



Cluster Operator Approach

An extension of spin wave theory

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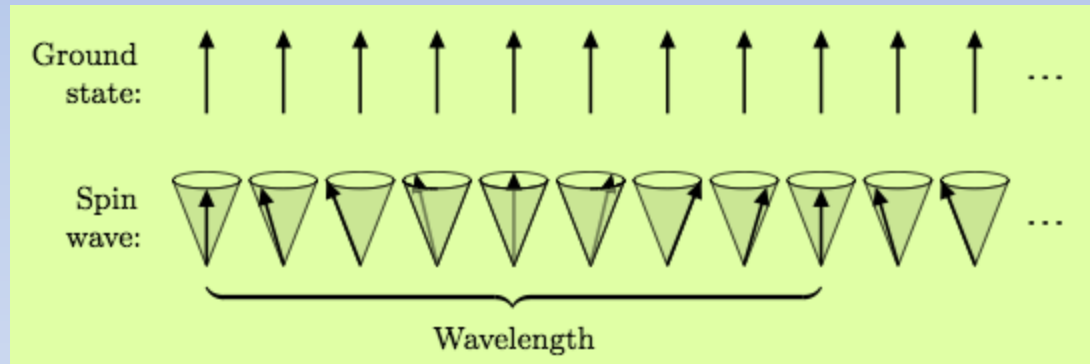
IPM school on spintronics and nanomagnetism
Nov. 2015

Spin wave theory

Ferromagnetic Heisenberg model on the spin-1/2 chain

$$\hat{H} = -J \sum_{\langle i,j \rangle} \hat{S}_i \cdot \hat{S}_j$$

$S \rightarrow \infty$



$$\hat{S}_i^\pm = S_i^x \pm iS_i^y$$

$$\hat{H} = -J \sum_i \hat{S}_i^z \hat{S}_{i+1}^z + \frac{1}{2} (\hat{S}_i^+ \hat{S}_{i+1}^- + \hat{S}_i^- \hat{S}_{i+1}^+)$$

Spin wave theory

Ferromagnetic Heisenberg model on the spin-1/2 chain

$$\hat{H} = -J \sum_{\langle i,j \rangle} \hat{S}_i \cdot \hat{S}_j$$

Holstein-Primakoff transformation:

$$\hat{S}_i^z = S - a_i^+ a_i$$

$$\hat{S}_i^+ = (2S - a_i^+ a_i)^{1/2} a_i$$

$$\hat{S}_i^- = a_i^+ (2S - a_i^+ a_i)^{1/2}$$

Linear SWT



$$\langle a_i^+ a_i \rangle \ll 2S$$

$$\hat{S}_i^z = S - a_i^+ a_i$$

$$\hat{S}_i^+ \cong (2S)^{1/2} a_i$$

$$\hat{S}_i^- \cong (2S)^{1/2} a_i^+$$

Spin wave theory

Ferromagnetic Heisenberg model on the spin-1/2 chain

$$\hat{H} = -J \sum_{\langle i,j \rangle} \hat{S}_i \cdot \hat{S}_j$$

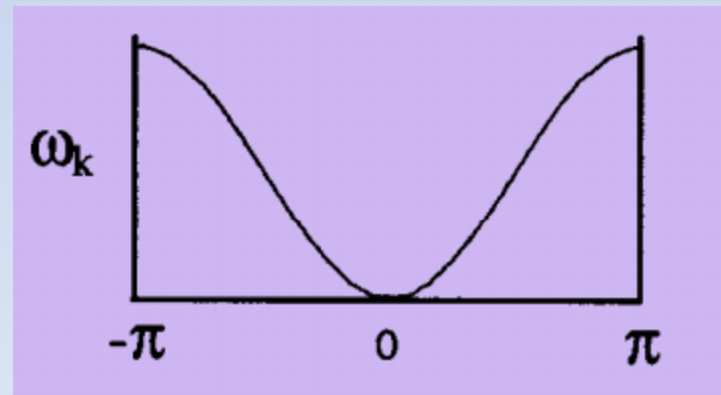
$$\hat{H}_{eff} = -JNS^2 + JS \sum_i (a_{i+1}^+ - a_i^+)(a_{i+1} - a_i)$$

Fourier Transformation: $a_i = \frac{1}{\sqrt{N}} \sum_k^{B.Z.} e^{-ik \cdot r_i} a_k$, $a_i^+ = \frac{1}{\sqrt{N}} \sum_k^{B.Z.} e^{ik \cdot r_i} a_k^+$

$$\hat{H}_{eff} = -JNS^2 + \sum_k^{B.Z.} \hbar \omega_k a_k^+ a_k$$

$$\hbar \omega_k = 2JS(1 - \cos k) = 4JS \sin^2(k/2)$$

$$k \rightarrow 0 \quad , \hbar \omega_k \rightarrow JSk^2$$



Multi-Spin flip excitations

Frustrated antiferromagnetic J_1 - J_2 Heisenberg model
on the Honeycomb lattice

$$H = J_1 \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \vec{S}_i \cdot \vec{S}_j$$

Classical $S \rightarrow \infty$ Limit :

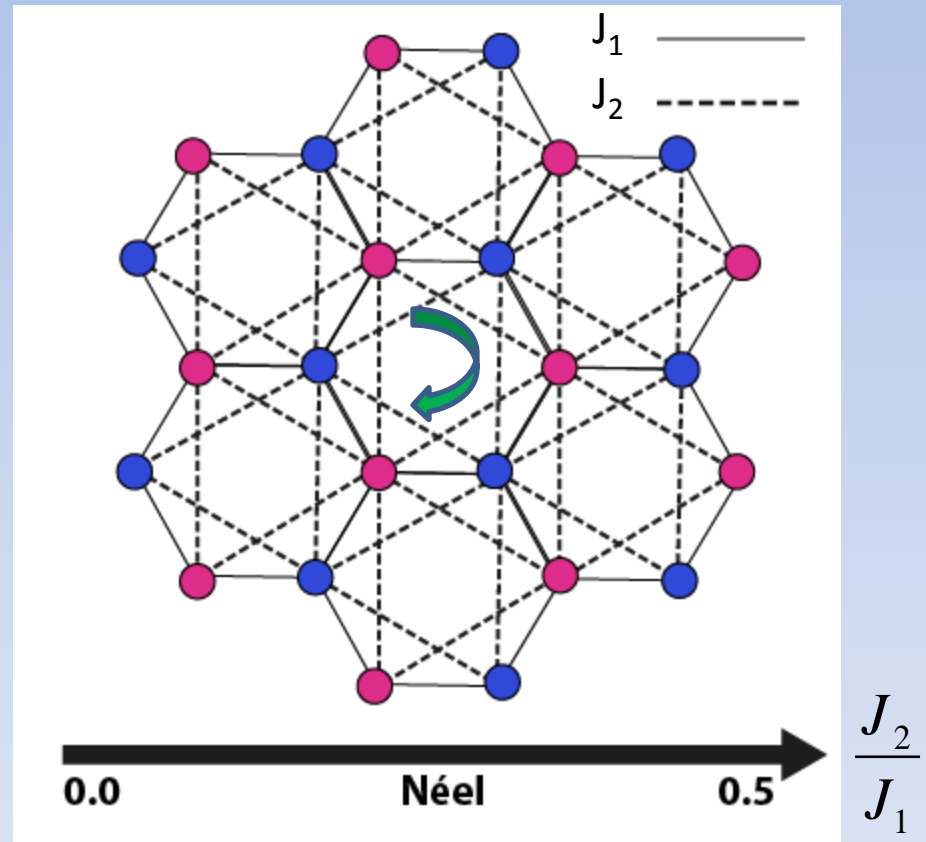
Single spin flip : $\Delta E_s = 6J_1 - 12J_2$

Plaquette flip : $\Delta E_h = 12J_1 - 48J_2$

$$\Delta E_h < \Delta E_s \Rightarrow \frac{1}{6} < \frac{J_2}{J_1} < \frac{1}{2}$$

Zero-Energy Plaquette Flip :

$$\Delta E_h = 0 \Rightarrow \frac{J_2}{J_1} = \frac{1}{4}$$



Classical Phase diagram

Multi-Spin flip excitations

Frustrated antiferromagnetic J_1 - J_2 Heisenberg model
on the Checkerboard lattice

Classical $S \rightarrow \infty$ Limit :

Single spin flip : $\Delta E_s^{Néel} = 2J_1 - J_2$,

$$\Delta E_s^{Collinear} = J_2$$

Plaquette flip : $\Delta E_p^{Néel} = 4(J_1 - J_2)$,

$$\Delta E_p^{Collinear} = 4(J_2 - J_1)$$

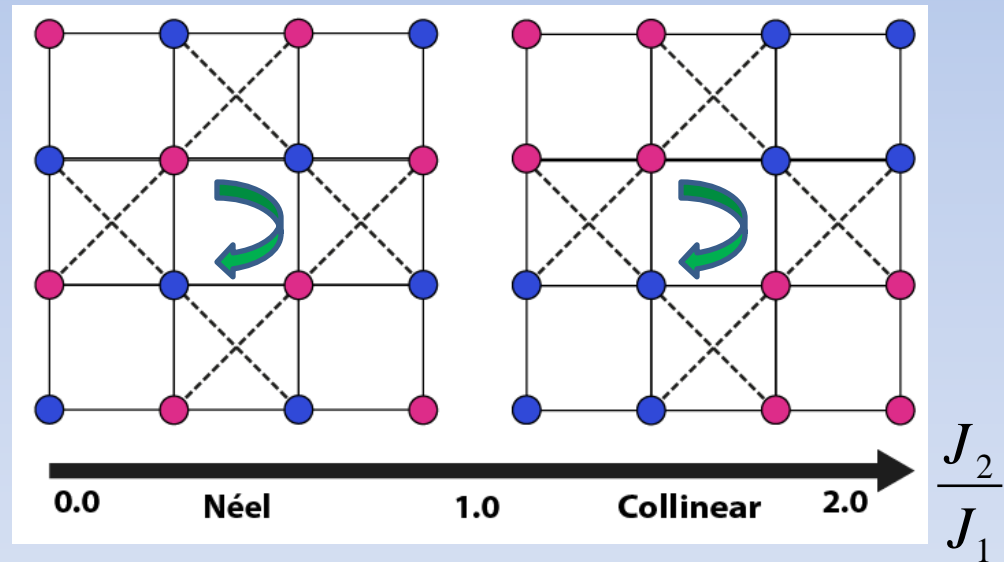
$$\Delta E_p < \Delta E_s \Rightarrow \frac{2}{3} < \frac{J_2}{J_1} < \frac{4}{3}$$

Zero-Energy Plaquette Flip :

$$\Delta E_p = 0 \Rightarrow \frac{J_2}{J_1} = 1$$

$$H = J_1 \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \vec{S}_i \cdot \vec{S}_j$$

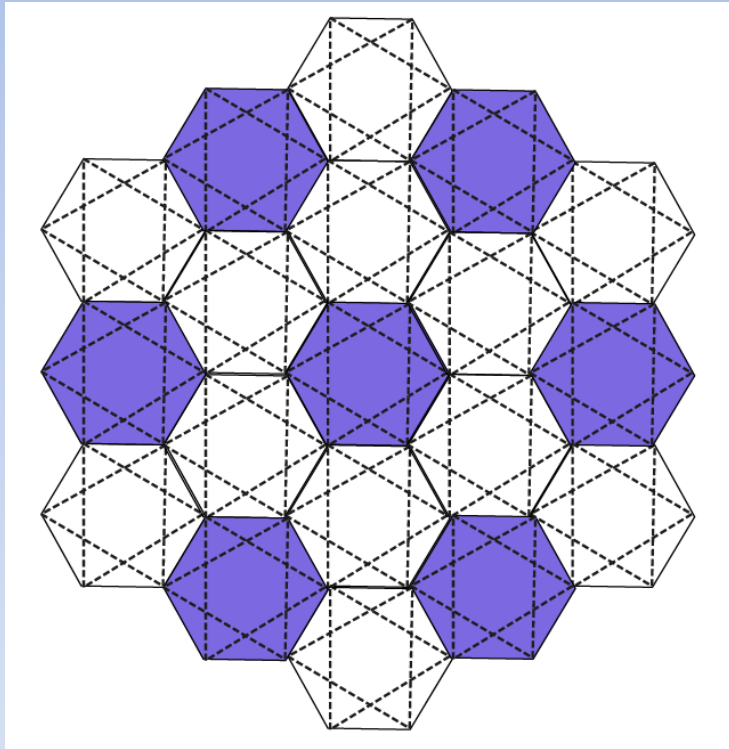
J_1 ———
 J_2 - - - -



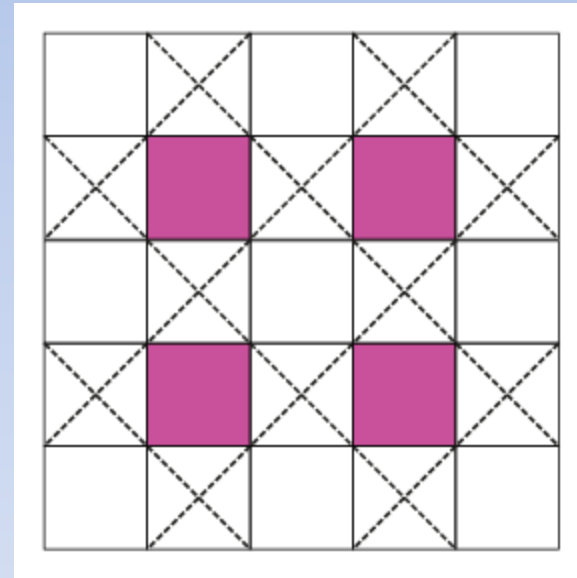
Classical Phase diagram

Cluster Operator Theory

Based on a plaquette ordered background
with plaquette-type excitations



Honeycomb Lattice



Checkerboard Lattice

Sachdev and Bhatt, PRB (1990) 43,9323

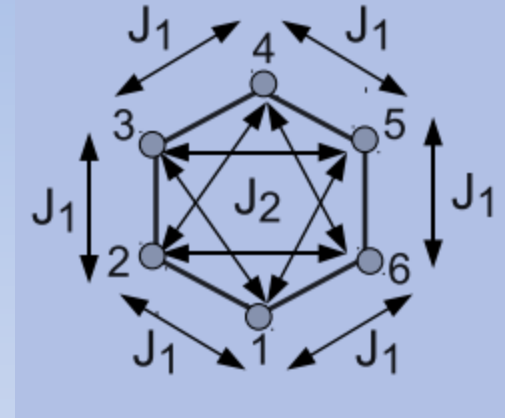
Zhitomirsky and Ueda, PRB (1996) 54,139007

Cluster Operator Theory

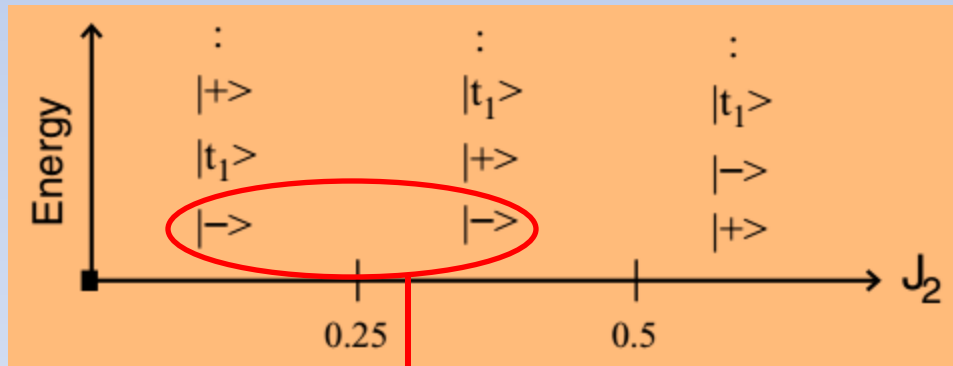
$J_1 - J_2$ Heisenberg model on the honeycomb Lattice

Single Hexagon Problem: (we set $J_1 = 1$)

$$H_{Single-Hex} = \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \vec{S}_i \cdot \vec{S}_j$$



$64 = 2^6$ states



R.Ganesh, et al, PRB (2013) 87,054413

Unique ground state of the single hexagon for $0.0 < J_2 < 0.5$,
the range that we predict existence of a plaquette ordered ground state.

Cluster Operator Theory

$J_1 - J_2$ Heisenberg model on the honeycomb Lattice

In the absence of interaction between plaquettes, all shaded plaquettes are in their unique groundstates.

Interaction between plaquettes:

$$H_{IJ} = J_1 S_1^I \cdot S_4^J + J_2 S_2^I \cdot S_4^J + J_2 S_6^I \cdot S_4^J + J_2 S_1^I \cdot S_3^J + J_2 S_1^I \cdot S_5^J$$

The interaction term hybridizes the ground state of each plaquette with its other excited states:

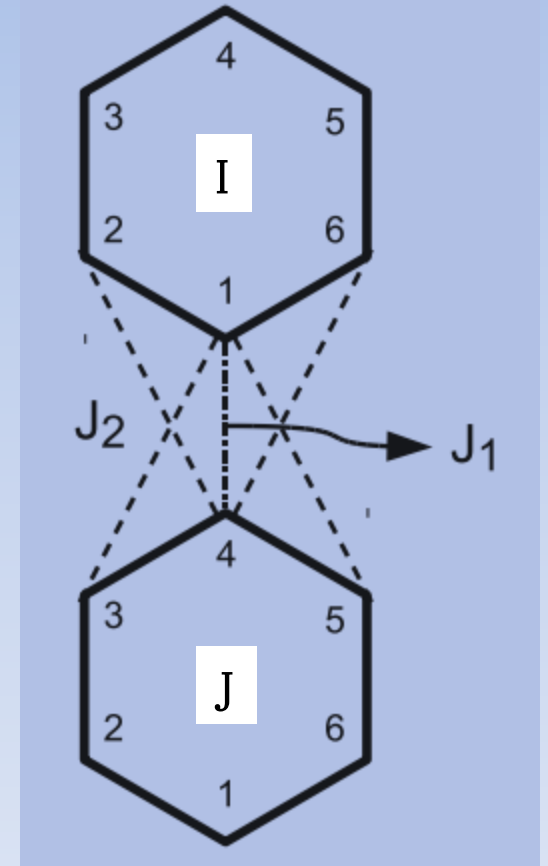
Amplitudes of possible interplaquette interactions:

$$\langle uv | H_{IJ} | -- \rangle$$

$$\langle u - | H_{IJ} | - v \rangle$$

$$\langle - v | H_{IJ} | u - \rangle$$

$$\langle -- | H_{IJ} | uv \rangle$$



Cluster Operator Theory

$J_1 - J_2$ Heisenberg model on the honeycomb Lattice

Effective Hamiltonian: A boson scheme

$$|u\rangle_I = b_{I,u}^+ |0\rangle, \quad u = 1, \dots, 64$$

Bose-condensation assumption of groundstate bosons:

$$b_{I,-} \equiv b_{I,-}^+ \equiv \bar{p}$$

To preserve the Hilbert space,
the total occupancy of bosons per plaquette should be unity:

$$N\bar{p}^2 + \sum_{I,u=2,\dots,64} b_{I,u}^+ b_{I,u} = N$$

Cluster Operator Theory

$J_1 - J_2$ Heisenberg model on the honeycomb Lattice

Effective Hamiltonian: A boson scheme

$$H_{eff} = \sum_I \epsilon_1 \bar{p}^2 + \sum_{I,u=2}^{64} \epsilon_u b_{I,u}^+ b_{I,u} - \mu [N \bar{p}^2 + \sum_{I,u=2}^{64} b_{I,u}^+ b_{I,u} - N] \\ + \bar{p}^2 \sum_{\langle I,J \rangle} \sum_{u,v=2}^{64} [\langle uv | H_{IJ} | -- \rangle b_{I,u}^+ b_{J,v}^+ + \langle u - | H_{IJ} | - v \rangle b_{I,u}^+ b_{J,v} + H.C.]$$

After going to momentum space and doing a Bogoliubov transformation:

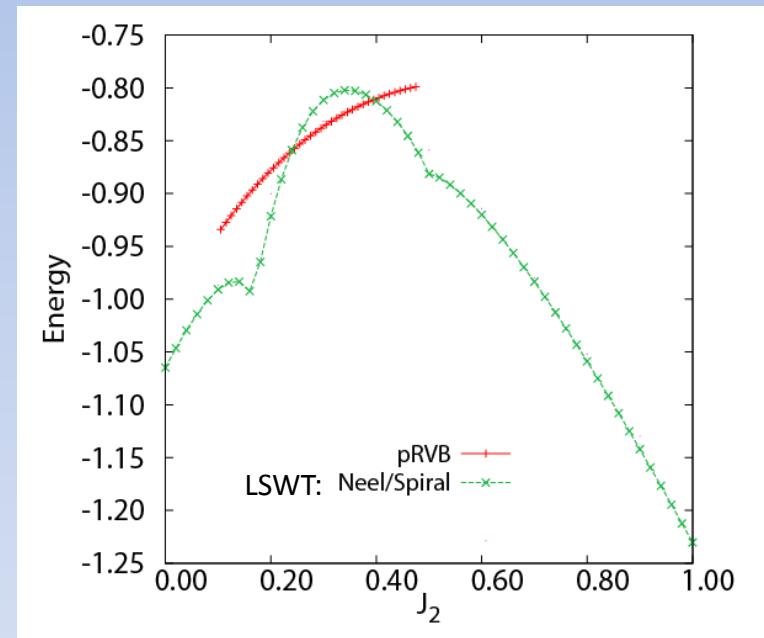
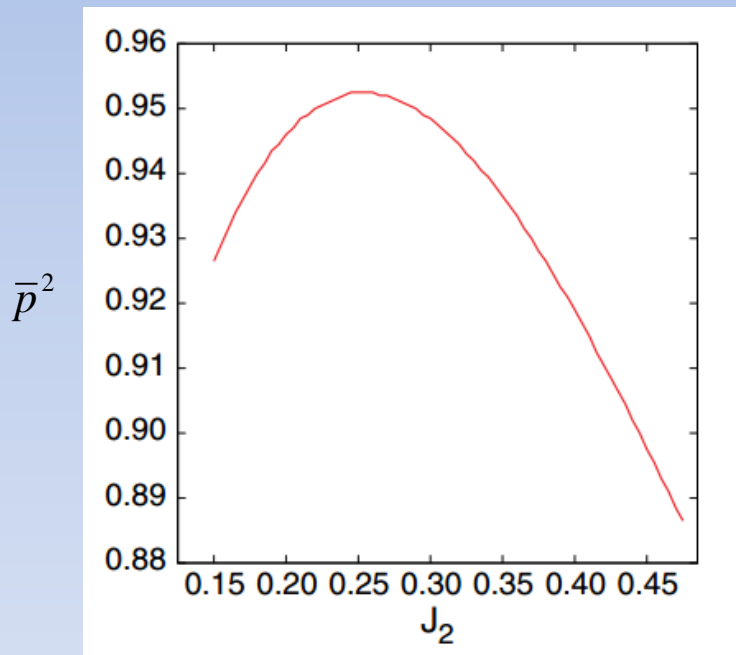
$$H_{eff} = N\mu + N\bar{p}^2 (\epsilon_- - \mu) - \frac{1}{2} N \sum_u (\epsilon_u - \mu) + \sum_{k,v} \left(\frac{1}{2} + \gamma_{k,v}^+ \gamma_{k,v} \right) \omega_{k,v}(\mu, \bar{p})$$

Self-consistent equations: $\frac{\partial \langle H \rangle}{\partial \mu} = 0, \quad \frac{\partial \langle H \rangle}{\partial \bar{p}} = 0$

Cluster Operator Theory

$J_1 - J_2$ Heisenberg model on the honeycomb Lattice

Results

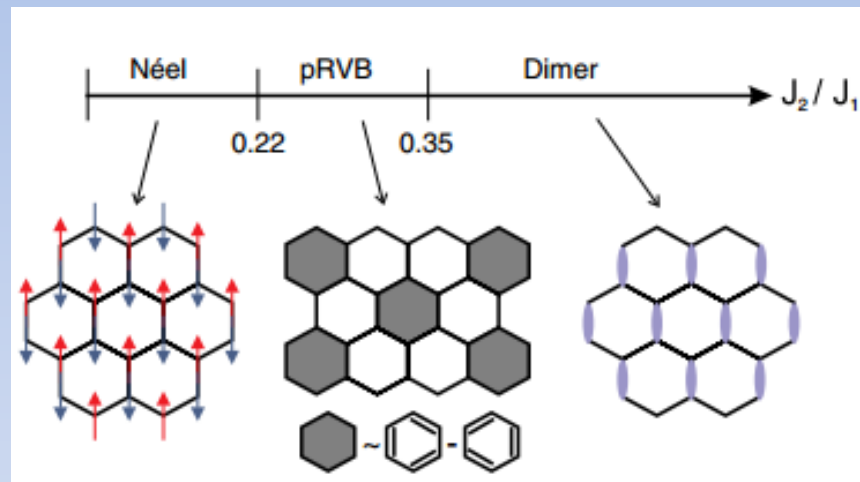


Plaquette order is strongest around $J_2/J_1=0.25$, where we showed that there is a zero-energy plaquette flip excitation in classical limit.

Cluster Operator Theory

$J_1 - J_2$ Heisenberg model on the honeycomb Lattice

Results



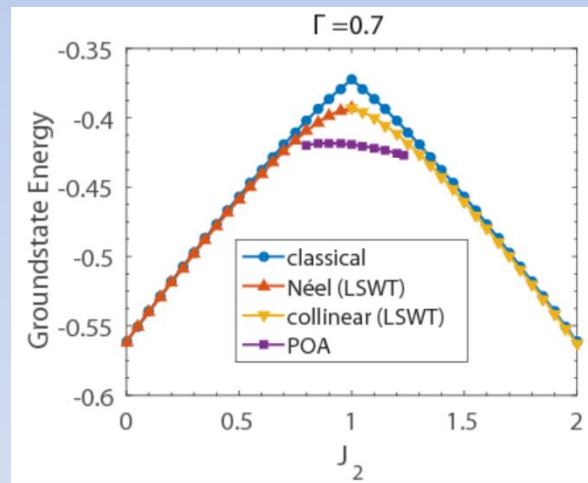
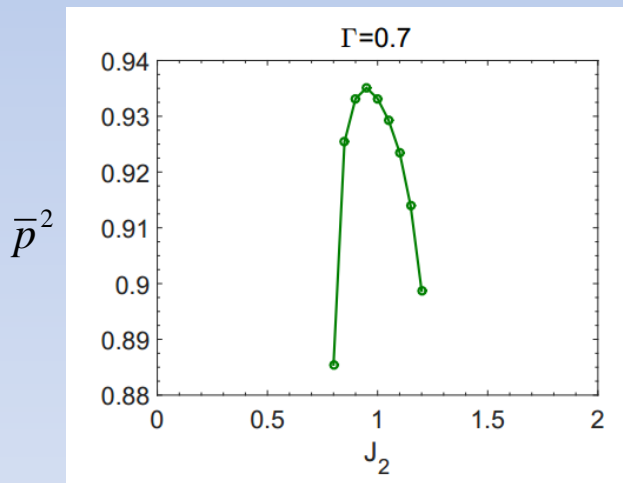
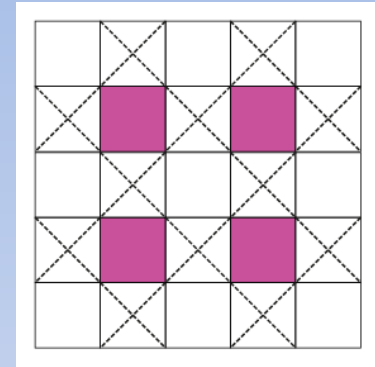
Phase diagram of the model obtained from DMRG calculation

Cluster Operator Theory

Transverse field J_1 - J_2 Ising model on the checkerboard lattice

$$H = J_1 \sum_{\langle i,j \rangle} S_i^z S_j^z + J_2 \sum_{\langle\langle i,j \rangle\rangle} S_i^z S_j^z - \Gamma \sum_i S_i^x$$

Results

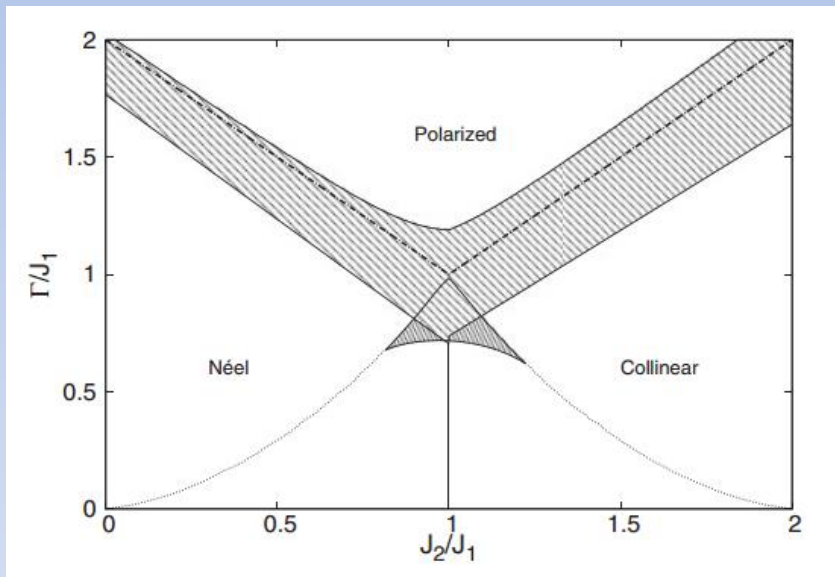


Plaquette order is strongest around $J_2/J_1=1.0$, where we showed that there is a zero-energy plaquette flip excitation in classical limit.

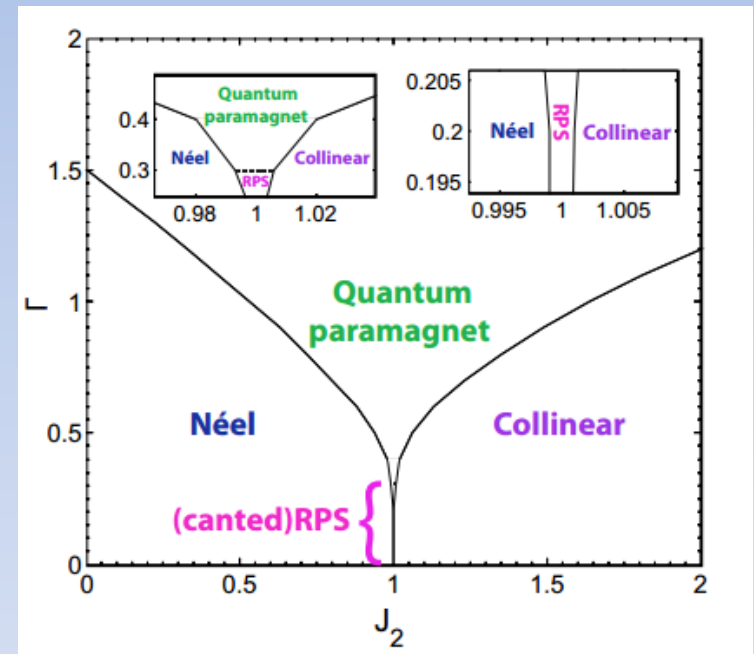
Cluster Operator Theory

Transverse field J_1 - J_2 Ising model on the checkerboard lattice

Results



Phase diagram of the model
obtained from LSWT,
L.P. Henry, et al,
PRB (2012) 85,134427



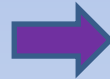
Phase diagram of the model
obtained from COA,
Sadzadeh, et.al.
Eur. Phys. J. B (2015) 88:259

Cluster Operator Approach

an analogy to spin wave theory

SWT

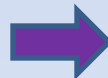
An initial classical
ordered ground state
($m=1$)
+
Single spin flip
Quantum fluctuations



Reduction of the order
parameter ($m < 1$)
+
Correction on the ground state
energy
+
Harmonic spectrum of low-
energy excitations

COA

An initial cluster
ordered ground state
($\bar{p}=1$)
+
Multi-spin
Quantum fluctuations



Reduction of the Bose
condensation density
($\bar{p} < 1$)
+
Correction on the ground state
energy
+
An-harmonic spectrum of low-
energy excitations

**Thanks for your attention
and**

**Special thanks to M. Sadrzadeh who
helped me in preparing this lecture.**