Grassmann Tensor Product State & the Emergence of Topological Superconductivity in 2D Strongly Correlated Doped Dirac Systems

(arXiv:1408.6820)

Zhengcheng Gu (Perimeter Institute)

Collaborators:

Dr. H. C. Jiang (Stanford)

Prof. G. Baskaran(C.I.T./PI)

Beijing. May. 2015
p+ip topological superconductivity in spinless fermion systems

A Majorana zero mode emerges in the vortex core

(N. Read and Green, Phys. Rev. B 61, 10267 (2000))

Vortex carries non-Abelian statistics

- Topological quantum computation. (Kitaev, 1997)

But hard to be realized in nature

- Electron carries spin, spinless fermion is artificial.
- In BCS theory, a strong spin polarization will kill the superconductivity -- instability towards phase separation.
- How about strong coupling systems: spin-charge separation?
Outline

- An old problem: stability of Nagaoka Ferromagnetic in infinite-U Hubbard model on honeycomb lattice
- Numerical approach: Grassmann tensor product state
- Analytic approach: a controlled quantum field theory
- A new mechanism of superconductivity in strongly correlated Dirac fermions
- Towards experimental realization
- Summary and outlook
The infinite-U Hubbard model:

Repulsive Hubbard model

\[
H = t \sum_{\langle ij \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + h.c. + U \sum_i n_{i\uparrow} n_{i\downarrow}
\]

\[
H_{t-J} = t \sum_{\langle ij \rangle, \sigma} \hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + h.c. + J \sum_{\langle ij \rangle} \left( \hat{S}_i \cdot \hat{S}_j - \frac{1}{4} n_i n_j \right) \quad \tilde{c}_{i\sigma} = \hat{c}_{i\sigma}(1 - \hat{c}_{i\bar{\sigma}}^\dagger \hat{c}_{i\bar{\sigma}})
\]

Infinite-U repulsive Hubbard model with a single hole:

A fully polarized ground state -- Nagaoka's Theorem
(Nagaoka, 1966)

Unfortunately, Nagaoka's Theorem can not be generalized into finite doping.

- Nevertheless, Nagaoka state is an eigenstate of the infinity-U Hubbard model. It could be a good starting point for understanding correlated systems with spin-charge separation.

- If Nagaoka state becomes unstable, there is a big chance for p+ip topological superconductivity.
Recent numerical results:

Infinite-U Hubbard model on square lattice (DMRG)

- HMF = Half-Metallic Ferromagnetic = Nagaoka Ferromagnetic

Contradict to other results, e.g., series expansion.

DMRG calculation claims that Nagoaka state is stable up to 20% doping on square lattice infinite-U Hubbard model

How about honeycomb geometry?

Repulsive Hubbard model on honeycomb lattice

- It is a Mott insulator with AF ordering at half-filling
- It might be a d+id/p+ip superconductor at finite doping due to repulsive interaction and geometry

We first investigate infinite-U Hubbard model on honeycomb lattice by using (Grassmann) tensor product state algorithm.
Meanfield approach to many body systems

- The key concept is to find an ideal trial wave function, e.g., for a spin $\frac{1}{2}$ system:

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

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

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

$$h_{MF}^c = 4$$

$$\beta_{MF}^c = 0.5$$

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

Meanfield theory has no long-range entanglement and fails for strongly correlated systems
Tensor product state (TPS)

Meanfield states: $\uparrow \rightarrow u^\uparrow; \quad \downarrow \rightarrow u^\downarrow \quad m_1 \quad m_2 \quad m_3 \quad m_4 \quad m_5 \quad m_6 \quad m_7$

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

MPS/DMRG (the best numerical method in 1D):

$\Psi(\{m_i\}) = \text{Tr} [A^{m_1} A^{m_2} A^{m_3} A^{m_4} \cdots]; \quad m_i = \uparrow, \downarrow \quad \uparrow \rightarrow A^\uparrow; \quad \downarrow \rightarrow A^\downarrow$

TPS $\uparrow \rightarrow T^{\uparrow}_{\downarrow \uparrow \downarrow \downarrow}; \quad \downarrow \rightarrow T^{\downarrow}_{\downarrow \uparrow \downarrow \downarrow}$ (F. Verstraete and J. I. Cirac 2004)
Properties of TPS:

- Entanglement entropy satisfies area law

\[ S(\rho_L) = \alpha L \]  

(F. Verstraete et al.)

- TPS faithfully represent symmetry protected topologically ordered states


- TPS faithfully represent non-chiral topologically ordered states


- TPS faithfully represent symmetry protected topologically ordered states


TPS have achieved great success in spin models

- Consistent with DMRG on frustrated magnets, e.g., J1-J2 model, Kagome Heisenberg model.

TPS for fermion systems

How to simulate fermion systems?

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

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

- A naive wavefunction

\[ m_i = 0,1 \]

Is it a fermionic wavefunction?

No

How to write down a wavefunction for fermionic systems?
A fermion wavefunction should give out the correct sign under different orderings.

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

**The magic of Grassmann algebra:**

\[
\begin{align*}
T_{A_{abc}}^{m_i} &= T_{A_{abc}}^{m_i} \theta_\alpha^P(a) \theta_\beta^P(b) \theta_\gamma^P(c), \\
T_{B_{a'b'c'}}^{m_j} &= T_{B_{a'b'c'}}^{m_j} \theta_\alpha' P(a') \theta_\beta' P(b') \theta_\gamma' P(c'), \\
G_{a'a'} &= \delta_{a'a'} d\theta_\alpha^P(a) d\theta_{\alpha'}^P(a').
\end{align*}
\]

\[
\Psi(\{m_i\}, \{m_j\}) = \sum_{\{a\}, \{a'\}} \int \prod_{i \in A} G_{a'a'} \prod_{i \in A} T_{A_{abc}}^{m_i} \prod_{j \in B} T_{B_{a'b'c'}}^{m_j}
\]

\[ P(m_i) + P(a) + P(b) + P(c) = 0(\text{mod}2) \]
Grassmann TPS as a powerful tool to represent fermionic topological phases


- In d+1D, Grassmann TPS even lead to a classification of symmetry protected topological phases in interacting fermion systems. A new type of topological superconductor beyond free fermion was predicted. New mathematics -- the group supercohomology theory was developed. (Zheng-Cheng Gu and Xiao-Gang Wen, PRB 90, 115141 (2014))
Algorithm

Imaginary time evolution:

\[
\langle \eta_{i} \eta_{j} | e^{-\beta H} | \eta_{i} \eta_{j} \rangle = \begin{vmatrix} m \end{vmatrix} \begin{vmatrix} m \end{vmatrix}
\]

\[
\begin{vmatrix} m \end{vmatrix} \begin{vmatrix} m \end{vmatrix} = \begin{vmatrix} m \end{vmatrix} \begin{vmatrix} m \end{vmatrix}
\]

Grassmann tensor renormalization:

\[
T_{A} T_{B} = T \approx \begin{vmatrix} \Lambda \end{vmatrix}
\]

※ exponentially hard (N. Schuch, etal., PRL, 2007)


\[
\frac{m}{\sqrt{\Lambda_{b}}} \frac{m}{\sqrt{\Lambda_{c}}} \frac{m}{\sqrt{\Lambda_{d}}}
\]

\[
\frac{m}{\sqrt{\Lambda_{b}}} \frac{m}{\sqrt{\Lambda_{c}}} \frac{m}{\sqrt{\Lambda_{d}}}
\]

\[
\frac{m}{\sqrt{\Lambda_{b}}} \frac{m}{\sqrt{\Lambda_{c}}} \frac{m}{\sqrt{\Lambda_{d}}}
\]

\[
\frac{m}{\sqrt{\Lambda_{b}}} \frac{m}{\sqrt{\Lambda_{c}}} \frac{m}{\sqrt{\Lambda_{d}}}
\]
A free fermion model:

**Free fermion model on honeycomb lattice:**

\[
H = -2\Delta \sum_{\langle i \in A, j \in B \rangle} c_i^\dagger c_j^\dagger + H.c. + \mu \sum_i n_i \quad (Z.C. Gu Phys. Rev. B 88, 115139 (2013))
\]

- The energy is correct even with extremely small D for gapped systems.
- Truncation error is slightly larger for critical systems.
A simple interacting fermion model:

Spinless fermion with nearest neighbor attractive interactions on honeycomb lattice:

\[ H = - \sum_{\langle ij \rangle} \left( \frac{c_i^\dagger c_j + h.c.}{\langle ij \rangle} \right) - V \sum_{\langle ij \rangle} n_i n_j \]


- Grassmann TPS ansatz is randomly initialized, no pre assumption of superconducting order parameter.

- The p+ip paring pattern emerges during imaginary time evolution.

<table>
<thead>
<tr>
<th>Doping</th>
<th>( n_f = 0.224 )</th>
<th>( n_f = 0.313 )</th>
<th>( n_f = 0.36 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \Delta_{a}^{SC} / \Delta_{b}^{SC} )</td>
<td>(-0.4996, 0.8656)</td>
<td>(-0.4995, 0.8657)</td>
<td>(-0.4995, 0.8656)</td>
</tr>
<tr>
<td>( \Delta_{b}^{SC} / \Delta_{c}^{SC} )</td>
<td>(-0.5005, 0.8660)</td>
<td>(-0.5006, 0.8659)</td>
<td>(-0.5006, 0.8659)</td>
</tr>
<tr>
<td>( \Delta_{c}^{SC} / \Delta_{a}^{SC} )</td>
<td>(-0.4999, 0.8664)</td>
<td>(-0.4999, 0.8665)</td>
<td>(-0.4999, 0.8666)</td>
</tr>
</tbody>
</table>
Infinite-U Hubbard model

The HFM state is unstable!

- Almost fully polarized $m \approx 0.99$ for doping $< 0.2$, but different from a simple HFM, and $m=0$ for doping $> 0.2$

- What's the true ground state?

$N = 2 \times 3^6$
relative error $< 0.4\%$
A $p+ip$ superconductor!

- $p+ip$ superconductivity coexists with ferromagnetic ordering!
- What's the mechanism?

$$\Delta E \sim 0.1\delta t$$
$$\Delta_t \sim 0.07\delta$$

<table>
<thead>
<tr>
<th>Doping</th>
<th>$\delta = 0.069$</th>
<th>$\delta = 0.102$</th>
<th>$\delta = 0.168$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta x, (y, z) / \Delta x, (y, z)$</td>
<td>(-0.500, 0.866)</td>
<td>(-0.500, 0.866)</td>
<td>(-0.500, 0.866)</td>
</tr>
<tr>
<td>$\Delta_t; a / \Delta_t; b$</td>
<td>(-0.500, 0.866)</td>
<td>(-0.500, 0.866)</td>
<td>(-0.500, 0.866)</td>
</tr>
<tr>
<td>$\Delta_t; b / \Delta_t; c$</td>
<td>(-0.500, 0.866)</td>
<td>(-0.500, 0.866)</td>
<td>(-0.499, 0.865)</td>
</tr>
<tr>
<td>$\Delta x, (y, z) / \Delta x, (y, z)$</td>
<td>(-0.500, 0.866)</td>
<td>(-0.500, 0.866)</td>
<td>(-0.500, 0.866)</td>
</tr>
<tr>
<td>$\Delta_t; c / \Delta_t; a$</td>
<td>(-0.500, 0.866)</td>
<td>(-0.500, 0.866)</td>
<td>(-0.500, 0.866)</td>
</tr>
</tbody>
</table>
Finite but small $J$(large $U$)?

Ground state energy (PBC)

$N = 2 \times 3^6$

relative error $\sim 0.2\%$

$t/J = 30$

- agree with DMRG results
- but no ferromagnetic order $m = 0$

$t/J = 50$

- agree with DMRG results
- but no ferromagnetic order $m = 0$
Stability and instability of p+ip superconductivity

- The p+ip order parameter decreases with increasing D.
- Non-Fermi liquid?

- The p+ip superconductivity can be stabilized by in-plane magnetic field.
  \[
  \frac{t}{J} = 30
  \]
A minimal field theory model for infinite-U Hubbard model:

Slave fermion is a good starting point: \( c_{i\sigma} = f_i^\dagger b_{i\sigma} \)

- Add a small Zeemann field to break the spin symmetry to U(1).

\[
\begin{align*}
    b^\uparrow &= \sqrt{\rho_0 + \delta \rho} e^{i\theta} & b^\downarrow &= 0 \\
    \mathcal{L}_{\text{eff}} &= \overline{\psi}_a \gamma^\mu (\partial_\mu - iA_\mu) \psi_a - \mu \overline{\psi}_a \gamma^0 \psi_a + \frac{\rho_0}{g} (\partial_\mu \theta - A_\mu)^2
\end{align*}
\]

- The linear dispersion relation for holon arises from the Dirac cone structure at 50% doping.

- In the XY limit, Ferromagnetic Goldstone mode has a linear dispersion in general.

Dual vortex representation in the dilute limit:

\[
\begin{align*}
    \mathcal{L}_{\text{eff}} &= \overline{\psi}_a \gamma^\mu (\partial_\mu - iA_\mu) \psi_a - \mu \overline{\psi}_a \gamma^0 \psi_a + \frac{i}{2\pi} \varepsilon^{\mu\nu\lambda} A_\mu \partial_\nu a_\lambda \\
    &+ \frac{g}{16\pi^2 \rho_0} (\varepsilon^{\mu\nu\lambda} \partial_\nu a_\lambda)^2 + |(\partial_\mu + ia_\mu)\phi|^2 + m^2 |\phi|^2,
\end{align*}
\]
Cheap vortices/skyrmion -- beyond dilute limit!

Vortices/skyrmion current -- charge current interaction:

\[ \mathcal{L}_{CC} = j_\mu \varepsilon^{\mu\nu\lambda} \partial_\nu a_\lambda \]

\[ j_\mu = i[\phi^* (\partial_\mu - ia_\mu)\phi - \phi (\partial_\mu - ia_\mu)\phi^*] \]

- Integral out emergent U(1) gauge field A:

\[ \varepsilon^{\mu\nu\lambda} \partial_\nu a_\lambda = 2\pi \bar{\psi}_a \gamma^\mu \psi_a \]

- Plug in the above constraint and integral out the vortex field:

\[
\begin{align*}
\mathcal{L}_{\text{eff}} &= \bar{\psi}_a \gamma^\mu \partial_\mu \psi_a - \mu \bar{\psi}_a \gamma^0 \psi_a \\
&\quad + \left( \frac{g}{4\rho_0} + \frac{4\pi^2}{m} \right) (\bar{\psi}_a \gamma^\mu \psi_a)^2 + \frac{4\pi^2}{m} \left[ \partial_\mu (\bar{\psi}_a \gamma^\nu \psi_a) \right]^2,
\end{align*}
\]

\[ [\partial_x (\bar{\psi}_a \gamma^0 \psi_a)]^2 \sim (n_i - n_{i+\delta_x})^2 \sim -2n_i n_{i+\delta_x} \] an attractive interaction!
A straightforward argument

Consider an almost fully polarized state

\[
H = t \sum_{\langle ij \rangle} (1 - n_{i\downarrow}) c_{i\uparrow}^\dagger c_{j\uparrow}(1 - n_{j\downarrow}) + h.c. \quad \langle n_{i\uparrow} \rangle = \delta_0 \ll 1
\]

\[
+ t \sum_{\langle ij \rangle} (1 - n_{i\uparrow}) c_{i\downarrow}^\dagger c_{j\downarrow}(1 - n_{j\uparrow}) + h.c.
\]

\[
\simeq t(1 - \delta_0)^2 \sum_{\langle ij \rangle} c_{i\uparrow}^\dagger c_{j\uparrow} + h.c. + t \sum_{\langle ij \rangle} c_{i\uparrow}^\dagger c_{j\uparrow} S_i^- S_j^+ + h.c.
\]

\[
(1 - n_{i\uparrow}) c_{i\downarrow}^\dagger = c_{i\uparrow} c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger = S_i^- c_{i\uparrow} \quad c_{j\downarrow}(1 - n_{j\uparrow}) = c_{j\downarrow} c_{j\uparrow} c_{j\uparrow}^\dagger = c_{j\uparrow} S_j^+
\]

Express in terms of kinetic energy and current operators

\[
H = t(1 - \delta_0)^2 \sum_{\langle ij \rangle} (c_{i\uparrow}^\dagger c_{j\uparrow} + h.c.)
\]

\[
+ \frac{1}{2} t \sum_{\langle ij \rangle} (c_{i\uparrow}^\dagger c_{j\uparrow} + c_{j\uparrow}^\dagger c_{i\uparrow})(S_i^- S_j^+ + S_j^- S_i^+)
\]

\[
+ \frac{1}{2} t \sum_{\langle ij \rangle} (c_{i\uparrow}^\dagger c_{j\uparrow} - c_{j\uparrow}^\dagger c_{i\uparrow})(S_i^- S_j^+ - S_j^- S_i^+)
\]

\[
+ \frac{1}{\kappa} (S_i^- S_j^+ - S_j^- S_i^+)^2
\]

\[
- 2t^2 \kappa n_{i\uparrow} n_{j\uparrow}
\]

\[
\vec{z} \cdot (\vec{S}_i \times \vec{S}_j)
\]

chirality current!
Spin-charge separation and Non-BCS mechanism: skyrmion current mediated superconductor

- The formal calculation in quantum field theory implies a new mechanism — skyrmion current mediated superconductivity.

- Such a mechanism relies on spin-charge separation and emergent U(1) gauge field, therefore it is beyond BCS theory.

- Condensation of skyrmion excitations leads to a potential non-fermi liquid!

\[ \mathcal{L}'_{\text{eff}} = \overline{\psi}_a \gamma^\mu (\partial_\mu - iA_\mu) \psi_a - \mu \overline{\psi}_a \gamma^0 \psi_a + \frac{1}{g'} (\varepsilon^{\mu\nu\lambda} \partial_\nu A_\lambda)^2, \]
Possible realizations: \( \text{InCu}_{2/3}\text{V}_{1/3}\text{O}_3 \).

- Doping: non Fermi liquid?
- Doping plus in-plane magnetic field: \( p+ip \) topological superconductor?

Other systems:

- \( ^3\text{He} \) absorbed on substrate. (PRL 109, 235306 (2012) )
- Organic layer on graphene. (Nature Physics 9, 368 (2013) )
Grassmann TPS are unbiased variational states to study strongly interacting electron systems.

We found strong numerical evidences that doped infinite-U Hubbard model on honeycomb lattice is a $p+ip$ superconductor coexisting with ferromagnetic order.

Based on a controlled quantum field theory calculation, we propose a non-BCS mechanism for such a superconductor.

We propose potential materials and experimental methods to realize a $p+ip$ superconductor.

Towards resolving the mechanism of high-Tc cuprates

$U/t$: SM 4 d+id 50 NF 1000? $p+ip$