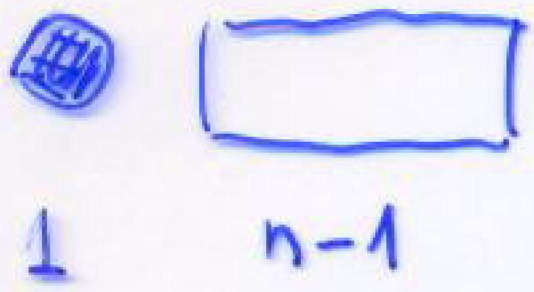
Renormalization in the "language" of the states ⇒ Matrix-Product States

$$|s_n\rangle|\beta\rangle \Longrightarrow \boxed{|s_n\rangle \otimes |\beta\rangle_{n-1}} \xrightarrow{\text{Projection}} |\alpha_n\rangle$$



tensor product

"glues" the different parts

$$\underset{m}{|\alpha\rangle_n} = \sum_\beta \underset{[m,\, m_s\cdot m]}{A_n^{\alpha(\beta,s_n)}}\ \underset{m_s}{|s_n\rangle} \otimes \underset{m}{|\beta_{n-1}\rangle}$$

projection operator

1) Change in notation

$$\underset{[M,M]}{A_n^{\alpha,\beta}}[s_n] \equiv A_n^{\alpha,\underbrace{(\beta,s_n)}_{m\times m_s\ \text{"vector"}}}$$

Position dependent matrices

2) Recursion relation → fixed point: $A_n[s] \to A[s]$, $n \to \infty$

Repeatedly applying RG

$$|\alpha\rangle_n = \sum_{s_n \dots s_1 \beta} \left(A[s_n] A[s_{n-1}] \dots A[s_1]\right)^{\alpha,\beta} |s_n s_{n-1} \dots s_1\rangle \otimes |\beta\rangle_0$$

where $|\beta_0\rangle$ is some initial state

$\Rightarrow$ Wavefunction $\equiv$ matrix product form

$\Rightarrow$ Trial wavefunction: linear combination of m^2 states:

$$|\alpha,\beta\rangle_n = \sum_{s_n \dots s_1} \left(A[s_n] A[s_{n-1}] A[s_1]\right)^{\alpha,\beta} |s_n s_{n-1} \dots s_1\rangle$$

by introducing matrix Q $[m,m]$

unnormalized state $|Q\rangle_n$

$$|Q_n\rangle = \sum_{\{s\}} \mathrm{tr}\left(Q\, A[s_n] A[s_{n-1}] \dots A[s_1]\right) |s_n \dots s_1\rangle$$

state uniform in the bulk, but linear combination of boundary conditions $|\alpha_n\rangle$ (left) and $|\beta_0\rangle$ (right)

- special case $Q = \mathbb{1}$ $\rightarrow$ translationally invariant state with periodic boundary condition (PBC)

- Projection preserves orthonormal bases: $\langle \alpha, \alpha' \rangle = \delta_{\alpha,\alpha'}$

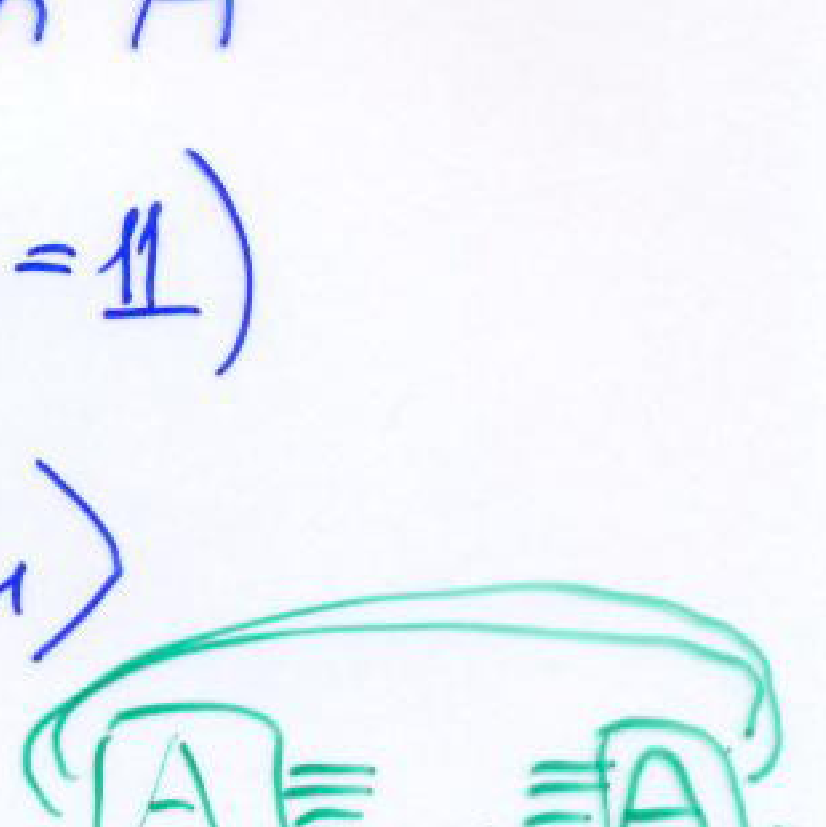
$$\delta_{\alpha,\alpha'} = \sum_{\substack{\beta\beta' \\ ss'}} \left(A^{\alpha',\beta'}[s']\right)^{*} A^{\alpha,\beta}[s] \langle s'|s\rangle\langle\beta'|\beta\rangle$$

$$= \sum_{s} \left(A[s]\, A^{+}[s]\right)^{\alpha,\alpha'}$$

$$\Rightarrow \sum_{s} A[s] A^{+}[s] = \mathbb{1} \rightarrow$$ constrain to reduc[e] # of free parameters in A

Expectation values (using $Q = \mathbb{1}$)

$$|1\rangle = \sum_{\{s_j\}} tr\left(A[s_n] \ldots A[s_1]\right) |s_n \ldots s_1\rangle$$



$$\langle 1|O|1\rangle = \sum_{\{s_j\},\{s_j'\}} tr\left(A^{*}[s_n'] \ldots A^{*}[s_1']\right) tr\left(A[s_n] \ldots A[s_1]\right) \times$$

$$\times \langle s_n' \dots s_1' | \mathcal{O} | s_n \dots s_1 \rangle$$

tensor product matrix:

$$(B \otimes C)^{(\alpha,\beta)(\tau,\nu)} = B^{\alpha,\tau} C^{\beta\nu}$$

notation: $A^{\alpha,\beta}$ $M \times M$ matrix

$A^{(\alpha,\beta)}$ $M^2 \times 1$ vector

- $tr(B)\, tr(C) = tr(B \otimes C)$
- $(BCD) \otimes (EFG) = (B \otimes E)(C \otimes F)(D \otimes G)$

$$\langle 1 | \mathcal{O} | 1 \rangle = \sum_{\{s_j\},\{s_j'\}} tr\Big[\big(A^*[s_n'] \otimes A[s_n]\big) \dots \big(A^*[s_1'] \otimes A[s_1]\big) \Big] \times$$

$$\times \langle s_n' \dots s_1' | \mathcal{O} | s_n \dots s_1 \rangle$$

mapping $\hat{M}$ $3 \times 3 \Longrightarrow m^2 \times m^2$

$$\hat{M} \equiv \sum_{s',s} M_{s's} \left(A^*[s'] \otimes A[s] \right)$$

$s \equiv (s_x, s_y, s_z) \Rightarrow \hat{S} = (\hat{S}_x, \hat{S}_y, \hat{S}_z)$ $\quad \mathbb{1} \Rightarrow \hat{1}$

norm and expectation value of spin at site j

$$\langle 1|1\rangle = \mathrm{tr}(\hat{1})^n$$

$$\langle 1|\vec{S}_j|1\rangle = \mathrm{tr}\left(\hat{1}^{n-1}\,\hat{S}\right) \quad \left(\text{cyclicity of trace}\right)$$

$$\langle s_j', s_i' | \vec{S}_i \vec{S}_j | s_j\, s_i\rangle \equiv \left(\vec{S}_i\cdot\vec{S}_j\right)_{s_j' s_i',\, s_j s_i}$$

$$= \left(\vec{S}\right)_{s_i' s_i} \cdot \left(\vec{S}\right)_{s_j', s_j}$$

$$\langle 1|\vec{S}_j \vec{S}_{j+1}|1\rangle = \mathrm{tr}\left(1^{n-2}\,\hat{S}\,\hat{S}\right)$$

$$\langle 1|\vec{S}_j \vec{S}_{j+\ell}|1\rangle = \mathrm{tr}\left(\hat{1}^{n-\ell-1}\,\hat{S}\,\hat{1}^{\ell-1}\,\hat{S}\right)$$

$$E_{MP} = \langle 1|H|1\rangle$$

Low-lying excited states: for translationally invariant systems $\Rightarrow$ Bloch state

$$|Q,k\rangle_n = \sum_{s_n \ldots s_1} \sum_{j=1}^{n} e^{ijk}\, \mathrm{tr}\left(A[s_n] \ldots A[s_{j+1}]\, Q\, A[s_j] \ldots A[s_1]\, X\, |s_n \ldots s_1\rangle\right.$$

like GS, $|1\rangle$, with disturbance Q at some site; disturbance run over all sites to form a state with definite momentum $\Rightarrow$ single "particle" excitation

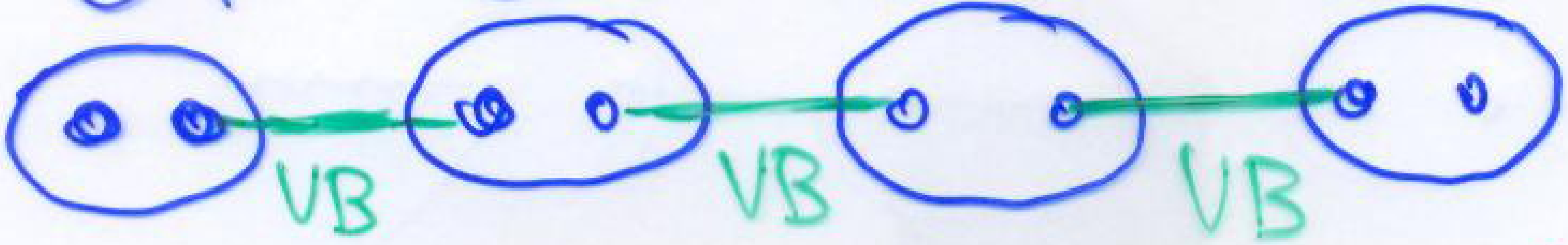
$$(Q', k|H|Q, k)_n\,, \quad (Q', k|Q k)_n$$

Evolution of states: (example)

$$\mathcal{H} = \sum_{i=1}^{n} \vec{S}_i \vec{S}_{i+1} - \beta \left(\vec{S}_i \vec{S}_{i+1} \right)^2$$

$\beta = -1/3$ exact MP [2,2]

S-1 S-1 S-1 S-1

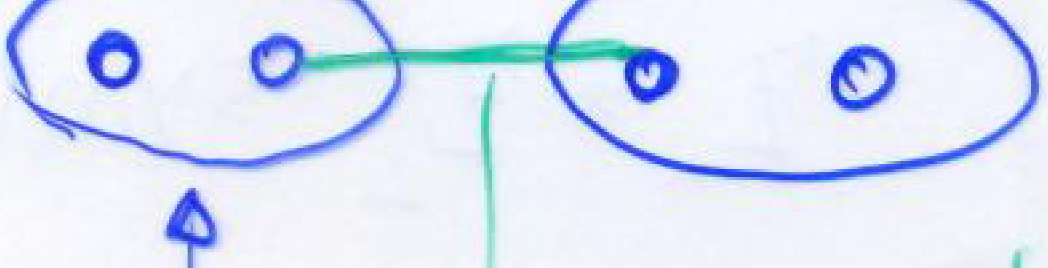


free endspin S-$1/2$ $\quad \psi_{\alpha\beta} = \frac{1}{\sqrt{2}}\{\psi_\alpha \psi_\beta \pm \psi_\beta \psi_\alpha\}$ free endspin S-$1/2$

$\beta = 0$ Haldane model short range VB

two spin-$1/2$ → singlet ($s=0$) $m_s^z = 1$

→ triplet ($s=1$) $m^z = -1, 0, 1$



$Z_2 \times Z_2$ SYMM.

triplet

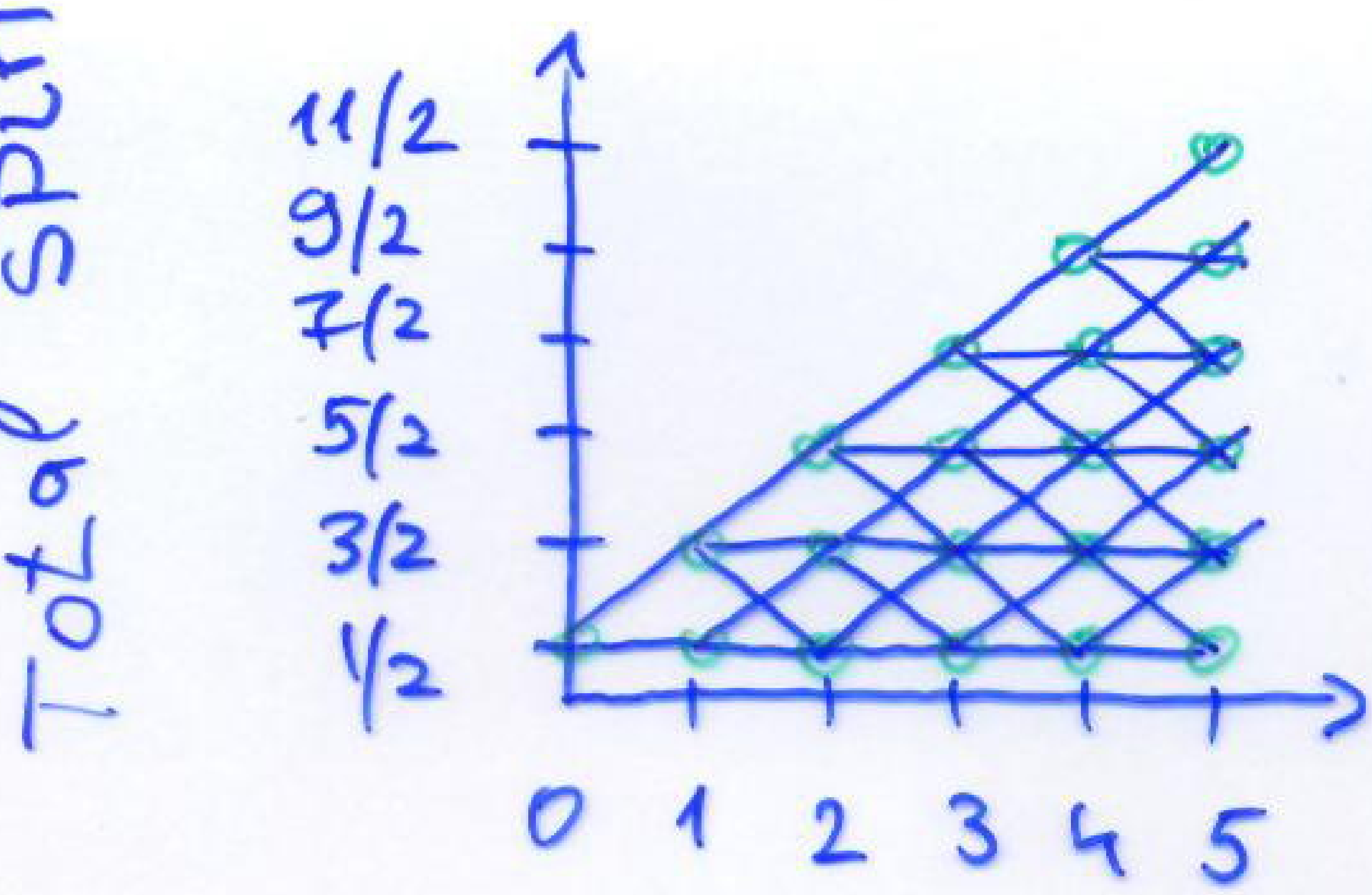
singlet bond

- first step

(S-½) × (S-1) $\quad \frac{1}{2} \otimes 1 = \frac{1}{2} \oplus \frac{3}{2}$ two irreducibl[e] representation[s]

- 2nd step

$$\left(\frac{1}{2} \oplus \frac{3}{2}\right) \otimes 1 = \frac{1}{2} \oplus \frac{3}{2} \oplus \frac{1}{2} \oplus \frac{3}{2} \oplus \frac{5}{2}$$



# of s-1 sites

total spin j

Z-component $m=-j \dots j$ $\Big\}$ $|j, m\rangle$

$|j', m'\rangle = |1/2, -1/2\rangle, |3/2, -1/2\rangle, |3/2, -3/2\rangle$
$|1/2, 1/2\rangle, |3/2, 1/2\rangle, |3/2, 3/2\rangle$

$m = 6$ states kept

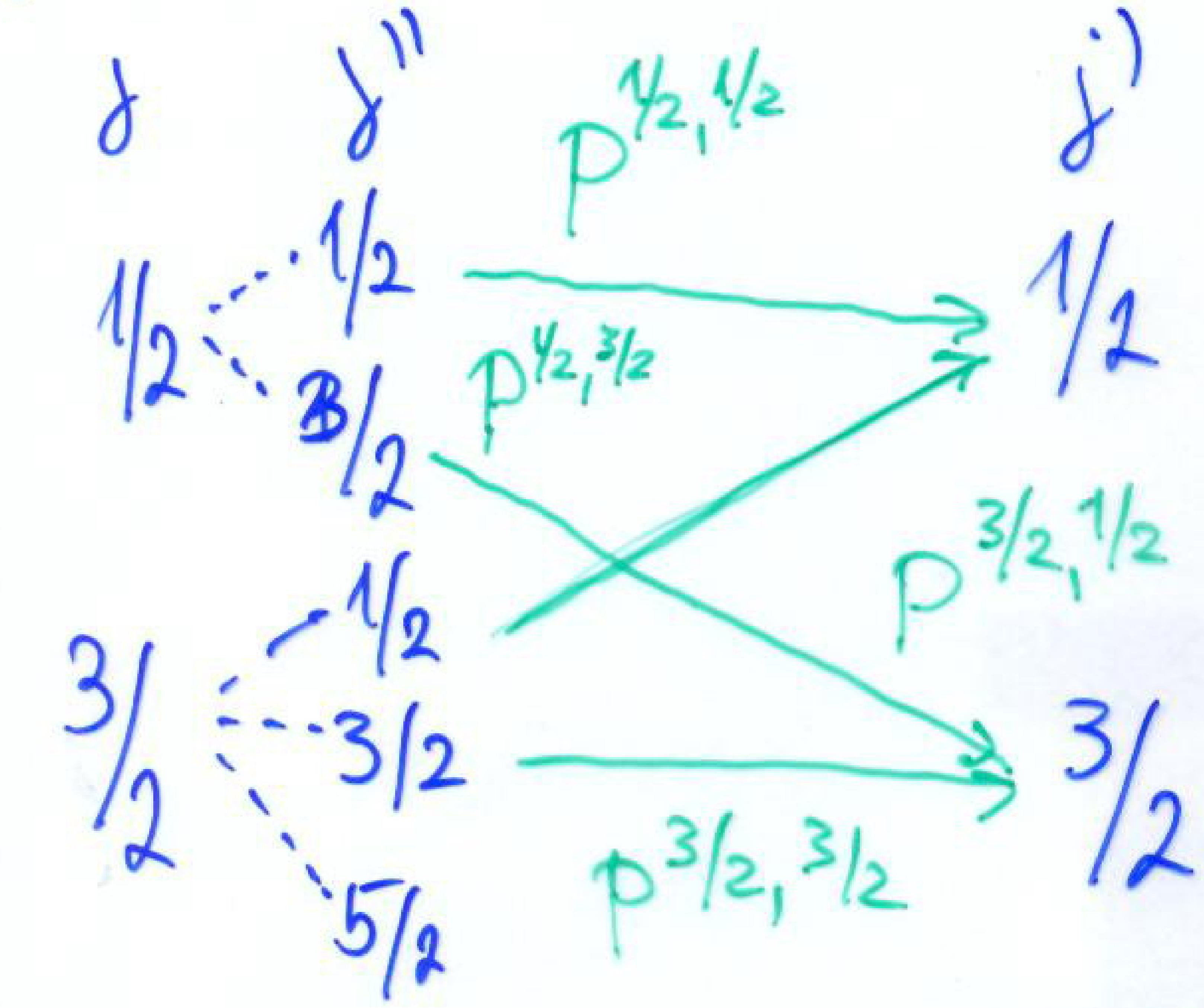
$j \equiv$ old state, j'' intermediate st., j' new state

$P^{j', j}$ Projection

$$|j, j'', m''\rangle = \sum_{m,s} \langle (j,m)(1,s) | j'', m''\rangle \left(|s\rangle \otimes |j,m\rangle \right)$$

Clebsch-Gordan coefficients

$|j'', m''\rangle$ 18 states $\Longrightarrow$ $|j', m'\rangle$ 6 states



Projection preserves total spin

$\Rightarrow j'' = j'$ and $m'' = m'$

$$|j, m'\rangle = \sum_j P^{j',j} \, |j, j, m'\rangle$$

since $j'' = j'$ & $m'' = m'$ $\Rightarrow |j, j', m'\rangle$ intermed. states

$$|j', m'\rangle = \sum_{s(jm)} A^{(j',m')(j,m)}[s] \left(|s\rangle \otimes |j, m\rangle \right)$$

where $A^{(j',m'),(j,m)}[s] = P^{j',j} \langle (j,m)(1\,s) | j', m' \rangle$

A has $3 \times 6 \times 6 = 108$ elements

$$P = \begin{pmatrix} P^{1/2\,1/2} & P^{1/2\,3/2} \\ P^{3/2\,1/2} & P^{3/2\,3/2} \end{pmatrix}$$

$\langle j_1, m_1 | j_2, m_2 \rangle = \delta_{j_1 j_2} \delta_{m_1 m_2}$

$\Rightarrow$ diagonal elements of $P^T P$ are 1 spin-$\frac{1}{2}$ & spin $\frac{3}{2}$ states are orthogonal

$$P = \begin{pmatrix} \cos\varphi & \cos\theta \\ \sin\varphi & \sin\theta \end{pmatrix}$$

φ, θ only free parameters in A for $m=6$

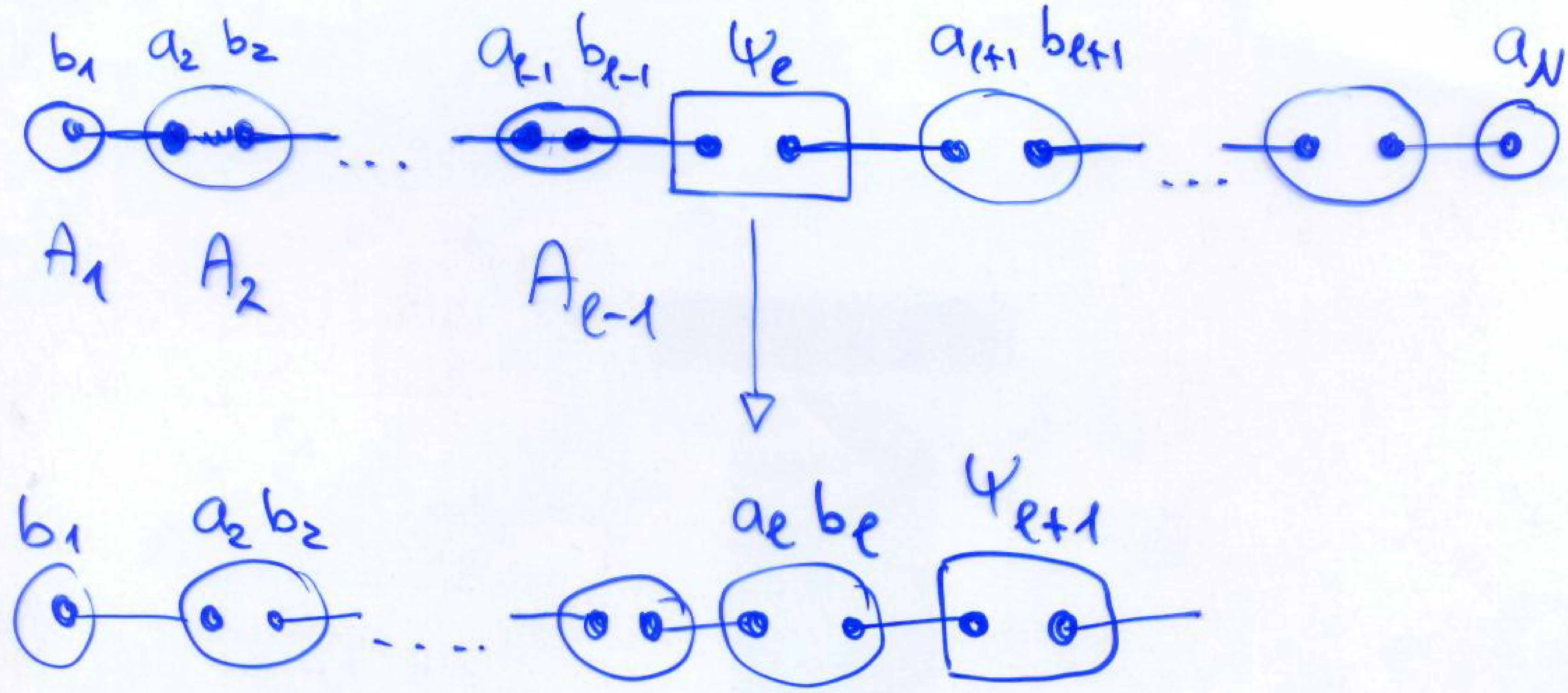
$$E_{MP}(\phi, \theta) = \langle 1 | H | 1 \rangle$$

- minimization of energy in terms of θ, φ use example Mathematica

- Variational method, upper bound on energy

- DMRG produces matrix product state in the thermodynamic limit for OBC $|\alpha\rangle_n$ & $|\beta_0\rangle$ are $[M,1]$ vectors

<u>DMRG</u> $\square \bullet \square$



- two auxiliary state spaces a_l, b_l of dimension M
- mapping $a_l \otimes b_l \to \mathcal{H}_l$

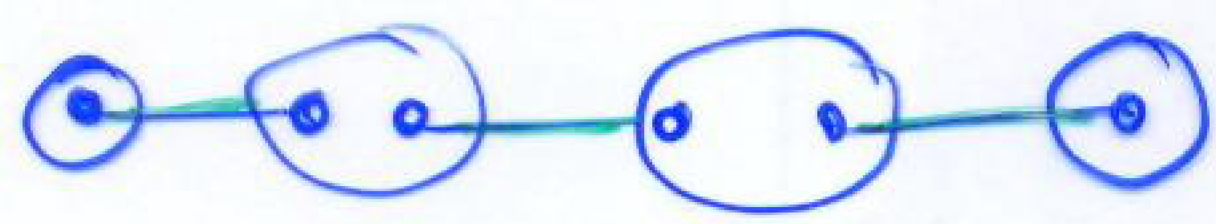
$\left(A_l[s]\right)_{\alpha\beta}$: $A_l = \sum_{s_l} \sum_{\alpha_l \beta_l} \left(A_l[s]\right)_{\alpha\beta} |s_l\rangle\langle\alpha_l \beta_l|$

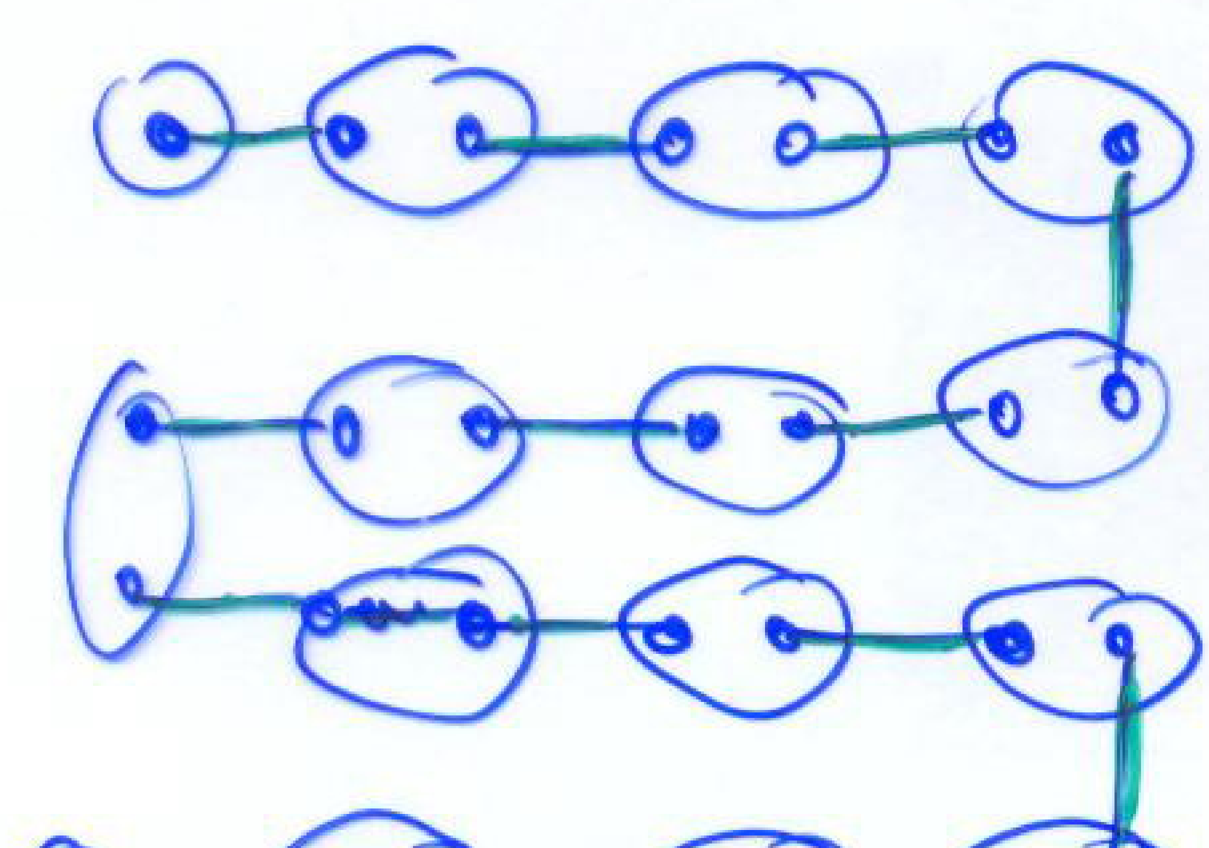
$|\alpha\rangle, |\beta\rangle$ states of the auxiliary state phase

- apply $A_1 \otimes A_2 \otimes \dots A_N$ to the product of maximally entangled states $|\varphi_1\rangle|\varphi_2\rangle \dots |\varphi_{N-1}\rangle$

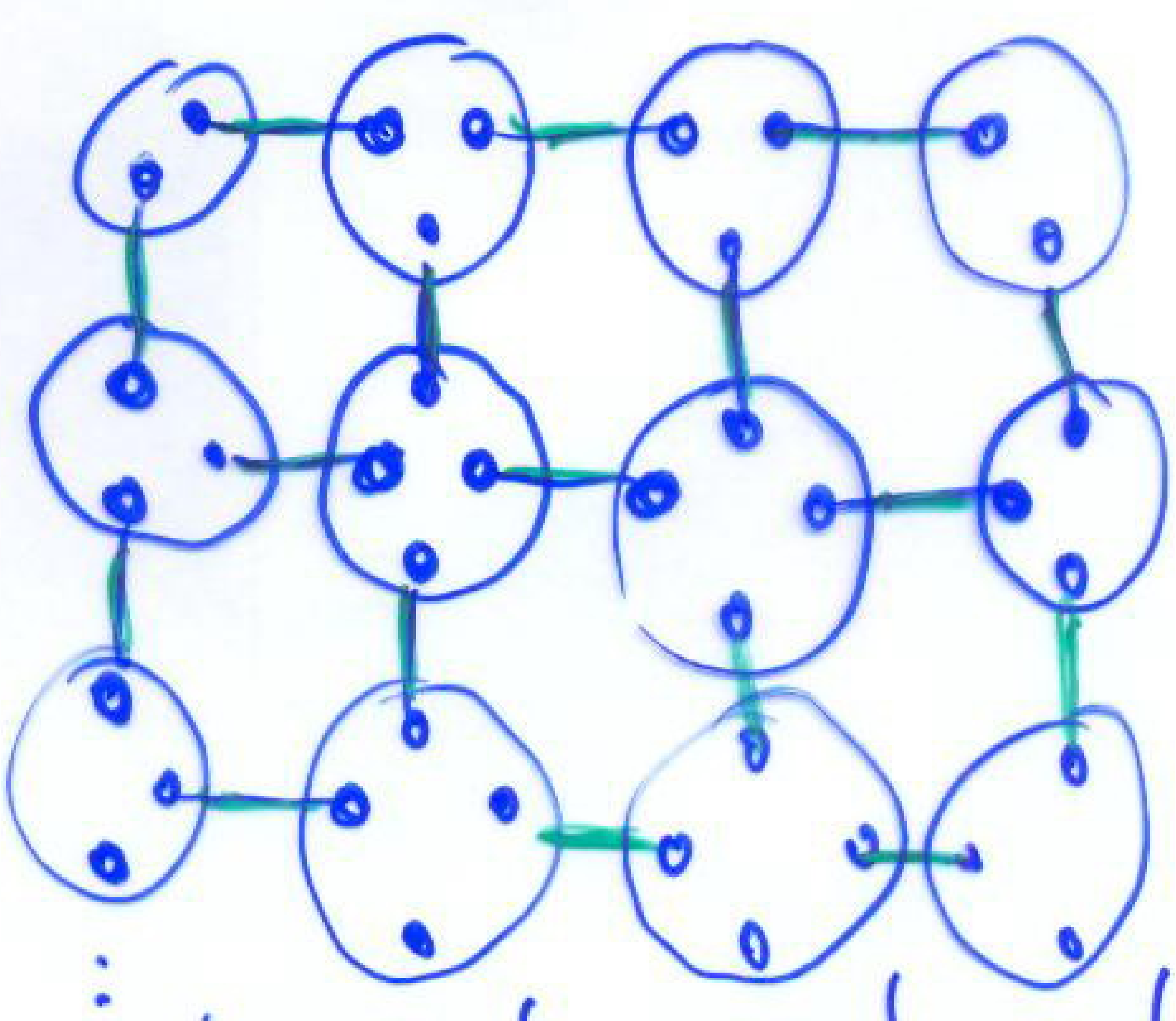
where $|\varphi_i\rangle = \sum_{\beta_i = \alpha_i + 1} |\beta_i\rangle|\alpha_{i+1}\rangle$

- this ensures that prefactors of $|s_1 \ldots s_N\rangle$ products of $A[s]$ matrices
- finite lattice algorithm: one keeps for site ℓ all A at other sites fixed and seeks ψ_ℓ that minimizes the total energy
- truly variational in the space generated by the maps A
- no guarantee to reach global minimum

1d  MPS (matrices)

2d 

MPS
2 auxiliary subsystems



4 auxilary subsystems
PEPS (tensors)