DMRG for Bilayer Graphene

**Figure:**
- **Y-axis:** Expectation Values
- **X-axis:** $w_0/w_1$
- **Graphs:**
  - $\langle \gamma^z \rangle$ (HF)
  - $\langle \gamma^z \rangle$ (DMRG)
  - $\langle \gamma^+ \rangle$ (DMRG)
  - $\langle \delta_{\gamma^z} \rangle$ (DMRG)

**Legend:**
- QAH
- SM

**References:**
- arXiv: 1909.06341
  - DEP
  - Xiangyu Cao
  - Mike Zaletel
  - Tomohiro Soejima
  - DEP
  - Nick Bultinck
  - Johannes Hauschild
  - Mike Zaletel

**Authors:**
- Daniel E. Parker

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Acknowledgements

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 $< \text{Band gap}$
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.
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 $\chi(D)$.

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

$$\hat{H}_{BM} = \hat{H}_{MLG}(\theta) + \hat{H}_{MLG}(-\theta) + \hat{T}$$

$$= \int_{mBZ} [d\mathbf{k}] \ f^\dagger_{k} h(\mathbf{k}) f_{k}$$

Bistritzer, MacDonald (2011); etc
The “IBM” Model

Interacting Bistritzer-MacDonald (IBM) model:
- start with the BM model $h(\mathbf{k})$
- add gate-screened Coulomb interactions

\[ \hat{H} := \hat{H}_{\text{BM}} + \hat{H}_{\text{Coulomb}} \]
\[ = \int_{mBZ} [d\mathbf{k}] f_k^\dagger h(\mathbf{k}) f_k + \int d[\mathbf{q}] V_{\mathbf{q}} : \hat{\rho}(\mathbf{k} + \mathbf{q})\hat{\rho}(\mathbf{k}) : \]
\[ V_{\mathbf{q}} = e^2 \frac{\tanh(|\mathbf{q}|d)}{2\epsilon_r\epsilon_0 |\mathbf{q}|} e^2 \]

$d \approx 10 \text{ nm}$ 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 atoms/moiré unit cell — far too many
- Project to flat bands:

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

- Kinetic scale (bandwidth of flat bands): \( t \approx 1 \text{ meV} \)
- Interaction scale (Coulomb): \( V \approx 10 \text{ meV} \)
- Band gap: \( \Delta E \approx 25 \text{ meV} \)
- \( t \ll V < \Delta E \implies \text{Projection is perturbatively valid.} \)
- 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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  1. Localized 2D Wannier orbitals
  2. Local action of $U_v(1)$ and $C_2T$

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- Solution I: let symmetry act non-locally
  - “Fidget spinner” Wannier functions
  - $Q_V = \sum_{i,j,n,m} Q_{ij}^{n,m} \hat{c}_{mi}^\dagger \hat{c}_{nj}$, $Q_{ij}^{n,m}$ long-ranged
  - Coulomb also long-ranged (not Hubbard-like)
  - Numerically, finite size will break symmetry!

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- **Solution II**: increase $8 \rightarrow 20$ bands
  - Top. obstruction is “fragile”
  - computationally infeasible

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Is there a better solution for DMRG?

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
1D Wannier Localization

Hybrid $xk$ Wannier orbitals: localize along $x$, periodic along $y$
1D Wannier Localization

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

$$|w_{\pm,n,k_y}\rangle = \sum_{b \in \text{flat bands}} \int [dk_x] U_{\pm,b} e^{ik \cdot R_n} \hat{f}^\dagger_{b,k} |0\rangle.$$
1D Wannier Localization

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

Coulomb interactions

BM Model

Project to flat bands

IBM Model

2D Wannier Localization

Hybrid Cylinder Model

2D Wannier Model

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

2D Wannier

(a) $\rho(x, y; +, k_y/G_y = 0)$

(b) $\rho(x, y; +, k_y/G_y = 0.5)$

$\rho(x, y; +, k_y/G_y = 0.5)$ (a) (b)
Hybrid Cylinder Model

\[
\begin{align*}
  k_y/G_y & \quad 1/2 \\
  1/3 & \\
  1/6 & \\
  0 & \quad \Phi_y \\
  -1/6 & \\
  -1/3 & \\
  -1/2 & \quad k_x/G_x
\end{align*}
\]
\[ w_{\pm,n,k_y} = \sum_{b \in \text{flat bands}} \int [dk_x] U_{\pm,b} e^{i k \cdot R_n} f_{b,k}^\dagger. \]
We have now mapped the BLG Hamiltonian to an infinite cylinder. Schematically,

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

Taking finite \( k_y \) cuts gives a quasi-1D model

(Intermediate) 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”

Long Range

1D Range \( R = (2 \times 2 \times 2) \times L_y \times \Delta x \)  \( D \approx 4R^2; \sim 230,000; \)  DMRG \( \sim O(D^2) \)
Obstruction: MPO Bond Dimension

- BM Model
- IBM Model
- Hybrid Cylinder Model
- Ground State $|\Psi\rangle$

Coulomb interactions

Project to flat bands

IBM Model

1D Wannier Localization

2D Wannier

Hybrid Cylinder Model

2D Lattice Model

Bond Dimension

'Practical' Limit

- Ising
- XXZ
- Long-Range Ising
- 2d Heisenburg
- BLG
- BLG+Spin+Valley

Bond Dimension

10^1

10^2

10^3

10^4

10^5

'Practical' Limit

iDMRG

Ground State $|\Psi\rangle$
Solution: MPO Compression

- BM Model
- Project to flat bands
- IBM Model
- 1D Wannier Localization
- Hybrid Cylinder Model
- MPO Compression
- Compressed Model
- Ground State $|\Psi\rangle$

Coulomb interactions

- 2D Wannier
- 1D Wannier Localization

Bond Dimension
- 'Practical' Limit

<table>
<thead>
<tr>
<th>Model</th>
<th>Bond Dimension</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ising</td>
<td>$10^1$</td>
</tr>
<tr>
<td>Long-Range Ising</td>
<td>$10^2$</td>
</tr>
<tr>
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<td>$10^3$</td>
</tr>
<tr>
<td>BLG</td>
<td>$10^4$</td>
</tr>
<tr>
<td>BLG+ Spin+Valley</td>
<td>$10^5$</td>
</tr>
</tbody>
</table>

Solution: MPO Compression
2. Matrix Product Operators and Compression
Matrix Product Operators

A local Hamiltonian

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

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

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

Rewrite the graph as an operator-valued matrix.
Matrix Product Operators

A local Hamiltonian

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

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

Rewrite the graph as an operator-valued matrix.
Given a Hamiltonian, what is the optimal MPO (smallest $D$)?

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

Finite MPOs: Directly analogous to MPS compression; see [1] & ITensor library [2].

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

References:
- Chan, Keselman, Nakatani, Li, White (2016)
- Fishman, White, Stoudenmire (2020)
- DEP, Cao, Zaletel (2020).
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**Compression**

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

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

Compression Algorithm

Idea: use a Schmidt decomposition that respects locality.

Any local operator can be written as

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

Compress by truncating the sum:

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

Theorem: For local $\hat{H}$ compress $\rightarrow \hat{H}'$, 

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

**Algorithm 1** iMPO Compression

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

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

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 $\hat{W}'$ to any local operator.
MPO Compression for tBLG

![Graph showing bond dimension vs. error]

- **ε(D)/ε(0)**
  - Green line: No Valley, No Spin
  - Blue line: Valley, Spin
- **∼ 1% error**

![Graph showing bond dimension vs. other metrics]

- **Δγ**
- **|1 − F| 1/2**
- **ε(D)/ε(0)**
- **δE/EC**
- **√DMRG Error**
MPO Compression enables DMRG for tBLG

![Graph showing bond dimension for different models]

- **Uncompressed** (blue circles)
- **Compressed** (red stars)

**Models**:
- Ising
- Long-Range Ising
- 2d Heisenburg
- BLG
- BLG+ Spin+Valley

**Bond Dimension**:
- ‘Practical’ Limit
- X-axis: Models
- Y-axis: Logarithmic scale

**Coulomb Interactions**
- Project to flat bands
- 1D Wannier Localization
- 2D Wannier Model

**Compression**
- MPO Compression
- iDMRG

**Ground State**:
- $|\Psi\rangle$
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:

$$T_{L_1} |w(\pm, n, k_y)\rangle = |w(\pm, n + 1, k_y)\rangle$$

$$T_{L_2} |w(\pm, n, k_y)\rangle = e^{i2\pi k_y} |w(\pm, n, k_y)\rangle$$

$$C_2 T |w(\pm, n, k_y)\rangle = |w(\mp, -n, k_y)\rangle$$

$$C_{2x} |w(\pm, n, k_y)\rangle = \mp i e^{-i2\pi k_y n} |w(\mp, n, -k_y)\rangle$$

$C_3$ is slightly broken by the rectangular BZ.
1-Particle Observables

Let

\[ P(k) = \begin{pmatrix} \langle w^\dagger_+, k w^+, k \rangle & \langle w^\dagger_+, k w^+, k \rangle \\ \langle w^\dagger_+, k w^+, k \rangle & \langle w^\dagger_+, k w^+, k \rangle \end{pmatrix} \]

\[ = \gamma^0(k)\sigma^0 + \gamma^x(k)\sigma^x + \gamma^y(k)\sigma^y + \gamma^z(k)\sigma^z \]

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

\[ P(k) \iff (\theta(k), \varphi(k)) \] (spherical coords.)

\( C_2T \) Order parameter

\[ C_2T \ \text{sym} \ \implies \gamma^z(k) = 0 \implies \theta(k) = \frac{\pi}{2} \]
Phase Transition & QAH Phase

Vary interlayer coupling

\[
\begin{align*}
  w_0 & \quad \text{AA regions} \\
  w_1 & \quad \text{AB regions}
\end{align*}
\]

\[\text{Ledwith, Tarnopolsky, Khalaf, Vishwanath (2020)}\]
Phase Transition & QAH Phase

Vary interlayer coupling

\[ \begin{aligned}
& w_0 \quad \text{AA regions} \\
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\end{aligned} \]

Low \( w_0/w_1 \)

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

\[ |\psi \rangle_{QAH} \approx \prod \hat{w}_{+,n,k_y}^\dagger |0 \rangle. \]

- Filled Chern +1 band implies quantum anomalous Hall state.
- Matches analytic solution at \( w_0 = 0 \)
Phase Transition & QAH Phase

Vary interlayer coupling

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High \( w_0/w_1 \) – more involved

- \( C_2 \mathcal{T} \) preserved

\[\text{Ledwith, Tarnopolsky, Khalaf, Vishwanath (2020)}\]
The Remarkable Accuracy of Hartree-Fock

▶ Only 2% difference between DMRG and HF in $\varphi_k$

▶ $|\Psi_{\text{DMRG}}\rangle = |\Psi_{\text{SD}}\rangle + \epsilon |\Psi^{(1)}\rangle$.

▶ Despite strong interactions, the ground state is essentially a Slater determinant!
The High $w_0/w_1$ Phase is Nematic

$C_2 \mathcal{T}$ preserved, so

\[
\begin{align*}
\theta(k) &= \frac{\pi}{2} \\
\varphi(C_2 \mathcal{T} k) &= -\varphi(k) + \pi
\end{align*}
\]

At $K^+$, $C_3$ acts as

\[
\varphi(C_3 K^+) = \varphi(K^+) + \pi/3,
\]

but

\[
\varphi(C_3 K^+) = \varphi(K^+) \approx \frac{\pi}{2}.
\]

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

\[ W(C) = \int_C A = \frac{1}{2} \int_{\partial C} \nabla \varphi \cdot dk = n\pi, \ n \in \mathbb{Z}. \]

- 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 $\neq$ BM Ground State

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

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

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**Many-body States**

- Slater Det. States
- Pert. theory

$\Psi_{\text{BM}}$ $\Psi_{\text{DMRG}}$ $\Psi_{\text{HF}}$
Compression enables DMRG for BLG

Transition from QAH to Nematic SM_y

Hartree-Fock is remarkably accurate!

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

BLG DMRG: 2009.02354.
Several states only slightly above the ground state. Partially explained by Eslam’s Ginsberg-Landau-like functional

$$E_{HF}[\varphi_k] = E_{HF}^{QAH} + \frac{1}{2} \int g_k (\nabla_k \varphi_k - 2a_k)^2 d^2k + \ldots$$

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

- twist angle disorder
- strain
- lattice relaxation

<table>
<thead>
<tr>
<th>State ($w_0/w_1 = 0.85$)</th>
<th>Energy [meV]</th>
</tr>
</thead>
<tbody>
<tr>
<td>DMRG SM_y</td>
<td>-28.24</td>
</tr>
<tr>
<td>QAH Ansatz</td>
<td>-28.04</td>
</tr>
<tr>
<td>SM_y Ansatz</td>
<td>-27.92</td>
</tr>
<tr>
<td>C2T - Stripe Ansatz</td>
<td>-28.08</td>
</tr>
<tr>
<td>Dirac (BM GS)</td>
<td>-20.62</td>
</tr>
</tbody>
</table>
\[ H_{\text{IBM}} = \sum_{k \in \text{mBZ}} f_k^\dagger h(k) f_k + \sum_{q} V(q) : \rho_q^\dagger \rho_{-q} : \]

\[
\rho_q = \sum_{k \in \text{mBZ}} f_k^\dagger \Lambda_q(k) f_k
\]

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

\[
V_q = e^2 \frac{\tanh(|q|/d)}{2\varepsilon_r \varepsilon_0 |q|}
\]

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \theta_{BM} )</td>
<td>( \sim 1.05 \degree )</td>
</tr>
<tr>
<td>( w_1 )</td>
<td>( \sim 109 \text{ meV} )</td>
</tr>
<tr>
<td>( w_0/w_1 )</td>
<td>[0, 1]</td>
</tr>
<tr>
<td>Gate distance</td>
<td>10 nm</td>
</tr>
<tr>
<td>Relative permittivity</td>
<td>12</td>
</tr>
<tr>
<td>( N_y )</td>
<td>6</td>
</tr>
<tr>
<td>( \Phi_y )</td>
<td>( \pi, \pi/10 )</td>
</tr>
<tr>
<td>( \chi )</td>
<td>( \leq 1024 )</td>
</tr>
<tr>
<td>( \Delta x )</td>
<td>10</td>
</tr>
<tr>
<td>( \epsilon_{\text{MPO}} )</td>
<td>( &lt; 10^{-2} \text{ meV} )</td>
</tr>
</tbody>
</table>

- Kinetic energy scale \( (t) \): \( < 1 \text{ meV} \)
- Interaction energy scale \( (V) \): \( < 10 \text{ meV} \)
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 $\chi$ is the original bond dimension. Compression preserves ground state physics.

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

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

under a single-bond truncation for some constant $C$.

One can show similar bounds for the ground state wavefunction, and expectation values of observables.
\[
\hat{H}_{\text{simple}} = \sum_{i<j<k<\ell} V_{ij\ell} c_i^\dagger c_j^\dagger c_k c_\ell
\]

\[
\hat{S} = \begin{pmatrix}
0 & \hat{1} & 0 & \hat{1} \\
0 & \hat{1} & \ddots & \ddots & \ddots \\
& \ddots & \ddots & \ddots & \ddots \\
& & \ddots & \ddots & \ddots & 0 \\
& & & & 0 & \hat{1} \\
& & & & 0 & 0
\end{pmatrix}
\]

\[
\hat{S}_i(\hat{O}[r_i\ldots]) = (\hat{O}[r_i - 1\ldots])
\]
\[ H = H_{\text{hop}} + H_{\text{int}} = H_{\text{hop}} + H_2 + H_3 + H_4 \]

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

\[ H_2 = \sum_{i<j} \tilde{V}_{ij}^{nn} i_n j_n \]

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

\[ H_4 = \sum_{i<j<k<\ell} \tilde{V}_{ijk\ell}^{cc} c_i^\dagger c_j^\dagger c_k c_\ell + \tilde{V}_{ijk\ell}^{cccc} c_i^\dagger c_j^\dagger c_k c_\ell + \tilde{V}_{ijk\ell}^{ccccc} c_i^\dagger c_j^\dagger c_k c_\ell, \]
Local Operators

Start with a local operator. e.g.

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

It is a sum of Pauli strings: \( \cdots \hat{1}_{-2}\hat{1}_{-1}\hat{X}_0\hat{X}_1\hat{1}_2\hat{1}_3 \cdots \).

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

$$\hat{H} = \hat{H}_L \hat{I}_R + \hat{I}_L \hat{H}_R + \sum_{i,j} M_{ij} \hat{h}_L^i \hat{h}_R^j.$$
**Matrix Product Operators**

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

\[
\hat{W} = \begin{pmatrix}
\hat{1} & \hat{X} & \hat{X} & 0 & \hat{h} & \hat{Z} \\
0 & 0 & 0 & \hat{J} & \hat{X} \\
0 & 0 & \hat{Z} & 0 \\
0 & 0 & 0 & \hat{K} & \hat{X} \\
\hat{1} & \hat{X} & \hat{X} & 0 & \hat{h} & \hat{Z} & \hat{X}
\end{pmatrix} = \Rightarrow \text{in} \Rightarrow \text{out}
\]

Bond Dimension 5

Matrix Product Operators

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.
Matrix Product Operators

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

For $\hat{H} = \sum_i J \hat{X}_i \hat{X}_i + K \hat{X}_i \hat{Z}_{i+1} \hat{X}_{i+2} + h \hat{Z}_i$, 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.
Matrix Product Operators

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

For \( \hat{H} = \sum_i J\hat{X}_i\hat{X}_i + K\hat{X}_i\hat{Z}_{i+1}\hat{X}_{i+2} + h\hat{Z}_i \),

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

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

$$\hat{W} = \begin{pmatrix}
\mathbb{1} & \hat{X} & \hat{X} & 0 \\
0 & 0 & 0 & \hat{Z} \\
0 & 0 & 0 & K\hat{X} \\
\mathbb{1} & & & \\
\end{pmatrix}$$
MPOs represent operators

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

\[ \hat{W} = \begin{pmatrix} \hat{1} & \hat{X} & \hat{X} & 0 & h \hat{Z} \\ 0 & 0 & 0 & 0 & J \hat{X} \\ 0 & 0 & 0 & 0 & K \hat{X} \\ 0 \end{pmatrix} \]

\[ \mathbf{v}_L \hat{W}^{(1)} = \begin{pmatrix} I_L \\ \hat{X}_1 \\ \hat{X}_1 \\ h \hat{Z}_1 \end{pmatrix}^T \]
MPOs represent operators

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

\[
\hat{W} = \begin{pmatrix}
\hat{I} & \hat{X} & \hat{X} & 0 & h \hat{Z} \\
0 & 0 & 0 & J \hat{X} \\
0 & 0 & \hat{Z} & 0 \\
0 & 0 & 0 & K \hat{X} \\
\hat{I}
\end{pmatrix}
\]

\[
v_L \hat{W}^{(1)} \hat{W}^{(2)} = \begin{bmatrix}
I_L \\
\hat{X}_2 \\
\hat{X}_2 \\
\hat{X}_1 \hat{Z}_2 \\
h \hat{Z}_1 + h \hat{Z}_1 + J \hat{X}_1 \hat{X}_2
\end{bmatrix}^T
\]
MPOs represent operators

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

\[ \hat{W} = \begin{pmatrix}
\hat{1} & \hat{X} & \hat{X} & 0 \\
0 & 0 & 0 & J\hat{X} \\
0 & 0 & \hat{Z} & 0 \\
0 & 0 & 0 & K\hat{X} \\
\hat{1} 
\end{pmatrix} \]

\[ \mathbf{v}_L \hat{W}^{(1)} \hat{W}^{(2)} \hat{W}^{(3)} = \\
\begin{bmatrix}
\hat{1} \\
\hat{X}_3 \\
\hat{X}_3 \\
\hat{X}_2\hat{Z}_3 \\
h\hat{Z}_1 + h\hat{Z}_2 + h\hat{Z}_3 + J\hat{X}_1\hat{X}_2 + J\hat{X}_2\hat{X}_3 + K\hat{X}_1\hat{Z}_2\hat{X}_3
\end{bmatrix}^T \]
MPOs represent operators

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

\[ \hat{W} = \begin{pmatrix} \hat{1} & \hat{X} & \hat{X} & 0 & h \hat{Z} \\ 0 & 0 & 0 & J \hat{X} \\ 0 & 0 & \hat{Z} & 0 \\ 0 & 0 & 0 & K \hat{X} \hat{1} \end{pmatrix} \]

\[ \mathbf{v}_L \hat{W}^{(1)} \ldots \hat{W}^{(n)} = \begin{bmatrix} \hat{I}_L \\ \hat{h}_L \\ \hat{H}_L \end{bmatrix}^T \]

— Unstarted

— Split

— Placed
MPOs represent operators

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

\[ \hat{W} = \begin{pmatrix}
\mathbb{I} & \hat{X} & \hat{X} & 0 & h\hat{Z} \\
0 & 0 & 0 & J\hat{X} & \hat{Z} \\
0 & 0 & h\hat{Z} & 0 & h\hat{Z} \\
0 & 0 & 0 & K\hat{X} & \mathbb{I}
\end{pmatrix} \]

\[ \mathbf{v}_L \hat{W}^{(1)} \cdots \hat{W}^{(n)} = \begin{bmatrix} \hat{I}_L \\ \hat{h}_L \\ \hat{H}_L \end{bmatrix}^T \]

\[ \hat{H} = \mathbf{v}_L \hat{W}^{(1)} \hat{W}^{(2)} \cdots \hat{W}^{(N)} \mathbf{v}_R \quad \text{where} \quad \mathbf{v}_R = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}^T \]
Many MPOs represent the same Hamiltonian.

\[
\hat{H} = \ldots \hat{W}^{(n)} \hat{W}^{(n+1)} \ldots \\
= \ldots (G G^{-1}) \hat{W}^{(n)} (G G^{-1}) \hat{W}^{(n+1)} (G G^{-1}) \ldots \\
= \ldots (G^{-1} \hat{W}^{(n)} G) (G^{-1} \hat{W}^{(n+1)} G) \ldots \\
= \ldots \hat{W}'^{(n)} \hat{W}'^{(n+1)} \ldots
\]

where \( \hat{W}' = G^{-1} \hat{W} G \), \( G G^{-1} = I \). This is a gauge choice. What gauge is best?
Gauge Transforms

Many MPOs represent the same Hamiltonian.

\[ \hat{H} = \cdots \hat{W}^{(n)} \hat{W}^{(n+1)} \cdots \]
\[ = \cdots (GG^{-1}) \hat{W}^{(n)} (GG^{-1}) \hat{W}^{(n+1)} (GG^{-1}) \cdots \]
\[ = \cdots (G^{-1} \hat{W}^{(n)} G) (G^{-1} \hat{W}^{(n+1)} G) \cdots \]
\[ = \cdots \hat{W}'^{(n)} \hat{W}'^{(n+1)} \cdots \]

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

**Compression Problem:** Given \( \hat{H} \), what is the optimal MPO (best approximation) \( \hat{W} \) at bond dim. \( \chi \)?
Almost Schmidt Decompositions

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

$$|\psi\rangle = \sum_{i,j} M_{ij} |\psi^i_L\rangle |\psi^j_R\rangle$$

can always be put in Schmidt form

$$|\psi\rangle = \sum_{a=1} s_a |\phi^a_L\rangle |\phi^a_R\rangle$$

with $$\langle \phi^a_L | \phi^b_L \rangle = \delta^{ab} = \langle \phi^a_R | \phi^b_R \rangle.$$
Almost Schmidt Decompositions

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\[ |\psi\rangle = \sum_{a=1} s_a |\phi^a_L\rangle |\phi^a_R\rangle \]

with \( \langle \phi^a_L | \phi^b_L \rangle = \delta^{ab} = \langle \phi^a_R | \phi^b_R \rangle \). Then

\[ |\psi'\rangle = \sum_{a=1}^{\chi} s_a |\phi^a_L\rangle |\phi^a_R\rangle \]

is the “optimal” rank-\( \chi \) approximation.
Almost Schmidt Decompositions

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

$$|\psi\rangle = \sum_{i,j} M_{ij} |\psi_i^L\rangle |\psi_j^R\rangle$$

can always be put in Schmidt form

$$|\psi\rangle = \sum_{a=1}^{s} s_a |\phi^a_L\rangle |\phi^a_R\rangle$$

with $\langle \phi^a_L | \phi^b_L \rangle = \delta^{ab} = \langle \phi^a_R | \phi^b_R \rangle$. Then

$$|\psi'\rangle = \sum_{a=1}^{\chi} s_a |\phi^a_L\rangle |\phi^a_R\rangle$$

is the “optimal” rank-$\chi$ approximation.

A local operator

$$\hat{H} = \hat{H}_L \hat{I}_R + \hat{I}_L \hat{H}_R + \sum_{i,j} M_{ij} \hat{h}_i^L \hat{h}_j^R$$

can be put in almost-Schmidt form

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

with $(\hat{O}^a_L | \hat{O}^b_L) = \delta^{ab} = (\hat{O}^a_R | \hat{O}^b_R)$.
Almost Schmidt Decompositions

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

\[ |\psi\rangle = \sum_{i,j} M_{ij} |\psi^i_L\rangle |\psi^j_R\rangle \]

can always be put in Schmidt form

\[ |\psi\rangle = \sum_{a=1}^{s} s_a |\phi^a_L\rangle |\phi^a_R\rangle \]

with \( \langle \phi^a_L | \phi^b_L \rangle = \delta^{ab} = \langle \phi^a_R | \phi^b_R \rangle \). Then

\[ |\psi'\rangle = \sum_{a=1}^{\chi} s_a |\phi^a_L\rangle |\phi^a_R\rangle \]

is the “optimal” rank-\( \chi \) approximation.

A local operator

\[ \hat{H} = \hat{H}_L \hat{I}_R + \hat{I}_L \hat{H}_R + \sum_{i,j} M_{ij} \hat{h}_i \hat{h}_j \]

can be put in almost-Schmidt form

\[ \hat{H} = \hat{H}_L \hat{I}_R + \hat{I}_L \hat{H}_R + \sum_{a=1}^{s} s_a \hat{O}_L^a \hat{O}_R^a \]

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

\[ \hat{H}' = \hat{H}_L \hat{I}_R + \hat{I}_L \hat{H}_R + \sum_{a=1}^{\chi} s_a \hat{O}_L^a \hat{O}_R^a \]

is the “optimal” rank-\( \chi \) 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?
How do we compute the almost-Schmidt form with MPOs?

\[ \hat{H} = \hat{H}_L \hat{l}_R + \hat{l}_L \hat{H}_R + \sum_{i,j} M_{i,j} \hat{h}_L^{i} \hat{h}_R^{i} \]

\[ = \begin{bmatrix} \hat{l}_L & \hat{h}_L & \hat{H}_L \end{bmatrix} \begin{bmatrix} 1 & M & 1 \\ \end{bmatrix} \begin{bmatrix} \hat{H}_R \\ \hat{h}_R \\ \hat{l}_R \end{bmatrix} \]

\[ = \cdots \hat{W}_L \hat{W}_L \hat{W}_L M \hat{W}_R \hat{W}_R \hat{W}_R \cdots \]
How do we compute the almost-Schmidt form with MPOs?

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

\[
\begin{bmatrix}
\hat{I}_L & \hat{h}_L & \hat{H}_L \\
1 & M & 1 \\
\end{bmatrix}
\begin{bmatrix}
\hat{H}_R \\
\hat{h}_R \\
\hat{I}_R \\
\end{bmatrix}
= \cdots \hat{W}_L \hat{W}_L \hat{W}_L \mathcal{M} \hat{W}_R \hat{W}_R \hat{W}_R \cdots
\]

SVD \( \mathcal{M} = USV^\dagger \) with \( S = \text{diag}(s_a) \), and let
\( \hat{W}_L' := U^\dagger \hat{W}_L U \), \( \hat{W}_R' := V^\dagger \hat{W}_R V \).
How do we compute the almost-Schmidt form with MPOs?

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

\[
\begin{bmatrix}
\hat{I}_L & \hat{h}_L & \hat{H}_L
\end{bmatrix}
\begin{bmatrix}
1 & M & \hat{H}_R \\
\hat{h}_R \\
\hat{I}_R
\end{bmatrix}
= \cdots \hat{W}_L \hat{W}_L \hat{W}_L \mathcal{M} \hat{W}_R \hat{W}_R \hat{W}_R \cdots
\]

SVD \(\mathcal{M} = U S V^\dagger\) with \(S = \text{diag}(s_a)\), and let

\[
\hat{W}_L' := U^\dagger \hat{W}_L U, \quad \hat{W}_R' := V^\dagger \hat{W}_R V .
\]

Then

\[
\hat{H} = \cdots \hat{W}_L' \hat{W}_L' \hat{W}_L' S \hat{W}_R' \hat{W}_R' \hat{W}_R' \cdots
\]

is an almost-Schmidt decomposition.

---

**Algorithm 5 iMPO Compression**

1: \textbf{procedure} \textsc{iCompress}(\hat{W}, \eta) \Comment{Cutoff \(\eta\)}
2: \hphantom{1:} \hat{W}_R \leftarrow \text{RightCan}[\hat{W}]
3: \hphantom{1:} \hat{W}_R \leftarrow R \hat{W}_R R^{-1} \text{ so that } [\hat{W}_R]_{1a} = 0
4: \hphantom{1:} \hat{W}_L, C \leftarrow \text{LeftCan}[\hat{W}_R]
5: \hphantom{1:} (U, S, V^\dagger) \leftarrow \text{SVD}[C]
6: \hphantom{1:} \hat{Q}, \hat{P} \leftarrow U^\dagger \hat{W}_L U, V^\dagger \hat{W}_R V
7: \hphantom{1:} \chi' \leftarrow \max\{a \in [1, \chi] : s_a > \eta\} \Comment{Defines \(P\)}
8: \hphantom{1:} \hat{W}_L'', S, \hat{W}_R'' \leftarrow p^\dagger \hat{W}_L' p, p^\dagger S p, p^\dagger \hat{W}_R' p
9: \hphantom{1:} \text{return } \hat{W}_L'' \Comment{One could also return } \hat{W}_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.
MPO Compression Algorithm

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

\[
\hat{H} = \hat{H}_L \hat{I}_R + \hat{I}_L \hat{H}_R + \sum_{i,j} M_{i,j} \hat{h}_L^i \hat{h}_R^j \\
= \begin{bmatrix}
\hat{I}_L & \hat{h}_L & \hat{H}_L
\end{bmatrix}
\begin{bmatrix}
1 & \ & \ \\
M & \hat{H}_R
\end{bmatrix}
\begin{bmatrix}
\hat{h}_R \\
\hat{I}_R
\end{bmatrix}
\]

\[
= \cdots \hat{W}_L \hat{W}_L' \hat{W}_L M \hat{W}_R \hat{W}_R' \hat{W}_R \cdots
\]

SVD \( M = USV^\dagger \) with \( S = \text{diag}(s_a) \), and let

\[
\hat{W}' := U^\dagger \hat{W}_L U, \ \hat{W}' := V^\dagger \hat{W}_R V.
\]

Then

\[
\hat{H} = \cdots \hat{W}' \hat{W}_L' \hat{W}_L S \hat{W}_R' \hat{W}_R' \hat{W}_R \cdots
\]

is an almost-Schmidt decomposition.

**Algorithm 6** iMPO Compression

1: procedure iCompress(\( \hat{W}, \eta \)) \( \triangleright \) Cutoff \( \eta \)
2: \( \hat{W}_R \leftarrow \text{RightCan}[\hat{W}] \)
3: \( \hat{W}_R \leftarrow R \hat{W}_R R^{-1} \) so that \([\hat{W}_R]_{1a} = 0\)
4: \( \hat{W}_L, C \leftarrow \text{LeftCan}[\hat{W}_R] \)
5: \( (U, S, V^\dagger) \leftarrow \text{SVD}[C] \)
6: \( \hat{Q}, \hat{P} \leftarrow U^\dagger \hat{W}_L U, V^\dagger \hat{W}_R V \)
7: \( \chi' \leftarrow \max\{a \in [1, \chi] : s_a > \eta\} \) \( \triangleright \) Defines \( \hat{P} \)
8: \( \hat{W}'_L', S, \hat{W}'_R' \leftarrow \hat{P}^\dagger \hat{W}_L' \hat{P}, \hat{P}^\dagger S \hat{P}, \hat{P}^\dagger \hat{W}_R' \hat{P} \)
9: return \( \hat{W}'_L' \) \( \triangleright \) One could also return \( \hat{W}'_R' \).

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.