Notes on "DMRG for interacting systems"

I. DMRG set up and symmetries (e.g. SU2)

II. Generalize to fermionic systems

III. Momentum as additional quantum number (or momentum space DMRG) — applying to FQHE

IV. Examples

\[ |\Psi\rangle = \sum_{ij} \psi_{ij} |i\rangle \otimes |j\rangle \]
1. Diagonalize $H_{\text{full}}$ to obtain $|\psi\rangle$.

2. Construct the reduced density matrix

$$
\rho_{ii'} = \sum_k \psi_{ik} \psi_{i'k}^* 
$$

(matrix representation $\Psi \sim M$, $\rho = MM^+$)

diagonalize $\rho$ and keep $m$ eigenvectors corresponding to $m$ largest eigenvalues. $\text{Tr} \rho = 1$.

3. Control truncation error $\varepsilon = 1 - \sum_{i=1}^{m} \rho_i$.

4. Construct $m$ new basis vectors from $2m$ states

$$
|d_e\rangle |S_{e+1}\rangle \Rightarrow |d_{e+1}\rangle 
$$

$$
|d_{e+1}\rangle = \sum A^{\ell+1}_{d_{e+1}, d_e} |S_{e+1}\rangle |d_e\rangle \otimes |S_{e+1}\rangle 
$$

Where each row is the eigenvector of $\tilde{\rho}$.

4. Update operators and truncate them, e.g.

$$
\tilde{H}_{\text{sys}} = \tilde{H}_{\text{sys}} \otimes I_{e+1} + \sum_{c, \ell} c_{ij} B_c^{\ell} \otimes B_j^{\ell+1}
$$

$H_{\text{sys}} = OHO^+$
0 is m×2m matrix, the rows of 0 are the kept states.

\[
\begin{pmatrix}
A^+ & A^- \\
\hat{d}_{e+1} & \alpha_e \\
\end{pmatrix}
\]

* SU2 symmetry

common eigenstates of \( \hat{S}^2 \), \( \hat{S}_z \) and \( H \).

basis states \( |s, m, \alpha\rangle \).

The matrix element can be obtained using Wigner–Eckart theorem.

\[
\langle \bar{s}', m', \alpha' | T^{(k)}_{g, i} | s, m, \alpha \rangle = (-1)^{S'} \frac{\langle \bar{s}' \alpha' | T^{(k)}_{i} | s, m \rangle}{\langle \bar{s}' \alpha' | T^{(k)}_{i} | s, m \rangle}
\]

\( T^{(k)}_{i} \) the irreducible tensor operator, \( i \)-other index, site for example. \( T^{(k)}_{g, i} \) it is \( g \) component \( (g = -k, -k+1, \ldots, k) \).

1. Set basis

\[
|SMd\rangle = \sum_{m, m_z} |s_{1} m_s s_{2} m_z, d\rangle \langle s_{1} m_s s_{2} m_z | SM\rangle
\]

clebsch–Gordan coefficients representing an additional unitary transformation to basis set of U1.
2. Identifying irreducible tensors

Definition \[ [\mathbf{S}_{\alpha i}, T^{(k)}_{\beta j}] = \frac{1}{\sqrt{2}} T^{(k)}_{\beta j} \]

\[ [\mathbf{S}_{\pm i}, T^{(k)}_{\pm j}] = \sqrt{(k \mp 1)(k \pm 8 + 1) + T^{(k)}_{\pm j}} \]

\[ T^{(1)} = -\frac{1}{\sqrt{2}} S^+ \]

\[ T^{(0)} = S^z \]

\[ T^{(-1)} = \frac{1}{\sqrt{2}} S^- \]

\[ \langle S^i T^{(0)} S \rangle = \sqrt{(2S+1)(S+1)} S \]

Two irreducible tensor operators \( T^{(k)} \), \( U^{(k)} \) can form a new irreducible operator \( X^{(k)} \)

\[ X^{(k)} = \sum_{\beta_1 \beta_2} (-1)^{k_1 + k_2 + \beta} \sqrt{2k+1} \begin{pmatrix} k_1 & k_2 & k \\ \beta_1 & \beta_2 & -\beta \end{pmatrix} T^{(k)}_{\beta_1} U^{(k)}_{\beta_2} \]

\[ \mathbf{S}_i \cdot \mathbf{S}_j = -T^{(1)}_{1 i} T^{(1)}_{1 j} - T^{(0)}_{1 i} T^{(0)}_{1 j} + T^{(1)}_{0 i} T^{(0)}_{0 j} \quad \text{rank-0} \]

Similarly, \( T^{(1)} : \)

\[ T^{(1)} = \frac{i}{\sqrt{2}} (-\frac{1}{\sqrt{2}})(\mathbf{S}_i \times \mathbf{S}_j)_x + i(\mathbf{S}_i \times \mathbf{S}_j)_y \]

\[ T^{(0)} = \frac{i}{\sqrt{2}} (\mathbf{S}_i \times \mathbf{S}_j)_z \]

\[ T^{(-1)} = \frac{i}{\sqrt{2}} \frac{1}{\sqrt{2}} [(\mathbf{S}_i \times \mathbf{S}_j)_x - i(\mathbf{S}_i \times \mathbf{S}_j)_y] \]

is useful for systems with three vector chiral terms.
3. Beside the transformation to total $S$ basis, and using the reduced matrix elements for irreducible tensor operators, everything else can be carried out similar to $U(1)$-DMRG.

* Example, $t$-$J$ model

$$H = \sum_{\langle ij \rangle} -t_{ij} (c_i^+ c_j + c_j^+ c_i) + \sum_{\langle ij \rangle} J_{ij} \left( \mathbf{S}_i \cdot \mathbf{S}_j - N_i N_j / 4 \right)$$

Irreducible tensor - rank -$\frac{1}{2}$

$$\begin{cases} T_{-\frac{1}{2}, i} = C_{i+} \\ T_{\frac{1}{2}, i} = -C_{i+} \end{cases}$$

Thus that the hopping term $H_t$ can be expressed as

$$H_t = \sum_{\langle ij \rangle} -t_{ij} \left( T_{-\frac{1}{2}, i} T_{-\frac{1}{2}, j} + T_{\frac{1}{2}, i} T_{\frac{1}{2}, j} - T_{-\frac{1}{2}, j} T_{\frac{1}{2}, i} - T_{\frac{1}{2}, i} T_{-\frac{1}{2}, j} \right)$$

Two irreducible $T^{(k_1)}$, $T^{(k_2)}$ can compose a new tensor $X^{(k)}$:

$$X^{(k)}_{\theta_1 \theta_2} = \sum_{\theta_1 \theta_2} T^{(k_1)}_{\theta_1 \theta_2} \cdot T^{(k_2)}_{\theta_1 \theta_2} \cdot S_{\theta_1 \theta_2} \cdot k, k = \sum_{\theta_1 \theta_2 \theta_3} \sqrt{2} k + 1 \cdot \sqrt{2} k + (k_1, k_2, k_3)$$

So $X^{(0)} = \sum_{\theta_1 \theta_2} T^{(1)}_{\theta_1 \theta_2} \cdot T^{(1)}_{\theta_1 \theta_2} \cdot \left( \begin{array}{cc} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{array} \right) = \frac{1}{\sqrt{2}} \left( T^{(1)}_{\frac{1}{2}, \frac{1}{2}} - T^{(1)}_{\frac{1}{2}, \frac{1}{2}} - T^{(1)}_{\frac{1}{2}, \frac{1}{2}} + T^{(1)}_{\frac{1}{2}, \frac{1}{2}} \right)$

Therefore, we have

$$H_t = \sum_{\langle ij \rangle} -\sqrt{2} t_{ij} \left( X^{(0)}_{\theta_1 \theta_2} + X^{(0)}_{\theta_1 \theta_2} \right)$$
II. DMRG for fermionic system

In DMRG, basis states usually form block structure according to their quantum numbers.

basis for system $|g_{n1}, g_{n2}, \ldots \rangle$

$g_{n1}$ ... maybe $S_z^\text{tot}$ of system
$g_{n2}$ ... maybe electron number $N_e^\text{tot}$ of system

operators are sparse matrices, which connect certain basis states with fixed change of quantum numbers.

$C_i^+$ gives $\Delta g_{n1} = \frac{1}{2}$, $\Delta g_{n2} = 1$, etc.

(In DMRG, you match the quantum number between operators and basis.)

Jordan-Wigner transformation is easy to implement in such a system

$C_i^+ = e^{i\pi \sum_{l<i} N_e} b_{i0}^+$

$b_{i0}$ is the corresponding bosonic creation operator, which adds one particle at site $i$ to the basis state (its a hardcore boson operator).
For \( C_{i_0}^+ \) in the system, the phase \( e^{i\pi \sum_{0<i} n_e} \) will be combined with \( b_i^+ \) when \( i \)-site is being included into system. But for \( C_{i_0}^+ \) in the environment, we incorporate part of sign

\[
(C_{i_0}^+|_{\text{env}}) = e^{i\pi \sum_{l<i} n_e}.
\]

When dealing with \( H_{\text{full}} \), all remaining signs for operators from environment or sys/env sites should be taken into account. They are easy to get since each basis has a good quantum number for electron number.

### III Momentum space DMRG set up

\[
H = \sum_j \xi_j C_j^+ C_j + \sum_{j_1,j_2,j_3,j_4} A_{j_1,j_2,j_3,j_4} C_{j_1}^+ C_{j_2}^+ C_{j_3} C_{j_4}
\]

\[
= \sum_j \xi_j C_j^+ C_j + \sum_{j_1,j_2,j_3,j_4} A_{j_1,j_2,j_3,j_4} C_{j_1}^+ C_{j_2}^+ C_{j_3} C_{j_4}
\]

\( C_j^+ \) creates an electron with momentum \( j \). The total momentum is conserved.
* Adding \( q_n^3 \) total momentum to basis quantum numbers.

\[
|q_{n1}, q_{n2}, q_{n3}, \ldots >
\]

\[
\uparrow \uparrow \uparrow \text{tot} \quad \uparrow \uparrow \downarrow \text{tot} \quad ...
\]

* Order the summation to speed up

\[
H = \sum_{j_1, j_2, q} R_{j_1 j_2, j_2 q, j_1 q} \quad C_{j_1}^+ C_{j_2}^+ C_{j_2-q} C_{j_1+q}
\]

\[
\{ \begin{array}{l} j_1 < j_2 \\ j_1 + q < j_2 - q \end{array} \}
\]

\[
R_{j_1 j_2 j_3 j_4} = A_{j_1 j_2 j_3 j_4} + A_{j_2 j_1 j_4 j_3}
\]

\[
- A_{j_2 j_1 j_3 j_4} - A_{j_1 j_2 j_4 j_3}
\]

\[
A_{j_1 j_2 j_3 j_4} = \int \phi_{j_1}^*(n) \phi_{j_2}^*(\vec{r}_2) V(n-\vec{r}_2) \phi_{j_3} (\vec{r}_2) \phi_{j_4} (\vec{r}_2)
\]

* Combining similar terms to reduce the number of operators, e.g.

\[
\text{define } \sum_{j_2, q} R_{j_1 j_2 j_2 q, j_1 q} \quad C_{j_2}^+ C_{j_2-q} C_{j_1+q} = C_3 (j_1)
\]

\[
H \rightarrow \sum_{j_1} \quad C_3 (j_1)
\]

Only when 3 \( C \) operators are all in system or environment!

(keep remaining terms unchanged).
* carefully including all terms to your $H_{\text{full}}$ (so many terms ...).

* benefit is that we can target states with different $q_{\text{tot}}$. It works for torus, infinite cylinder (or finite) or sphere.

* Exact diagonalization program for FQHE (torus example)

The single particle wavefunction, \( \Psi_{N_i, j}(x, y) = \left( \frac{1}{2N! \pi^{N/2} L_y l} \right)^{1/2} e^{i \frac{x_j^2}{2l^2} y - \frac{(x_j - x)^2}{2l^2}} \mathcal{H}_N \left( \frac{x_j - x}{\ell} \right) \) (infinite system \( L_x = \infty \)).

But, we should use the finite one: \( L_x L_y = 2\pi l^2 N_s \)

\[
\sum_{j=1}^{+\infty} e^{i \frac{x_j^2}{2l^2} y - \frac{(x - x_{jk})^2}{2l^2}} \mathcal{H}_N \left( \frac{x_j - x}{\ell} \right)
\]

\( x_{jk} = \frac{2\pi j \ell^2}{L_y} + k L_x \) (forcing the periodic condition).

\[ V_{ij}^{x_{ij}, j_4} = \frac{1}{2} \int d^2 \tau_1 d^2 \tau_2 \Psi_{N_i}^* \Psi_{N_j} \mathcal{V} \left( \tau_1 - \tau_2 \right) \Psi_{N_{j_1}} \Psi_{N_{j_3}} \Psi_{N_{j_4}} \]

set up ED code for \( N_s = 6 \) (flux number) and \( N_e = 2 \) (electron number).

totally \( \frac{N_s!}{N_e! (N_s - N_e)!} \) states \( \Rightarrow \frac{6 \cdot 5}{2} = 15 \)

110000 --- too many, wait, use \( k_{\text{total}} \) momentum!
k=0 sector \ (mod N_5),

\[
\begin{align*}
0 & : 001 \quad 1 + 5 = 0 \\
001 & : 010 \quad 2 + 4 = 0
\end{align*}
\]

only 2 states

\[
H = \begin{pmatrix}
R_{1551} & fR_{1542} \\
*fR_{1542} & R_{2442}
\end{pmatrix}
\]

f-fermion sign \ (f=1) 
check (if \ Ne > 2).

\[
0 \quad \frac{\partial}{\partial z} \quad \frac{\partial}{\partial \phi}
\]

are there particles in between to give fermionic signs?

k=1 sector

\[
\begin{align*}
0 & : 10000 \\
001 & : 0001 \\
000 & : 110
\end{align*}
\]

\[
\begin{pmatrix}
R_{0110} & f_1R_{0152} & f_2R_{0143} \\
* & R_{2552} & f_3R_{2543} \\
* & * & R_{3443}
\end{pmatrix}
\]

3-fold degenerating Laughlin FSHE

excitation gap is finite and robust
more electrons, separating orbits to A & B

\[ \left| \tilde{\psi}_A \right> = \left| n_0, n_1, n_2, \ldots, n_{N_{3/2}} \right> \ldots \]

occupation number for a set of orbitals in A.

a table for finding \( \tilde{\psi}_A \) from \( \{ n_j \} \).

so once you use \( C_{j_1} C_{j_2} \ldots |\tilde{\psi}_A> \) etc

you can get new index |\tilde{\psi}'> quickly.

\textbf{total basis} \( |\phi> = |\tilde{\psi}_A> \otimes |\tilde{\psi}_B> \)

\textbf{new index}, adding one basis when \( \Phi_n(i_A) + \Phi_n(j_B) = \text{desired momentum} \ k \).

\textbf{a table for finding} \( \tilde{\psi} \) quickly from \( \left( i_A, i_B \right) \).

Set up matrix elements, then we can diagonalize \( H \)

for a chosen total momentum \( k. \) \( |\Psi> = \sum_{i_A} \sum_{i_B} \gamma_{i_A} |i_A> \otimes |i_B> \)

\( E(k) \) gives information of topological degeneracy.
Energy spectrum for torus system with varying tunneling $t$. Predicted by Xiao-Gang Wen & G.-Q. Wu.

Fractional Quantum Hall Bilayers at Half-Filling: Non-Abelian Phase

Tunneling-driven
* Calculating topological Chern number
adding generalized boundary phase \( \theta \) \((\alpha, \beta)\)

\[
\Gamma (L \times \hat{x}) \Psi_j (x, y) = e^{i \theta \hat{x} \cdot \hat{y}} \Psi_j (x, y)
\]

\[
\Gamma (L \hat{y} \hat{y}) = e^{i \beta \hat{y}}
\]

\( \Gamma \) is the single-particle magnetic translational operator in the \( x \) or \( y \) directions.

\[
\Psi_{Nj} (x, y) = \left( \frac{1}{(2^N N! \pi^{N/2} L_y L_x)} \right)^{1/2} e^{i \frac{\hat{X}_{jk}'}{\hbar^2} \hat{p}^2 - \frac{(x - X_{jk})^2}{2\hbar^2}} \cdot H_N \left( \frac{X_{jk} - x}{\hbar} \right)
\]

\( \Psi_{Nj} \) is the momentum index in Landau gauge.

\[
X_{jk}' = \frac{2\pi k^2}{L_y} + \frac{2x^2}{L_x} + \beta \hbar^2
\]

Nontrivial: changing \( \beta = 0 \) to \( \frac{2\pi}{L_y} \), will increase \( j \rightarrow j+1 \) (representing the center of the orbital).

Obtain many-body wavefunction as before

\[
| \Psi (\alpha, \beta) \rangle = \sum \Psi_{ij} (\alpha, \beta) | \hat{T}_A (\alpha, \beta) \rangle | | \hat{T}_B (\alpha, \beta) \rangle
\]

(One should also do unitary transformation, so that

\[
\Psi \rightarrow e^{-i \alpha (x + \hbar \tilde{X}) - \frac{\beta (y + \hbar \tilde{Y})}{\hbar}}
\]

Hamiltonian

\[
-i \frac{\partial}{\partial x} \rightarrow -i \frac{\partial}{\partial x} + \alpha, -i \frac{\partial}{\partial y} \rightarrow -i \frac{\partial}{\partial y} + \beta
\]

\[
C = \frac{i}{4\pi} \int dx \, dy \left( \frac{\partial \Psi}{\partial \theta_x} \frac{\partial \Psi^*}{\partial \theta_y} - \frac{\partial \Psi^*}{\partial \theta_x} \frac{\partial \Psi}{\partial \theta_y} \right) \text{ with } \frac{\partial \Psi}{\partial \theta_x} = \alpha L_x \frac{\partial \Psi}{\partial \theta_y} = \beta L_y
\]
For one component FHHE with no disorder, if there is a spectrum gap between ground states and excited states, we have \( \gamma_{ij}(x, \beta) = \gamma_{ij}(0, 0) \) (interaction does not depend on boundary phases although \( \gamma_{ij} \) (orbitals) does).

All Berry phase comes from the rotation of the basis vectors, the Chern number = filling number = \( N_e / N_g \).

The bilayer case is nontrivial.

\[ \begin{align*}
\theta_x^2 & \rightarrow 2 \\
\theta_y^2 & \rightarrow 0 \\
\theta_x^1 & \rightarrow 1 \\
\theta_y^1 & \rightarrow \theta_x^1
\end{align*} \]

if \((\theta_x', \theta_y^2)\) change, but \((\theta_x^2 = \theta_y^1 = 0)\), the interlayer interaction will depend on boundary phases, we can obtain \( \delta \)-drag Hall conductance.

\[
C^{\alpha \beta} = \frac{i}{4\pi} \iint d\theta_x d\theta_y \left\{ \frac{\partial \psi^\alpha}{\partial \theta_x^\beta} \frac{\partial \psi^\beta}{\partial \theta_y^\alpha} - \frac{\partial \psi^\alpha}{\partial \theta_y^\beta} \frac{\partial \psi^\beta}{\partial \theta_x^\alpha} \right\}
\]

forms 2x2 Chern number matrix:

for 331 Halperin state: \( C = \frac{1}{8} \left( \begin{array}{cc} 3 & -1 \\ -1 & 3 \end{array} \right) \) inverse of \( k \) matrix. \( K = \left( \begin{array}{cc} 3 & 1 \\ 1 & 3 \end{array} \right) \).
IV Examples

* DMRG inserting flux to detect topological degeneracy

\[ S_i^+ S_j^- \rightarrow e^{i \theta y} S_i^+ S_j^- \]

if the bond crosses the \( y \)-boundary (e.g. \( i_y = 2y \), \( j_y = 1 \))

using \( \Psi(\theta y - \Delta \theta) \) as the initial wavefunction for new \( \theta y \). Updating \( H(\theta y) \) locally when we sweep pass different points.

Measuring \( \langle S_i^z \rangle \) for different \( \theta y \), comparing entanglement spectrum as function of \( \theta y \).

* Spontaneous Quantum Hall Effect

Using complex code to work with minimum entangled state if time-reversal symmetry is spontaneously broken

(In real code, ground state would have additional double degeneracy).
Topological entanglement spectrum and entropy for detecting topological order (FQHE) root configuration

$1000, 1000$ for $1/3$ FQHE

$\{111000, 111000\}$ for Read-Rezayi $\frac{13}{5}$

$\{10101, 10101, 10101\}$

**TABLE 1:** In this table, we analyze the counting rules of the edge excitations in the "...11100111001100..." sector, which has multiplicities 1, 1, 3, 6, ... at $\Delta L = 0, 1, 2, 3, ...$

<table>
<thead>
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<th>$\Delta L = 0$</th>
<th>$\Delta L = 1$</th>
<th>$\Delta L = 2$</th>
<th>$\Delta L = 3$</th>
<th>$\Delta L = 4$</th>
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</tbody>
</table>

$\uparrow$
### Table II

In this table, we analyze the counting rule of the edge excitations in the ...111001110011|00 ... sector, which has multiplicities 1, 2, 5, 9, ... at ΔL = 0, 1, 2, 3, ...

<table>
<thead>
<tr>
<th>ΔL = 0</th>
<th>ΔL = 1</th>
<th>ΔL = 2</th>
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</table>

### Table III

In this table, we analyze the counting rule of the edge excitations in the ...10101101101101|0000 ... sector, which has multiplicities 1, 3, 6, 13, ... at ΔL = 0, 1, 2, 3, ...

<table>
<thead>
<tr>
<th>ΔL = 0</th>
<th>ΔL = 1</th>
<th>ΔL = 2</th>
<th>ΔL = 3</th>
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### Table IV

In this table, we analyze the counting rule of the edge excitations in the ...10101101101100|00 ... sector, which has multiplicities 1, 2, 5, 10, ... at ΔL = 0, 1, 2, ...

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</tr>
</tbody>
</table>

### III. Results for finite-layer thickness

In a two dimensional system, the ideal Coulomb interaction between electrons has $V(q) = 1/q$. The finite thickness in the normal direction of an experimental quantum Hall system modifies the short-distance part of the ideal 2D interaction, yielding
Infinite Cylinder $L = 24$

$T, T', T' \ldots$ and $T, T', T' \ldots$ (I3)

Entanglement Spectrum:

Ground State: $T = TOTOT Totot TOTOT TOTOT$

On Cylinder, we also find another

 Detected by Entanglement Spectrum:

Read-Rezayi State

Entanglement Spectrum: $T2/5$ FQHE as
Largest system (Ne=24)

Better spectrum for Moore-Read state

Ne=22

Halfpern 331 State

Moore-Read vs. Halfpern 331 Entanglement spectrum and entropy