Derivation of order parameters through reduced density matrices

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Order parameters (OP) and critical phenomena

Simplest example: magnetization of a ferromagnet

- OP: base of the Landau-Ginzburg theory of phase transitions

  A phase is characterized by its (broken) symmetries

The free energy is a functional of the coarse-grained OP associated to the broken symmetry. All other microscopic details can be ignored

- Renormalization group approach & universality
  OP: Appropriate variable to construct effective (field) theories
  Example: magnetization $\Rightarrow$ φ^4 field theory

How to identify the/an order parameter ?

Spectrum and spontaneous symmetry breaking

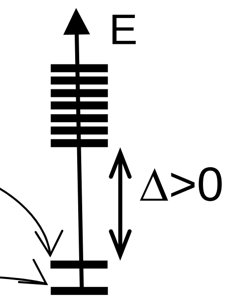
Quantum lattice models at T=0
Spontaneous breakdown some discrete symmetries
Gapped spectrum

- Ferro. Ising chain in transverse field

$$H = -\sum_{\langle ij\rangle} \sigma_i^z \sigma_j^z - h \sum_i \sigma_i^x$$

$$|1\rangle = \tfrac{1}{\sqrt{2}}\left(|\uparrow\ \uparrow\ \uparrow\rangle - |\downarrow\ \downarrow\ \downarrow\rangle\right)$$

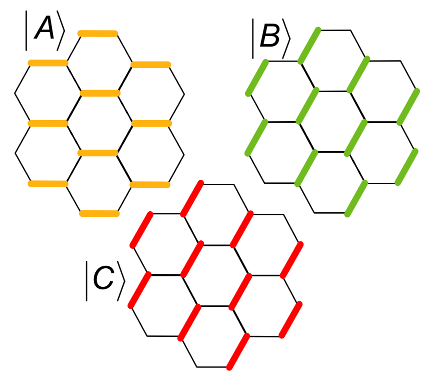
$$|0\rangle = \tfrac{1}{\sqrt{2}}\left(|\uparrow\ \uparrow\ \uparrow\rangle + |\downarrow\ \downarrow\ \downarrow\rangle\right)$$

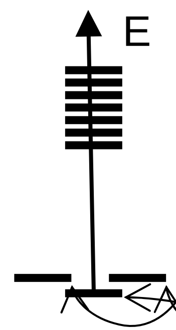


Order parameter : σ_0^z

but $\langle 0|\sigma_0^z|0\rangle = \langle 1|\sigma_0^z|1\rangle = 0$

- Valence-bond crystal on the hexagonal lattice





$$|2\rangle \sim |A\rangle + e^{-\frac{2i\pi}{3}}|B\rangle + e^{-\frac{4i\pi}{3}}|C\rangle$$

$$|1\rangle \sim |A\rangle + e^{\frac{2i\pi}{3}}|B\rangle + e^{\frac{4i\pi}{3}}|C\rangle$$

$$|0\rangle \sim |A\rangle + |B\rangle + |C\rangle$$

$\Rightarrow$ **Eigenstates ≠ symmetry-breaking states**

Order parameter – definitions

- Definition 1

$$\hat{O}_{triv} = \frac{1}{|G|}\sum_{g\in G} g\ \hat{O}\ g^{-1} \quad \text{trivial rep. component of } \hat{O}$$

$$\exists\ |A\rangle = \sum_{i=1}^{n} \alpha_i |i\rangle \text{ such that } \langle A|\hat{O}|A\rangle - \langle A|\hat{O}_{triv}|A\rangle \neq 0$$

- Definition 2 (not involving G)

$$\exists\ |A\rangle = \cdots, \text{ such that } \langle A|\hat{O}|A\rangle - \frac{1}{n}\sum_{i=1}^{n}\langle i|\hat{O}|i\rangle \neq 0$$

- Definition 3

$$\exists\ |A\rangle, |B\rangle = \cdots, \text{ such that } \langle A|\hat{O}|A\rangle - \langle B|\hat{O}|B\rangle \neq 0$$

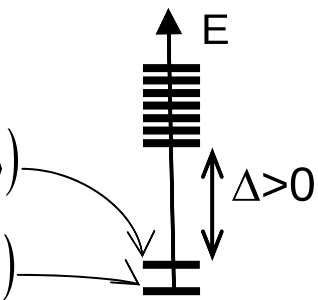
Correlations and order parameter

- Example of the ferromagnetic Ising chain

$$H = -\sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z - h \sum_i \sigma_i^x$$

$$|1\rangle = \tfrac{1}{\sqrt{2}}\left(|\uparrow \ \uparrow \ \uparrow\rangle - |\downarrow \ \downarrow \ \downarrow\rangle\right)$$

$$|0\rangle = \tfrac{1}{\sqrt{2}}\left(|\uparrow \ \uparrow \ \uparrow\rangle + |\downarrow \ \downarrow \ \downarrow\rangle\right)$$



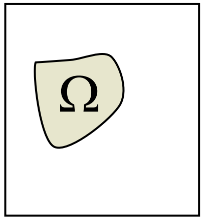
Eigenstates have no magnetization but long-range correlations

$$\langle 0|\sigma_0^z|0\rangle = \langle 1|\sigma_0^z|1\rangle = 0$$

$$\langle 0|\sigma_0^z \sigma_r^z|0\rangle \sim \langle 1|\sigma_0^z \sigma_r^z|1\rangle \sim \text{cst}$$

$\Rightarrow$ Look for all possible correlations to find the order parameter ?

Order parameter and Reduced Density Matrices



- A local (in Ω) observable is an OP if it can distinguish two ground-states:

$$|A\rangle = \sum_i \alpha_i |i\rangle \;;\; |B\rangle = \sum_i \beta_i |i\rangle$$ linear combinations of the eigenstates

Such that:
(in the thermodynamic limit)

$$\langle A|\hat{O}|A\rangle \neq \langle B|\hat{O}|B\rangle$$

- Question: For a given Ω, does such $\{\alpha_i, \beta_i, \hat{O}\}$ exist ?

Hint: all the information is contained in the reduced density matrices

$$\hat{\rho}\underbrace{\left(|i\rangle,|j\rangle\right)}_{\text{Eigenstates of the (whole) system}} = \mathrm{Tr}_{\overline{\Omega}}\left[\,|i\rangle\langle j|\,\right] = \sum_{|e\rangle} \langle e|i\rangle\langle j|e\rangle$$

Eigenstates of the (whole) system

State of the exterior $\overline{\Omega}$

Local difference between states - definitions

- We introduce the difference between *two* states (with respect to Ω):

$$\mathrm{diff}\left(|A\rangle,|B\rangle,\Omega\right)=\mathrm{Max}_{\substack{\hat{O}\text{ defined on }\Omega \\ \text{normalized } \|\hat{O}\|\leq 1}}\left|\langle A|\hat{O}|A\rangle-\langle B|\hat{O}|B\rangle\right|$$

= how different are $|A\rangle$ and $|B\rangle$, seen from Ω

- Properties of "diff":

$$0\leq \mathrm{diff}\left(|A\rangle,|B\rangle,\Omega\right)\leq 2$$

$$\Omega\subset\Omega' \Rightarrow \mathrm{diff}\left(|A\rangle,|B\rangle,\Omega\right)\leq \mathrm{diff}\left(|A\rangle,|B\rangle,\Omega'\right)$$

- Example 1
  Ferromagnet

$$|A\rangle=|\uparrow\ \uparrow\ \uparrow\rangle\ ,\ |B\rangle=|\downarrow\ \downarrow\ \downarrow\rangle$$

$$\Omega=\{1\},\ diff=2,\ \hat{O}^{opt}=2S_0^z$$

- Example 2
  Dimerized states

$$|A\rangle=|(1\ \ 2)\ \ (3\ \ 4)\ \ (5\ \ 6)\rangle$$

$$|B\rangle=|1)\ \ (2\ \ 3)\ \ (4\ \ 5)\ \ (6\rangle$$

(dimer) $=\frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle-|\downarrow\uparrow\rangle\right)$

Singlet, total spin S=0

$$\Omega=\{1\},\ diff=0$$

$$\Omega=\{1,2\},\ diff=\tfrac{3}{2},\ \hat{O}^{opt}=2\vec{S}_1\cdot\vec{S}_2+\tfrac{1}{2}$$

- How to compute "diff($|A\rangle$,$|B\rangle$,Ω)" in general ?

Computation of $\mathrm{diff}\left(|A\rangle,|B\rangle,\Omega\right)$

… one has to diagonalize the difference of the reduced density matrices :

$$\mathrm{diff}\left(|A\rangle,|B\rangle,\Omega\right) = \mathrm{Max}_{\substack{\hat{O}\text{ defined on }\Omega \\ \text{normalized }\|\hat{O}\|\leq 1}} \left| \langle A|\hat{O}|A\rangle - \langle B|\hat{O}|B\rangle \right|$$

$$= \mathrm{Max}_{\substack{\hat{O}\text{ defined on }\Omega \\ \text{normalized }\|\hat{O}\|\leq 1}} \mathrm{Tr}_{\Omega}\left[\hat{O}\left(\rho_{AA}^{\Omega} - \rho_{BB}^{\Omega}\right)\right]$$

$$= \cdots$$

$$= \sum |\lambda_n| \quad \text{where} \quad \rho_{AA}^{\Omega} - \rho_{BB}^{\Omega} = \sum \lambda_n |n\rangle\langle n|$$

$$\hat{O}^{opt} = \sum \mathrm{sign}(\lambda_n)|n\rangle\langle n|$$

- How to obtain the broken symmetry states |A⟩ and |B⟩ ?

Finding the broken symmetry states

- Optimization over the states $|A\rangle$ and $|B\rangle$

$|1\rangle, |2\rangle, \cdots, |d\rangle$: degenerate ground states

$$\widetilde{D}_\Omega\left(|1\rangle, |2\rangle, \cdots, |d\rangle\right) = \mathrm{Max}_{\substack{|A\rangle = \sum \alpha_i |i\rangle \\ |B\rangle = \sum \beta_i |i\rangle \\ \langle A|A\rangle = 1, \langle B|B\rangle = 1}} \; diff\left(|A\rangle, |B\rangle, \Omega\right)$$

$$D_\Omega\left(|1\rangle, |2\rangle, \cdots, |d\rangle\right) = \mathrm{Max}_{\substack{|A\rangle = \sum \alpha_i |i\rangle \\ \langle A|A\rangle = 1}} \; diff\left(|A\rangle, |ref\rangle, \Omega\right) \quad \text{with} \quad |ref\rangle = \frac{1}{\sqrt{d}} \sum_{i=1}^{d} |i\rangle$$

Possible iterative method to find the maximum :
A $\Rightarrow$ Ô $\Rightarrow$ A $\Rightarrow$ Ô … (diff increasing)

- Simple case when d=2:
  Two possibilities:

$$|A\rangle = \tfrac{1}{\sqrt{2}}\left(|1\rangle + |2\rangle\right), \; |B\rangle = \tfrac{1}{\sqrt{2}}\left(|1\rangle - |2\rangle\right)$$

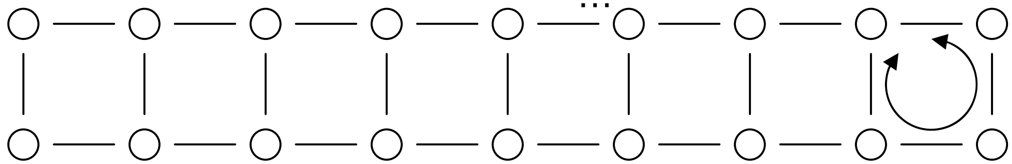
$$|A\rangle = \tfrac{1}{\sqrt{2}}\left(|1\rangle + \boxed{i}\,|2\rangle\right), \; |B\rangle = \tfrac{1}{\sqrt{2}}\left(|1\rangle - \boxed{i}\,|2\rangle\right)$$

Time reversal symmetry breaking

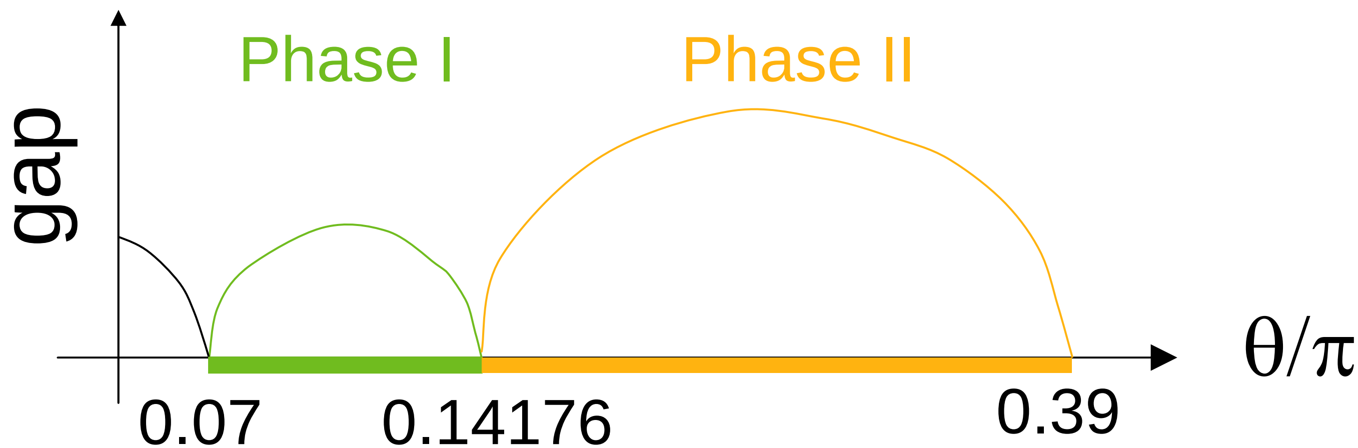
- Applications ?

Spin-1/2 ladder with ring exchange interactions

Läuchli, Schmid, Troyer, PRB 67, 100409(R) (2003)
Hikihara, Momoi, Hu, PRL 90, 087204 (2003).
Momoi, Hikihara, Nakamura, Xiao Hu, PRB 67, 174410 (2003)
...

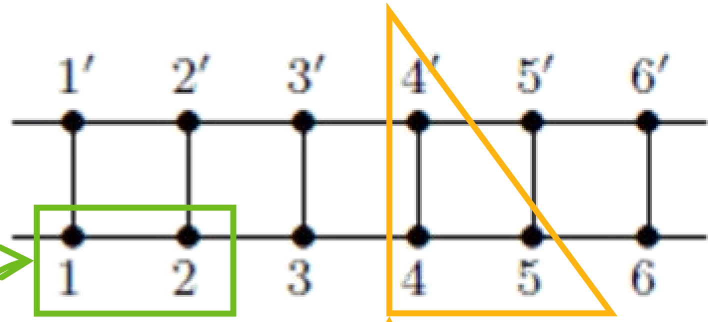


$$\mathcal{H} = \cos\theta \sum_{-} \vec{S}_i \cdot \vec{S}_j + \sin\theta \sum_{\square} (P_4 + P_4^{-1})$$



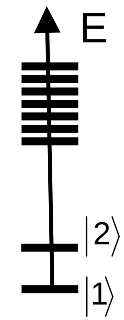
2-fold degeneracy in both phases (wave-vectors k=0 and k=π)
What are the corresponding order parameters ?

Optimal order parameters on minimal area



$$\text{diff}_1 = \text{diff}\left(|1\rangle + |2\rangle, |1\rangle - |2\rangle\right)$$

$$\text{diff}_2 = \text{diff}\left(|1\rangle + i|2\rangle, |1\rangle - i|2\rangle\right)$$



Phase I   Phase II

Area Ω	$\theta = 0.12\pi$		$\theta = 0.19\pi$	
	diff1	diff2	diff1	diff2
$\{1\}$	0^*	0^*	0^*	0^*
$\{1,2\}$	0.5698	0^*	~~0.0029~~	0^*
$\{1,1'\}$	0^*	0^*	0^*	0^*
$\{1,2'\}$	0^*	0^*	0^*	0^*
$\{1,2,1'\}$	0.5698	~~0.0267~~	~~0.0029~~	0.3340
$\{1,2,3\}$	0.6579	~~0.0670~~	~~0.0033~~	0.2365
$\{1,2,1',2'\}$	0.5698	~~0.0462~~	~~0.0029~~	0.5785

Numerical results on 14x2 system - periodic BC

- Phase I: leg dimer order

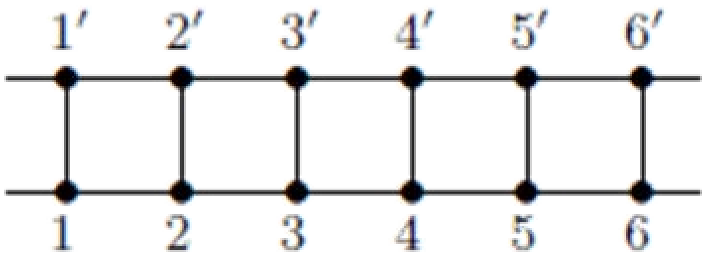
$$\hat{O}^{opt}_{\{1,2\}} = 2\vec{S}_1 \cdot \vec{S}_2 + \frac{1}{2}$$

- Phase II: scalar chiral order (broken time-reversal sym.)

$$\hat{O}^{opt}_{\{1,2,1'\}} = \frac{4}{\sqrt{3}} \vec{S}_1 \cdot \left(\vec{S}_2 \times \vec{S}_{1'}\right)$$

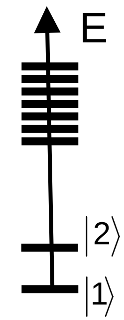
$\Rightarrow$ Reproduced known results !

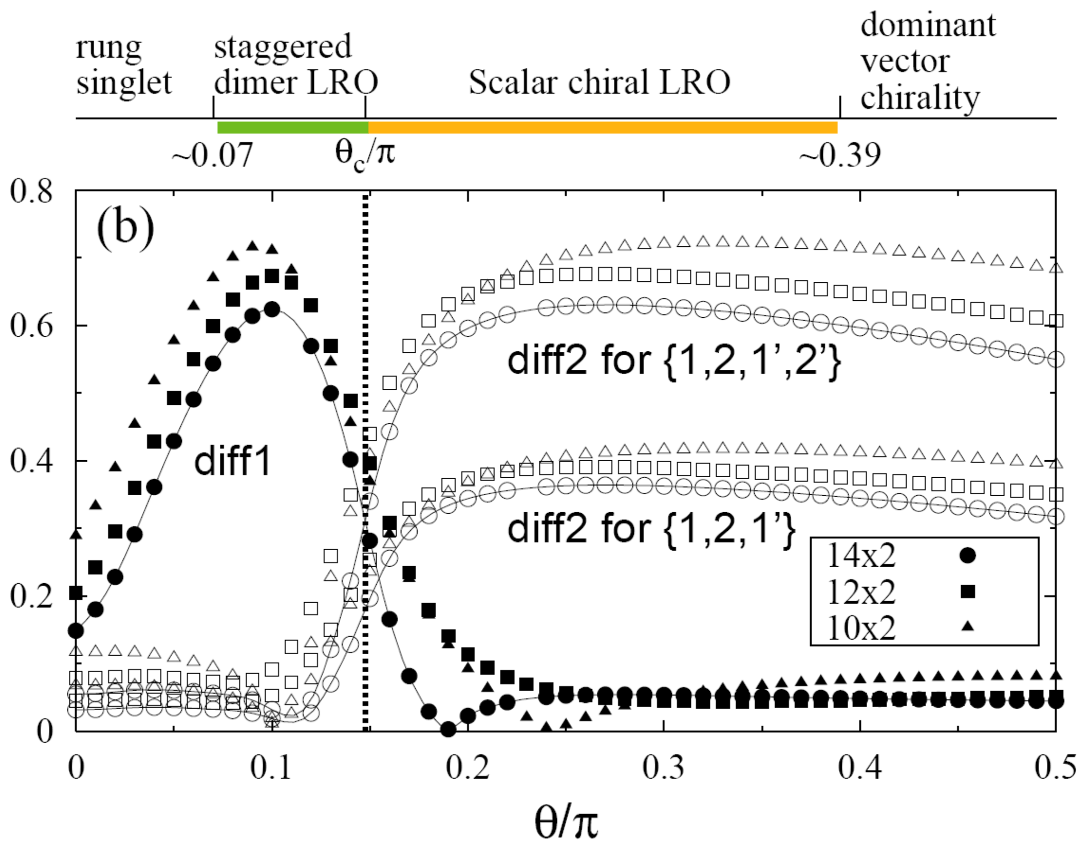
Locating the phase transition with "diff"



$$\mathrm{diff}_1 = \mathrm{diff}\left(|1\rangle + |2\rangle, |1\rangle - |2\rangle\right)$$

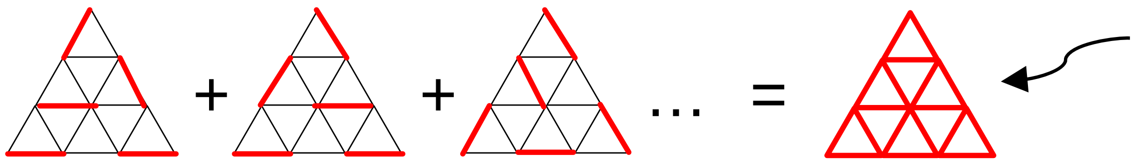
$$\mathrm{diff}_2 = \mathrm{diff}\left(|1\rangle + i|2\rangle, |1\rangle - i|2\rangle\right)$$





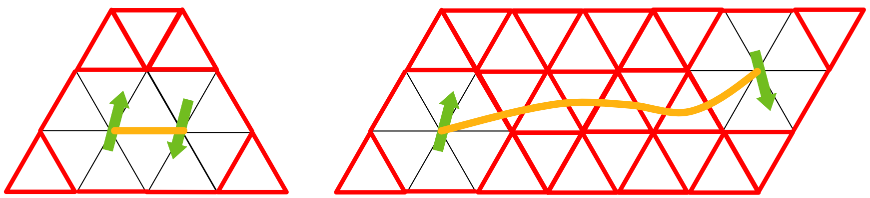
Short-ranged RVB states (Z_2 liquids)

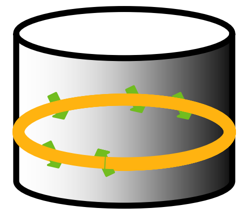
- Unique ground-state ?



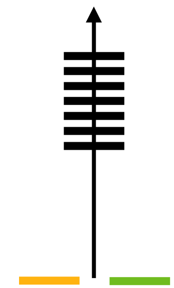
Spatially *uniform* state
[Anderson 1973]

Creation, propagation and annihilation of a pair of spinons





Topological degeneracy
(X. G. Wen 1991) ↔ **fractionalization**
See also Oshikawa & Senthil cond-mat/0506008



2-fold degeneracy

- Many examples/candidates

Spin models, Bose-Hubbard models, dimer models, etc.

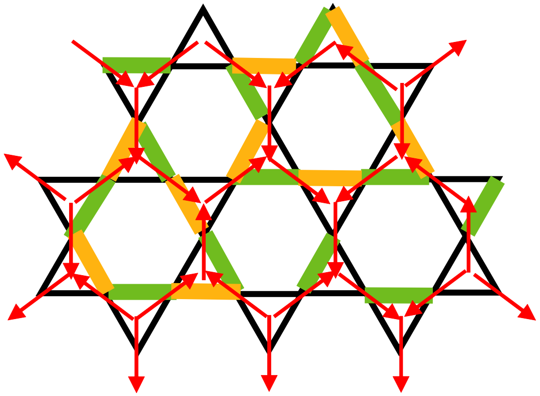
Read & Sachdev PRL **1991**; Kitaev, cond-mat **1997**; GM *et al.* PRB **1999**; Nayak & Shtengel PRB **2001**; Capriotti *et al.* PRL **2001**; Moessner & Sondhi PRL **2001**; Balents, Fisher & Girvin PRB **2002**; GM, Serban & Pasquier PRL **2002**; Moessner & Sondhi PRB **2003**; Fouet et al. PRB **2003**; X. G. Wen PRL **2003**; Ioffe *et al.* Nature **2002**; Douçot, Fegeil'man & Ioffe PRL **2003**; Senthil & Motrunich PRB **2002**, PRL **2002**; S. Fujimoto PRB **2005**; Raman, Moessner & Sondhi PRB **2005**

an exactly solvable example…

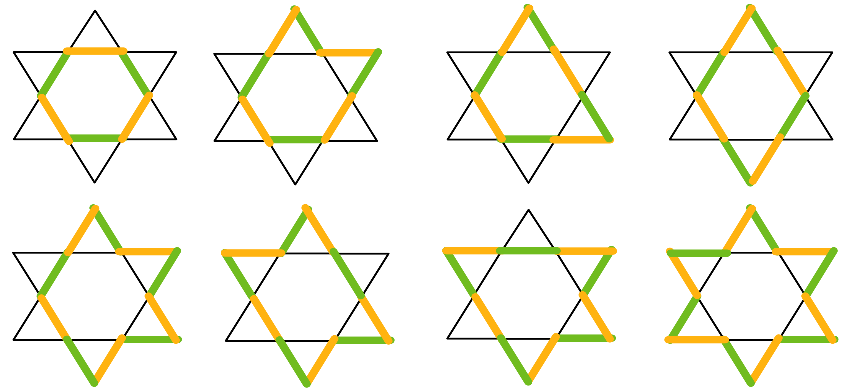
« Toy » dimer model realizing a short-range RVB liquid

[GM, Serban & Pasquier PRL 2002]

- Quantum dimers on the kagome lattice

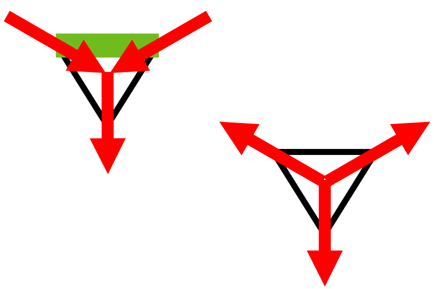


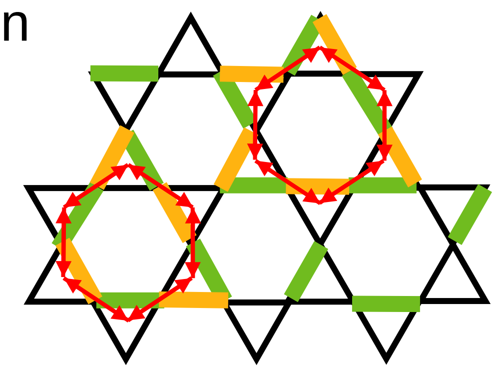
- Hamiltonian: all single-hexagon dimer hopping (with the same amplitude)



Looks like a very complicated model… but

- Arrow representation

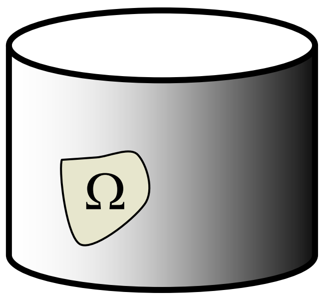




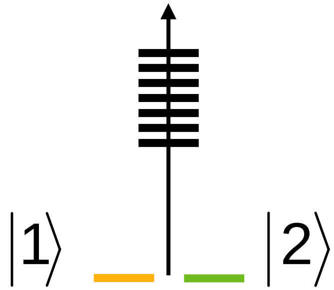
$\tau^z(i) =$ Flips the arrow ***i***

$$H = -\sum_{h \in \text{hexagon}} \underbrace{\prod_{i=1}^{6} \tau_i^z}_{\text{dimer hoping}}$$

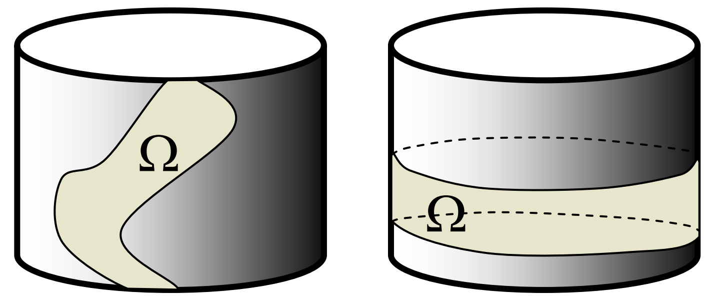
trivial in the τ^z variables !



Local area



2-fold degeneracy



Non-local areas

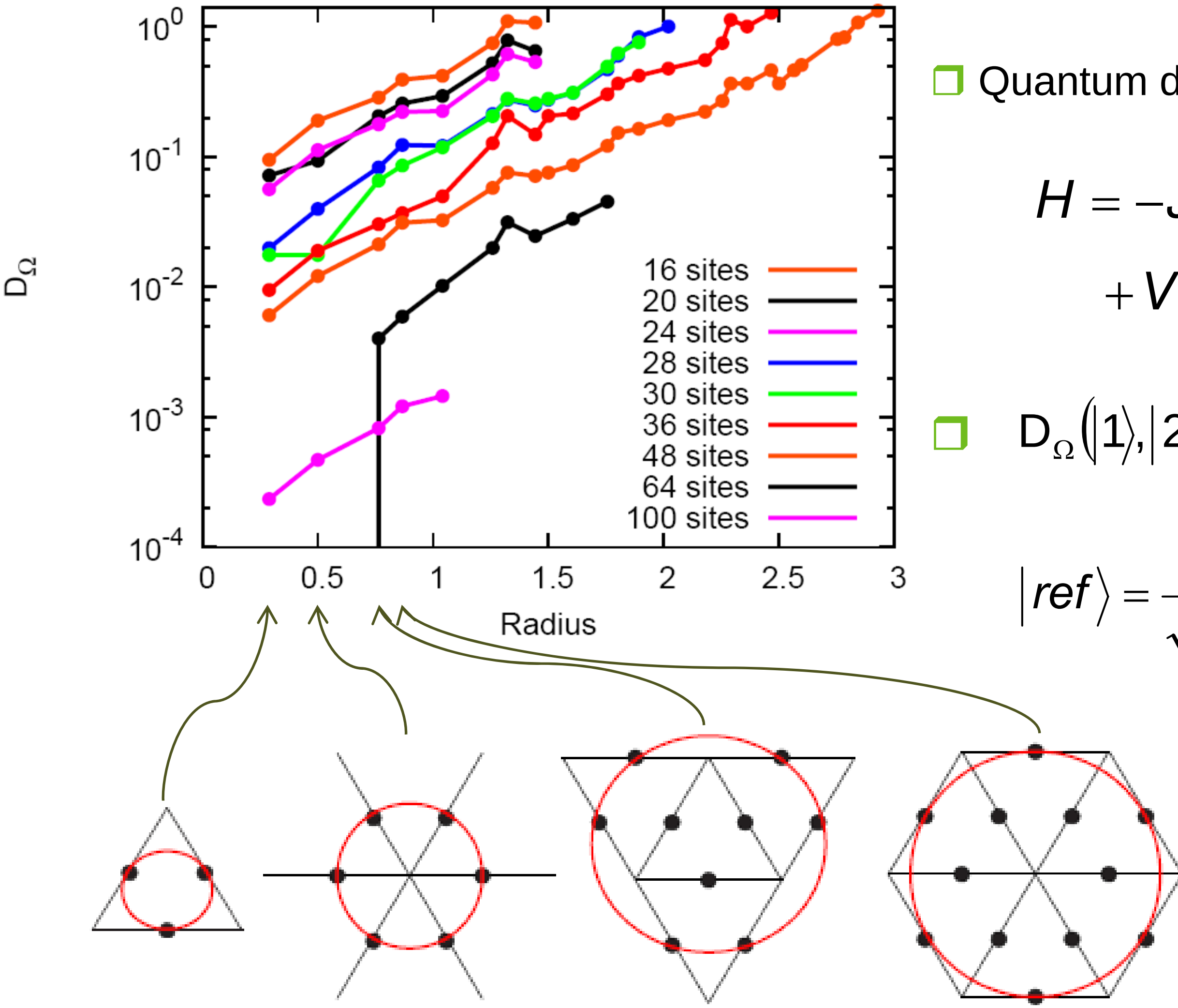
For any **local** area:

- $D\left(|1\rangle,|2\rangle,\Omega\right) = \mathrm{Max}_{\substack{|A\rangle=\sum \alpha_i |i\rangle \\ |B\rangle=\sum \beta_i |i\rangle \\ \langle A|A\rangle=1,\ \langle B|B\rangle=1}} \ diff\left(|A\rangle,|B\rangle,\Omega\right) = 0$

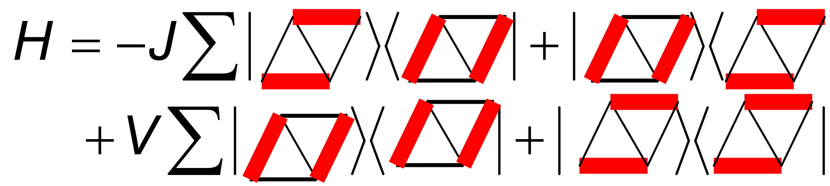
- $|A\rangle = \sum \alpha_i |i\rangle, \quad \mathrm{Tr}_{\overline{\Omega}}\left[\,|A\rangle\langle A|\,\right]$ is independent of $\{\alpha_i\}$

- Different ground-states are undistinguishable with local observables
  Protection against decoherence for a qubit
  [Kitaev 1997; Ioffe *et al.* Nature 2002; Ioffe, Feigel'man PRB 2002;
  GM Pasquier, Mila, Lhuillier PRB 2005]

RVB liquid on the triangular lattice



- Quantum dimer model [Moessner & Sondhi 2001]

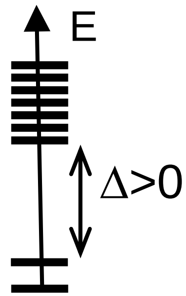


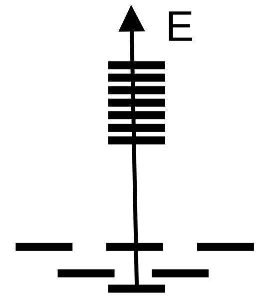
- $$D_\Omega\left(|1\rangle,|2\rangle,|3\rangle,|4\rangle\right) = \mathrm{Max}_{\substack{|A\rangle=\sum \alpha_i |i\rangle \\ \langle A|A\rangle=1}} \mathit{diff}\left(|A\rangle,|ref\rangle,\Omega\right)$$

$$|ref\rangle = \frac{1}{\sqrt{d}}\sum_{i=1}^{d}|i\rangle$$

- Calculations at the Rokhsar-Kivelson point (J=V=1) using direct enumeration and Pfaffians.

Conclusions

- If you see this : 

or this 

Use RDM's to compute D_Ω and $\hat{O}_\Omega^{opt}$

- Application to other systems

- Other dimer liquids (work in progress)
- Kagome s=1/2 ?
- …

Equivalence between def. 1 and def. 2

$\hat{O}_{triv} = \frac{1}{|G|}\sum_{g\in G} g\,\hat{O}\,g^{-1}$ commutes with any $g \in G$

$H = H_0 + \lambda \hat{O}_{triv}$ perturbed Hamiltonian (same symmetries as H_0)

$\lambda << 1 \Rightarrow$ no phase transition $\Rightarrow$ stable ground state degeneracy

Degenerate perturbation theory described by $\langle i|\hat{O}_{triv}|j\rangle$

Stability of the degeneracy $\Rightarrow \langle i|\hat{O}_{triv}|j\rangle = c\delta_{ij}$

$|\Psi\rangle = \sum_{i=1}^{n} \alpha_i |i\rangle$; $g|i\rangle = \sum_{i=1}^{n} R_{ij}(g)|i\rangle$ with $R(g)$ an $n \times n$ unitary matrix

$\Rightarrow \langle\Psi|\hat{O}_{triv}|\Psi\rangle = \frac{1}{n}\sum_{i=1}^{n}\langle i|\hat{O}|i\rangle$ indep. of the α_i