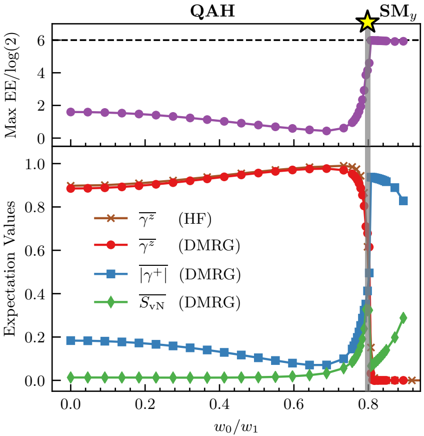
DMRG for Bilayer Graphene



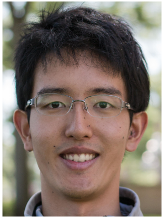
arXiv: 1909.06341
DEP
Xiangyu Cao
Mike Zaletel

arXiv: 2009.02354
Tomohiro Soejima
DEP
Nick Bultinck
Johannes Hauschild
Mike Zaletel

Daniel E. Parker

24 September 2020

Acknowledgements



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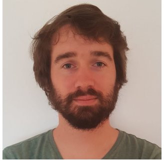

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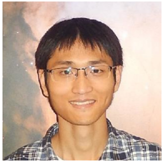

Xiangyu Cao
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Mike Zaletel
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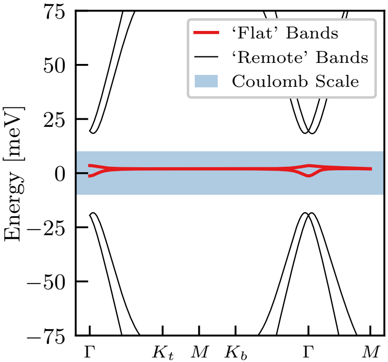
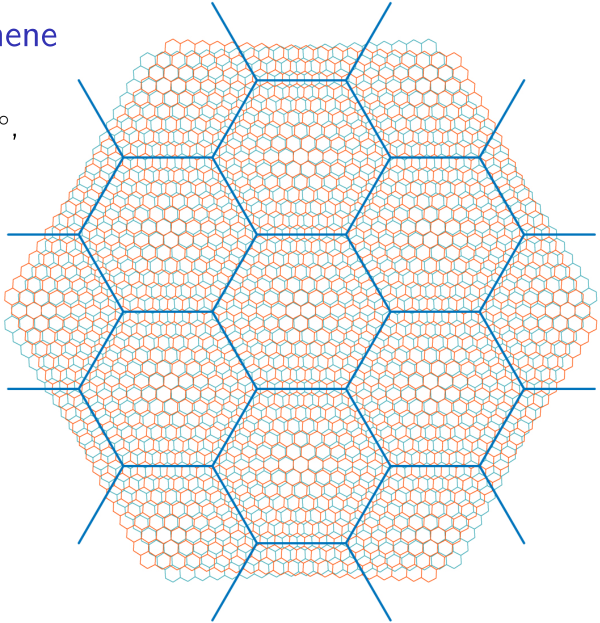
Outline

1. One Way to Simulate tBLG
2. Matrix Product Opreators & Compression
3. tBLG Physics from DMRG

Magic Angle Twisted Bilayer Graphene

1. Two layers of graphene, twisted at $\sim 1.05^\circ$, gives narrow bands
2. Bandwidth $\ll$ Coulomb scale $<$ Band gap
3. Many intriguing phases result!





Bistritzer & MacDonald 2011; Cao *et al* 2018; and many, many others!
Fig: Quanta Magazine

Phases of tBLG

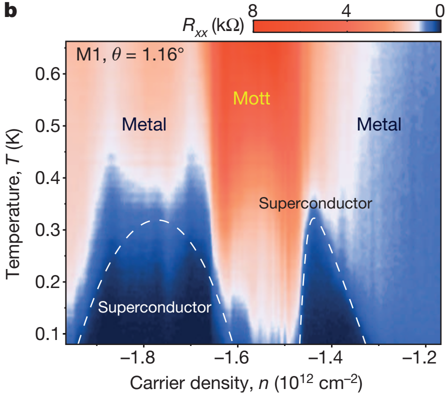
tBLG hosts many intriguing phases

- Correlated insulators
- quantum anomalous Hall (Chern) insulators
- orbital magnets & various ferromagnetic states
- semimetallic phases

  ⋮

- superconductivity

Roughly 1 zillion theory papers with various mechanisms.



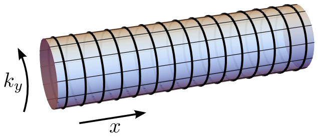
Goal: compute the ground state with unbiased, non-perturbative numerics.

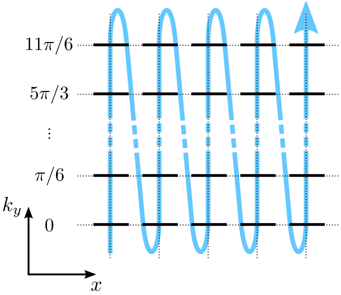
Cao *et al* 2018; and many, many others!

1. One Way to Simulate tBLG
or
Computing the Right Model

Denity Matrix Renormalization Group (DMRG)

- Non-perturbative method to find ground states of 1D quantum systems
- Essentially exact for area law (gapped) systems and usually accurate for gapless ones.
- Can handle 2d systems in an infinite cylinder geometry:
  - $\infty \times L_y$
  - $L_y \sim 6 - 12$.
- Requires Hamiltonians written as Matrix Product Operators
- States are encoded as matrix product states
- The complexity of matrix product states (operators) is parameterized by the bond dimension χ (D).



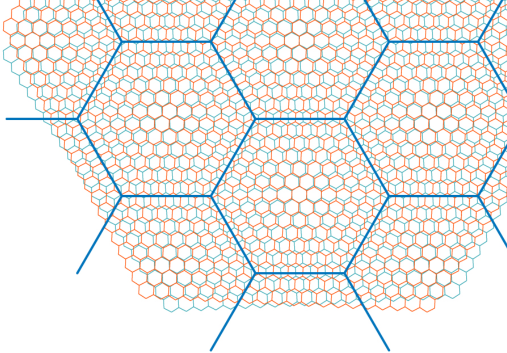


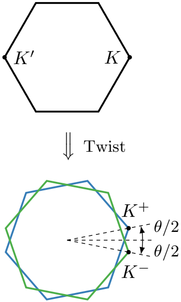
White (1992); Pirvu, Murg, Cirac, Verstraete (2010); etc. Figure from Motruk, Zaletel, Mong, Pollmann (2015)

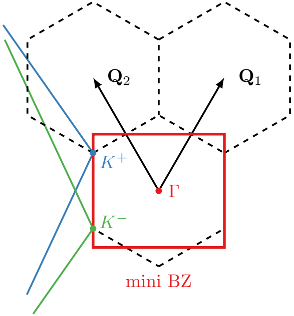
Lightning review: BM Model

The Bistritzer-MacDonald (BM) model is a standard non-interacting model for twisted bilayer graphene.

Graphene unit cell $\ll$ moiré unit cell, so Graphene Brillouin Zone $\gg$ moire (mini) BZ.

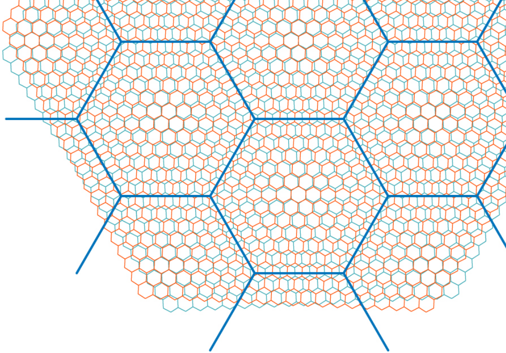






Bistritzer, MacDonald (2011); etc

Lightning review: BM Model



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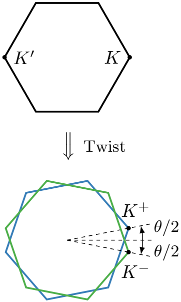
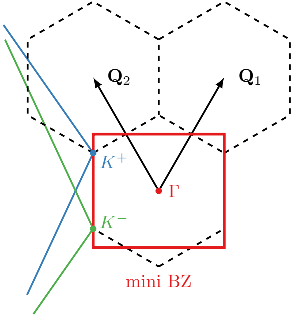
$$\widehat{H}_{\mathrm{BM}} = \underbrace{\widehat{H}_{\mathrm{MLG}}(\theta)}_{\text{top layer}} + \underbrace{\widehat{H}_{MLG}(-\theta)}_{\text{bottom layer}} + \underbrace{\widehat{T}}_{\text{interlayer tunneling}}$$

$$= \int_{\mathrm{mBZ}} [d\boldsymbol{k}]\ \boldsymbol{f}^{\dagger}_{\boldsymbol{k}} h(\boldsymbol{k}) \boldsymbol{f}_{\boldsymbol{k}}$$



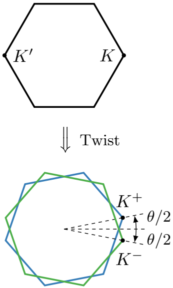


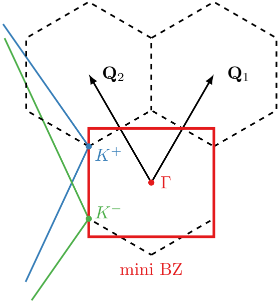
Bistritzer, MacDonald (2011); etc

The "IBM" Model

Interacting Bistritzer-MacDonald (IBM) model:

- start with the BM model $h(\boldsymbol{k})$
- add gate-screened Coulomb interactions

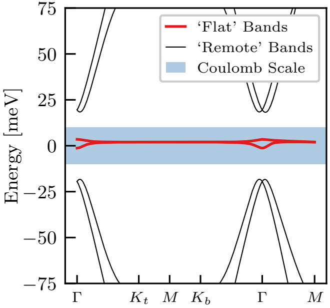




$$\widehat{H} := \widehat{H}_{\mathrm{BM}} + \widehat{H}_{\mathrm{Coulomb}}$$

$$= \int_{\mathrm{mBZ}} [d\boldsymbol{k}] \boldsymbol{f}^\dagger_{\boldsymbol{k}} h(\boldsymbol{k}) \boldsymbol{f}_{\boldsymbol{k}} + \int d[\boldsymbol{q}] V_{-\boldsymbol{q}} : \hat{\rho}(\boldsymbol{k}+\boldsymbol{q})\hat{\rho}(\boldsymbol{k}) :$$

$$V_{\boldsymbol{q}} = e^2 \frac{\tanh(|\boldsymbol{q}|\, d)}{2\epsilon_r \epsilon_0 |\boldsymbol{q}|}.$$

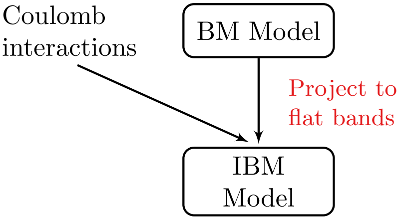


$d \approx 10\,\mathrm{nm}$ is gate distance, $\epsilon_R \approx 12$ is permitivity

Can we compute the ground state?

Bultinck, Khalaf, Liu, Chatterjee, Vishwanath, Zaletel (2019); Kang, Vafek (2020); etc.

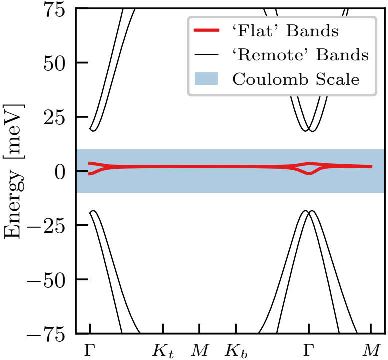
Projection to Narrow Bands



- 10,000 atoms/moiré unit cell — far too many
- Project to flat bands:

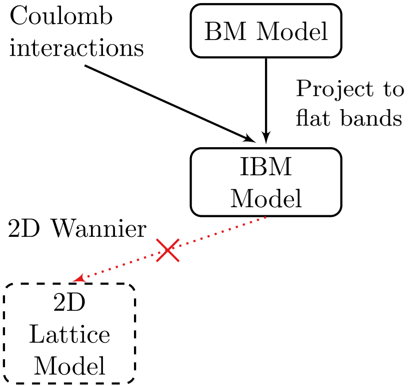
$$H_{\mathrm{IBM}} = \mathcal{P}^{\dagger}[H_{\mathrm{BM}} + H_{\mathrm{Coulomb}}]\mathcal{P}$$

- Kinetic scale (bandwidth of flat bands): $t \approx 1\,\mathrm{meV}$
- Interaction scale (Coulomb): $V \approx 10\,\mathrm{meV}$
- Band gap: $\Delta E \approx 25\,\mathrm{meV}$
- $t \ll V < \Delta E \implies$ Projection is perturbatively valid.
- Now 8 fermions/moiré unit cell
  - 2 bands
  - K and K' valleys
  - spin $\uparrow, \downarrow$



Topological Obstruction to 2D Wannierization

- Most numerical methods require a discrete lattice
- Straightforward solution: find localized Wannier orbitals via Fourier transform.



Po, Zou, Vishwanath, Senthil (2018, 2018, 2019); Song, Wang, Shi, Li, Fang, Bernevig (2019); Ahn, Park, Yang (2019); Kang, Vafek (2018); Koshino, Yuan, Koretsune, Ochi, Kuroki, Fu (2018); etc

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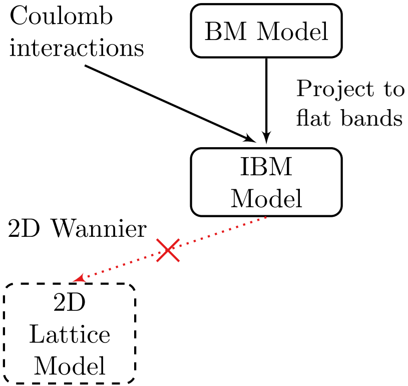

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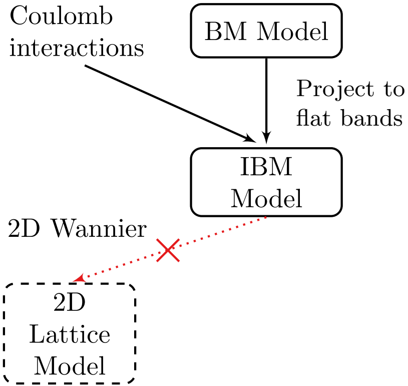
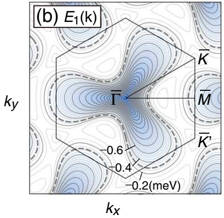
  - "Fidget spinner" Wannier functions
  - $Q_v = \sum_{i,j,n,m} Q^{ij}_{n,m} \hat{c}^\dagger_{mi} \hat{c}_{nj}$, $Q^{ij}_{n,m}$ long-ranged
  - Coulomb also long-ranged (not Hubbard-like)
  - Numerically, finite size will break symmetry!





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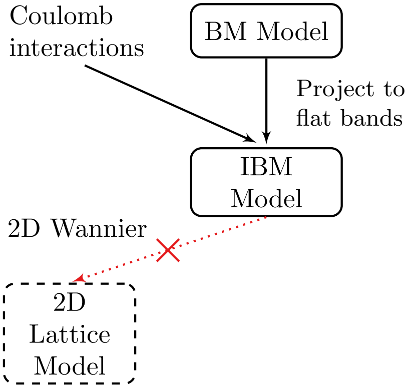
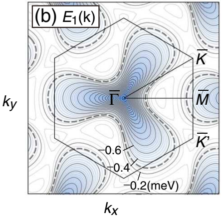
  - Top. obstruction is "fragile"
  - computationally infeasible





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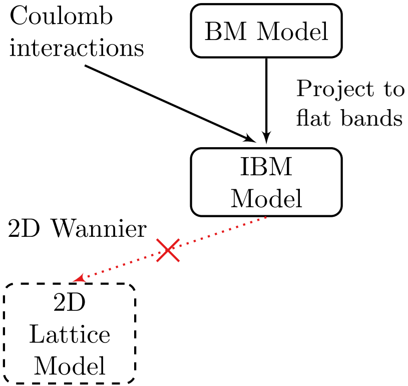

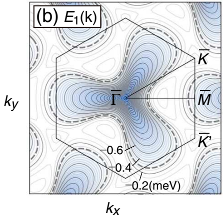

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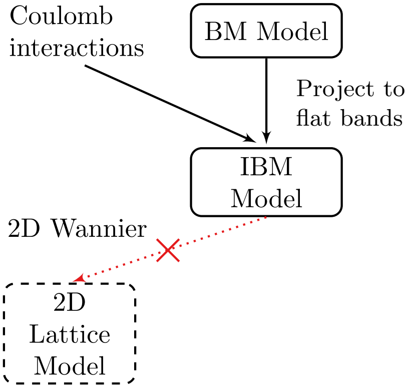
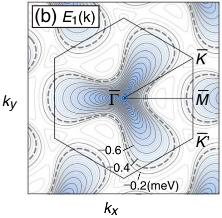
Is there a better solution for DMRG?





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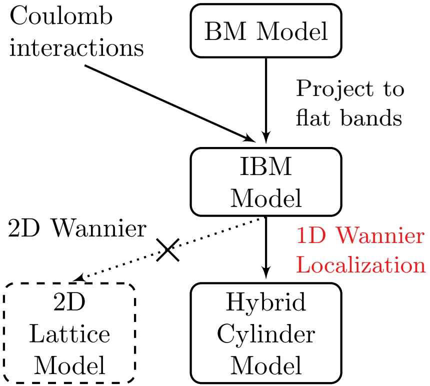
1D Wannier Localization

Hybrid xk Wannier orbitals: localize along x, periodic along y



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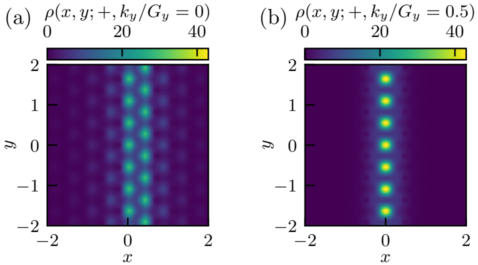
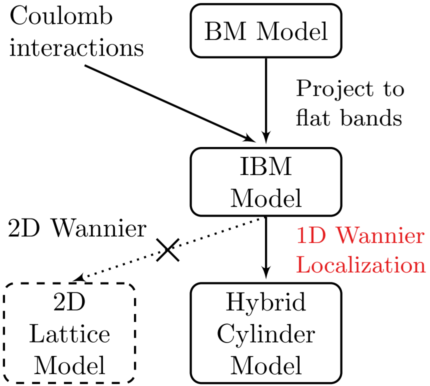
$$|w_{\pm,n,k_y}\rangle = \sum_{b\in \text{ flat bands}} \int [dk_x]\, U_{\pm,b}\, e^{i\boldsymbol{k}\cdot\boldsymbol{R}_n} \hat{f}^\dagger_{b,\boldsymbol{k}}\, |0\rangle\,.$$





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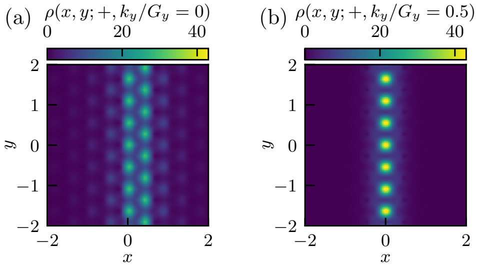
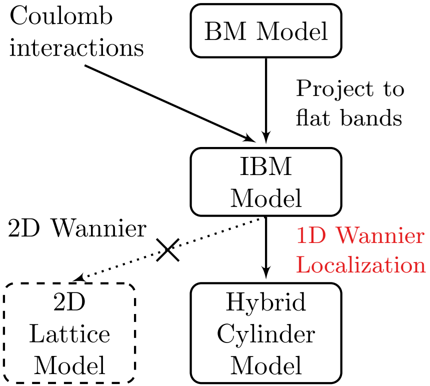
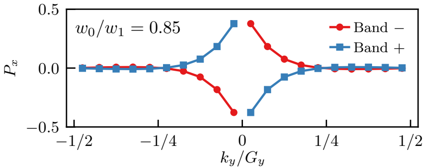
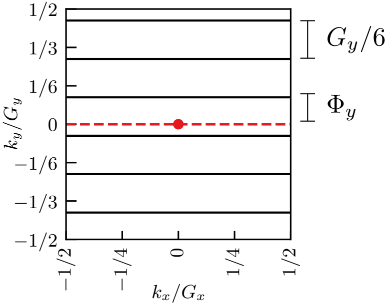


Bands labelled by Chern number $C = \int dk_y \frac{dP_x}{dk_y} = \pm 1$.





Hybrid Cylinder Model



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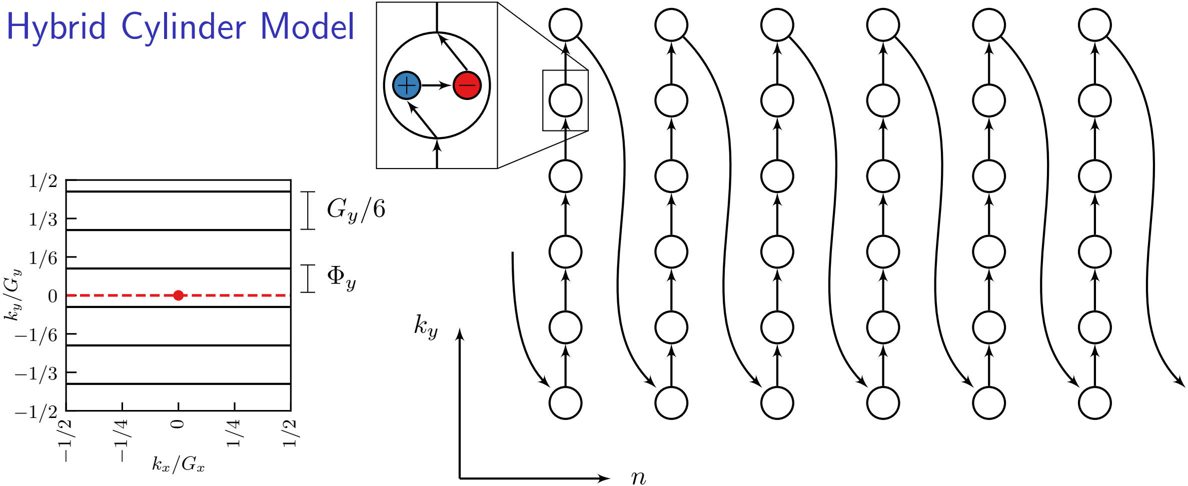


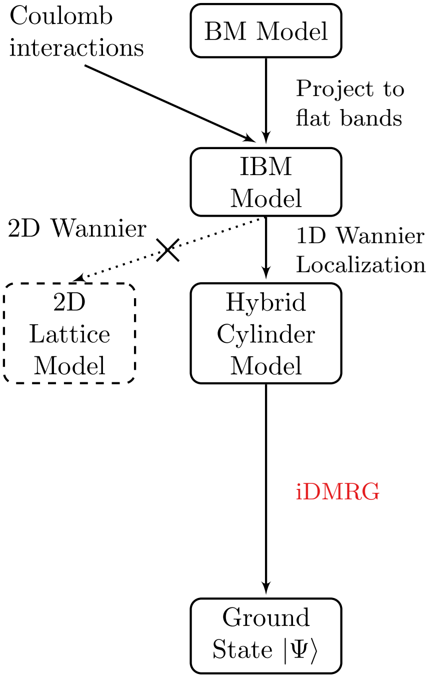
$$w^{\dagger}_{\pm,n,k_y} = \sum_{b \in \text{ flat bands}} \int [dk_x]\; U_{\pm,b}\, e^{i\boldsymbol{k}\cdot\boldsymbol{R}_n} \hat{f}^{\dagger}_{b,\boldsymbol{k}}.$$

Infinite 2D DMRG

- We have now mapped the BLG Hamiltonian to an infinite cylinder. Schematically,

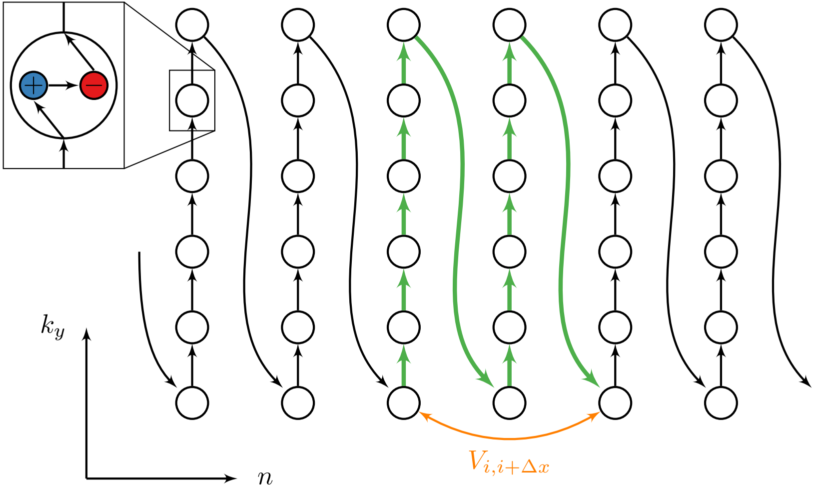
$$H_{\text{cyl}} = \text{FT}_x \left[\mathcal{P}^\dagger [H_{\text{BM}} + H_{\text{Coulomb}}] \mathcal{P} \right]$$

- Taking finite k_y cuts gives a quasi-1D model
- (Infinite) Density Matrix Renormalization Group
  - For any* quasi-1D model, can find $|\Psi_0\rangle$ and E_0.
  - Several good libraries, such as `TenPy`
- Finite DMRG for BLG — see Kang and Vafek
- In principle we can find the ground state
- DMRG scales as $O(D^2)$ where D is the Hamiltonian's "bond dimension"



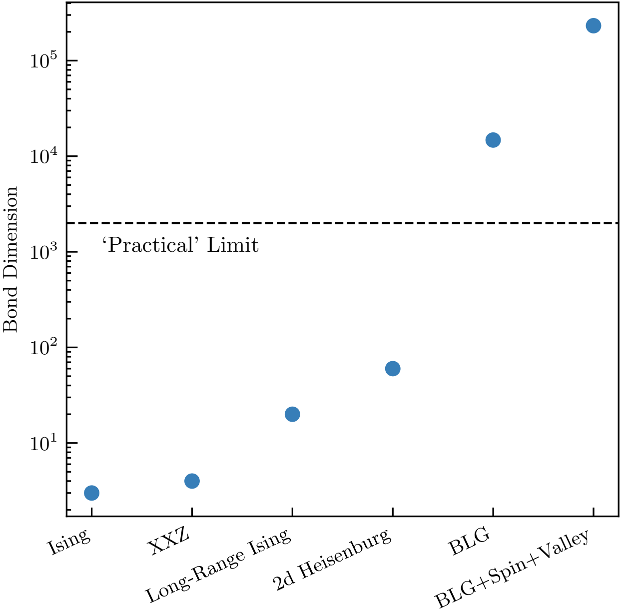
Kang, Vafek (arXiv: 2002.10360).

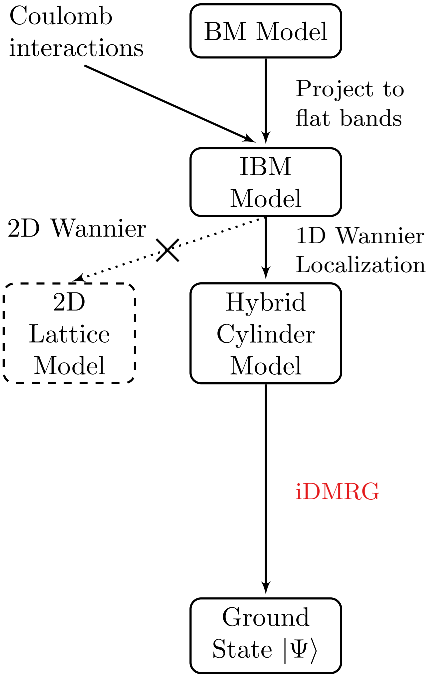
Long Range



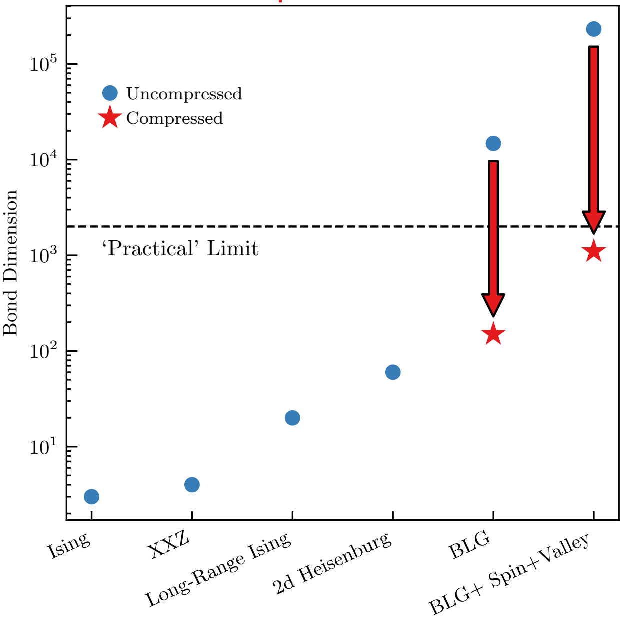
1D Range $R = \underbrace{(2 \times 2 \times 2)}_{\text{orbitals}} \times \underbrace{L_y}_{\text{cuts}} \times \underbrace{\Delta x}_{\text{range}}$ $D \approx 4R^2; \sim 230,000;$ DMRG $\sim O(D^2)$

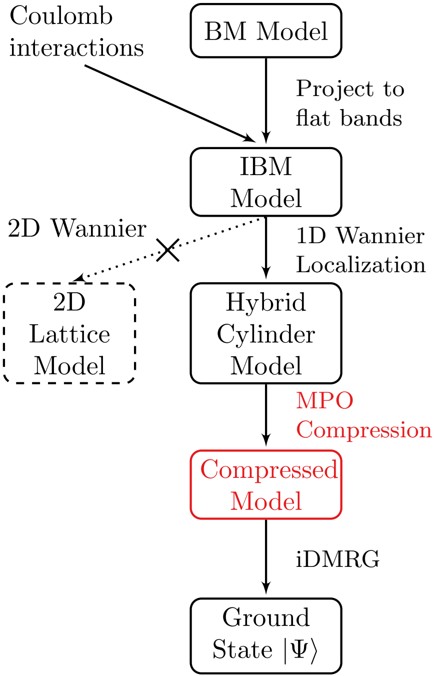
Obstruction: MPO Bond Dimension





Solution: MPO Compression





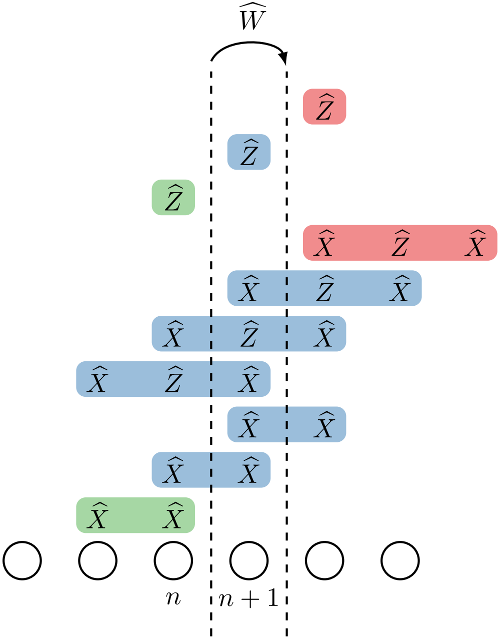
2. Matrix Product Operators and Compression

Matrix Product Operators

A local Hamiltonian

$$\widehat{H} = \sum_i J\widehat{X}_i\widehat{X}_i + K\widehat{X}_i\widehat{Z}_{i+1}\widehat{X}_{i+2} + h\widehat{Z}_i$$

is a sum of Pauli strings: $\cdots\widehat{\mathbb{1}}_{-2}\widehat{\mathbb{1}}_{-1}\widehat{X}_0\widehat{X}_1\ \widehat{\mathbb{1}}_2\ \widehat{\mathbb{1}}_3\cdots$



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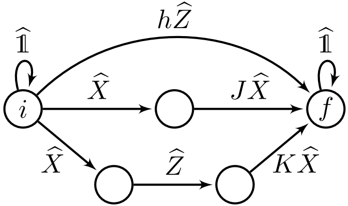
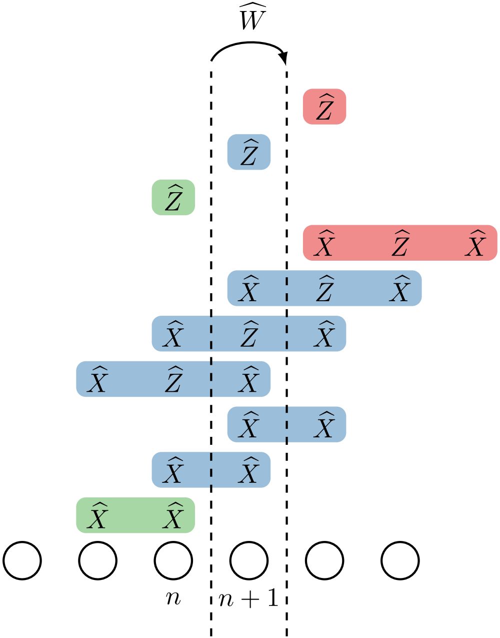


A Matrix Product Operator is a machine to place one more site.



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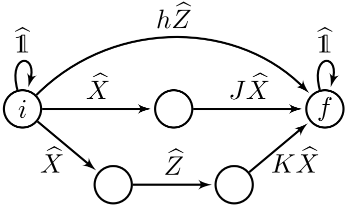

$\Uparrow$ out

$$\widehat{W} = \left(\begin{array}{c|ccc|c} \widehat{\mathbb{1}} & \widehat{X} & \widehat{X} & 0 & h\widehat{Z} \\ \hline & 0 & 0 & 0 & J\widehat{X} \\ & 0 & 0 & \widehat{Z} & 0 \\ & 0 & 0 & 0 & K\widehat{X} \\ \hline & & & & \widehat{\mathbb{1}} \end{array}\right)$$

$\Longrightarrow$ in

Bond Dimension 5

A Matrix Product Operator is a machine to place one more site.
Rewrite the graph as an operator-valued matrix.

Compression

Given a Hamiltonian, what the optimal MPO (smallest D)?

e.g. $\widehat{H} = \sum_i J\widehat{X}_i\widehat{X}_{i+1} + K\widehat{X}_i\widehat{Z}_{i+1}\widehat{X}_{i+2} + h\widehat{Z}_i$

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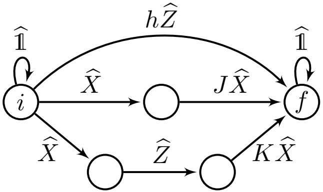

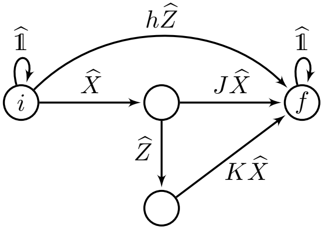

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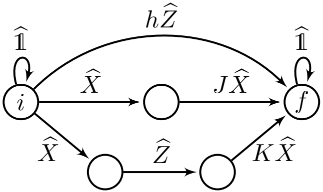
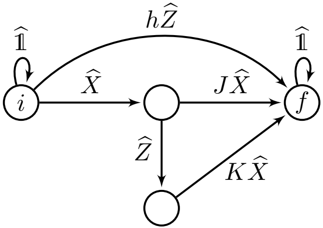




Finite MPOs Directly analagous to MPS compression; see [1] & `ITensor` library [2]

Infinite MPOs More involved due to *locality*; see [3].

[1] Chan, Keselman, Nakatani, Li, White (2016); [2] Fishman, White, Stoudenmire (2020); [3] **DEP**, Cao, Zaletel (2020).

Compression Algorithm

Idea: use a Schmidt decomposition that respects *locality*.

Any local operator can be written as

$$\widehat{H} = \widehat{H}_L \widehat{I}_R + \widehat{I}_L \widehat{H}_R + \sum_{a=1} s_a \hat{\mathcal{O}}_L^a \hat{\mathcal{O}}_R^a.$$

Compress by truncating the sum:

$$\widehat{H}' = \widehat{H}_L \widehat{I}_R + \widehat{I}_L \widehat{H}_R + \sum_{a=1}^{D} s_a \hat{\mathcal{O}}_L^a \hat{\mathcal{O}}_R^a.$$

Theorem: For local $\widehat{H} \xrightarrow{compress} \widehat{H}'$,

$$\left|E_{\mathrm{GS}} - E'_{\mathrm{GS}}\right| < C\epsilon; \quad \epsilon^2 := \sum_{a=D+1} s_a^2.$$

Algorithm 1 iMPO Compression

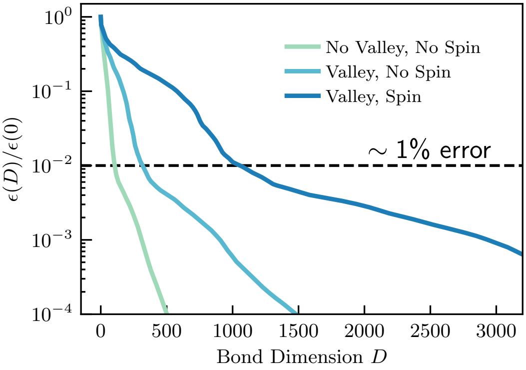
Require: $\widehat{W}$ is a first-order infinite MPO.

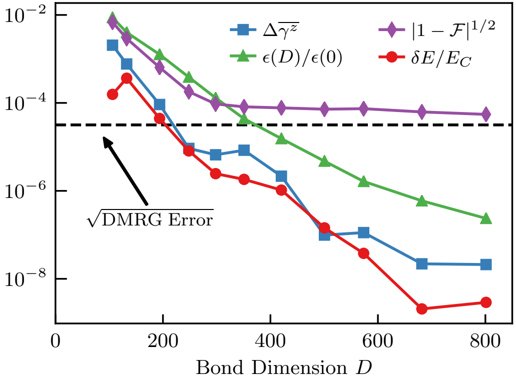
1: **procedure** ICOMPRESS($\widehat{W}, \eta$) ▷ Cutoff η
2: $\widehat{W}_R \leftarrow$ RIGHTCAN[$\widehat{W}$]
3: $\widehat{W}_R \leftarrow R\widehat{W}_R R^{-1}$ so that $[\widehat{W}_R]_{1a} = 0$
4: $\widehat{W}_L, C \leftarrow$ LEFTCAN[$\widehat{W}_R$]
5: $(U, S, V^\dagger) \leftarrow$ SVD[C]
6: $\widehat{Q}, \widehat{P} \leftarrow U^\dagger \widehat{W}_L U\,,\ V^\dagger \widehat{W}_R V$
7: $\chi' \leftarrow \max\{a \in [1, \chi] : s_a > \eta\}$ ▷ Defines $\mathbb{P}$
8: $\widehat{W}''_L, S, \widehat{W}''_R \leftarrow \mathbb{P}^\dagger \widehat{W}'_L \mathbb{P}, \mathbb{P}^\dagger S \mathbb{P}, \mathbb{P}^\dagger \widehat{W}'_R \mathbb{P}$
9: **return** $\widehat{W}''_L$ ▷ One could also return $\widehat{W}''_R$.

Physically, the singular values s_a fall off (exponentially) quickly, so we can chop off the small ones.

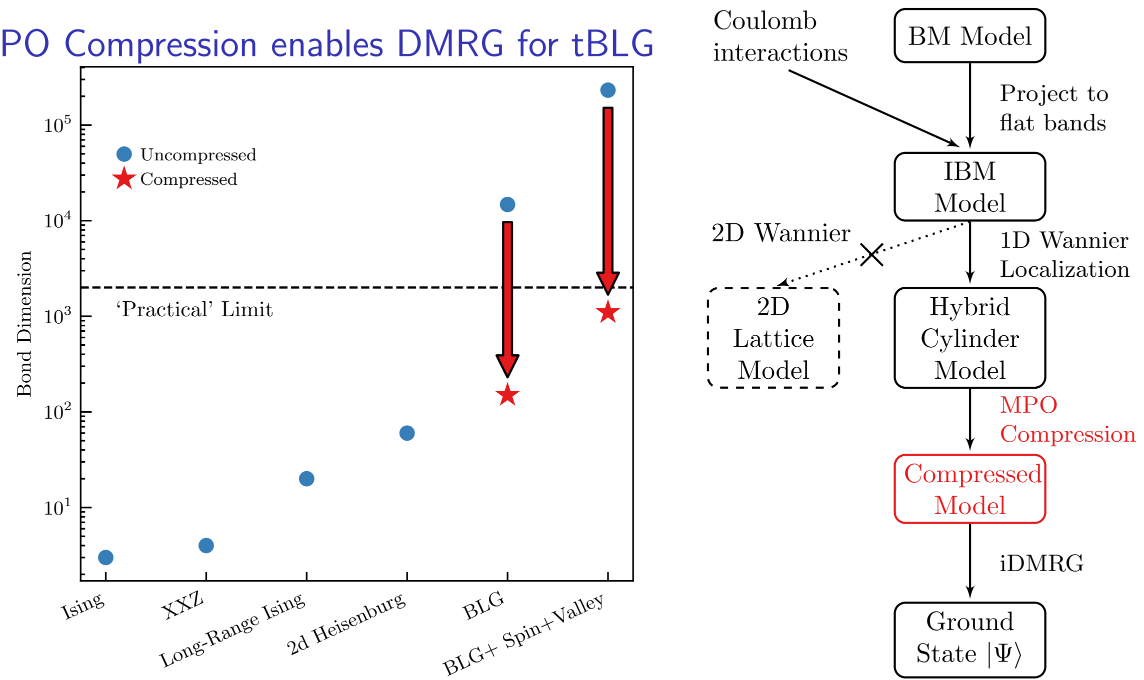
We can compute low bond dimension approximations $\widehat{W}'$ to any local operator.

MPO Compression for tBLG





MPO Compression enables DMRG for tBLG



3. tBLG Physics from DMRG

Wannier Basis and Symmetry Actions

Restrict to the spinless, 1-valley case at half-filling.
We use $N_y = 6$ momentum cuts at

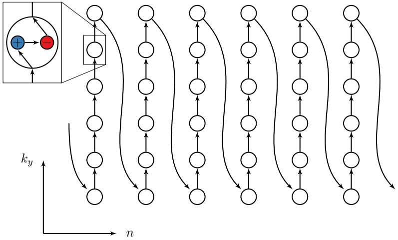
$$k_y/G_y = \frac{n + \Phi_y/(2\pi)}{N_y} \pmod 1$$

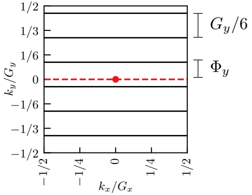
This gives a cylinder radius of $12 = N_y \times 2$.

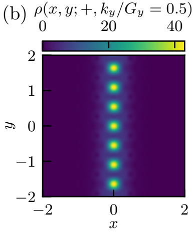
Symmetries:

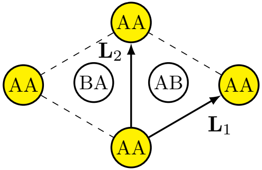
$$T_{L_1} |w(\pm, n, k_y)\rangle = |w(\pm, n+1, k_y)\rangle$$
$$T_{L_2} |w(\pm, n, k_y)\rangle = e^{i2\pi k_y} |w(\pm, n, k_y)\rangle$$
$$C_2\mathcal{T} |w(\pm, n, k_y)\rangle = |w(\mp, -n, k_y)\rangle$$
$$C_{2x} |w(\pm, n, k_y)\rangle = \mp i e^{-i2\pi k_y n} |w(\mp, n, -k_y)\rangle$$

C_3 is slightly broken by the rectangular BZ.

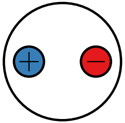








1-Particle Observables



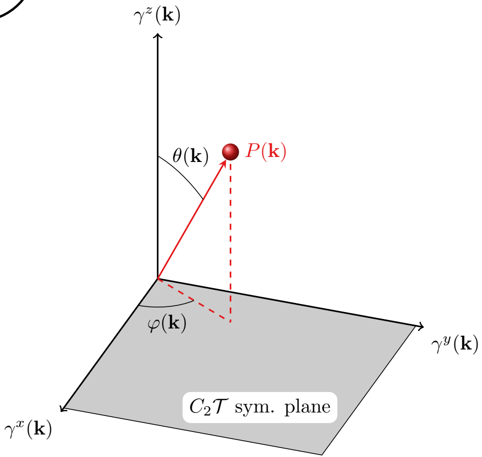
Let

$$P(\boldsymbol{k}) = \begin{pmatrix} \langle w^\dagger_{+,\boldsymbol{k}} w_{+,\boldsymbol{k}} \rangle & \langle w^\dagger_{-,\boldsymbol{k}} w_{+,\boldsymbol{k}} \rangle \\ \langle w^\dagger_{+,\boldsymbol{k}} w_{-,\boldsymbol{k}} \rangle & \langle w^\dagger_{-,\boldsymbol{k}} w_{-,\boldsymbol{k}} \rangle \end{pmatrix}$$

$$= \gamma^0(\boldsymbol{k})\sigma^0 + \gamma^x(\boldsymbol{k})\sigma^x + \gamma^y(\boldsymbol{k})\sigma^y + \gamma^z(\boldsymbol{k})\sigma^z$$

If one electron per $\boldsymbol{k}$, then $|\gamma^x|^2 + |\gamma^y|^2 + |\gamma^z|^2 = 1$, which gives a unit sphere:

$$P(\boldsymbol{k}) \iff (\theta(\boldsymbol{k}), \varphi(\boldsymbol{k})) \quad \text{(spherical coords.)}$$



$C_2\mathcal{T}$ Order parameter

$$C_2\mathcal{T} \text{ sym} \implies \gamma^z(\boldsymbol{k}) = 0 \implies \theta(\boldsymbol{k}) = \frac{\pi}{2}$$

Phase Transition & QAH Phase

Vary interlayer coupling

$$\begin{cases} w_0 & \text{AA regions} \\ w_1 & \text{AB regions} \end{cases}$$

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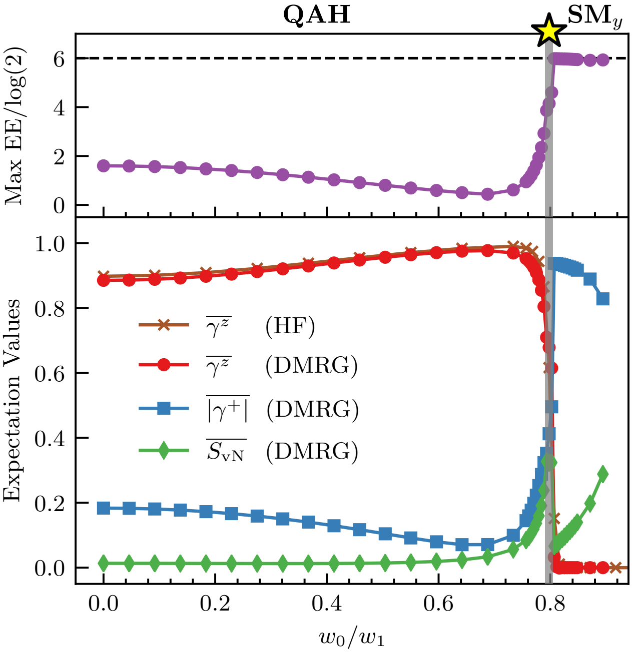
Low w_0/w_1

- Broken $C_2\mathcal{T}$ ($\overline{\gamma^z} \neq 0$)
- Almost completely polarized, so

$$|\Psi\rangle_{\mathrm{QAH}} \approx \prod \hat{w}^\dagger_{+,n,k_y} |0\rangle \,.$$

- Filled Chern +1 band implies quantum anomalous Hall state.
- Matches analytic solution at $w_0 = 0$



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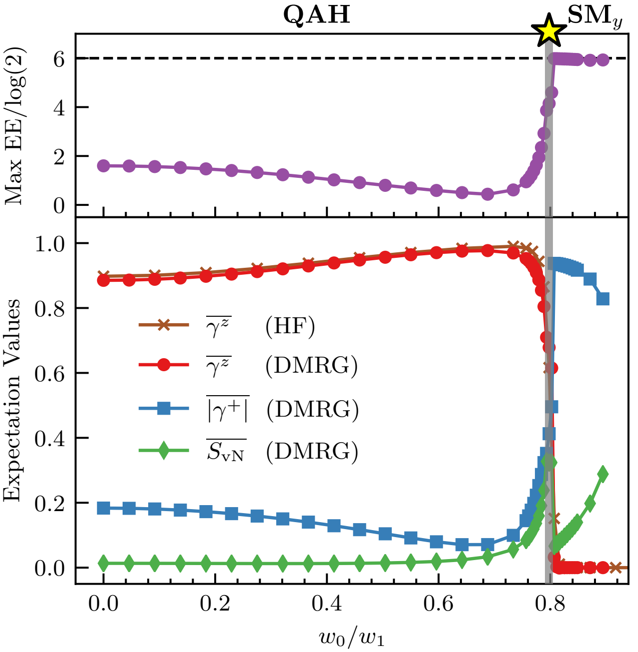
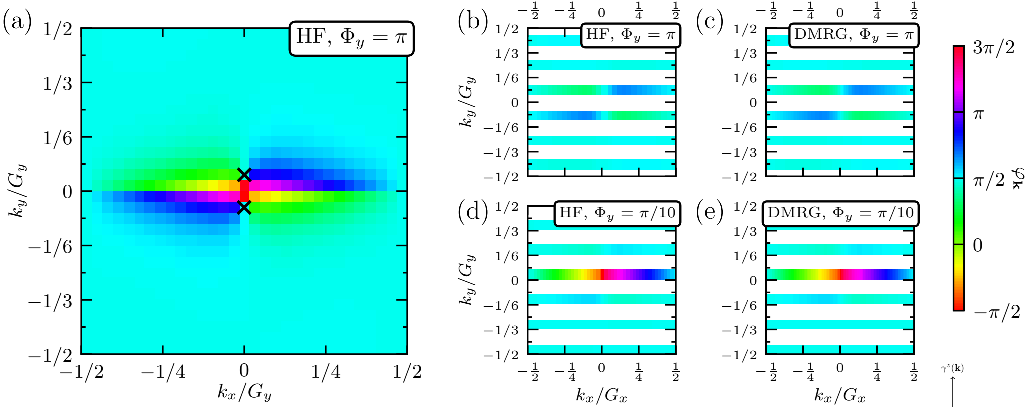
High w_0/w_1 – more involved

- $C_2\mathcal{T}$ preserved

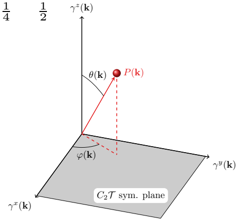


Ledwith, Tarnopolsky, Khalaf, Vishwanath (2020)

The Remarkable Accuracy of Hartree-Fock



- Only 2% difference between DMRG and HF in $\varphi_{\boldsymbol{k}}$
- $|\Psi_{\mathrm{DMRG}}\rangle = |\Psi_{\mathrm{SD}}\rangle + \epsilon\,|\Psi^{(1)}\rangle$.
- Despite strong interactions,
  the ground state is essentially a Slater determinant!



The High w_0/w_1 Phase is Nematic

$C_2\mathcal{T}$ preseved, so

$$\begin{cases} \theta(\boldsymbol{k}) & = \frac{\pi}{2} \\ \varphi(C_2\mathcal{T}\boldsymbol{k}) & = -\varphi(\boldsymbol{k}) + \pi \end{cases}$$

At K^+, C_3 acts as

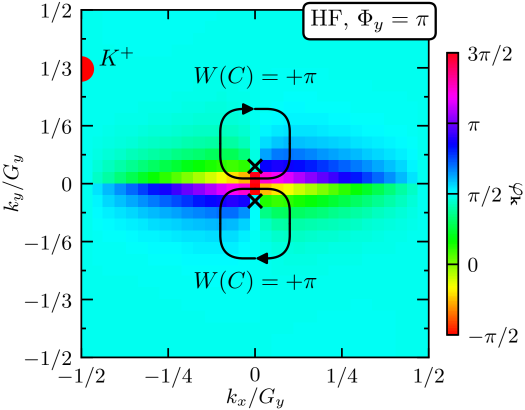
$$\varphi(C_3K^+) = \varphi(K^+) + \pi/3,$$

but

$$\varphi(C_3K^+) = \varphi(K^+) \approx \frac{\pi}{2}.$$

Therefore C_3 is broken; we pick out a preferred orientation.

The high w_0/w_1 phase is nematic.

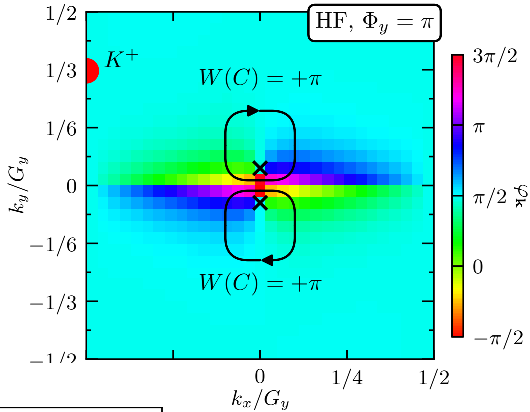


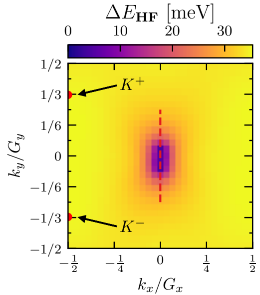
NEMATIC (semimetal)

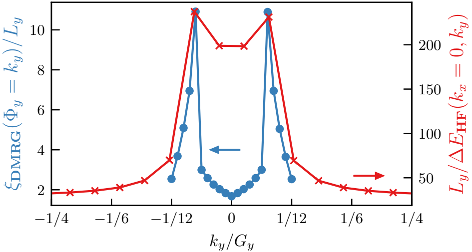
- Wilson loops are quantized

$$W(C) = \int_C \mathcal{A} = \frac{1}{2}\int_{\partial C} \boldsymbol{\nabla}\varphi \cdot \, d\boldsymbol{k} = n\pi, n \in \mathbb{Z}.$$

- We find two Dirac nodes with $+\pi$, so this phase is a nematic semimetal.
- The Dirac nodes appear in both HF and DMRG.

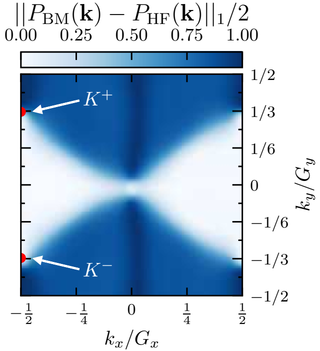




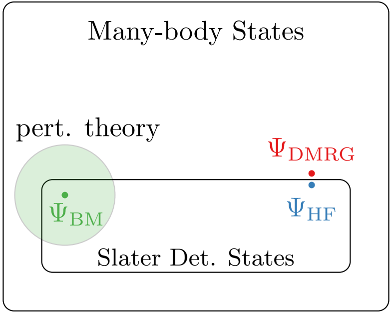


Nematic Semimetal$_y$ $\neq$ BM Ground State

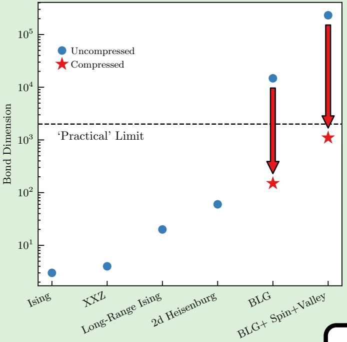
- The nematic semimetal is NOT close to the BM ground state
- Both do have Dirac nodes
- However, nodes positioned near Γ (BM) vs $K^{\pm}$ (Nematic SM)
- The trace distance between the states is large



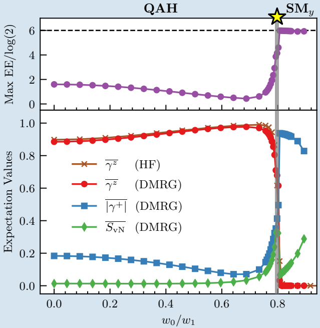
Even though the ground state $\Psi_{\rm DMRG}$ is close to a Slater-Determinant $\Psi_{\rm HF}$, it does not seem to be (perturbatively) close to the non-interacting ground state $\Psi_{\rm BM}$.



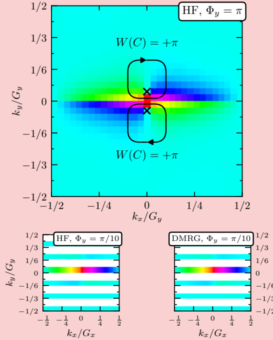
Compression enables DMRG for BLG



Transition from QAH to Nematic SM_y



Hartree-Fock is remarkably accurate!



Compression: 1909.06341. **BLG DMRG:** 2009.02354.

Future Work

- 2 Valleys
- Spin
- Excitations
- Superconductivity
- Strain
- Other moire systems

Extra Slide: Ground State Competition

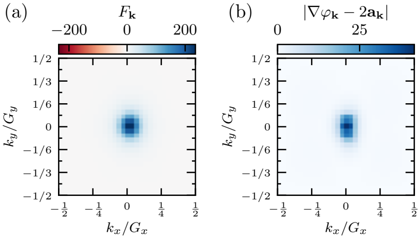
Several states only slightly above the ground state. Partially explained by Eslam's Ginsberg-Landau-like functional

$$E_{\mathrm{HF}}[\varphi_{\mathrm{k}}] = E_{\mathrm{HF}}^{\mathrm{QAH}} + \frac{1}{2}\int g_{\mathrm{k}}(\nabla_{\mathrm{k}}\varphi_{\mathrm{k}} - 2\boldsymbol{a}_{\boldsymbol{k}})^2 d^2\boldsymbol{k} + \cdots$$

The true physical ground state may be controlled by "second order effects":

- twist angle disorder
- strain
- lattice relaxation

State ($w_0/w_1 = 0.85$)	Energy [meV]
DMRG SM_y	-28.24
QAH Ansatz	-28.04
SM_y Ansatz	-27.92
$C_2\mathcal{T}$ - Stripe Ansatz	-28.08
Dirac (BM GS)	-20.62



Extra Slide: IBM Model

$$H_{\text{IBM}} = \sum_{\boldsymbol{k}\in\text{mBZ}} \boldsymbol{f}^{\dagger}_{\boldsymbol{k}} h(\boldsymbol{k}) \boldsymbol{f}_{\boldsymbol{k}} + \sum_{\boldsymbol{q}} V(\boldsymbol{q}) : \rho^{\dagger}_{\boldsymbol{q}} \rho_{-\boldsymbol{q}} :$$

$$\rho_{\boldsymbol{q}} = \sum_{\boldsymbol{k}\in\text{mBZ}} \boldsymbol{f}^{\dagger}_{\boldsymbol{k}} \Lambda_{\boldsymbol{q}}(\boldsymbol{k}) \boldsymbol{f}_{\boldsymbol{k}}$$

$$[\Lambda_{\boldsymbol{q}}(\boldsymbol{k})]_{ab} = \langle \psi_{a,\boldsymbol{k}} | e^{-i\boldsymbol{q}\cdot\boldsymbol{r}} | \psi_{b,\boldsymbol{k}+\boldsymbol{q}} \rangle$$

$$V_{\boldsymbol{q}} = e^2 \frac{\tanh(|\boldsymbol{q}|\, d)}{2\epsilon_r \epsilon_0 \, |\boldsymbol{q}|}$$

Parameter	**Value(s)**
θ_{BM}	$\sim 1.05^\circ$
w_1	~ 109 meV
w_0/w_1	[0, 1]
Gate distance	10 nm
Relative permitivity	12
N_y	6
Φ_y	$\pi, \pi/10$
χ	≤ 1024
Δx	10
ϵ_{MPO}	$< 10^{-2}$ meV
Kinetic energy scale (t)	< 1 meV
Interaction energy scale (V)	< 10 meV

Extra Slide: MPO Compression — Technical Comments

- MPO compression is analogous to the MPS case, but distinct.
- We must preserve locality, unlike MPS
- Computing canonical forms is tricky.
- Cannot use the standard transfer matrix technique from MPS's because locality implies that there is no dominant eigenvalue, but instead a Jordan block structure.
- Canonicalization and compression are both $O(\chi^3)$ where χ is the original bond dimension.
- Compression preserves ground state physics.

Proposition: If $\widehat{H}$ has ground state energy E_0 and $\widehat{H}'$ has ground state E_0', then

$$\left|\left|E_0 - E_0'\right|\right| < C\epsilon; \quad \epsilon^2 = \sum_{a=\chi+1}^{\infty} s_a^2$$

under a single-bond truncation for some constant C.

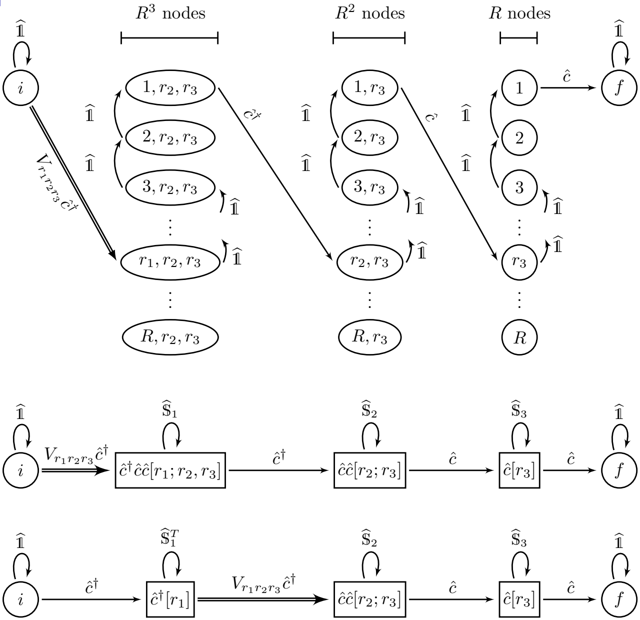
One can show similar bounds for the ground state wavefunction, and expectation values of observables.

Extra Slide: MPO Construction

$$\widehat{H}_{\text{simple}} = \sum_{i<j<k<\ell} V_{ijk\ell} c_i^\dagger c_j^\dagger c_k c_\ell$$

$$\widehat{\mathbb{S}} = \begin{pmatrix} 0 & \widehat{\mathbb{1}} & & & \\ & 0 & \widehat{\mathbb{1}} & & \\ & & \ddots & \ddots & \\ & & & 0 & \widehat{\mathbb{1}} \\ & & & & 0 \end{pmatrix}$$

$$\widehat{\mathbb{S}}_i(\widehat{O}[r_i\ldots]) = (\widehat{O}[r_i - 1\ldots])$$



Extra Slide: MPO Construction II

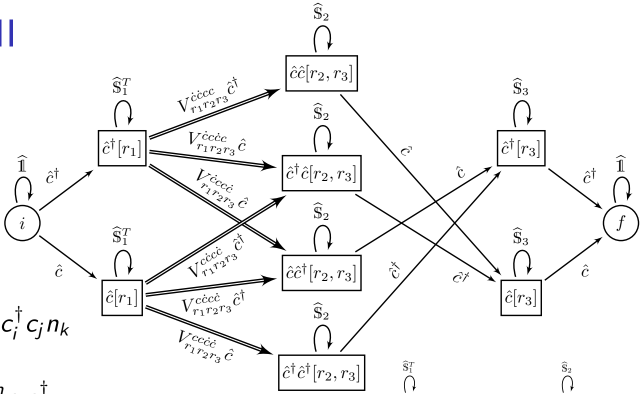
$$H = H_{\text{hop}} + H_{\text{int}} = H_{\text{hop}} + H_2 + H_3 + H_4$$

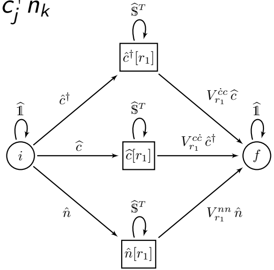
$$H_{\text{hop}} = \sum_{i<j} \tilde{V}_{ij}^{\dot{c}c} c_i^\dagger c_j + \sum_{i<j} \tilde{V}_{ij}^{c\dot{c}} c_i c_j^\dagger$$

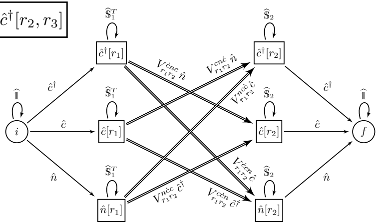
$$H_2 = \sum_{i<j} \tilde{V}_{ij}^{nn} n_i n_j$$

$$H_3 = \sum_{i<j<k} \tilde{V}_{ijk}^{\dot{c}nc} c_i^\dagger n_j c_k + \tilde{V}_{ijk}^{n\dot{c}c} n_i c_j^\dagger c_k + \tilde{V}_{ijk}^{\dot{c}cn} c_i^\dagger c_j n_k + \tilde{V}_{ijk}^{nc\dot{c}} n_i c_j c_k^\dagger + \tilde{V}_{ijk}^{cn\dot{c}} c_i n_j c_k^\dagger + \tilde{V}_{ijk}^{c\dot{c}n} c_i c_j^\dagger n_k$$

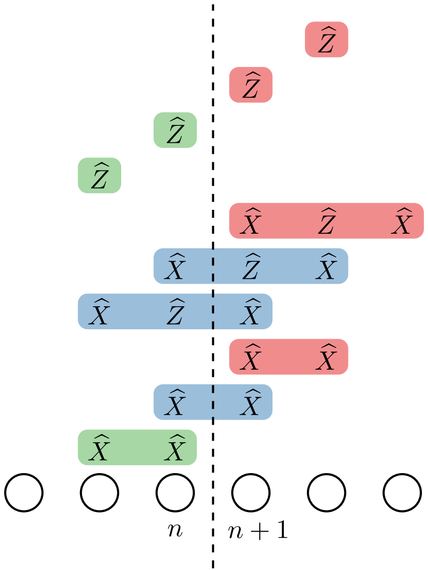
$$H_4 = \sum_{i<j<k<\ell} \tilde{V}_{ijk\ell}^{\dot{c}\dot{c}cc} c_i^\dagger c_j^\dagger c_k c_\ell + \tilde{V}_{ijk\ell}^{\dot{c}c\dot{c}c} c_i^\dagger c_j c_k^\dagger c_\ell + \tilde{V}_{ijk\ell}^{\dot{c}cc\dot{c}} c_i^\dagger c_j c_k c_\ell^\dagger + \tilde{V}_{ijk\ell}^{cc\dot{c}\dot{c}} c_i c_j c_k^\dagger c_\ell^\dagger + \tilde{V}_{ijk\ell}^{c\dot{c}cc} c_i c_j^\dagger c_k c_\ell^\dagger + \tilde{V}_{ijk\ell}^{c\dot{c}\dot{c}c} c_i c_j^\dagger c_k^\dagger c_\ell,$$







Local Operators



Start with a local operator. e.g.

$$\widehat{H} = \sum_i J\widehat{X}_i\widehat{X}_i + K\widehat{X}_i\widehat{Z}_{i+1}\widehat{X}_{i+2} + h\widehat{Z}_i.$$

It is a sum of Pauli strings: $\cdots \widehat{\mathbb{1}}_{-2}\widehat{\mathbb{1}}_{-1}\widehat{X}_0\widehat{X}_1\widehat{\mathbb{1}}_2\widehat{\mathbb{1}}_3\cdots$.
Making a cut gives three categories:

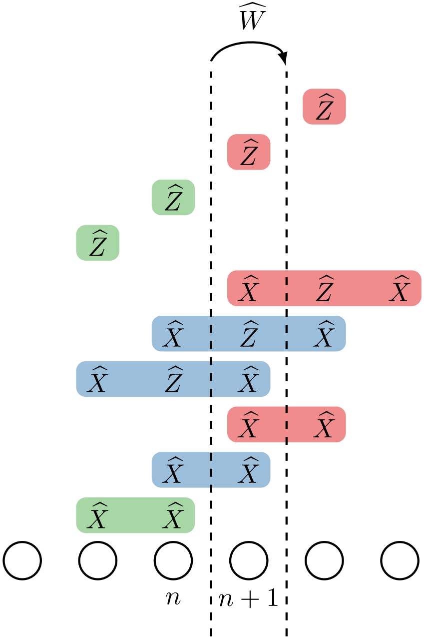
1. Left of the cut
2. Straddling the cut
3. Right of the cut

We can decompose the Hamiltonian as

$$\widehat{H} = \widehat{H}_L\widehat{I}_R + \widehat{I}_L\widehat{H}_R + \sum_{i,j} M_{ij}\hat{h}^i_L\hat{h}^j_R.$$

Matrix Product Operators

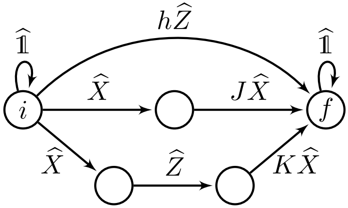
A Matrix Product Operator is a ‘machine’ to place one more site.

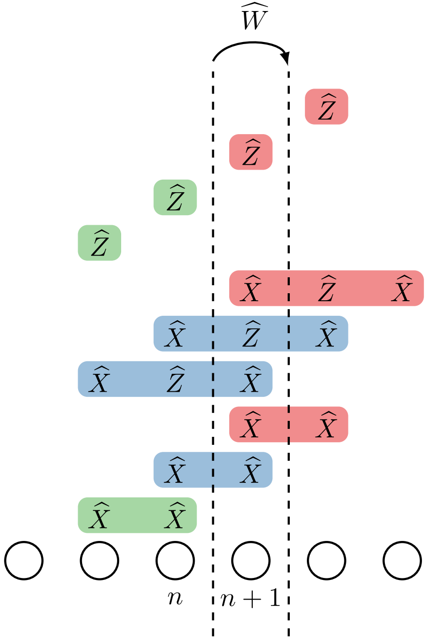


Matrix Product Operators

A Matrix Product Operator is a 'machine' to place one more site.

For $\widehat{H} = \sum_i J\widehat{X}_i\widehat{X}_i + K\widehat{X}_i\widehat{Z}_{i+1}\widehat{X}_{i+2} + h\widehat{Z}_i$,





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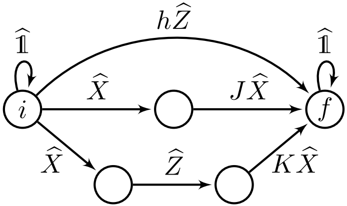


$$\widehat{W} = \left(\begin{array}{c|ccc|c} \widehat{1} & \widehat{X} & \widehat{X} & 0 & h\widehat{Z} \\ \hline & 0 & 0 & 0 & J\widehat{X} \\ & 0 & 0 & \widehat{Z} & 0 \\ & 0 & 0 & 0 & K\widehat{X} \\ \hline & & & & \widehat{1} \end{array}\right)$$

$\Uparrow$ out

$\Longrightarrow$ in

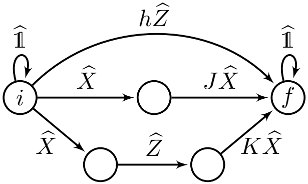
Bond Dimension 5

We can use the graph-matrix correspondence to write this as an operator-valued matrix — a Matrix Product Operator.

The size of the matrix is the bond dimension.

MPOs represent operators

$$\widehat{H} = \sum_i J\widehat{X}_i\widehat{X}_i + K\widehat{X}_i\widehat{Z}_{i+1}\widehat{X}_{i+2} + h\widehat{Z}_i$$

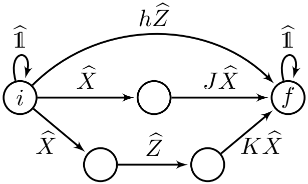


$$\widehat{W} = \left(\begin{array}{c|ccc|c} \widehat{\mathbb{1}} & \widehat{X} & \widehat{X} & 0 & h\widehat{Z} \\ \hline & 0 & 0 & 0 & J\widehat{X} \\ & 0 & 0 & \widehat{Z} & 0 \\ & 0 & 0 & 0 & K\widehat{X} \\ \hline & & & & \widehat{\mathbb{1}} \end{array}\right)$$

$$\boldsymbol{v}_L = \left[\begin{array}{c} 1 \\ \hline 0 \\ 0 \\ 0 \\ \hline 0 \end{array}\right]^T$$

MPOs represent operators

$$\widehat{H} = \sum_i J\widehat{X}_i\widehat{X}_i + K\widehat{X}_i\widehat{Z}_{i+1}\widehat{X}_{i+2} + h\widehat{Z}_i$$

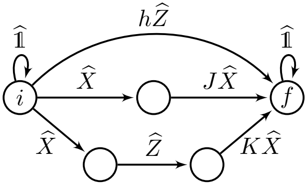


$$\widehat{W} = \left(\begin{array}{c|ccc|c} \widehat{\mathbb{1}} & \widehat{X} & \widehat{X} & 0 & h\widehat{Z} \\ \hline & 0 & 0 & 0 & J\widehat{X} \\ & 0 & 0 & \widehat{Z} & 0 \\ & 0 & 0 & 0 & K\widehat{X} \\ \hline & & & & \widehat{\mathbb{1}} \end{array}\right)$$

$$\boldsymbol{v}_L \widehat{W}^{(1)} = \left[\begin{array}{c} I_L \\ \hline \widehat{X}_1 \\ \widehat{X}_1 \\ 0 \\ \hline h\widehat{Z}_1 \end{array}\right]^T$$

MPOs represent operators

$$\widehat{H} = \sum_i J\widehat{X}_i\widehat{X}_i + K\widehat{X}_i\widehat{Z}_{i+1}\widehat{X}_{i+2} + h\widehat{Z}_i$$

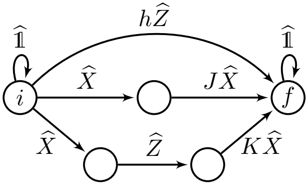


$$\widehat{W} = \left(\begin{array}{c|ccc|c} \widehat{\mathbb{1}} & \widehat{X} & \widehat{X} & 0 & h\widehat{Z} \\ \hline & 0 & 0 & 0 & J\widehat{X} \\ & 0 & 0 & \widehat{Z} & 0 \\ & 0 & 0 & 0 & K\widehat{X} \\ \hline & & & & \widehat{\mathbb{1}} \end{array}\right)$$

$$\boldsymbol{v}_L \widehat{W}^{(1)} \widehat{W}^{(2)} = \left[\begin{array}{l} I_L \\ \hline \widehat{X}_2 \\ \widehat{X}_2 \\ \widehat{X}_1\widehat{Z}_2 \\ \hline h\widehat{Z}_1 + h\widehat{Z}_1 + J\widehat{X}_1\widehat{X}_2 \end{array}\right]^T$$

MPOs represent operators

$$\widehat{H} = \sum_i J\widehat{X}_i\widehat{X}_i + K\widehat{X}_i\widehat{Z}_{i+1}\widehat{X}_{i+2} + h\widehat{Z}_i$$



$$\widehat{W} = \left(\begin{array}{c|ccc|c} \widehat{\mathbb{1}} & \widehat{X} & \widehat{X} & 0 & h\widehat{Z} \\ \hline & 0 & 0 & 0 & J\widehat{X} \\ & 0 & 0 & \widehat{Z} & 0 \\ & 0 & 0 & 0 & K\widehat{X} \\ \hline & & & & \widehat{\mathbb{1}} \end{array}\right)$$

$$\boldsymbol{v}_L \widehat{W}^{(1)}\widehat{W}^{(2)}\widehat{W}^{(3)} = \left[\begin{array}{c} \widehat{\mathbb{1}} \\ \hline \widehat{X}_3 \\ \widehat{X}_3 \\ \widehat{X}_2\widehat{Z}_3 \\ \hline h\widehat{Z}_1 + h\widehat{Z}_2 + h\widehat{Z}_3 + J\widehat{X}_1\widehat{X}_2 + J\widehat{X}_2\widehat{X}_3 + K\widehat{X}_1\widehat{Z}_2\widehat{X}_3 \end{array}\right]^T$$

MPOs represent operators

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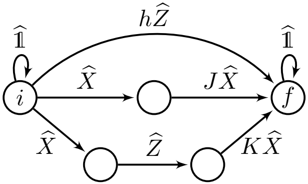

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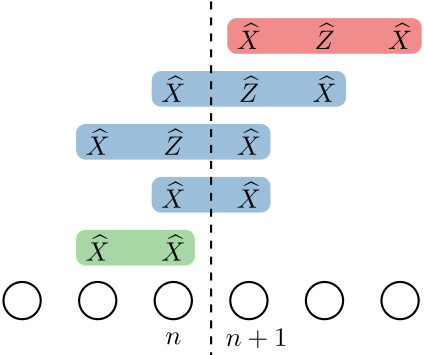
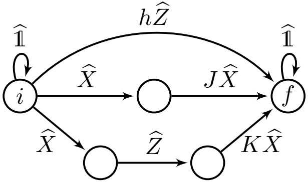
$$\boldsymbol{v}_L \widehat{W}^{(1)} \ldots \widehat{W}^{(n)} = \begin{bmatrix} \widehat{I}_L \\ \hline \widehat{\boldsymbol{h}}_L \\ \hline \widehat{H}_L \end{bmatrix}^T \begin{array}{l} \longleftarrow \text{Unstarted} \\ \longleftarrow \text{Split} \\ \longleftarrow \text{Placed} \end{array}$$



MPOs represent operators

$$\widehat{H} = \sum_i J\widehat{X}_i\widehat{X}_i + K\widehat{X}_i\widehat{Z}_{i+1}\widehat{X}_{i+2} + h\widehat{Z}_i$$



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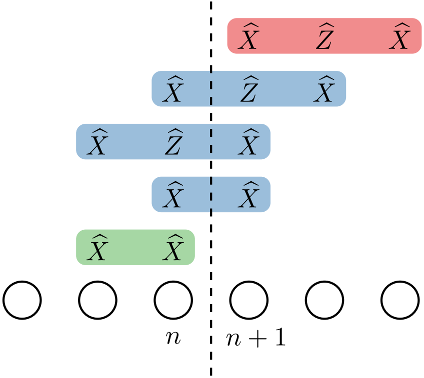
$$\boldsymbol{v}_L \widehat{W}^{(1)} \dots \widehat{W}^{(n)} = \begin{bmatrix} \widehat{I}_L \\ \hline \widehat{\boldsymbol{h}}_L \\ \hline \widehat{H}_L \end{bmatrix}^T$$

$\longleftarrow$ Unstarted

$\longleftarrow$ Split

$\longleftarrow$ Placed

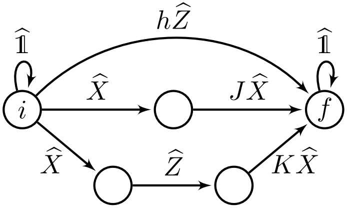


$$\widehat{H} = \boldsymbol{v}_L \widehat{W}^{(1)} \widehat{W}^{(2)} \dots \widehat{W}^{(N)} \boldsymbol{v}_R \quad \text{where} \quad \boldsymbol{v}_R = \begin{bmatrix} 0 \\ \hline 0 \\ \hline 1 \end{bmatrix}^T$$

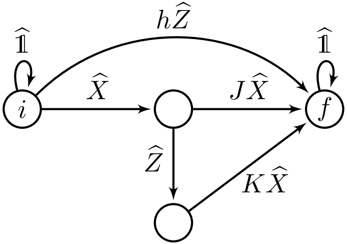
Gauge Transforms

Many MPOs represent the same Hamiltonian.

$$\begin{aligned}\widehat{H} &= \cdots \widehat{W}^{(n)}\widehat{W}^{(n+1)}\cdots \\ &= \cdots (GG^{-1})\widehat{W}^{(n)}(GG^{-1})\widehat{W}^{(n+1)}(GG^{-1})\cdots \\ &= \cdots (G^{-1}\widehat{W}^{(n)}G)(G^{-1}\widehat{W}^{(n+1)}G)\cdots \\ &= \cdots \widehat{W}'^{(n)}\widehat{W}'^{(n+1)}\cdots\end{aligned}$$



where $\widehat{W}' = G^{-1}\widehat{W}G$, $GG^{-1} = I$. This is a gauge choice. What gauge is best?



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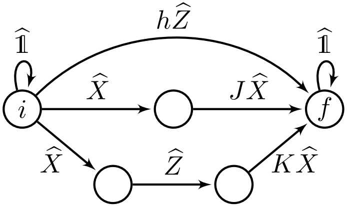
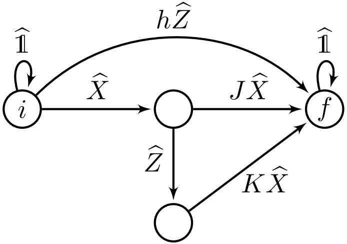


where $\widehat{W}' = G^{-1}\widehat{W}G$, $GG^{-1} = I$. This is a gauge choice. What gauge is best?

Compression Problem: Given $\widehat{H}$, what is the optimal MPO (best approximation) $\widehat{W}$ at bond dim. χ?



Almost Schmidt Decompositions

A state split into left (L) and right (R)

$$|\psi\rangle = \sum_{i,j} M_{ij} |\psi_L^i\rangle |\psi_R^j\rangle$$

can always be put in Schmidt form

$$|\psi\rangle = \sum_{a=1} s_a |\phi_L^a\rangle |\phi_R^a\rangle$$

with $\langle\phi_L^a|\phi_L^b\rangle = \delta^{ab} = \langle\phi_R^a|\phi_R^b\rangle$.

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$$|\psi'\rangle = \sum_{a=1}^{\chi} s_a |\phi_L^a\rangle |\phi_R^a\rangle$$

is the "optimal" rank-χ approximation.

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is the "optimal" rank-χ approximation.

A local operator

$$\widehat{H} = \widehat{H}_L \widehat{I}_R + \widehat{I}_L \widehat{H}_R + \sum_{i,j} M_{i,j} \hat{h}_L^i \hat{h}_R^j$$

can be put in almost-Schmidt form

$$\widehat{H} = \widehat{H}_L \widehat{I}_R + \widehat{I}_L \widehat{H}_R + \sum_{a=1} s_a \hat{\mathcal{O}}_L^a \hat{\mathcal{O}}_R^a$$

with $(\hat{\mathcal{O}}_L^a|\hat{\mathcal{O}}_L^b) = \delta^{ab} = (\hat{\mathcal{O}}_R^a|\hat{\mathcal{O}}_R^b)$.

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with $(\hat{\mathcal{O}}_L^a|\hat{\mathcal{O}}_L^b) = \delta^{ab} = (\hat{\mathcal{O}}_R^a|\hat{\mathcal{O}}_R^b)$. Then

$$\widehat{H}' = \widehat{H}_L \widehat{I}_R + \widehat{I}_L \widehat{H}_R + \sum_{a=1}^{\chi} s_a \hat{\mathcal{O}}_L^a \hat{\mathcal{O}}_R^a$$

is the "optimal" rank-χ approximation that *preserves locality*.

MPO Compression Algorithm

How do we *compute* the almost-Schmidt form with MPOs?

MPO Compression Algorithm

How do we *compute* the almost-Schmidt form with MPOs?

$$\widehat{H} = \widehat{H}_L \widehat{I}_R + \widehat{I}_L \widehat{H}_R + \sum_{i,j} M_{i,j} \hat{h}_L^i \hat{h}_R^j$$

$$= \left[\ \widehat{I}_L \ \middle|\ \widehat{\boldsymbol{h}}_L \ \middle|\ \widehat{H}_L\ \right] \begin{bmatrix} 1 & & \\ & M & \\ & & 1 \end{bmatrix} \begin{bmatrix} \widehat{H}_R \\ \hline \widehat{\boldsymbol{h}}_R \\ \hline \widehat{I}_R \end{bmatrix}$$

$$= \cdots \widehat{W}_L \widehat{W}_L \widehat{W}_L \ \mathcal{M} \ \widehat{W}_R \widehat{W}_R \widehat{W}_R \cdots$$

MPO Compression Algorithm

How do we *compute* the almost-Schmidt form with MPOs?

$$\widehat{H} = \widehat{H}_L \widehat{I}_R + \widehat{I}_L \widehat{H}_R + \sum_{i,j} M_{i,j} \hat{h}_L^i \hat{h}_R^j$$

$$= \left[\begin{array}{c|c|c} \widehat{I}_L & \widehat{\boldsymbol{h}}_L & \widehat{H}_L \end{array}\right] \begin{bmatrix} 1 & & \\ & M & \\ & & 1 \end{bmatrix} \left[\begin{array}{c} \widehat{H}_R \\ \hline \widehat{\boldsymbol{h}}_R \\ \hline \widehat{I}_R \end{array}\right]$$

$$= \cdots \widehat{W_L} \widehat{W_L} \widehat{W_L} \; \mathcal{M} \; \widehat{W_R} \widehat{W_R} \widehat{W_R} \cdots$$

SVD $\mathcal{M} = USV^\dagger$ with $S = \mathrm{diag}(s_a)$, and let $\widehat{W_L'} := U^\dagger \widehat{W_L} U$, $\widehat{W_R'} := V^\dagger \widehat{W_R} V$.

MPO Compression Algorithm

How do we *compute* the almost-Schmidt form with MPOs?

$$\widehat{H} = \widehat{H}_L \widehat{I}_R + \widehat{I}_L \widehat{H}_R + \sum_{i,j} M_{i,j} \hat{h}_L^i \hat{h}_R^j$$

$$= \left[\begin{array}{c|c|c} \widehat{I}_L & \hat{\boldsymbol{h}}_L & \widehat{H}_L \end{array} \right] \begin{bmatrix} 1 & & \\ & M & \\ & & 1 \end{bmatrix} \left[\begin{array}{c} \widehat{H}_R \\ \hline \hat{\boldsymbol{h}}_R \\ \hline \widehat{I}_R \end{array} \right]$$

$$= \cdots \widehat{W}_L \widehat{W}_L \widehat{W}_L \ \mathcal{M} \ \widehat{W}_R \widehat{W}_R \widehat{W}_R \cdots$$

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$$\widehat{H} = \cdots \widehat{W}_L' \widehat{W}_L' \widehat{W}_L' \ S \ \widehat{W}_R' \widehat{W}_R' \widehat{W}_R' \cdots$$

is an almost-Schmidt decomposition.

Algorithm 5 iMPO Compression

1: **procedure** ICOMPRESS($\widehat{W}, \eta$) ▷ Cutoff η
2: $\widehat{W}_R \leftarrow$ RIGHTCAN$[\widehat{W}]$
3: $\widehat{W}_R \leftarrow R\widehat{W}_R R^{-1}$ so that $[\widehat{W}_R]_{1a} = 0$
4: $\widehat{W}_L, C \leftarrow$ LEFTCAN$[\widehat{W}_R]$
5: $(U, S, V^\dagger) \leftarrow$ SVD$[C]$
6: $\widehat{Q}, \widehat{P} \leftarrow U^\dagger \widehat{W}_L U \,,\ V^\dagger \widehat{W}_R V$
7: $\chi' \leftarrow \max\{a \in [1, \chi] : s_a > \eta\}$ ▷ Defines $\mathbb{P}$
8: $\widehat{W}_L'', S, \widehat{W}_R'' \leftarrow \mathbb{P}^\dagger \widehat{W}_L' \mathbb{P}, \mathbb{P}^\dagger S \mathbb{P}, \mathbb{P}^\dagger \widehat{W}_R' \mathbb{P}$
9: **return** $\widehat{W}_L''$ ▷ One could also return $\widehat{W}_R''$.

MPO Compression Algorithm

How do we *compute* the almost-Schmidt form with MPOs?

$$\hat{H} = \hat{H}_L \hat{I}_R + \hat{I}_L \hat{H}_R + \sum_{i,j} M_{i,j} \hat{h}_L^i \hat{h}_R^j$$

$$= \left[\ \hat{I}_L \ \middle|\ \hat{\boldsymbol{h}}_L \ \middle|\ \hat{H}_L \ \right] \begin{bmatrix} 1 & & \\ & M & \\ & & 1 \end{bmatrix} \begin{bmatrix} \hat{H}_R \\ \hline \hat{\boldsymbol{h}}_R \\ \hline \hat{I}_R \end{bmatrix}$$

$$= \cdots \widehat{W}_L \widehat{W}_L \widehat{W}_L \ \mathcal{M} \ \widehat{W}_R \widehat{W}_R \widehat{W}_R \cdots$$

SVD $\mathcal{M} = USV^\dagger$ with $S = \mathrm{diag}(s_a)$, and let $\widehat{W}'_L := U^\dagger \widehat{W}_L U$, $\widehat{W}'_R := V^\dagger \widehat{W}_R V$.Then

$$\hat{H} = \cdots \widehat{W}'_L \widehat{W}'_L \widehat{W}'_L \ S \ \widehat{W}'_R \widehat{W}'_R \widehat{W}'_R \cdots$$

is an almost-Schmidt decomposition.

Algorithm 6 iMPO Compression

```
1: procedure ICOMPRESS(Ŵ, η)                                ▷ Cutoff η
2:     Ŵ_R ← RIGHTCAN[Ŵ]
3:     Ŵ_R ← R Ŵ_R R^{-1} so that [Ŵ_R]_{1a} = 0
4:     Ŵ_L, C ← LEFTCAN[Ŵ_R]
5:     (U, S, V†) ← SVD[C]
6:     Q̂, P̂ ← U† Ŵ_L U , V† Ŵ_R V
7:     χ' ← max{a ∈ [1, χ] : s_a > η}                       ▷ Defines ℙ
8:     Ŵ''_L, S, Ŵ''_R ← ℙ† Ŵ'_L ℙ, ℙ† S ℙ, ℙ† Ŵ'_R ℙ
9:     return Ŵ''_L                          ▷ One could also return Ŵ''_R.
```

Physically, the singular values s_a fall off (exponentially) quickly, so we can chop off the small ones.

Upshot: practical algorithm to greatly reduce bond dimension of an MPO.