TECHNISCHE UNIVERSITÄT DRESDEN

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SFB 1143

Tensor Networks (SS2021)

Lecture 9: Fermionic systems

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§ 2.5 Spin-fermion mapping

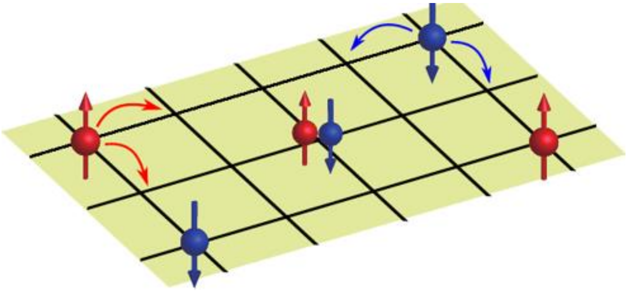
- In physics we are often interested in electronic systems, e.g., the Hubbard model:

$$H = -t \sum_{\langle ij \rangle, \sigma = \uparrow, \downarrow} \left(c_{i\sigma}^{\dagger} c_{j\sigma} + c_{j\sigma}^{\dagger} c_{i\sigma} \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

Fermionic operators:

$$\left\{ c_{i\sigma}, c_{j\sigma'}^{\dagger} \right\} = \delta_{ij} \delta_{\sigma\sigma'}$$

$$\left\{ c_{i\sigma}, c_{j\sigma'} \right\} = \left\{ c_{i\sigma}^{\dagger}, c_{j\sigma'}^{\dagger} \right\} = 0$$



§ 2.5 Spin-fermion mapping

- The many-fermion Hilbert space (i.e. Fock space) has a special structure due to the anticommutation relations.

Consider spinless fermions first: $\{c, c^\dagger\} = 1$

Single-site case:

$|0\rangle$ $\qquad$ $|1\rangle = c^\dagger|0\rangle$

$c|0\rangle = 0$ $\Rightarrow$ $|0\rangle$: vacuum

§ 2.5 Spin-fermion mapping

Single-site case: $|0\rangle$ $|1\rangle = c^\dagger|0\rangle$

- Particle number operator: $n \equiv c^\dagger c$

$$n|0\rangle = 0|0\rangle \qquad n|1\rangle = 1|1\rangle$$

- Fermion parity operator: $(-1)^n = \exp(i\pi n)$

$$(-1)^n|0\rangle = 1|0\rangle \qquad (-1)^n|1\rangle = -1|1\rangle$$

- Projectors: $|0\rangle\langle 0| = cc^\dagger$ $|1\rangle\langle 1| = c^\dagger c$

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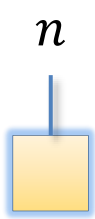
- States: $|n\rangle = \left(c^\dagger\right)^n |0\rangle \qquad (n = 0,1)$

$$|\psi\rangle = \sum_{n=0,1} \psi_n |n\rangle$$



Superselection rule: States with different fermion parity cannot mix (i.e., only eigenstates of fermion parity make sense!)

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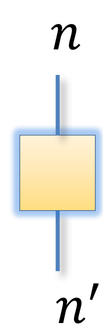
- Operators: $c^\dagger = |1\rangle\langle 0|$ $\qquad c = |0\rangle\langle 1|$

$$O = \sum_{n,n'=0,1} O_{n,n'} \, |n\rangle\langle n'|$$



$$c^\dagger \to \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \sigma^+$$

$$c \to \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \sigma^-$$

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N-site case: $|n_1, n_2, \dots, n_N\rangle \equiv \left(c_1^\dagger\right)^{n_1} \left(c_2^\dagger\right)^{n_2} \cdots \left(c_N^\dagger\right)^{n_N} |0\rangle$

$n_j = 0{,}1$

$c_j |0\rangle = 0 \ \forall j$

Anticommutation relations:

$$\left\{c_i, c_j^\dagger\right\} = \delta_{ij}$$

$$\left\{c_i, c_j\right\} = \left\{c_i^\dagger, c_j^\dagger\right\} = 0$$

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Acting operators on states:

$$c_j\left|n_1, \dots n_j, \dots, n_N\right\rangle = c_j\left(c_1^\dagger\right)^{n_1} \cdots \left(c_j^\dagger\right)^{n_j} \cdots \left(c_N^\dagger\right)^{n_N}|0\rangle$$

$$= (-1)^{n_1+\cdots+n_{j-1}}\left(c_1^\dagger\right)^{n_1} \cdots c_j\left(c_j^\dagger\right)^{n_j} \cdots \left(c_N^\dagger\right)^{n_N}|0\rangle$$

$$= (-1)^{n_1+\cdots+n_{j-1}}\left(c_1^\dagger\right)^{n_1} \cdots \delta_{n_j,1}\left(c_j^\dagger\right)^{n_j-1} \cdots \left(c_N^\dagger\right)^{n_N}|0\rangle$$

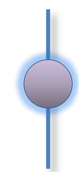
$$= (-1)^{n_1+\cdots+n_{j-1}}\delta_{n_j,1}\left|n_1, \dots n_j - 1, \dots, n_N\right\rangle$$

$$\Rightarrow \quad c_j = \sum_{\{n\}}(-1)^{\sum_{l=1}^{j-1} n_l}\,\delta_{n_j,1}\left|n_1, \dots n_j - 1, \dots, n_N\right\rangle\left\langle n_1, \dots n_j, \dots, n_N\right|$$

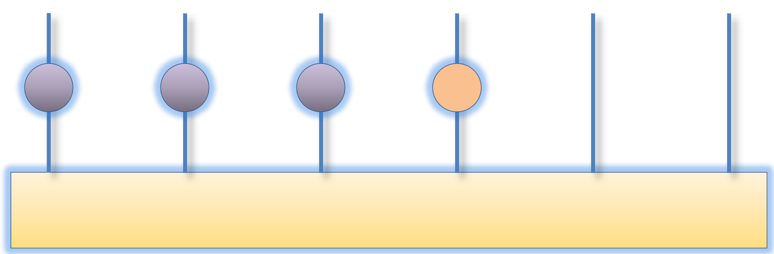
§ 2.5 Spin-fermion mapping

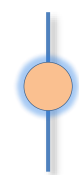
$$c_j = \sum_{\{n\}} (-1)^{\sum_{l=1}^{j-1} n_l} \delta_{n_j,1} |n_1, \dots n_j - 1, \dots, n_N\rangle\langle n_1, \dots n_j, \dots, n_N|$$

$$|\psi\rangle = \sum_{n_1,\dots,n_N=0,1} \psi(n_1, \dots, n_N)\, |n_1, \dots, n_N\rangle$$


$= \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$

$c_j|\psi\rangle \rightarrow$




$= \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$

§ 2.5 Spin-fermion mapping

- Spin-fermion mapping: states

$$|0\rangle \overset{!}{\rightarrow} |\downarrow\rangle \qquad |1\rangle \overset{!}{\rightarrow} |\uparrow\rangle$$

$$|n_1, n_2, \dots, n_N\rangle \overset{!}{\rightarrow} \underline{|s_1, s_2, \dots, s_N\rangle}$$

$$s_j = 2n_j - 1$$

§ 2.5 Spin-fermion mapping

- Spin-fermion mapping: operators

$$c_j = (-\sigma^z) \otimes \cdots \otimes (-\sigma^z) \otimes \sigma^- \otimes I \otimes \cdots \otimes I$$

$$= \left[\prod_{l=1}^{j-1} (-\sigma_l^z)\right] \sigma_j^-$$

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- Spin-fermion mapping: operators

$$c_j = \left[\prod_{l=1}^{j-1}(-\sigma_l^z)\right]\sigma_j^- \qquad c_j^\dagger = \left[\prod_{l=1}^{j-1}(-\sigma_l^z)\right]\sigma_j^+$$

$$c_j^\dagger c_j = \frac{1}{2}(\sigma_j^z + 1)$$

This is the famous Jordan-Wigner transformation! It is very useful for doing DMRG with fermions.

§ 2.5 Spin-fermion mapping

- In one dimension, fermion models with local interactions are mapped to spin models with local interactions.

Example: $t - V$ model (with open boundary condition)

$$H = -t \sum_{j=1}^{N-1} \left(c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j\right) + V \sum_{j=1}^{N-1} n_j n_{j+1}$$

$$\Rightarrow \quad c_j^\dagger c_{j+1} = \sigma_j^+ \left[\prod_{l=1}^{j-1} (-\sigma_l^z)\right] \left[\prod_{k=1}^{j} (-\sigma_k^z)\right] \sigma_{j+1}^-$$

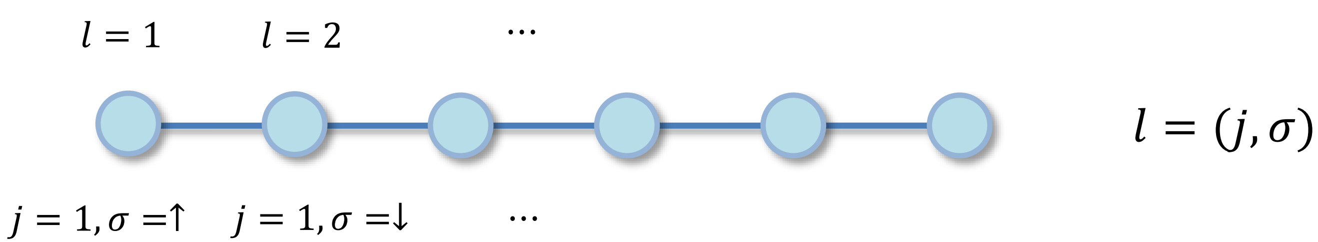
$$= \sigma_j^+ (-\sigma_j^z) \sigma_{j+1}^- = \sigma_j^+ \sigma_{j+1}^-$$

§ 2.5 Spin-fermion mapping

Example: Hubbard model

$$H = -t \sum_{j,\sigma=\uparrow,\downarrow} \left(c_{j\sigma}^{\dagger} c_{j+1,\sigma} + c_{j+1,\sigma}^{\dagger} c_{j\sigma} \right) + U \sum_{j} n_{j\uparrow} n_{j\downarrow}$$

$$c_{j\uparrow} = \left[\prod_{k=1}^{j-1} (-\sigma_k^z)(-\tau_k^z) \right] \sigma_j^- \qquad c_{j\downarrow} = \left[\prod_{k=1}^{j-1} (-\sigma_k^z)(-\tau_k^z) \right] (-\sigma_j^z) \tau_j^-$$



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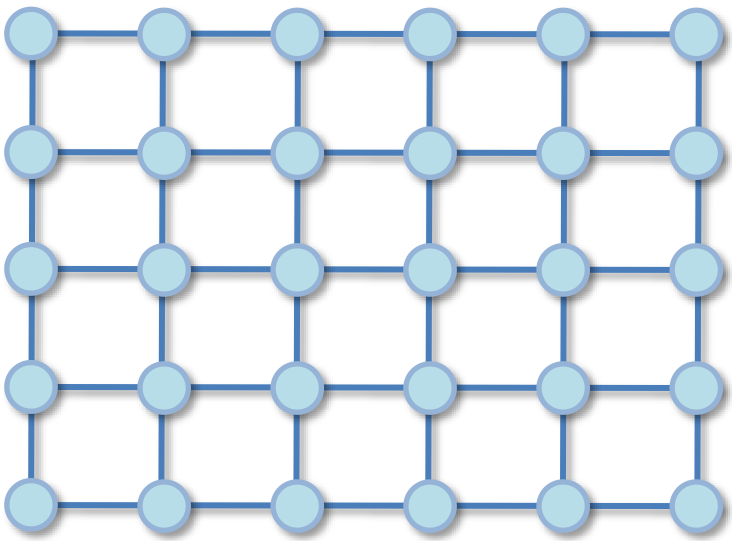
Challenging cases:

- Higher dimensional models:



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Challenging cases:

- Quantum chemistry calculations

$$H = \sum_{j,l=1}^{N} c_j^{\dagger} T_{jl} c_l + \sum_{i,j,l,m=1}^{N} V_{ijlm} c_i^{\dagger} c_j^{\dagger} c_l c_m$$

§ 2.5 Spin-fermion mapping

Challenging cases:

- Quantum chemistry calculations

$$H = \sum_{j,l=1}^{N} c_j^\dagger T_{jl} c_l + \sum_{i,j,l,m=1}^{N} V_{ijlm} c_i^\dagger c_j^\dagger c_l c_m$$

Bottleneck: large entanglement (MPS bond dimension not enough), large MPO bond dimension for H …

Current techniques: choose suitable 1D path, choose/optimize single-particle basis, use symmetry …

§ 2.6 Free fermion case

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

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

Motivation:

- ➢ Hartree-Fock solution
- ➢ Starting point for introducing correlations (e.g. Gutzwiller projection)
- ➢ Benchmark model for tensor network numerics

§ 2.6 Free fermion case

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

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

§ 2.6 Free fermion case

- Covariance/correlation matrix:

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

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- Covariance/correlation matrix:

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

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

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

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