When Gutzwiller meets DMRG: a microscopic-wavefunction-guided approach to 2D correlated electrons

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Reference: [1] arXiv: 2203.07321; [2] Science Bulletin 67, 918 (2022). Method: [3] PRB 101, 16135 (2020); [4] PRB 104, L020409 (2021); [5] PRB 105, L081101 (2022).

When Gutzwiller meets DMRG

Martin C. Gutzwiller (1925-2014)





□ A pioneer in correlated electrons

- Wrote down and studied a model, which is now called (single-band) Hubbard model.
- The most promising method for the Hubbard model was devised by M. Gutzwiller."
 - P. W. Anderson in 1987

One of creators of quantum chaos theory



Steven R. White



- Density Matrix Renormalization Group
 (DMRG) was invented by Steven White
 in 1992.
- Most accurate computational method for many-particle quantum systems in 1D.

Two dimensions: difficulty vs. versatility



The unique 2D

+

+

 $\underline{d} = 4 - \epsilon$, $\epsilon = 2$: absence of long-

ranged orders, strong fluctuations;

 $\underline{d > 1}$: absence of powerful tools,

growing quantum entanglement





Outline

- **Dimensionality crossover from 1D to 2D: any paradigm?**
- **D** Methodology: Gutzwiller guided (boosted) DMRG
- □ Method benchmark: Kitaev honeycomb model
- **Example: AFM Heisenberg model on the Kagome lattice**

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Any paradigm for correlated electrons in 2D?

Paradigm

A model of something, or a very clear and typical example of something.

(Cambridge Business English Dictionary @ Cambridge University Press)

Paradigms in physics

- **philosophy** + method
- **reductionism, emergence principle**
- **Hamiltonian / Lagrangian**
- **Given theory**

Classic paradigms in condensed matter physics

- Landau: symmetry breaking, order parameter
- **BCS:** Cooper pair, BCS wave function (macroscopic quantum phenomenon)
- Laughlin: wave function, quasi-particle carrying a fractional charge

Situation: so far not a universal one

Dimensionality crossover: $1D \rightarrow 2D$

A facilitated issue: Is there any paradigm from 1D to 2D?

D Epistemology: learn something unknown from known.

1D is well understood owing to powerful tools: Bosonization, CFT, DMRG, ...

Efforts to dimensionality expansion: from 1D to 2D

- □ Bosonization → various 2D versions of Bosonization
- □ CFT → CFT in higher dimensions, conformal bootstrap, ...
- □ DMRG → tensor networks, PEPS, PESS (simplex), ...

Dimensionality expansion is much more difficult than its reduction
□ A huge gap between 1D and 2D: dramatically increasing entanglement, ...
□ A typical example for : "1→2" is

much more significant than " $0 \rightarrow 1$ ".

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Methodology

DMRG guided (boosted) by Gutzwiller projected wave functions

- **Convert a Gutzwiller projected state to a matrix product state (MPS)**
- **DMRG** initialized with such a converted state
- □ More advantages of the Gutzwiller-MPS conversion
 - **Compare Gutzwiller projected state with a DMRG-optimzed MPS directly**
 - **Compute entanglement features for Gutzwiller projected states**





"The most promising method for the Hubbard model was devised by M. Gutzwiller."
 - P. W. Anderson in 1987





Most accurate computational method for many-particle quantum systems in 1D.

How to convert: from projected Fermi sea to MPS

Ying-Hai Wu, Lei Wang, Hong-Hao Tu, PRL 124, 246401 (2020), arXiv:1910.11011

|0>

single-particle operators

matrix product identity

Gutzwiller projection on an MPS

 $\begin{array}{c} - + = \uparrow \checkmark \\ - + = \downarrow \checkmark \\ \checkmark \\ \end{array}$ $|\Psi\rangle = P_G |\Psi_0\rangle$ **Gutzwiller projection** P_G d_N^{\dagger} d_1^{\dagger} $|0\rangle_c$ 2S+12S+12S+1

 $|\Psi_0\rangle = \sum_{s} \operatorname{sgn}(s) A^{s_1}[1] A^{s_2}[2] \cdots A^{s_{N-1}}[N-1] A^{s_N}[N] |s\rangle$ $|\Psi\rangle = \sum_{\tau} \operatorname{sgn}(\tau) B^{\tau_1}[1] B^{\tau_2}[2] \cdots B^{\tau_{L-1}}[L-1] B^{\tau_L}[L] |\tau\rangle$ $B^{\tau_j} = \begin{cases} \prod_{\alpha} A^{s_l}[l]|_{l=(j,\alpha)}, & \text{if } \sum_{\alpha} s_{l=(j,\alpha)} = 1, \\ 0, & \text{otherwise.} \end{cases}$

Ying-Hai Wu, Lei Wang, Hong-Hao Tu, PRL 124, 246401 (2020), arXiv:1910.11011 Hui-Ke Jin, Hong-Hao Tu, YZ, PRB 101, 16135 (2020), arXiv:2001.04611

How to convert: paired fermions — various methods

① MPO-MPS by pairing function

$$|\Psi_0\rangle = \prod_{kl} (1 + g_{kl} c_k^{\dagger} c_l^{\dagger}) |0\rangle_c = \prod_k \hat{W}_k |0\rangle_c$$

Ying-Hai Wu, Lei Wang, Hong-Hao Tu, PRL 124, 246401 (2020), arXiv:1910.11011

2 MPO-MPS by filling up Bogoliubov quasi-holes: much more efficiently



Hui-Ke Jin, Hong-Hao Tu, YZ, PRB 101, 16135 (2020), arXiv:2001.04611

How to convert: paired fermions — various methods

- **(1) MPO-MPS by pairing function**
- **② MPO-MPS by filling up Bogoliubov holes**
- **③** Paffian method:
 - ① stable against the gap closing
 - **(2)** does not rely on the choice of maximally localized Wannier orbitals



Hui-Ke Jin, Rong-Yang Sun, YZ, Hong-Hao Tu, PRB 105, L081101 (2022), arXiv:2111.09101

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Benchmark in 2D: Kitaev honeycomb model

- **D** Exactly solvable model of great interest
- **Gapless states are not well solved by usual DMRG**
- Parton wave function is known
- **Different topological sectors**



Model Hamiltonian

$$\mathcal{H}_{3} = \sum_{\langle jk \rangle \in a} J_{a} \sigma_{j}^{a} \sigma_{k}^{a} + J_{3} \sum_{\langle jkl \rangle \in \Delta} \sigma_{j}^{x} \sigma_{k}^{y} \sigma_{l}^{z}$$

$$\sigma_j^a \ (a = x, y, z)$$



A. Kitaev, Ann. Phys. 321, 2 (2006)

Kitaev honeycomb model: from Gutzwiller to MPS

Accumulated truncation error:

$$\epsilon_{\text{trunc}}(\tilde{D}) = 1 - \prod_{m=1}^{2N} F^{(m)}(\tilde{D}),$$
$$F^{(m)}(\tilde{D}) = 1 - \sum_{j=1}^{2N} \epsilon_j^{(m)}(\tilde{D}),$$

Relative energy deviation:

$$\delta E_g(\Phi_y) = \frac{\langle \Psi_G(\Phi_y) | \mathcal{H}_3 | \Psi_G(\Phi_y) \rangle - E_g(\Phi_y)}{|E_g(\Phi_y)|}$$



$$J_y = J_z = 1; L_x = 10, L_y = 4, \Phi_y = -1$$

		$J_x = 4$			
	$ ilde{D}$	$J_3 = 0$	$J_3 = 0.1$	$J_3 = 0.2$	$J_3=0$
€trunc	100	1.7×10^{-1}	9.2×10^{-2}	5.7×10^{-2}	1.1×10^{-4}
	200	2.4×10^{-2}	1.0×10^{-2}	5.0×10^{-3}	1.0×10^{-6}
	400	2.5×10^{-3}	5.6×10^{-4}	2.4×10^{-4}	3.4×10^{-7}
	600	4.2×10^{-4}	8.0×10^{-5}	3.0×10^{-5}	3.4×10^{-7}
	800	1.1×10^{-4}	1.9×10^{-5}	7.4×10^{-6}	3.4×10^{-7}
	1000	3.4×10^{-5}	6.8×10^{-6}	2.9×10^{-6}	3.4×10^{-7}
δE_g	100	1.3×10^{-2}	7.2×10^{-3}	3.9×10^{-3}	8.6×10^{-5}
	200	1.1×10^{-3}	4.9×10^{-4}	1.8×10^{-4}	6.8×10^{-8}
	400	8.8×10^{-5}	2.4×10^{-5}	9.2×10^{-6}	4.9×10^{-8}
	600	1.6×10^{-5}	4.0×10^{-6}	1.3×10^{-6}	4.9×10^{-8}
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	1000	1.6×10^{-6}	3.3×10^{-7}	1.3×10^{-7}	4.9×10^{-8}

Hui-Ke Jin, Hong-Hao Tu, YZ, arXiv:2009.04129, PRB Lett (2021)

Kitaev honeycomb model: Gutzwiller guided DMRG

Cylinder geometry:
$$L_x = L_y = 6$$
, $J_3 = 0$



Small initial bond dimension: D
= 200;
Final bond dimension after DMRG sweeps: D = 8000 (random), 6500 (Gutzwiller);
The eigenvalue (Φ_y = ±1) is preserved;
The random-MPS initialized DMRG always converges to an MPS in Φ_y = -1 sector, a local minimum.

 $[E_g(\Phi_y = -1) - E_g(\Phi_y = 1) \approx 0.084]$



Hui-Ke Jin, Hong-Hao Tu, YZ, arXiv:2009.04129, PRB Lett (2021)

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Quantum Spin Liquid: terminology



Liquid

 vs. "solids": ordered spins, glassy spins, VBS, etc
 fluctuating vs. static/ordering /freezing

Spin

 charge degrees of freedom are freezing, Mott insulator
 low energy physics depicted by spin degrees of freedom

Quantum

- vs. "thermal": vanishing entropy density
- highly quantum entangled ground states

Definition

* Quantum spin liquid is defined as a Mott insulator which does not order magnetically even down to zero temperature due to quantum fluctuations.

Mott insulator

Pristine Mott insulator: odd number electrons/spins per unit cell.
 Can not be adiabatically connected to a trivial band insulator.
 Mottness is more than being an insulator.

Emergent particles and fields

□ **Spinons:** *S*=1/2, charge neutral, mobile objects

G "Fractionalization"

Gauge field: to accomplish physical spin degrees of freedom

 \Box These spinons are generally accompanied by gauge fields, U(1) or Z₂.



$$\square S = rac{1}{2}$$
 , $S_z = \pm rac{1}{2}$

\Box one magnon ($\Delta S = 1$) \rightarrow two spinons

Some most updated views

D Long-ranged entanglement of spins



- **D** Topological order
 - Gapped spin liquid states must have topological order. [M. B. Hastings (2004)]



- □ (Continuous or discrete) symmetry fractionalization
 - □ From symmetry protected topological order (SPT) to symmetry enriched topological order (SET).

A recommend review



Routes to quantum spin liquid

† Enhance quantum spin fluctuations





charge fluctuations multi-spin exchanges



degenerate orbitals spin-orbital or pseudospin



ka go me, ka go me

笼子缝,笼子缝 笼子中的鸟儿 无时无刻都想要跑来 就在那黎明前的夜晚 鹤与龟滑倒了 背后面对你的是谁? かごめかごめ かごの中の鸟は いついつ出やる 夜明けのばんに 鹤と亀が滑った 後ろの正面谁? ka go me ka go me ka go no na ka no to ri wa yi tsu yi tsu de ya ru yo a ke no ba n ni tsu ru to ka me ga su be tta wu shi ro no shoumen da re

Quantum fluid of spins on a basket weave lattice?





AFM Heisenberg model on Kagome lattice

Materials: herbertsmithite and its relatives

Name	Formula	Group	Lattice	Order
Botallackite	$Cu_4(OH)_6Cl_2$	$P2_1/m$	Т	AF (7.2 K)
Atacamite	$Cu_4(OH)_6Cl_2$	Pnma	Р	AF (9 K)
Clinoatacamite	$Cu_4(OH)_6Cl_2$	$P2_1/n$	Р	AF (6.5 K)
→ Claringbullite	$Cu_4(OH)_6ClF$	$P6_3/mmc$	Р	AF (17 K)
→ Barlowite	$Cu_4(OH)_6BrF$	$P6_3/mmc$	Р	AF (15 K)
Bobkingite	$Cu_5(OH)_8Cl_2W_2$	C2/m	Р	?
→ Herbertsmithite	$ZnCu_3(OH)_6Cl_2$	$R\bar{3}m$	Κ	AF (\cdots)
Tondiite	$MgCu_3(OH)_6Cl_2$	$R\bar{3}m$	Κ	AF (\cdots)
Kapellasite	$ZnCu_3(OH)_6Cl_2$	$P\bar{3}m1$	Κ	$F(\cdot \cdot \cdot)$
Haydeeite	$MgCu_3(OH)_6Cl_2$	$P\bar{3}m1$	Κ	F (4.2 K)
Zn-brochantite	$ZnCu_3(OH)_6SO_4$	$P2_{1}/a$	\mathbf{K}^*	AF (\cdots)



An incomplete list of numeric papers

Exact diagonalization: up to 48 sites

Leung and Elser (93); Lecheminant et al. (97); Mila (98); Waldtmann et al. (98); Sindzingre and Lhuillier (09); Lauchli et al. (11); Nakano and Sakai (11); Lauchli et al. (19); etc.

DMRG/iDMRG

Wietek and Lauchli (20); Jiang et al. (08); Yan et al. (11); Depenbrock et al. (12); Jiang et al. (12); Nishimoto et al. (13); He et al. (17); etc.

Tensor network

Mei et al. (17); Liao et al. (17); Jahromi et al. (20); Evenbly and Vidal (10); etc.

VMC

Ran et al. (07); Iqbal et al. (13,14,15); etc.

Issue: to gap or not to gap

AFM Heisenberg model on Kagome lattice

Model Hamiltonian

$$H = J \sum_{\langle ij \rangle_1} \mathbf{S}_i \cdot \mathbf{S}_j + J' \left(\sum_{\langle ij \rangle_2} \mathbf{S}_i \cdot \mathbf{S}_j + \sum_{\langle ij \rangle_3} \mathbf{S}_i \cdot \mathbf{S}_j \right)$$

Effective Hamiltonian: mean-field ansatz

$$H_{\rm MF} = \sum_{\langle ij \rangle_1} \sum_{\sigma=\uparrow,\downarrow} (\chi_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + {\rm H.c.})$$

A few example ansatzes: \Box DSL: $[0, \pi]$ (two Driac cones) \Box CSL: $[\pi/2, 0]$ (Chern # C = 2) \Box SFS: [0, 0] (spinon FS)

YC8

Rong-Yang Sun, Hui-Ke Jin, Hong-Hao Tu, YZ, arXiv: 2203.07321

 $[\Phi_3, \Phi_6]$

DMRG calculations initialized with various parton ansatzes



Alternative strategy: "Attack from right"

Model Hamiltonian

$$H = J \sum_{\langle ij \rangle_1} \mathbf{S}_i \cdot \mathbf{S}_j + J' \left(\sum_{\langle ij \rangle_2} \mathbf{S}_i \cdot \mathbf{S}_j + \sum_{\langle ij \rangle_3} \mathbf{S}_i \cdot \mathbf{S}_j \right)$$

 Start with a relative large *J*' that hosts stable CSL ground states;
 Then reduce *J*' adiabatically and monitor the evolution of ground states.

Rong-Yang Sun, Hui-Ke Jin, Hong-Hao Tu, YZ, arXiv: 2203.07321

Emergent Chiral Spin Liquid: Fractional Quantum Hall Effect in a Kagome Heisenberg Model

Shou-Shu Gong, Wei Zhu & D. N. Sheng

Department of Physics and Astronomy, California State University, Northridge, California 91330, USA.

SCIENTIFIC REPORTS | 4:6317 | DOI: 10.1038/srep06317



Chiral spin liquid

VOLUME 59, NUMBER 18

PHYSICAL REVIEW LETTERS

2 NOVEMBER 1987

Equivalence of the Resonating-Valence-Bond and Fractional Quantum Hall States

V. Kalmeyer Department of Physics, Stanford University, Stanford, California 94305

and

R. B. Laughlin Department of Physics, Stanford University, Stanford, California 94305, and University of California, Lawrence Livermore National Laboratory, Livermore, California 94550 (Received 24 July 1987)

We present evidence that the ground state of the frustrated Heisenberg antiferromagnet in two dimensions is well described by a fractional quantum Hall wave function for bosons. This is compatible with the resonating-valence-bond concept of Anderson in being a liquid with neutral spin- $\frac{1}{2}$ excitations. Our results suggest strongly that the resonating-valence-bond and fractional quantum Hall states are the same thing. We also argue that the excitation spectrum has an energy gap.



□ Topological order ⇔ gapped QSL □ Symmetry breaking: time reversal, parity

PHYSICAL REVIEW B

VOLUME 39, NUMBER 16

1 JUNE 1989

Chiral spin states and superconductivity

X. G. Wen, Frank Wilczek,* and A. Zee Institute for Theoretical Physics, University of California, Santa Barbara, California 93106 (Received 9 December 1988)



scalar spin chirality

 $E_{123} \equiv \langle \sigma_1 \cdot (\sigma_2 \times \sigma_3) \rangle$







Possible chiral spin liquid on the Kagome lattice

VOLUME 70, NUMBER 17

PHYSICAL REVIEW LETTERS

26 April 1993

Possible Spin-Liquid States on the Triangular and Kagomé Lattices

Kun Yang, L. K. Warman, and S. M. Girvin Physics Department, Indiana University, Bloomington, Indiana 47405 (Received 23 November 1992)

The frustrated quantum spin-one-half Heisenberg model on the triangular and kagomé lattices is mapped onto a single species of fermion carrying statistical flux $\theta = \pi$. The corresponding Chern-Simons gauge theory is analyzed at the Gaussian level and found to be massive. This provides a new motivation for the spin-liquid Kalmeyer-Laughlin wave function. Good overlap of this wave function with the numerical ground state is found for small clusters.



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A QUICK PREVIEW OF RESULTS



Identify the topological order: v = 1/2 Laughlin state

Effective Hamiltonian

Entanglement spectra (ES): SU(2)₁ WZW



4 exact boundary zero modes: $d_{L\sigma}^{\dagger}$ and $d_{R\sigma}^{\dagger}$

Anyon eigen-basis (MES)

$$|\Psi_1\rangle = \hat{P}_G d_{L\uparrow}^{\dagger} d_{L\downarrow}^{\dagger} |\Phi\rangle, \quad |\Psi_2\rangle = \hat{P}_G d_{L\uparrow}^{\dagger} d_{R\downarrow}^{\dagger} |\Phi\rangle$$

Li, Haldane (08); Qi, Katsura, Ludwig (12)



AFM Heisenberg model on Kagome lattice



AFM Heisenberg model on Kagome lattice



More on spin chirality and its correlation



Evaluation of spin chirality: (1) $\chi = |\chi_0 \chi_{r_{max}}|^{1/2}$; (2) Real MPS: re-diagonalization; (3) Complex MPS.

1 (a) J' = 0.2:

- (1) Larger circumference L_y will enhance χ ;
- 2 Larger *D* will enhance χ ;
- (3) Larger aspect ratio L_y/L_x will enhance χ ;
- (b) & (c) J' = 0: (1) Larger $L_y \rightarrow \text{larger } \chi$; (2) Larger $D \rightarrow \text{larger } \chi$.

Ordered states



Take-home messages

□ A promising method: Gutzwiller + DMRG
 □ The performance of DMRG in 2D can be dramatically improved
 □ Challenging AFM Heisenberg model on the Kagome lattice
 □ Chiral spin liquid: ν = 1/2 Laughlin state
 □ Two topological sectors + Kramers' degeneracy in each topological sector

