Wednesday, September 16th

Valence bond states: link models

Quantum Information and Condensed Matter Physics

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Annals of Physics 323 (2008) 2115-2131. arXiv:0710.2349
Annals of Physics 324 (2009) 1875-1896. arXiv:0811.1049

What is this talk about?

We look for a 2D spin system in a square lattice with a ground state such that:

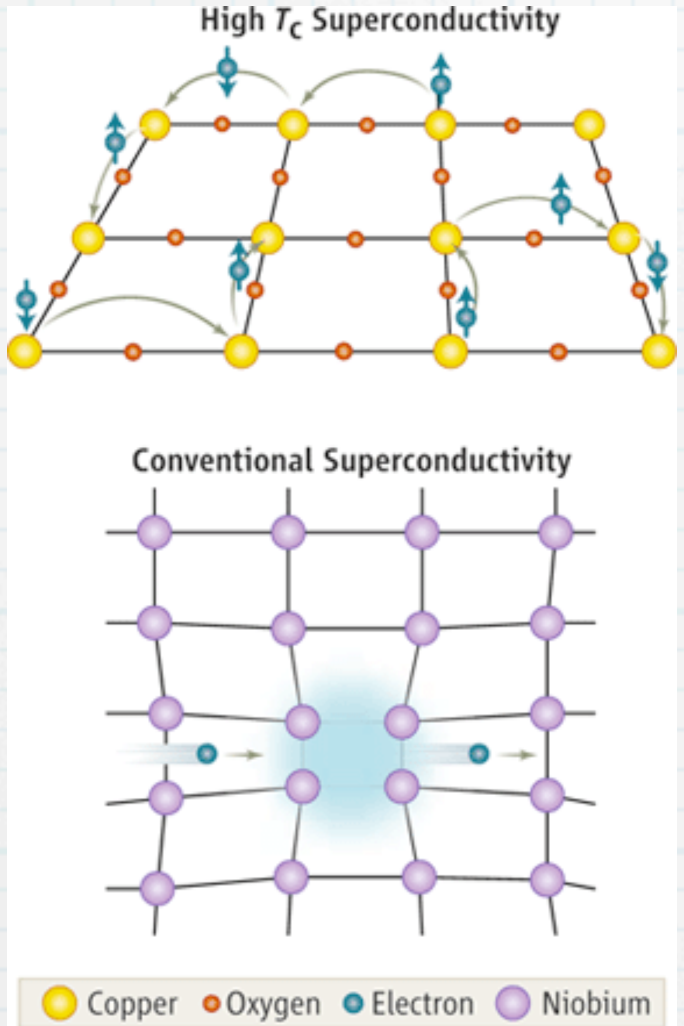
i. Real singlet state of SU(2) (non-chiral).
ii. Homogeneous, translationally and rotationally invariant.
iii. With a local spin-1 representation.
iv. Unique ground state of a nearest neighbor Heisenberg-like hamiltonian.

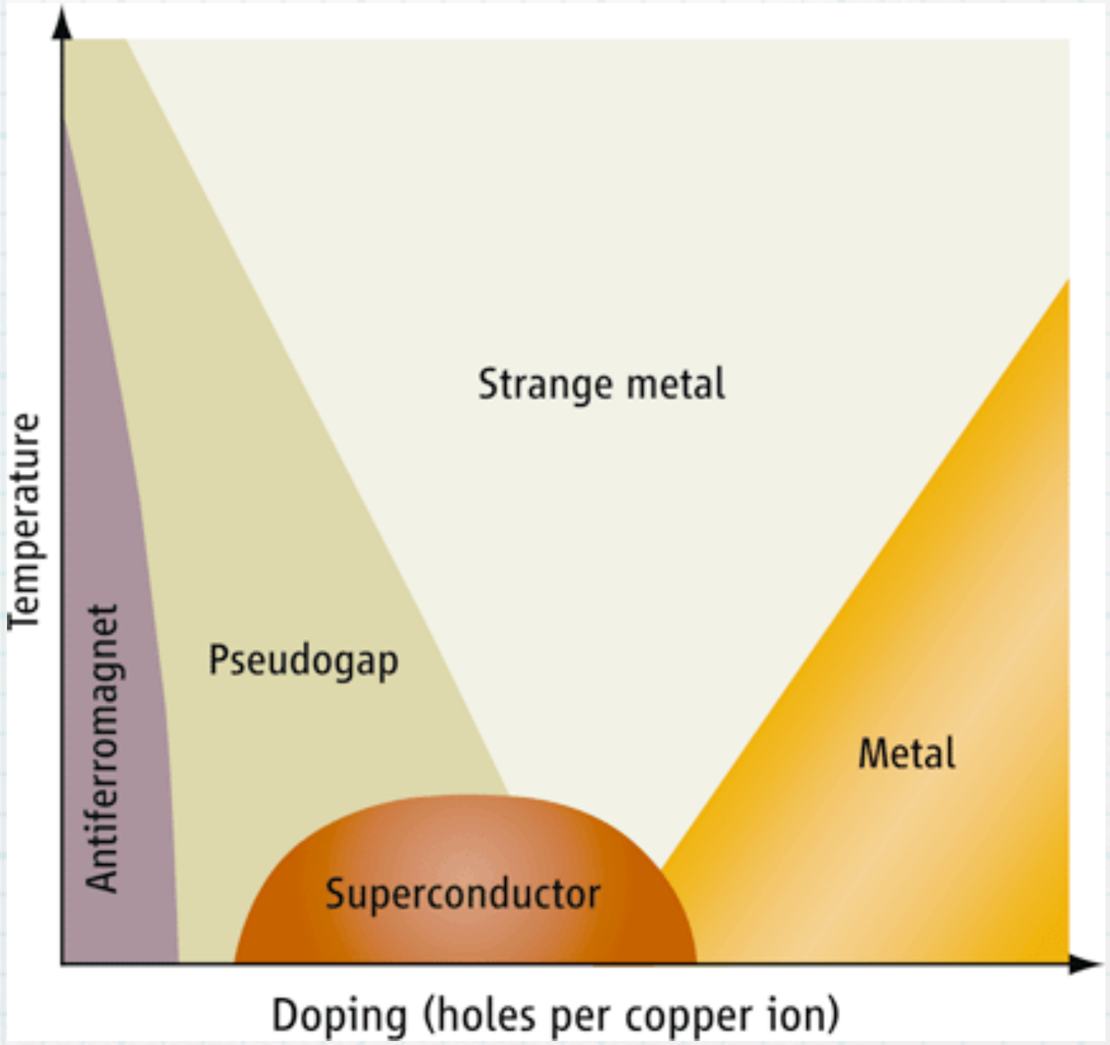
Contents

* Motivation.
  - Quantum spin liquids. (Why are VBS interesting?).
  - Example of spin liquids in 1D (AKLT model)
  - Entanglement of spins on a square lattice.
* 2D multipartite valence bond states.
* Ground state properties and correlations.
  - Field theory: bosonization
  - Numerical methods: D.M.R.G., C.O.R.E, exact diagonalization
* Antiferromagnetic Mott-Hubbard insulator. Neutron scattering

Quantum spin liquids

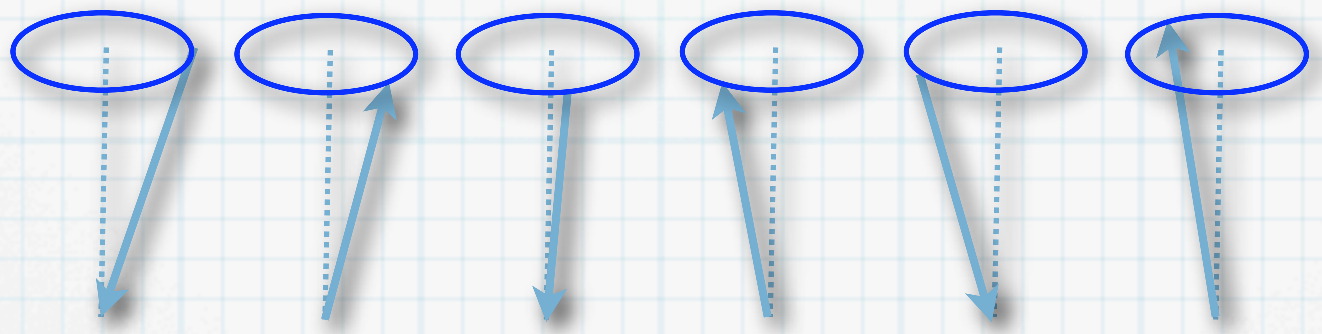
What is the responsible mechanism that causes certain materials to exhibit high-temperature superconductivity?





Spin liquids ground states believed to be related to high-temperature superconductivity [P. Anderson, Science, 235: 1196-1198, 1987]

Quantum spin liquids



$$\langle \hat{S}_m^\alpha \hat{S}_n^\alpha \rangle \rightarrow \text{const} \neq 0$$

Neel state and anti-ferromagnetic spin wave

What are the possible ground states of 2D Heisenberg-like models when magnetic long-range order has been destroyed?

* A spin liquid is a quantum state without magnetic long-range order.
* A spin liquid is a state without any spontaneous broken symmetry.

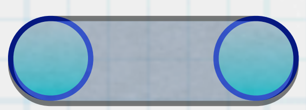
Quantum spin liquids

Example of 1D spin liquid- AKLT model

[I. Affleck, T. Kennedy, E.H. Lieb, H. Tasaki. Phys. Rev. Lett. 59, 799 (1987)]

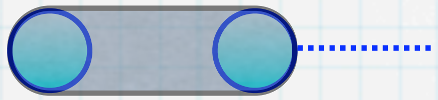
$$|\alpha\rangle = \begin{cases} |\uparrow\rangle \\ |\downarrow\rangle \end{cases}$$

$$|\alpha\rangle\epsilon_{\alpha\beta}|\beta\rangle = |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$$



$$\Psi_{\alpha\beta} = \frac{|\alpha\rangle|\beta\rangle + |\beta\rangle|\alpha\rangle}{\sqrt{2}} = \begin{cases} \sqrt{2}|+1\rangle & \alpha = \beta = \uparrow \\ |0\rangle & \alpha \neq \beta \\ \sqrt{2}|-1\rangle & \alpha = \beta = \downarrow \end{cases}$$

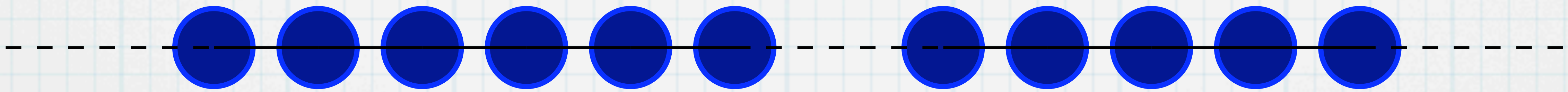
Quantum spin liquids



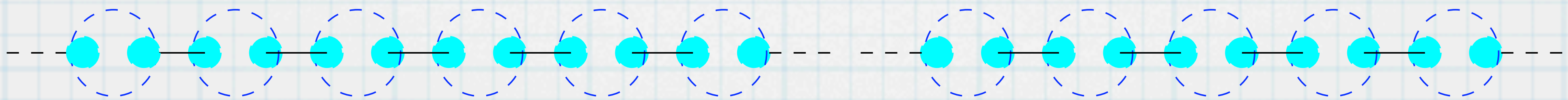
$$(\Psi \cdot \epsilon)_{\alpha\beta} = \frac{1}{\sqrt{3}} \left(\sigma^x_{\alpha\beta} |x\rangle + \sigma^y_{\alpha\beta} |y\rangle + \sigma^z_{\alpha\beta} |z\rangle \right) = \sum_s A^s_{\alpha\beta} |s\rangle$$

$$|x\rangle \propto |\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle = |+1\rangle + |-1\rangle$$

$$|y\rangle \propto |\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle = |+1\rangle - |-1\rangle \qquad |z\rangle \propto |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle = |0\rangle$$

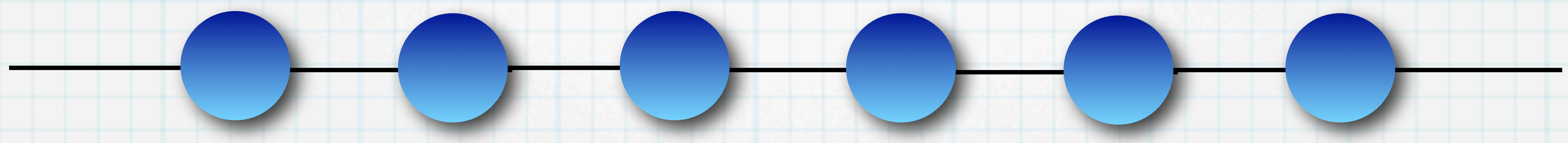


$\sigma^{s_{i-2}} \sigma^{s_{i-1}} \sigma^{s_i} \sigma^{s_{i+1}} \qquad \sigma^{s_{j-1}} \sigma^{s_j} \sigma^{s_{j+1}}$



Quantum spin liquids

Antiferromagnetic spin-1 chain



No long-range order: $\langle \hat{S}_n^\alpha \hat{S}_m^\beta \rangle = \delta_{\alpha\beta} \, (-1)^{m+n} \, e^{-|m-n|/\xi}$

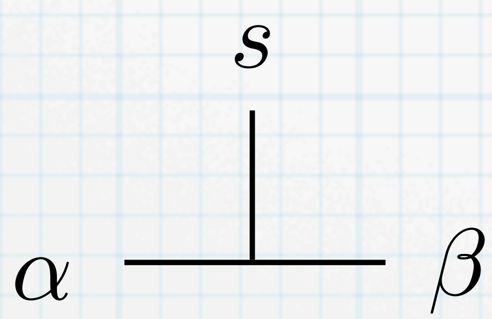
Singlet state: $\langle \hat{S}_n^x \rangle = \langle \hat{S}_n^y \rangle = \langle \hat{S}_n^z \rangle = 0$

Translationally invariant

Quantum spin liquids

Some properties:

i) Composition rules.-



$$\frac{1}{2} \otimes \frac{1}{2} = 0 \oplus 1$$

$$0 \otimes \frac{1}{2} = \frac{1}{2} \qquad \frac{1}{2} \otimes 1 = \frac{1}{2} \qquad \Rightarrow SU(2)_2$$

ii) Boundary conditions and degeneracy.-

Periodic boundary conditions = Unique state
Open boundary conditions = 4-fold degeneracy

Quantum spin liquids

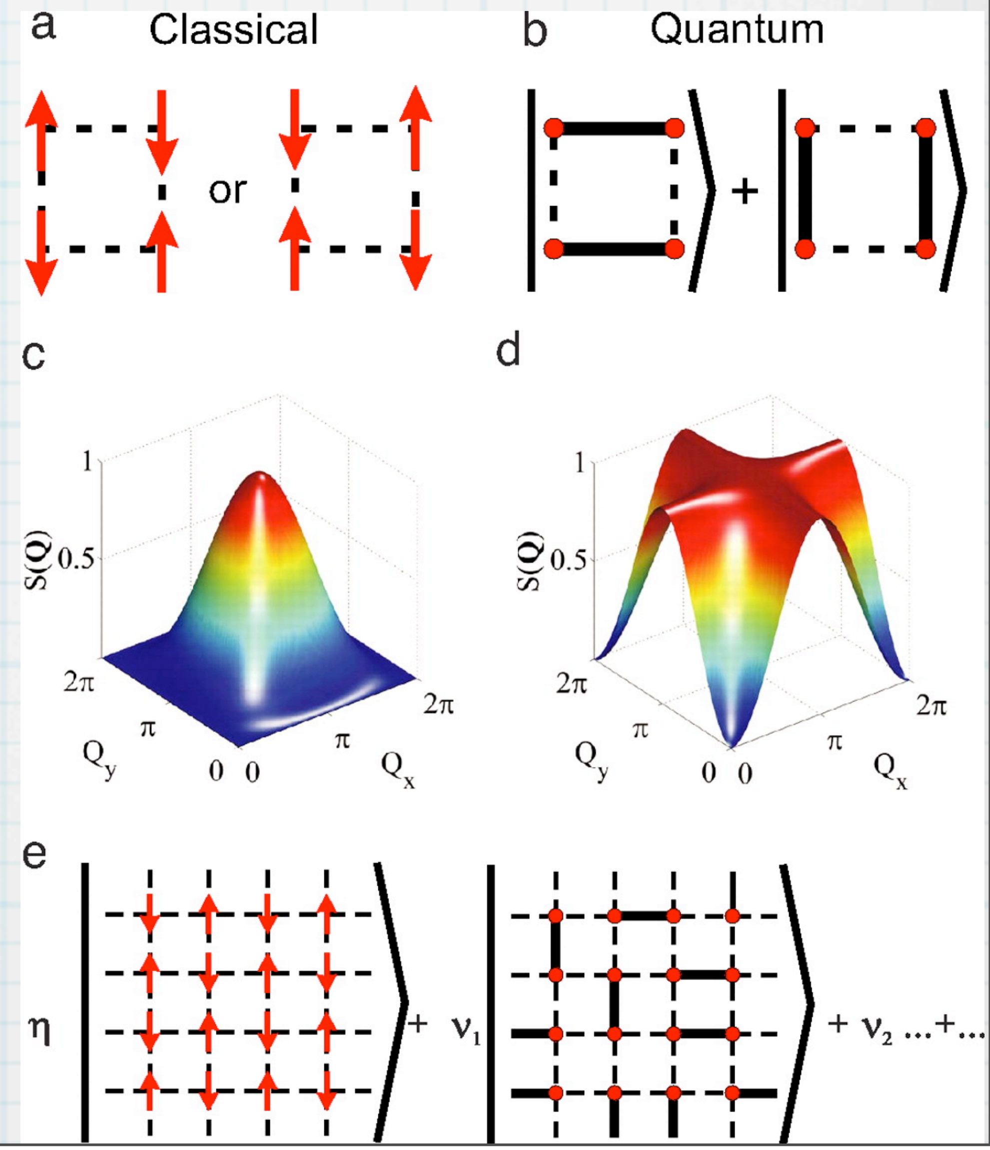
iii) Two-point correlation function.- Exponential decay.
Correlation length smaller than the lattice spacing

iv) Non-local order parameter.-

String order parameter and entanglement length
den Nijs, Rommelse (1989)
Cirac, Martin-Delgado, Popp, Verstraete (2005)

Entanglement of spins on a square lattice

Experiment shows an anti-ferromagnetic ground state substantially different from "Neel order + minor QM corrections"
[N.B. Christensen et al., PNAS, 104: 15264-15269, 2007]



- 2D spin-1/2 system (cuprates)
- "substantial deviation" occurred at length scale about "distance between two sites"
- deviation believed to be entanglement related

2D multipartite valence bond state

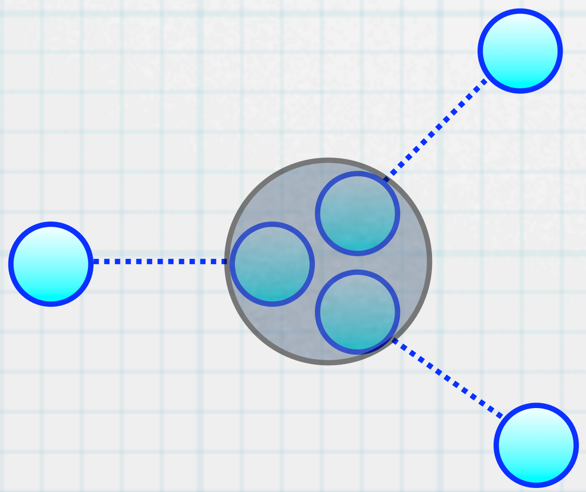
Requirements:

i) Real singlet state of SU(2) (non-chiral).

ii) Homogeneous, translationally and rotationally invariant.

iii) With a local spin-1 representation.

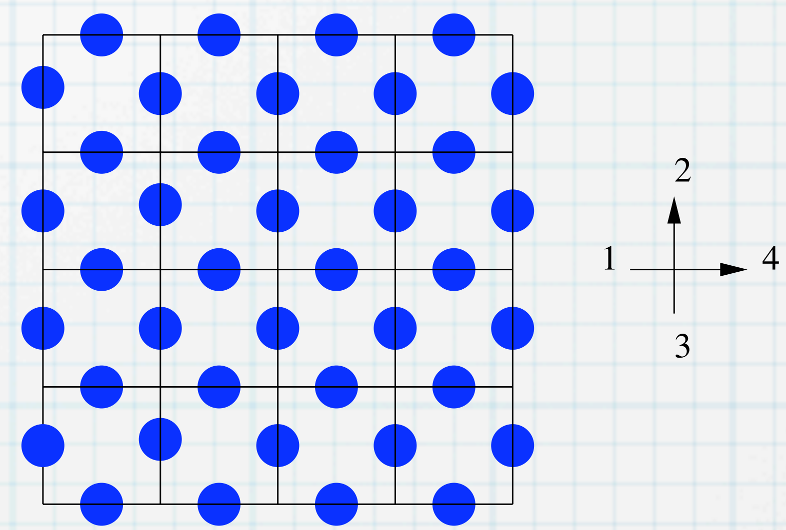
iv) Ground state of a nearest neighbor Hamiltonian.



Minimum spin representation: 3/2

2D multipartite valence bond state

We place the physical Hilbert space at every link of the lattice

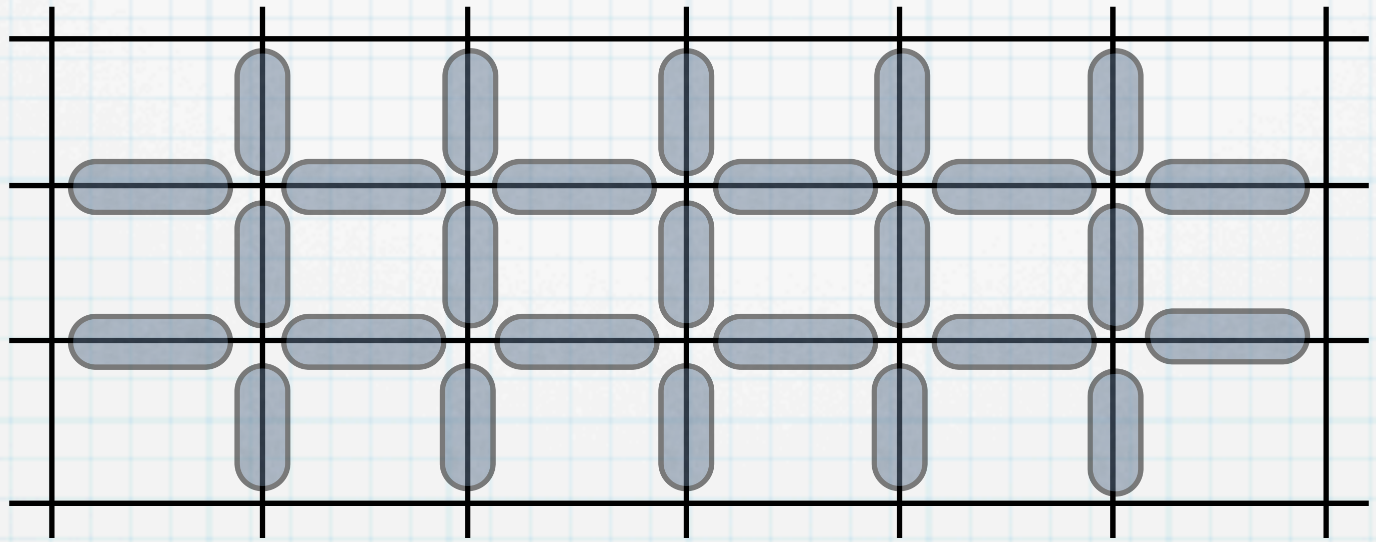


Local spin-1 representation

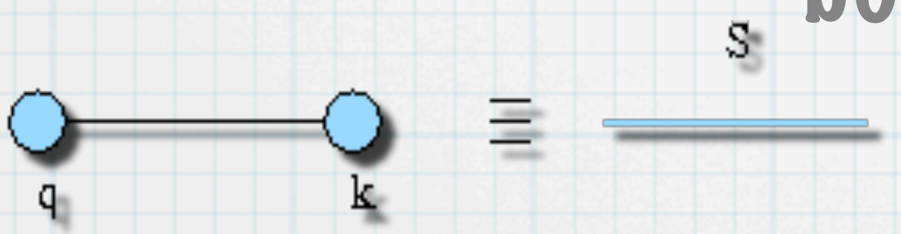
$$|\alpha\rangle = \begin{cases} |\uparrow\rangle \\ |\downarrow\rangle \end{cases}$$

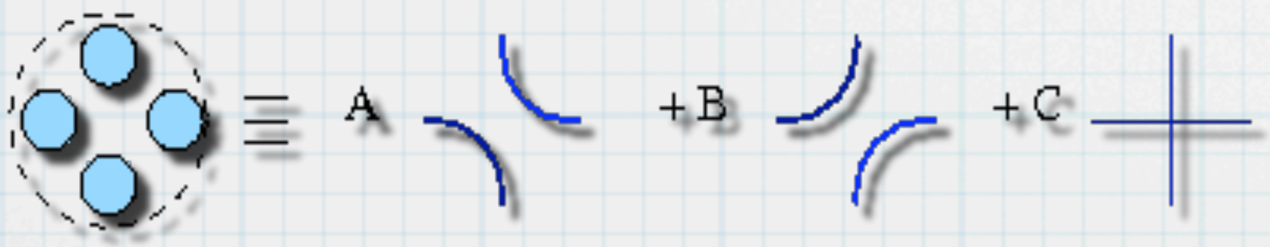
$$\Psi_{\alpha\beta} = \frac{|\alpha\rangle|\beta\rangle + |\beta\rangle|\alpha\rangle}{\sqrt{2}} = \begin{cases} \sqrt{2}|+1\rangle & \alpha = \beta = \uparrow \\ |0\rangle & \alpha \neq \beta \\ \sqrt{2}|-1\rangle & \alpha = \beta = \downarrow \end{cases}$$

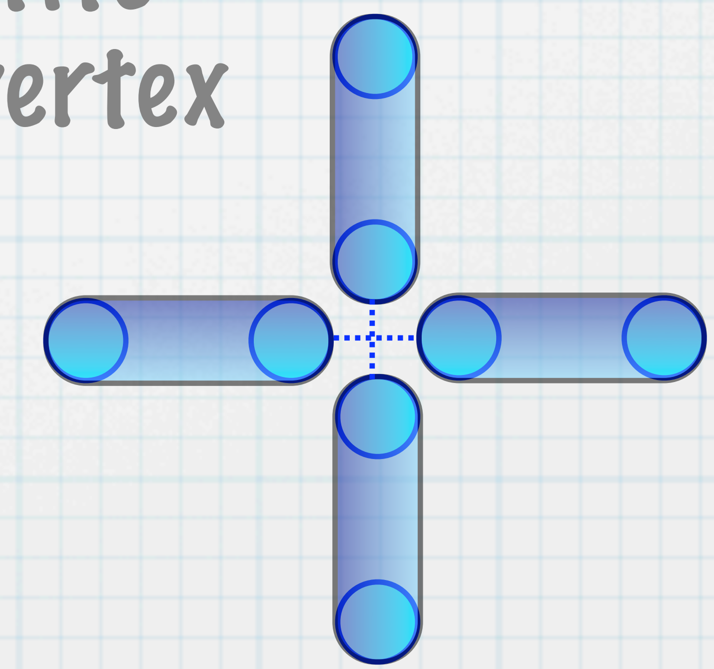
2D multipartite valence bond state



We need a multipartite bond state at every vertex



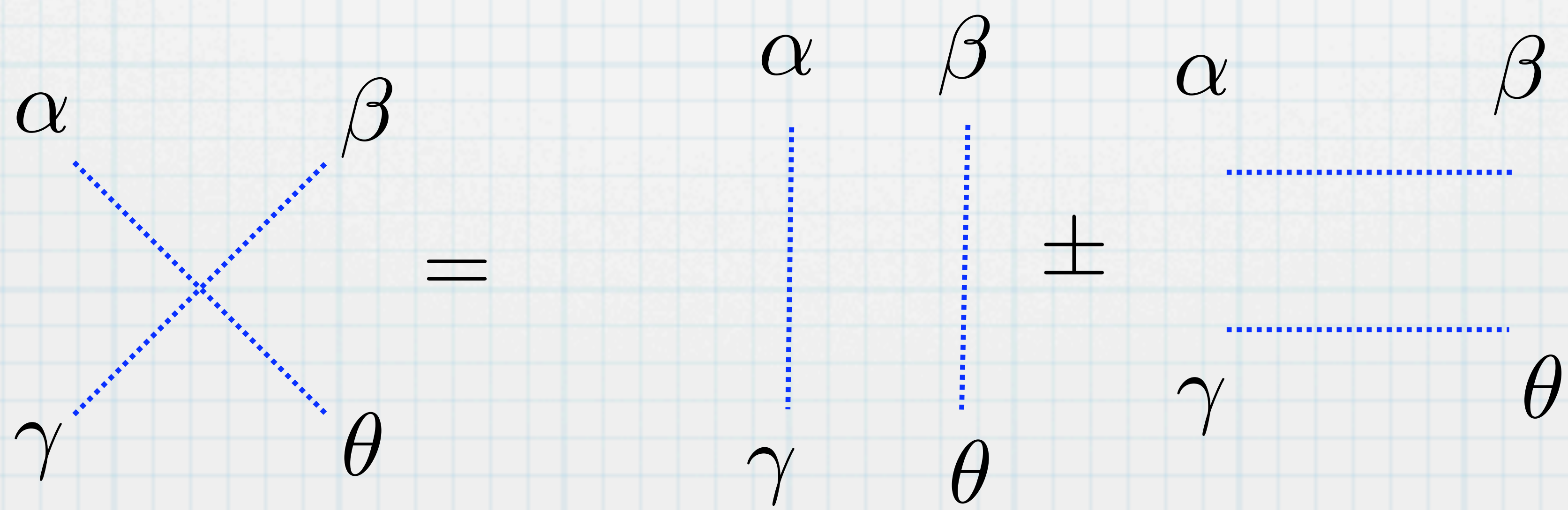




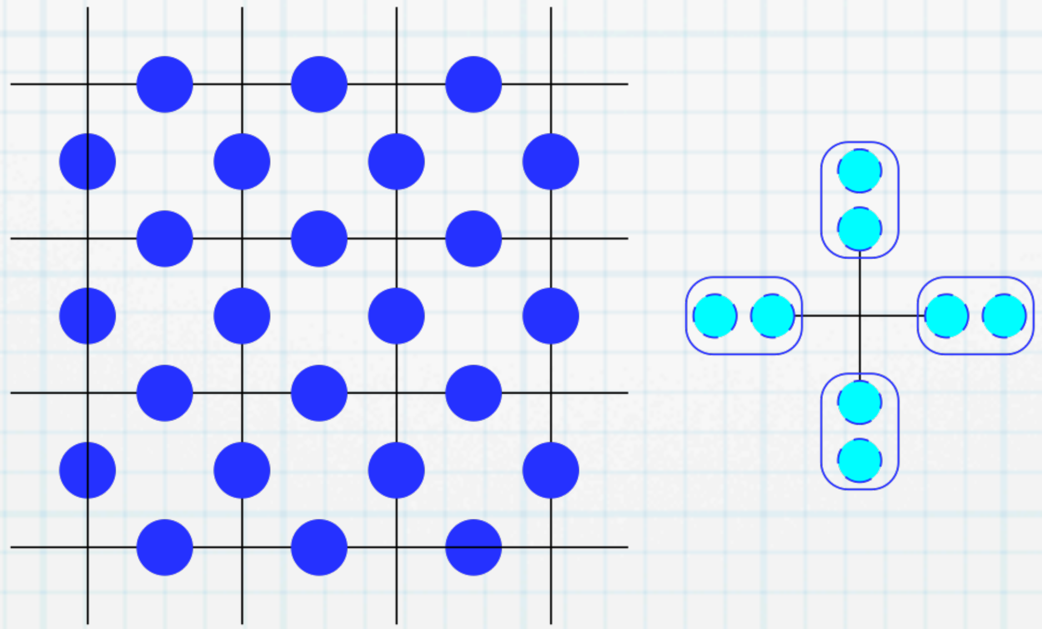
2D multipartite valence bond state

* Real singlet state of SU(2) (non-chiral).
* Homogeneous, translationally and rotationally invariant.

$$|\alpha\rangle \epsilon_{\alpha\beta} |\beta\rangle = |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$$



2D multipartite valence bond state



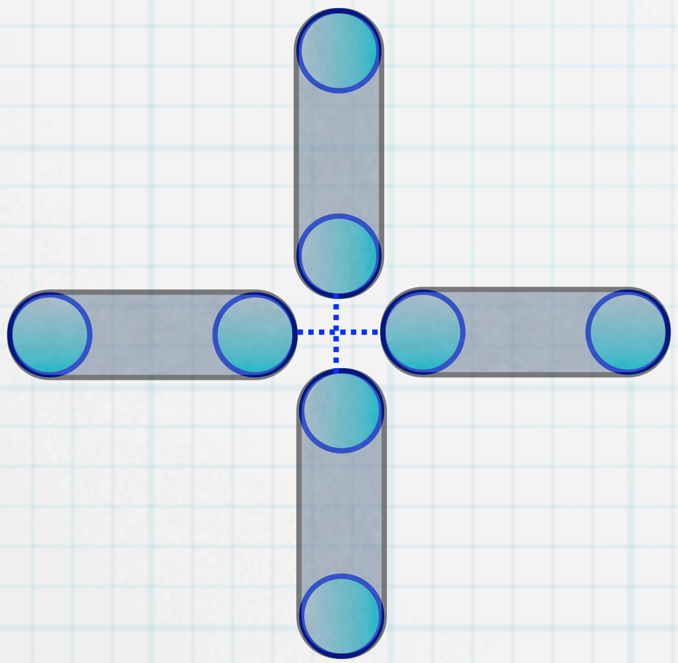
i. The physical Hilbert space is placed at the links of the lattice.

ii. The Hamiltonian is made out of nearest neighbor Heisenberg-like interactions.

iii. It is homogeneous, translationally and rotationally invariant.

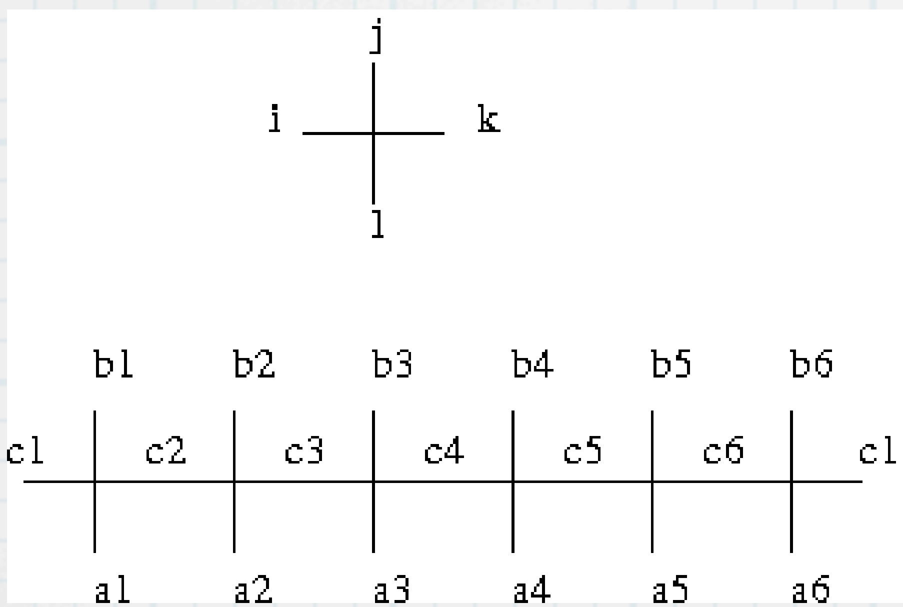
iv. The ground state is a real singlet state of SU(2) (non-chiral).

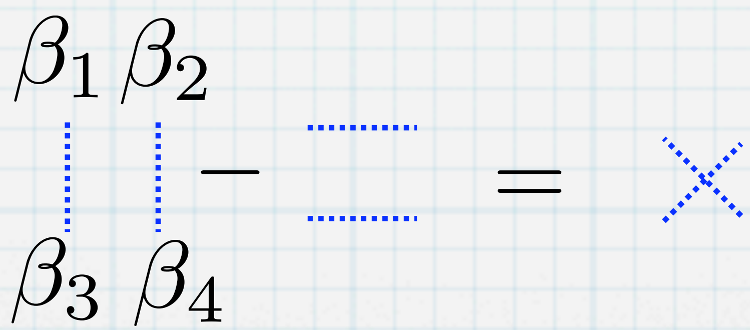
Ground state properties and correlations



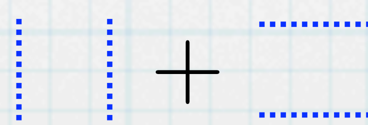
Locally:- $\psi_{\alpha_1\beta_1}\psi_{\alpha_3\beta_3}\Gamma^{\beta_1\beta_2}_{\beta_3\beta_4}\psi_{\beta_2\alpha_2}\psi_{\beta_4\alpha_4}$

$$\langle \mathrm{VBS}|\mathrm{VBS}\rangle = \sum_{\text{configuration}} \prod_{\text{lattice}} R^{ij}_{lk} = \mathcal{Z}_{2D}$$





Uncorrelated chains



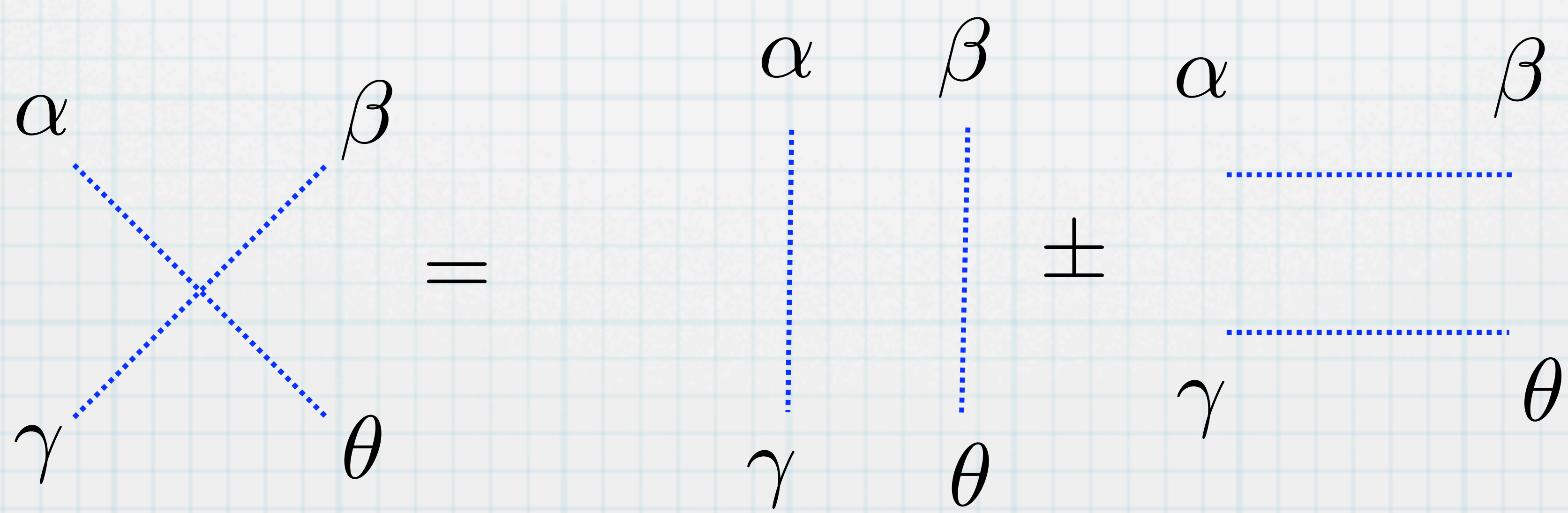
Critical theory

Ground state properties and correlations

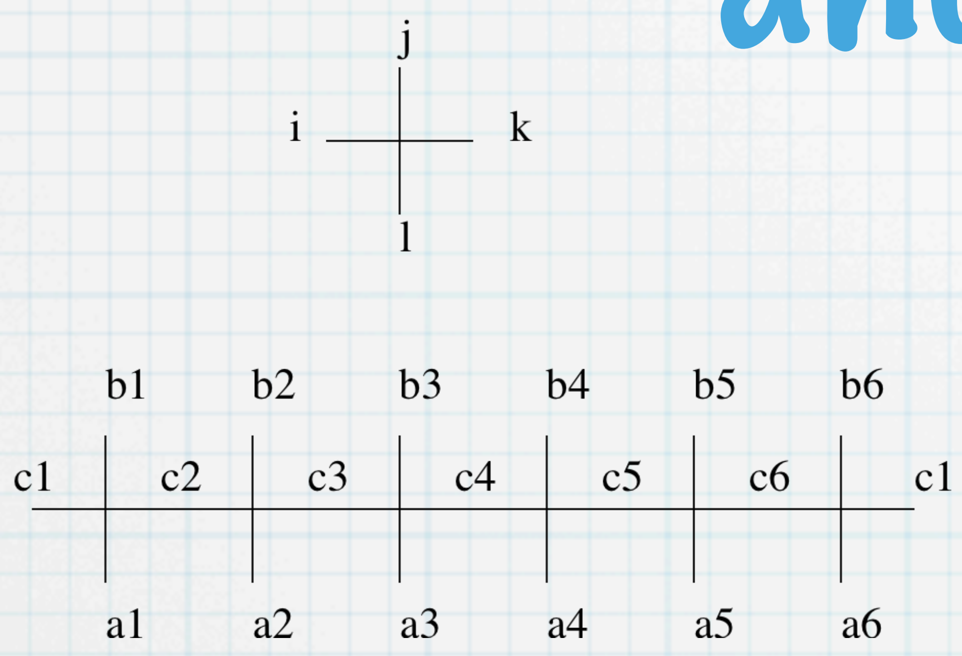
Some generalization:-

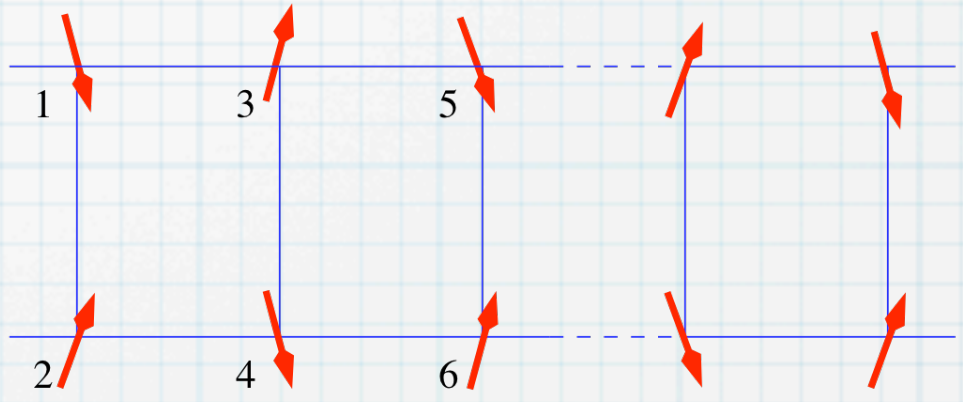
$$\Psi = a(s)\sigma^0|0\rangle + a(t)\left(\sigma^x|x\rangle + \sigma^y|y\rangle + \sigma^z|z\rangle\right)$$

$$a(s) = \frac{\sqrt{1+3\Lambda}}{2} \qquad a(t) = i\,\frac{\sqrt{1-\Lambda}}{2}$$



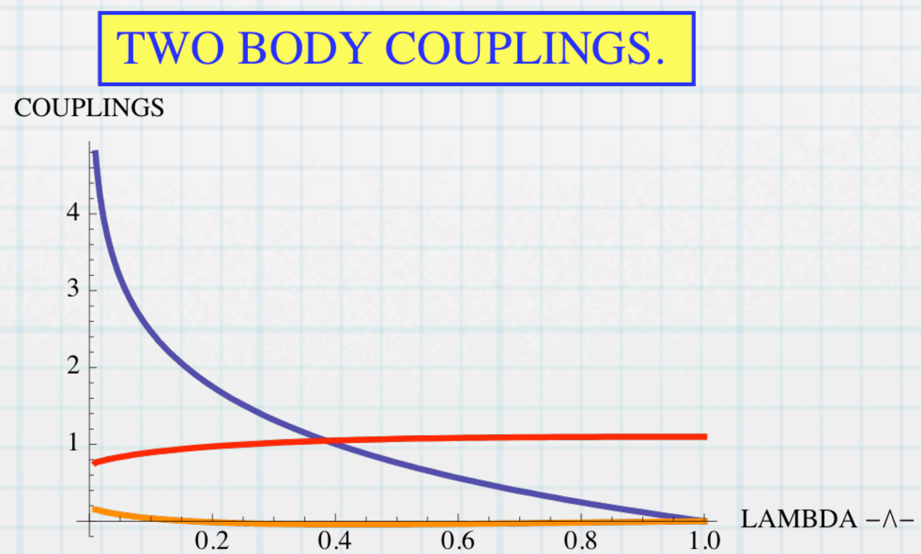
Ground state properties and correlations





$$H = \beta_1 \left((\vec{S}_1 \cdot \vec{S}_2) + (\vec{S}_3 \cdot \vec{S}_4) \right) + \beta_2 \left((\vec{S}_1 \cdot \vec{S}_3) + (\vec{S}_2 \cdot \vec{S}_4) \right) + \beta_3 \left((\vec{S}_1 \cdot \vec{S}_4) + (\vec{S}_2 \cdot \vec{S}_3) \right)$$
$$+\beta_4 \left((\vec{S}_1 \cdot \vec{S}_2)(\vec{S}_3 \cdot \vec{S}_4) \right) + \beta_5 \left((\vec{S}_1 \cdot \vec{S}_3)(\vec{S}_2 \cdot \vec{S}_4) \right) + \beta_6 \left((\vec{S}_1 \cdot \vec{S}_4)(\vec{S}_2 \cdot \vec{S}_3) \right)$$

Any expectation value is obtained via a mapping of the 2D quantum state to a 2D classical statistical model and from there to a 1d quantum mechanical problem using a transfer matrix defined from the 2D quantum state.



Ground state properties and correlations

First analysis: Continuum limit:-

[A.M. Tsvelik. Phys. Rev. B42, 10499 (1990)]

$$H = \sum_{\mu=\{x,y,z\}} H_{m_t}[\check{a}^\mu] + H_{m_s}[\check{a}^0]$$

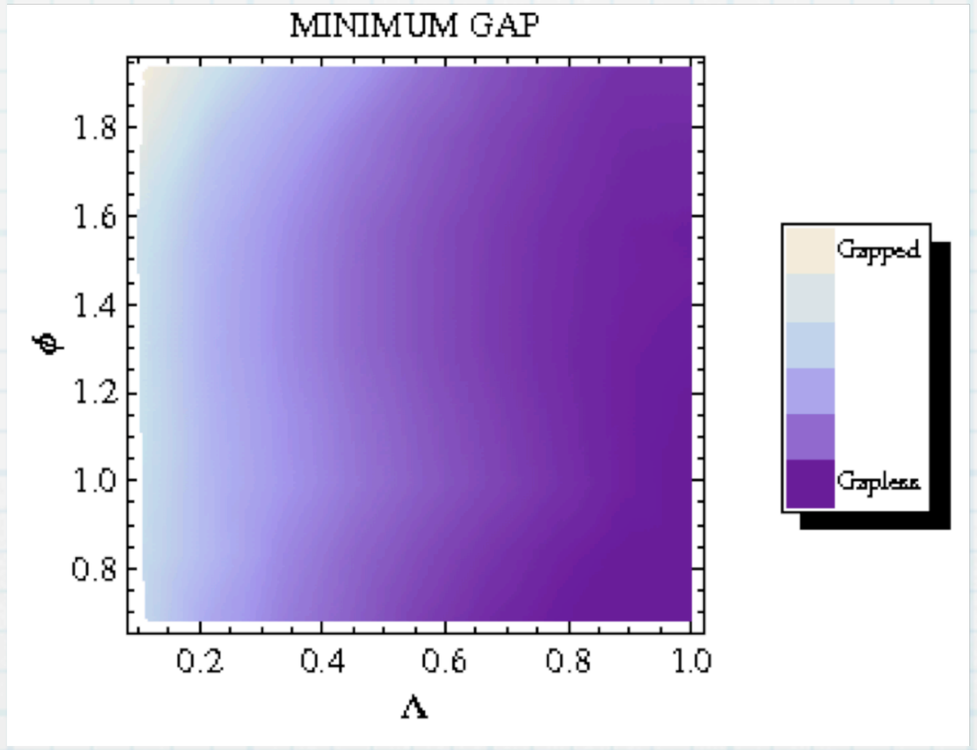
$$H = \frac{iv_{\rm eff}}{2} \int dx \, (\check{a}_L \partial_x \check{a}_L - \check{a}_R \partial_x \check{a}_R) + im \int dx \, (\check{a}_L \check{a}_R)$$

The ladder problem is equivalent to four Ising models.
The only relevant operator is a mass term.

Ground state properties and correlations

Relevance of the parameters:

Inverse of the gap in the ladder = Correlation length in the 2D VBS.



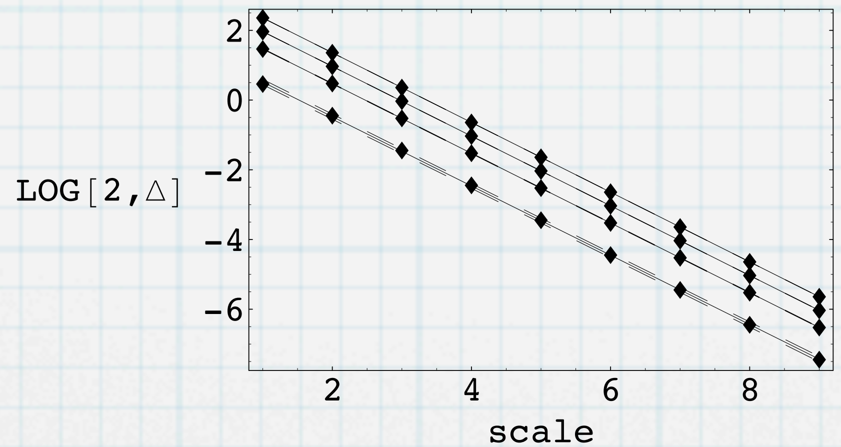
D.M.R.G. results with a sample of 100 points

Ground state properties and correlations

Two points correlation function: Exponential or algebraic decay?

$$g(\vec{r}_i - \vec{r}_j) = \langle 0|\vec{S}_i \cdot \vec{S}_j|0\rangle \simeq e^{-\frac{|\vec{r}_i - \vec{r}_j|}{\xi}}$$

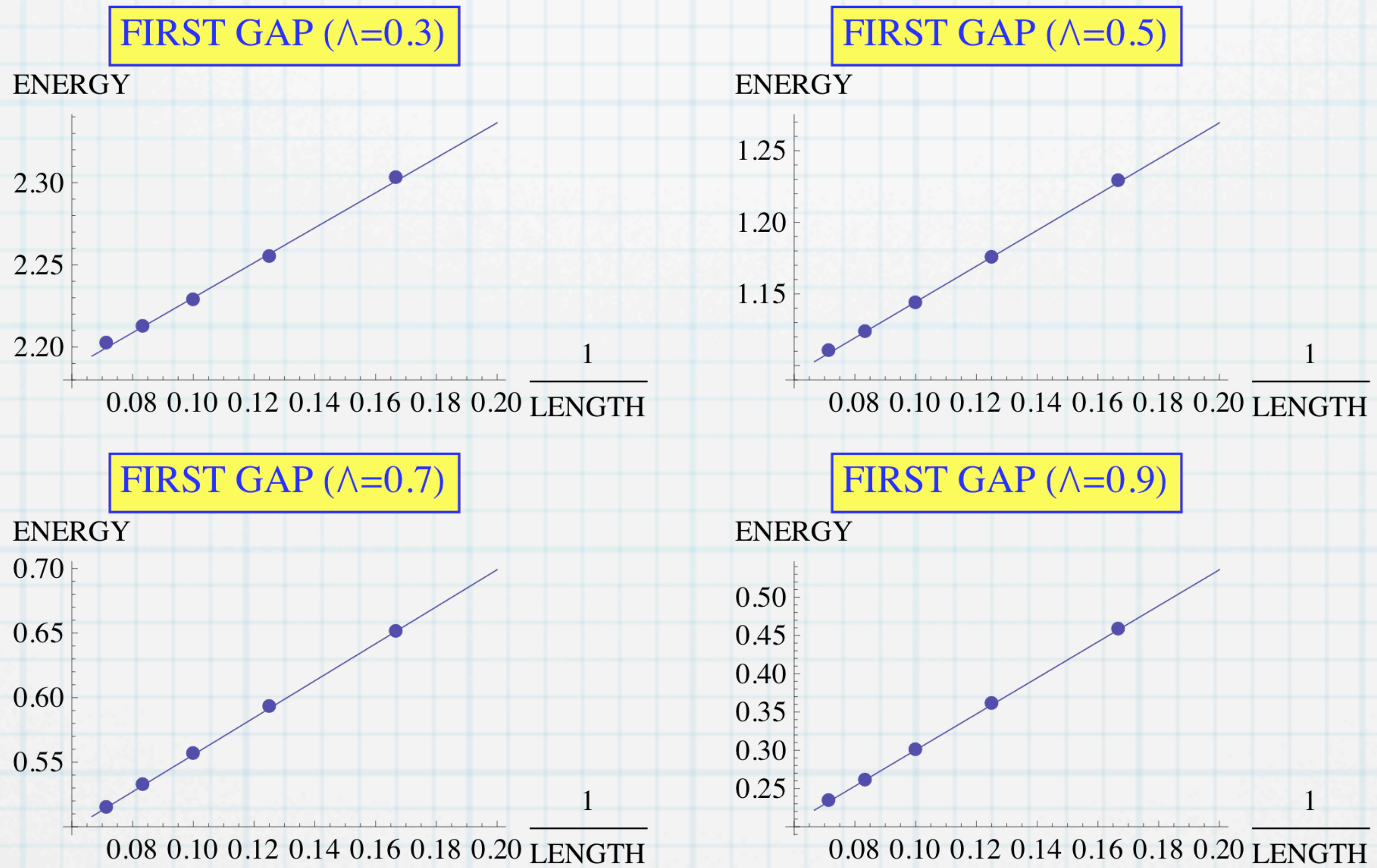
$$\Delta \simeq \frac{1}{\xi} \simeq N^{-\theta} \qquad \theta \simeq 0.99(4)$$



Numerical results obtained from CORE calculations
Data, fitted curve and 95% confidence interval

Ground state properties and correlations

Two points correlation function: Exponential or algebraic decay?

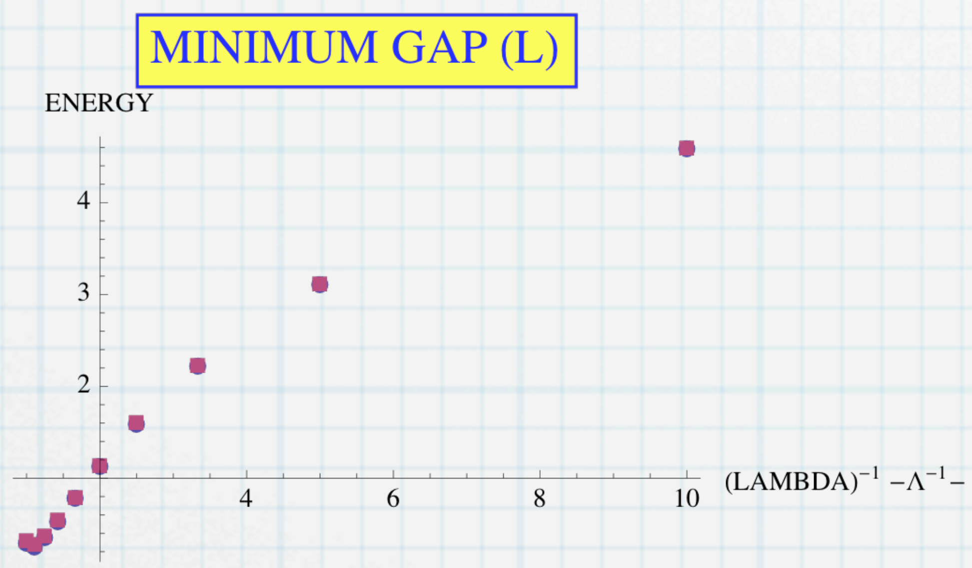


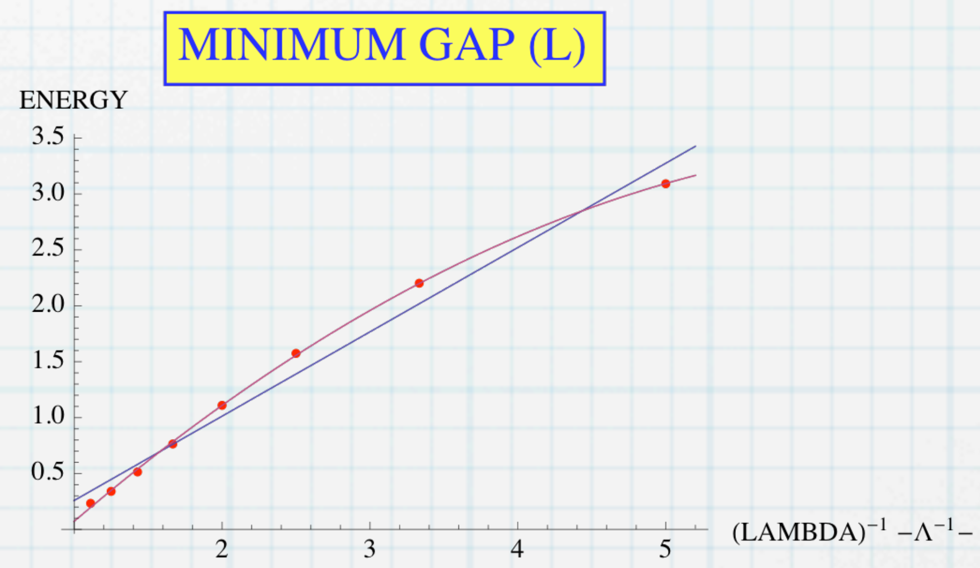
Results from D.M.R.G., C.O.R.E and exact diagonalization of the first energy gap as a function of the length and scale. All plots show a clear linear dependence of the gap with the inverse of the length of the ladder.

Ground state properties and correlations

Two points correlation function:

Relevance of the parameters





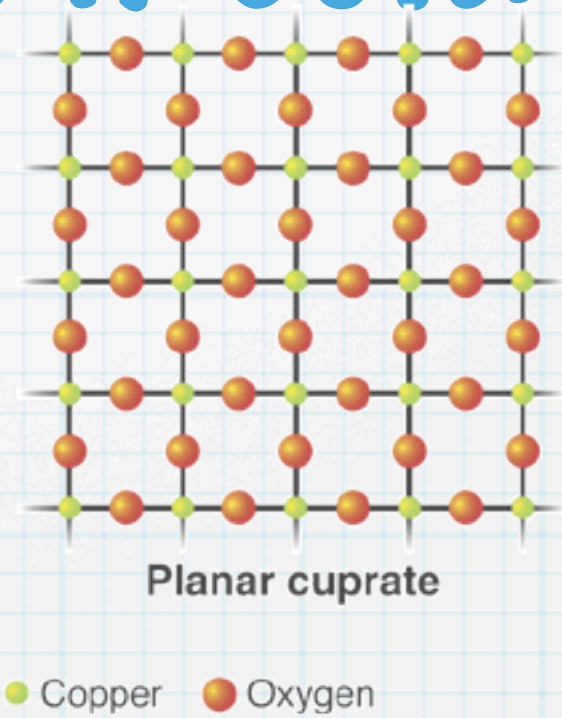
The plots does not show a linear dependence of the gap with the perturbation

Antiferromagnetic Mott-Hubbard insulator.

Copper oxide

$Bi_2Sr_2Ca_nCu_{n+1}O_{2n+6}$

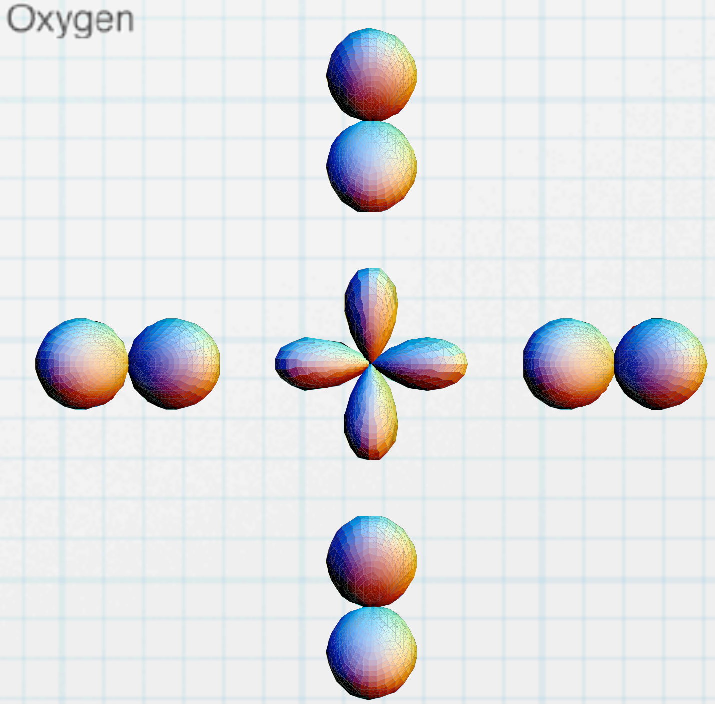
Universal structure.-



Ionic configuration.-

Cu^{2+} d^9

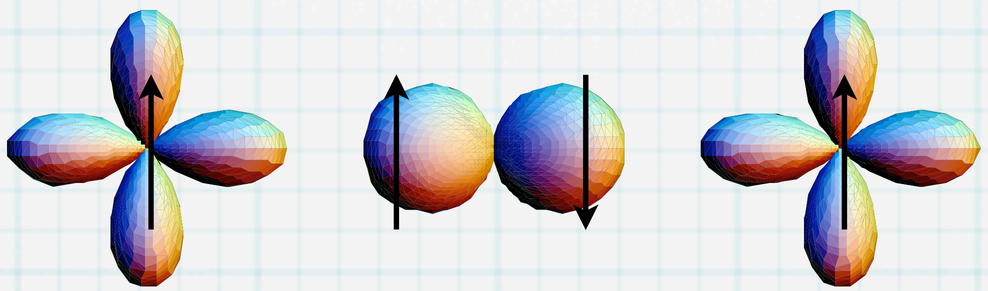
O^{2-} p^6



Antiferromagnetic Mott-Hubbard insulator.

Super-exchange mechanism: Anderson 1950

Hybridisation of ionic orbital by covalent mixing

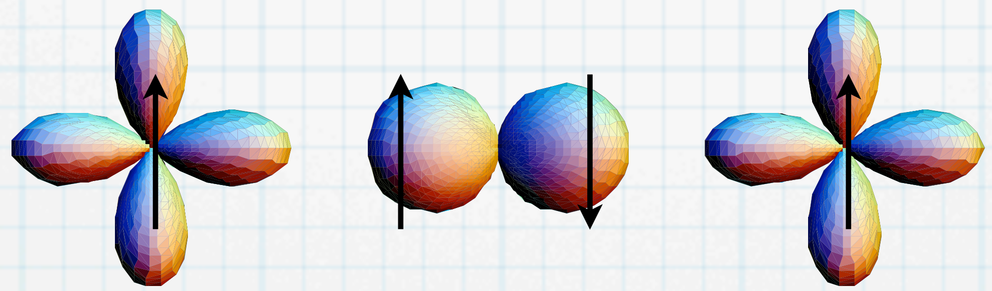


Orbital energies: $E_p = \langle \sigma_p | \mathcal{H} | \sigma_p \rangle$ $\quad E_d = \langle \sigma_d | \mathcal{H} | \sigma_d \rangle$

Covalent mixing amplitude: $\lambda \simeq \dfrac{\langle \sigma_p | \mathcal{H} | \sigma_d \rangle}{E_p - E_d}$

Antiferromagnetic Mott-Hubbard insulator.

Triplet (parallel) configuration



$$|\downarrow_p\rangle \xrightarrow{\text{covalent-mixing}} \frac{|\downarrow_p\rangle + \lambda|\downarrow_{d_L}\rangle + \lambda|\downarrow_{d_R}\rangle}{\sqrt{1+2\lambda^2}}$$

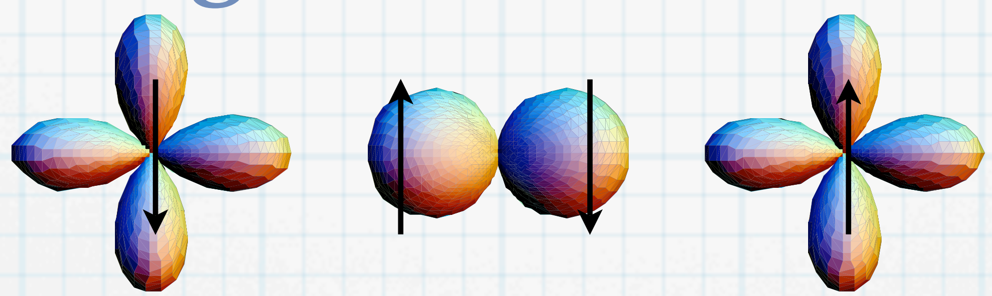
$$|\uparrow_p\rangle \xrightarrow{\text{Pauli principle}} |\uparrow_p\rangle.$$

$$E_{\uparrow\uparrow} \simeq \frac{1}{1+2\lambda^2}[(\langle\downarrow_p| + \lambda\langle\downarrow_{d_L}| + \lambda\langle\downarrow_{d_R}|)\langle\uparrow_p|\mathcal{H}|\uparrow_p\rangle(|\downarrow_p\rangle + \lambda|\downarrow_{d_L}\rangle + \lambda|\downarrow_{d_R}\rangle)]$$

$$= 2E_p + \frac{2\lambda^2}{1+2\lambda^2}(E_p - E_d).$$

Antiferromagnetic Mott-Hubbard insulator.

Singlet (anti-parallel) configuration



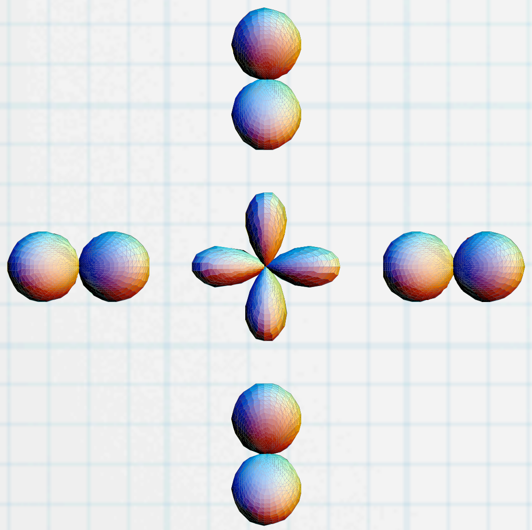
$$|\downarrow_p\rangle \xrightarrow{\text{covalent-mixing}} \frac{|\downarrow_p\rangle + \lambda|\downarrow_{d_R}\rangle}{\sqrt{1+\lambda^2}}$$

$$|\uparrow_p\rangle \xrightarrow{\text{covalent-mixing}} \frac{|\uparrow_p\rangle + \lambda|\uparrow_{d_L}\rangle}{\sqrt{1+\lambda^2}}.$$

$$E_{\downarrow\uparrow} = 2E_p + \frac{2\lambda^2}{1+\lambda^2}(E_p - E_d)$$

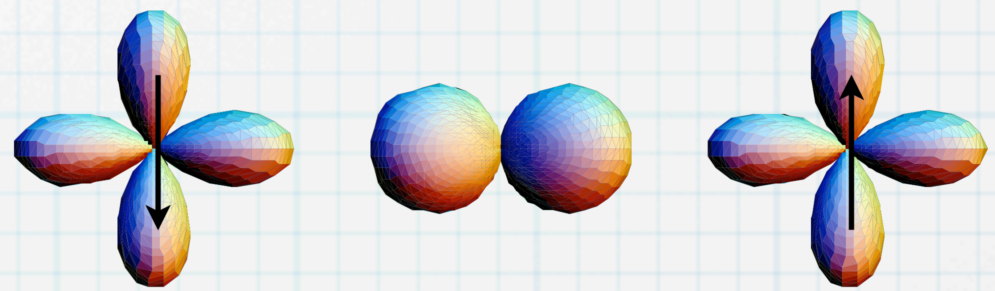
Super-exchange splitting.- $E_{\uparrow\uparrow} - E_{\downarrow\uparrow} \simeq \dfrac{2\lambda^4(E_d - E_p)}{(1+2\lambda^2)(1+\lambda^2)}$

Antiferromagnetic Mott-Hubbard insulator.

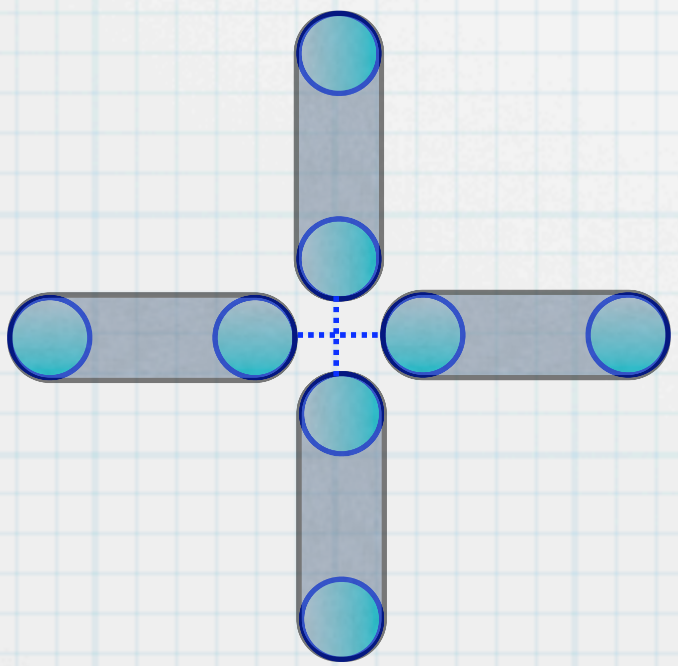


Interpretations:-

1) $$\hat{H}_{eff} = J \sum_{n,m} \vec{S}_n \vec{S}_m$$



2)

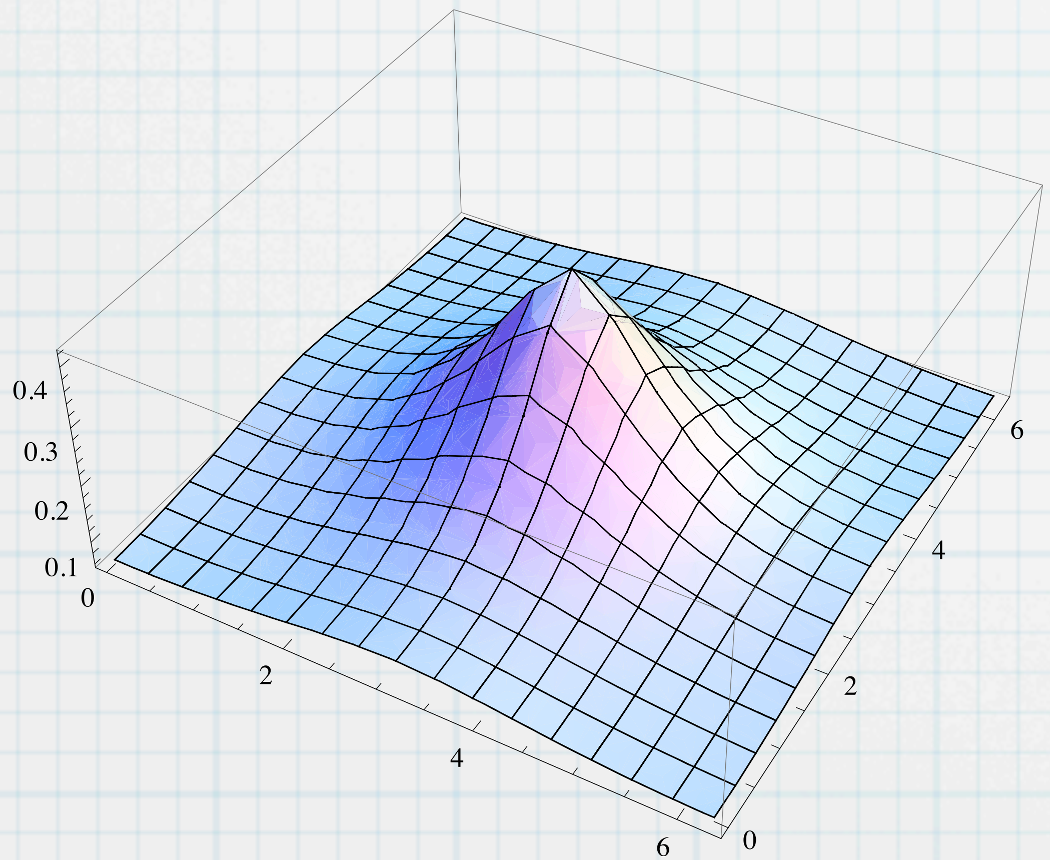


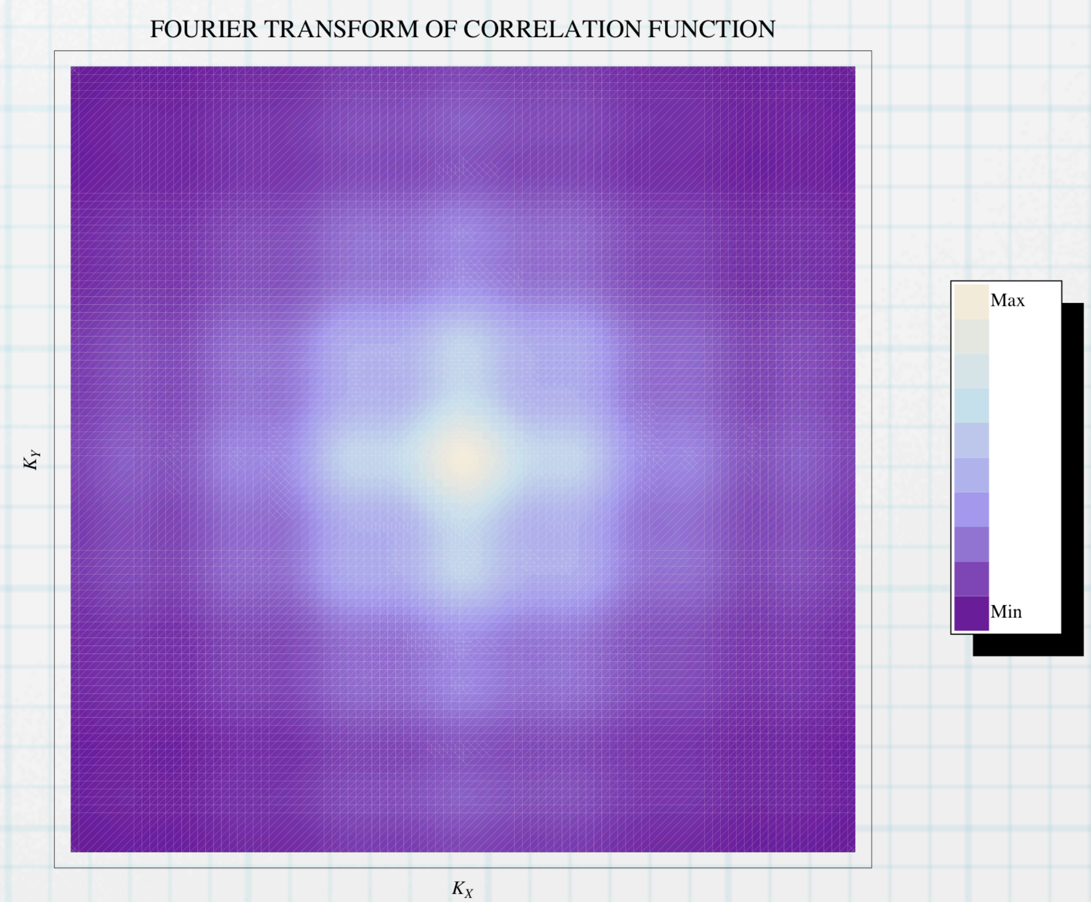
The structure of the state at the link describes the splitting in the amplitude of probability of finding the system in a triplet or singlet configuration.

Neutron scattering experiment

Structure factor:

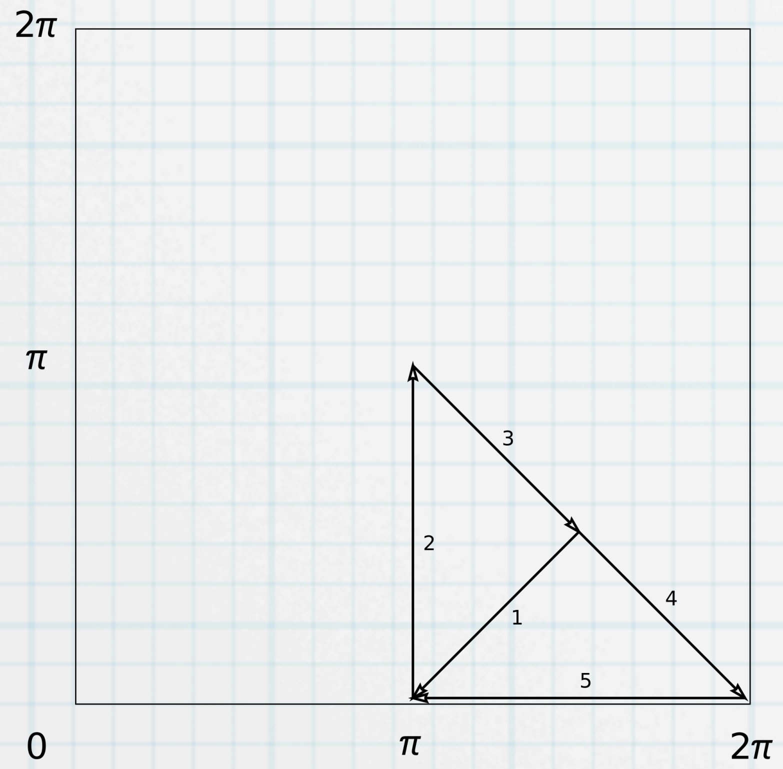
$$S(\vec{q}) = \frac{1}{N}\sum_{i,j}\langle 0|\vec{S}_i \cdot \vec{S}_j|0\rangle \exp\left(i\vec{q}\cdot(\vec{r}_i - \vec{r}_j)\right)$$

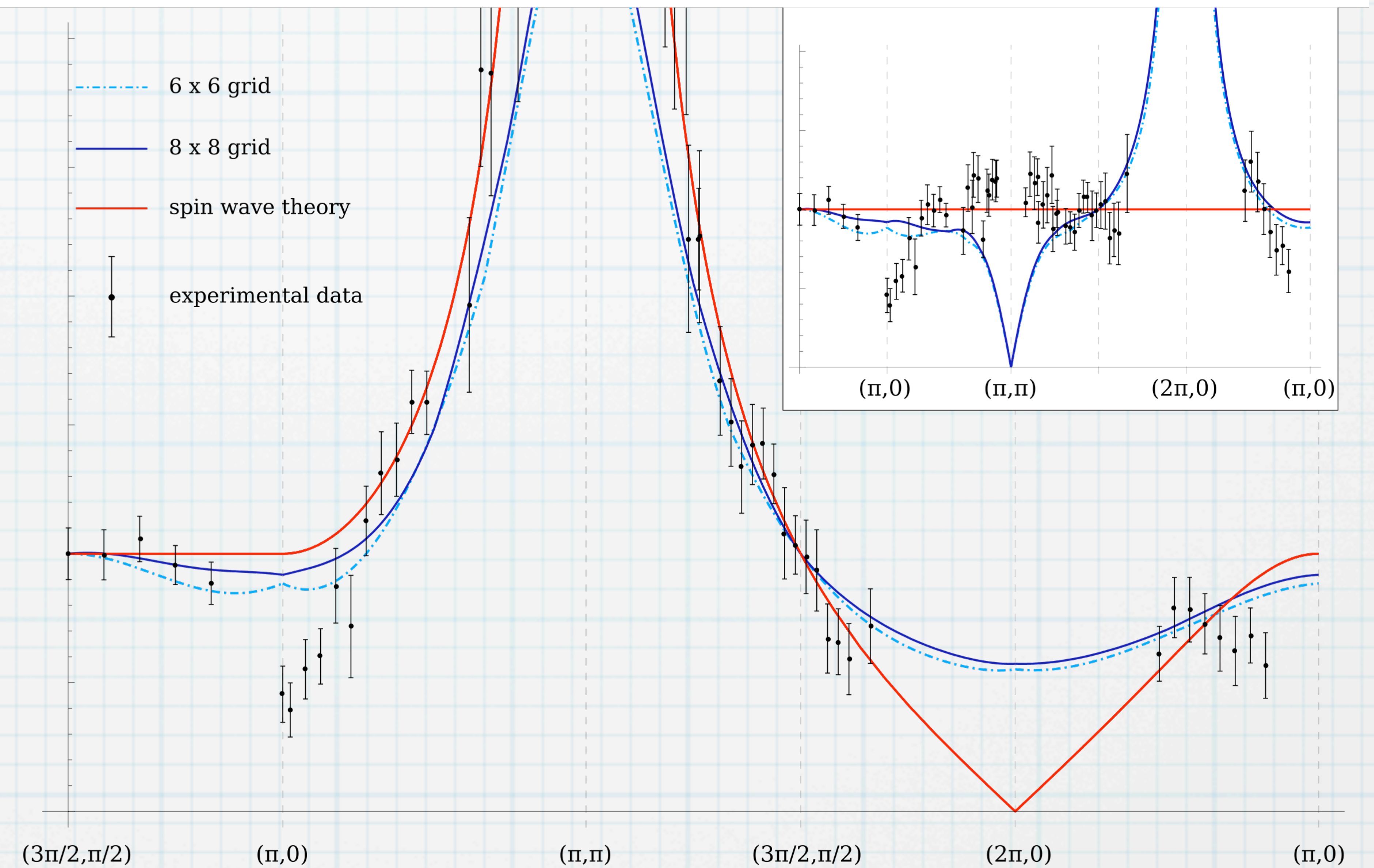




The structure factor can be measured by neutron scattering.

Neutron scattering experiment





Features of the predictions of linear spin wave theory, multipartite valence bond state and the experimental data. G. Aeppli's group provided the experimental data. [PNAS 104 (39) (2007) 15264-15269]

2D multipartite valence bond state

Conclusions and Outlook:

* Non-local properties of the state.
* Low energy excitations.
* Relation with integrable models.
* Application for quantum information tasks.

Collaborators and References

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Annals of Physics 323 (2008) 2115-2131. arXiv:0710.2349
Annals of Physics 324 (2009) 1875-1896. arXiv:0811.1049