28pXZC-11

量子hard-square模型の基底状態と励起ギャップ

桂 法称（学習院大理）

Acknowledgment:
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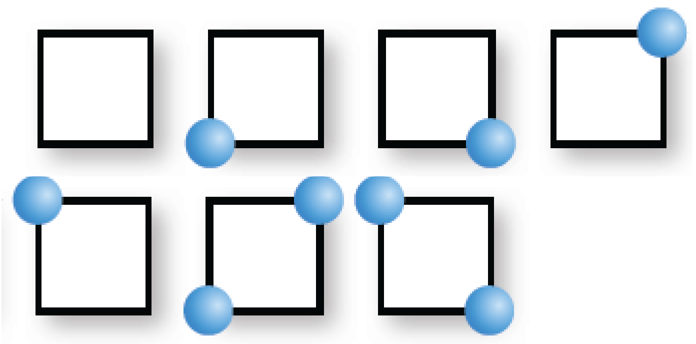
田中 宗 (東京大), 田村亮 (NIMS)



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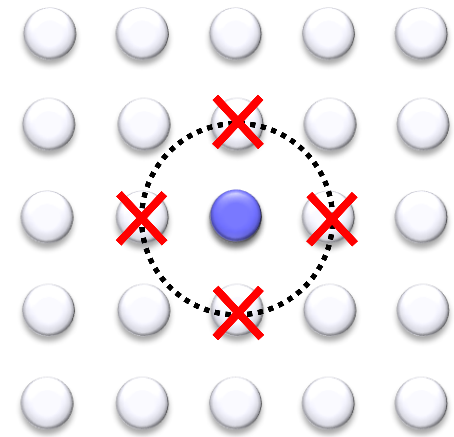
- H. Katsura, *Phys. Rev. A,* **88**, 065602 (2013).

Classical hard-square model

- Allowed states ⇔ config. of hard-squares
- 'Grand canonical' partition function:

$$\Xi(z) = \sum_n g(n) z^n$$

z: activity(fugacity)
$g(n)$: # allowed config. of n squares



- Phase transition at $z_c \simeq 3.796$

  $z < z_c$: liquid phase, $z > z_c$: solid phase
  Ising universality class (c=1/2 CFT)

Gaunt & Fisher, *J. Chem. Phys.* **43**, 2840 (1965).
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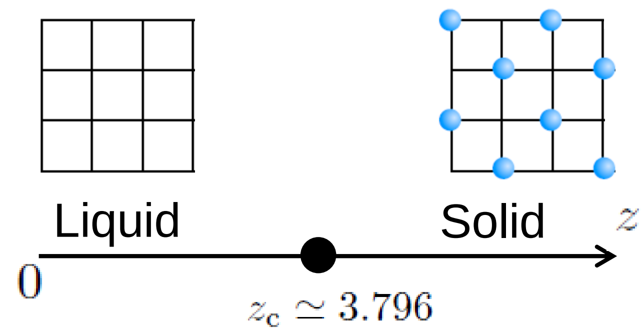
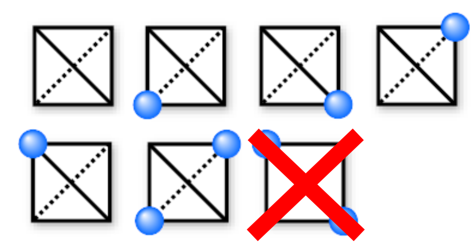


- Generalized hard-square model

  Hard-hexagon model → *integrable!*
  Phase transition at $z_c = (11 + 5\sqrt{5})/2 = 11.09$
  3-state Potts universality (c=4/5 CFT)

R. J. Baxter, *J. Phys. A,* **13**, L61 (1980) & his textbook.



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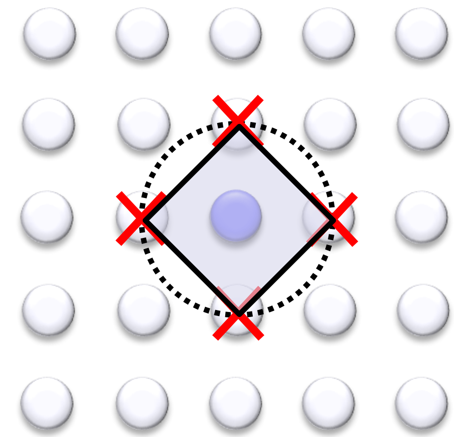

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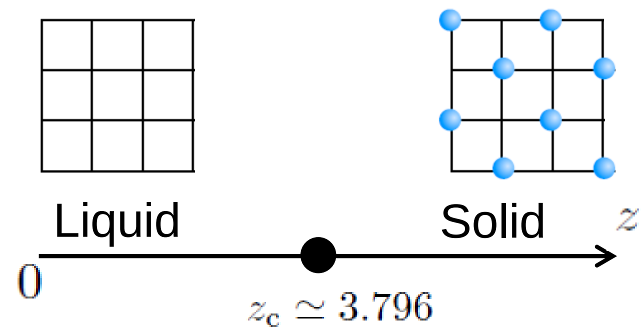

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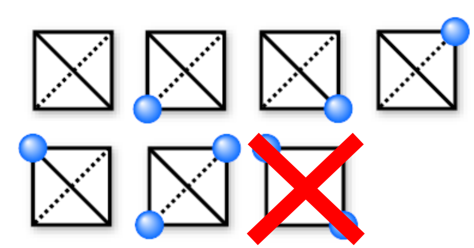

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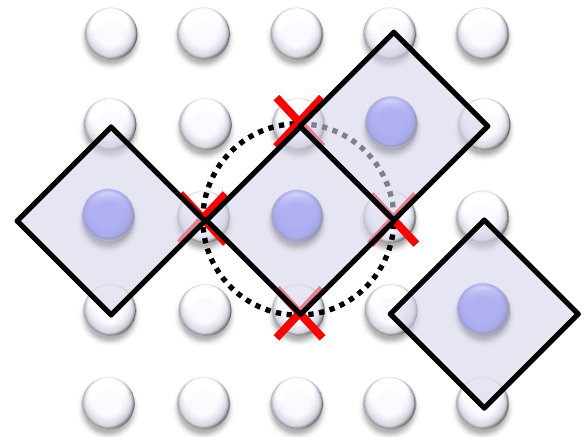

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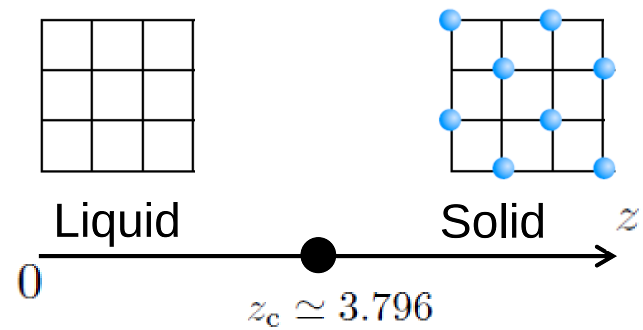

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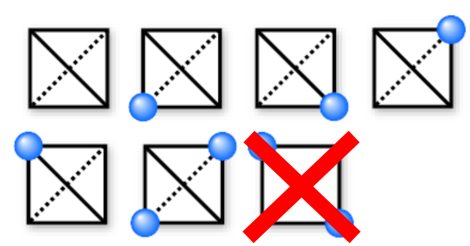

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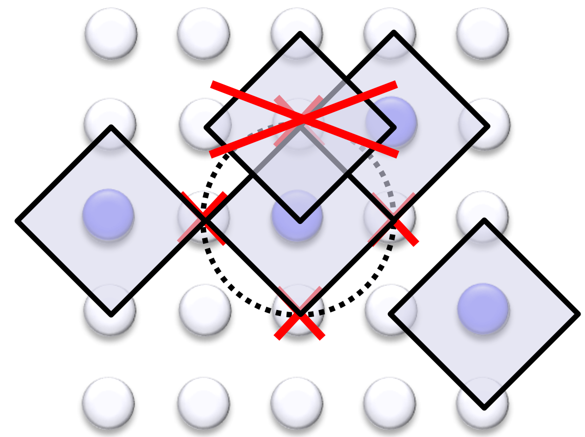

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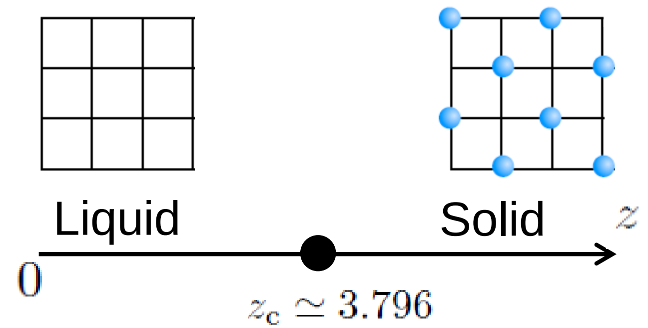

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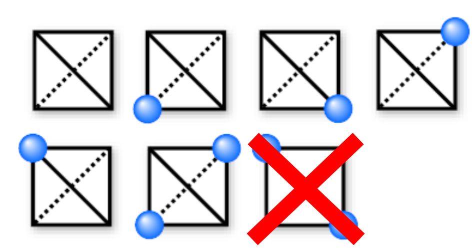


Quantum hard-square model

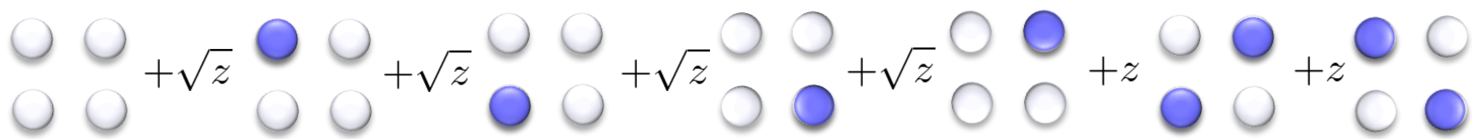
- **Ground state**

  → Superposition of allowed states

$$|\Psi(z)\rangle = \sum_{\mathcal{C}\in\mathcal{S}} z^{n_\mathcal{C}/2}|\mathcal{C}\rangle$$

$\mathcal{S}$: set of allowed configurations
$\mathcal{C}$: classical configuration in $\mathcal{S}$
$n_\mathcal{C}$: # particles in $\mathcal{C}$

Ex.) *N*=4



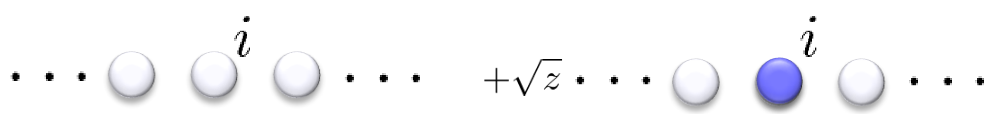
Normalization

$$\langle\Psi(z)|\Psi(z)\rangle = \Xi(z)$$

Classical partition function!

- **Cook up your Hamiltonian!**

  Rokhsar-Kivelson construction



$$H_i = \begin{pmatrix} z & -\sqrt{z} \\ -\sqrt{z} & 1 \end{pmatrix}_i \qquad H_i\,|\Psi(z)\rangle = 0 \quad \text{for all } i.$$

$|\Psi(z)\rangle$ is a ground state of $H=\sum_i H_i$ if *H* is positive semi-definite.

Quantum hard-square model (contd.)

- **Hamiltonian**

  Particle ⇔ spin

   ⇔ n=0 ⇔ ↓,  ⇔ n=1 ⇔ ↑

$$H = \sum_{i\in\Lambda} H_i, \quad H_i = [-\sqrt{z}\sigma_i^x + n_i + z(1-n_i)]\mathcal{P}_{\langle i\rangle}$$

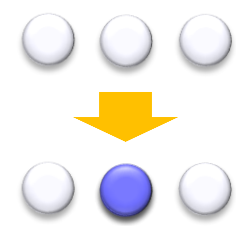
  Λ: Lattice (Can be any graph in any dim.)

  Projection operator:

$$\mathcal{P}_{\langle i\rangle} = \prod_{j \text{ next to } i} (1-n_j)$$

  - A spin can only be flipped if all of its neighboring spins are down.

  In 1d, $\mathcal{P}_{\langle i\rangle} = (1-n_{i-1})(1-n_{i+1})$.

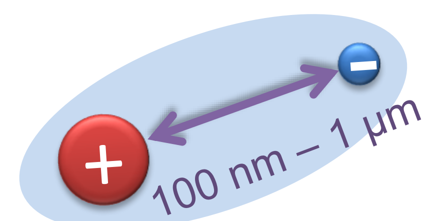


- **Motivation: Rydberg atoms**

  Atoms in states of high principal quantum number.

  They are interacting via the van der Waals-type int.

$$H_{\mathrm{Ryd}} = \Omega \sum_i \sigma_i^x + \Delta \sum_i n_i + \frac{V}{2}\sum_{i\neq j}\frac{n_i n_j}{|\boldsymbol{R}_i - \boldsymbol{R}_j|^6}$$



  The g.s. of *H* is a good variational w.f. for H_{Ryd}!

  - I. Lesanovsky, *PRL* **106**, 025301 (2011); **108**, 105301 (2012).
  - S. Ji, C. Ates & I. Lesanovsky, *PRL* **107**, 060406 (2011).

Results

- **Ground state**

  H is positive semi-definite and |*Ψ*(*z*)> is the **unique** g.s. of *H*.

  Positivity (*Energy*≧0)

  $$H_i = h_i^\dagger(z) h_i(z) \geq 0, \quad h_i(z) = [\sigma_i^- - \sqrt{z}(1-n_i)]\mathcal{P}_{\langle i \rangle}$$

  Uniqueness

  All the off-diagonal elements of *H* are non-positive and satisfy the connectivity condition. Thus Perron-Frobenius theorem applies to *H*.

- **Entanglement in the g.s**

- **Excited states**

  1d model

  Exact expressions for the 1st excited state & the gap. $E_1 = \dfrac{3+z-\sqrt{z^2+6z+1}}{2}$

  I. Lesanovsky, *PRL* **108**, 105301 (2012).

- **Rigorous proof of the gap** (Knabe's method)

  1d model

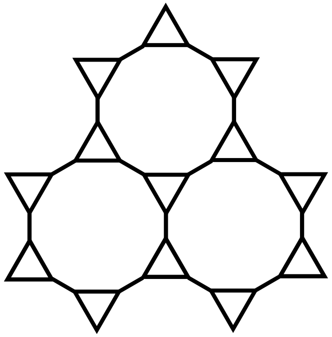
  Nonzero gap if $z < 1$ (not optimal).

  2d models

  kagome & 3-12 (Fisher) lattices: nonzero gap if $z < 1$.

  Honeycomb lattice: nonzero gap if $z < 0.62143\ldots$

  Square lattice: nonzero gap if $z < 2\sqrt{3} - 3 = 0.46410\ldots$



3-12 lattice

Knabe's method

S. Knabe, *J. Stat. Phys*. **52**, 627 (1988).

- **Hamiltonian**

$$H = \sum_{i\in\Lambda} P_i, \quad (P_i)^2 = P_i$$

Sum of projection operators
e.g., AKLT, Rokhsar-Kivelson, …

- **Assumptions**

1. Appropriate boundary conditions (if necessary).
2. The existence of (at least) one zero-energy g.s.
3. $[P_i, P_j]$ is nonzero if j is n.n. to i, and zero otherwise.

- **Lower bound on the gap**

The energy gap is at least ε if and only if $H^2 \geqq \varepsilon H$.

$$H^2 = \sum_i (P_i)^2$$

$$+ \sum_{D(i,j)=1} (P_iP_j + P_jP_i)$$

$$+ 2 \sum_{D(i,j)>1} P_iP_j$$

$H = \sum_i P_i \geq 0$

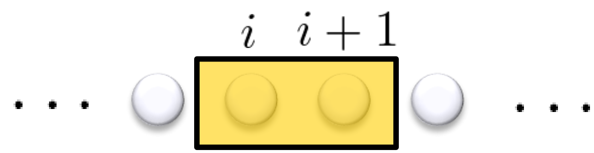
?? Unwanted term!

Positive semi-definite
$D(i,j)$: lattice distance

Knabe's method (contd.)

- **One-dimensional case (with PBC)**

$$H = \sum_{i=1}^{N} P_i, \quad P_{N+1} = P_1$$



2-site cluster Hamiltonian

$$h_{2,i} = P_i + P_{i+1} \qquad (h_{2,i})^2 \geq \epsilon_2 h_{2,i}$$

Local gap:
ϵ_2 is the gap of $h_{2,i}$.

$$\sum_{i=1}^{N}(h_{2,i})^2 = 2\sum_{i=1}^{N} P_i + \sum_{i=1}^{N}(P_i P_{i+1} + \text{h.c.})$$

Unwanted term

$$H^2 - \sum_{i=1}^{N}(h_{2,i})^2 + H = 2\sum_{D(i,j)>1} P_i P_j \geq 0$$

$$H^2 \geq 2\left(\epsilon_2 - \frac{1}{2}\right) H$$

An extension to *n*-site case is straightforward.

Application to 1d hard-square model

$$P_i = \frac{1}{1+z}[-\sqrt{z}\sigma_i^x + n_i + z(1-n_i)]\mathcal{P}_{\langle i \rangle}$$

Diagonalization of 8 × 8 matrix gives $\epsilon_2 = \frac{1}{1+z}$

→ The existence of the gap if $z < 1$.

Note) This may not be optimal…

Lower bound of gap

$$\Delta \geq \frac{1-z}{1+z}$$

Summary

Exact results for quantum hard-square models

- **Hamiltonian**

$$H = \sum_{i \in \Lambda} H_i, \quad H_i = [-\sqrt{z}\sigma_i^x + n_i + z(1-n_i)]\mathcal{P}_{\langle i \rangle}$$

H is positive semi-definite.

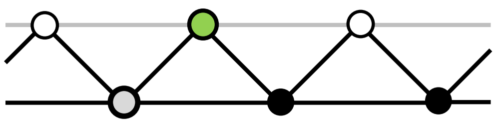
- **Ground state**
  Unique zero-energy g.s. for any lattice in any dim.
- **Existence of the gap**

1d chain, kagome, 3-12	$z < 1$
Honeycomb lattice	$z < 0.62143\ldots$
Square lattice	$z < 0.46410\ldots$

Sufficient but not optimal…
Better lower bound?

Future directions

- Construction of *quantum* RSOS models
  Implication for 2d *classical* stat. mech. models?
- Exact 1st excited states in 2d models
- Supersymmetric generalization
  Super weird ver. of Bose-Fermi mixture
  Anomalous degeneracy in 1d → *Super-Yangian??*



補足用スライド

- **Hamiltonian for 1d chain**

ANNNI model with transverse & longitudinal fields

$$H = \sum_{i=1}^{L} [-\sqrt{z}\sigma_i^x + (1-3z)n_i + \underline{v n_i n_{i+1}} + z n_{i-1} n_{i+1}]$$

$v \longrightarrow \infty$ → n.n. exclusion constraint

- **Hamiltonian for 3-12 (Fisher) lattice**

$$H = \sum_i [-\sqrt{z}\sigma_i^x + (1-4z)n_i] + v \sum_{\langle i,j \rangle} n_i n_j + z \sum_{\langle\langle i,j \rangle\rangle} n_i n_j$$

$v \longrightarrow \infty$ → n.n. exclusion constraint

NOTE) In other 2d lattices, Hamiltonian involves presumably unphysical 3-body, 4-body, … interactions.