Grassmann tensor product state approach to strongly correlated systems

Zheng-cheng Gu (KITP)

Collaborators:

Prof. Xiao-gang Wen (MIT)

Prof. Frank Verstraete (University of Vienna)

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Outline

- Why Tensor Product States(TPS)?
- Tensor-Entanglement Renormalization Group (TERG)
- Grassmann TPS and Grassmann TERG
- t-J model on honeycomb lattice
- Summary and outlook

Landau's paradigm of phases and phase transitions

Symmetry breaking

- Bose Einstein Condensation(BEC)
- BCS theory for conventional superconductivity
- Various of magnetic orders in spin systems

Fermi Liquid theory for electron systems.

- Band Insulators and Topological Insulators
- Metal, Semiconductors
- Integer Quantum Hall

Methods-trial wavefunctions

Mean-field description for symmetry breaking phases and phase transitions:

- The key concept is to find an ideal trial wavefunction, e.g., for a spin ½ system:

$$|\Psi_{trial}\rangle = \otimes \left(u^{\uparrow}|\uparrow\rangle_i + u^{\downarrow}|\downarrow\rangle_i\right)$$

- After minimizing the energy, we can find various symmetry ordered phases.

Energy Level Filling description for electron systems:

- The key concept is also to find an ideal trial wavefunction, e.g., for a spinless fermion system:

$$|\Psi_f\rangle = \exp\left(\frac{1}{2}\sum_{ij} u_{ij} c_j^{\dagger} c_i^{\dagger}\right)|0\rangle = \prod_m \left(1 + \lambda_m c_{m+}^{\dagger} c_{m-}^{\dagger}\right)|0\rangle$$

$$\propto \prod_m \left(v_m c_{m+}^{\dagger} + u_m c_{m-}\right)\left(u_m c_{m+} - v_m c_{m-}^{\dagger}\right)|0\rangle \quad \text{with} \quad |u_m|^2 + |v_m|^2 = 1; \frac{v_m}{u_m} = \lambda_m$$

quasi-particles

Beyond mean-field and ELF states: topological order

Fractional Quantum Hall(FQH)

- v=1/3 Laughlin State: $\Psi_3 = \prod_{i<j}(z_i - z_j)^3 e^{-\frac{1}{4}\sum_i |z_i|^2}$

High Temperature Superconductivity(High Tc)

- Gapped spin liquids: e.g. Z2 spin liquid

Topological order

- Can have the same (global)symmetry.
- Ground state degeneracies depend on the topology of the space.
- Ground state degeneracies are robust against any perturbations.
- Excitations carry fractional statistics.
- Protected chiral edge states(chiral topological order)

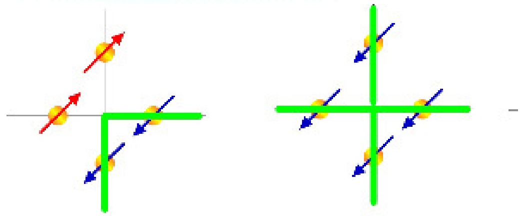
An exact solvable model

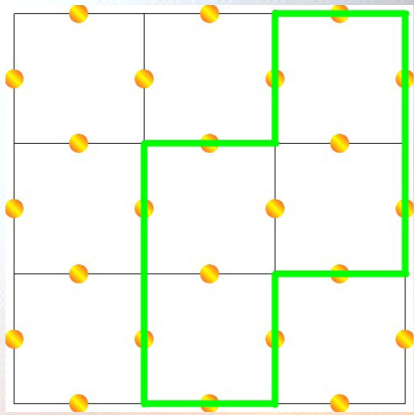
Z2 gauge model:

$$H = U\sum_v \left(1 - \prod_{l\in v}\sigma_l^z\right) - g\sum_p \prod_{l\in p}\sigma_l^x$$

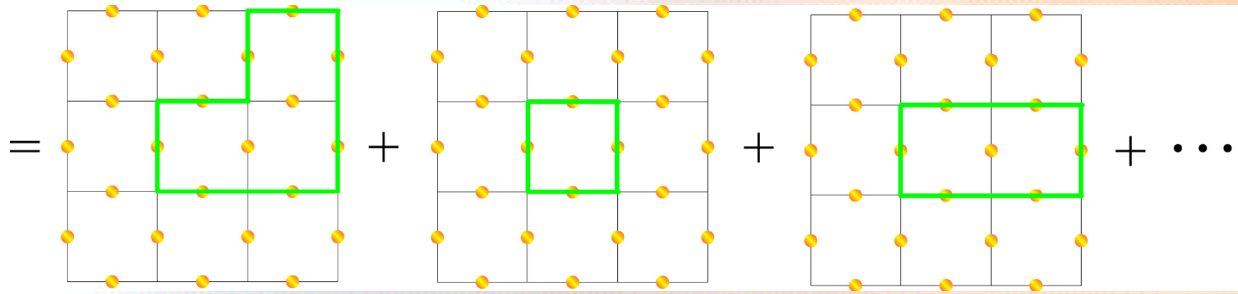
- same topological order as Z2 spin liquid

(Kitaev 2003, M. Levin and X.G. Wen 2005)





$$|\Psi_{Z_2}\rangle = \sum |X_{\text{close}}\rangle \qquad |\uparrow\rangle \to \text{no string}; \quad |\downarrow\rangle \to \text{one string}$$



- Four fold ground state degeneracy on torus; fractional statistics

What's the essential physics for topological order?

Long-range entanglement

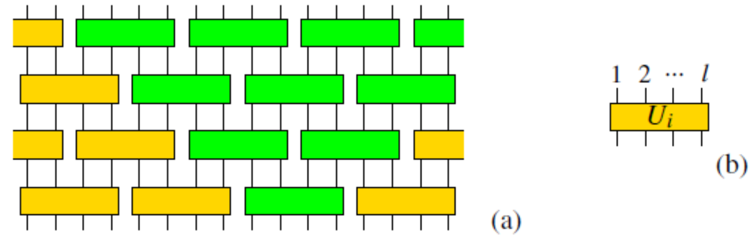
Short-range entanglement:

- *A state has only short-range entanglement if and only if it can be transformed into a direct-product state through a (finite) local unitary evolution.*

$$U^{(1)}_{pwl}U^{(2)}_{pwl}U^{(3)}_{pwl}\cdots U^{(M)}_{pwl}|\Psi\rangle = \text{direct product state}$$

$$U^{(i)}_{pwl} = \prod_k U^{(i)}_k$$

Long-range entanglement:



- *States could not be transformed into a direct-product state through (finite) local unitary evolutions.*
- *Topological order describes the equivalent classes defined by (finite) local unitary evolutions.* (classifications: Xie *etal*. 2010)

Is there any efficient and local representation for topological order?(Analogy of order parameter)

Tensor Product States(TPS)

Mean-field states: $\uparrow \longrightarrow u^{\uparrow}; \quad \downarrow \longrightarrow u^{\downarrow}$

$$\Psi(\{m_i\}) = u^{m_1} u^{m_2} u^{m_3} u^{m_4} \cdots; \quad m_i = \uparrow, \downarrow$$

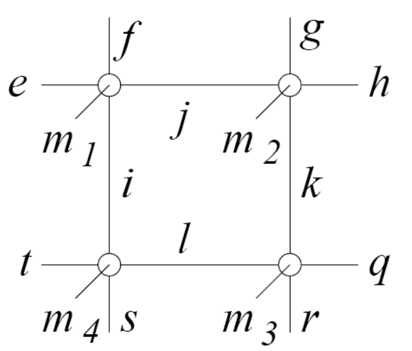
TPS: $\uparrow \longrightarrow T^{\uparrow}_{rlud}; \quad \downarrow \longrightarrow T^{\downarrow}_{rlud}$

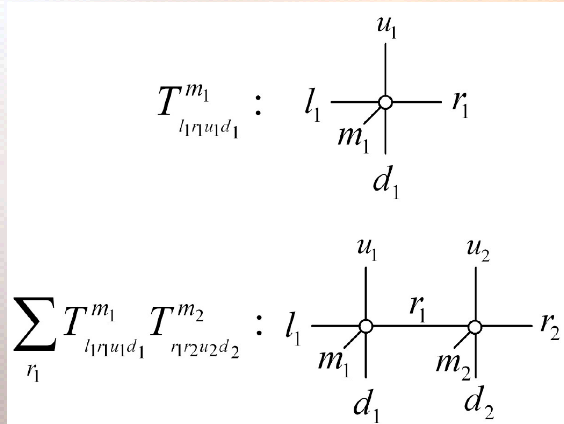
$$\Psi(\{m_i\}) = \sum_{ijkl\cdots} T^{m_1}_{ejfi} T^{m_2}_{jhgk} T^{m_3}_{lqkr} T^{m_4}_{tlis} \cdots$$

- Those Local complex tensors T's are the generalizations of the local order parameters u's which are complex numbers.

(F. Verstraete and J. I. Cirac 2004)

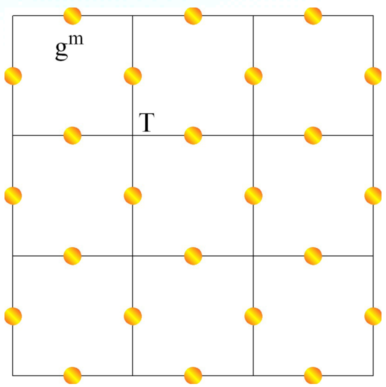
Graphic representation





TPS representations for topologically ordered states

TPS representation for ground state of Z2 gauge model

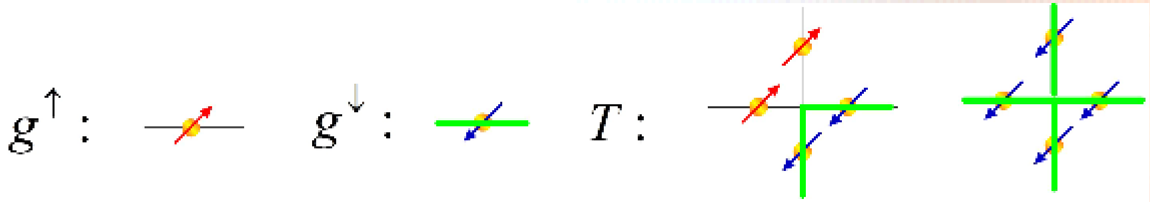


$$|\Psi_{Z_2}\rangle = \sum_{m_1, m_2, \ldots} \mathrm{tTr}[\otimes_v T \otimes_l g^{m_l}] |m_1, m_2, \ldots\rangle$$

$$T_{\alpha\beta\gamma\delta} = \begin{cases} 1 & \text{if} \quad \alpha+\beta+\gamma+\delta \quad \text{even} \\ 0 & \text{if} \quad \alpha+\beta+\gamma+\delta \quad \text{odd} \end{cases}$$

$$g^{\uparrow}_{00} = 1, \quad g^{\downarrow}_{11} = 1, \quad \text{others} = 0,$$

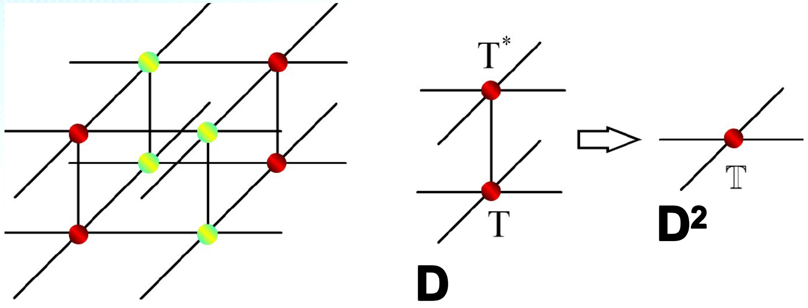
with internal indices like α running over 0, 1

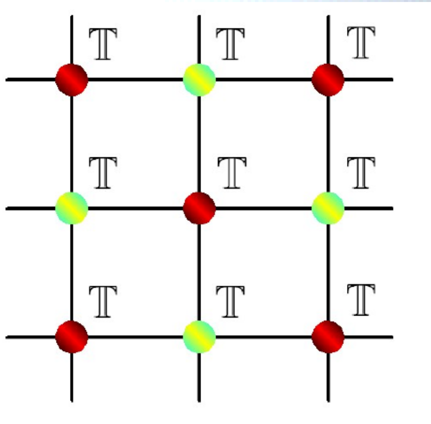


- It's easy to study local (Hamiltonian) perturbations of the system in TPS representation(Xie Chen, *etal,2010*)
- All the string-net states (classify all non-chiral topological order in bosonic systems) have exact TPS representations. (Z.C. Gu, *etal*., 2008, O. Buerschaper, *etal*., 2008)

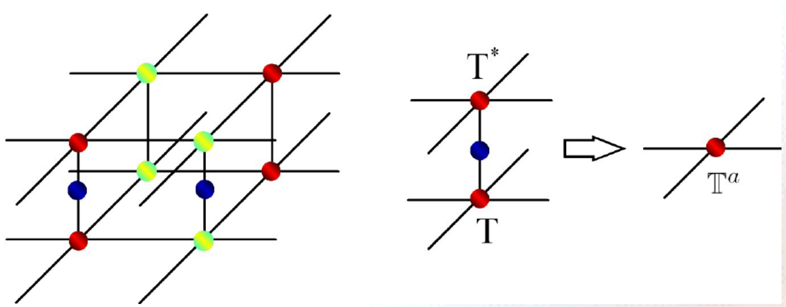
Calculate physical quantities

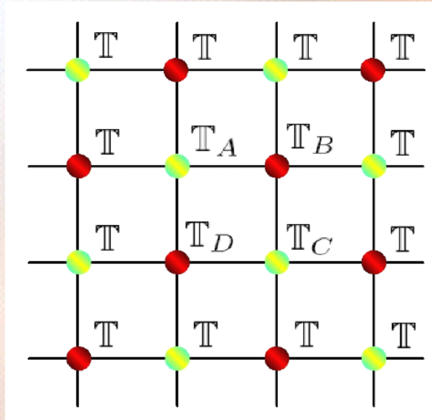
calculate the norm





calculate the energy

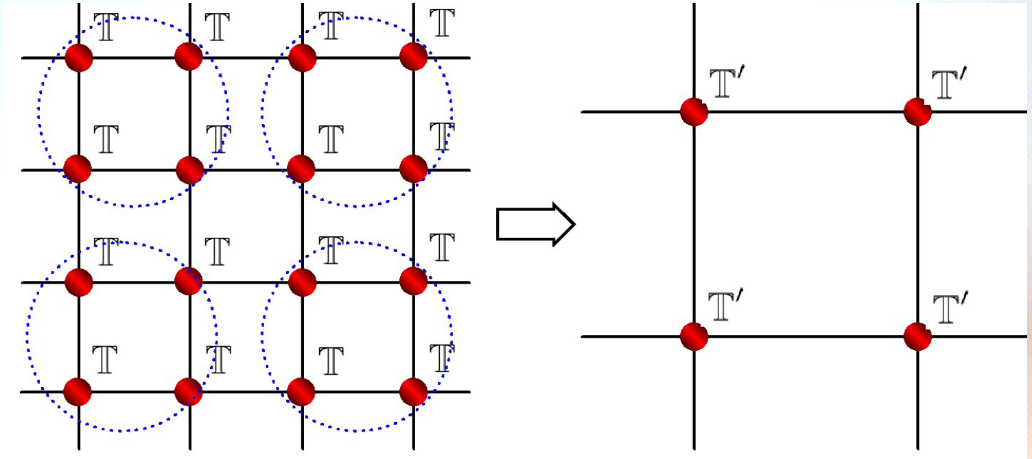


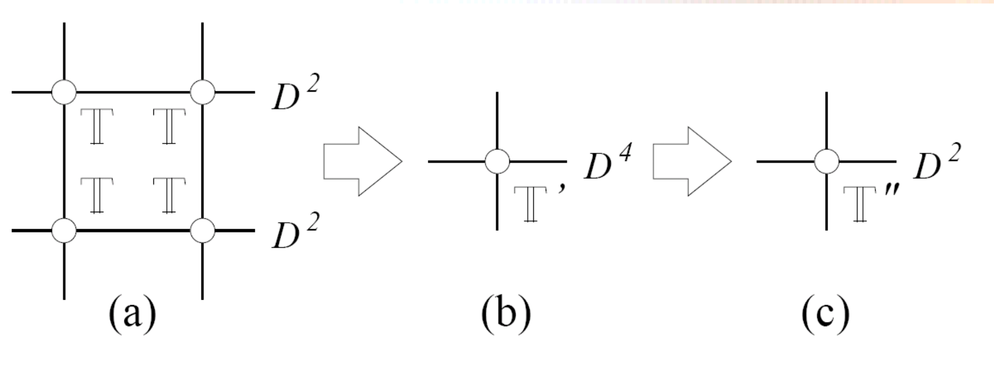


- Calculate the norm and energy for 2D tensor-net are exponential hard in general.(N. Schuch, *etal.*,2007)

Tensor-Entanglement Renormalization Group algorithm

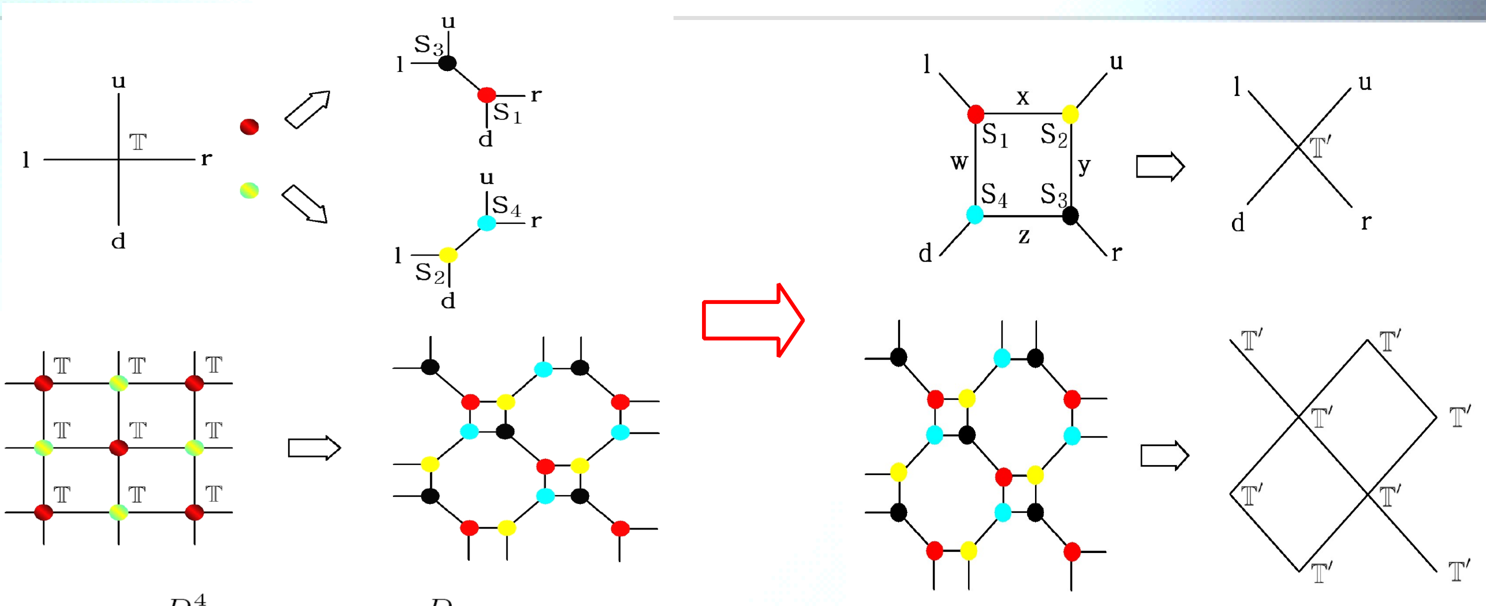
Basic idea





$$\mathrm{tTr}[\mathbb{T}\otimes\mathbb{T}\cdots] \approx \mathrm{tTr}[\mathbb{T}''\otimes\mathbb{T}''\cdots]$$

Detail implementation: Keep long-range entanglement



$$\mathbb{T}_{lrud} = \sum_{i=1}^{D^4} S^1_{rdi} S^3_{lui} \simeq \sum_{i=1}^{D_{cut}} S^1_{rdi} S^3_{lui}$$

$$\mathbb{T}_{lrud} = \sum_{i=1}^{D^4} S^2_{dli} S^4_{uri} \simeq \sum_{i=1}^{D_{cut}} S^2_{dli} S^4_{uri}$$

$$\mathbb{T}'_{lrud} = \sum_{xyzw} S_{1xwl} S_{3zyr} S_{2yxu} S_{4wzd}$$

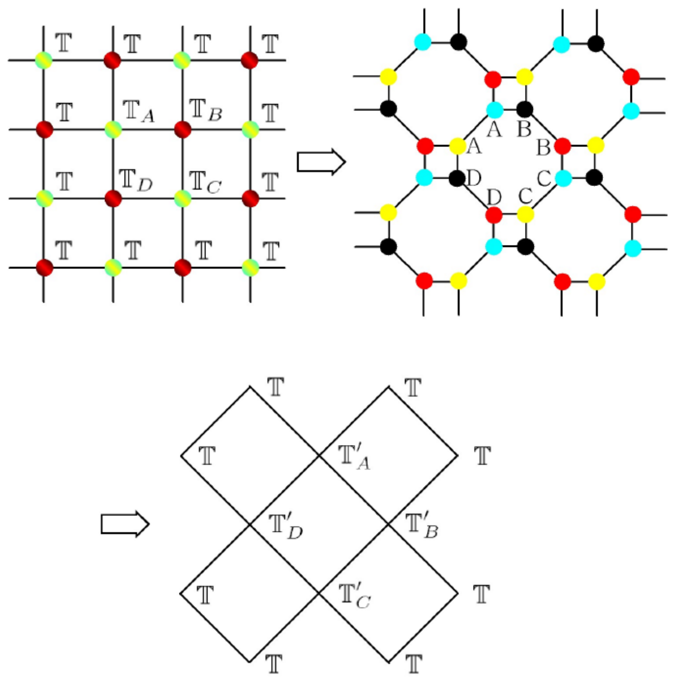
M. Levin, etal. 2007, Z. C. Gu, etal, 2008

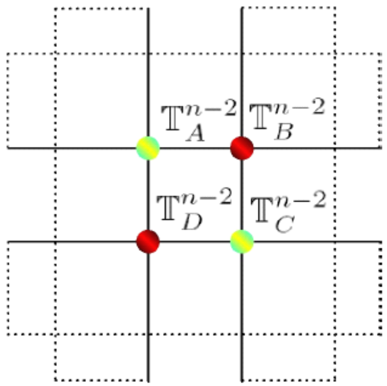
$$M^{\text{red}}_{rd;lu} = \mathbb{T}_{lrud} \quad M^{\text{red}} = USV^{\dagger}$$

$$S_{1rdi} = \sqrt{S_i} U_{rd,i}, S_{3lui} = \sqrt{S_i} V^{\dagger}_{i,lu}$$

- All the tensors that represent string-net states are fixed point tensors.(States not faraway from fixed point have controlled errors)
- Recent development: SRG(T Xiang 2009), wavefunction RG(Xie, Gu, Wen, 2010)

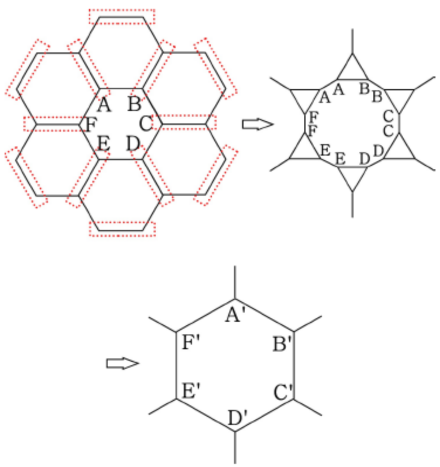
Calculate the energy of TPS

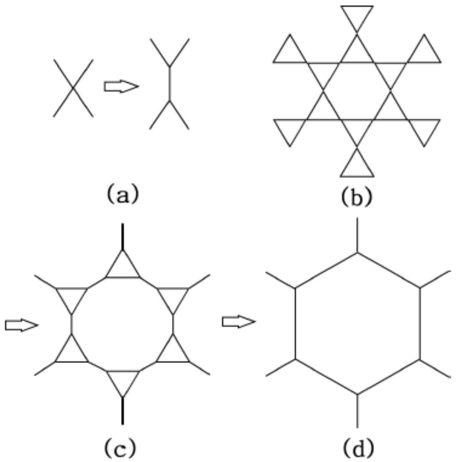


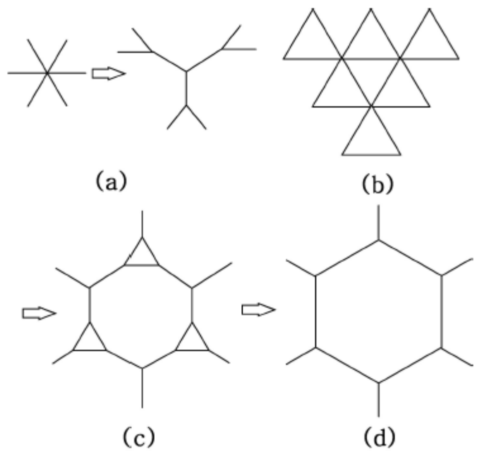


- The number of impurity tensors does not increase!

Other lattice geometry



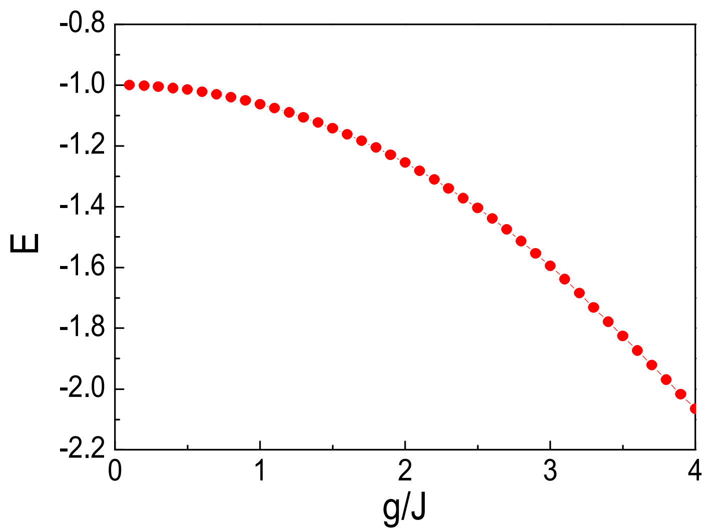


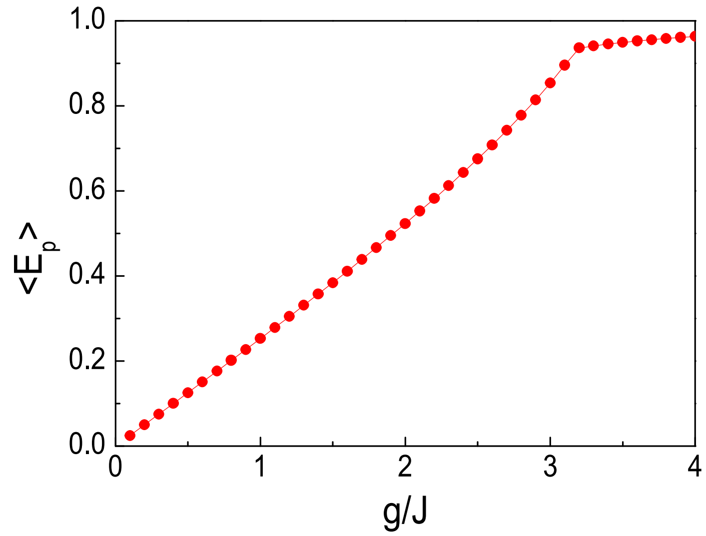


Example: topological order

Z2 gauge model with string tension:

$$H = U\sum_v\left(1-\prod_{l\in v}\sigma_l^z\right) - g\sum_p\prod_{l\in p}\sigma_l^x - J\sum_l\sigma_l^z$$





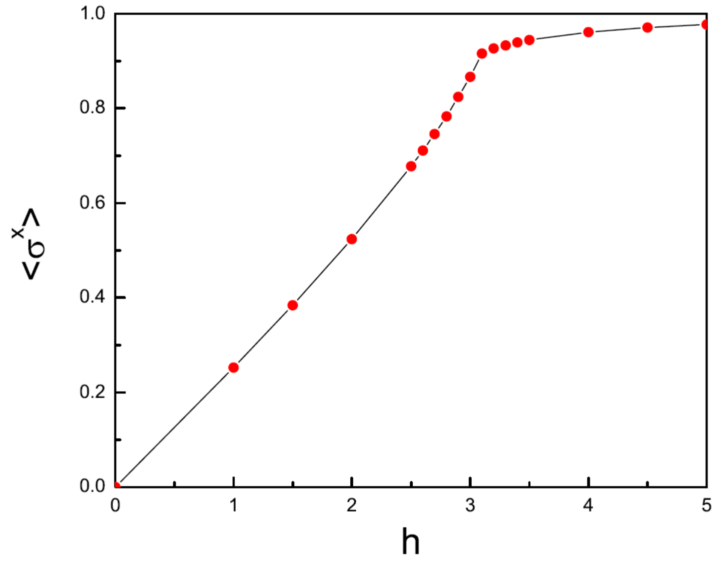
- The transition point is g/J=3.1, consistent with QMC result with g/J=3.044

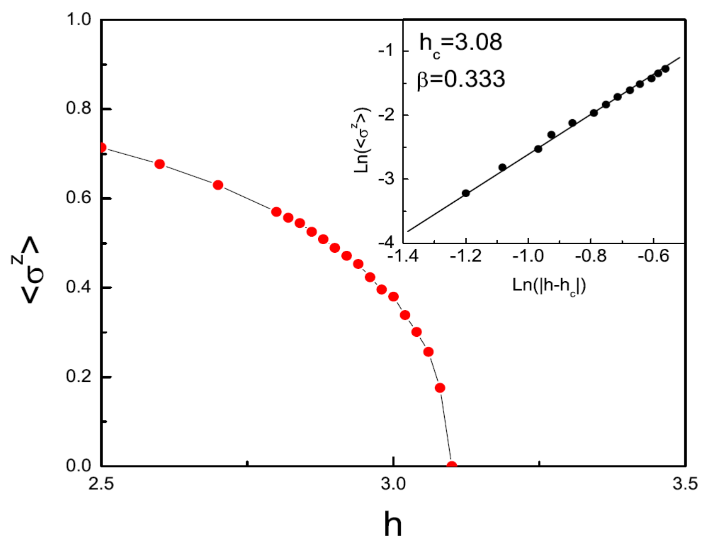
Example: symmetry breaking order

Transverse Ising model:

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

$D = 2 \qquad D_{\text{cut}} = 18$





- System size: $N=2^{18}$

$$\langle \sigma^z \rangle = A|h - h_c|^\beta$$

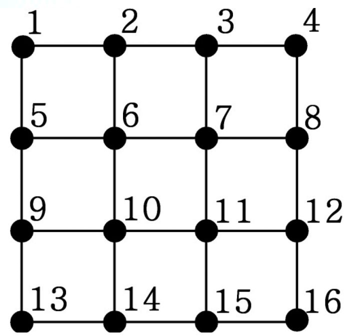
$$\beta^{QMC} \simeq 0.327 \qquad h_c^{QMC} \simeq 3.044$$

Much better than simple mean-field!

How to handle fermion ?

How to simulate fermion systems?

- Treat fermion systems as ordinary hardcore boson/spin systems.



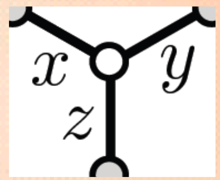
$$c_j^\dagger|0\rangle \rightarrow \prod_{i<j}(-1)^{n_i} b_j^\dagger|0\rangle = \prod_{i<j}(-1)^{n_i}|1\rangle$$

$$|0\rangle \rightarrow |0\rangle$$

Fermion hopping terms are non-local in two and higher dimensions.

- Mapping a local fermion system to local spin systems.

(The inverse construction of honeycomb Kitaev model,



$$\hat{H} = -\sum_{\alpha-link}\sum_{i-site} J_\alpha \hat{\sigma}_i^\alpha \hat{\sigma}_{i+\hat{e}_\alpha}^\alpha$$

can be generalized to arbitrary lattices and arbitrary local fermion models.)

Hard to use translational invariant TPS to study ground state.

Is there better recipe?

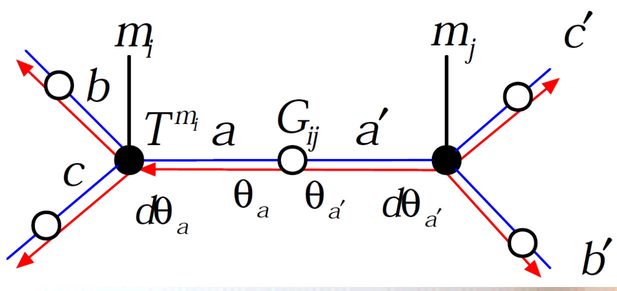
Grassmann TPS

General construction:

0,1

$$T^{m_i}_{abc} \rightarrow \mathbf{T}^{m_i}_{abc} = \sum_{n_a n_b n_c} T^{m_i}_{abc;n_a n_b n_c} \mathrm{d}\theta_a^{n_a} \mathrm{d}\theta_b^{n_b} \mathrm{d}\theta_c^{n_c}$$

$$\delta_{aa'} \rightarrow \mathbf{G}_{aa'} = \delta_{aa'}(1 + \theta_a \theta_{a'})$$



$$|\Psi\rangle = \sum_{m_i} \sum_{\{a\}} \int \prod_{\text{cite}} [c_i^\dagger]^{m_i} \mathbf{T}^{m_i}_{abc} \prod_{\text{link}} \mathbf{G}_{aa'} |0\rangle$$

$$m_i + n_a + n_b + n_c = 0(mod2)$$

$$\theta_i \theta_j = -\theta_j \theta_i, \qquad \mathrm{d}\theta_i \mathrm{d}\theta_j = -\mathrm{d}\theta_j \mathrm{d}\theta_i$$

$$\int \mathrm{d}\theta_i \theta_j = \delta_{ij} \qquad \int \mathrm{d}\theta_i 1 = 0.$$

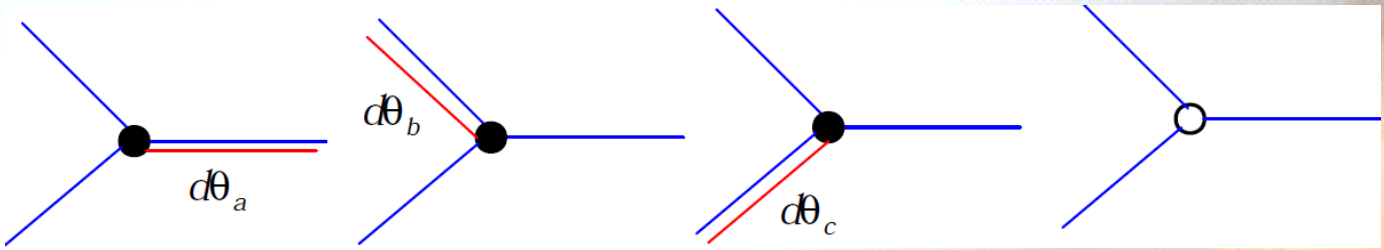
- The fermion wavefunction gives out the correct sign under different orderings.

$$|m_1 m_2 m_3 \cdots\rangle = [c_1^\dagger]^{m_1} [c_2^\dagger]^{m_2} [c_3^\dagger]^{m_3} \cdots |0\rangle \quad \Psi_f(\{m_i\}) = \langle m_1 m_2 m_3 \cdots | \Psi \rangle$$

- Calculate local physical quantities only evolve local Grassmann tensors.

Energy level filling (EFL) states can be easily represented as Grassmann tensor product states:

$$|\Psi_f\rangle = \exp\left(\sum_{\langle ij\rangle} u_{ij} c_j^\dagger c_i^\dagger\right)|0\rangle \qquad T_i^1 = \sum_{I\in i} \mathrm{d}\theta_I, \quad T_i^0 = 1, \qquad G_{ij} = 1 + u_{ij}\theta_J\theta_I$$



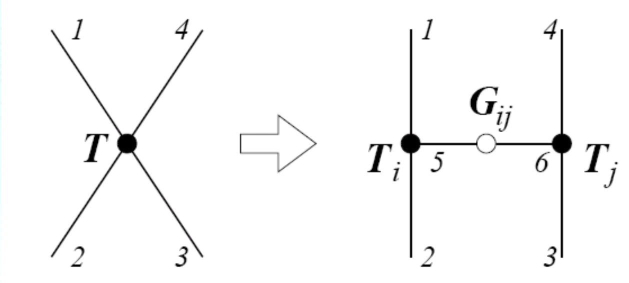
Grassmann tensor product states can represent all non-chiral topologically ordered states in fermionic systems.

- Fermionic analogy of toric code(Z2 gauge model), e.g., quantum double of Laughlin v=1/3 state.(Gu *etal*. 2010)

- These states could never be realized in boson/spin systems.

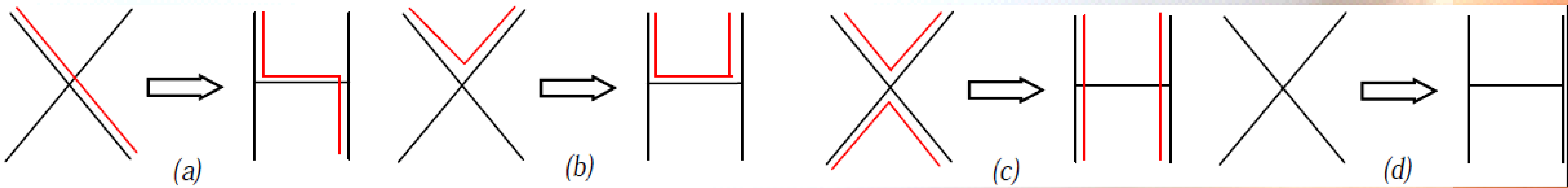
fPEPS (Christina V. Kraus *etal*. 2009) **be represented as Grassmann tensor product states.**

Grassmann tensor renormalization

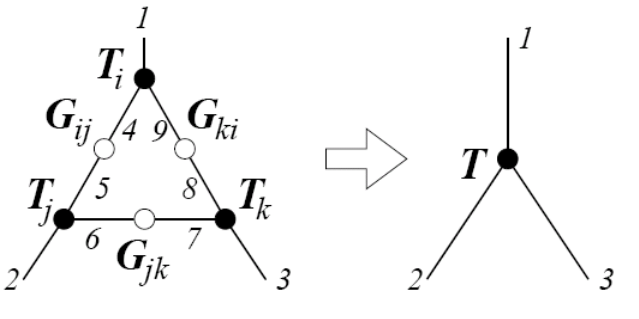


$$n_5 = \sum_{\alpha_1} n_1^{\alpha_1} + \sum_{\alpha_2} n_2^{\alpha_2} \mod 2$$

$$n_6 = \sum_{\alpha_3} n_3^{\alpha_3} + \sum_{\alpha_4} n_4^{\alpha_4} \mod 2.$$



Z2 fusion rule!



Take care of the sign !!!

$$\mathbb{T}^{\{n_1\}\{n_2\}\{n_3\}}_{p_1p_2p_3} = \sum_{p_4p_5p_6p_7p_8p_9} \sum_{n_4n_5n_6n_7n_8n_9} (-)^{(n^8 n^9)} \delta_{n^4n^5}\delta_{n^6n^7}\delta_{n^8n^9}\delta_{p_4p_5}\delta_{p_6p_7}\delta_{p_8p_9}$$

$$\times \quad \mathbb{T}^{\{n^1\}\{n^4\}\{n^9\}}_{i;p_1p_4p_9}\mathbb{T}^{\{n^2\}\{n^6\}\{n^5\}}_{j;p_2p_6p_5}\mathbb{T}^{\{n^3\}\{n^8\}\{n^7\}}_{k;p_3p_8p_7}$$

A simple test:

Short range paring state on honeycomb lattice:

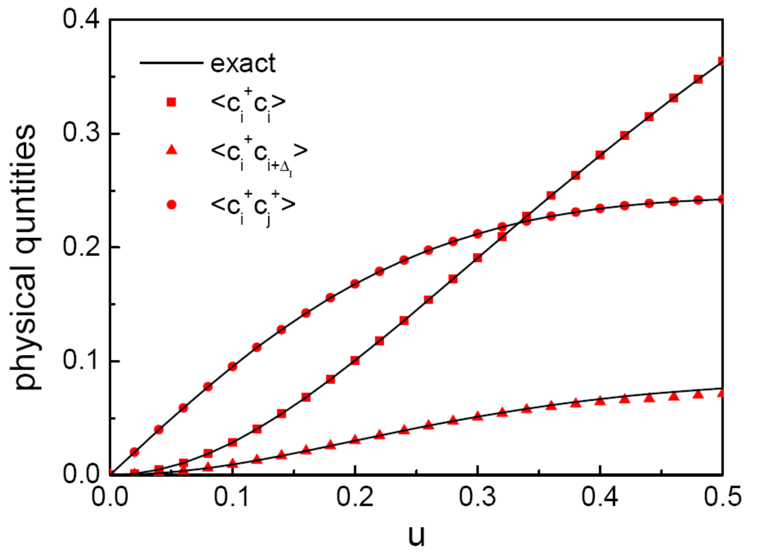
$$|\Psi_f\rangle = \exp\left(\sum_{\langle ij\rangle} u_{ij} c_j^\dagger c_i^\dagger\right)|0\rangle \qquad T_i^1 = \sum_{I\in i} d\theta_I, \quad T_i^0 = 1, \quad G_{ij} = 1 + u_{ij}\theta_J\theta_I$$

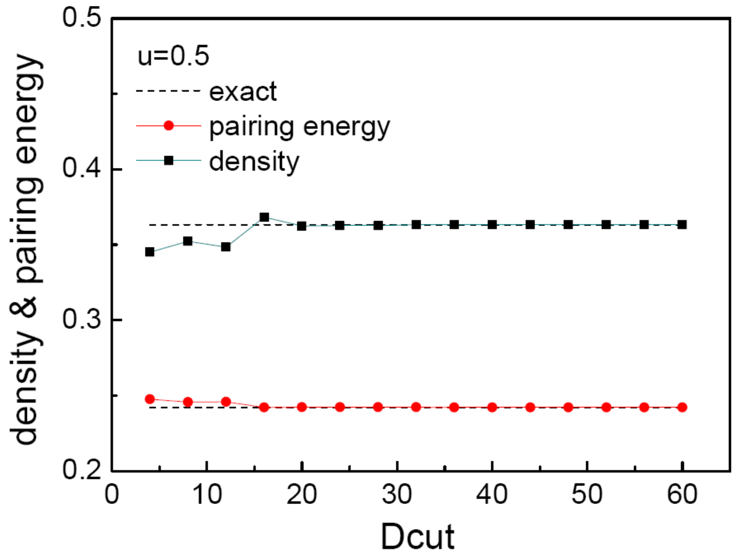
Parent Hamiltonian

$$H = -2u \sum_{\langle i\in A j\in B\rangle} c_i^\dagger c_j^\dagger + H.c. + \sum_i (1-3|u|^2) n_i - \sum_{i,I=1,\ldots,6} |u|^2 c_{i+\Delta_I}^\dagger c_i$$

$N=2*3^6$

$D_{cut}=32$





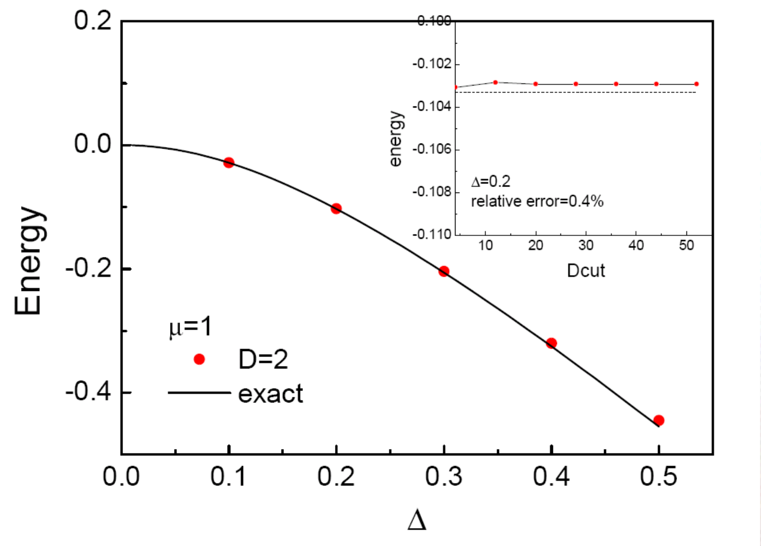
A free fermion example:

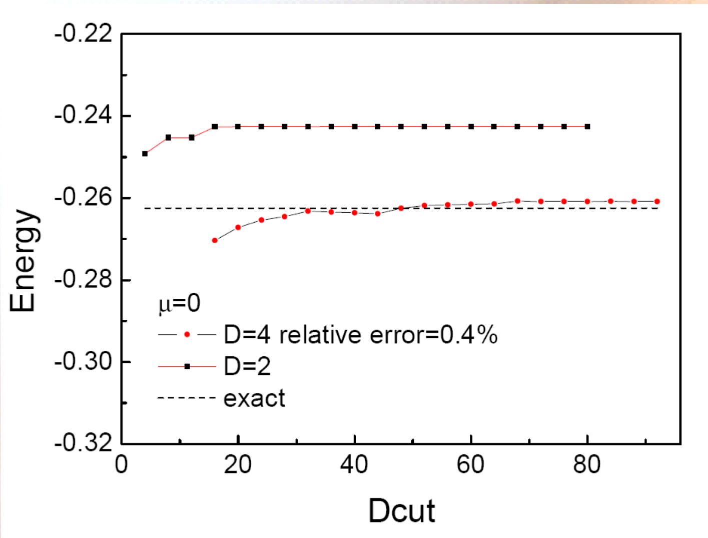
Free fermion model on honeycomb lattice:

$$H = -2\Delta \sum_{\langle i \in A j \in B \rangle} c_i^\dagger c_j^\dagger + H.c. + \mu \sum_i n_i$$

N=2*3^6 D_{cut}=60

- Imaginary time evolution is performed to find the ground state.



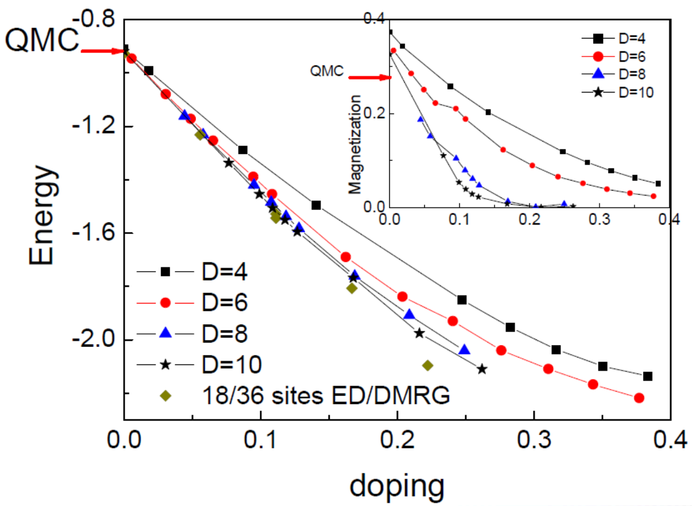


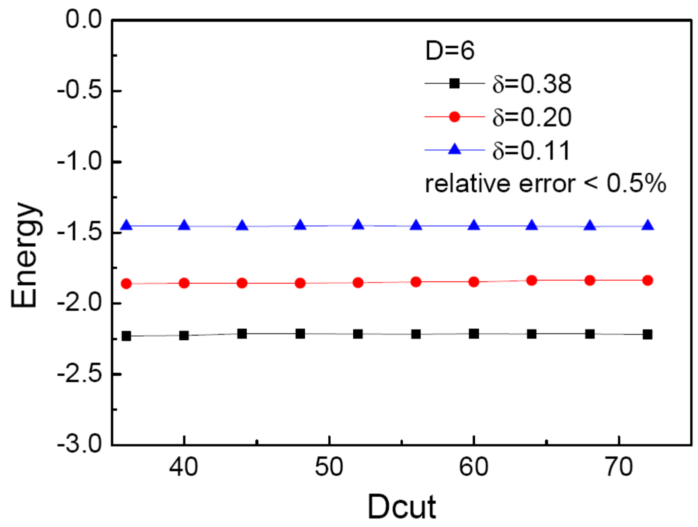
- The energy is correct even with extremely small D.
- Truncation error is larger for critical systems.

A more challenge example:

Honeycomb lattice t-J model (t=3J)

$$H_{t\text{-}J} = -t\sum_{\langle ij\rangle\sigma}\tilde{c}^{\dagger}_{i\sigma}\tilde{c}_{j\sigma} + H.c. + J\sum_{\langle ij\rangle}(\hat{S}_i\hat{S}_j - \frac{1}{4}\hat{n}_i\hat{n}_j) - \mu\sum_i \hat{n}_i \qquad \tilde{c}_{i\sigma} = \hat{c}_{i\sigma}(1-\hat{c}^{\dagger}_{i\bar{\sigma}}\hat{c}_{i\bar{\sigma}})$$

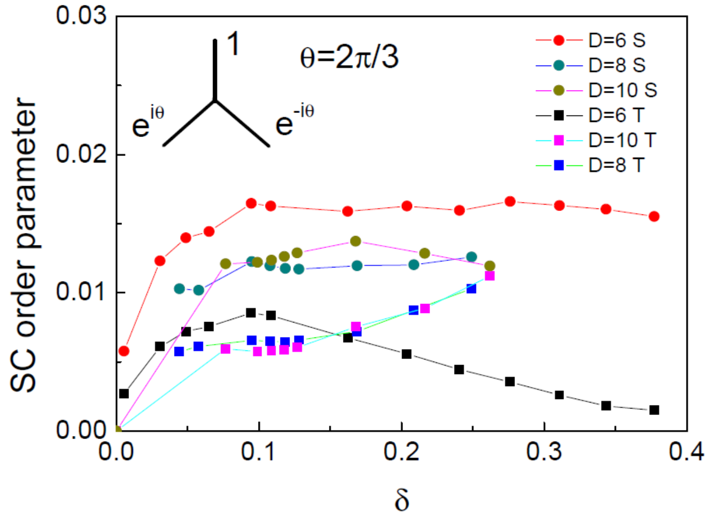


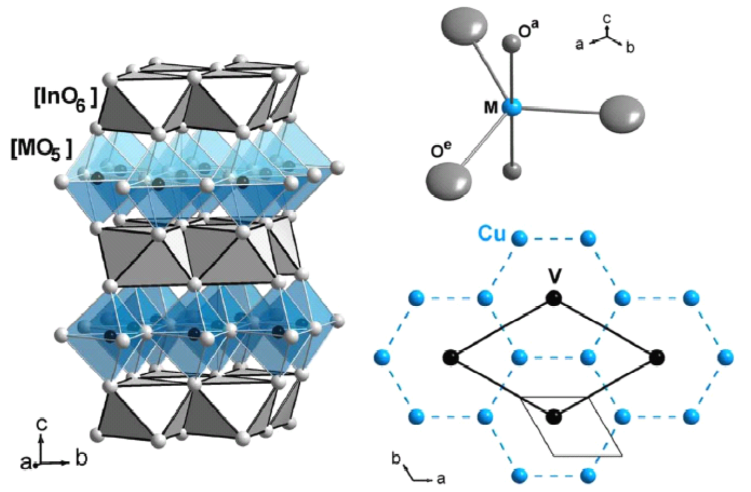


(In collaboration with Hongchen Jiang, Donna Sheng, etal.)

- Energy and magnetization are agree with QMC at half filling.
- Energy is pretty good comparing with ED for low doping.

Is it a superconductor?





- A robust chiral SC phase is found in a large doping regime.
- Coexist with AF at low doping.
- With both singlet and triplet paring.
- Triplet d vector anti-parallel with Neel vector.

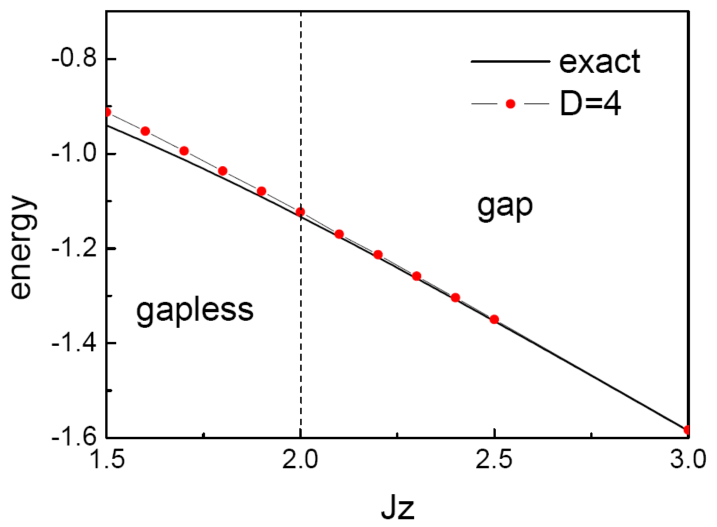
- **Possible realizations: AF S=1/2 honeycomb lattice in InCu2/3V1/3O3.** (Phys. Rev. B 78, 024420 (2008))
- Dope: chiral superconductor?
- Pressure: spin liquid? (Nature 464, 847 (2010))

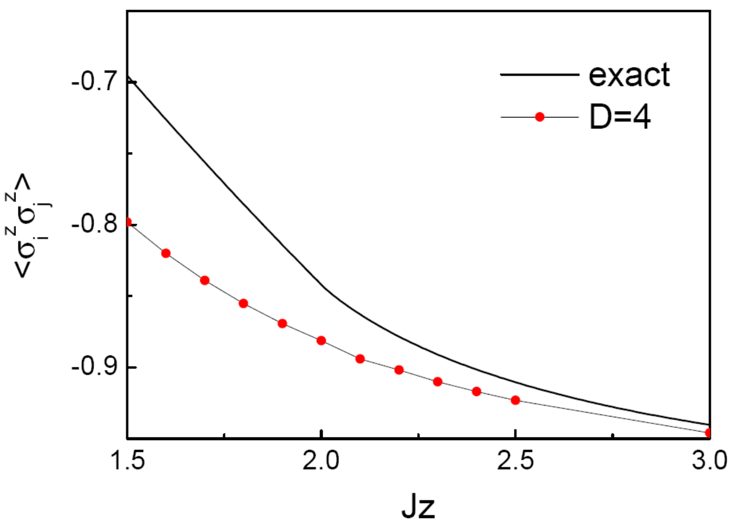
A spin model with emergent fermion:

Honeycomb Kitaev model

$$\hat{H} = -\sum_{\alpha-link}\sum_{i-site} J_\alpha \hat{\sigma}_i^\alpha \hat{\sigma}_{i+\hat{e}_\alpha}^\alpha$$

Jx=1, Jy=1, Jz=1.5~3





- **The energy is agree with exact result in the gapped phase.**
- **It's hard to realize the incommensurate Dirac cone phase with small inner dimension D.**

Summaries and future works

- Grassmann tensor product states provide a unified framework to describe symmetry breaking order states and topologically ordered states
- We generalize the TERG method to Grassmann TPS.
- We demonstrate our algorithm on the honeycomb t-J model and a novel chiral superconducting phase is predicted at finite doping, possible realization is discussed.
- Potential to solve the twenty-years puzzle, a Doped-Mott-Insulator is a superconductor!
- Generalize Grassmann representation to MERA,TTN
- Generalize to anyonic tensor product states.

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