# Correlated Valence-Bond States

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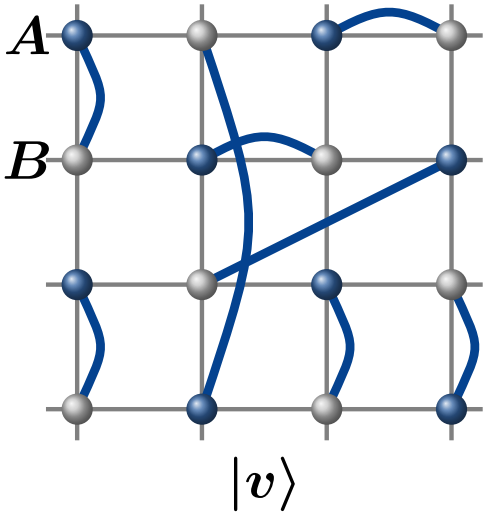
# Valence Bond (VB) States for S=1/2 spins

**VB state:** a set of singlets between A and B sublattice sites on a bipartite lattice

$$|v\rangle = \bigotimes_{ij} (i,j)$$

$$(i,j) = \frac{1}{2}\left[|\uparrow_i\downarrow_j\rangle - |\downarrow_i\uparrow_j\rangle\right]$$




$|v\rangle$

**VB basis:** overcomplete & non-orthogonal

- expansion of an arbitrary singlet state (not unique)

$$|\psi\rangle_{S=0} = \sum_v f_v |v\rangle \qquad (f_v > 0)$$

- Possible VB superposition states in 2D

  - Neel ordered states
  - Spin liquids
  - Valence-bond solid (VBS) states

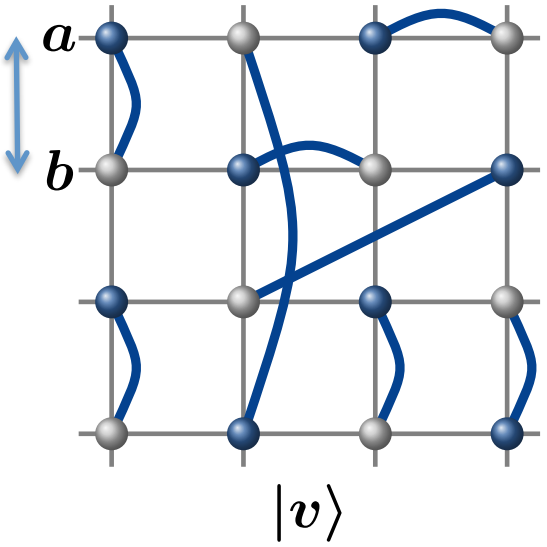
# Amplitude-Product (AP) States

## Variational states

[Liang, Doucot, Anderson (1988)]

$$|\psi\rangle = \sum_v f_v |v\rangle$$

$|r| = 1$




The wavefunction coefficients for a bond configuration:

$$f_v = h(a_1, b_1)h(a_2, b_2)\cdots h(a_{N/2}, b_{N/2})$$

Assume: $h(a, b) = h(|r|)$

$$f_v = \prod_r h(r)^{n_r(v)} \qquad (f_v > 0)$$

where $n_r(v)$ is the number of bonds of length r in $|v\rangle$

## Variational parameters: h(r)

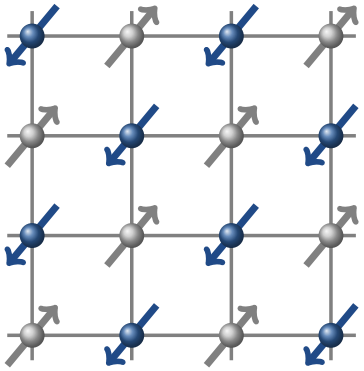
$$\frac{\langle\psi_h|H|\psi_h\rangle}{\langle\psi_h|\psi_h\rangle} \geq E_0$$

# Néel Ordered States

- The sublattice magnetization is non-zero

$$\vec{m}_s = \frac{1}{N}\sum_i \phi_i \vec{S}_i \neq 0$$

$$\phi_i = +1 \quad \text{if } i \in A$$
$$\phi_i = -1 \quad \text{if } i \in B$$



## Example:

- The ground state of the Heisenberg antiferromagnet on the square lattice

  MC [Reger, Young (1988)] + spin wave theory

$$\langle m_s^z \rangle \approx 0.3 \qquad N \to \infty$$

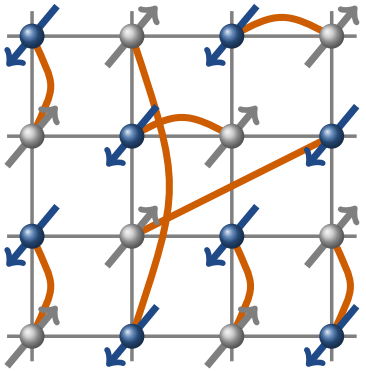
## Bond amplitudes for 2D Néel state:

- Variational optimization of h(r) for the square-lattice Heisenberg model

  [Jie, Sandvik (2007)]

$$h(|r|) \propto \frac{1}{|r|^3}$$

consistent with mean field calculations [Beach (2007)]

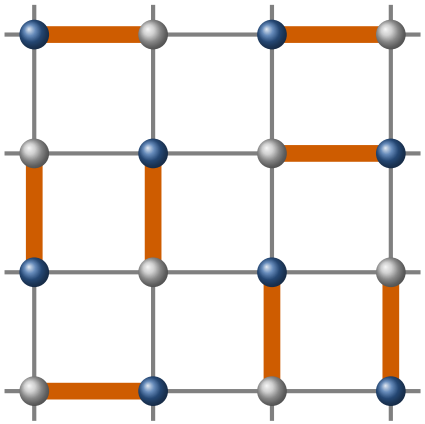


# Spin Liquids and Valence-Bond Solids (VBS)

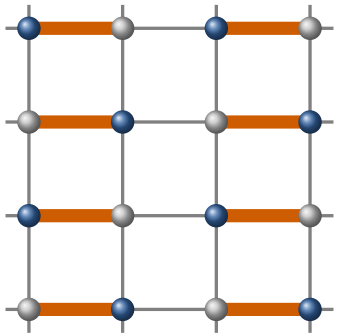
## Short-bond AP states describe non-Néel states

- $h(r) \propto 1/r^{\alpha}$ with large $\alpha$
- $h(r)$ decays exponentially
- $h(r) = \delta(r-1)$

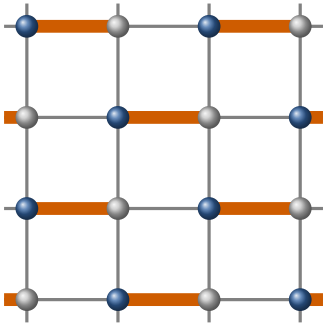
## Spin liquids



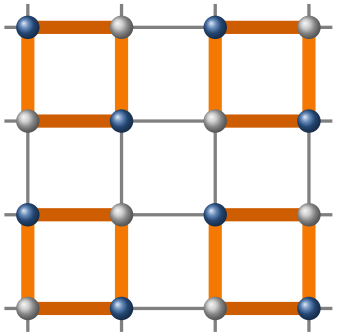
## VBS (cannot be described by AP states)



columnar



staggered



plaquette

# Goal & Motivation

## Goal

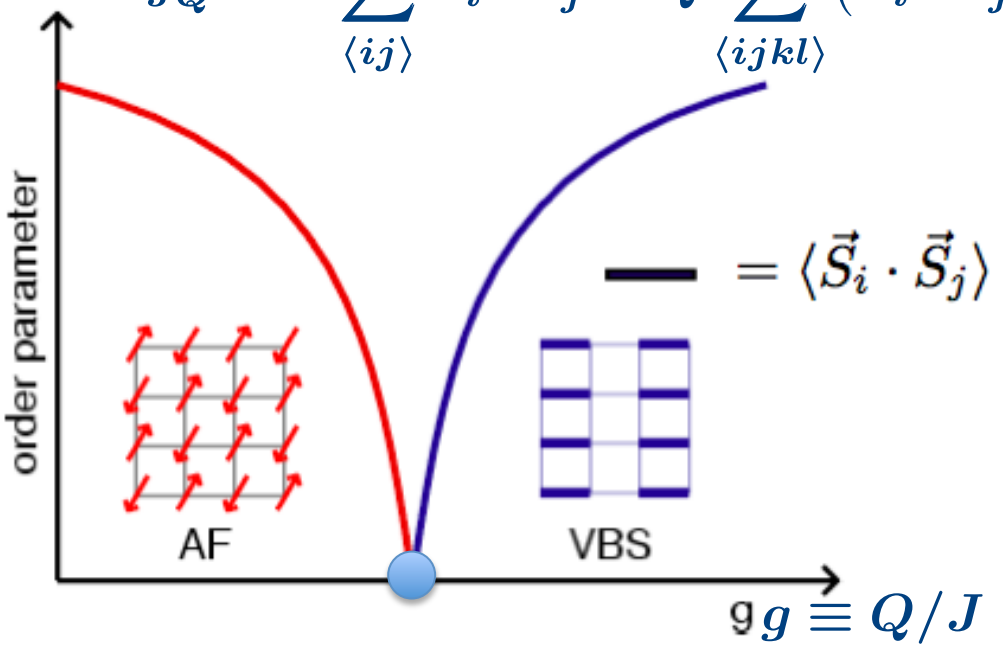
Construct generalized AP states that can describe VBS order in 2D

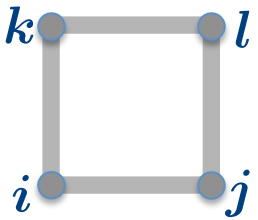
## Motivation

Néel-VBS transitions in 2D have received much interest recently in the context of unconventional quantum phase transitions beyond the LGW paradigm.

**Example:** the J-Q model [A.W. Sandvik, PRL 98, 227202 (2007)]

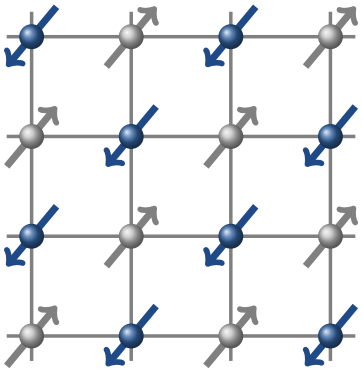
$$H_{JQ} = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j - Q \sum_{\langle ijkl \rangle} (\vec{S}_i \cdot \vec{S}_j - \frac{1}{4})(\vec{S}_k \cdot \vec{S}_l - \frac{1}{4})$$



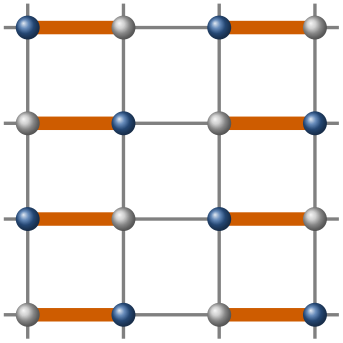



# Order-Order Transition

Neel



VBS



broken **Spin rotation symmetry** not broken

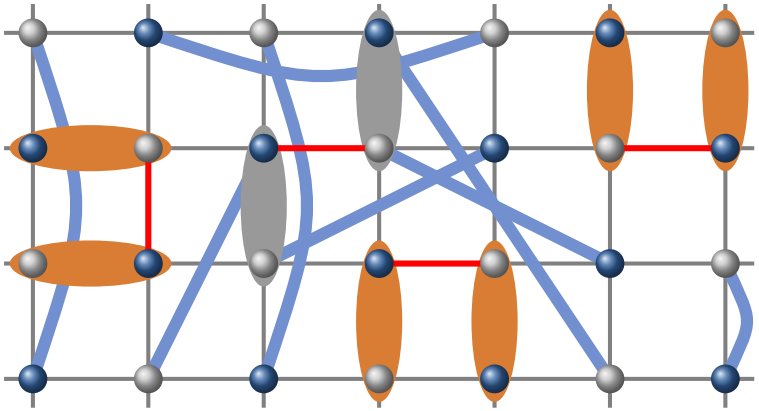
not broken **Lattice symmetry** broken

[T. Senthil, et. al. Science 303, 1490 (2004)]

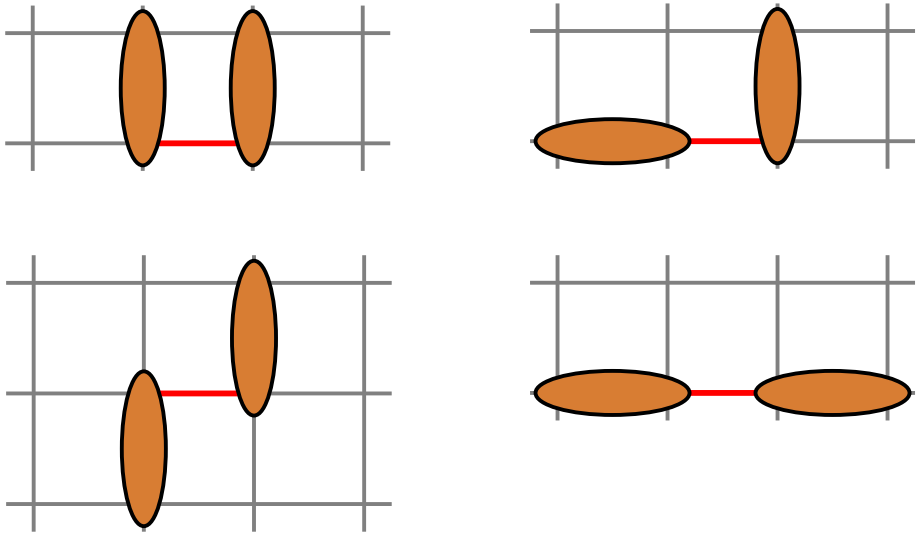
# Correlated Amplitude Product (CAP) States

**Idea:** Impose bond correlations

$$f_v = \prod_r h(r)^{n_r(v)} \prod_b w_b^{n_b(v)}$$



**Possible dimer correlations in 2D:**



$w_b > 1$ favored

$w_b < 1$ unfavored

$w_b = 1$ neutral

# Monte Carlo Sampling

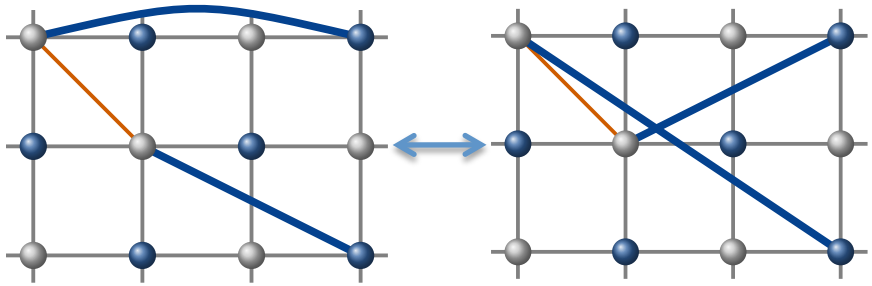
## Expectation value of O in a CAP state

$$\langle O\rangle \equiv \langle\psi|O|\psi\rangle = \frac{\sum_{v'v} W_{v'v}\frac{\langle v'|O|v\rangle}{\langle v'|v\rangle}}{\sum_{v'v} W_{v'v}}$$

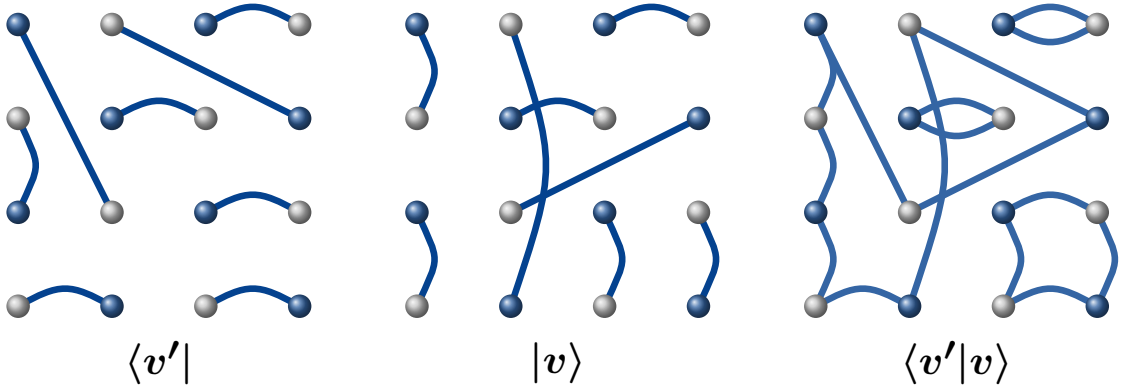
where $W_{v'v} = f_{v'} f_v \langle v'|v\rangle$

## Calculate <O> stochastically according to $W_{v'v}$ [Liang, Doucot, Anderson (1988)]

bond-pair updates



## $\langle v'|O|v\rangle$ depends on loop structure of transition graphs




$$\langle v'|v\rangle = 2^{N_{\text{loop}}-N/2}$$

# Observables on transition graphs

## Two-spin correlation

$$\frac{\langle v'|\boldsymbol{S}_i \cdot \boldsymbol{S}_j|v\rangle}{\langle v'|v\rangle} = \begin{cases} \pm 3/4, & \text{if } i,j \text{ in the same loop} \\ 0, & \text{if } i,j \text{ in different loops} \end{cases}$$

## Staggered magnetization

$$\frac{\langle v'|\mathbf{m}_s^2|v\rangle}{\langle v'|v\rangle} = \frac{3}{4}\sum_\ell \mathcal{L}_\ell^2$$

$$\frac{\langle v'|m_s^4|v\rangle}{\langle v'|v\rangle} = \sum_\ell \mathcal{L}_\ell^2 + \frac{15}{16}\left(\sum_\ell \mathcal{L}_\ell^2\right)^2 - \frac{5}{8}\sum_\ell \mathcal{L}_\ell^4$$

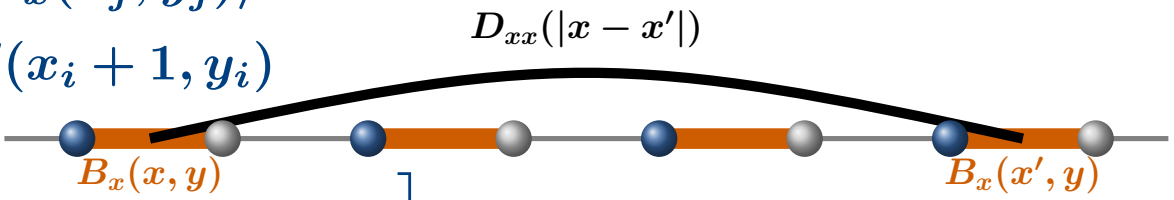
$\mathcal{L}_\ell$ : the size (the number of sites) of the loop

## Dimer correlation function

$$D_{xx}(x,y) = \langle B_x(x_i,y_i)B_x(x_j,y_j)\rangle$$

$$B_x(x_i,y_i) = S(x_i,y_i)\cdot S(x_i+1,y_i)$$

$$D_{xx}^* = D_{xx}(x,y) - \frac{1}{2}\left[D_{xx}(x-1,y) + D_{xx}(x+1,y)\right]$$



# Order parameter

## Neel order $\langle m_s^2 \rangle \neq 0$

fourth-order cumulant of $m_s$

$$U = \frac{5}{2}\left(1 - \frac{3}{5}\frac{\langle {m_s}^4 \rangle}{\langle {m_s}^2 \rangle^2}\right)$$

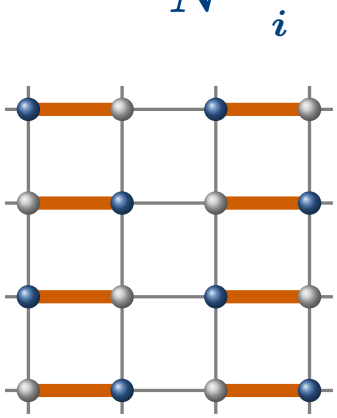
AF ordered phase: $U \to 1$ disordered phase: $U \to 0$

## VBS order parameter

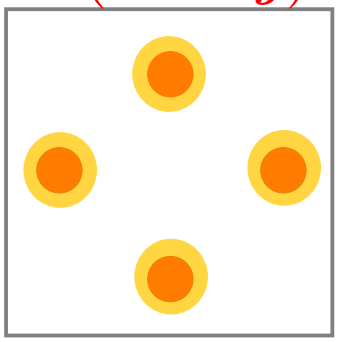
$$D_x = \frac{1}{N}\sum_i (-1)^{x_i} S(x_i, y_i) \cdot S(x_i + 1, y_i)$$

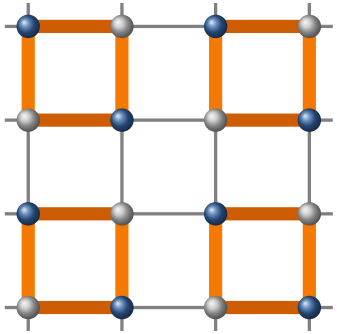
$$D_y = \frac{1}{N}\sum_i (-1)^{y_i} S(x_i, y_i) \cdot S(x_i, y_i + 1)$$

$$d_{x(y)} = \frac{\langle v' | D_{x(y)} | v \rangle}{\langle v' | v \rangle}$$



$P(d_x, d_y)$





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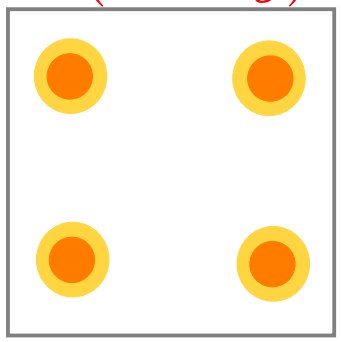
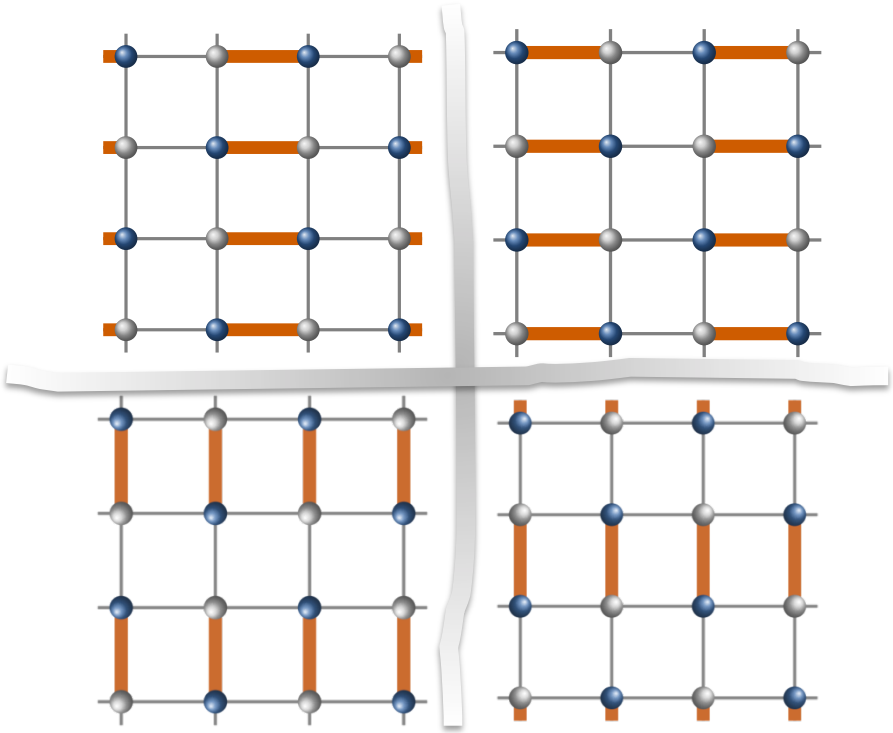
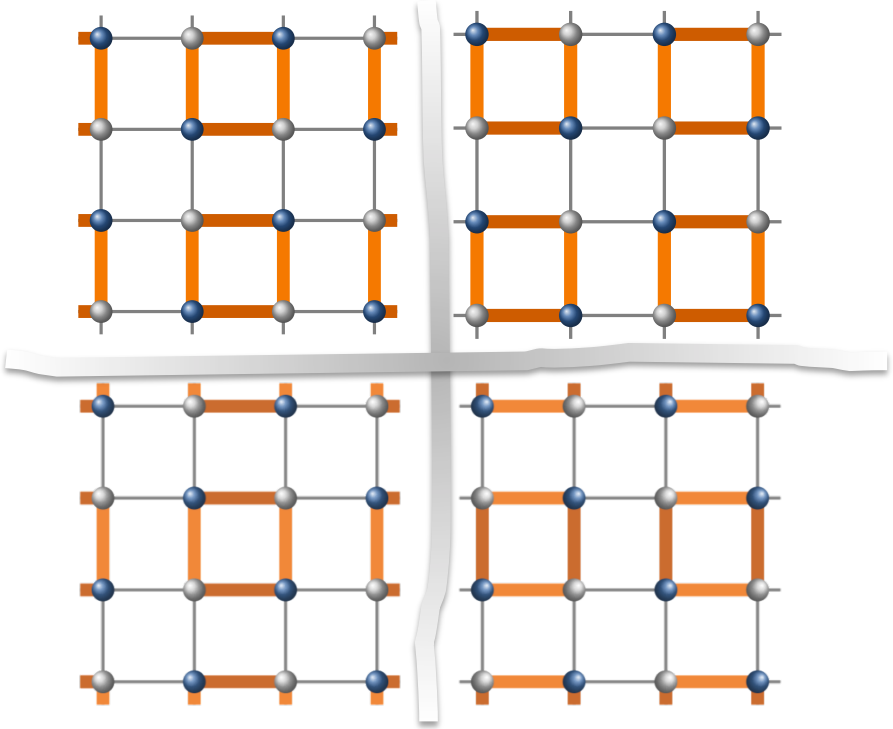


# VBS orderings

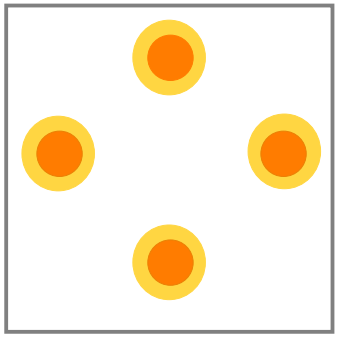
## Columnar order

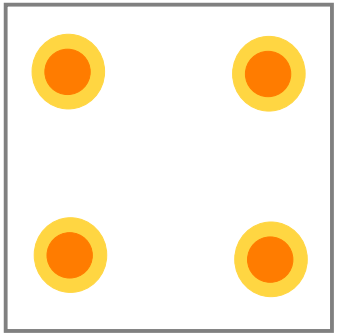


## Plaquette order



$P(d_x, d_y)$





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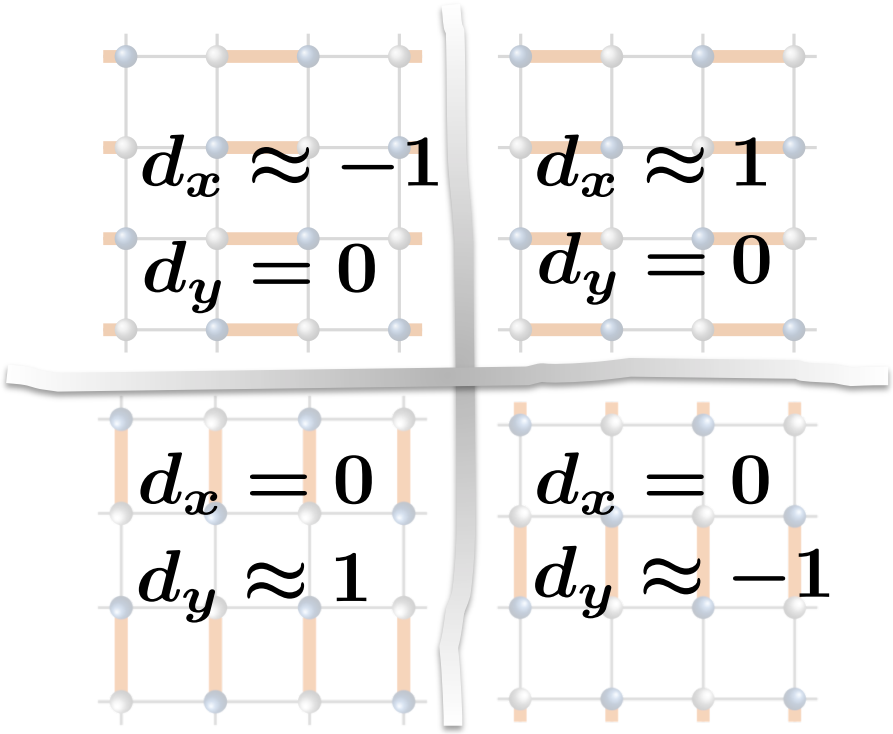


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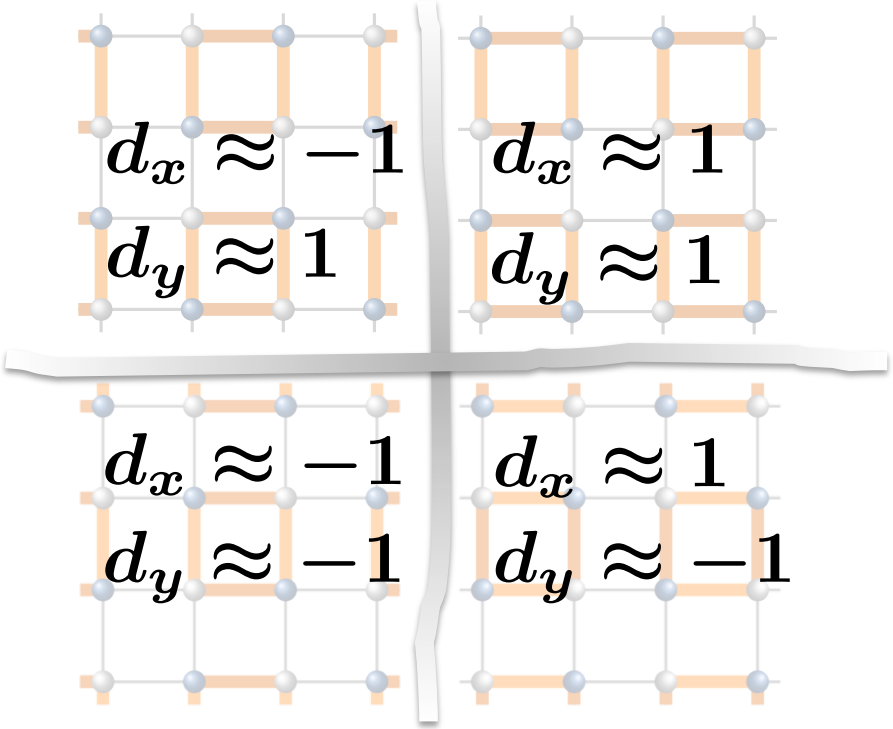


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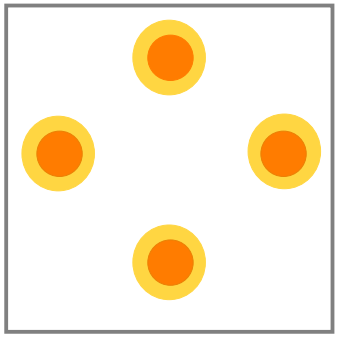
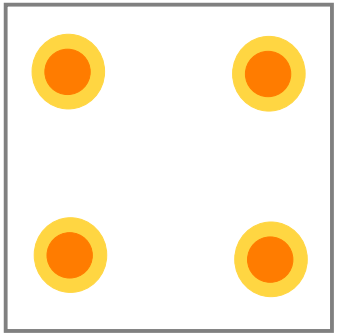
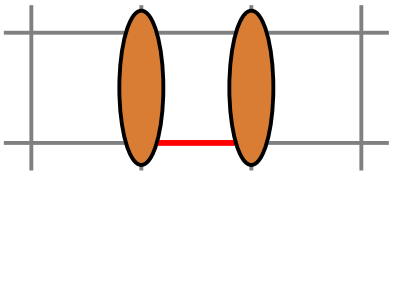




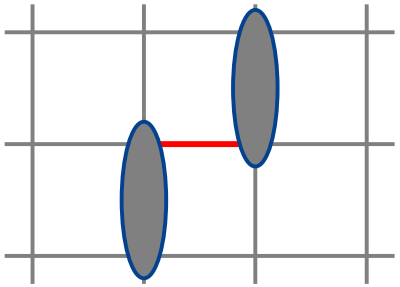
# Case for a First Order Néel-VBS transition

$$f_v = \prod_r h(r)^{n_r(v)} \prod_b w_b^{n_b(v)} \qquad h(r) = 1/r^3$$

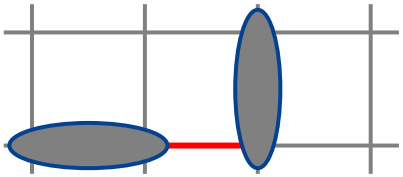
**Bond correlation factors**



$w = p > 1$



$w = 1/p$



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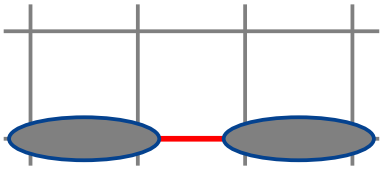

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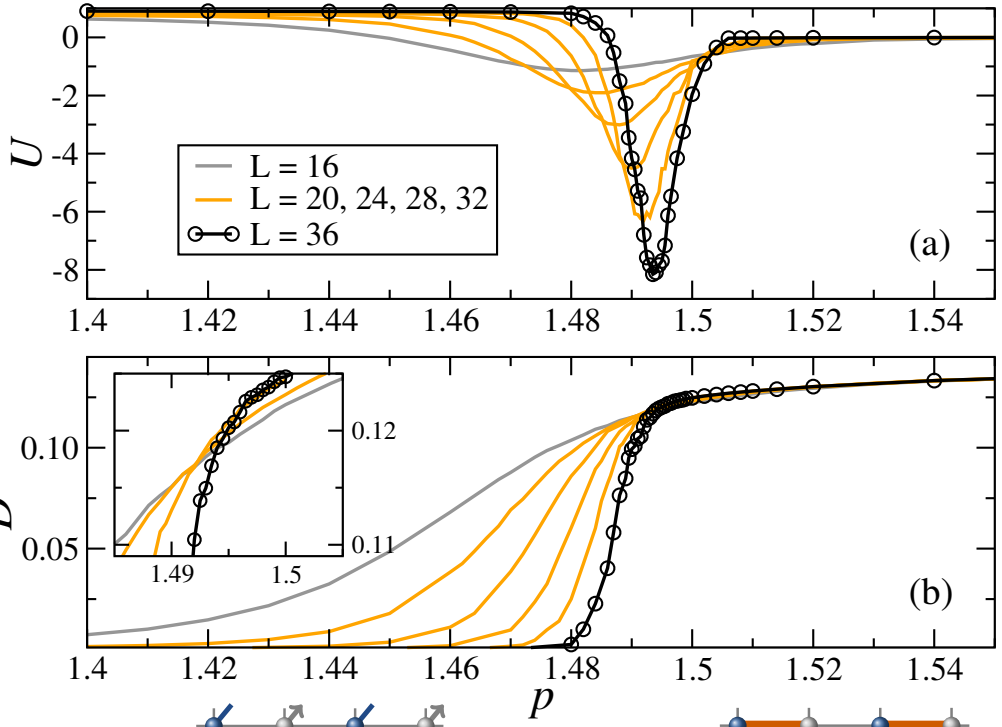


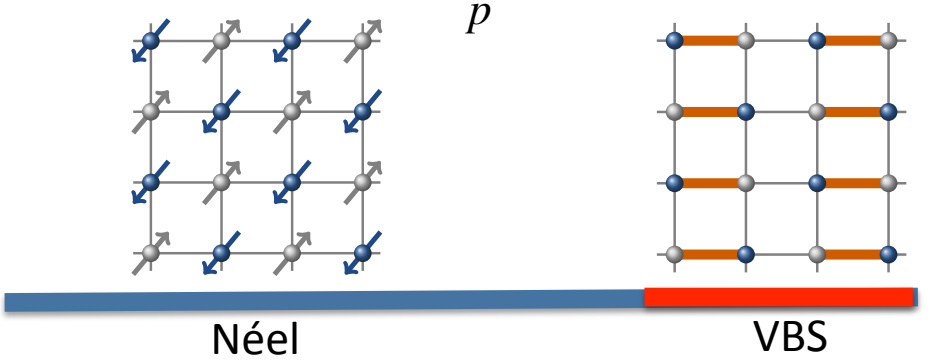

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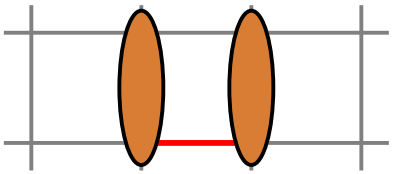
**Bond correlation factors**



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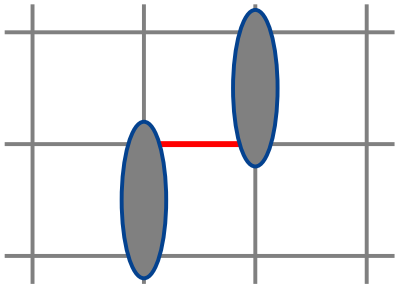

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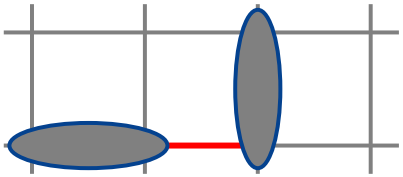

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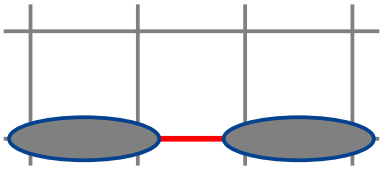

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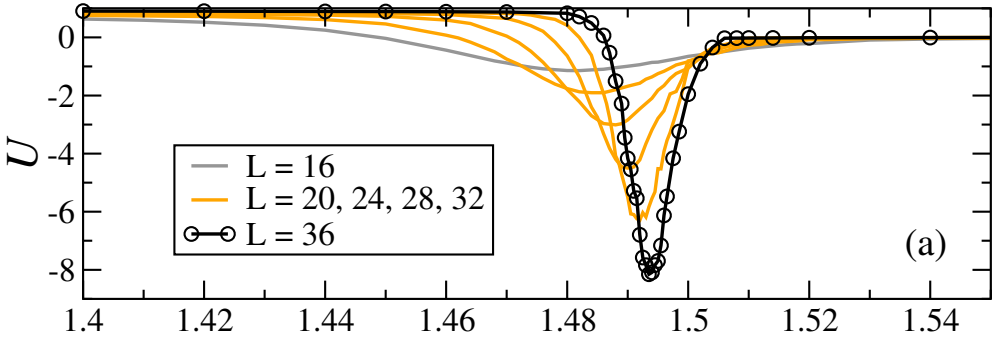
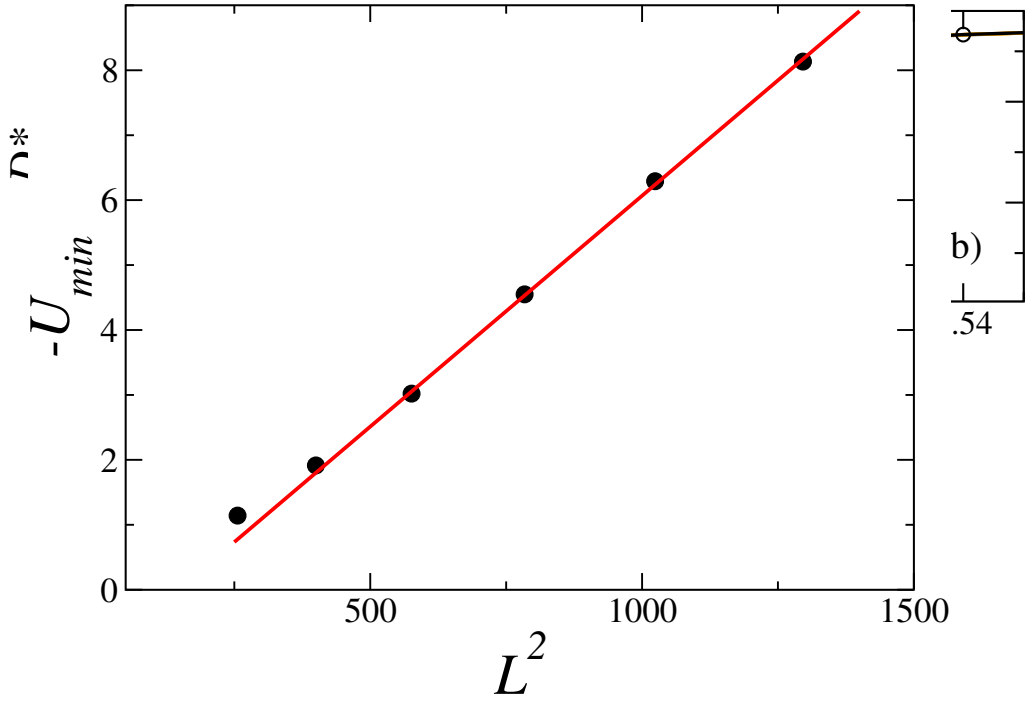
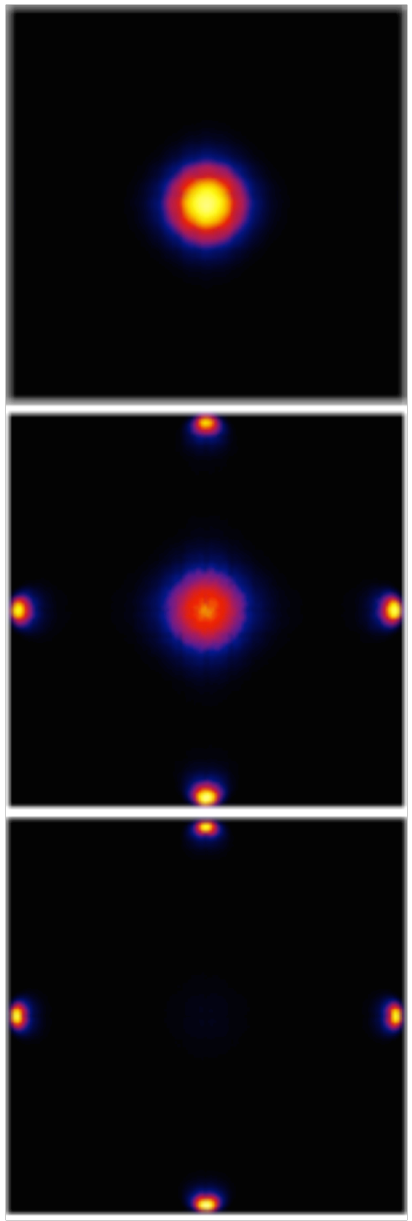


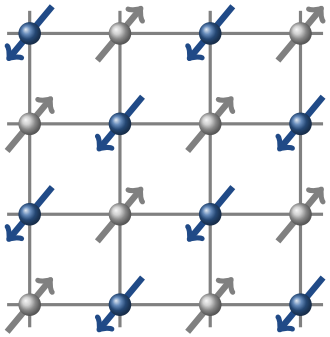
# Case for a First Order Néel-VBS transition

$h(r) = 1/r^3$

P($d_x$, $d_y$)

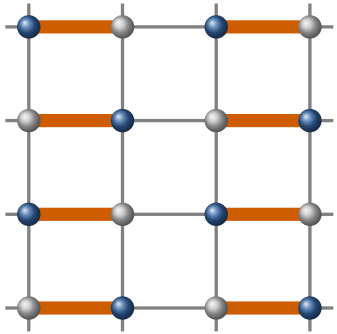


Neel

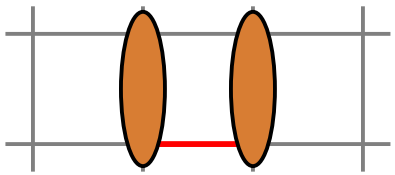


Neel-VBS coexistence

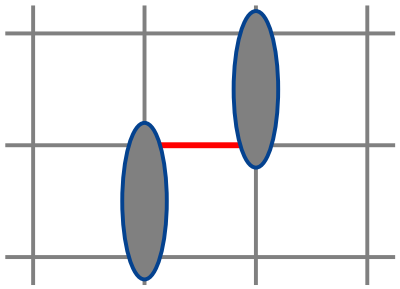
$Z_4$ symmetry broken



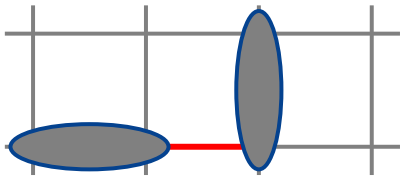
## Bond correlation factors



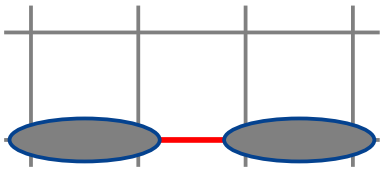
$w = p > 1$



$w = 1/p$



$w = 1/p$

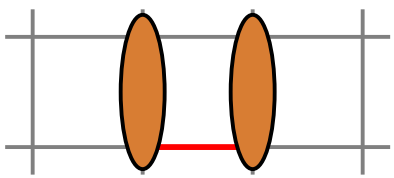


$w = 1/p$

# Case for a Second Order Néel-Liquid-VBS transition

$$h(r) = 1/r^3$$

**Bond correlation factors**



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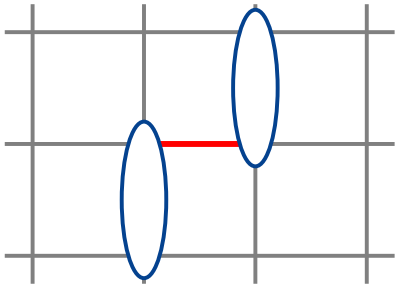
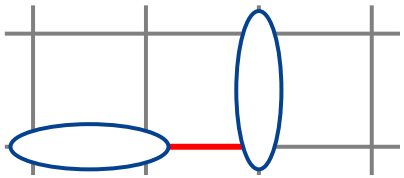
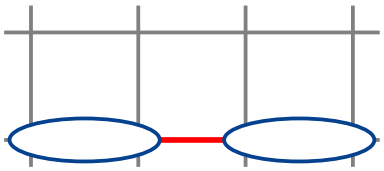


$w = 1$



$w = 1$



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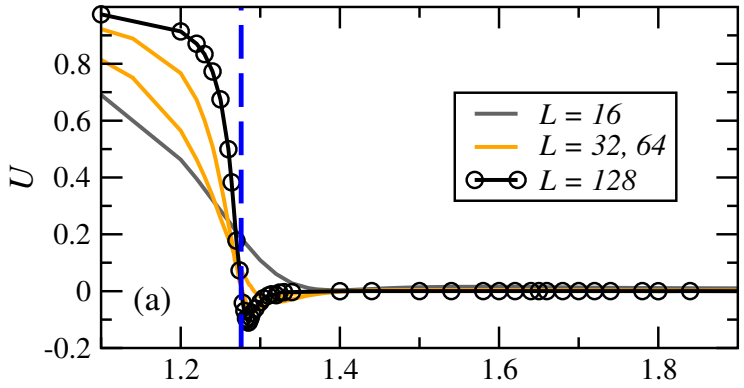
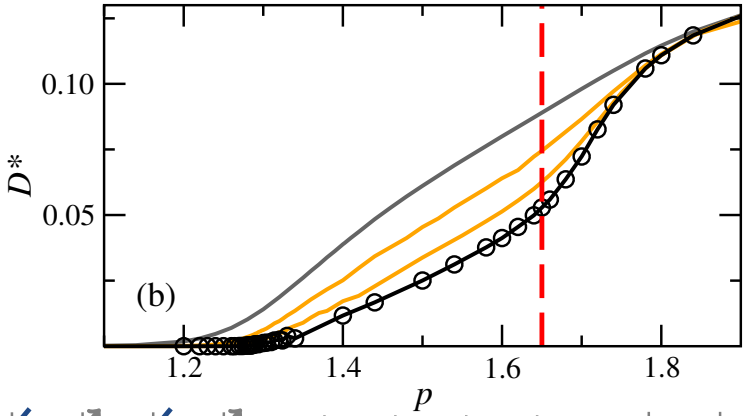
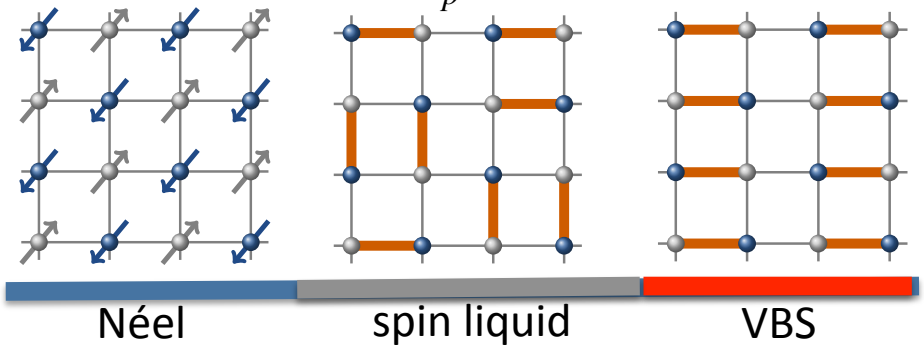


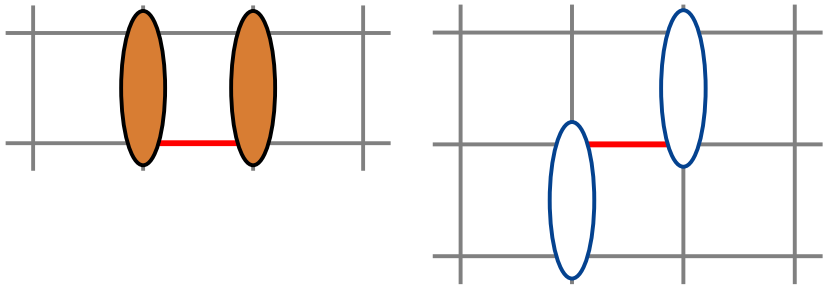



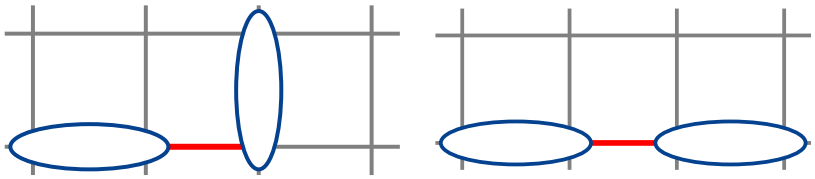
# Case for a Second Order Néel-Liquid-VBS transition

$$h(r) = 1/r^3$$

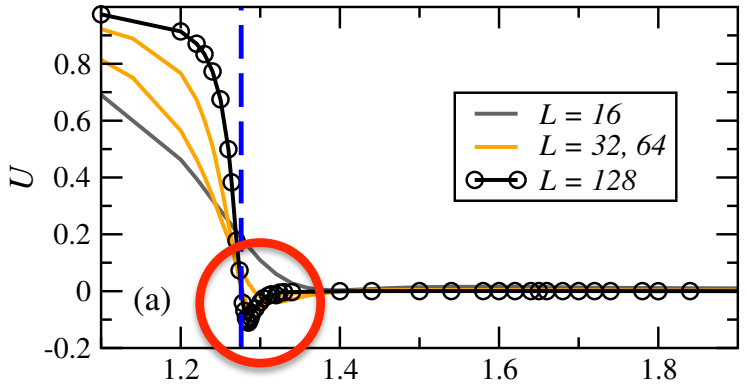
**Bond correlation factors**

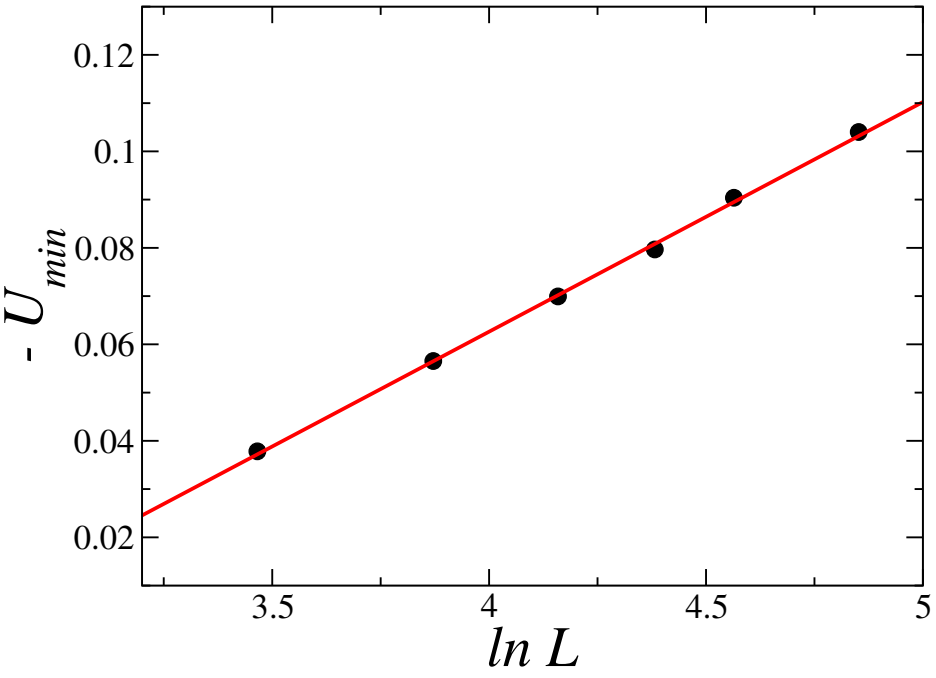


$w = p > 1$ $\quad$ $w = 1$



$w = 1$ $\quad$ $w = 1$



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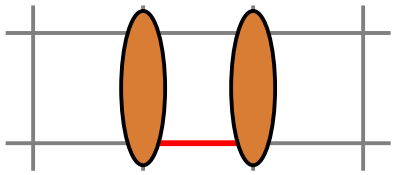
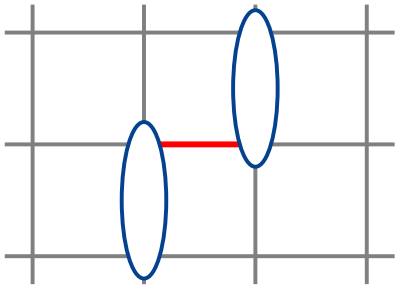
$$h(r) = 1/r^3$$

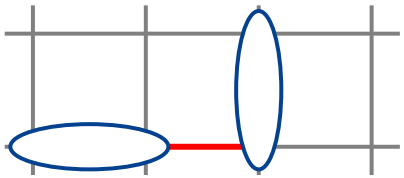
**Bond correlation factors**



$w = p > 1$



$w = 1$



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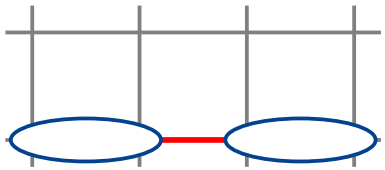

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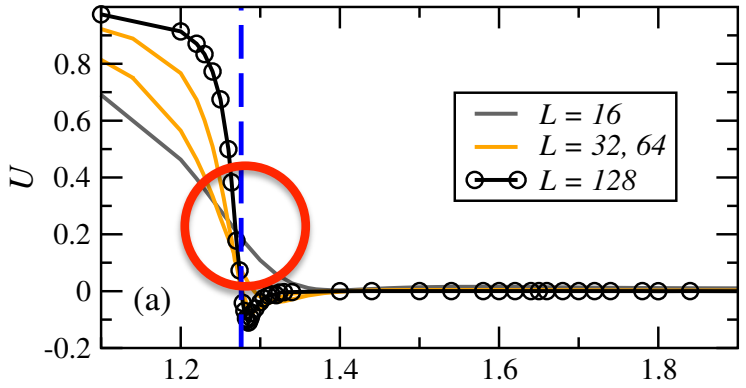
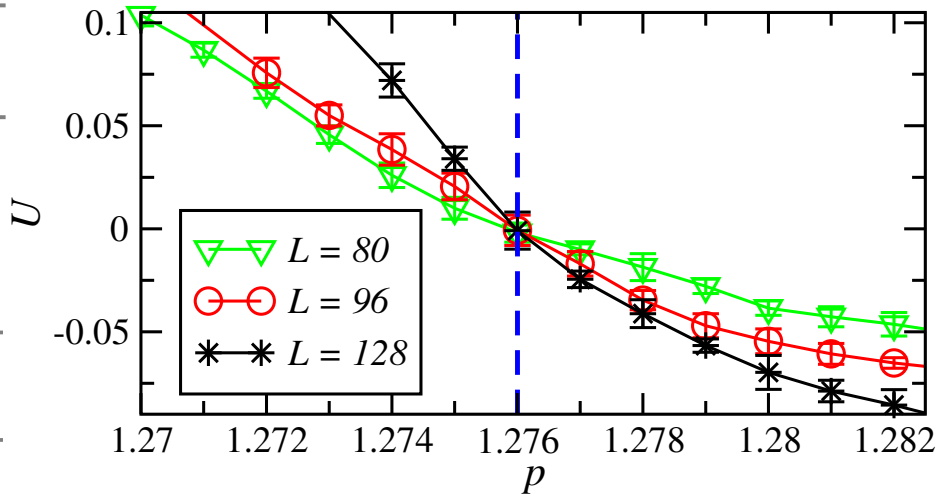
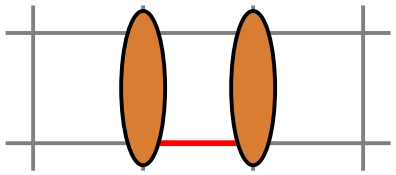


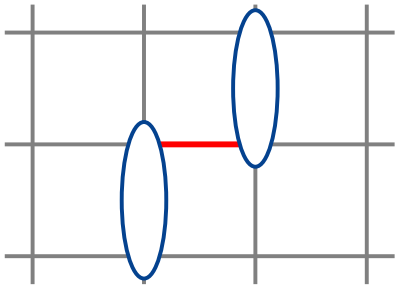
# Case for a Second Order Néel-Liquid-VBS transition

$$h(r) = 1/r^3$$

**Bond correlation factors**



$w = p > 1$



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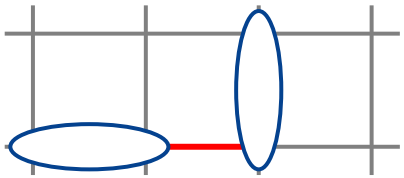

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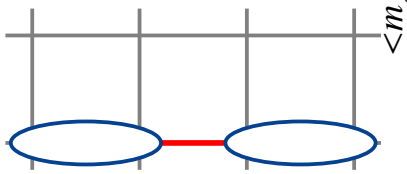

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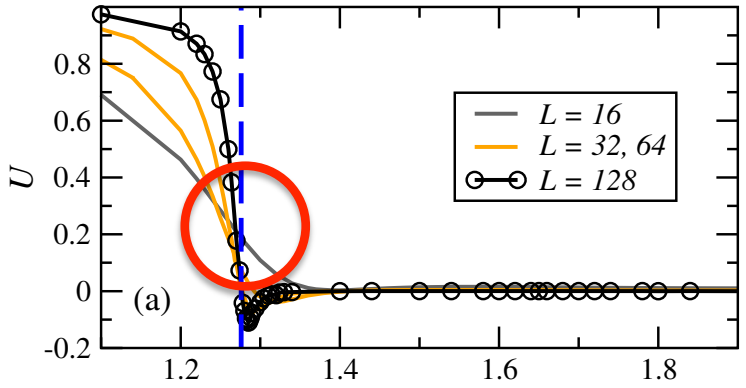
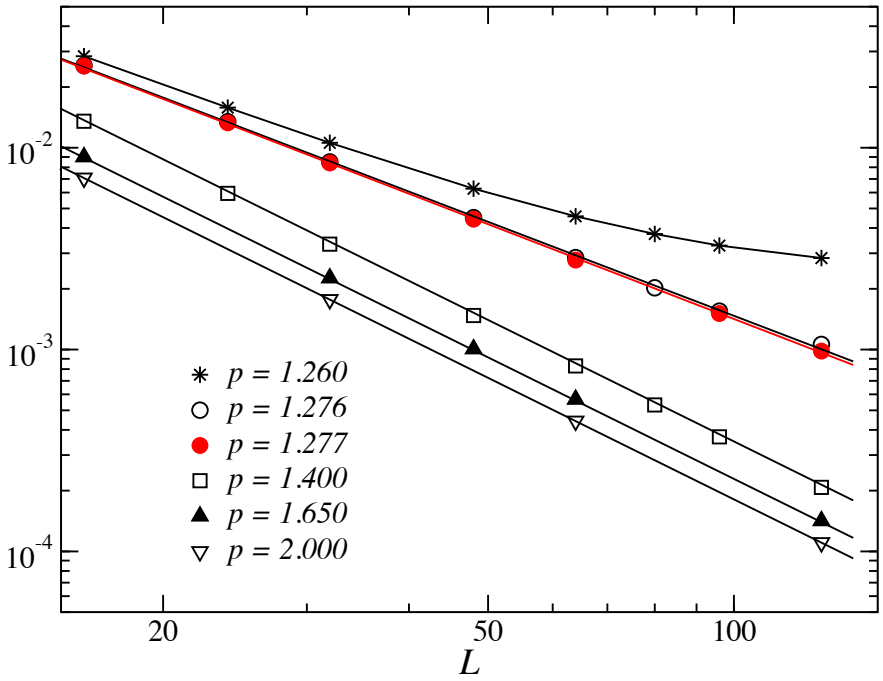
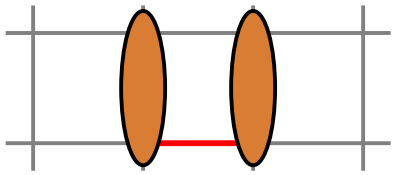


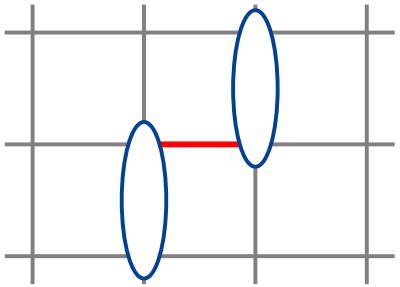
# Case for a Second Order Néel-Liquid-VBS transition

$$h(r) = 1/r^3$$

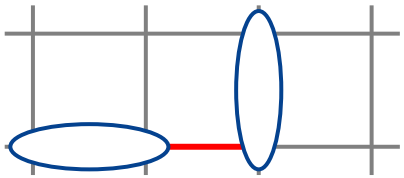
**Bond correlation factors**



$w = p > 1$



$w = 1$



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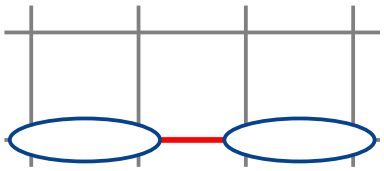

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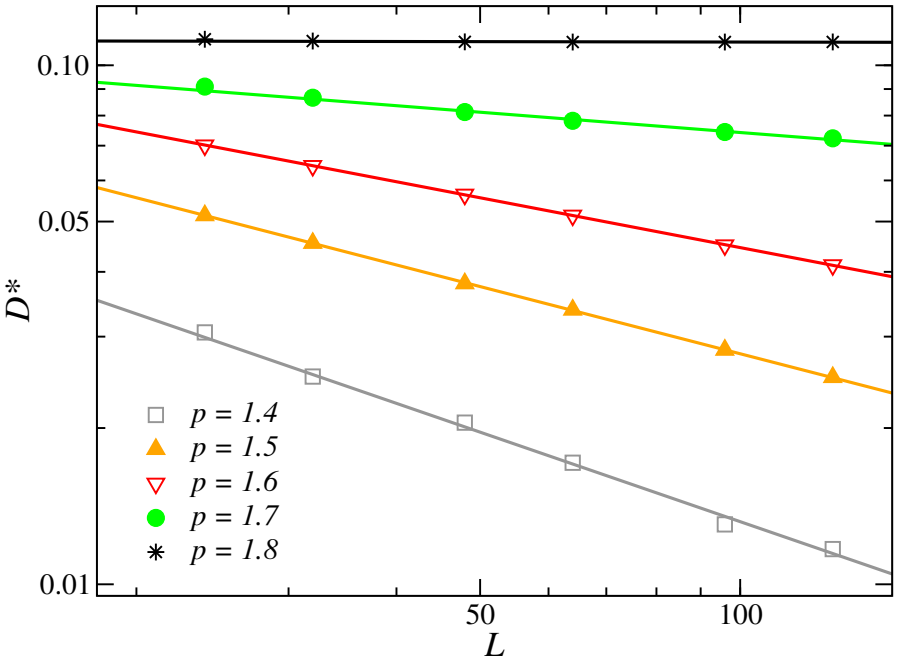
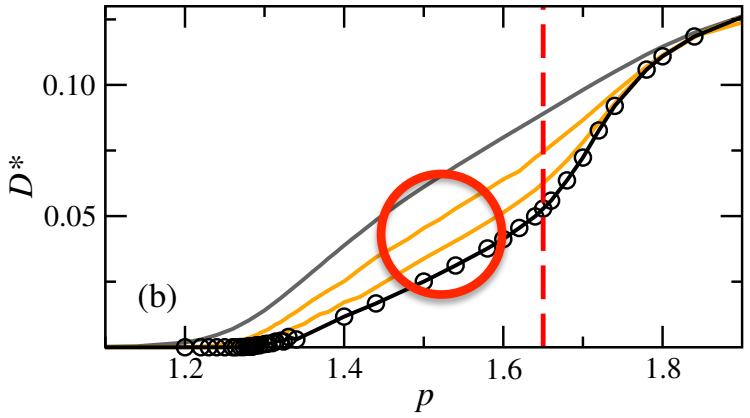
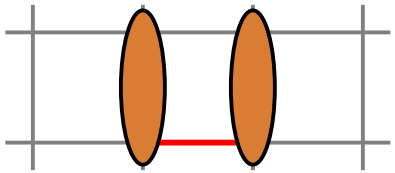


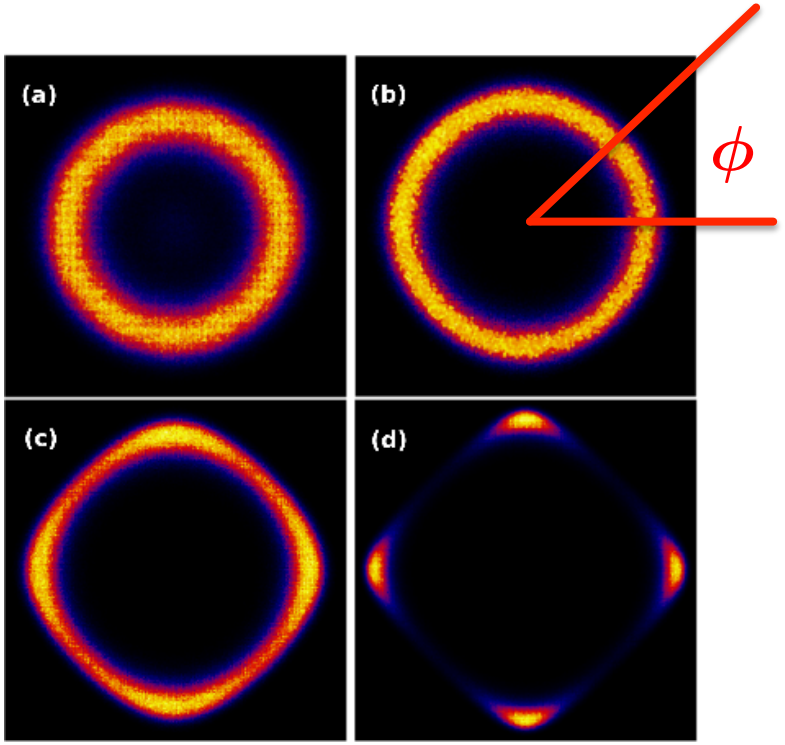
# Case for a Second Order Néel-Liquid-VBS transition

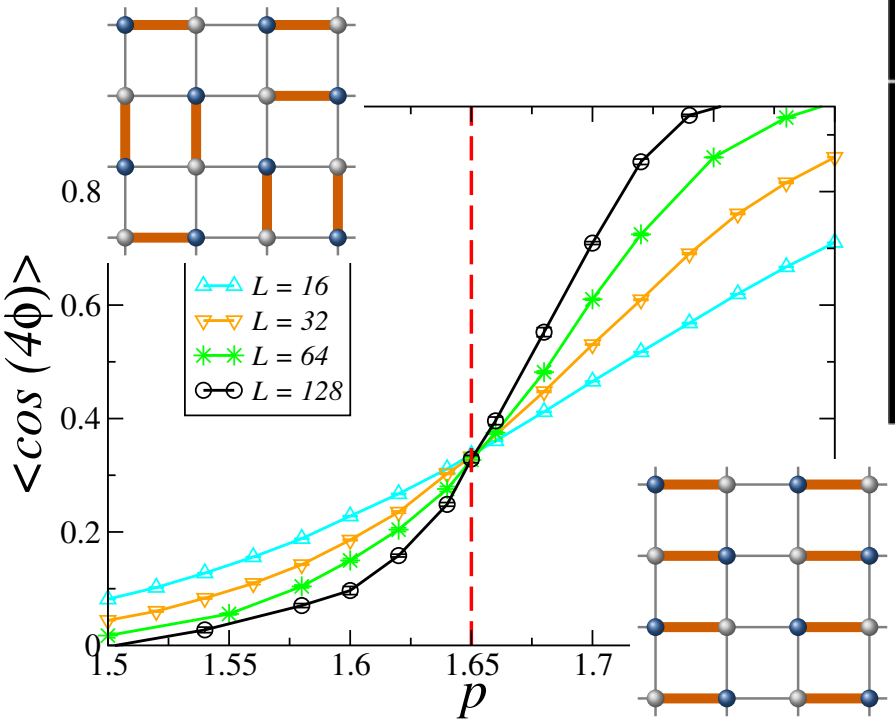
$$h(r) = 1/r^3$$



$$w = p > 1$$

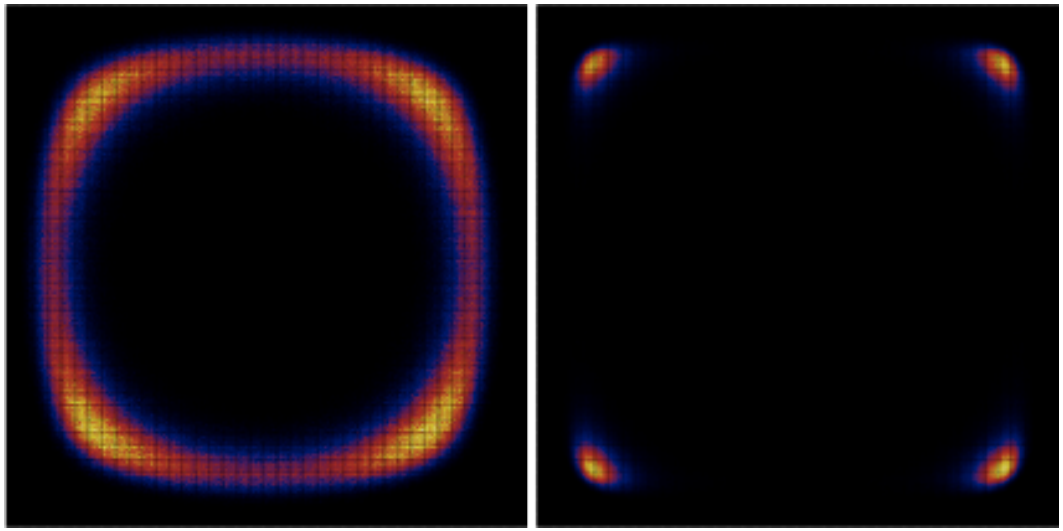
Distribution $P(d_x, d_y)$



# Outlook

- Study the nature of the transition from a Neel state to a plaquette VBS.
- Find a parametrization of the correlated AP states such that a QDC point is obtained.



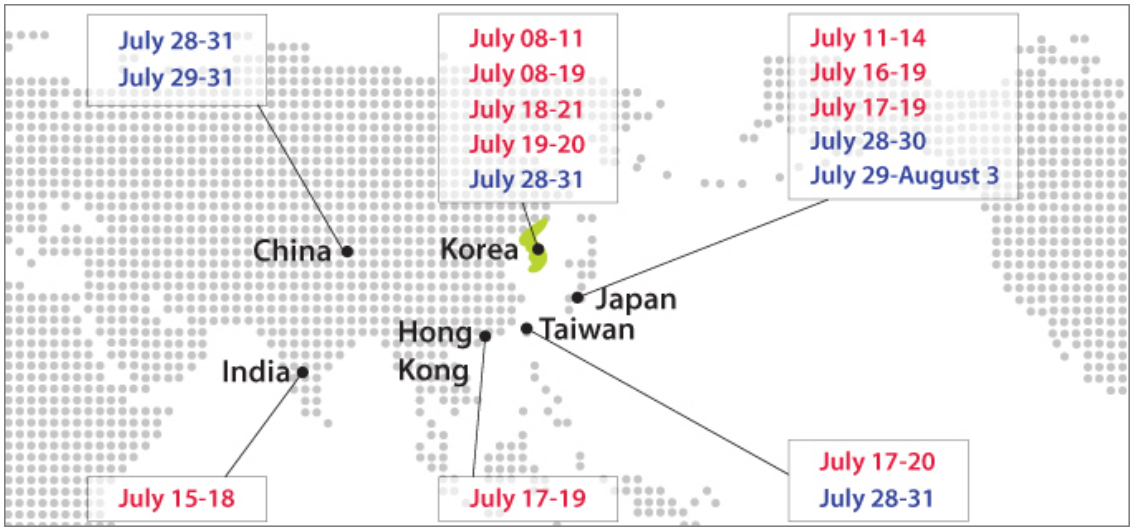
# Upcoming...

## ❑Statistical Physics of Quantum Matter

--satellite meeting to STATPHYS 25

- ❑ **When:** ***July 28-31***
- ❑ **Where:** ***Taipei, Taiwan***

quantum Monte Carlo simulations, tensor-product states, novel quantum states and quantum phase transitions, entanglement, quantum dynamics, frustrated quantum magnets, cold-atom systems...



# Valence-Bond vs. Spin Representation

- **Define**

$$|Z\rangle = |s_1^z, \cdots, s_N^z\rangle$$

- **A VB state**

$$|v\rangle = \frac{-1}{2^{N/4}} \sum_{\alpha=1}^{2^{N/2}} (-1)^{A_\uparrow} \; |Z_\alpha\rangle$$

where $A_\uparrow$ is the number of $\uparrow$ on the sublattice A.

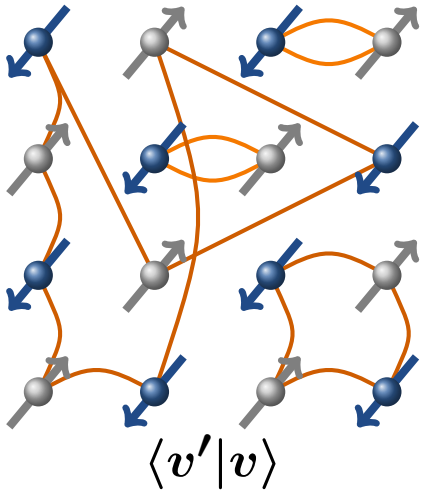
e.g.: $(i,j) = (|\uparrow_i\downarrow_j\rangle - |\downarrow_i\uparrow_j\rangle)/\sqrt{2}$

- **Overlap**

$$\langle v'|v\rangle = \frac{1}{2^{N/2}} \sum_{\alpha,\beta} \langle Z_\beta|Z_\alpha\rangle (-1)^{A_\uparrow^\alpha + A_\uparrow^\beta}$$

only the terms with $Z_\alpha = Z_\beta$ contribute.

$$\Rightarrow \quad \langle v'|v\rangle = 2^{N_{\text{loop}} - N/2}$$

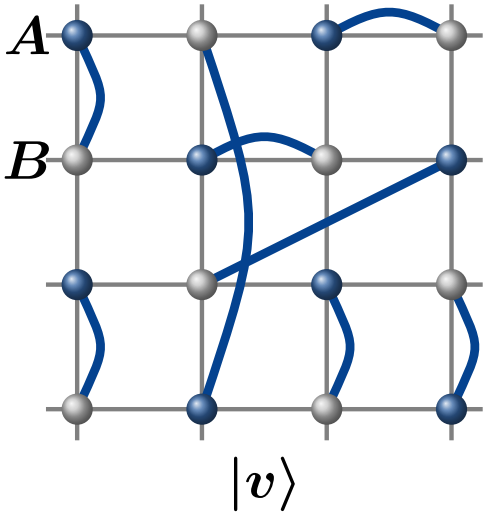


# Valence Bond (VB) States for S=1/2 spins

**VB state:** a set of singlets between A and B sublattice sites on a bipartite lattice

$$|v\rangle = \bigotimes_{ij} (i,j)$$

$$(i,j) = \frac{1}{2}\left[|\uparrow_i\downarrow_j\rangle - |\downarrow_i\uparrow_j\rangle\right]$$




$|v\rangle$

**VB basis:** overcomplete & non-orthogonal

- expansion of an arbitrary singlet state (not unique)

$$|\psi\rangle_{S=0} = \sum_v f_v |v\rangle$$

- useful for
  - quantum Monte Carlo [A.W. Sandvik (2005)]
  - definition of entanglement entropy
    - valence bond entropy [Alet et. al. (2007); YCL & A.W. Sandvik (2010)]
    - Renyi entanglement entropy [M.B. Hastings , R. Melko et. al. (2010)]
    - loop entropy [YCL & A.W. Sandvik (2010)]
  - definition of variational states [Liang, Doucot, Anderson (1988)]