Grassmann tensor product state approach to strongly correlated systems

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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 $\frac{1}{2}$ system:

$$|\Psi_{trial}\rangle = \bigotimes (u^\dagger |\uparrow \rangle_i + u^\dagger |\downarrow \rangle_i)$$

• 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:

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

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

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:**

- same topological order as Z2 spin liquid

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

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

\[|\Psi_{Z2}\rangle = \sum |X_{\text{close}}\rangle\]

\[|\uparrow\rangle \rightarrow \text{no string}; \quad |\downarrow\rangle \rightarrow \text{one string}\]

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- 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.

\[ U_{pwl}^{(1)}U_{pwl}^{(2)}U_{pwl}^{(3)} \cdots U_{pwl}^{(M)} |\Psi\rangle = \text{direct product state} \]

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 et al. 2010)

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

**Mean-field states:** \[ u^\uparrow; \quad u^\downarrow \]

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

**TPS:**

\[ T_{rlud}^\uparrow; \quad T_{rlud}^\downarrow \]

\[ \Psi(\{m_i\}) = \sum_{ijkl\cdots} T_{e j f i}^m T_{j h g k}^m T_{l g k r}^m T_{tlis}^m \cdots \]

- 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 $Z_2$ gauge model

$$|\Psi_{Z_2}\rangle = \sum_{m_1, m_2, \ldots} t \text{Tr} [\otimes_v T \otimes_l g^m] |m_1, m_2, \ldots\rangle$$

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

$$g^\uparrow_{00} = 1, \quad g^\uparrow_{11} = 1, \quad \text{others} = 0,$$

with internal indices like $\alpha$ running over $0, 1$

$g^\uparrow$, $g^\downarrow$, $T$

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

- Calculate the norm and energy for 2D tensor-net are exponential hard in general. (N. Schuch, et al., 2007)
Tensor-Entanglement Renormalization Group algorithm

Basic idea

\[ t \text{Tr}[T \otimes T \cdots] \approx t \text{Tr}[T' \otimes T'' \cdots] \]
Detail implementation: Keep long-range entanglement

\[ T_{trud} = \sum_{i=1}^{D} S^1_{rdi} S^3_{lui} \approx \sum_{i=1}^{D_{cut}} S^1_{rdi} S^3_{lui} \]

\[ T'_{trud} = \sum_{xyzw} S_{1xw} S_{3zyr} S_{2yxu} S_{4wzd} \]

\[ M_{rd;lu}^{\text{red}} = T_{trud} \quad M^{\text{red}} = U S V^\dagger \]

- 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:

\[ D = 2 \quad D_{\text{cut}} = 18 \]

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

- System size: \( N = 2^{18} \)

Much better than simple mean-field!
How to handle fermion?

How to simulate fermion systems?

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

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

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,

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

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:

\[ T_{abc}^{m_i} \rightarrow T_{abc}^{m_i} = \sum_{n_a n_b n_c} T_{abc; n_a n_b n_c}^{m_i} d\theta_a^{n_a} d\theta_b^{n_b} d\theta_c^{n_c} \]

\[ \delta_{aa'} \rightarrow G_{aa'} = \delta_{aa'} (1 + \theta_a \theta_{a'}) \]

\[ |\Psi\rangle = \sum_{m_i} \sum_{\{a\}} \int \prod_{\text{cite}} [c_i]^{m_i} T_{abc}^{m_i} \prod_{\text{link}} G_{aa'} |0\rangle \]

\[ m_i + n_a + n_b + n_c = 0 (mod 2) \]

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

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

- Calculate local physical quantities only evolve local Grassmann tensors.
Energy level filling (EFL) states can be easily represented as Grassmann tensor product states:

$$|\Psi_f\rangle = \exp \left( \sum_{\langle ij \rangle} u_{ij} c_j^\dagger c_i^\dagger \right) |0\rangle$$

$$T_i^1 = \sum_{I \in i} d\theta_I, \quad T_i^0 = 1, \quad G_{ij} = 1 + u_{ij} \theta_J \theta_I$$

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 et al. 2010)

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

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

\[ n_5 = \sum_{\alpha_1} n_1^{\alpha_1} + \sum_{\alpha_2} n_2^{\alpha_2} \mod 2 \]
\[ n_6 = \sum_{\alpha_3} n_3^{\alpha_3} + \sum_{\alpha_4} n_4^{\alpha_4} \mod 2. \]

\[ T_{p_1 p_2 p_3}^{\{n_1\} \{n_2\} \{n_3\}} = \sum_{p_4 p_5 p_6 p_7 p_8 p_9} \sum_{n_4 n_5 n_6 n_7 n_8 n_9} (-1)^{n_8 n_9} \delta_{n_4 n_5} \delta_{n_6 n_7} \delta_{n_8 n_9} \delta_{p_4 p_5} \delta_{p_6 p_7} \delta_{p_8 p_9} \]

Z2 fusion rule!

Take care of the sign !!!
A simple test:

Short range paring state on honeycomb lattice:

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

Parent Hamiltonian

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

\[ N=2 \times 3^6 \quad D_{\text{cut}}=32 \]
A free fermion example:

Free fermion model on honeycomb lattice:

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

\[ N = 2 \times 3^6 \quad D_{\text{cut}} = 60 \]

- 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)

\[
H_{t-J} = -t \sum_{\langle ij \rangle \sigma} \tilde{c}_i^\dagger \tilde{c}_j \sigma + \text{H.c.} + J \sum_{\langle ij \rangle} (\hat{S}_i \hat{S}_j - \frac{1}{4} \hat{n}_i \hat{n}_j) - \mu \sum_i \hat{n}_i \quad \tilde{c}_i \sigma = \hat{c}_i \sigma(1 - \hat{c}_i^\dagger \hat{c}_i \sigma)
\]

(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?
A spin model with emergent fermion:

Honeycomb Kitaev model

\[ \hat{H} = - \sum_{\alpha\text{-link}} \sum_{i\text{-site}} J_{\alpha} \hat{\sigma}_i^\alpha \hat{\sigma}_{i+\vec{e}_\alpha} \]

\[ J_x = 1, \quad J_y = 1, \quad J_z = 1.5 \sim 3 \]

- 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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