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)

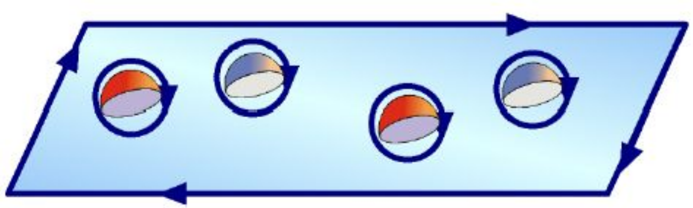
Prof. G. Baskaran(C.I.T./PI)

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

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

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

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.

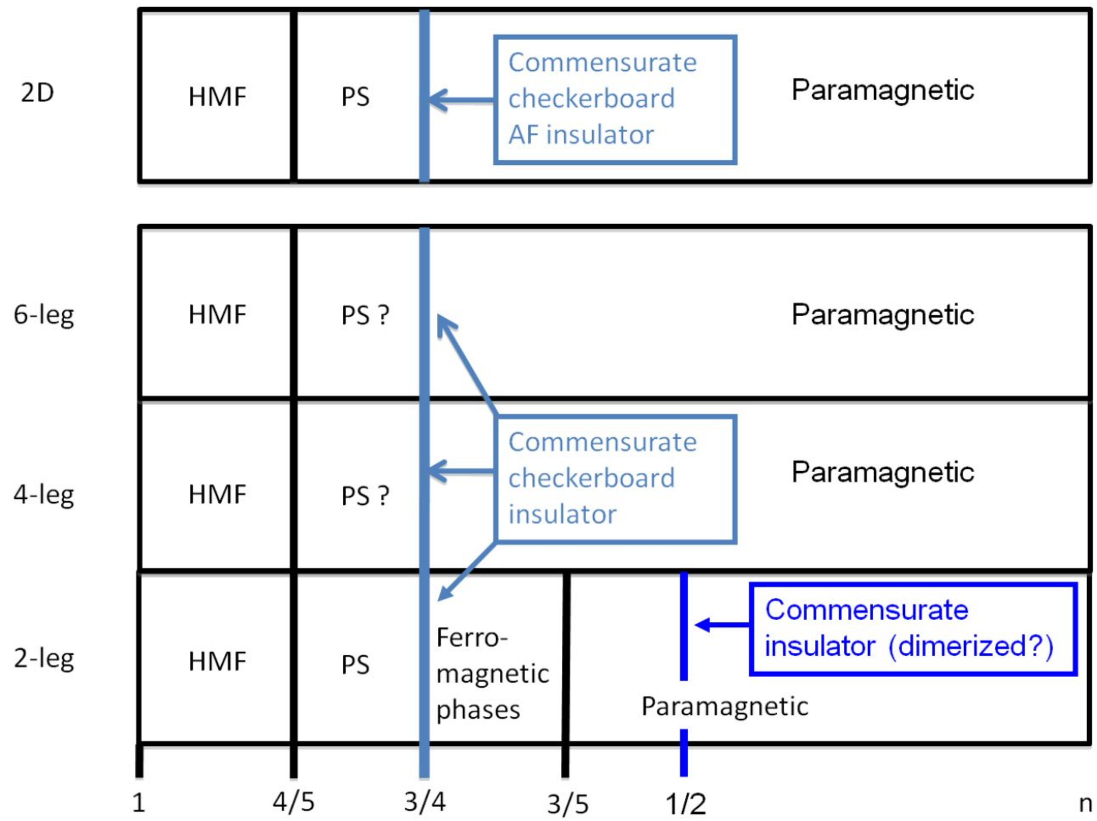
- Nevertheless, Nagaoka state is an eigenstate of the infinity-U Hubbard model. It could be a good starting point for understanding correlated systems with spin-charge separation.

- 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



Li Liu,Hong Yao, S White and S Kevilson, Phys. Rev. Lett.108, 126406 (2012)

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

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

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

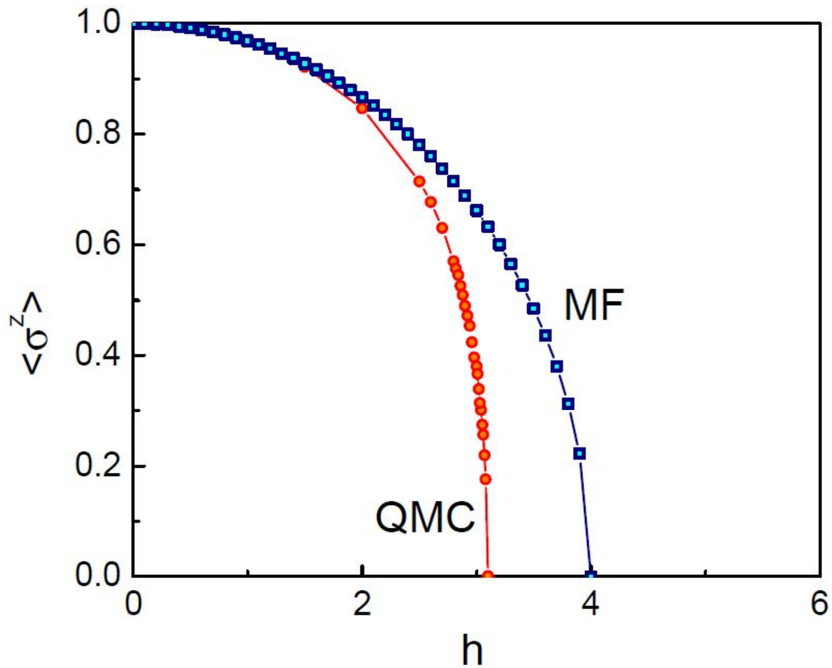
- The key concept is to find an ideal trial wave function, e.g., for a spin ½ system:

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

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

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

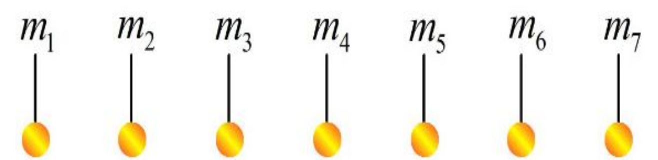
$$\begin{aligned} h_{MF}^c &= 4 \\ \beta_{MF}^c &= 0.5 \\ \langle\sigma_z\rangle &\propto |h-h_c|^{\beta} \end{aligned}$$



Meanfield theory has no long-range entanglement and fails for strongly correlated systems

Tensor product state(TPS)

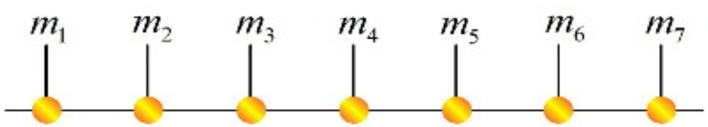
Meanfield states: $\uparrow \longrightarrow u^{\uparrow}; \quad \downarrow \longrightarrow u^{\downarrow}$



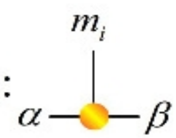
$$\Psi(\{m_i\}) = u^{m_1} u^{m_2} u^{m_3} u^{m_4} \cdots; \quad m_i = \uparrow, \downarrow$$

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

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

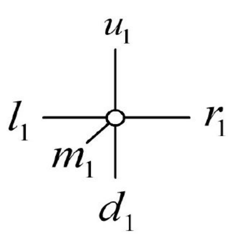


$A^{m_i}_{\alpha\beta}$:

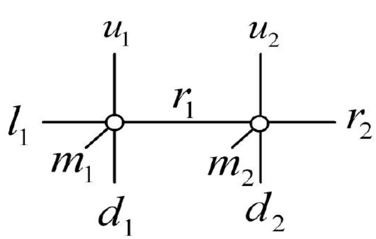


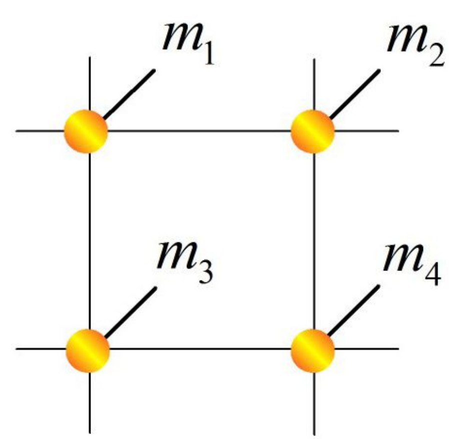
TPS $\uparrow \longrightarrow T^{\uparrow}_{lrud}; \quad \downarrow \longrightarrow T^{\downarrow}_{lrud}$ (F. Verstraete and J. I. Cirac 2004)

$T^{m_1}_{l_1 r_1 u_1 d_1}$:

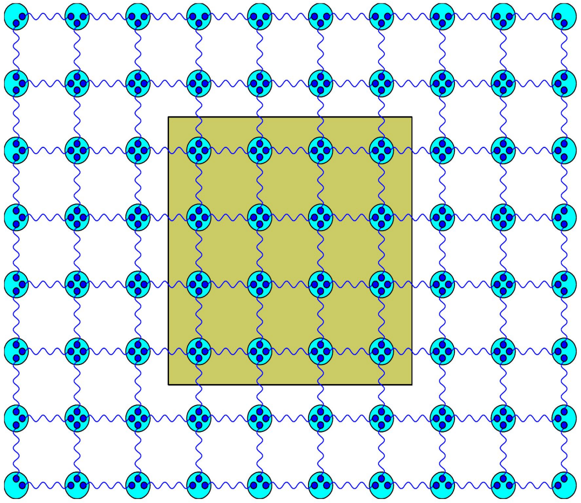


$\sum_{r_1} T^{m_1}_{l_1 r_1 u_1 d_1} T^{m_2}_{r_1 r_2 u_2 d_2}$:





Properties of TPS:



- Entanglement entropy satisfies area law

$$S(\rho_L) = \alpha L$$ (F. Verstraete *etal.*)

$$|\Psi_0\rangle = \prod_{link} |I\rangle \quad |I\rangle = \sum_{l=1}^{D} |ll\rangle$$

$$|\Psi_{TPS}\rangle = \prod_i P_i |\Psi_0\rangle \quad P_i = T^{m_i}_{lrud} |m_i\rangle\langle lrud|$$

- TPS faithfully represent non-chiral topologically ordered states (Z.C. Gu, *etal*., PRB, 2008, O. Buerschaper, *etal*., PRB, 2008)

- TPS faithfully represent symmetry protected topologically ordered states (X. Chen, Z.C.Gu, Z.X.Liu, X.G. Wen Science 338, 1604, 2012)

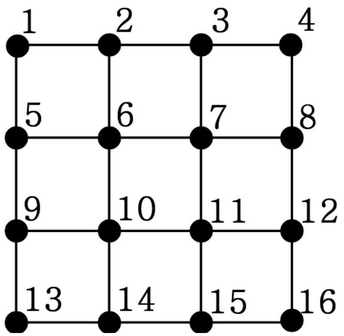
TPS have achieved great success in spin models

- Consistent with DMRG on frustrated magnets, e.g., J1-J2 model, Kagome Heisenberg model. (Ling Wang, Z C Gu, F Verstraete, X.G. Wen arXiv:1112.3331, Z.Y. Xie, *etal* Phys. Rev. X 4, 011025 (2014))

TPS for fermion systems

How to simulate fermion systems?

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

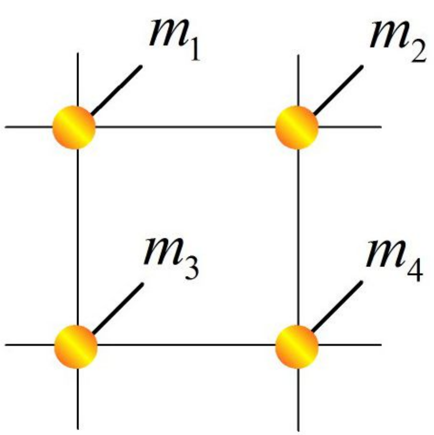


$$c_j^\dagger|0\rangle \rightarrow \prod_{i<j}(-1)^{n_i} b_j^\dagger|0\rangle = \prod_{i<j}(-1)^{n_i}|1\rangle$$
$$|0\rangle \rightarrow |0\rangle$$

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

- A naive wavefunction

$$m_i = 0,1$$



Is it a fermionic wavefunction?

No

How to write down a wavefunction for fermionic systems?

fPEPS/Grassmann TPS

C V Kraus *etal*. 2009

Z C Gu *etal*. 2010

- 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:

$$\theta_\alpha \theta_\beta = -\theta_\beta \theta_\alpha, \qquad \mathrm{d}\theta_\alpha \mathrm{d}\theta_\beta = -\mathrm{d}\theta_\beta \mathrm{d}\theta_\alpha,$$

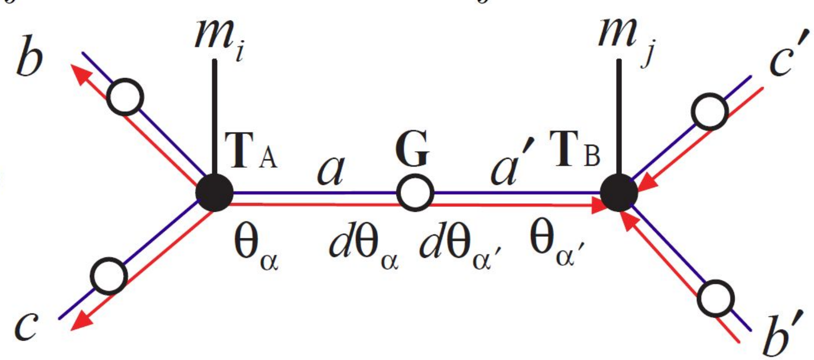
$$\int \mathrm{d}\theta_\alpha \theta_\beta = \delta_{\alpha\beta} \qquad \int \mathrm{d}\theta_\alpha 1 = 0.$$

0,1

$$\mathbf{T}_{A}{}_{abc}^{m_i} = T_{A}{}_{abc}^{m_i} \theta_\alpha^{P(a)} \theta_\beta^{P(b)} \theta_\gamma^{P(c)},$$

$$\mathbf{T}_{B}{}_{a'b'c'}^{m_j} = T_{B}{}_{a'b'c'}^{m_j} \theta_{\alpha'}^{P(a')} \theta_{\beta'}^{P(b')} \theta_{\gamma'}^{P(c')},$$

$$\mathbf{G}_{aa'} = \delta_{aa'} \mathrm{d}\theta_\alpha^{P(a)} \mathrm{d}\theta_{\alpha'}^{P(a')}.$$



$$\Psi(\{m_i\},\{m_j\}) = \sum_{\{a\},\{a'\}} \int \prod_{\langle ij \rangle} \mathbf{G}_{aa'} \prod_{i \in A} \mathbf{T}_{A}{}_{abc}^{m_i} \prod_{j \in B} \mathbf{T}_{B}{}_{a'b'c'}^{m_j}$$

$$P(m_i) + P(a) + P(b) + P(c) = 0(mod2)$$

Grassmann TPS as a powerful tool to represent fermionic topological phases

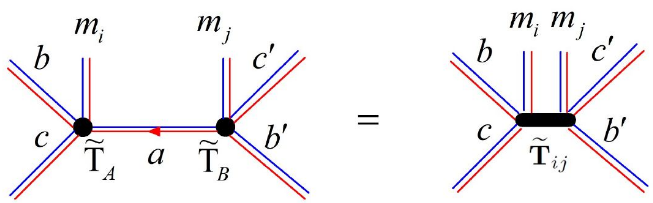
- In 2+1D, Grassmann TPS faithfully represent different patterns of fermionic long-range entanglement, which leads to a classification of non-chiral (intrinsic) topological phases in interacting fermion systems.
(Zheng-Cheng Gu, *etal*, arXiv:1010.1517(2010), Zheng-Cheng Gu, *etal,* Phys. Rev. B 90, 085140 (2014))

- 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

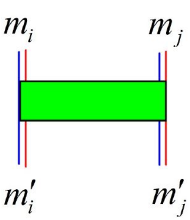
(Z.C. Gu Phys. Rev. B 88, 115139 (2013))

Imaginary time evolution:

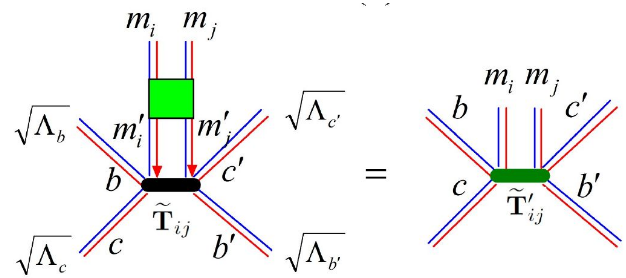


(a)

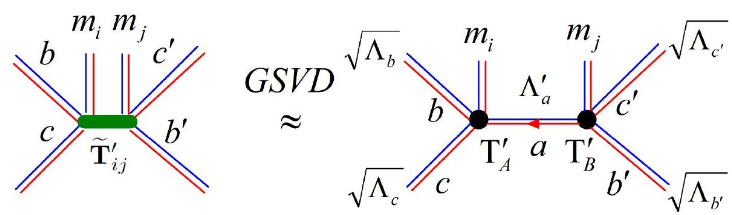
$$\langle \eta_i' \eta_j' | e^{-\delta\tau h_{ij}} | \eta_i \eta_j \rangle =$$



(b)

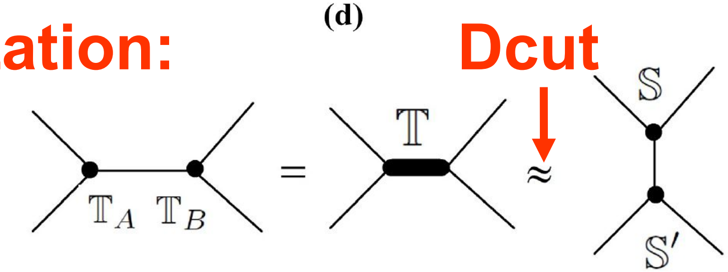


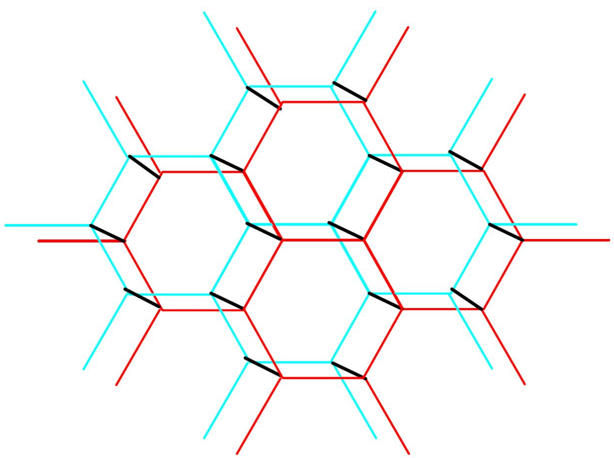
(c)

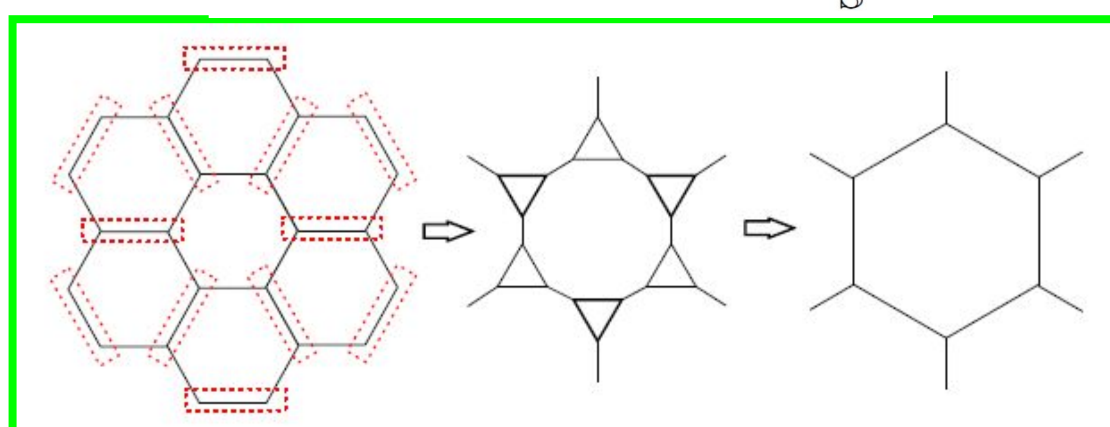


(d)

Grassmann tensor renormalization:





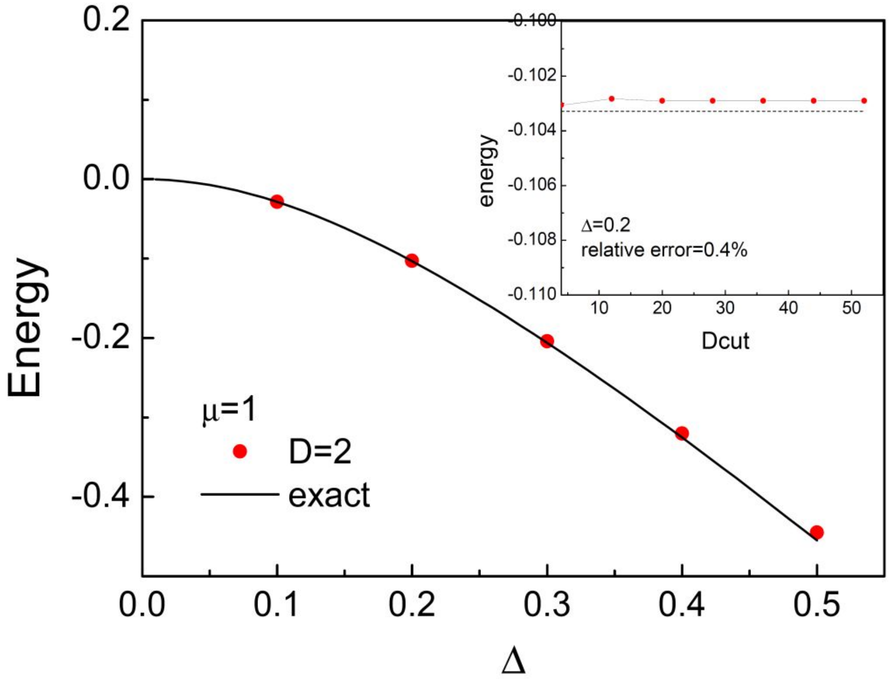


- exponentially hard
(N. Schuch, *etal.*, PRL, 2007)

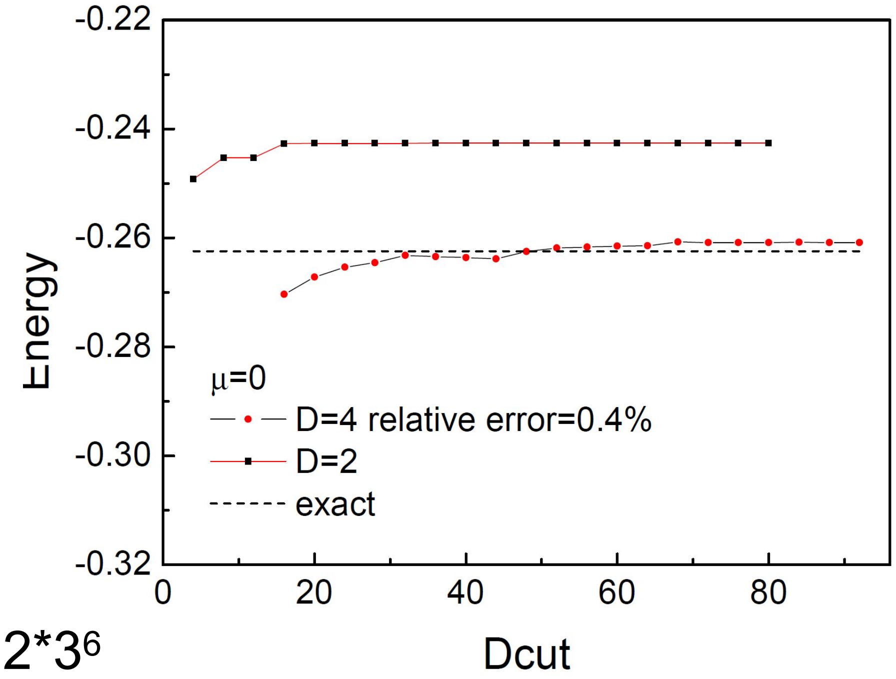
A free fermion model:

Free fermion model on honeycomb lattice:

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



N=2*3^6



- 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:

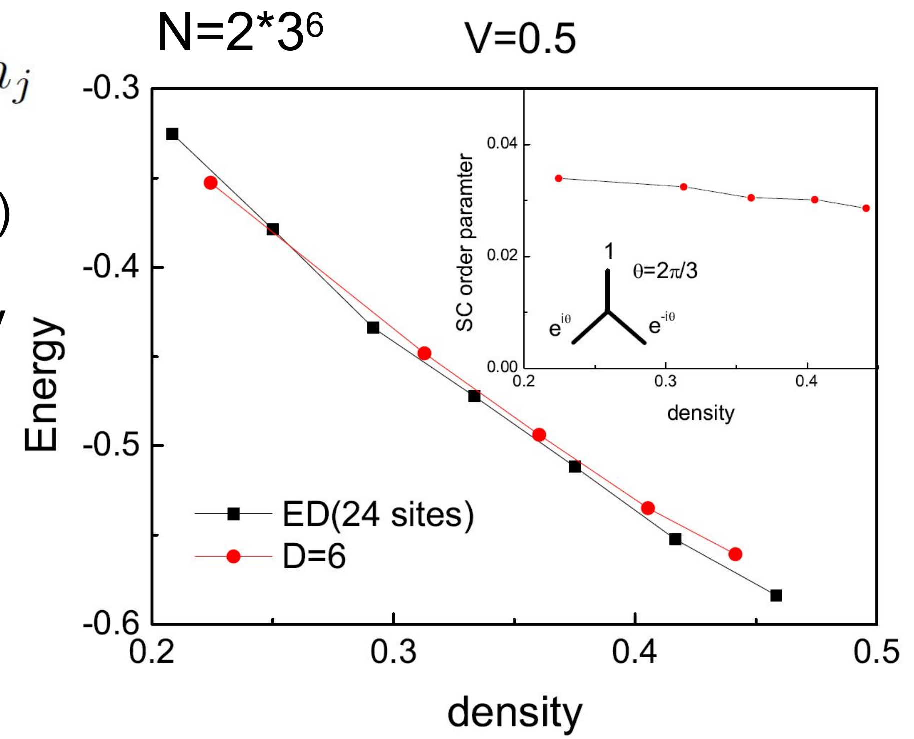
Spinless fermion with nearest neighbor attractive interactions on honeycomb lattice:

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

(Z.C. Gu Phys. Rev. B 88, 115139 (2013))

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

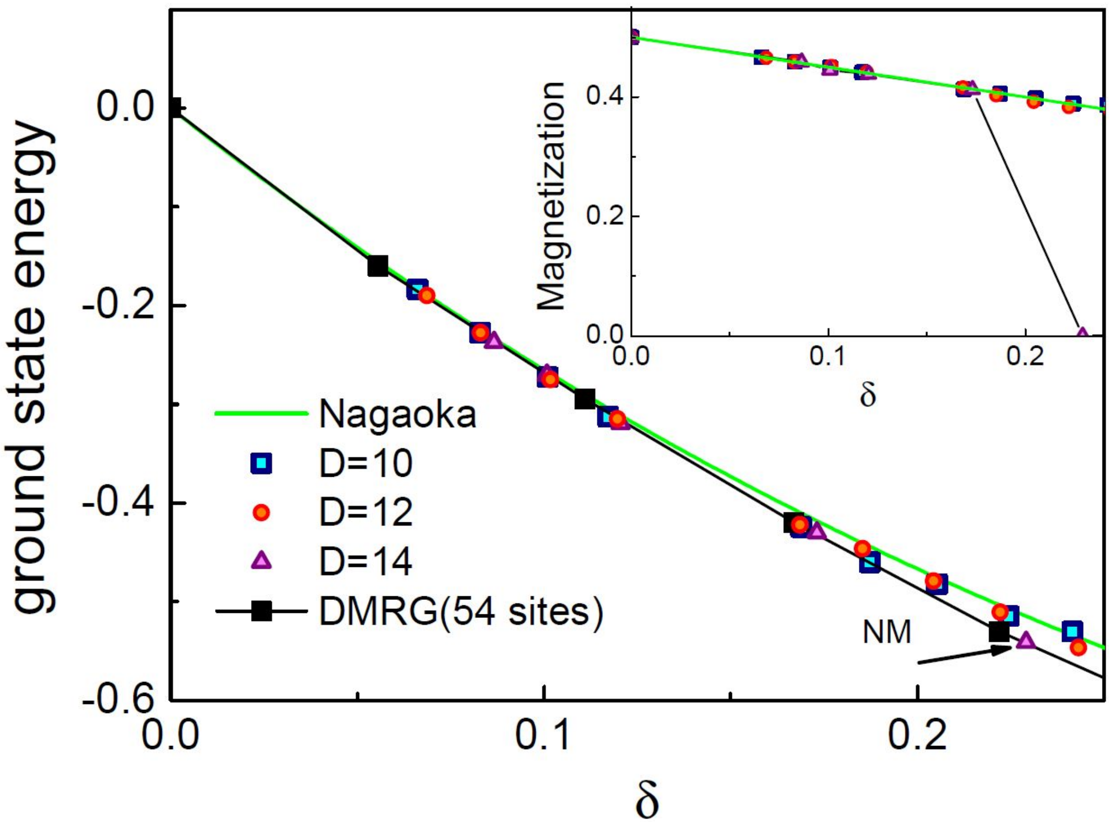
- The p+ip paring pattern emerges during imaginary time evolution.



Doping	$n_f = 0.224$	$n_f = 0.313$	$n_f = 0.36$
$\Delta_a^{SC}/\Delta_b^{SC}$	(-0.4996,0.8656)	(-0.4995,0.8657)	(-0.4995,-0.8656)
$\Delta_b^{SC}/\Delta_c^{SC}$	(-0.5005,0.8660)	(-0.5006,0.8659)	(-0.5006,-0.8659)
$\Delta_c^{SC}/\Delta_a^{SC}$	(-0.4999,0.8664)	(-0.4999,0.8665)	(-0.4999,-0.8666)

Infinite-U Hubbard model

The HFM state is unstable!



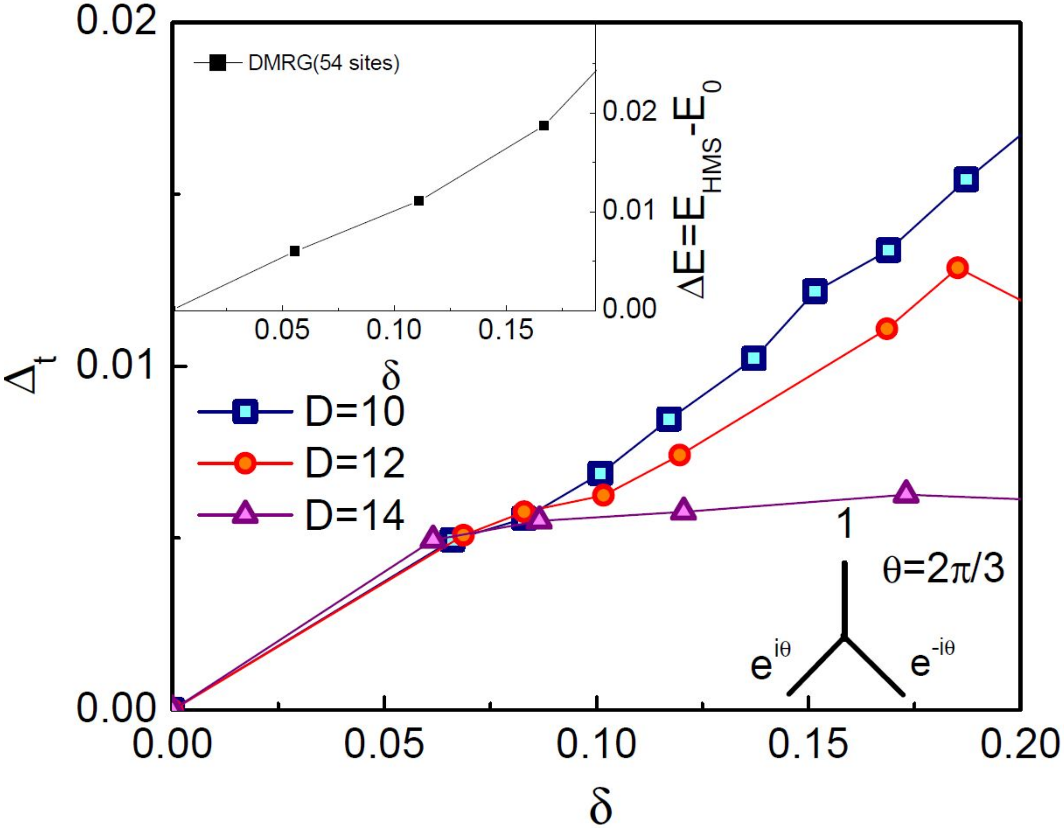
N=2*3^6

relative error < 0.4%

- Almost fully polarized m~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?

A p+ip superconductor!



- p+ip superconductivity coexists with ferromagnetic ordering!

- What's the mechanism?

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

$$\Delta_t \sim 0.07\delta$$

Doping	$\delta = 0.069$	$\delta = 0.102$	$\delta = 0.168$
$\Delta_{t;a}^{x,(y,z)}/\Delta_{t;b}^{x,(y,z)}$	(-0.500,0.866)	(-0.500,0.866)	(-0.500,0.866)
$\Delta_{t;b}^{x,(y,z)}/\Delta_{t;c}^{x,(y,z)}$	(-0.500,0.866)	(-0.500,0.866)	(-0.499,0.865)
$\Delta_{t;c}^{x,(y,z)}/\Delta_{t;a}^{x,(y,z)}$	(-0.500,0.866)	(-0.500,0.866)	(-0.500,0.866)

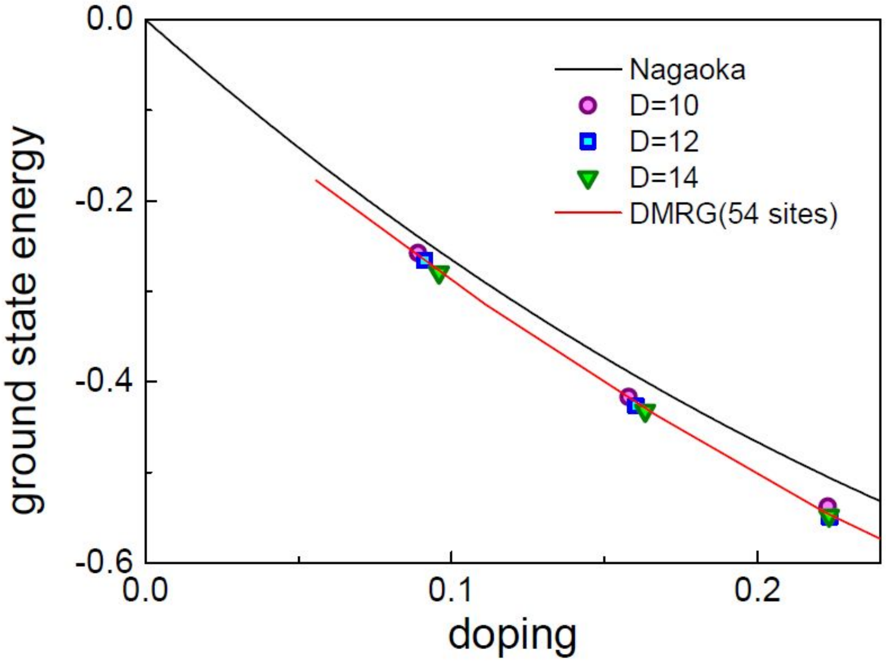
Finite but small J(large U)?

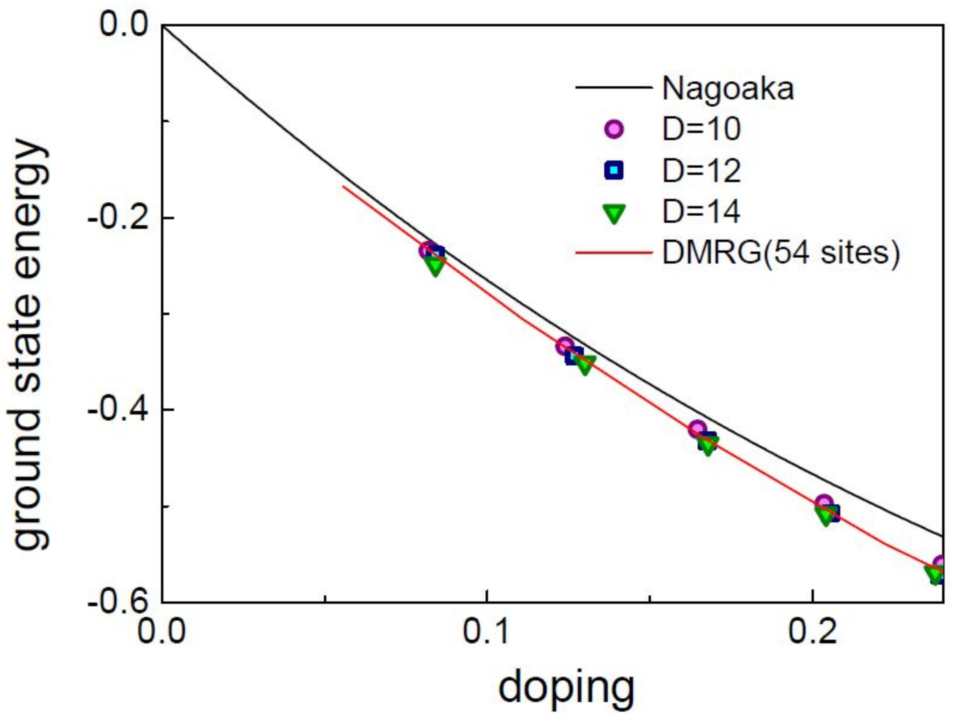
ground state energy(PBC)

N=2*3[6]

relative error ~ 0.2%

t/J=30



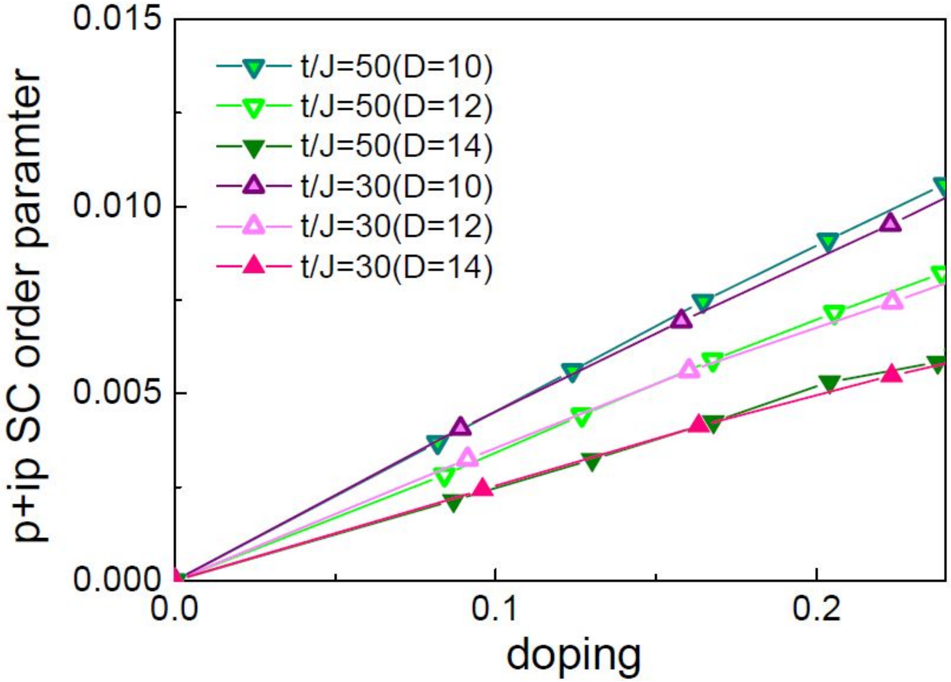


t/J=50

- agree with DMRG results
- but no ferromagnetic order

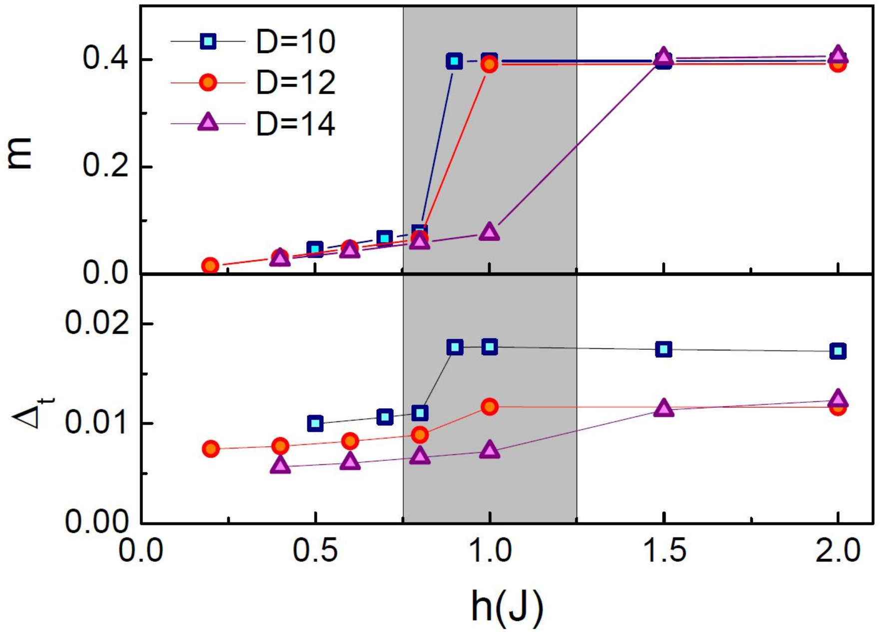
m=0

Stability and instability of p+ip superconductivity



- the p+ip superconductivity can be stabilized by in-plane magnetic field

t/J=30



- the p+ip order parameter decreases with increasing D
- non Fermi liquid?

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).

$$b_\uparrow = \sqrt{\rho_0 + \delta\rho}\, e^{i\theta} \qquad b_\downarrow = 0$$

$$\mathcal{L}_{\rm eff} = \overline{\psi}_a \gamma^\mu (\partial_\mu - iA_\mu)\psi_a - \mu \overline{\psi}_a \gamma^0 \psi_a + \frac{\rho_0}{g}(\partial_\mu \theta - A_\mu)^2$$

- 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:

$$\mathcal{L}_{\rm eff} = \overline{\psi}_a \gamma^\mu (\partial_\mu - iA_\mu)\psi_a - \mu \overline{\psi}_a \gamma^0 \psi_a + \frac{i}{2\pi}\varepsilon^{\mu\nu\lambda} A_\mu \partial_\nu a_\lambda$$
$$+ \frac{g}{16\pi^2 \rho_0}(\varepsilon^{\mu\nu\lambda}\partial_\nu a_\lambda)^2 + |(\partial_\mu + i a_\mu)\phi|^2 + m^2|\phi|^2,$$

Cheap vortices/skyrmion -- beyond dilute limit!

Vortices/skyrmion current -- charge current interaction:

$$\mathcal{L}_{\rm CC} \;=\; j_\mu \varepsilon^{\mu\nu\lambda}\partial_\nu a_\lambda$$

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

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

$$\varepsilon^{\mu\nu\lambda}\partial_\nu a_\lambda = 2\pi\overline{\psi}_a\gamma^\mu\psi_a$$

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

$$\begin{aligned}\mathcal{L}_{\rm eff} \;=&\; \overline{\psi}_a\gamma^\mu\partial_\mu\psi_a - \mu\overline{\psi}_a\gamma^0\psi_a \\ &+ \;(\frac{g}{4\rho_0} + \frac{4\pi^2}{m})(\overline{\psi}_a\gamma^\mu\psi_a)^2 + \frac{4\pi^2}{m}\left[\partial_\mu(\overline{\psi}_a\gamma^\nu\psi_a)\right]^2,\end{aligned} \tag{1}$$

$$[\partial_x(\overline{\psi}_a\gamma^0\psi_a)]^2 \sim (n_i - n_{i+\hat{\delta}_x})^2 \sim -2n_i n_{i+\hat{\delta}_x}$$

an attractive interaction!

A straightforward argument

Consider an almost fully polarized state

$$
\begin{aligned}
H &= t\sum_{\langle ij\rangle}(1-n_{i\downarrow})c^\dagger_{i\uparrow}c_{j\uparrow}(1-n_{j\downarrow})+h.c. \qquad \langle n_i^{\downarrow}\rangle = \delta_0 \ll 1\\
&+ t\sum_{\langle ij\rangle}(1-n_{i\uparrow})c^\dagger_{i\downarrow}c_{j\downarrow}(1-n_{j\uparrow})+h.c.\\
&\simeq t(1-\delta_0)^2\sum_{\langle ij\rangle}c^\dagger_{i\uparrow}c_{j\uparrow}+h.c.+t\sum_{\langle ij\rangle}c^\dagger_{i\uparrow}c_{j\uparrow}S_i^-S_j^+ + h.c.
\end{aligned}
$$

$$
(1-n_{i\uparrow})c^\dagger_{i\downarrow} = c_{i\uparrow}c^\dagger_{i\uparrow}c^\dagger_{i\downarrow} = S_i^- c^\dagger_{i\uparrow} \qquad c_{j\downarrow}(1-n_{j\uparrow}) = c_{j\downarrow}c_{j\uparrow}c^\dagger_{j\uparrow} = c_{j\uparrow}S_j^+
$$

Express in terms of kinetic energy and current operators

$$
\begin{aligned}
H &= t(1-\delta_0)^2\sum_{\langle ij\rangle}(c^\dagger_{i\uparrow}c_{j\uparrow}+h.c.)\\
&+ \frac{1}{2}t\sum_{\langle ij\rangle}(c^\dagger_{i\uparrow}c_{j\uparrow}+c^\dagger_{j\uparrow}c_{i\uparrow})(S_i^-S_j^+ + S_j^-S_i^+)\\
&+ \frac{1}{2}t\sum_{\langle ij\rangle}(c^\dagger_{i\uparrow}c_{j\uparrow}-c^\dagger_{j\uparrow}c_{i\uparrow})(S_i^-S_j^+ - S_j^-S_i^+),
\end{aligned}
$$

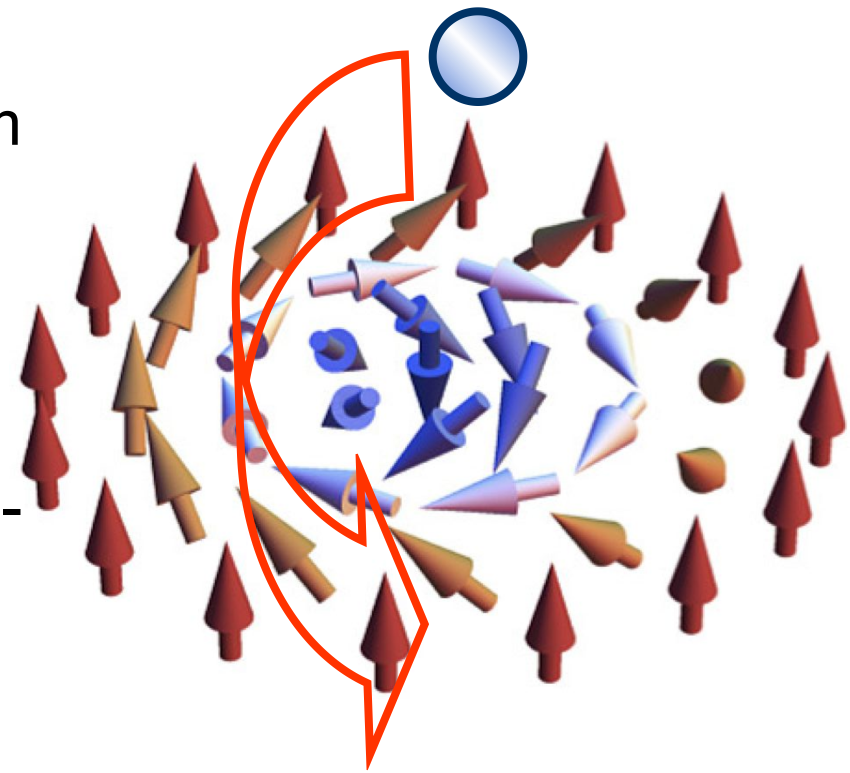
$$
+\ \frac{1}{\kappa}(S_i^-S_j^+ - S_j^-S_i^+)^2
$$

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

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

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.

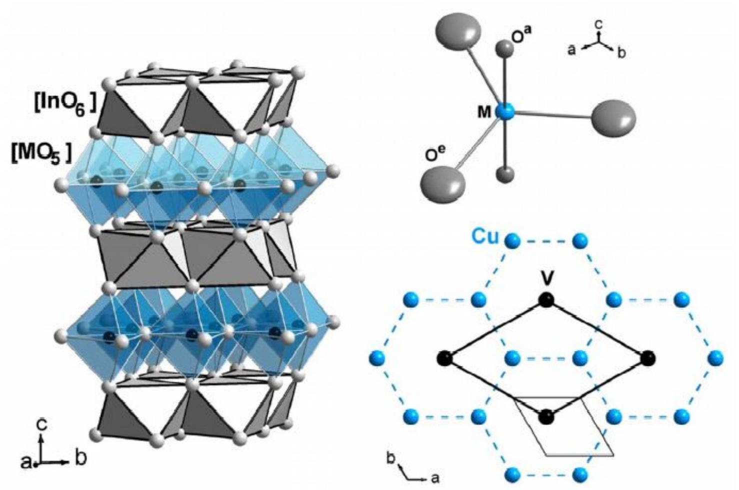
- Such a mechanism relies on spin-charge separation and emergent U(1) gauge field, therefore it is beyond BCS theory.

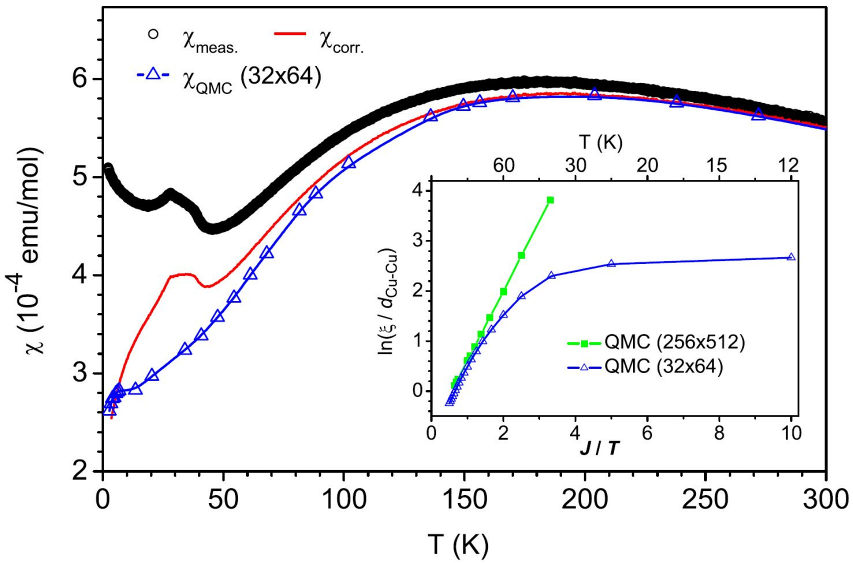
- Condensation of skyrmion excitations leads to a potential non-fermi liquid!

$$\mathcal{L}'_{\text{eff}} = \overline{\psi}_a \gamma^\mu (\partial_\mu - iA_\mu)\psi_a - \mu \overline{\psi}_a \gamma^0 \psi_a + \frac{1}{g'}(\varepsilon^{\mu\nu\lambda}\partial_\nu A_\lambda)^2,$$

Possible realizations: $InCu_{2/3}V_{1/3}O_3$.

- S=1/2 AF on honeycomb lattice.(Phys. Rev. B 78, 024420 (2008))
- Doping: non Fermi liquid?
- Doping plus in-plane magnetic field: p+ip topological superconductor?





Orther systems:

- 3He absorbed on substrate.(PRL 109, 235306 (2012))
- Organic layer on graphene.(Nature Physics 9, 368 (2013))

Summaries and future works

- 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.

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

(Z.C. Gu, *etal*., Phys. Rev. B 88, 155112 (2013),Z C Gu *etal*. in preparation)

- Towards resolving the mechanism of high-Tc cuprates