Title: Emergence of p+ip topological superconducting ground state in infinite-U Hubbard model on honeycomb lattice

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Abstract: In this talk, I will show the emergence of p+ip topological superconducting ground state in infinite-U Hubbard model on honeycomb lattice, from both state-of-art Grassmann tensor-network numerical approach and quantum field theory approach.

Emergence of p+ip superconducting ground state in

infinite-U Hubbard model

Zhengcheng Gu (PI)

Collaborators:

Prof. G. Baskaran(PI)
Prof. D. N. Sheng (California State U.)
Dr. H. C. Jiang (UC Berkeley)

PI. Feb. 2014

Outline

- Background for p+ip superconducting state of spinless fermion and infinite-U repulsive Hubbard model.

- Tensor product state(TPS) and its generalization for interacting fermion systems.

- Benchmark with free fermion and simple interacting fermion models.

- Infinite-U Hubbard model on honeycomb lattice: p+ip superconducting order coexists with ferromagnetic order.

- Mechanism: A quantum field theory approach.

- Summary and outlook.

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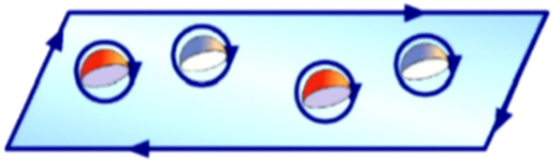
p+ip superconductor of spinless fermion

A Majorana zero mode emerges in the vortex core

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



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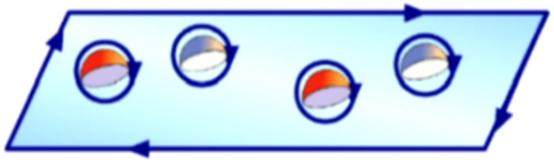

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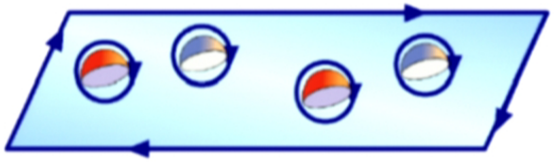

Vortex carries non-Abelian statistics

- 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 superconductivity.

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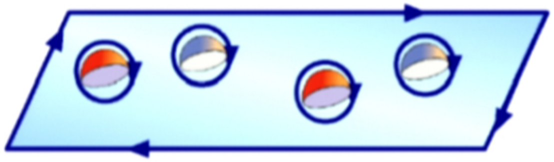

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- Electron carries spin, spinless fermion is artificial.
- In BCS theory, a strong spin polarization will kill superconductivity.
- How about a strong coupling model with non-BCS mechanism?

The infinite-U Hubbard model:

Repulsive Hubbard model

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

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

Infinite-U repulsive Hubbard model with a single hole: Nagaoka's Theorem (Nagaoka, 1966)

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Infinite-U repulsive Hubbard model with a single hole: Nagaoka's Theorem (Nagaoka, 1966)

- Kinetic energy driven Ferromagnetic ordering.
- The infinite-U limit is an important starting point to understand the strong coupling physics, e.g., the mechanism of high-Tc cuprates.

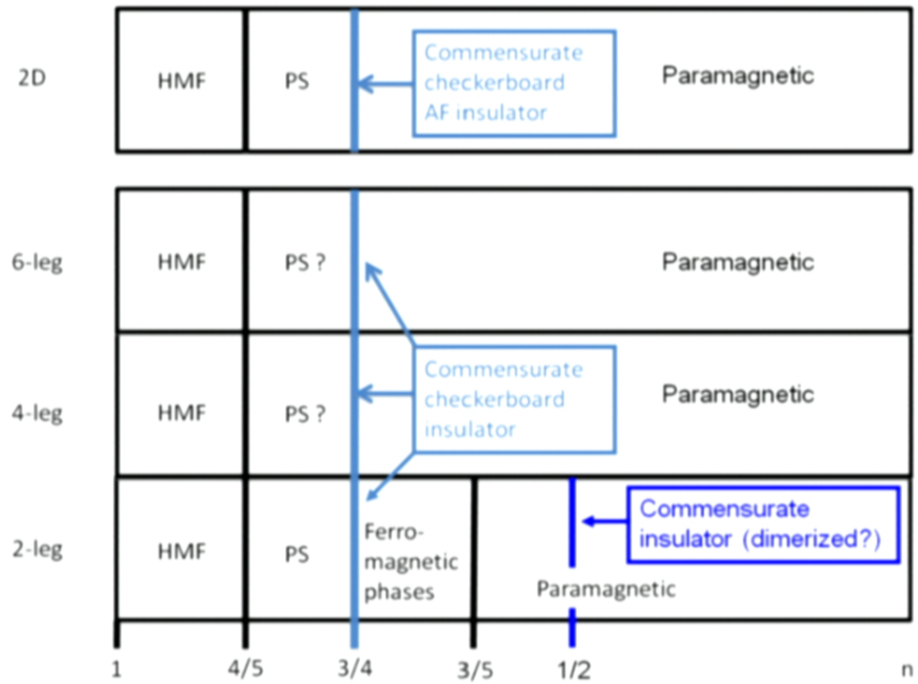
Unfortunately, Nagaoka's Theorem is very hard to be generalized to finite doping.

- Nevertheless, Nagaoka state is an eigenstate of infinite-U Hubbard model, can be stabilized by adding small magnetic field.

Recent numerical results:

Hubbard model on square lattice(DMRG)

- HMF=Half-Metallic Ferromagnetic=Nagaoka Ferromagnetic



Li Liu,*etal* Phys. Rev. Lett.108, 126406 (2012)

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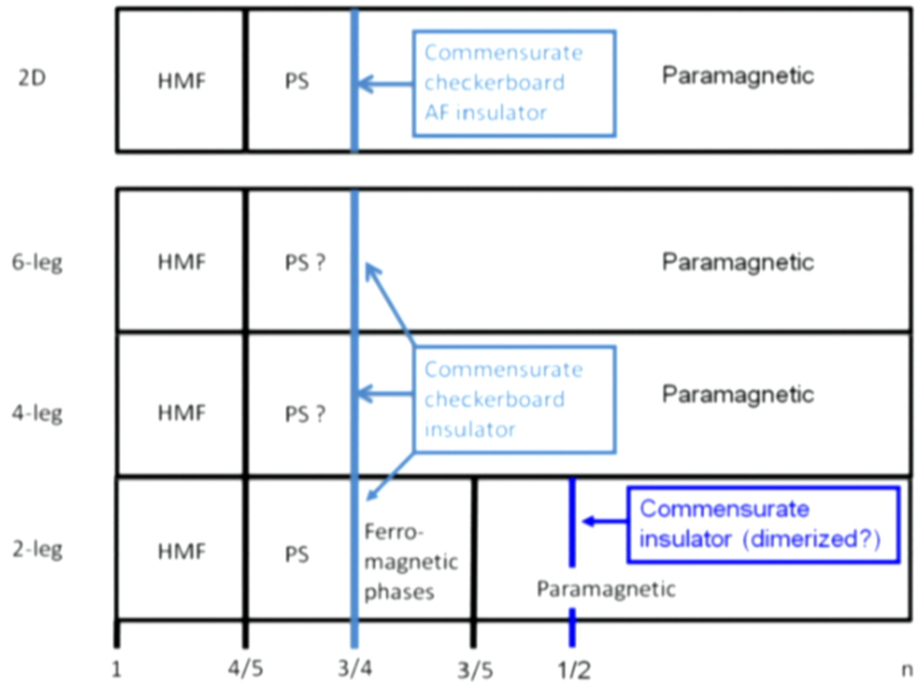

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- It might be a p+ip superconductor at finite doping due to geometry

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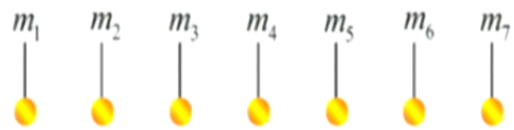
We investigate infinite-U Hubbard model on honeycomb lattice by performing a thermodynamic calculation with (Grassmann) tensor product states and a finite size calculation with DMRG.

What is a TPS

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

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



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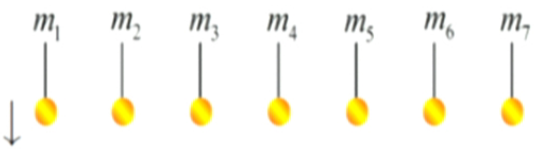

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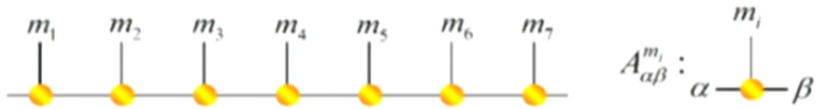
MPS/DMRG(the best numerical method in 1D):

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



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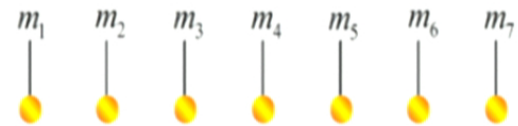

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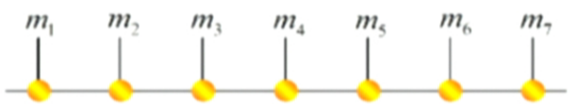

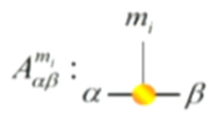

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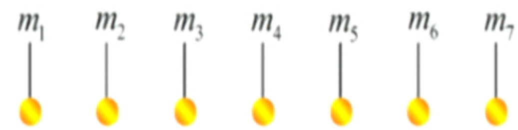

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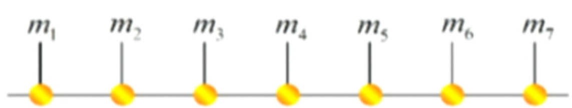
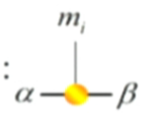


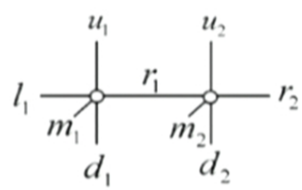
$A^{m_i}_{\alpha\beta}$:

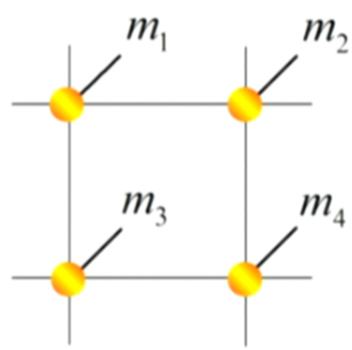


TPS: $\uparrow \longrightarrow T^{\uparrow}_{lrud}; \quad \downarrow \longrightarrow T^{\downarrow}_{lrud}$ (F. Verstraete and J. I. Cirac 2004)

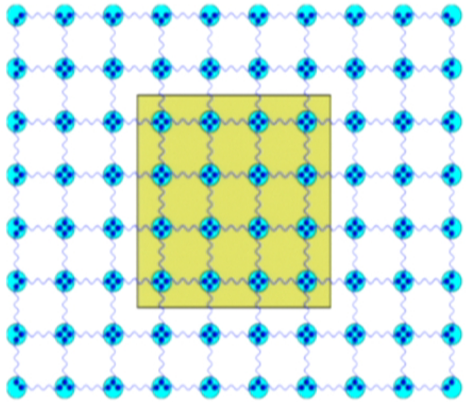
$T^{m_1}_{l_1 r_1 u_1 d_1}$:

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





Properties of TPS:



- Entanglement entropy satisfies area law

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

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

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

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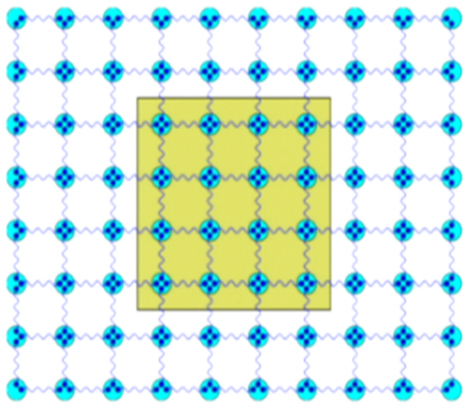

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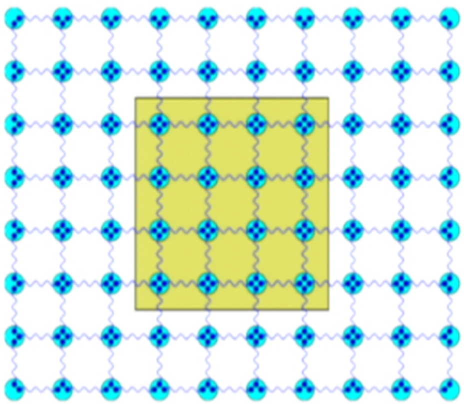

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- Systems with topological

$$S(\rho_L) = \alpha L - \gamma$$ A. Kitaev *etal.* 2006, M. Levin *etal.* 2006

TPS are faithful representation for topologically ordered states (Z.C. Gu, *etal.*, PRB, 2008, O. Buerschaper, *etal.*, PRB, 2008)

TPS have achieved great success in spin models.

- Consistent with QMC on sign free problems. (Z.C. Gu, *etal.*, Phys. Rev. B 78, 205116 (2008), Ling Wang *etal.*, Phys. Rev. B 83, 134421 (2011))
- Consistent with DMRG on frustrated magnets, e.g., J1-J2 model. (Ling Wang, Zheng-Cheng Gu, Frank Verstraete, Xiao-Gang Wen, arXiv:1112.3331)

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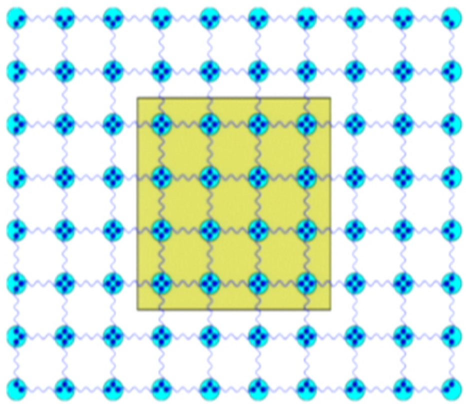

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TPS for fermion systems

How to simulate fermion systems?

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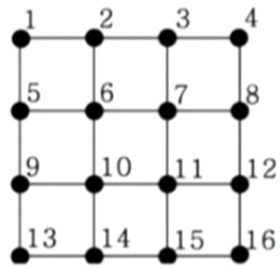
- Treat fermion systems as ordinary hardcore boson/spin systems.



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

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

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:

0,1

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

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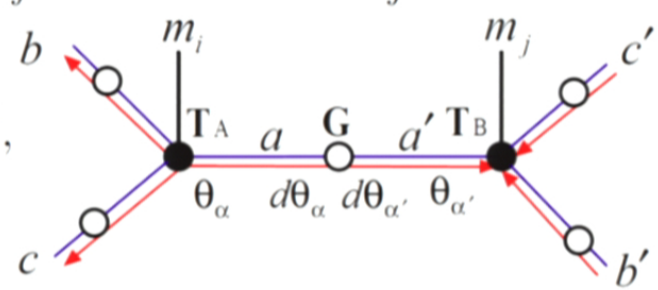

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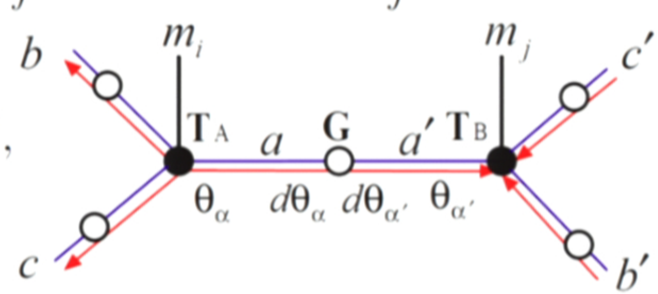

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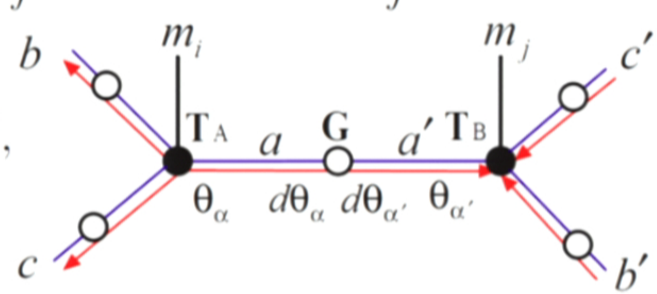

$$\Psi(\{m_i\},\{m_j\}) = \sum_{\{a\},\{a'\}}\int\prod_{\langle ij\rangle}\mathbf{G}_{aa'}\prod_{i\in A}\mathbf{T}_{A_{abc}}^{m_i}\prod_{j\in B}\mathbf{T}_{B_{a'b'c'}}^{m_j}$$

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

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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))

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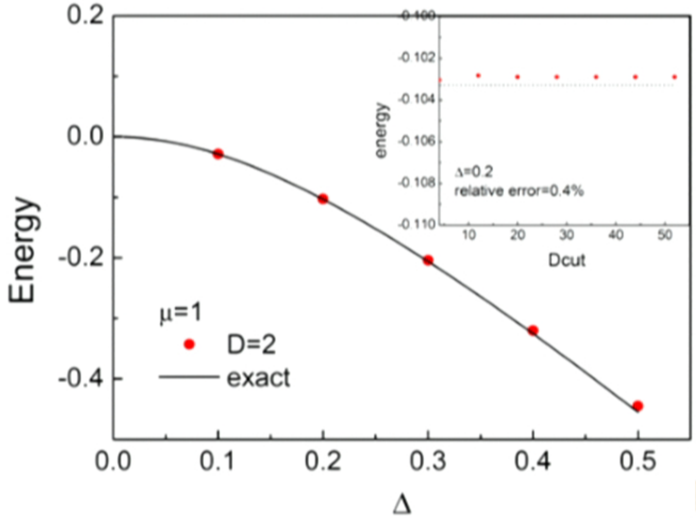
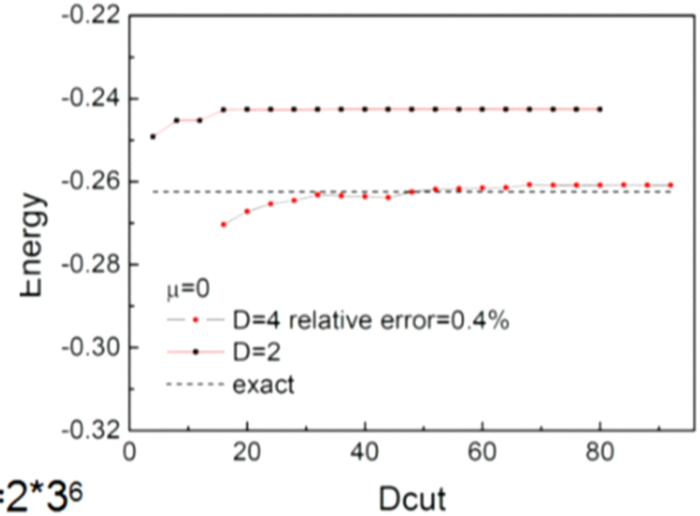


N=2*3^6

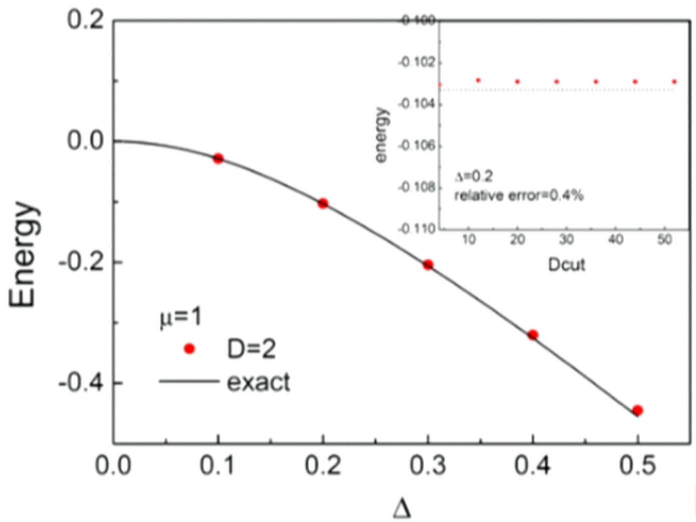


A free fermion model:

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))

- We use imaginary time evolution method to find the ground state.
- We use Grassmann tensor-entanglement renormalization algorithm to compute the ground state energy.(Z. C. Gu *etal*., arXiv:1004.2563)



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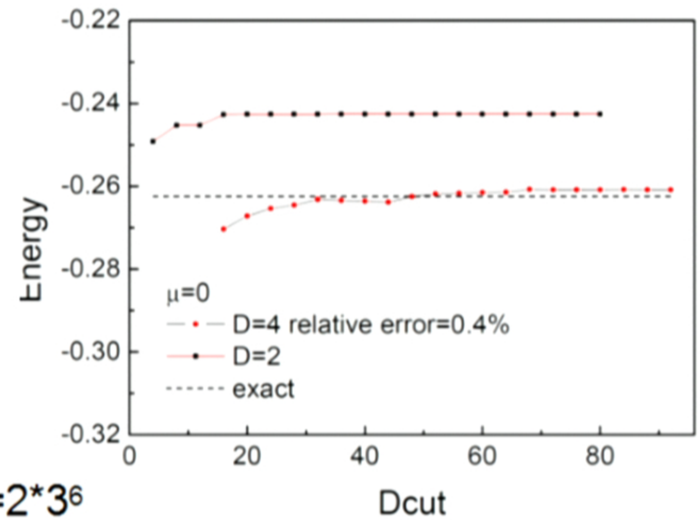

- The energy is correct even with extremely small D for gapped systems.
- Truncation error is slightly larger for critical systems.

A simple interacting fermion model:

Spinless fermion with nearest neighbor attractive interactions on honeycomb lattice:

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

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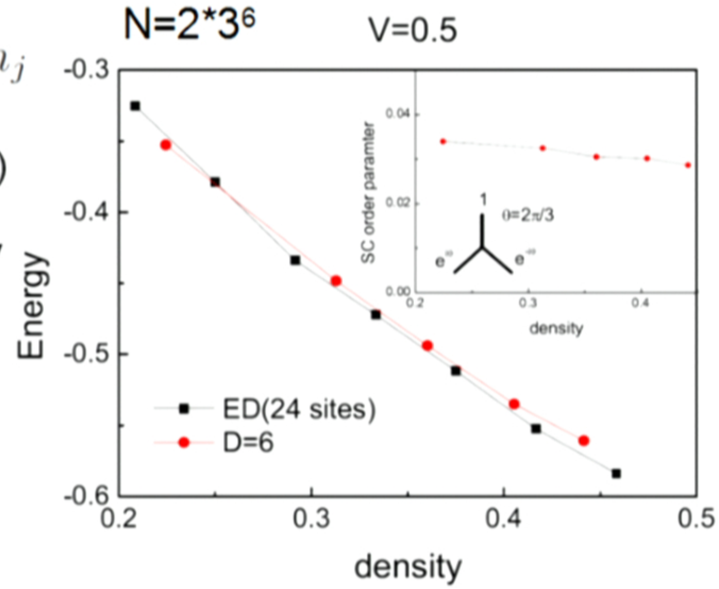
- Grassmann TPS ansatz is randomly initialized, no reassumption of superconducting order parameter.
- The p+ip paring pattern emerges during imaginary time evolution.



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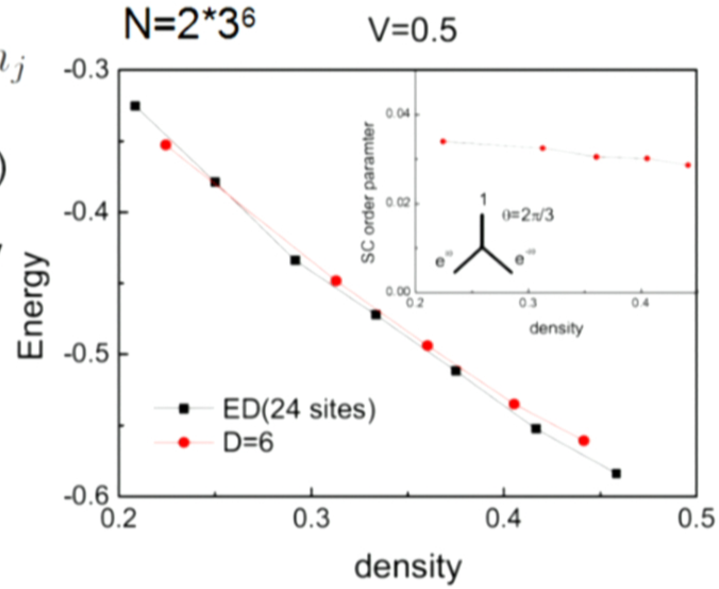
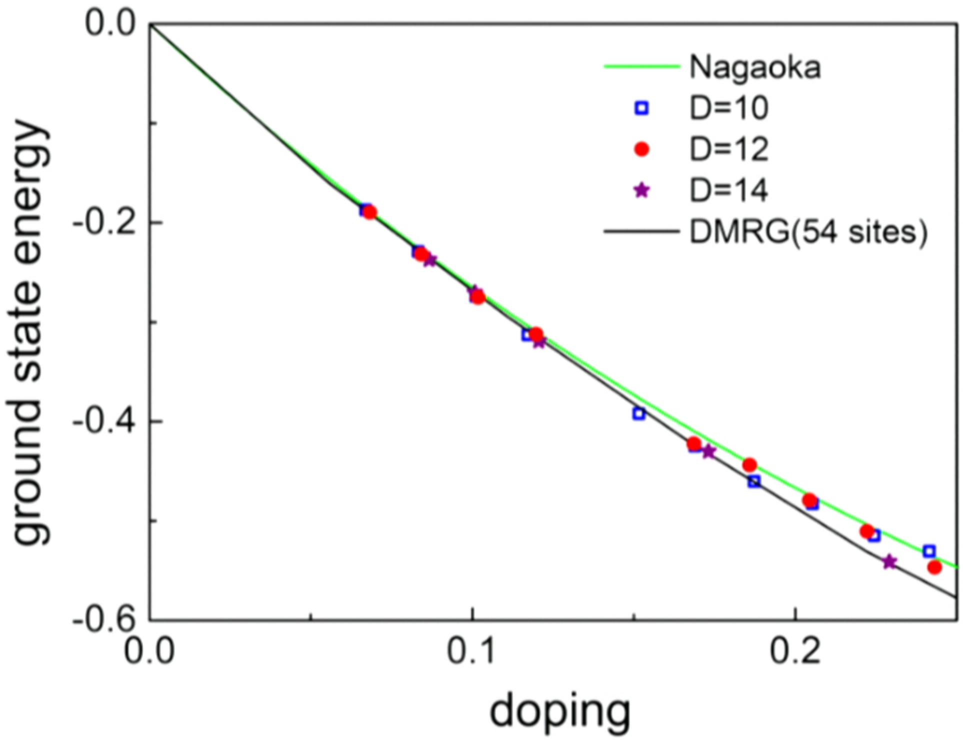


Doping	$n_f = 0.224$	$n_f = 0.313$	$n_f = 0.36$
$\Delta_a^{SC}/\Delta_b^{SC}$	(-0.4996,0.8656)	(-0.4995,0.8657)	(-0.4995,-0.8656)
$\Delta_b^{SC}/\Delta_c^{SC}$	(-0.5005,0.8660)	(-0.5006,0.8659)	(-0.5006,-0.8659)
$\Delta_c^{SC}/\Delta_a^{SC}$	(-0.4999,0.8664)	(-0.4999,0.8665)	(-0.4999,-0.8666)

Outline

- Background for p+ip superconducting state of spinless fermion and infinite-U repulsive Hubbard model.
- Tensor product state(TPS) and its generalization for interacting fermion systems.
- Benchmark with free fermion and simple interacting fermion models.
- Infinite-U Hubbard model on honeycomb lattice: p+ip superconducting order coexists with ferromagnetic order.
- Mechanism: A quantum field theory approach.
- Summary and outlook.

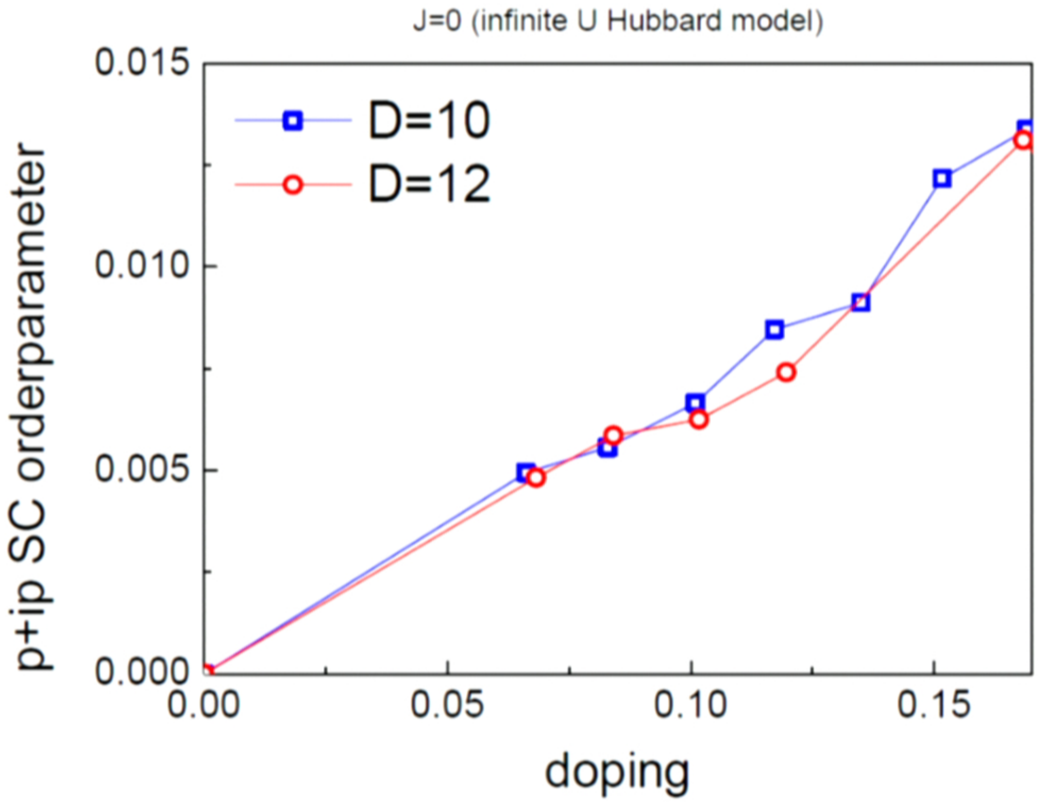
The Nagaoka state is unstable on honeycomb lattice!



- Almost fully polarized but different from a simple Nagaoka state.
- What's the true ground state?

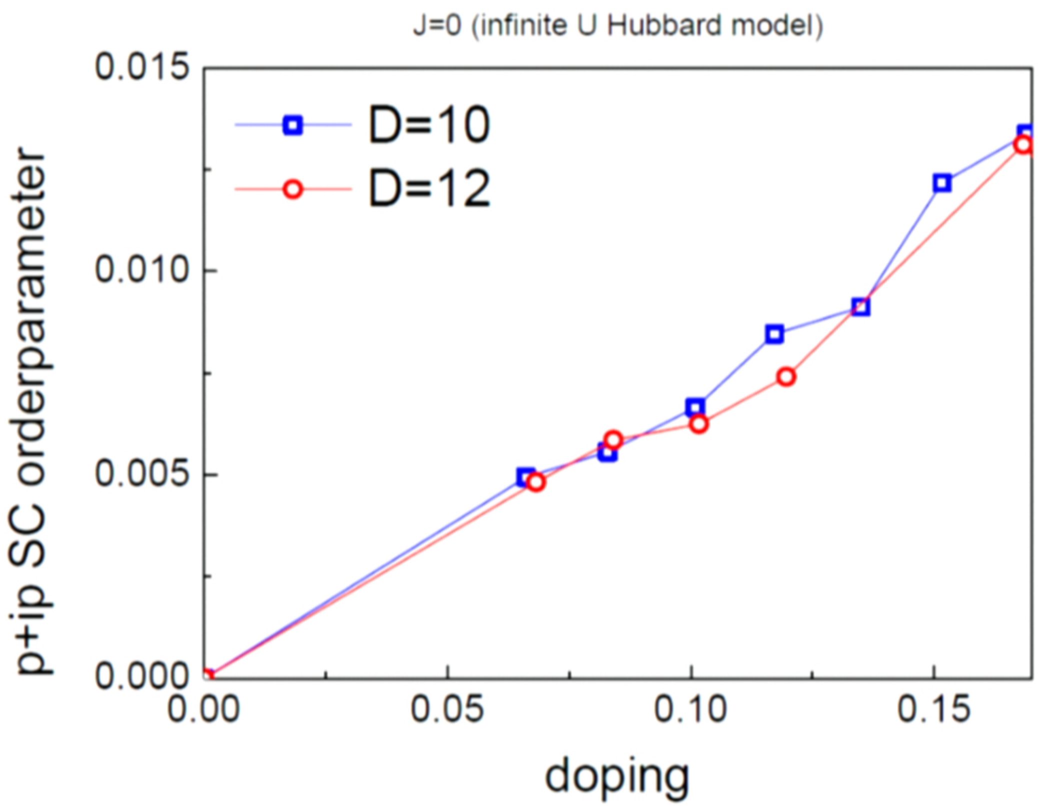
A p+ip superconductor!

A p+ip superconductor!



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

A p+ip superconductor!



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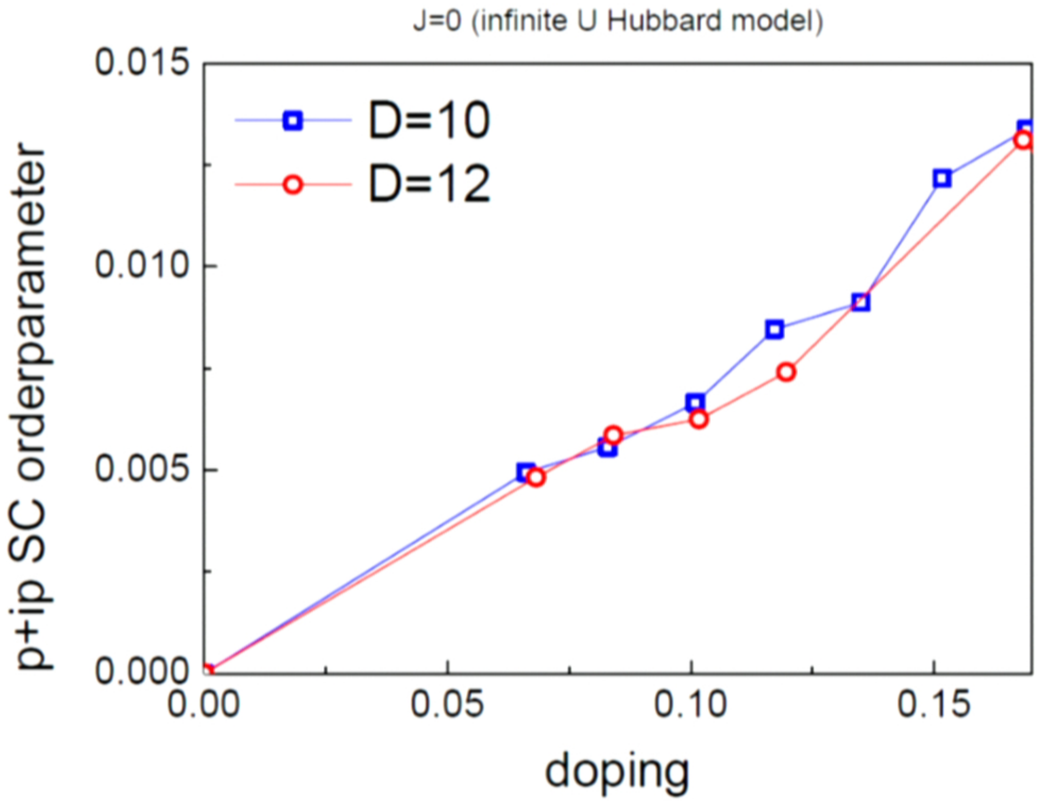

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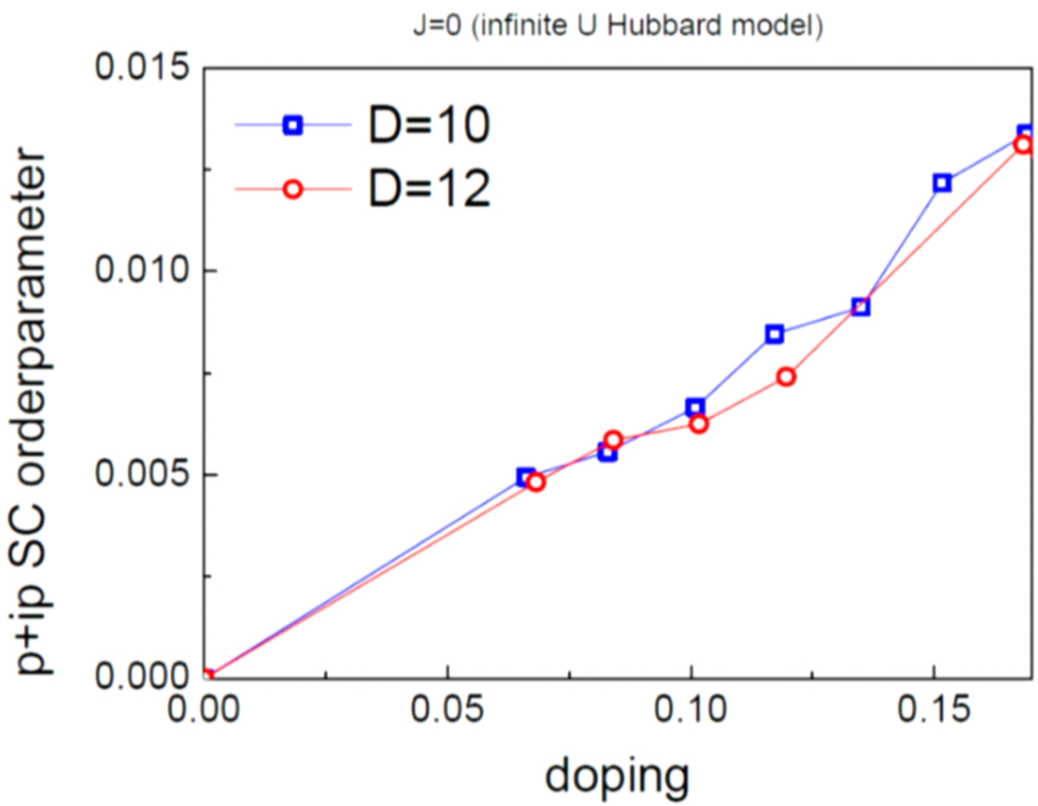

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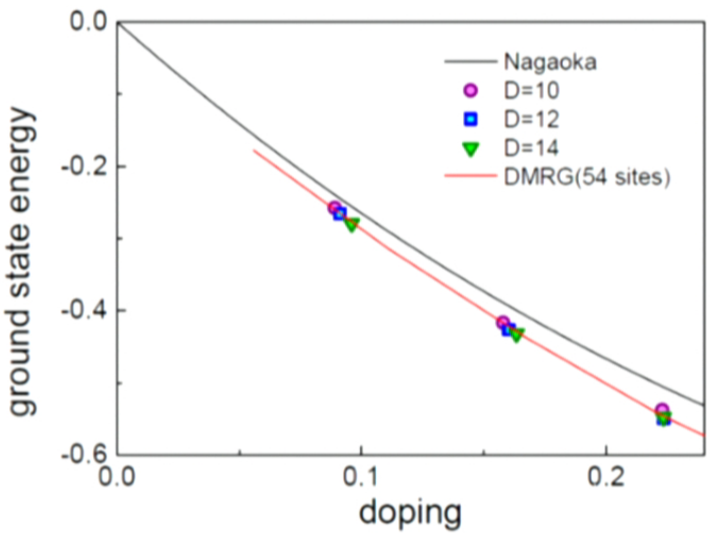
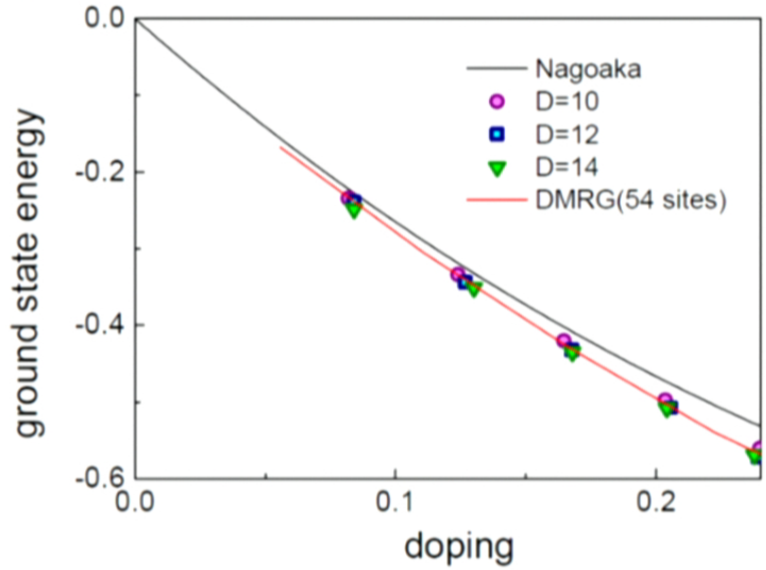
- What's the mechanism?

Finite but small J(large U)?

ground state energy(PBC)

t/J=30

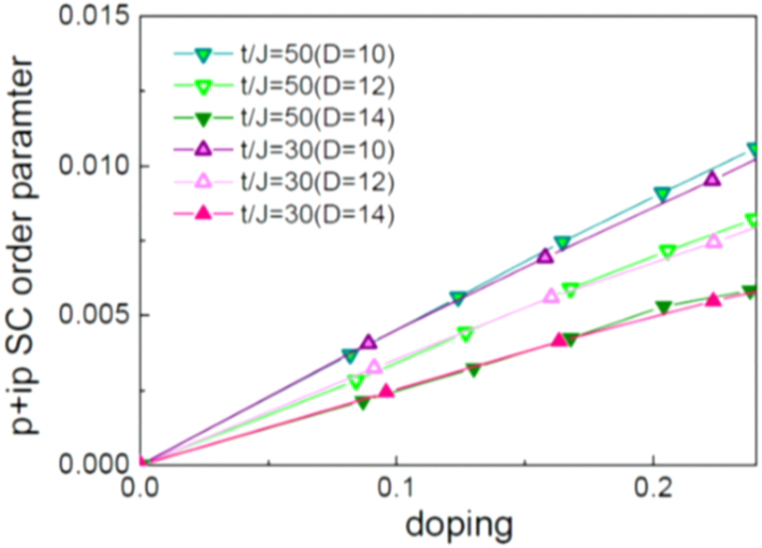




t/J=50

- agree with DMRG results
- but no ferromagnetic order

Stability and instability of p+ip superconductivity



- the p+ip order parameter decreases with increasing D
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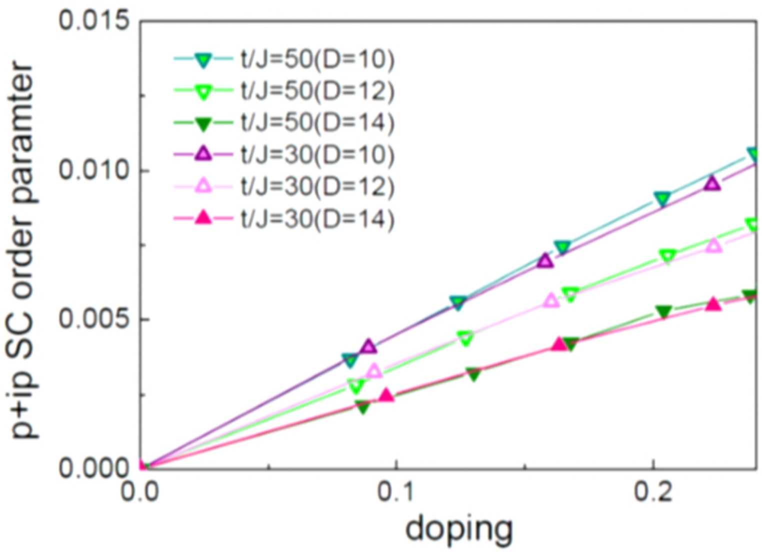
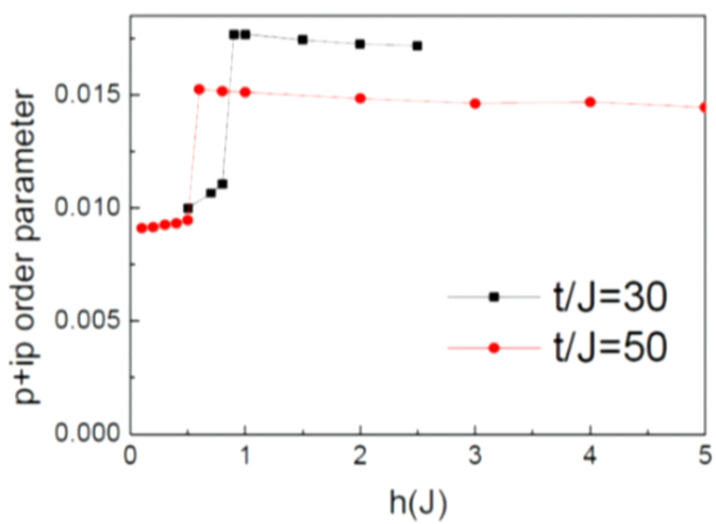


- the p+ip superconductivity can be stabilize by parallel magnetic field

D=10



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$$\theta = \eta + \zeta$$

smooth part → η; singular(vortex) part → ζ

Integrating out the smooth part leads to: $\partial_\mu \xi^\mu = 0$

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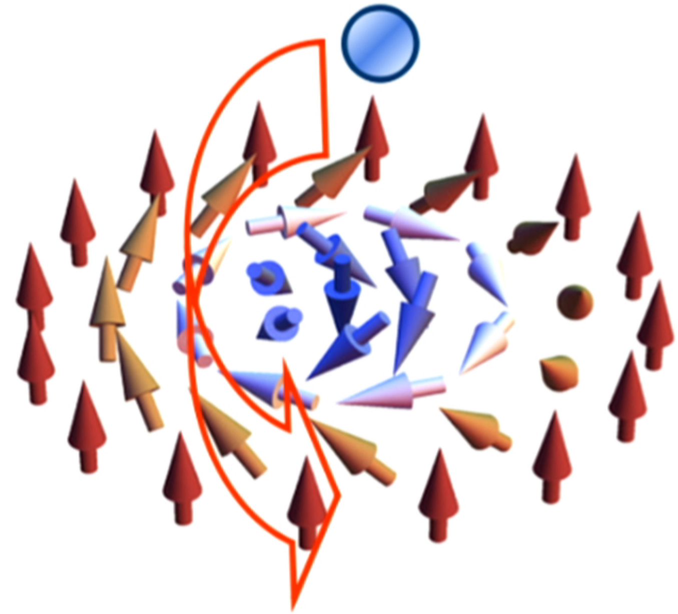
Imposing the constraints generates a Yukawa term: $\sum_\mu \partial_\mu\zeta f^* f$

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

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

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



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

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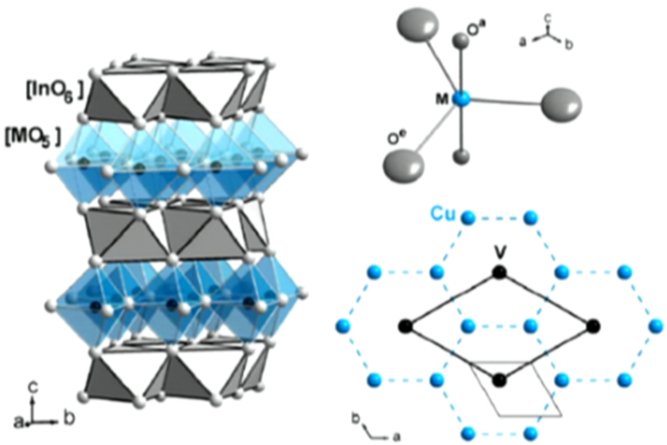

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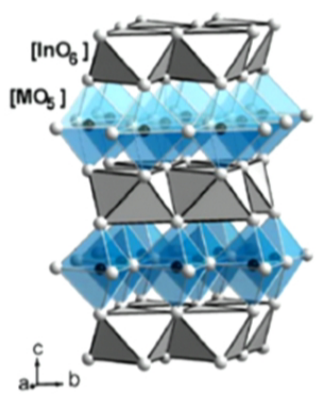
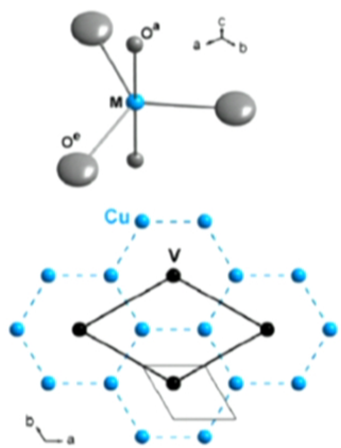
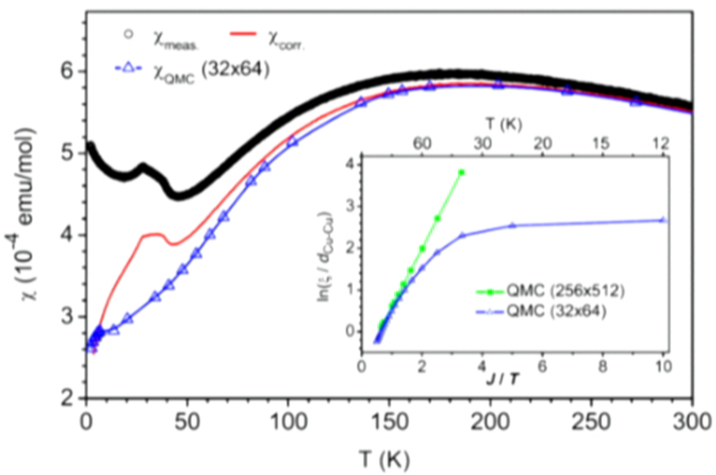






- Quasi long range order with T_N=37K

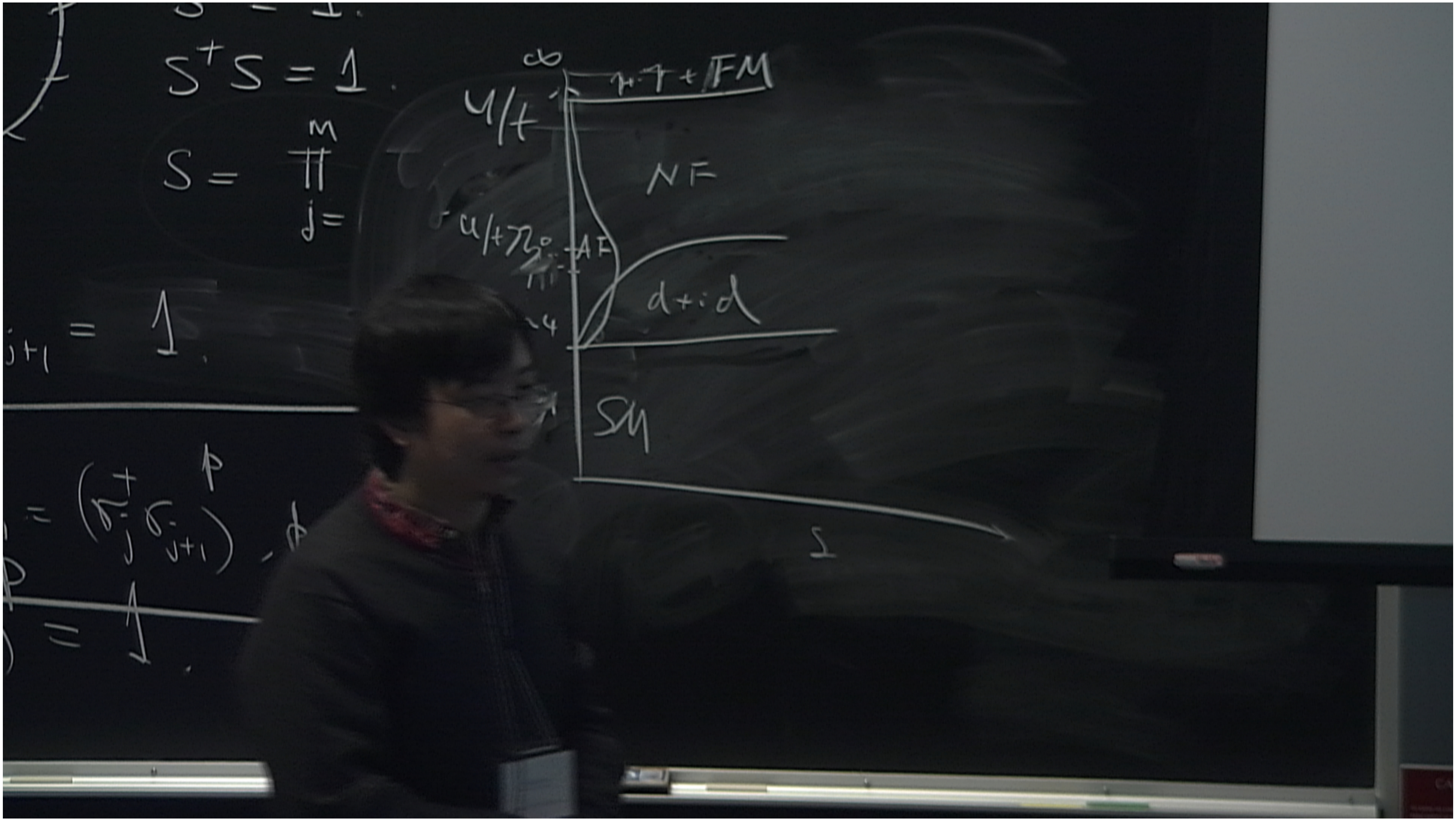
Summaries and future works

- Grassmann TPS are possible 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.



S⁺S = 1
U/t
FM
NF
AF
d+id
SM