TECHNISCHE UNIVERSITÄT DRESDEN

DRESDEN concept

SFB 1143

# Tensor Networks (SS2021)

## Lecture 10: Fermionic systems + MPO-MPS evolution

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# § 2.6 Free fermion case

- The free fermionic case, being exactly solvable, is invaluable for gaining some insights.

$$H = \sum_{j,l=1}^{N} c_j^\dagger T_{jl} c_l$$

Diagonalization:

$$H = c^\dagger T c = c^\dagger U^\dagger \left(U T U^\dagger\right) U c = d^\dagger \varepsilon d = \sum_{m=1}^{N} \varepsilon_m d_m^\dagger d_m$$

Ground state: $|\psi\rangle = \prod_{m=1}^{M} d_m^\dagger \, |0\rangle$ $(\varepsilon_m < 0 \text{ for } 1 \le m \le M)$

# § 2.6 Free fermion case

- Covariance/correlation matrix:

$$G_{lj} = \langle\psi|c_j^\dagger c_l|\psi\rangle$$

Review: I. Peschel & V. Eisler, J. Phys. A 42, 504003 (2009).

# § 2.6 Free fermion case

- Covariance/correlation matrix:

$$G_{lj} = \langle\psi|c_j^\dagger c_l|\psi\rangle$$

$$\Rightarrow \quad \left(UGU^\dagger\right)_{m'm} = \sum_{j,l=1}^{N} U_{m'l}\,\langle\psi|c_j^\dagger c_l|\psi\rangle\, U_{jm}^\dagger$$

$$= \langle\psi|d_m^\dagger d_{m'}|\psi\rangle$$

$$= \begin{pmatrix} I_{M\times M} & \\ & 0_{(N-M)\times(N-M)} \end{pmatrix}_{m'm}$$

# § 2.6 Free fermion case

- Covariance/correlation matrix:

$$G_{lj} = \langle\psi|c_j^\dagger c_l|\psi\rangle$$

- ➢ The same unitary diagonalizes the single-particle Hamiltonian $T$ and the correlation matrix $G$.

- ➢ For free fermions ($|\psi\rangle$: Gaussian state), higher order correlation functions are obtained from $G$ via Wick's theorem.

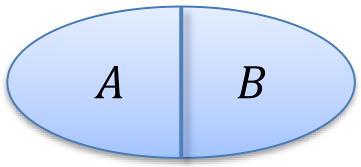
- ➢ For general pure state, the single-particle basis which diagonalizes $G$ defines natural orbitals.

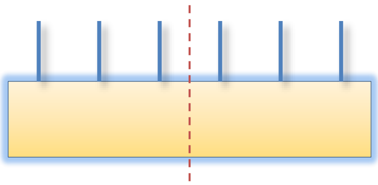
# § 2.6 Free fermion case

- Use the correlation matrix to obtain the reduced density matrix of free fermions:

$$G^A_{lj} = \langle\psi|c_j^\dagger c_l|\psi\rangle = \mathrm{tr}_A(\rho^A c_j^\dagger c_l)$$

submatrix of $G$ with $j, l \in A$

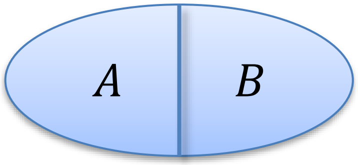


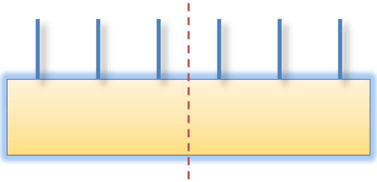
# § 2.6 Free fermion case

- Use the correlation matrix to obtain the reduced density matrix of free fermions:

$$G_{lj}^{A} = \langle\psi|c_j^{\dagger} c_l|\psi\rangle = \mathrm{tr}_A(\rho^A c_j^{\dagger} c_l)$$




Diagonalize $G^A$:



$$G^A = V^{\dagger} \Lambda V$$

$$G_{lj}^{A} = \sum_{p=1}^{N_A} V_{lp}^{\dagger} \Lambda_p V_{pj} \qquad \Lambda_p \in [0,1]$$

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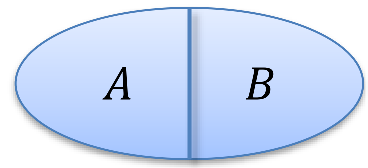
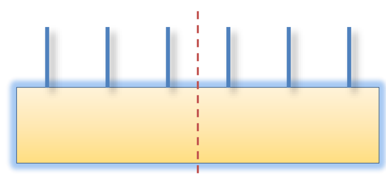
$$G^A_{lj} = \langle\psi|c_j^\dagger c_l|\psi\rangle = \mathrm{tr}_A(\rho^A c_j^\dagger c_l)$$




$$G^A_{lj} = \sum_{p=1}^{N_A} V^\dagger_{lp}\Lambda_p V_{pj}$$



$$\Rightarrow \Lambda_p\delta_{pp'} = \sum_{j,l=1}^{N_A} V_{pl}G^A_{lj}V^\dagger_{jp'} = \sum_{j,l=1}^{N_A} V_{pl}\mathrm{tr}_A(\rho^A c_j^\dagger c_l)V^\dagger_{jp'} = \mathrm{tr}_A(\rho^A f_{p'}^\dagger f_p)$$

# § 2.6 Free fermion case

$$\Lambda_p \delta_{pp'} = \sum_{j,l=1}^{N_A} V_{pl} G_{lj}^A V_{jp'}^\dagger = \sum_{j,l=1}^{N_A} V_{pl} \mathrm{tr}_A(\rho^A c_j^\dagger c_l) V_{jp'}^\dagger = \mathrm{tr}_A(\rho^A f_{p'}^\dagger f_p)$$

$$\Rightarrow \quad \rho^A = \prod_{p=1}^{N_A} [\Lambda_p f_p^\dagger f_p + (1-\Lambda_p) f_p f_p^\dagger] \qquad \Lambda_p \in [0,1]$$

↓

$\rho^A > 0$ and $(\rho^A)^2 \leq \rho^A$

# § 2.6 Free fermion case

$$\rho^A = \prod_{p=1}^{N_A} [\Lambda_p f_p^\dagger f_p + (1 - \Lambda_p) f_p f_p^\dagger]$$

Schmidt vectors:

$$|\alpha\rangle \equiv \left|n_1, n_2, \dots, n_{N_A}\right\rangle$$
$$= \left(f_1^\dagger\right)^{n_1} \left(f_2^\dagger\right)^{n_2} \cdots \left(f_{N_A}^\dagger\right)^{n_{N_A}} |0\rangle$$

Eigenvalues of $\rho^A$:

$$\rho^A |\alpha\rangle = \prod_{p=1}^{N_A} [\Lambda_p n_p + (1 - \Lambda_p)(1 - n_p)]\, |\alpha\rangle$$

Entanglement spectrum: eigenvalues of $-\ln \rho^A$

# § 2.6 Free fermion case

$$\rho^A = \prod_{p=1}^{N_A} [\Lambda_p f_p^\dagger f_p + (1 - \Lambda_p) f_p f_p^\dagger]$$

Entanglement/modular Hamiltonian:

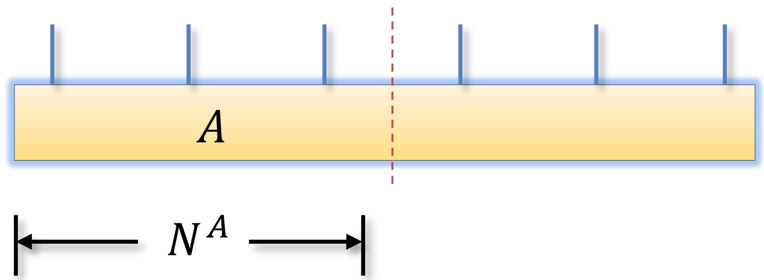
$$\rho^A \propto \exp\left[ -\sum_{p=1}^{N_A} \tilde{\varepsilon}_p f_p^\dagger f_p \right]$$

$$\tilde{\varepsilon}_p = -\ln\left(\frac{\Lambda_p}{1 - \Lambda_p}\right)$$

- Zero mode ($\tilde{\varepsilon}_p = 0$) indicates degeneracy in entanglement spectrum.

# § 2.6 Free fermion case

- The Schmidt decomposition can be computed exactly for free fermionic systems.




$$|\psi\rangle = \sum_{\alpha=1}^{\chi} \lambda_\alpha |\alpha^A\rangle \otimes |\alpha^B\rangle \qquad \chi \sim 2^{N_A}$$

➢ Each Schmidt vector $|\alpha^A\rangle$ is a free fermionic state.

# § 2.6 Free fermion case

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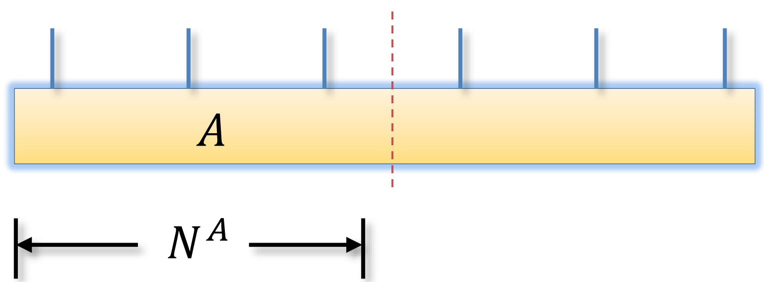


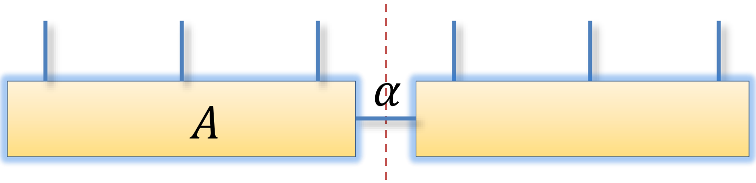

1D gapless case (partially filled Fermi sea):

$$S(N_A) = -\mathrm{tr}_A(\rho^A \ln \rho^A) \sim \begin{cases} \dfrac{c}{6} \ln N_A & \text{OBC} \\ \dfrac{c}{3} \ln N_A & \text{PBC} \end{cases}$$

$c$ = # of gapless modes

# § 2.6 Free fermion case

- MPS approximation: truncating reduced density matrix




$$\rho^A = \prod_{p=1}^{N_A} [\Lambda_p f_p^\dagger f_p + (1 - \Lambda_p) f_p f_p^\dagger]$$

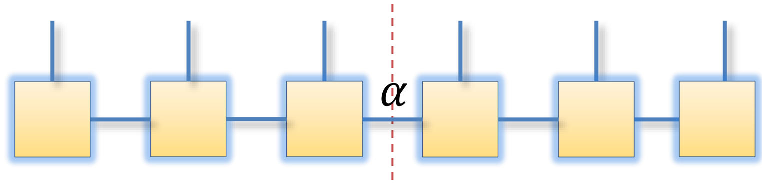
- Gaussian truncation: remove some modes with small contributions to $\rho^A$ → preserving Gaussian nature

- SVD truncation: remove some states $|\alpha\rangle$ corresponding to small eigenvalues of $\rho^A$ → more accurate

M. T. Fishman & S. R. White, Phys. Rev. B 92, 075132 (2015).

# § 2.6 Free fermion case

- Successively truncating $\rho$ for all bipartitions produces an MPS:

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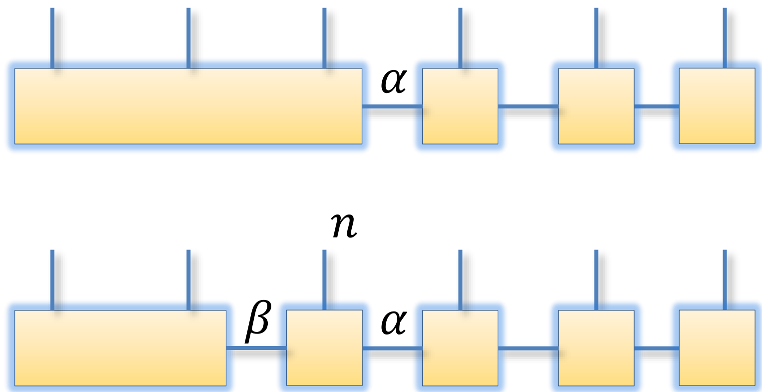


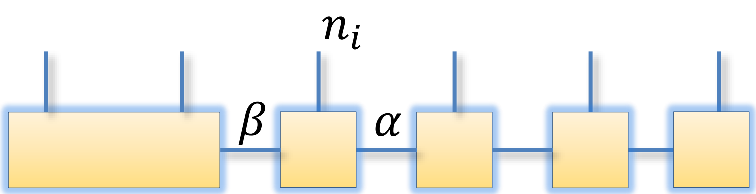

$\langle \alpha | \alpha' \rangle = \delta_{\alpha\alpha'}$

$\langle \beta | \beta' \rangle = \delta_{\beta\beta'}$

$$|\alpha\rangle = \sum_{\beta,n} A^n_{\beta\alpha} |\beta\rangle \otimes |n\rangle \quad \Rightarrow \quad A^n_{\beta\alpha} = (\langle\beta| \otimes \langle n|)|\alpha\rangle$$

G. Petrica, B.-X. Zheng, G. K.-L. Chan & B. K. Clark, Phys. Rev. B 103, 125161 (2021).

# § 2.6 Free fermion case




$$A^{n_i}_{\beta\alpha} = (\langle\beta| \otimes \langle n_i|)|\alpha\rangle$$

Example: $|\alpha\rangle = f_1^\dagger \cdots f_M^\dagger |0\rangle_{1\to i}$ $\quad |n_i = 0\rangle = |0\rangle_i$ $\quad |\beta\rangle = \tilde{f}_1^\dagger \cdots \tilde{f}_M^\dagger |0\rangle_{1\to i-1}$

$$f_p^\dagger = \sum_{j=1}^{i} c_j^\dagger V_{jp}^\dagger \qquad \tilde{f}_q^\dagger = \sum_{j=1}^{i-1} c_j^\dagger \tilde{V}_{jq}^\dagger$$

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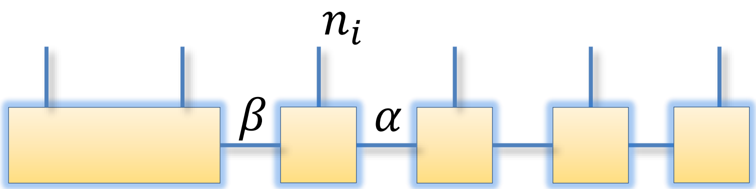


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$$f_p^\dagger = \sum_{j=1}^{i} c_j^\dagger V_{jp}^\dagger \qquad \tilde{f}_q^\dagger = \sum_{j=1}^{i} c_j^\dagger \tilde{V}_{jq}^\dagger$$

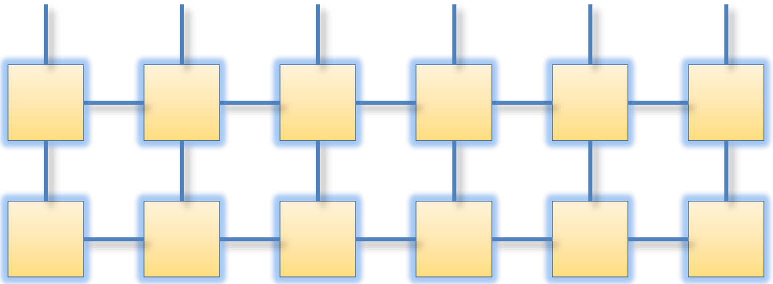
$$\Rightarrow \quad A^{n_i=0}_{\beta\alpha} = \langle 0|\tilde{f}_M \cdots \tilde{f}_1 f_1^\dagger \cdots f_M^\dagger|0\rangle = \det[(\tilde{V}V^\dagger)_{M\times M}]$$

G. Petrica, B.-X. Zheng, G. K.-L. Chan & B. K. Clark, Phys. Rev. B 103, 125161 (2021).

# § 3.1 MPO-MPS evolution

- In tensor network calculations, we often encounter the following MPO-MPS evolution:

$$|\psi'\rangle = W|\psi\rangle$$



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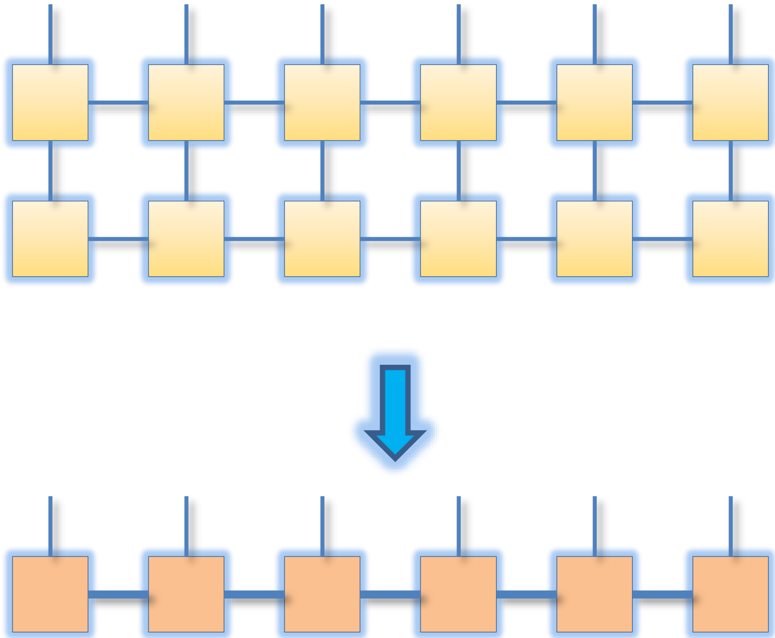

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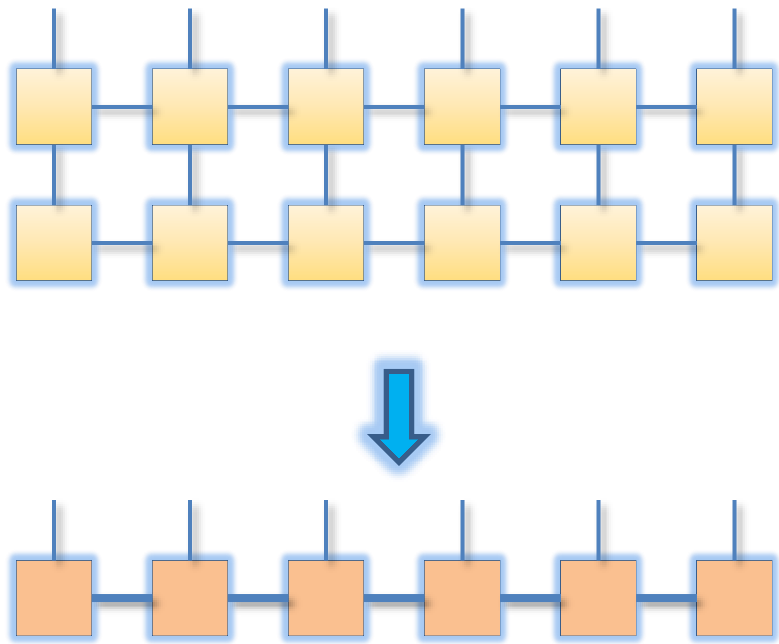
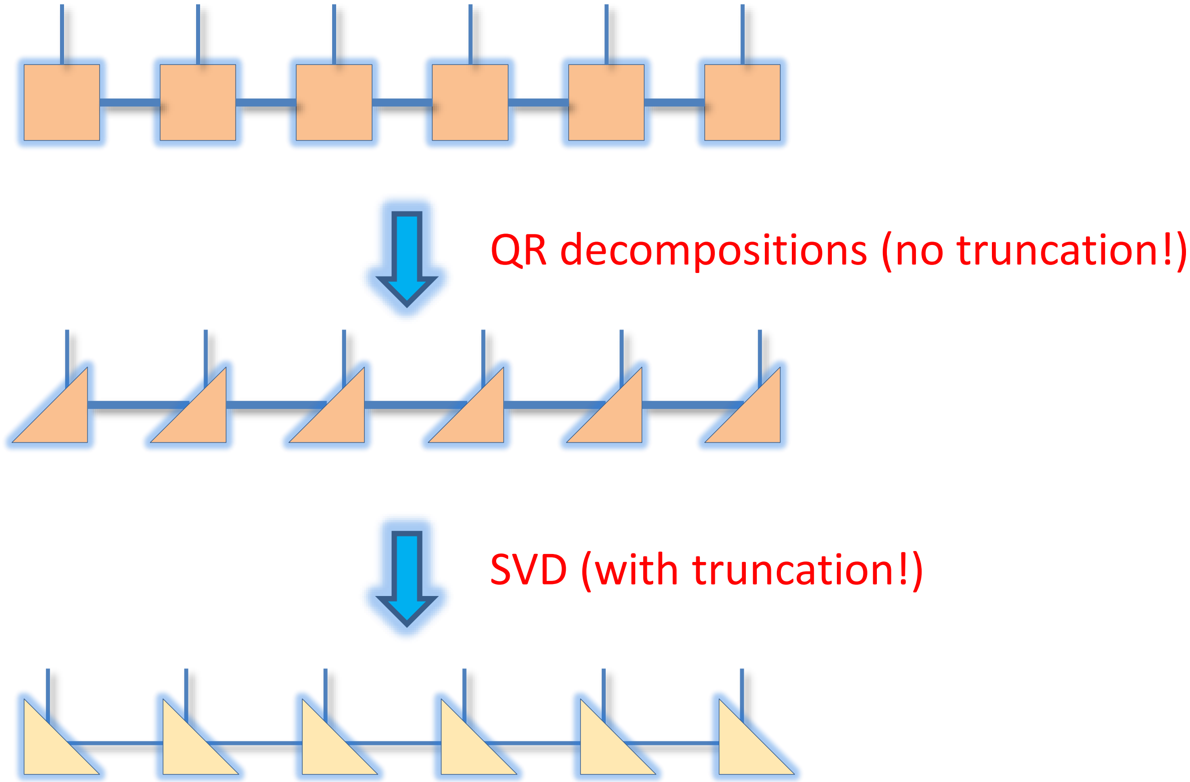


Bond dimension increases!
How to truncate?

# § 3.1 MPO-MPS evolution

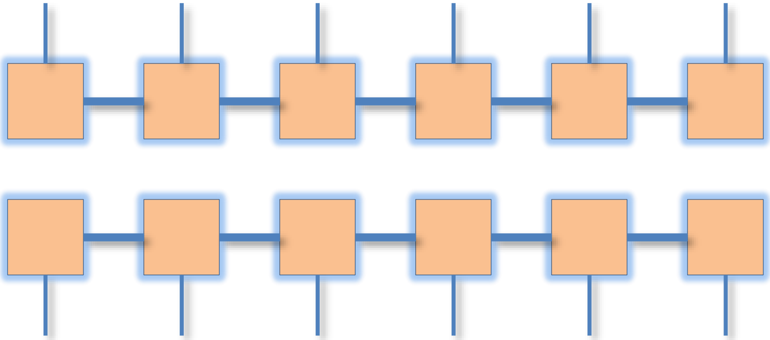
- Use bond canonical form (truncating reduced density matrices)



# § 3.1 MPO-MPS evolution

- The SVD truncation is often enough. If you are not satisfied, you may supplement it with further DMRG optimization:

$|\psi'\rangle\langle\psi'| =$



Maximize $|\langle\psi'|\psi(D)\rangle|^2 = \langle\psi(D)|\psi'\rangle\langle\psi'|\psi(D)\rangle$!

See also https://tensornetwork.org/mps/algorithms/denmat_mpo_mps/