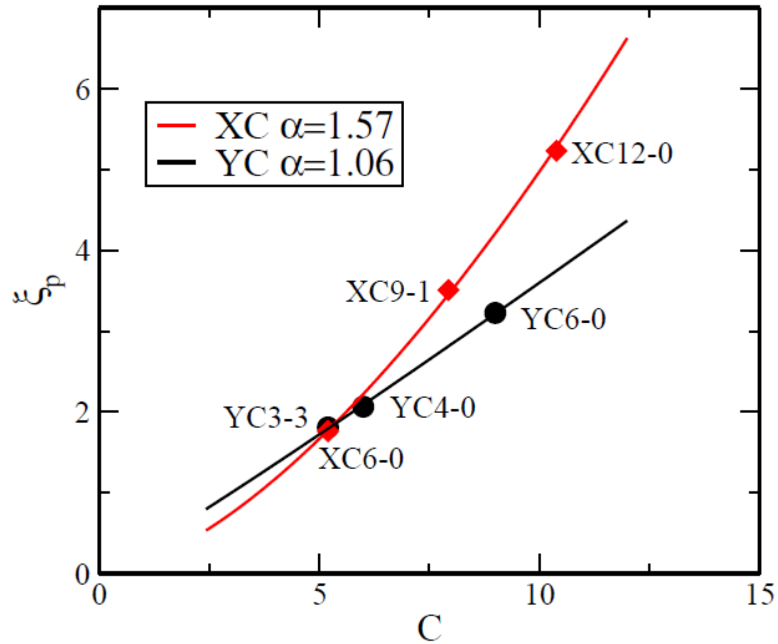
Wider cylinder has stronger PVB order than narrow ones.

Define PVB order $P_A = E_A + E_B \exp\left(\frac{2\pi}{3} i\right) + E_C \exp\left(\frac{4\pi}{3} i\right)$

E_A is the sum of six bonds around hexagon A. For SL phase, $P_A=0$.



Decay of PVB order from the cylinder
Edge to center.



PVB order correlation length versus
Cylinder width.

$$\xi_p \sim C^\alpha$$

Since α>1, it appears that PVB correlation length increase faster than the cylinder width. Indicate **long range PVB order** in the 2D limit.

Result holds for the entire intermediate phase.

Entropy analysis for J2=0.3 on various cylinders.

$S = aL + \cdots$ 2D gapped system (area law)

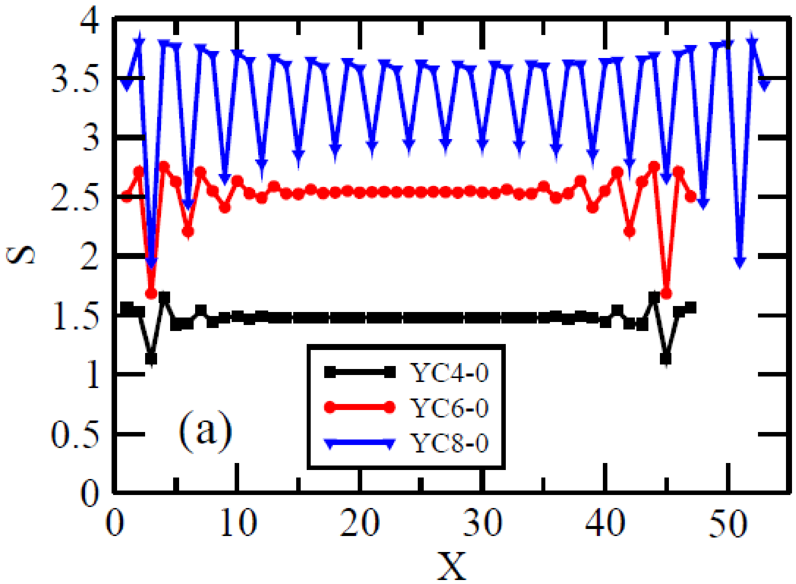
$S = aL - \gamma + \cdots$ 2D gapped system with topological order

$S = aL + b\ln L + c(L)\ln[\sin(\frac{\pi x}{L})] + \cdots$ 2D gapless system.

L is boundary length. X is subsystem size.

γ is topological entanglement entropy.

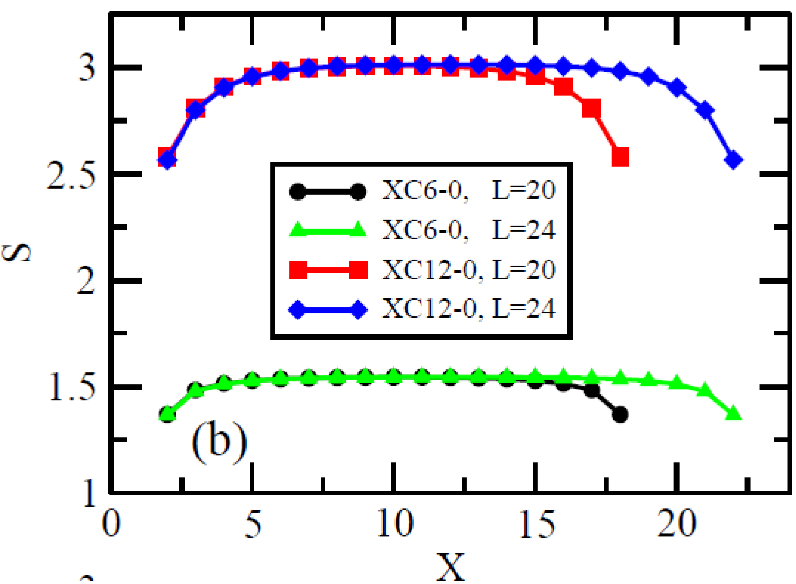
Entanglement entropy versus Subsystem size.



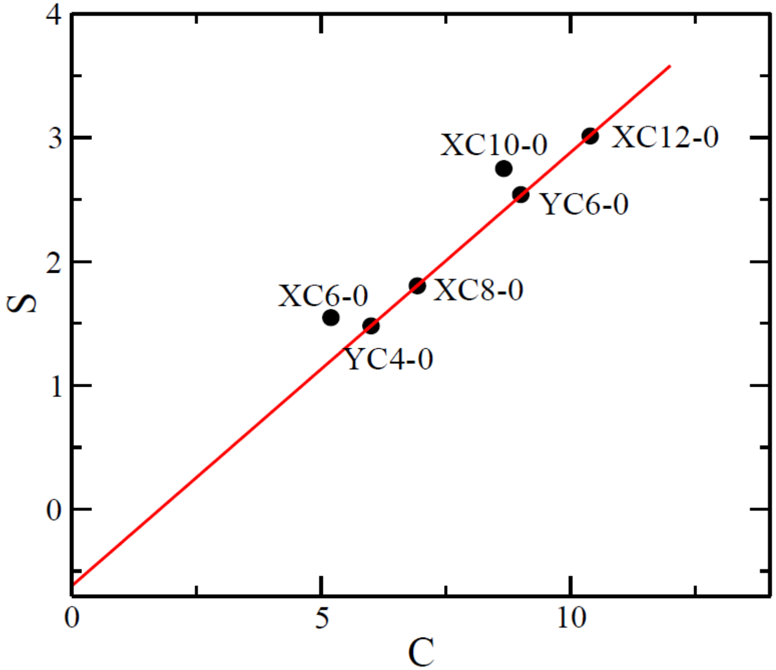
(1) Oscillation of entropy from cylinder edge indicate decay of PVB order.

(2) YC4-0 has shorted PVB correlation length than YC6-0 cylinder.

(3) YC8-0 has strong PVB order resulting in oscillations of entropy.

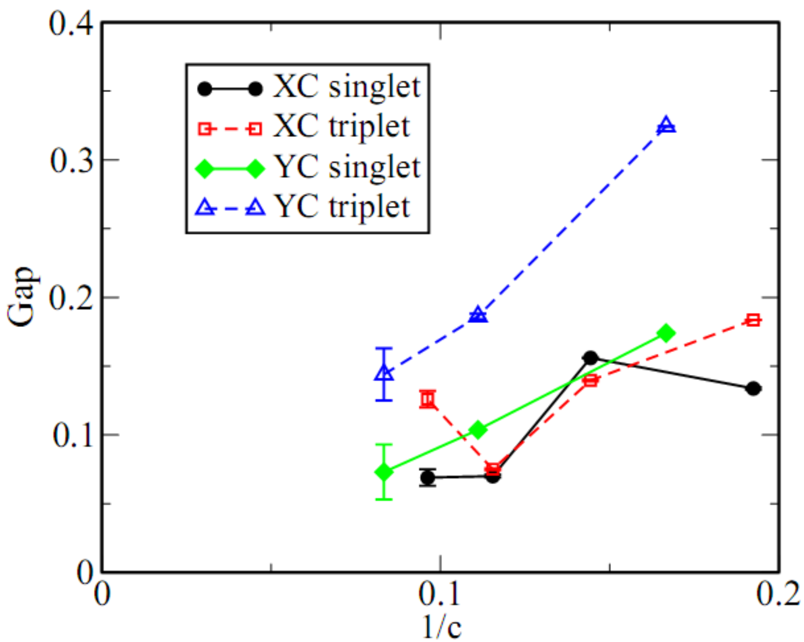


XC6-0 and XC12-0 entropy saturate independent of subsystem size x.



Extrapolate to get the entanglement entropy 0.619 close to ln(2)=0.693.

Since PVB correlation length is comparable to the cylinder width, it may NOT indicate TEE for a Z2 spin liquid.



Spin gaps for J_2=0.3

Estimate triplet gap in 2D limit is 0.11~0.12
Singlet gap is 0~0.07.

Conclusion

- For $0<J2<0.26$, AFM order.
- For $J2>0.36$, staggered valence bond crystal (SVBC).
- $0.26<J2<0.36$ has plaquette valence bond order (PVB).
- For intermediate phase has non-zero triplet gap.