Title: Efficient simulation of magic angle twisted bilayer graphene using the density matrix renormalization group

Speakers: Daniel Parker

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Abstract: Twisted bilayer graphene (tBLG) is a host to a variety of electronic phases, most notably superconductivity when doped away from putative correlated insulator phases. In order to understand the nature of those phases, numerical simulations such as Hartree-Fock calculation and density matrix renormalization group (DMRG) techniques are essential.

Due to the long-range Coulomb interaction and its fragile topology, however, tBLG is difficult to study with standard DMRG techniques.

In this work, we present how a recently developed MPO compression algorithm can be used to make the problem tractable, and how 1D Wannier localization can be used to circumvent the fragile topology.

As a test case, we apply this technique to the toy model of spinless/single-valley model of tBLG. We find that the ground state is essentially a k-space Slater determinant, confirming the validity of previous Hartree-Fock calculations. If time permits, I will also present our ongoing effort to apply this technique to spinful/valleyful model for tBLG.

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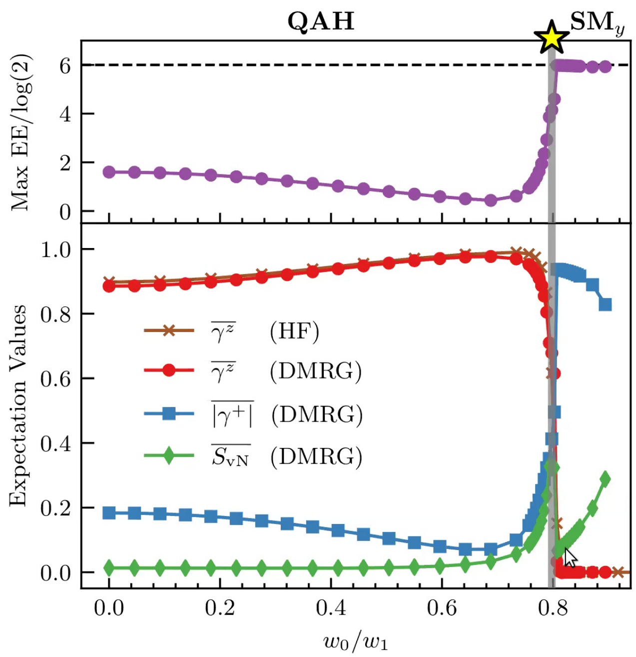
DMRG for Bilayer Graphene



arXiv: 1909.06341

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arXiv: 2009.02354

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Acknowledgements

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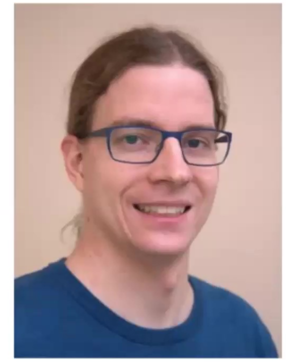

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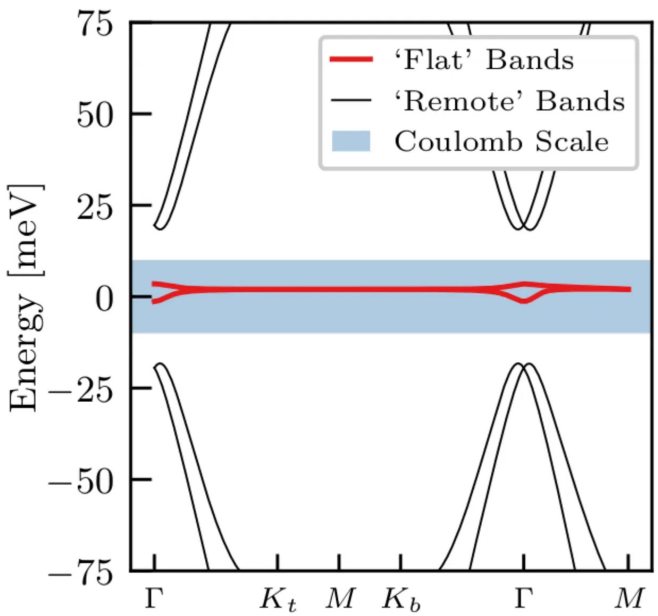
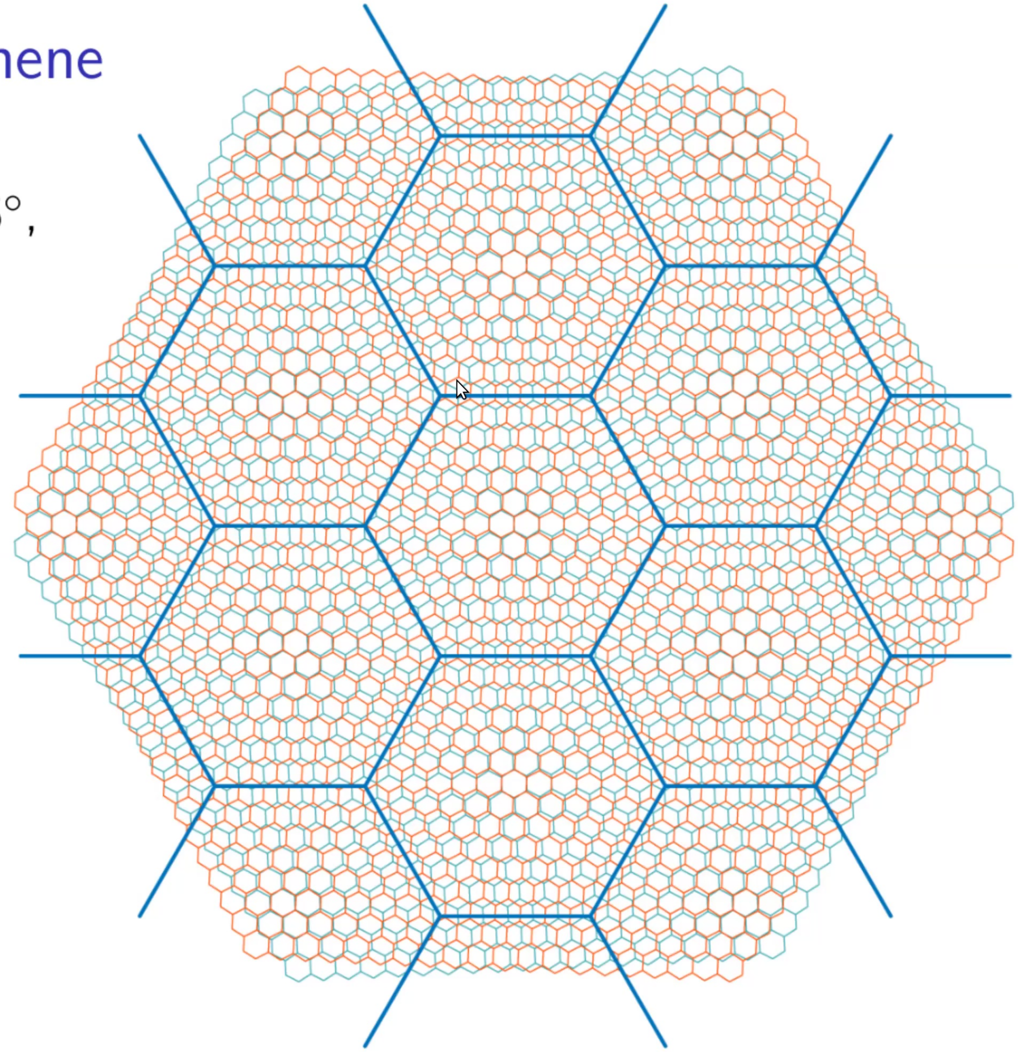
Outline

1. One Way to Simulate tBLG
2. Matrix Product Operators & 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

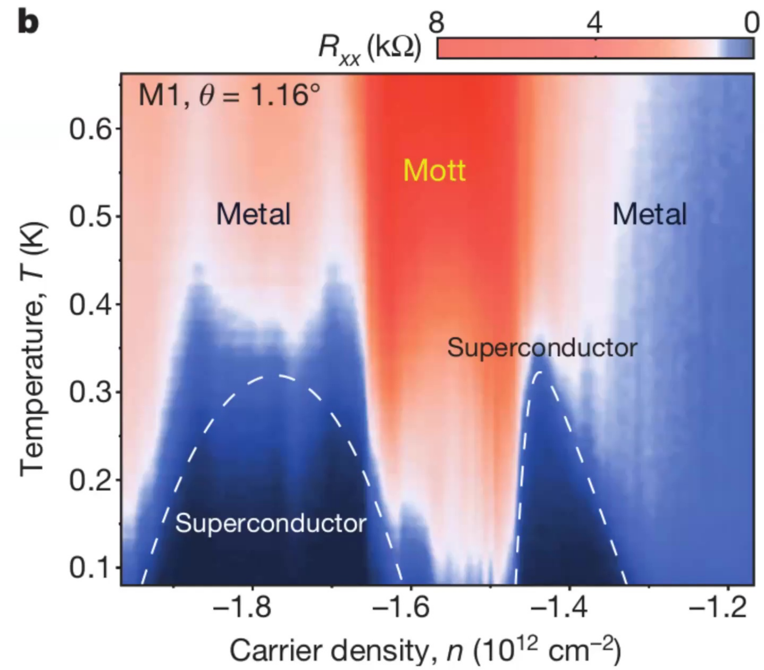
tBLG hosts many intriguing phases

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

  ⋮

- superconductivity

Roughly 1 zillion theory papers with various mechanisms.



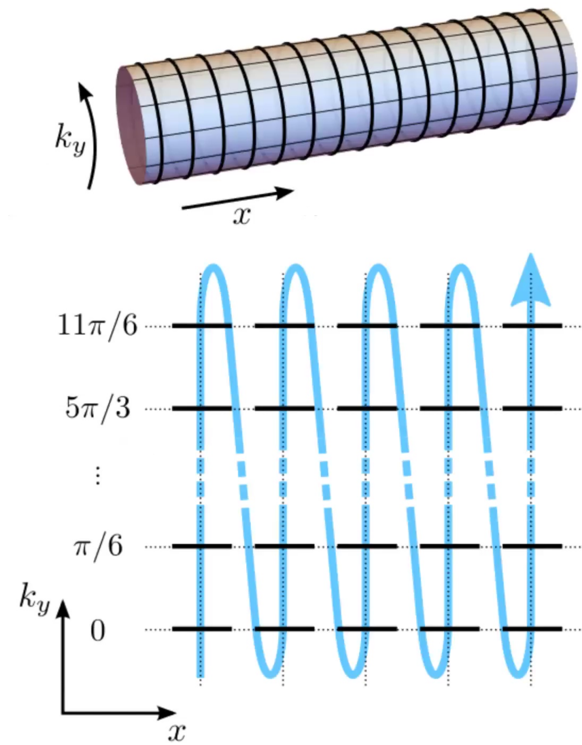
> **Goal**: compute the ground state with unbiased, non-perturbative numerics.

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

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

Density 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).

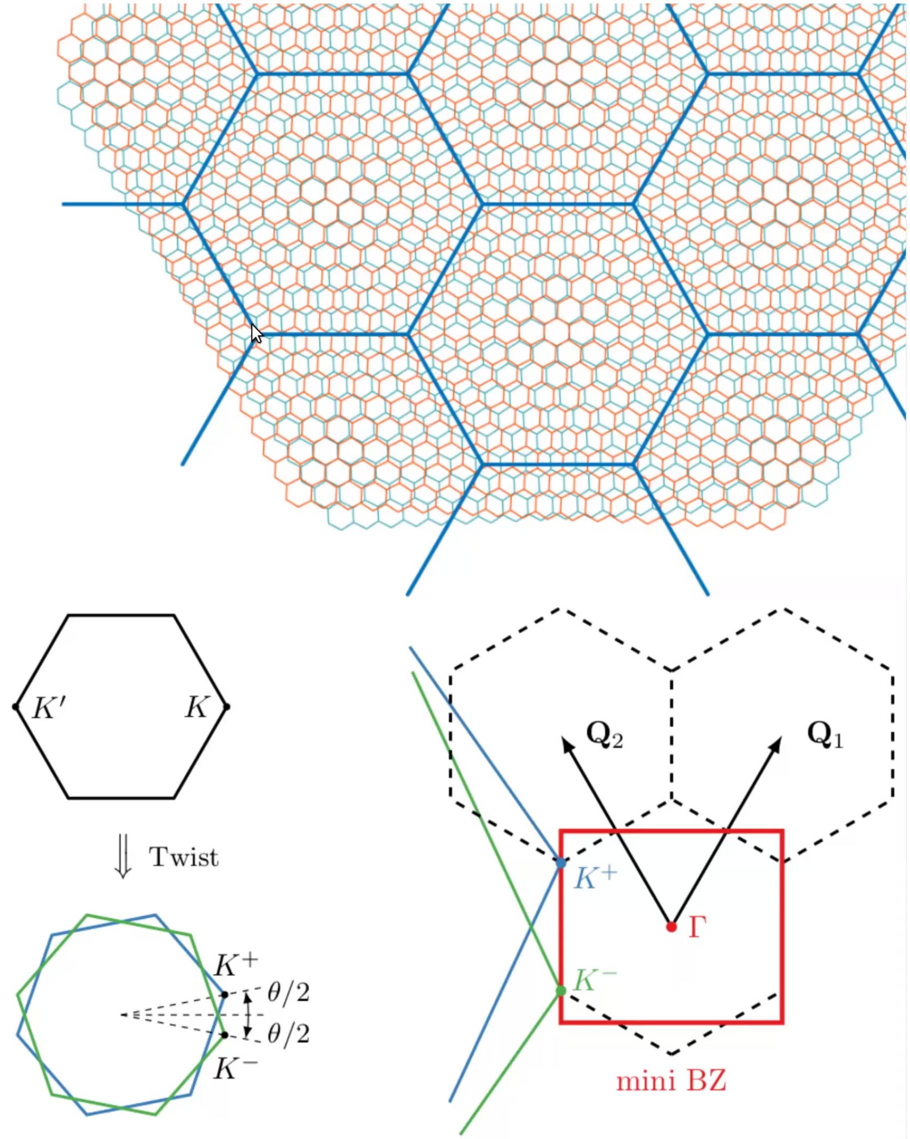


White (1992); Pirvu, Murg, Cirac, Verstraete (2010); etc. Figure from Motruk, Zaletel, Mong, Pollmann (2015)

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 $\gg$ moiré (mini) BZ.



Bistritzer, MacDonald (2011); etc

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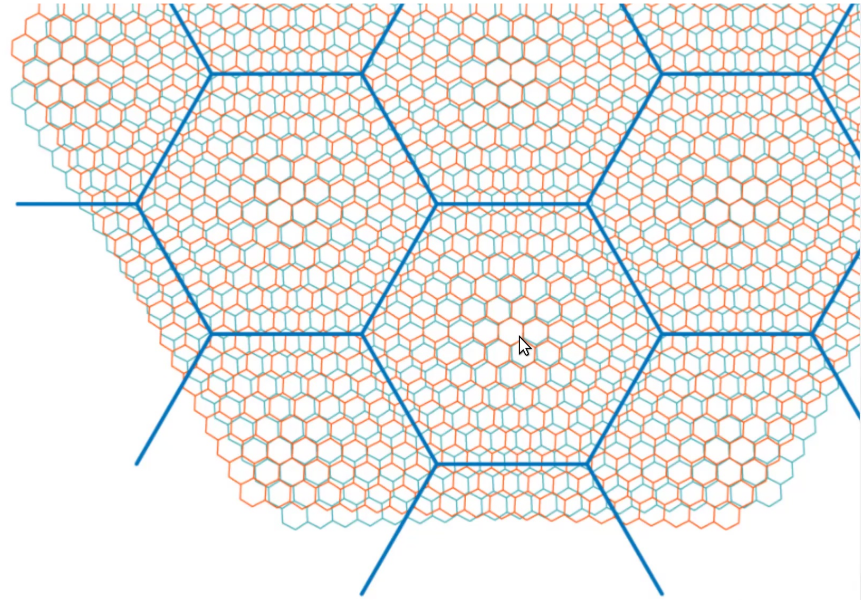
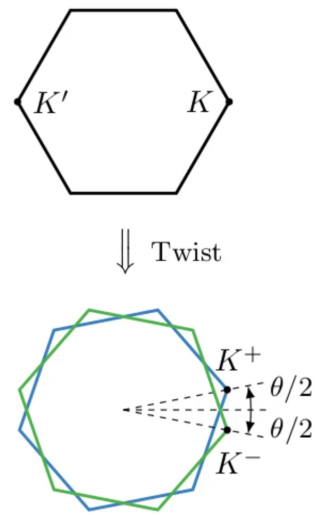
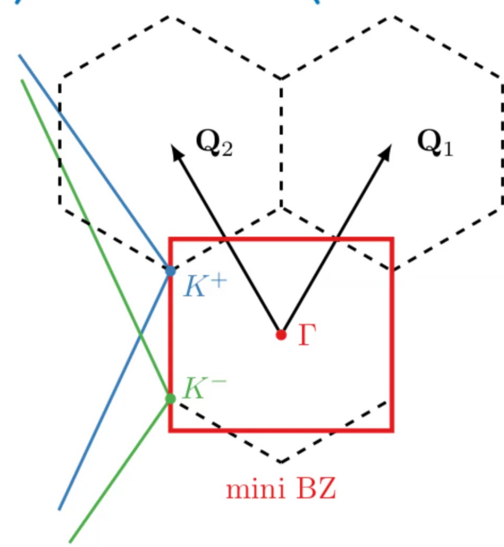
$$\widehat{H}_{\mathrm{BM}} = \underbrace{\widehat{H}_{\mathrm{MLG}}(\theta)}_{\text{top layer}} + \underbrace{\widehat{H}_{MLG}(-\theta)}_{\text{bottom layer}} + \underbrace{\widehat{T}}_{\text{interlayer tunneling}}$$

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

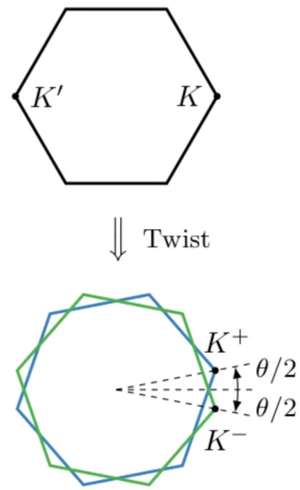
Bistritzer, MacDonald (2011); etc

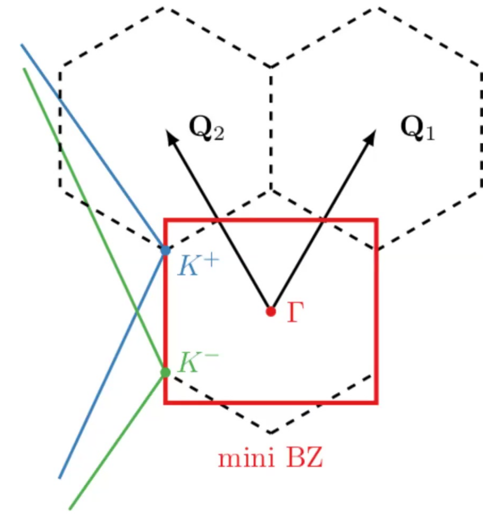






The "IBM" Model





Interacting Bistritzer-MacDonald (IBM) model:

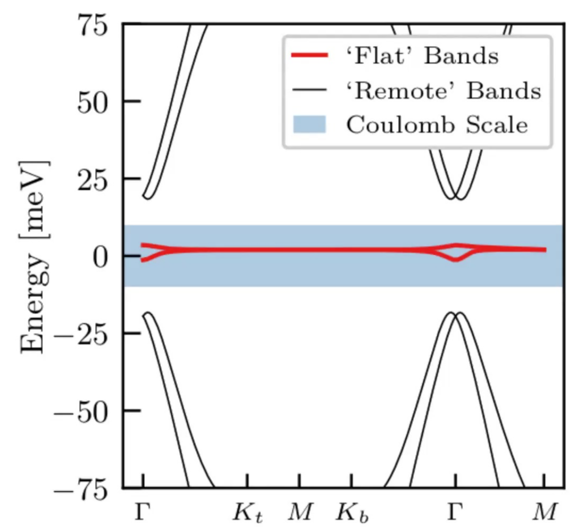
- start with the BM model $h(\boldsymbol{k})$
- add gate-screened Coulomb interactions

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

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

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

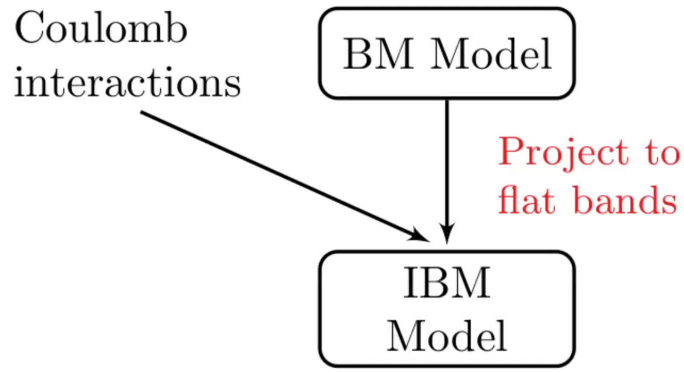
$d \approx 10\,\text{nm}$ is gate distance, $\epsilon_R \approx 12$ is permitivity



Can we compute the ground state?

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

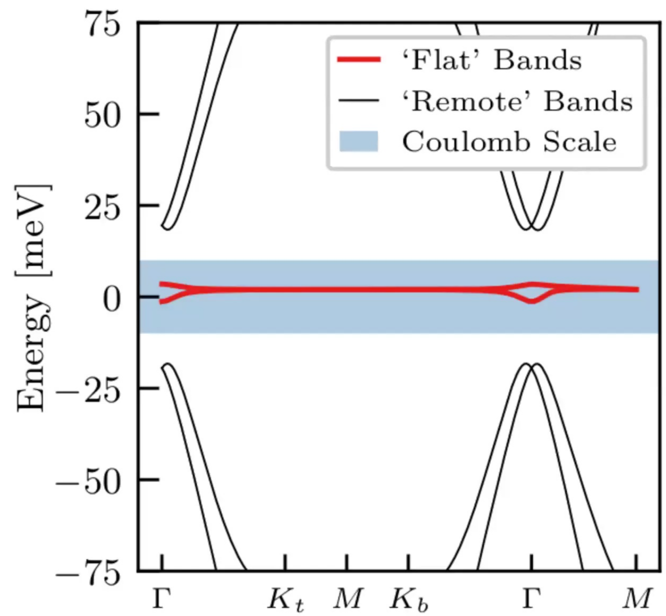
Projection to Narrow Bands



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

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

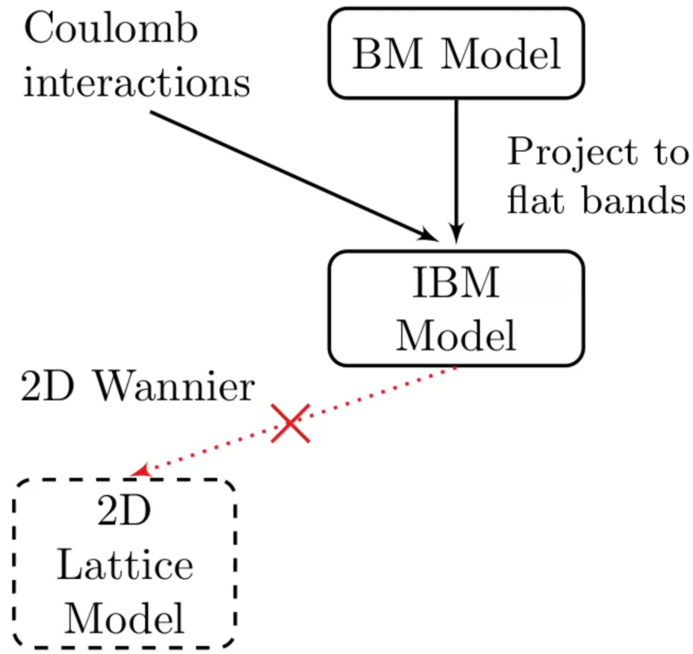
- Kinetic scale (bandwidth of flat bands): $t \approx 1\,\mathrm{meV}$
- Interaction scale (Coulomb): $V \approx 10\,\mathrm{meV}$
- Band gap: $\Delta E \approx 25\,\mathrm{meV}$
- $t \ll V < \Delta E \implies$ Projection is perturbatively valid.
- Now 8 fermions/moiré unit cell
  - 2 bands
  - K and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

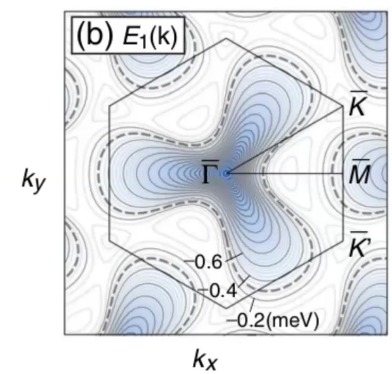


Topological Obstruction to 2D Wannierization

- Most numerical methods require a discrete lattice
- Straightforward solution: find localized Wannier orbitals via Fourier transform.
- Topological obstruction: cannot have both
  1. Localized 2D Wannier orbitals
  2. Local action of $U_v(1)$ and $C_2\mathcal{T}$
- Solution I: let symmetry act non-locally
  - "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!
- Solution II: increase $8 \to 20$ bands
  - Top. obstruction is "fragile"
  - computationally infeasible

Is there a better solution for DMRG?



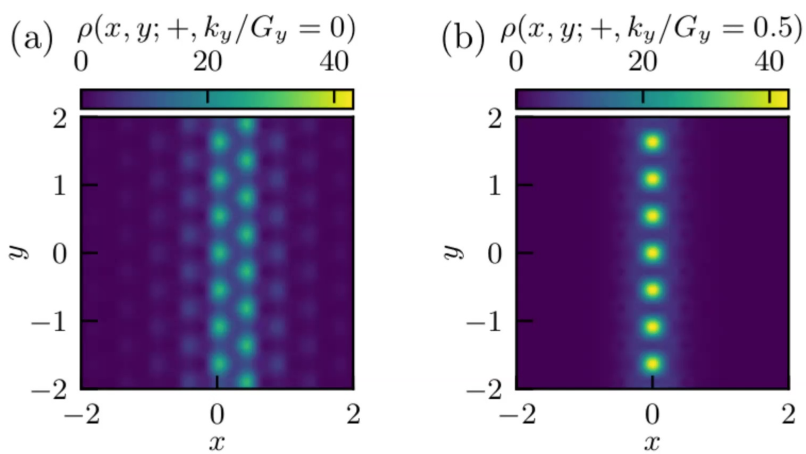


Zou, Po, Vishwanath, Senthil (2018, 2018, 2019); Song, Wang, Shi, Li, Fang, Bernevig (2019); Ahn, Park, Yang (2019); Kang, Vafek (2018); Koshino, Yuan, Koretsune, Ochi, Kuroki, Fu (2018); etc

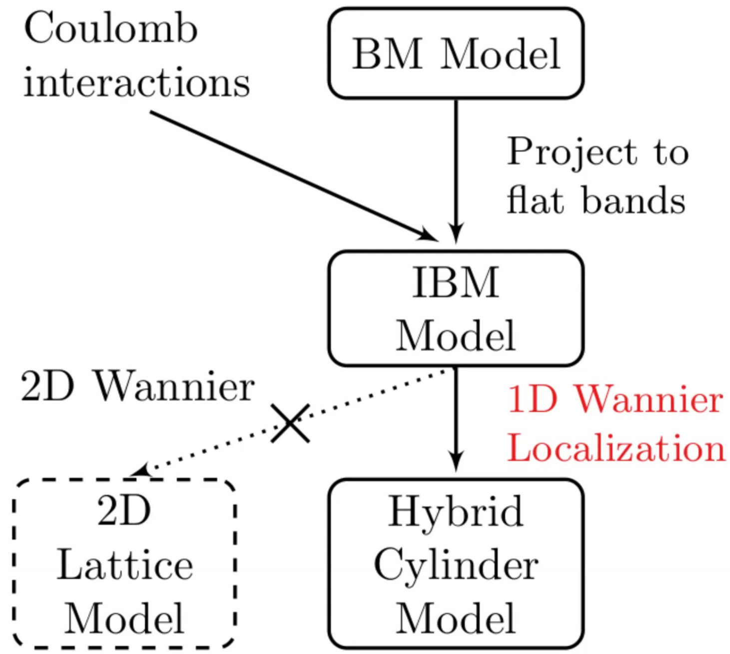
1D Wannier Localization

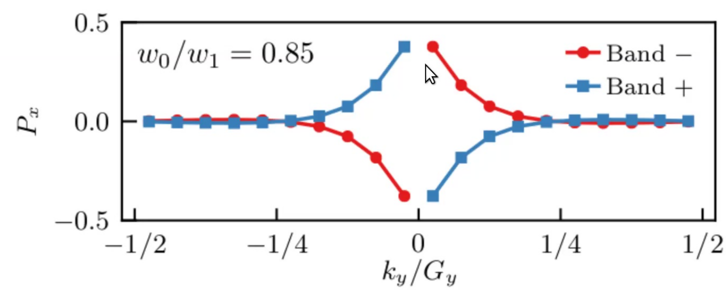
Hybrid xk Wannier orbitals: localize along x, periodic along y

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

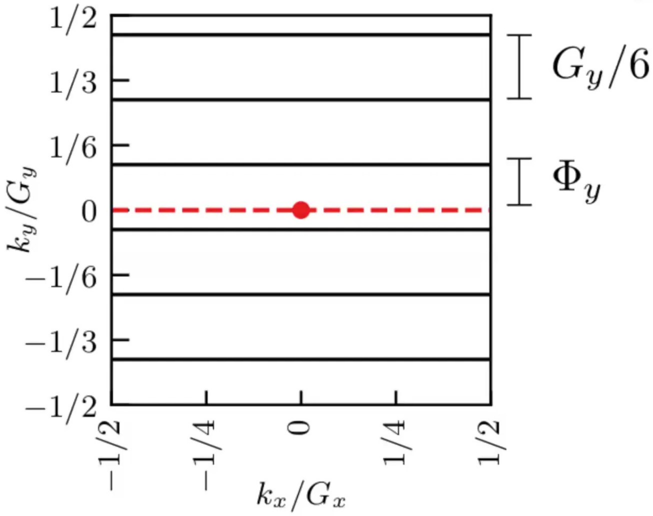


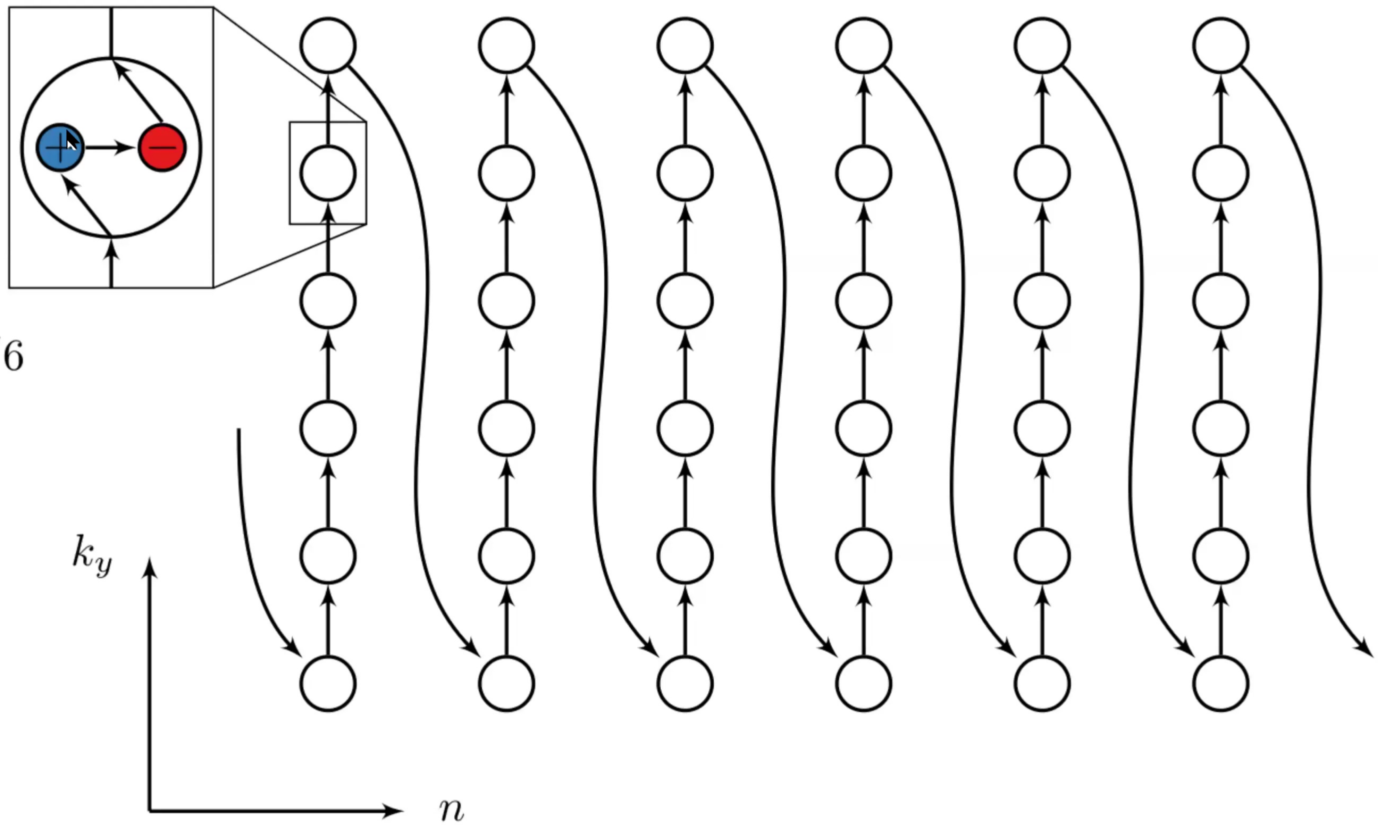
Bands labelled by Chern number $C = \int dk_y \, \frac{dP_x}{dk_y} = \pm 1$.





Hybrid Cylinder Model





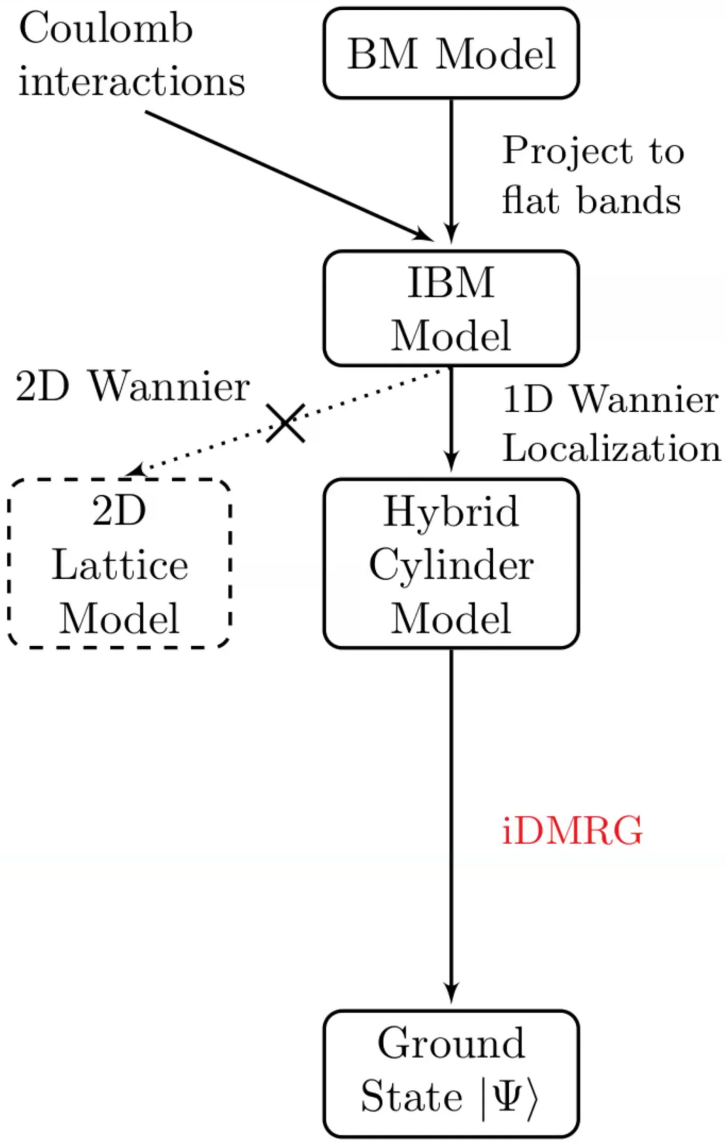
$$w^\dagger_{\pm,n,k_y} = \sum_{b \in \text{ flat bands}} \int [dk_x]\, U_{\pm,b}\, e^{i\boldsymbol{k}\cdot\boldsymbol{R}_n} \hat{f}^\dagger_{b,\boldsymbol{k}}.$$

Infinite 2D DMRG

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

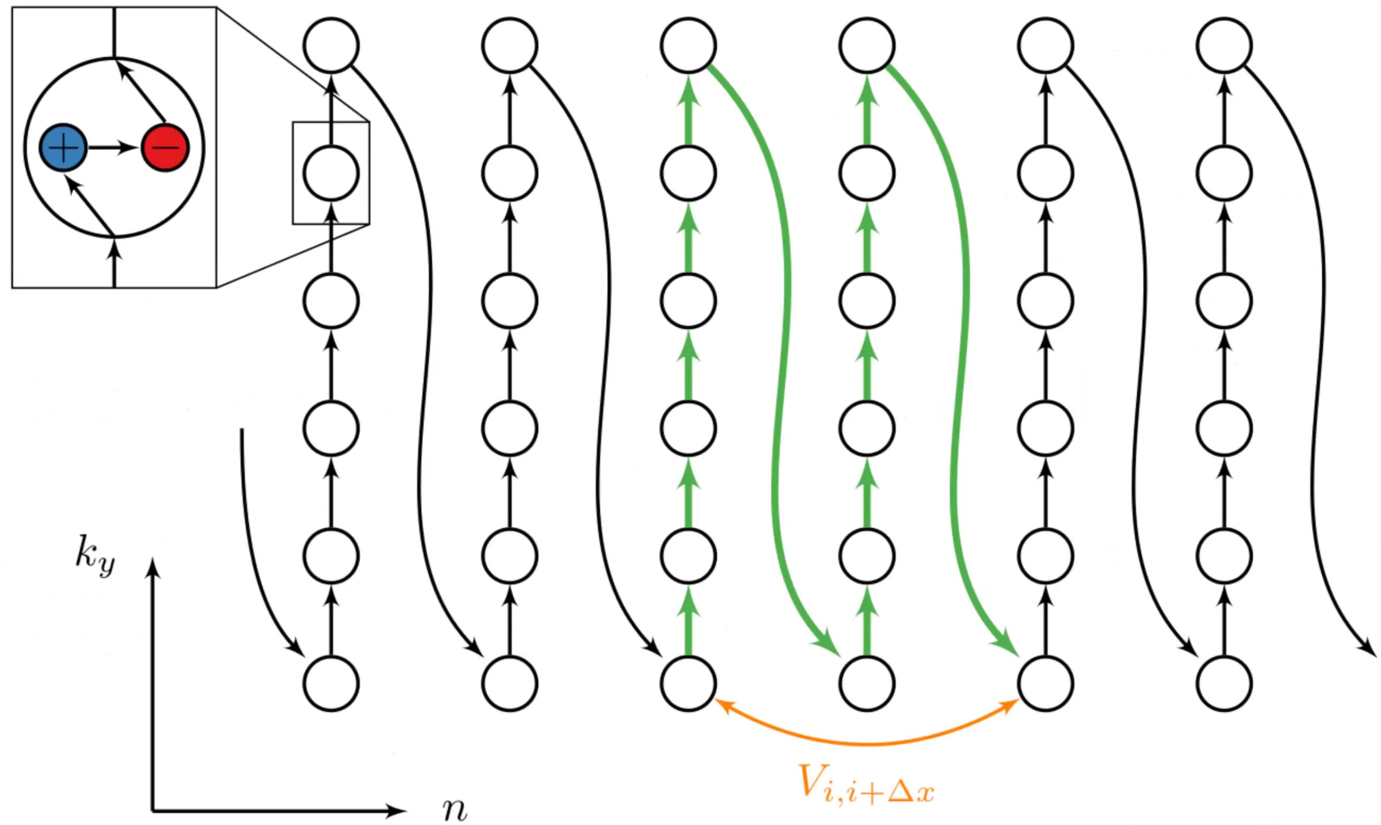
$$H_{\text{cyl}} = \mathrm{FT}_x \left[\mathcal{P}^\dagger [H_{\text{BM}} + H_{\text{Coulomb}}] \mathcal{P} \right]$$

- 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"



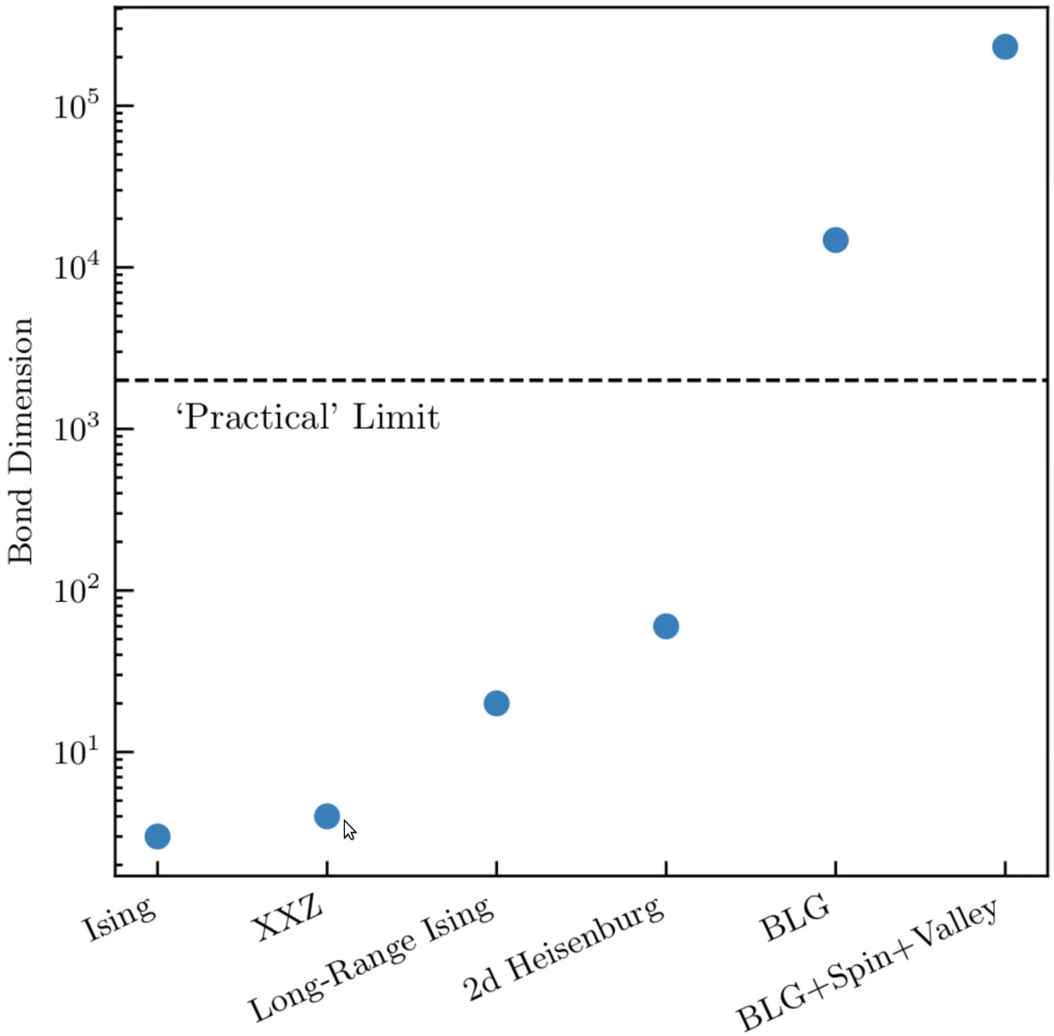
Kang, Vafek (arXiv: 2002.10360); https://tenpy.readthedocs.io/

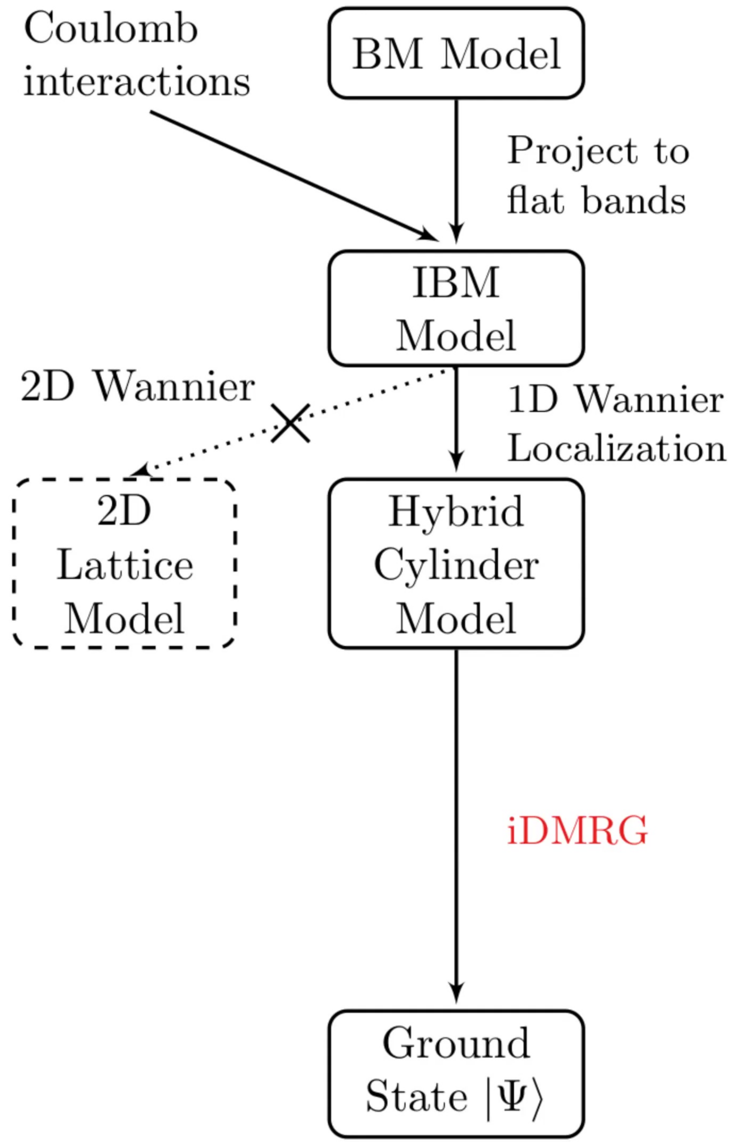
Long Range



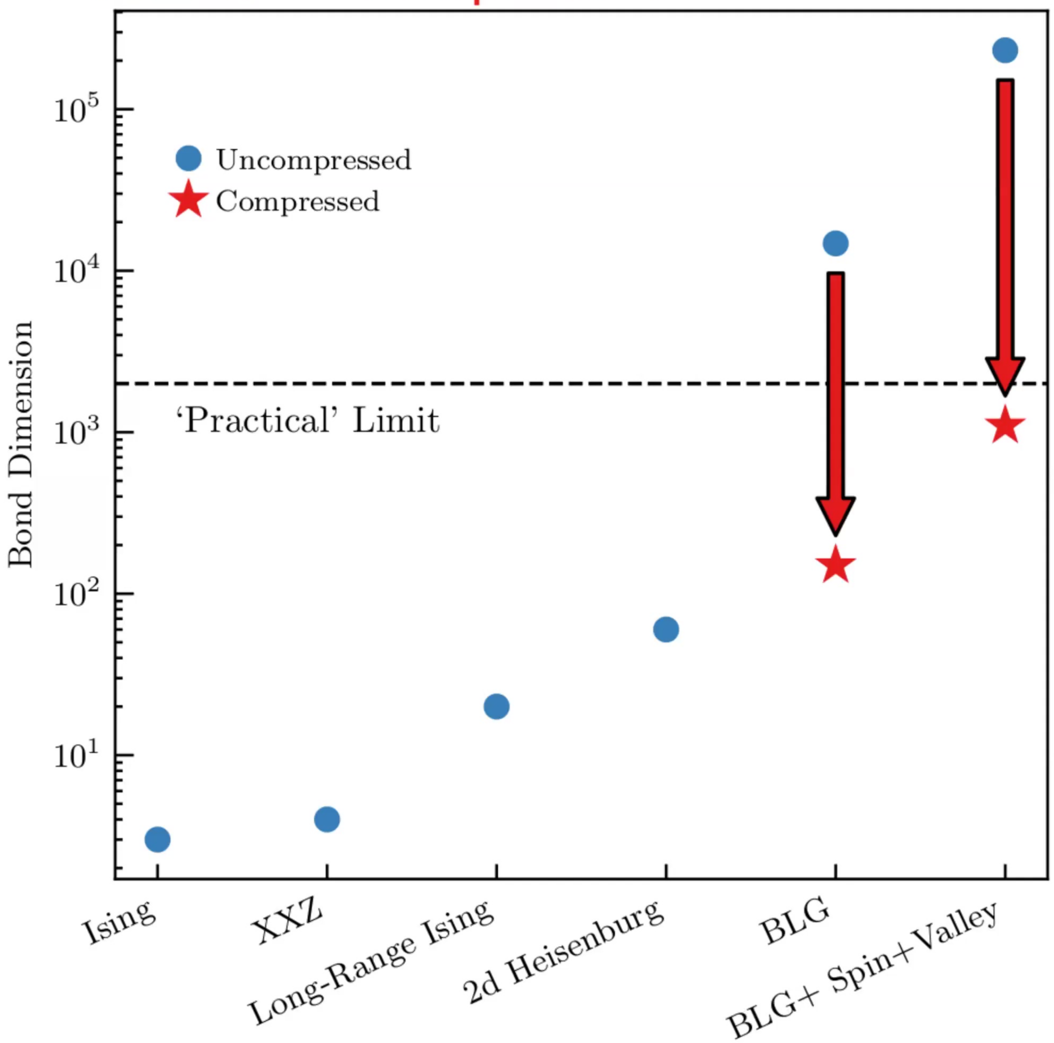
1D Range $R = \underbrace{(2 \times 2 \times 2)}_{\text{orbitals}} \times \underbrace{L_y}_{\text{cuts}} \times \underbrace{\Delta x}_{\text{range}}$; $D \approx 4R^2 \sim 230,000$; DMRG $\sim O(D^2)$

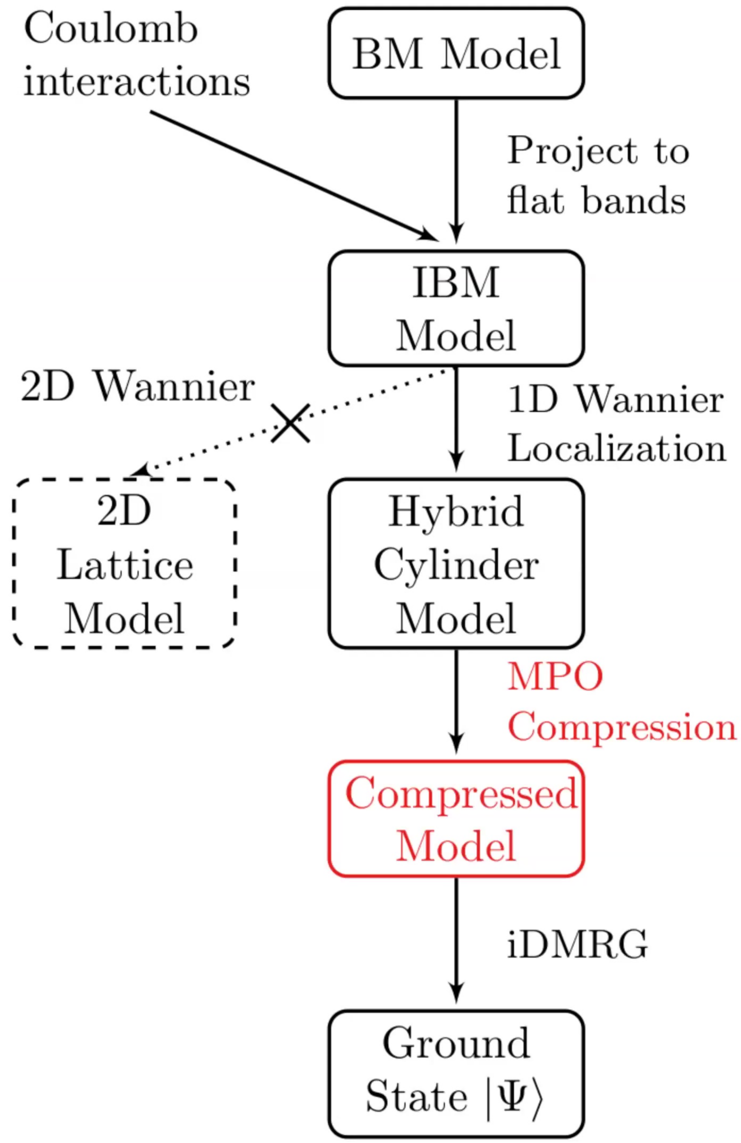
Obstruction: MPO Bond Dimension





Solution: MPO Compression





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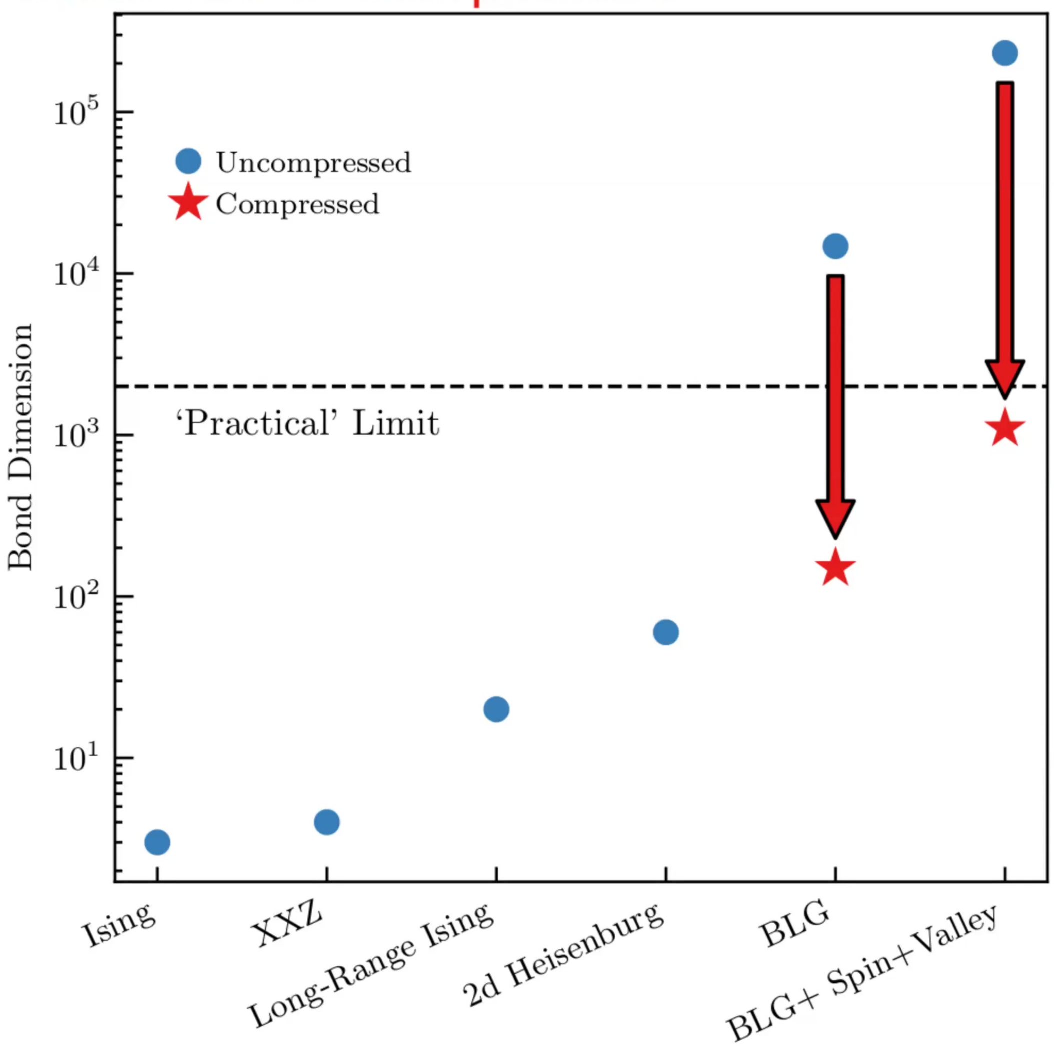
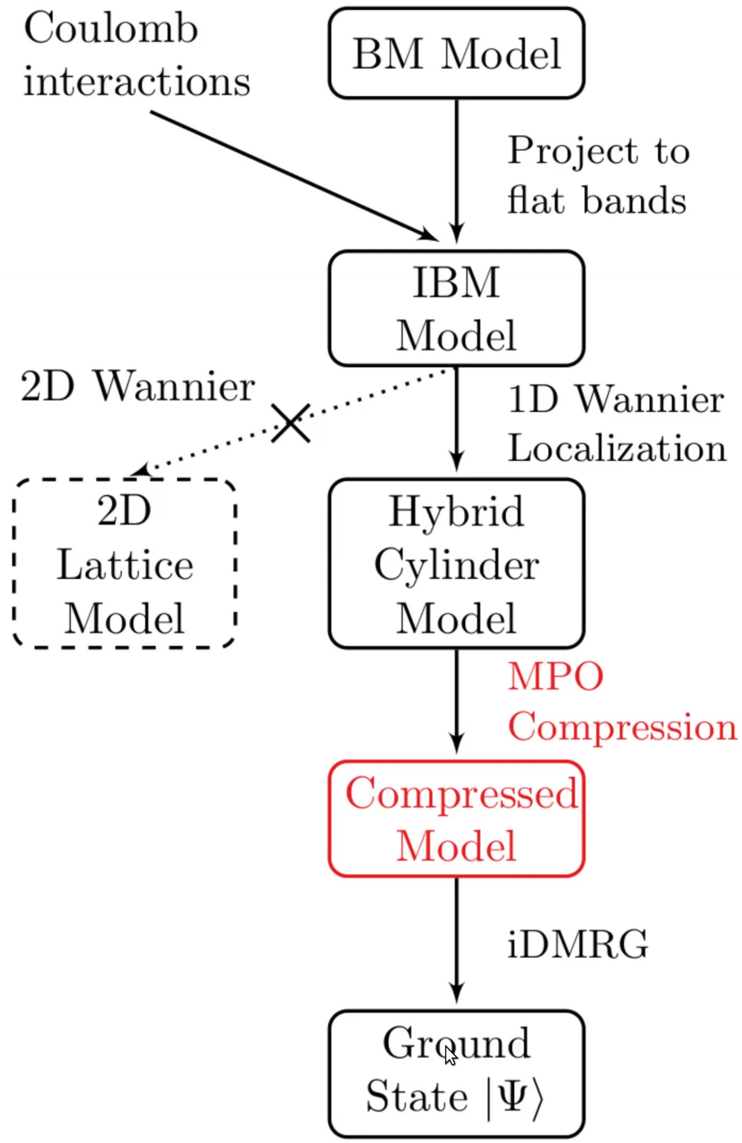




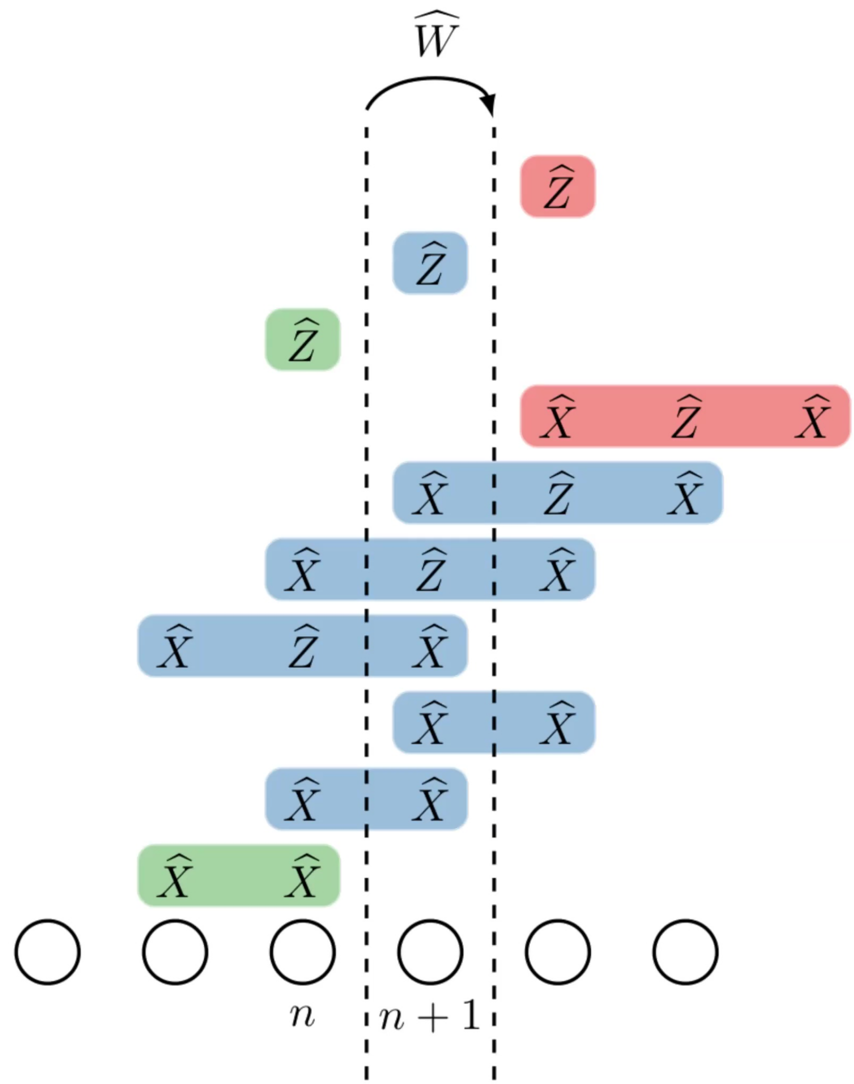
2. Matrix Product Operators and Compression

Matrix Product Operators

A local Hamiltonian

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

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



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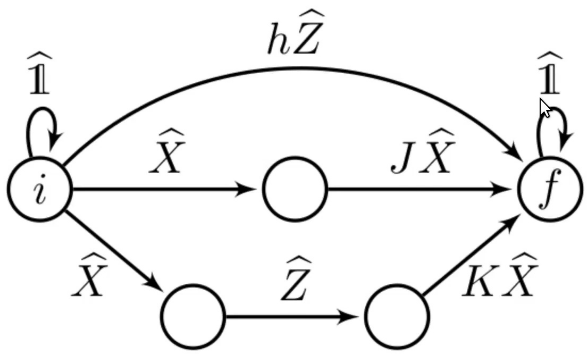
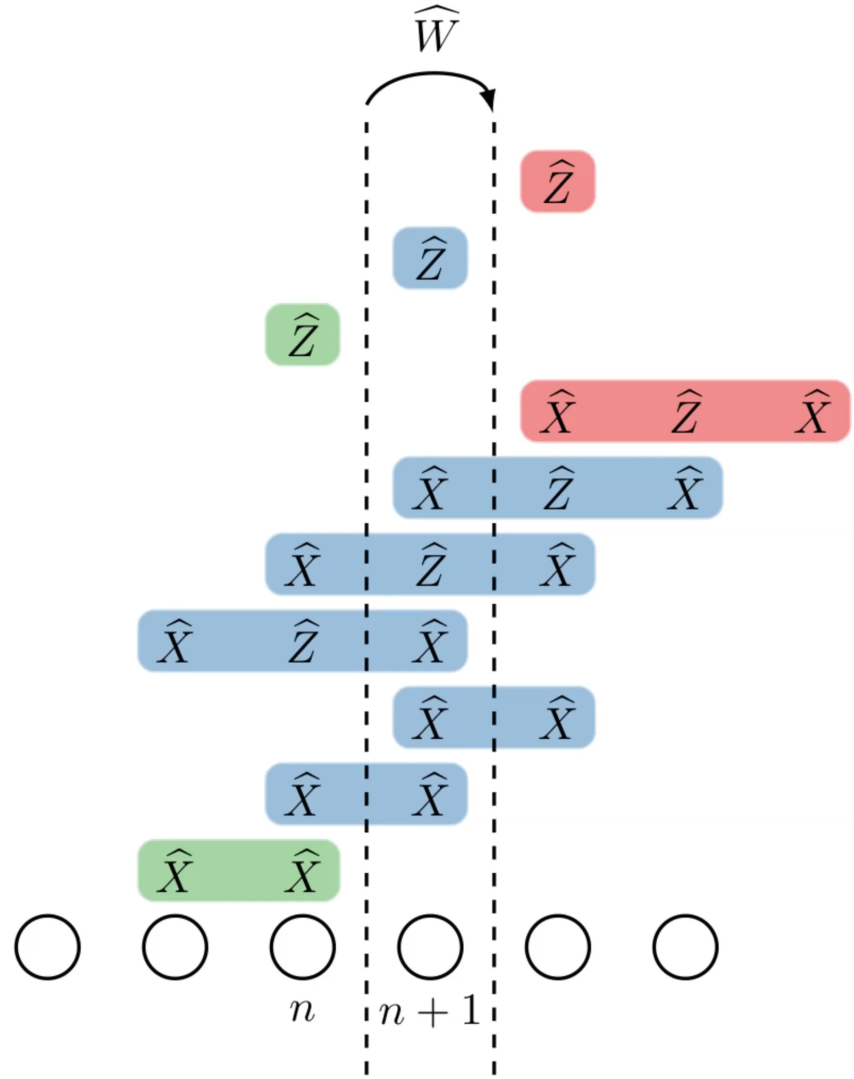


A Matrix Product Operator is a machine to place one more site.



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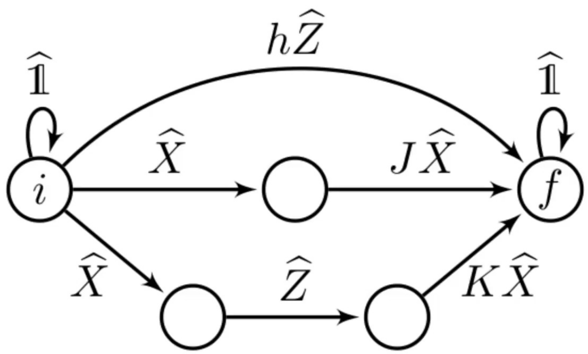


⇑ out

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

⟹ in

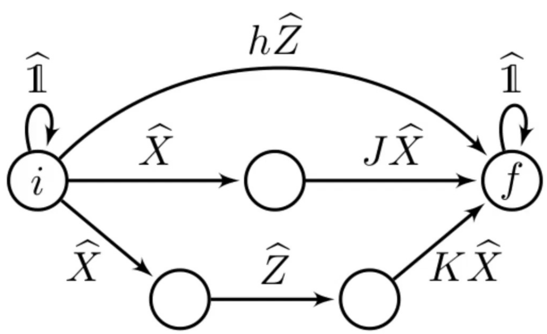
Bond Dimension 5

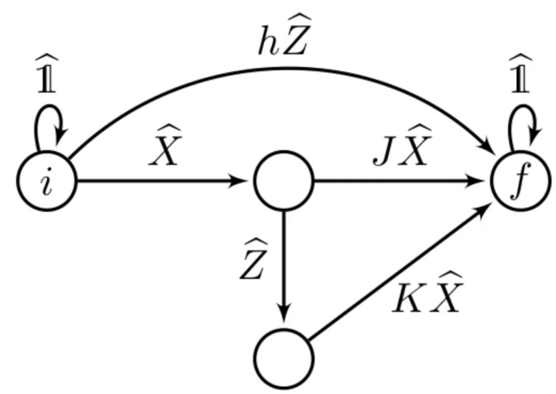
A Matrix Product Operator is a machine to place one more site.
Rewrite the graph as an operator-valued matrix.

Compression

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

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





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

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

Compress by truncating the sum:

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

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

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

Algorithm 1 iMPO Compression

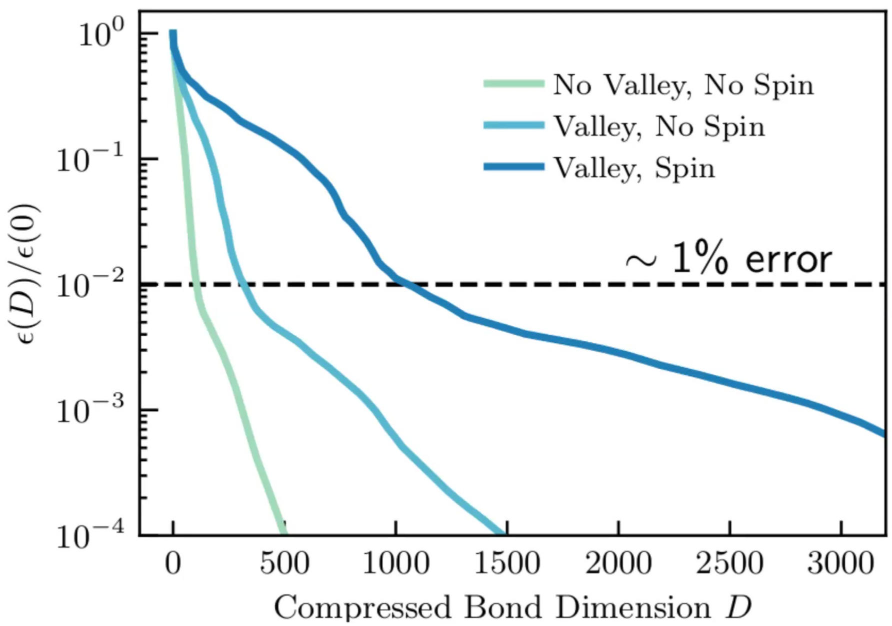
Require: $\widehat{W}$ is a first-order infinite MPO.

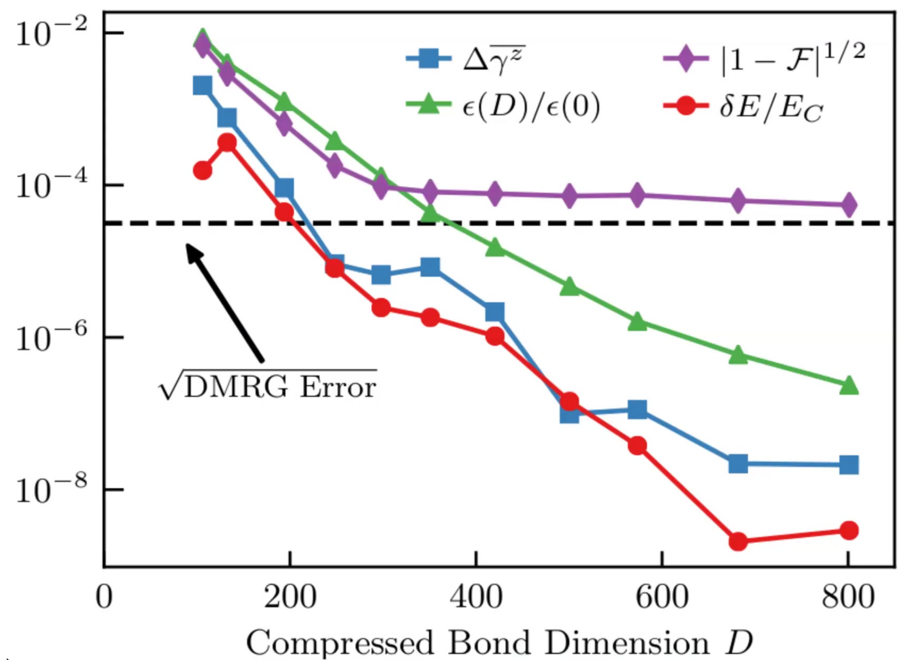
```
procedure ICompress(Ŵ, η)                                  ▷ Cutoff η
    Ŵ_R ← RightCanLocalOp[Ŵ]
    Ŵ_R ← R Ŵ_R R^{-1} so that ∀a, [Ŵ_R]_{1a} = 0
    Ŵ_L, C ← LeftCanLocalOp[Ŵ_R]
    (U, S, V†) ← SVD[C]
    Q̂, P̂ ← U† Ŵ_L U , V† Ŵ_R V
    χ' ← max{a ∈ [1, χ] : s_a > η}                          ▷ Defines ℙ
    Ŵ''_L, S, Ŵ''_R ← ℙ† Ŵ'_L ℙ, ℙ† S ℙ, ℙ† Ŵ'_R ℙ
    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.

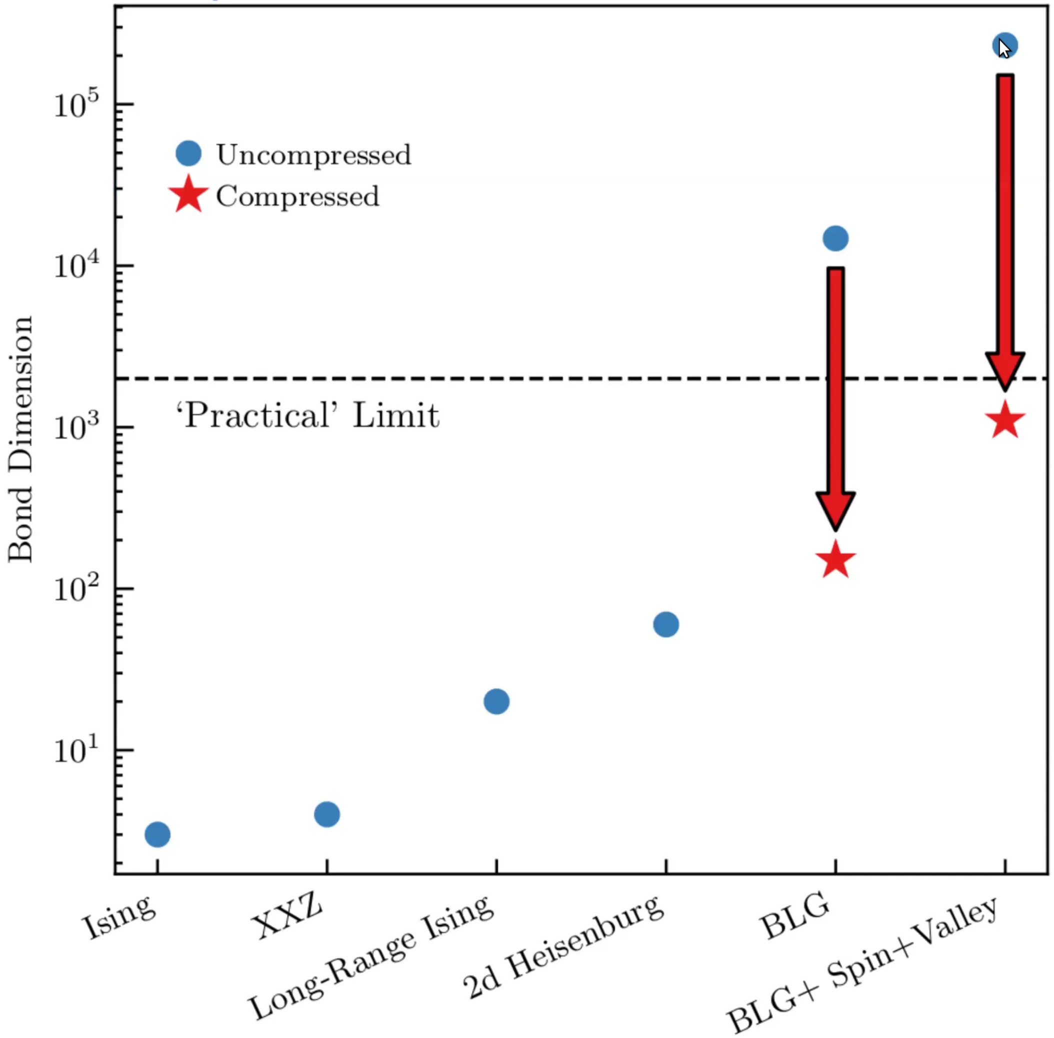
We can compute low bond dimension approximations $\widehat{W}'$ to any local operator.

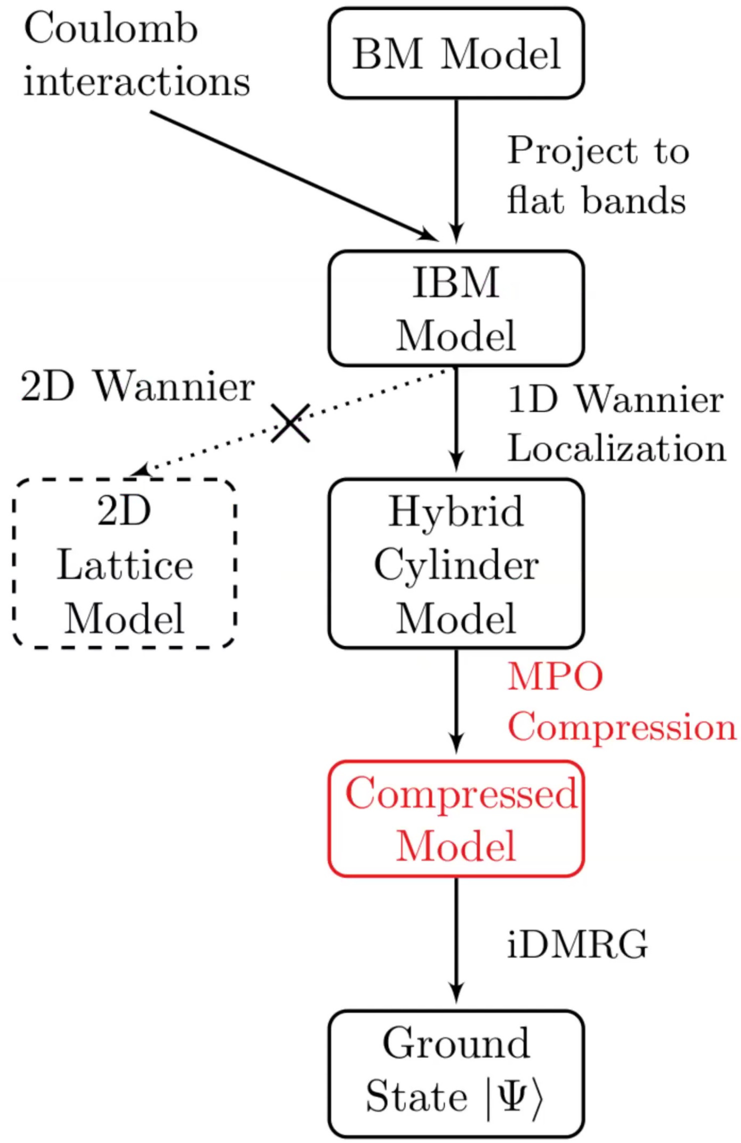
MPO Compression for tBLG



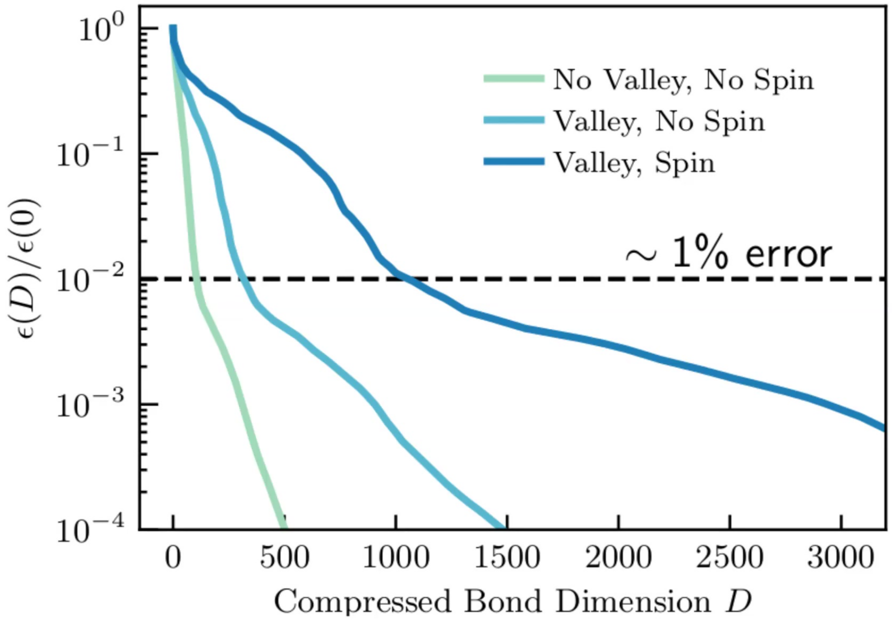


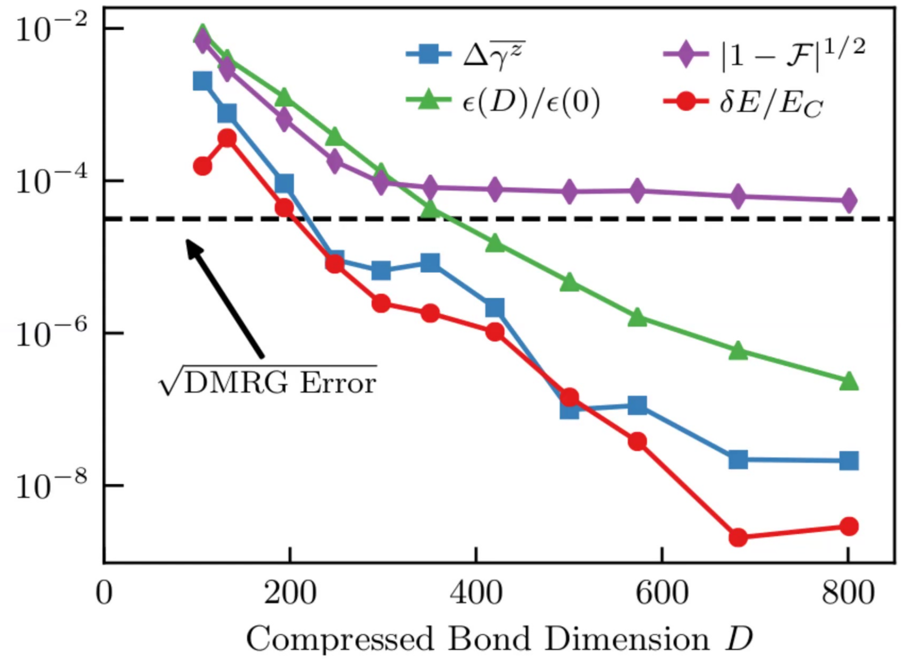
MPO Compression enables DMRG for tBLG





MPO Compression for tBLG





Compression Algorithm

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

Any local operator can be written as

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

Compress by truncating the sum:

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

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

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

Algorithm 1 iMPO Compression

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

procedure ICOMPRESS($\widehat{W}, \eta$) ▷ Cutoff η
- $\widehat{W}_R \leftarrow$ RIGHTCANLOCALOP$[\widehat{W}]$
- $\widehat{W}_R \leftarrow R\widehat{W}_R R^{-1}$ so that $\forall a$, $[\widehat{W}_R]_{1a} = 0$
- $\widehat{W}_L, C \leftarrow$ LEFTCANLOCALOP$[\widehat{W}_R]$
- $(U, S, V^\dagger) \leftarrow \text{SVD}[C]$
- $\widehat{Q}, \widehat{P} \leftarrow U^\dagger \widehat{W}_L U\ ,\ V^\dagger \widehat{W}_R V$
- $\chi' \leftarrow \max\{a \in [1, \chi] : s_a > \eta\}$ ▷ Defines $\mathbb{P}$
- $\widehat{W}''_L, S, \widehat{W}''_R \leftarrow \mathbb{P}^\dagger \widehat{W}'_L \mathbb{P}, \mathbb{P}^\dagger S \mathbb{P}, \mathbb{P}^\dagger \widehat{W}'_R \mathbb{P}$
- **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.

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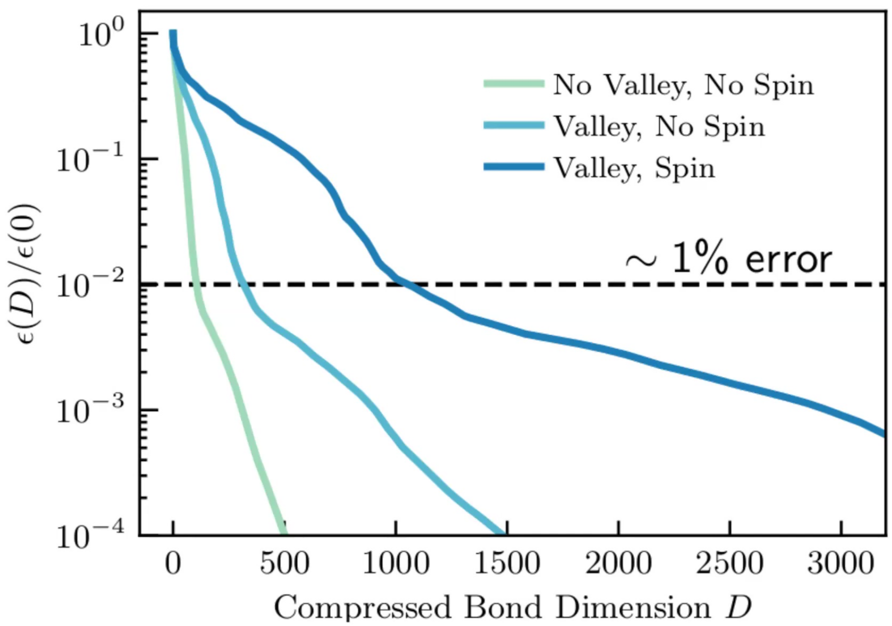
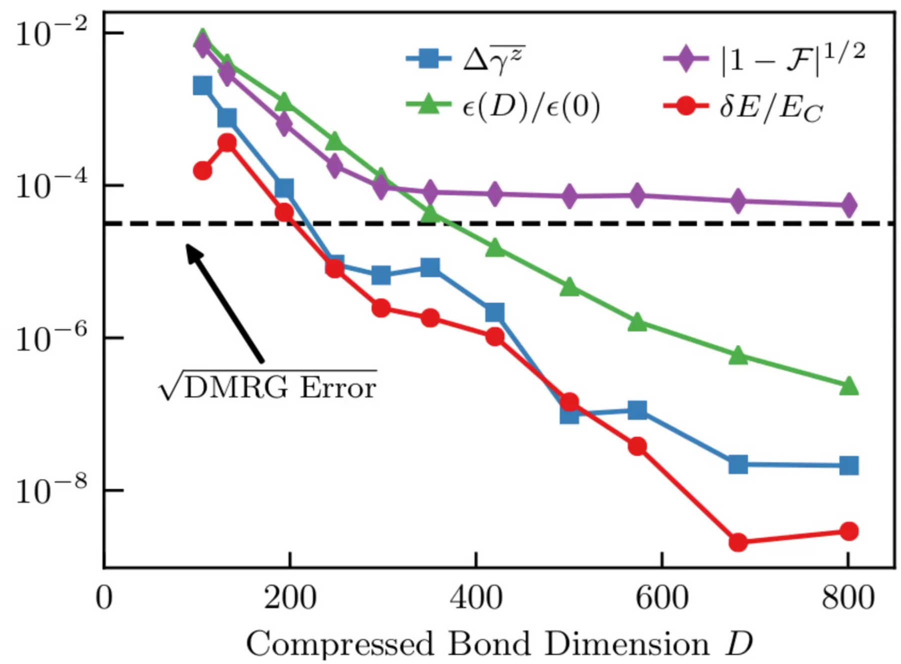




3. tBLG Physics from DMRG

Wannier Basis and Symmetry Actions

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

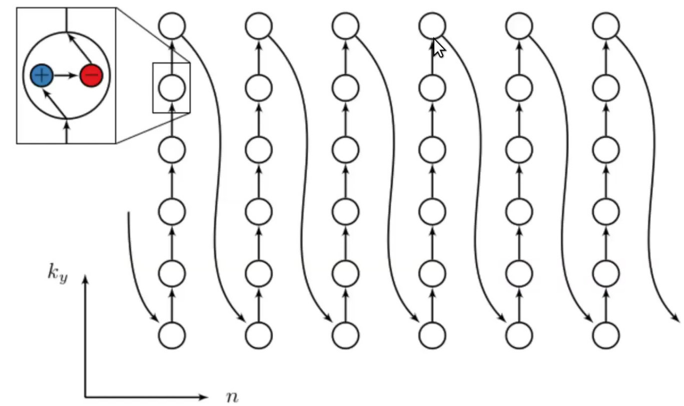
$$k_y/G_y = \frac{n + \Phi_y/(2\pi)}{N_y} \quad (\mathrm{mod}\ 1)$$

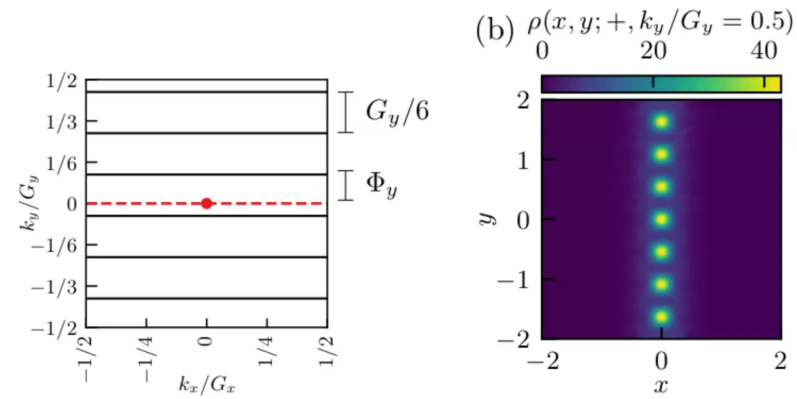
This gives a cylinder radius of $12 = N_y \times 2$.

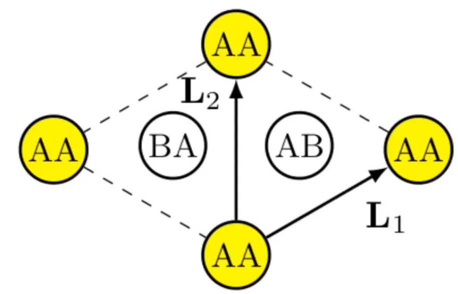
Symmetries:

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

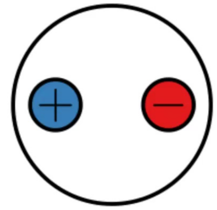
C_3 is slightly broken by the rectangular BZ.







1-Particle Observables



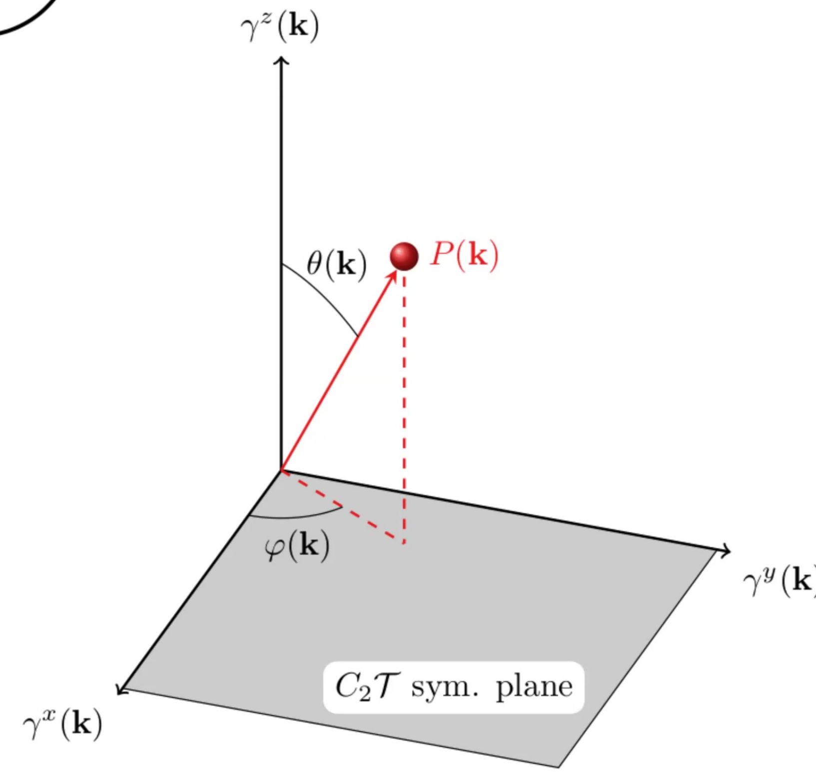
Let

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

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

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

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



$C_2\mathcal{T}$ 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

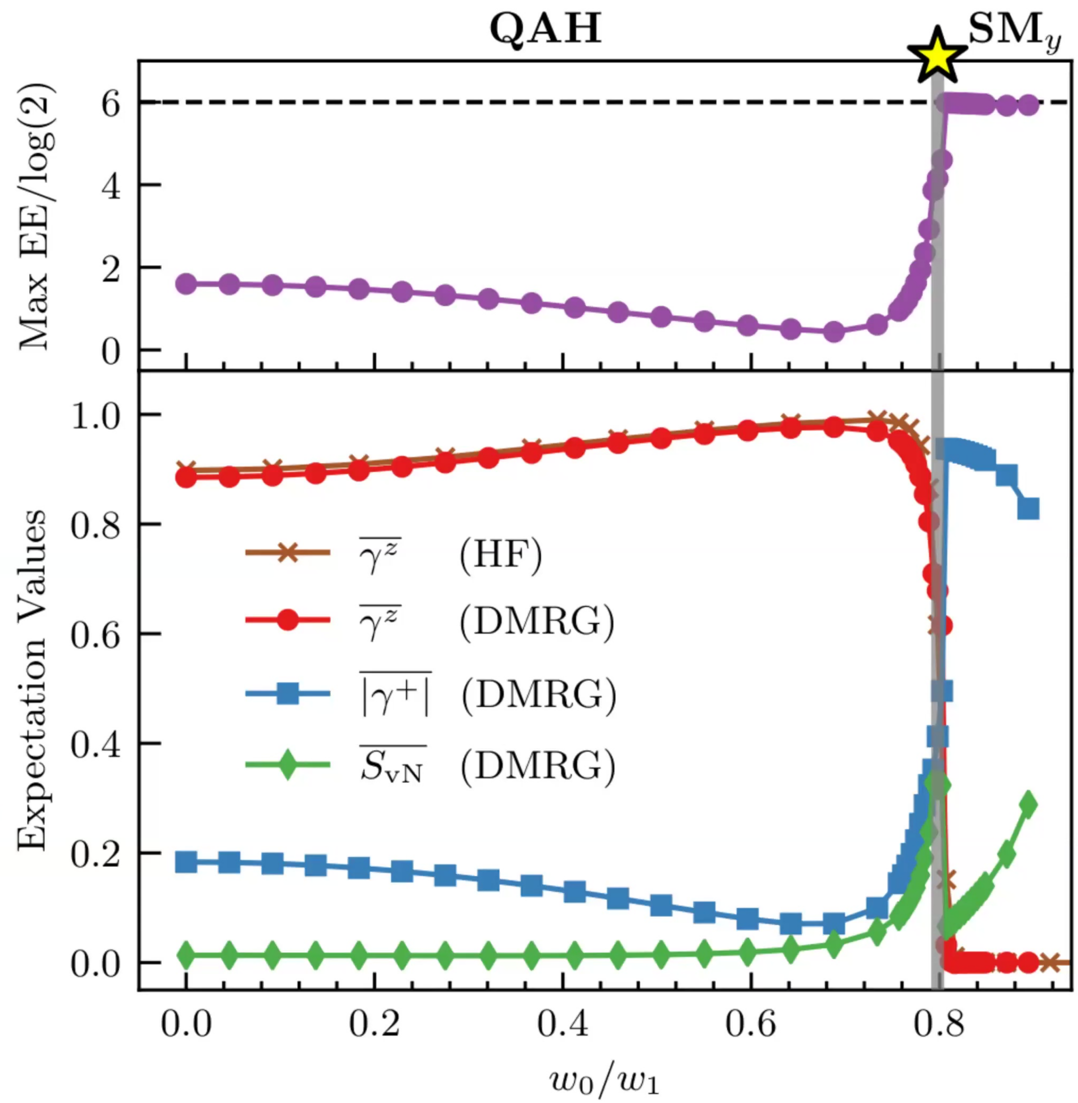
$$\begin{cases} w_0 & \text{AA regions} \\ w_1 & \text{AB regions} \end{cases}$$

Low w_0/w_1

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

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

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



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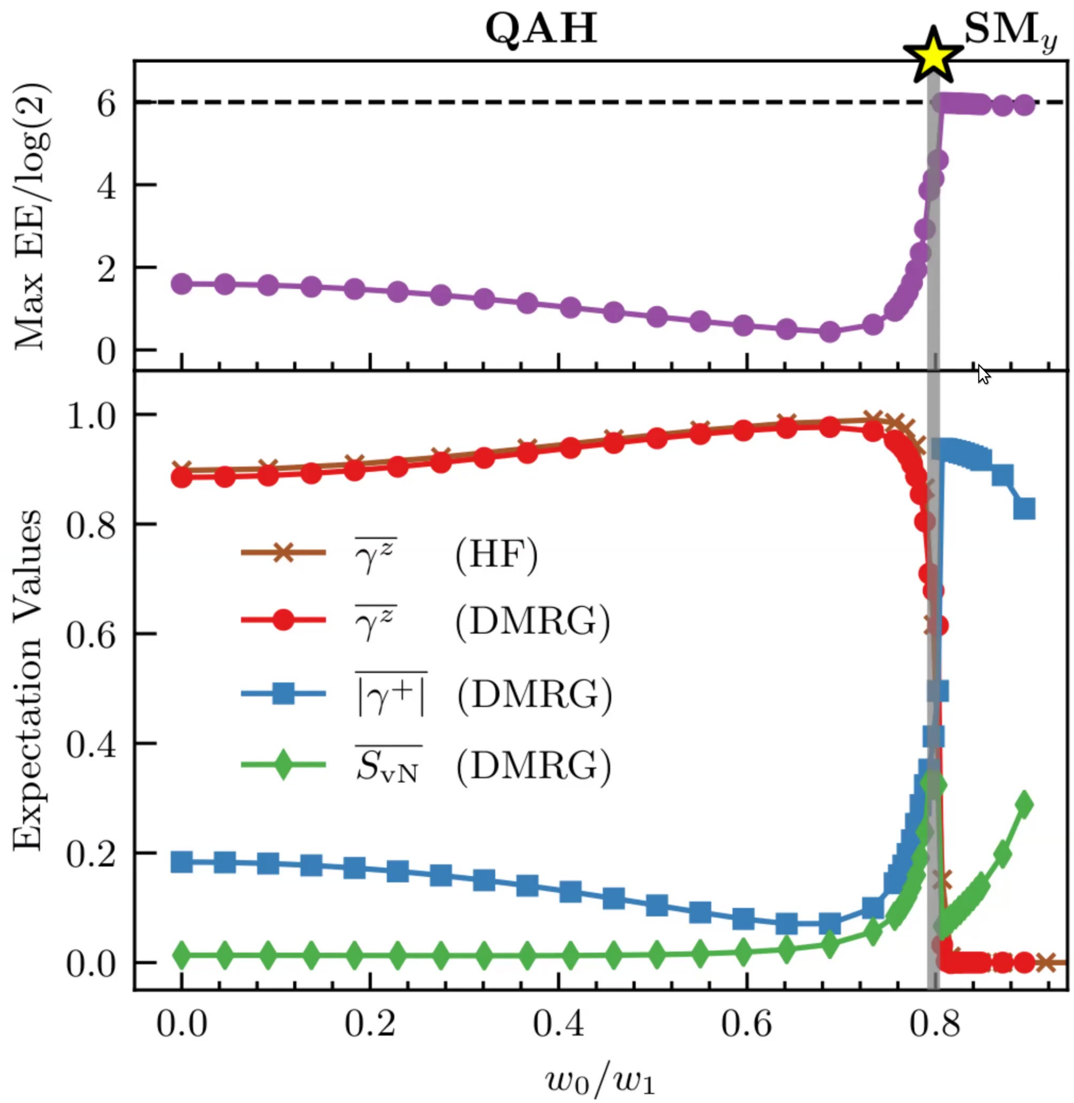

Ledwith, Tarnopolsky, Khalaf, Vishwanath (2020)

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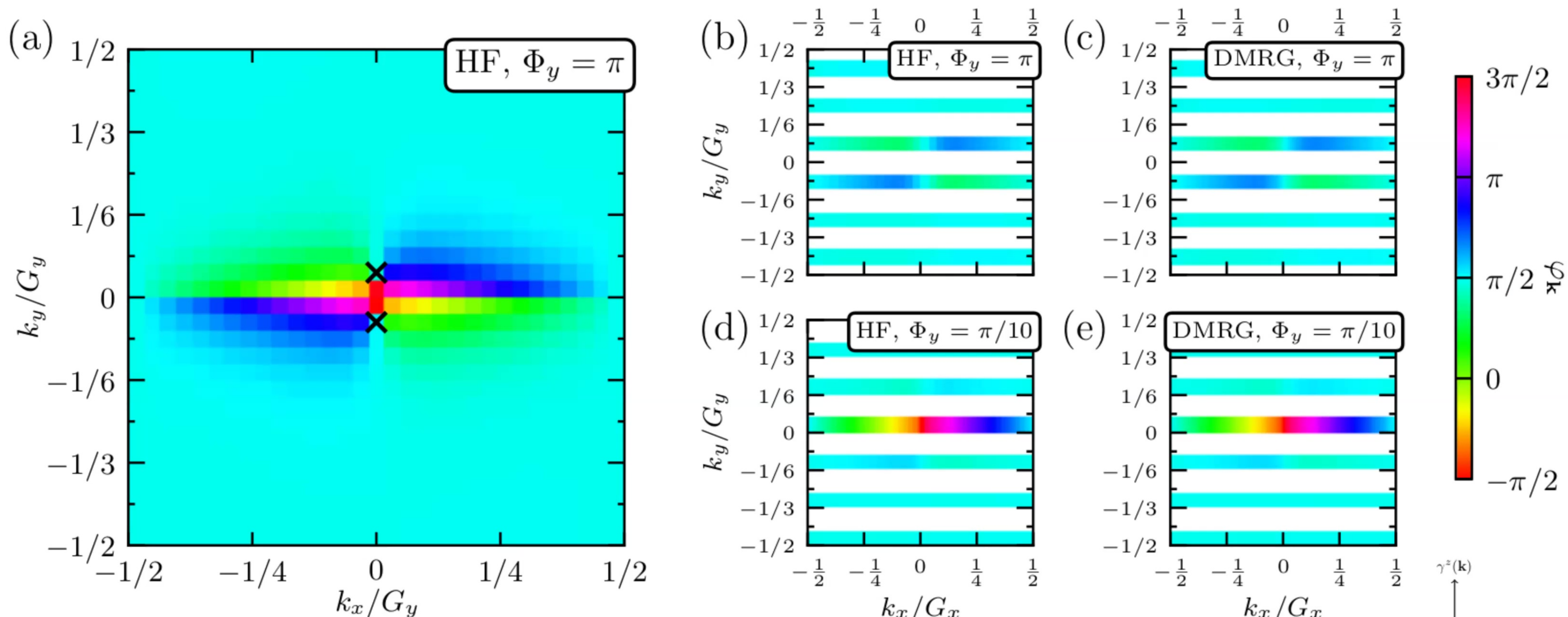

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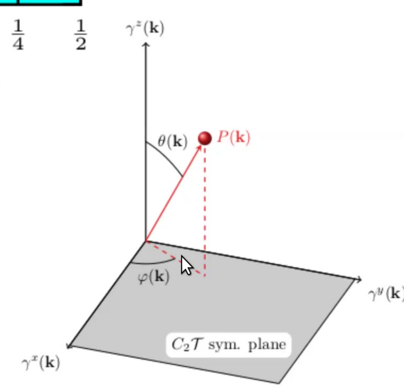

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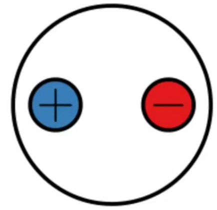

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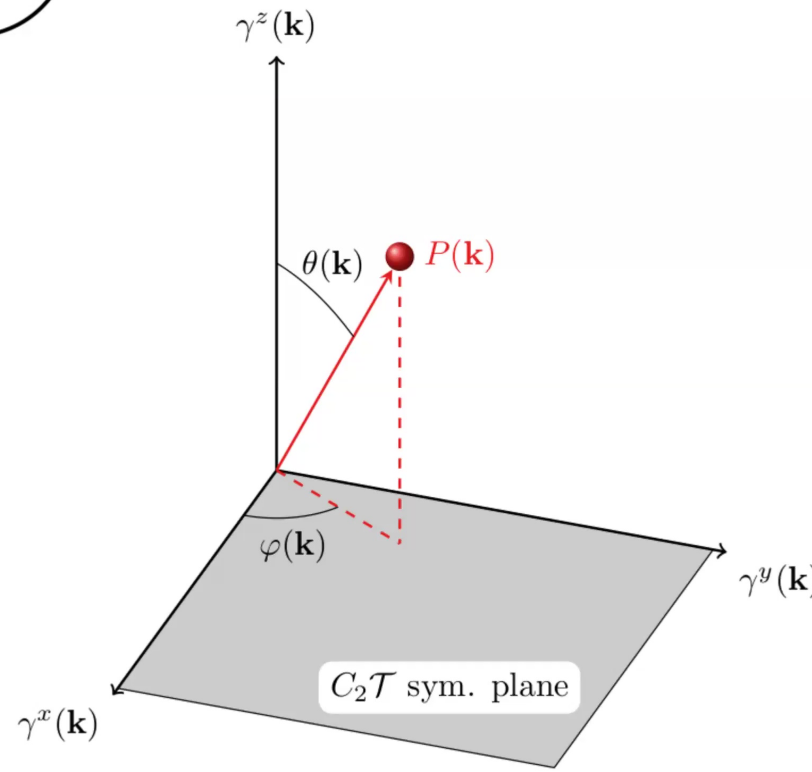

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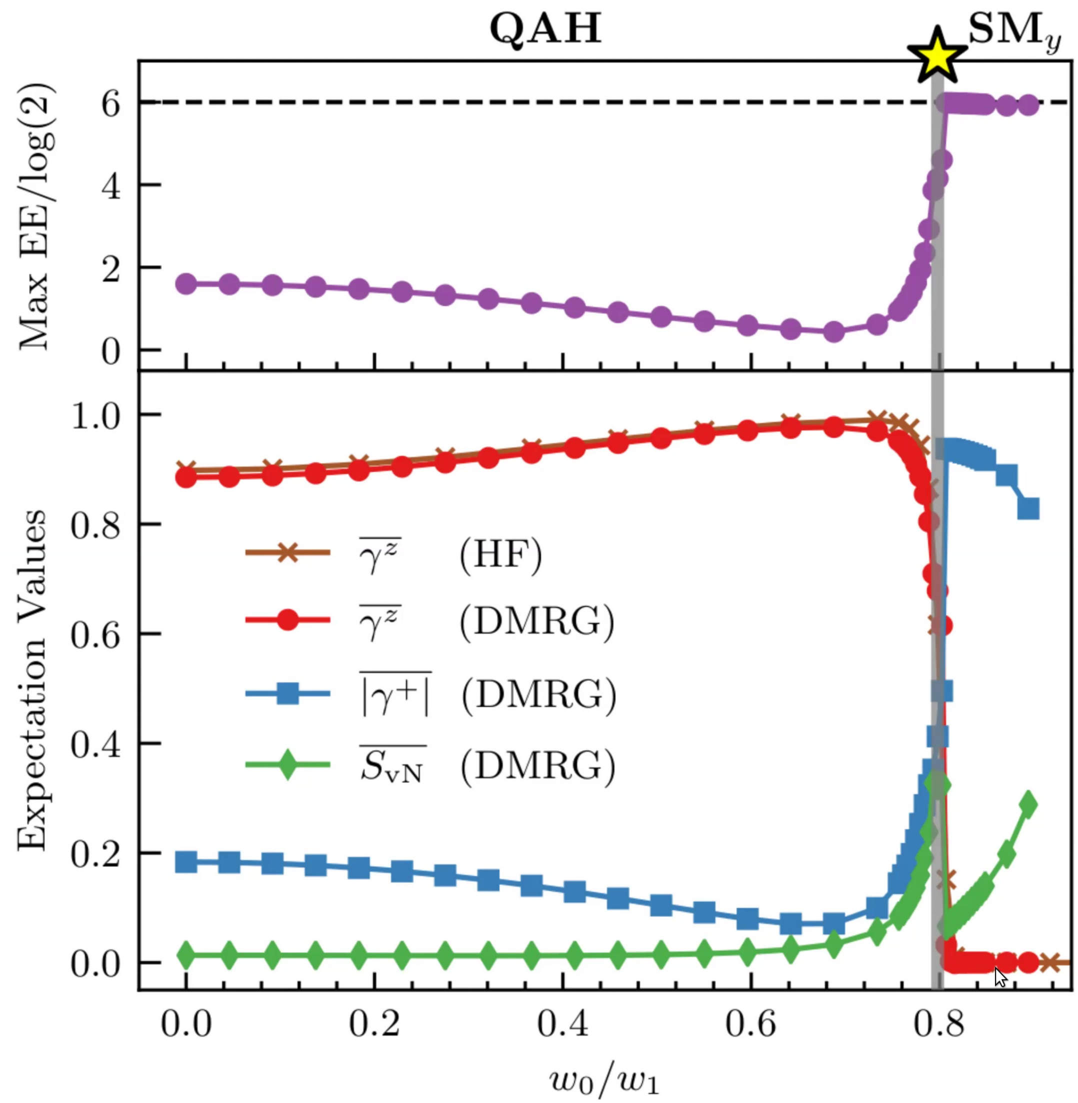

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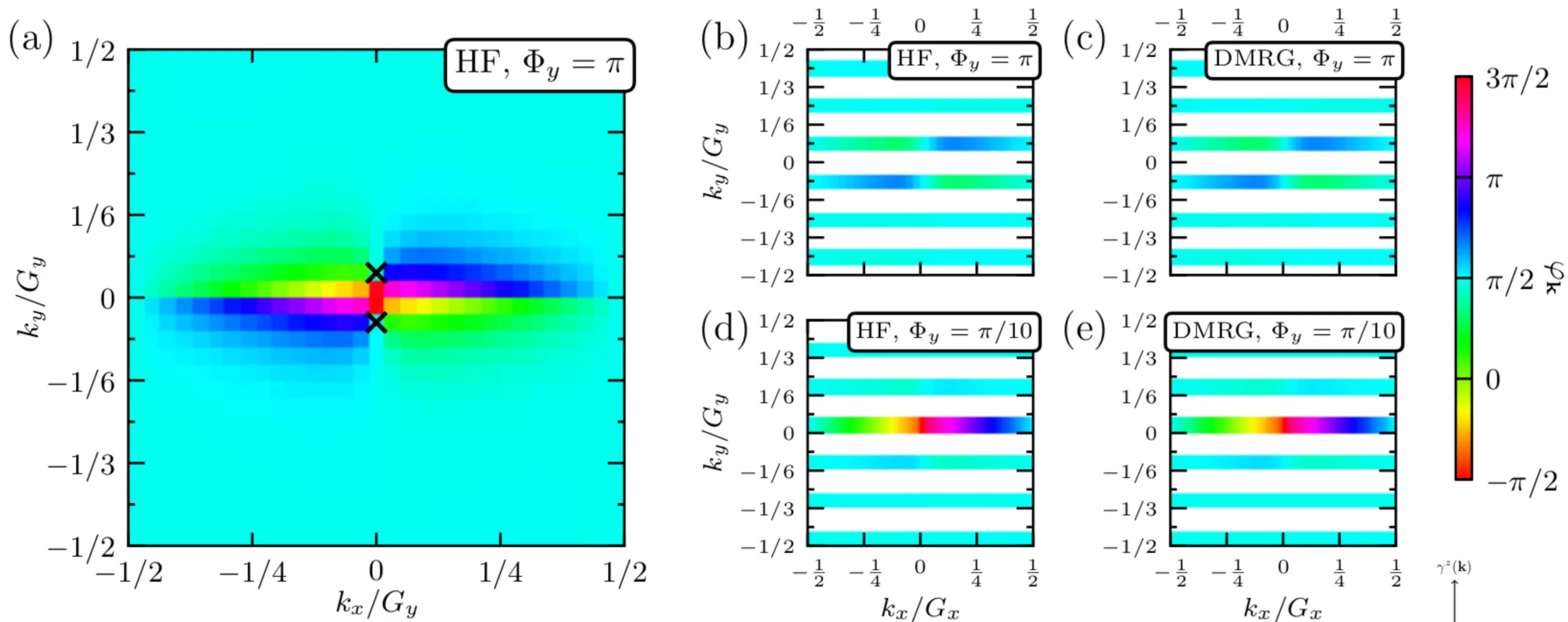

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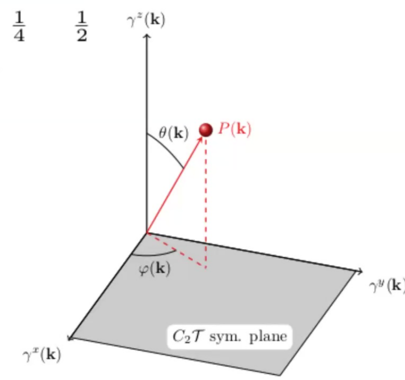


The High w_0/w_1 Phase is Nematic

$C_2\mathcal{T}$ 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

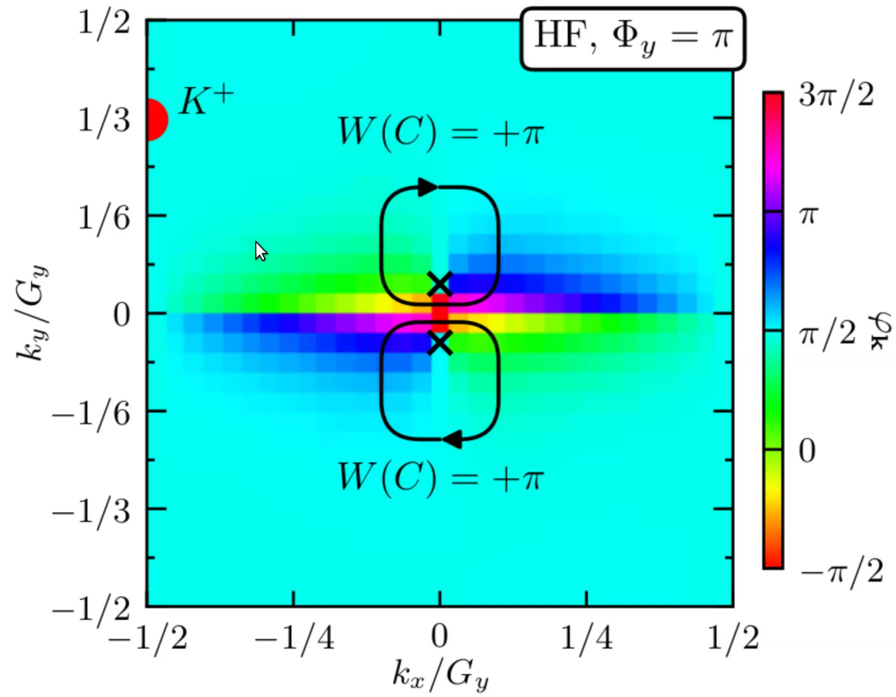
$$\varphi(C_3K^+) = \varphi(K^+) + \pi/3,$$

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.

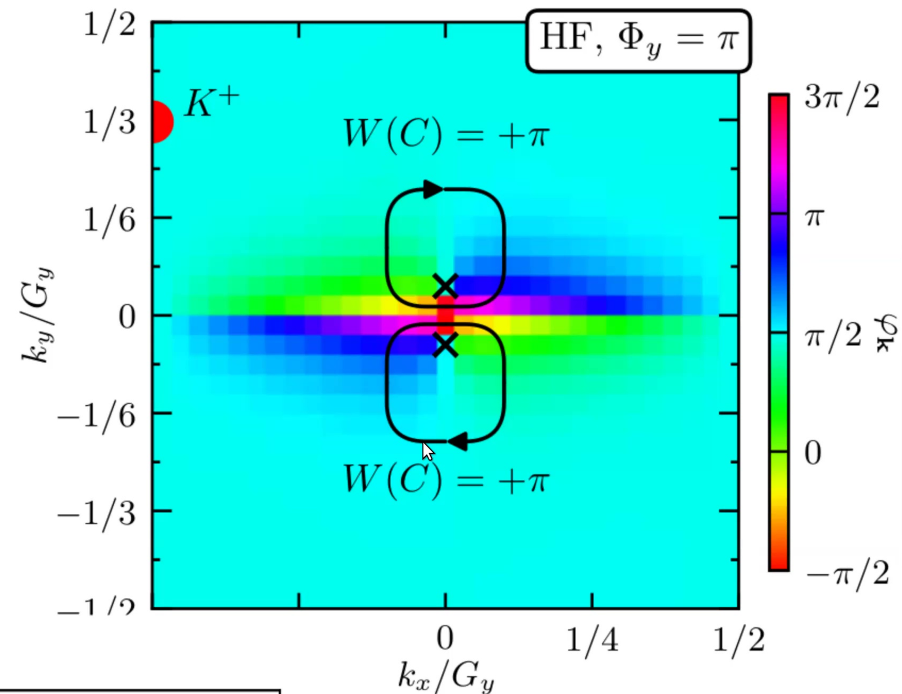


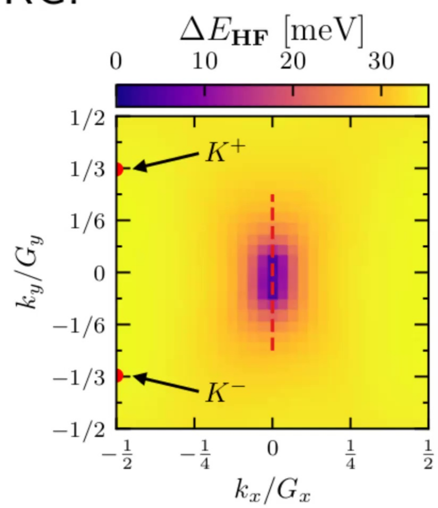
NEMATIC (semimetal)

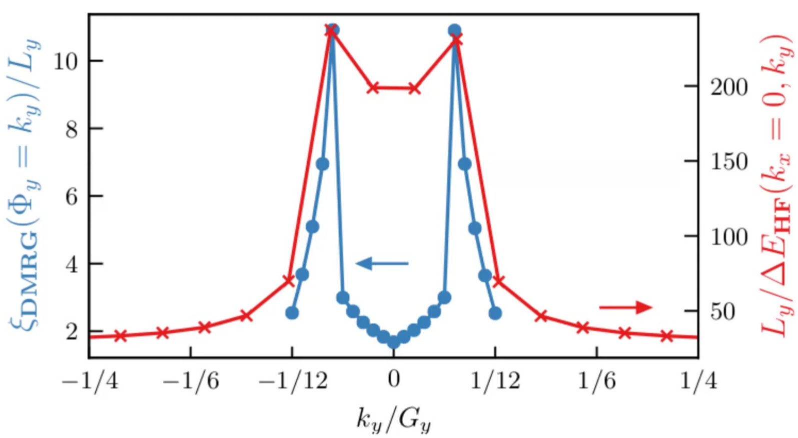
- Wilson loops are quantized

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

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



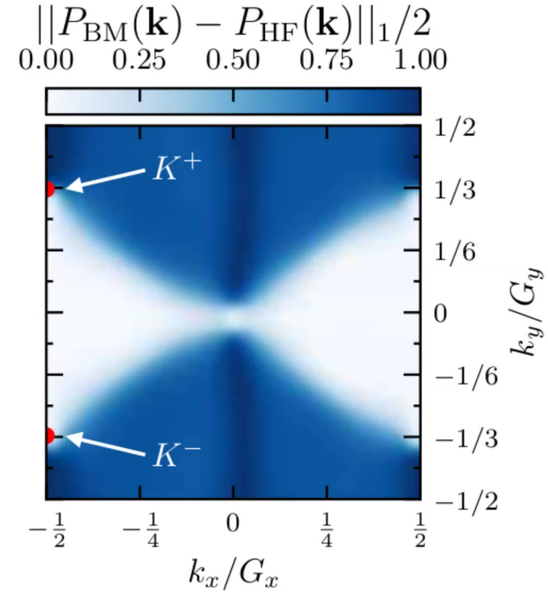


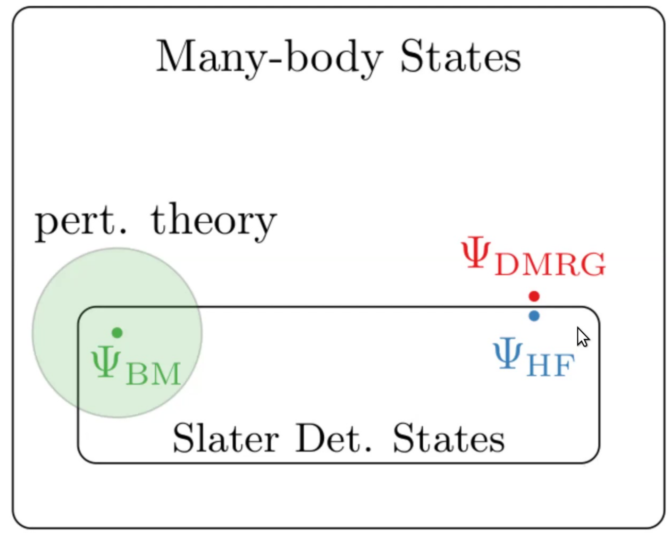


Nematic Semimetal$_y$ $\neq$ BM Ground State

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

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





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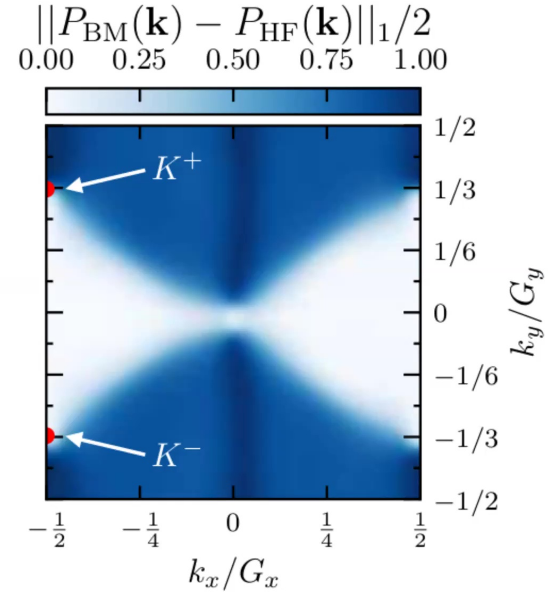

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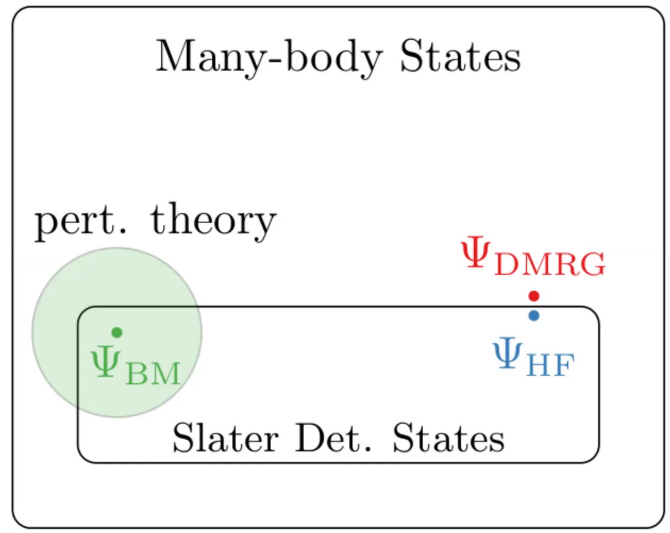
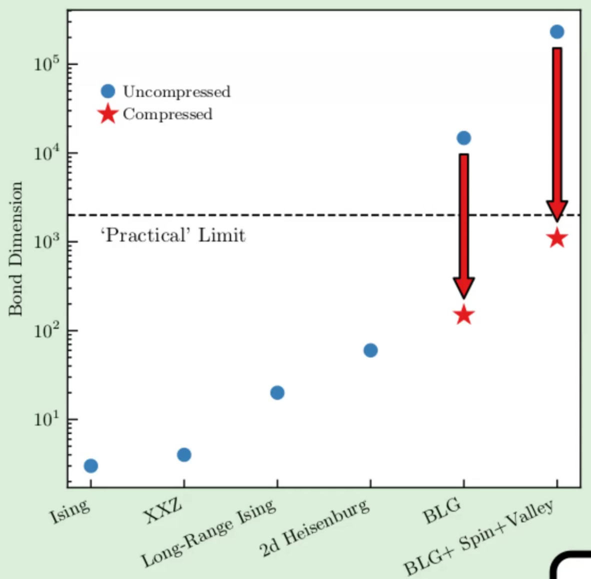
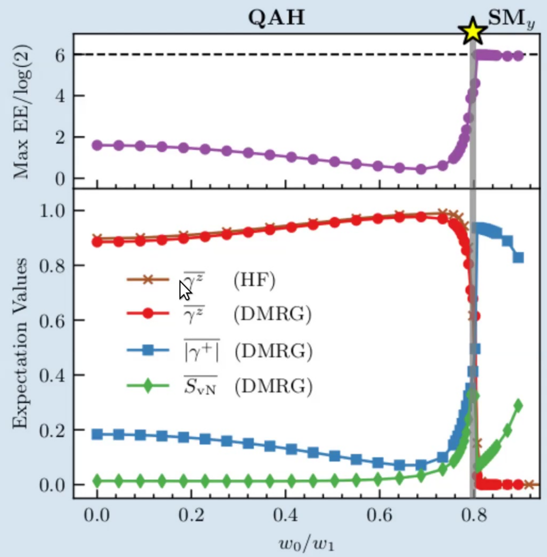


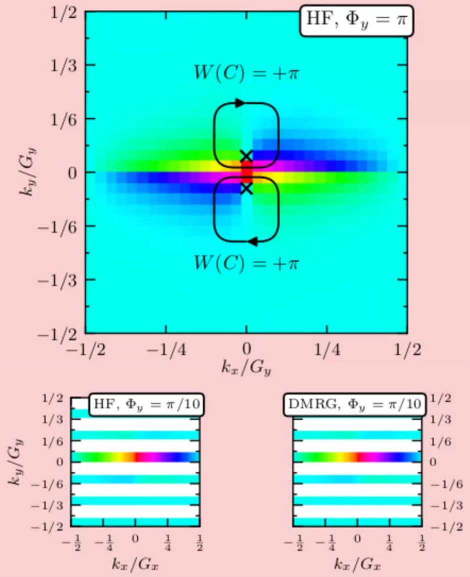
Compression enables DMRG for BLG



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 moiré systems

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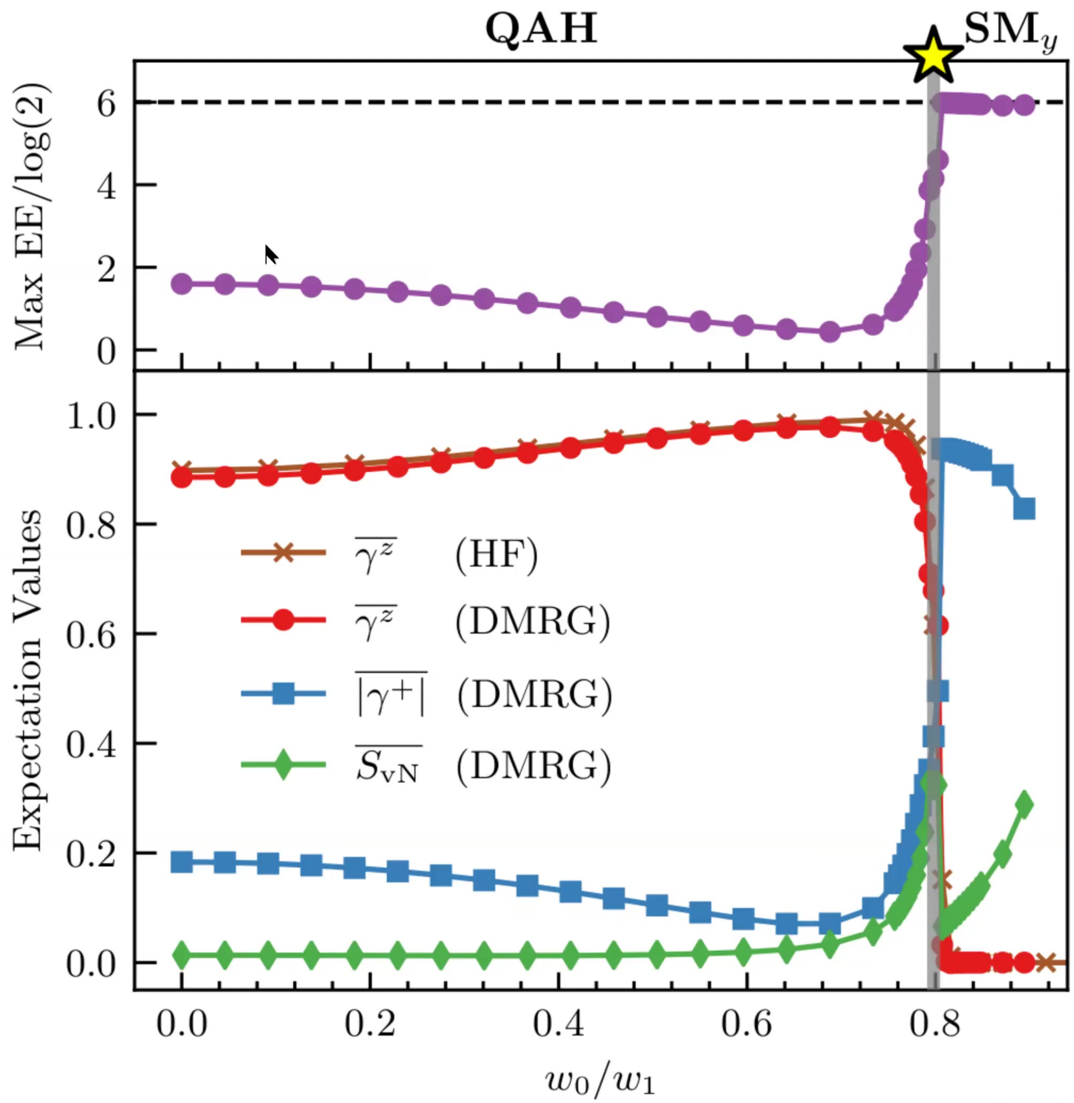

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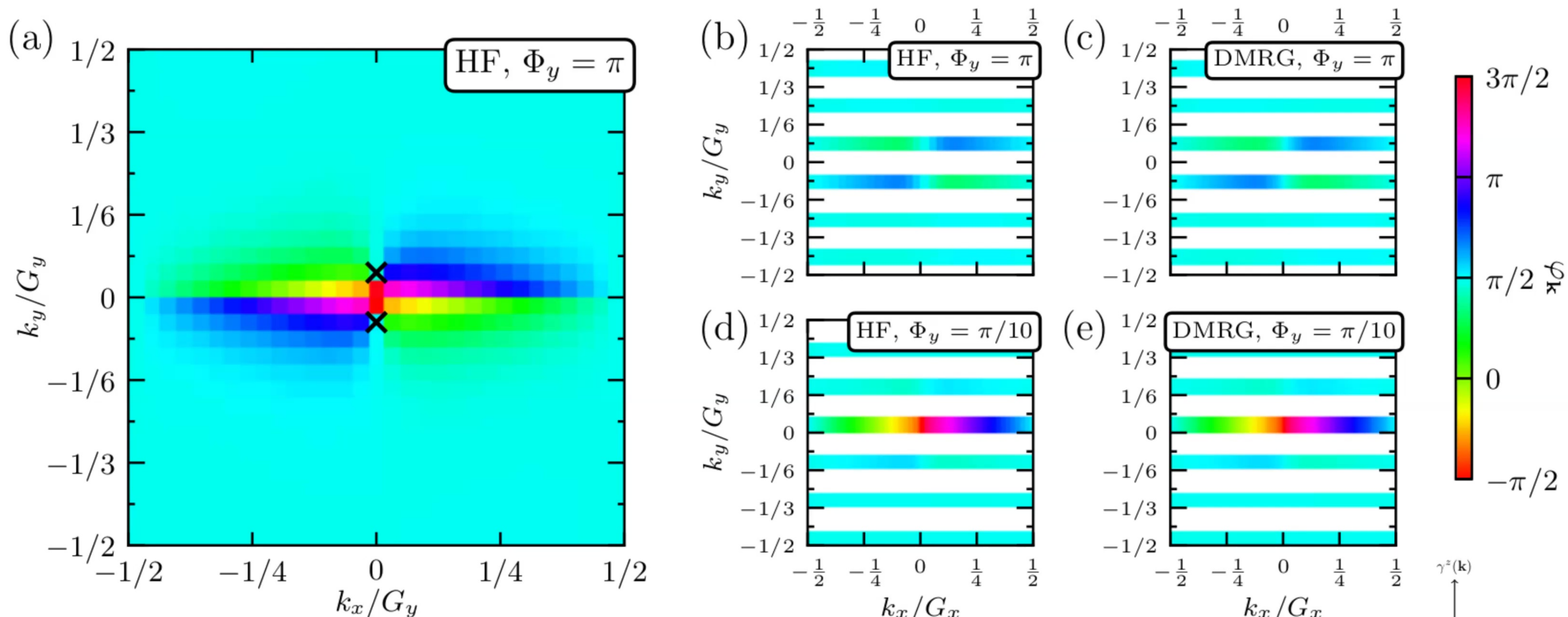

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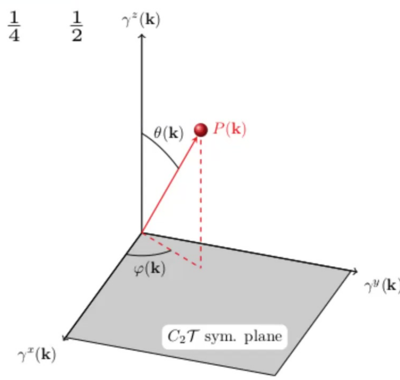

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