Tensor Networks

Iztok Pizorn
Frank Verstraete

University of Vienna

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Matrix product states (MPS)

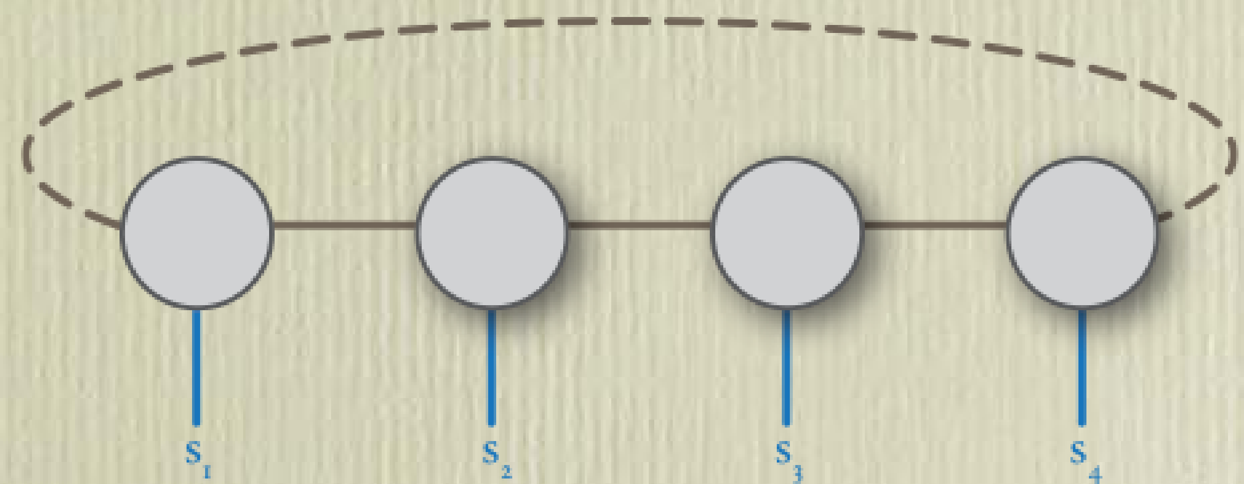
- Introduction to matrix product states
- Ground states of finite systems
- Ground states of infinite systems
- Real-time evolution
- Projected dynamics

Introduction to MPS

S Östlund & S Rommer PRL (95);
M Fannes, B Nachtergaele, RF Werner (92)

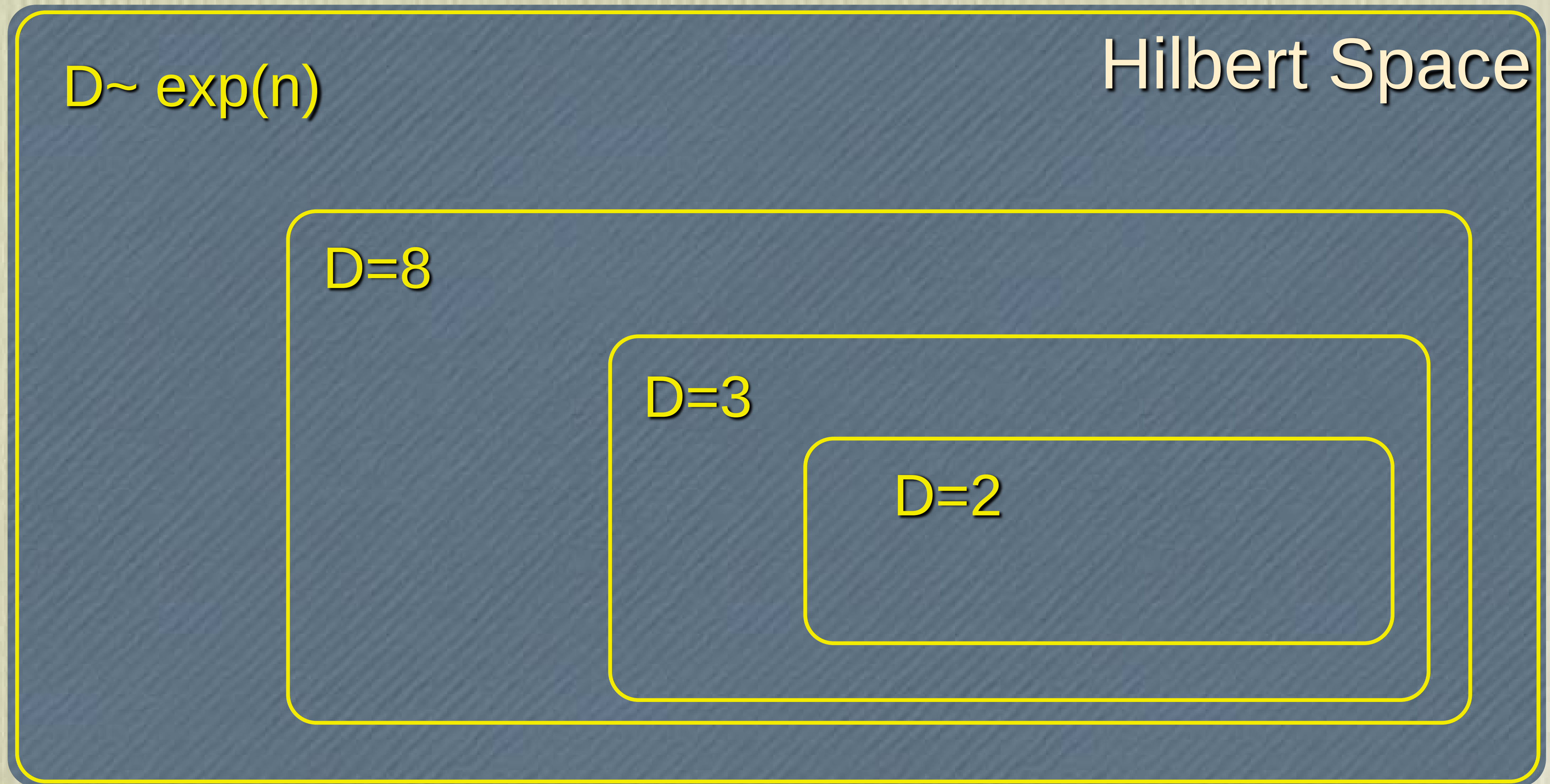
$$|\Psi\rangle = \sum_{s_1, s_2, \dots, s_n} c_{s_1, s_2, \dots, s_n} |s_1\rangle |s_2\rangle \cdots |s_n\rangle$$

$$|\Psi\rangle = \sum_{s_1, s_2, \dots, s_n} \mathrm{tr}\left[\mathbf{A}^{[1]s_1} \cdot \mathbf{A}^{[2]s_2} \dots \mathbf{A}^{[n]s_n}\right] |s_1\rangle |s_2\rangle \cdots |s_n\rangle$$



in total: 2n matrices $\mathbf{A}^{[j]s_j} \in \mathbb{R}^{D \times D}$ $2nD^2$

MPS bond dimension



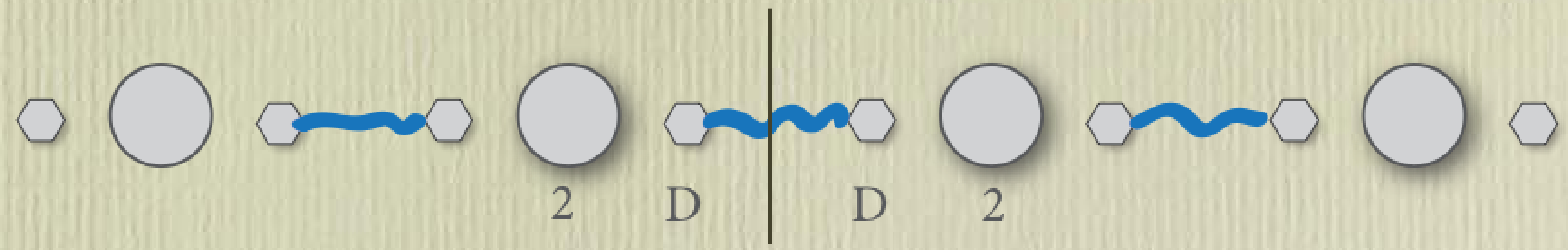
Exact description of an arbitrary quantum state requires exponentially large matrices A

Matrix product states only describe a certain subset of the full Hilbert space

But what kind of states are we really interested in?

Physical background

F Verstraete, D Porras & JI Cirac, PRL (04)



Bond dimension D puts a bound to entanglement: $S = -\mathrm{tr}\left(\rho_R \log_2 \rho_R\right)$
entanglement entropy at most log2(D)

typically $S \sim n$

Area law: $S(n) \leq \underbrace{c \log n}_{\text{critical}} + c'$

All gapped 1d systems at zero temperature can be well described by matrix product states!

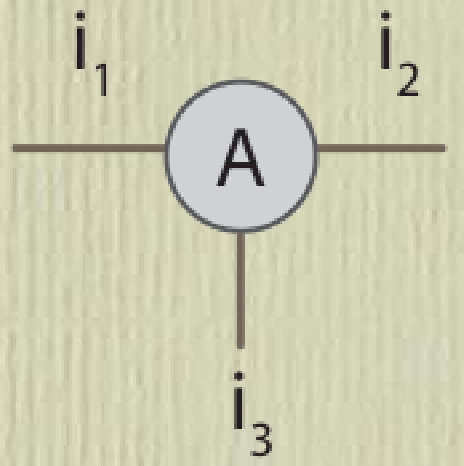
*Find matrices **A** such that the total energy is minimal!*

Why tensor networks

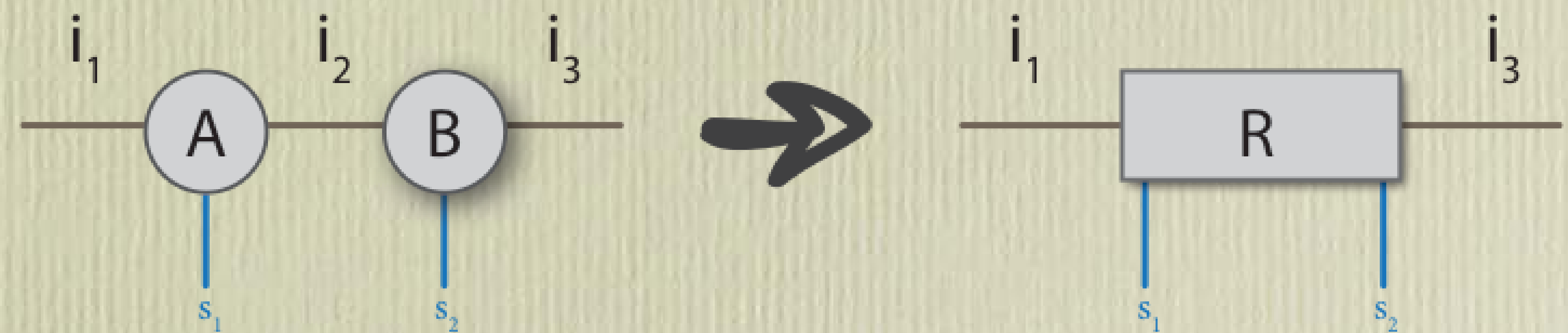
- Density matrix renormalization group (DMRG)
  - successful simulation of strongly correlated 1d systems
- 1D: matrix product states ~ DMRG
- 2D: PEPS & friends
  - early stage but promising
  - quantum monte carlo & “sign problem”

Obsolete when we get a quantum computer (Chris Monroe’s talk)

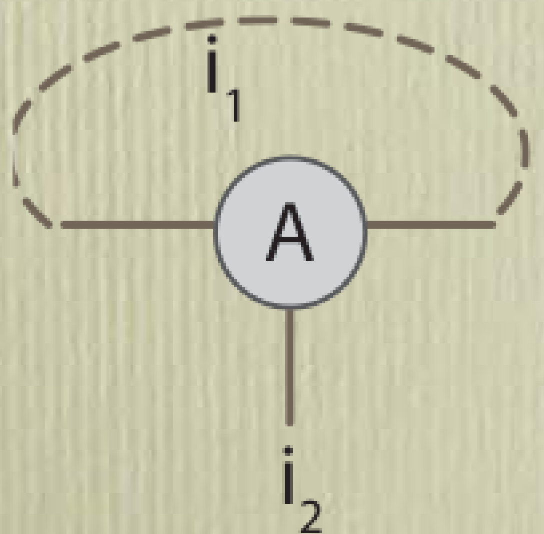
On notation



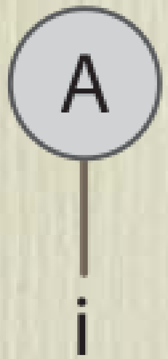
A_{i_1,i_2,i_3} or A_{i_2,i_1,i_3} or ...



$$\sum_{i_2} A_{i_1,i_2,s_1} B_{i_2,i_3,s_2} = R_{i_1,i_3,s_1,s_2}$$



$$\sum_{i_1} A_{i_1,i_2}$$

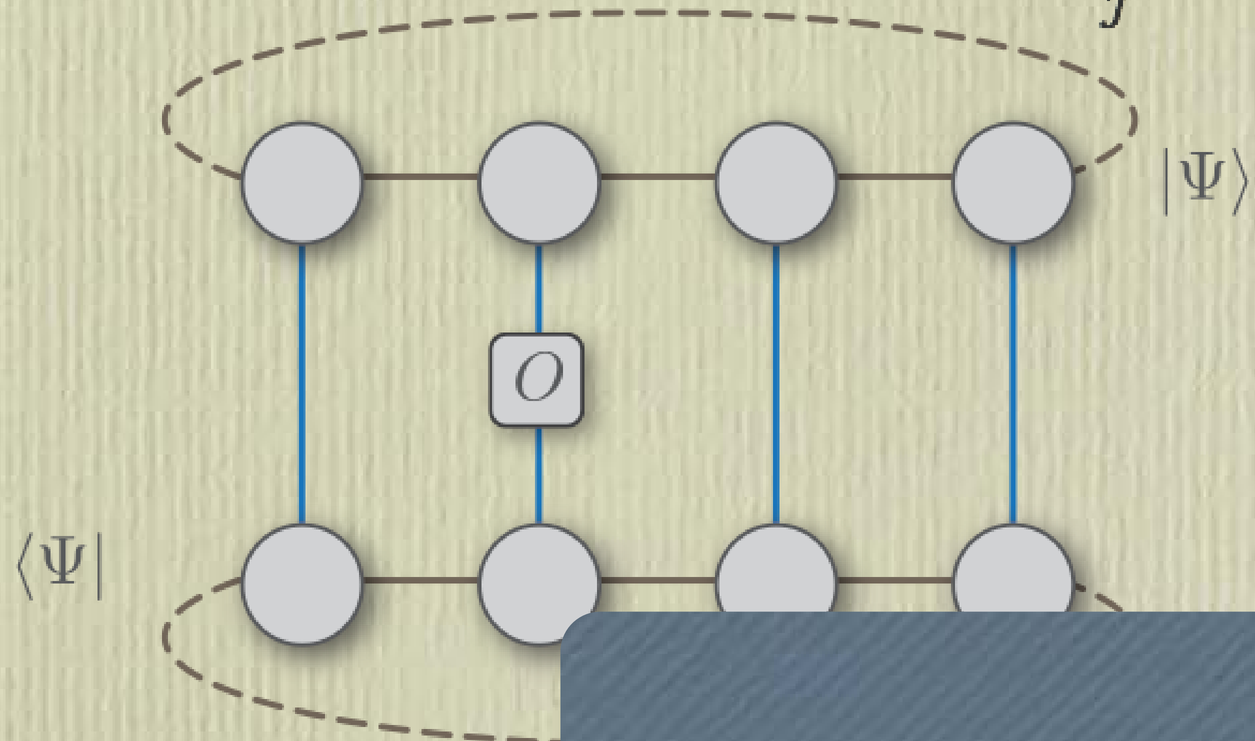


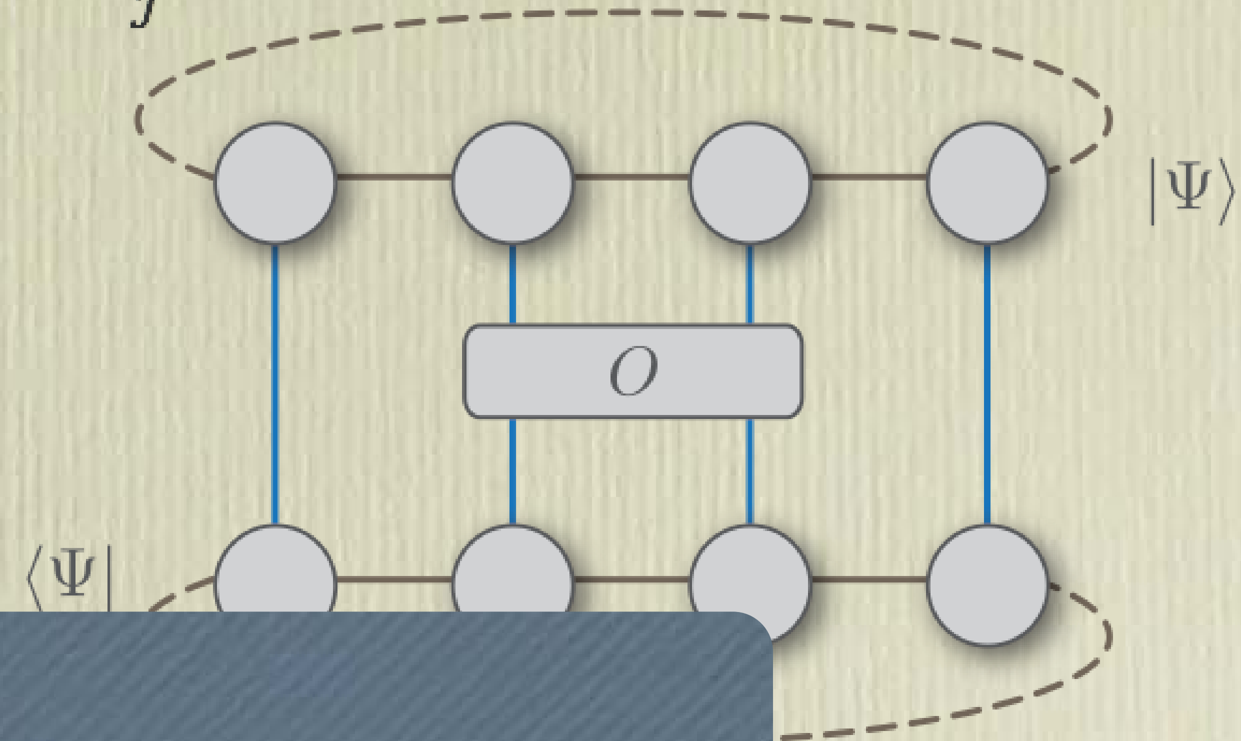
A_i

Observables and MPS

$$H = \sum_j Z_j + \sum_j W_{j,j+1}$$

$$H = h \sum_j \sigma_j^z + \sum_j \sigma_j^x \sigma_{j+1}^x$$





One-sit … erators

$\langle\Psi$ … $|\Psi\rangle$

Exp … ator

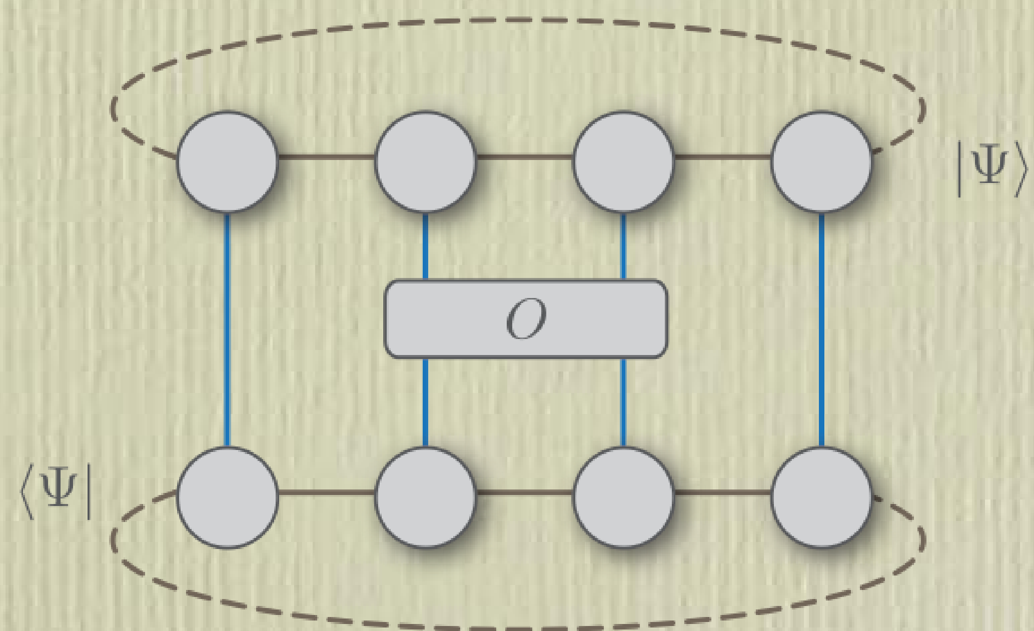
Simulate ground states

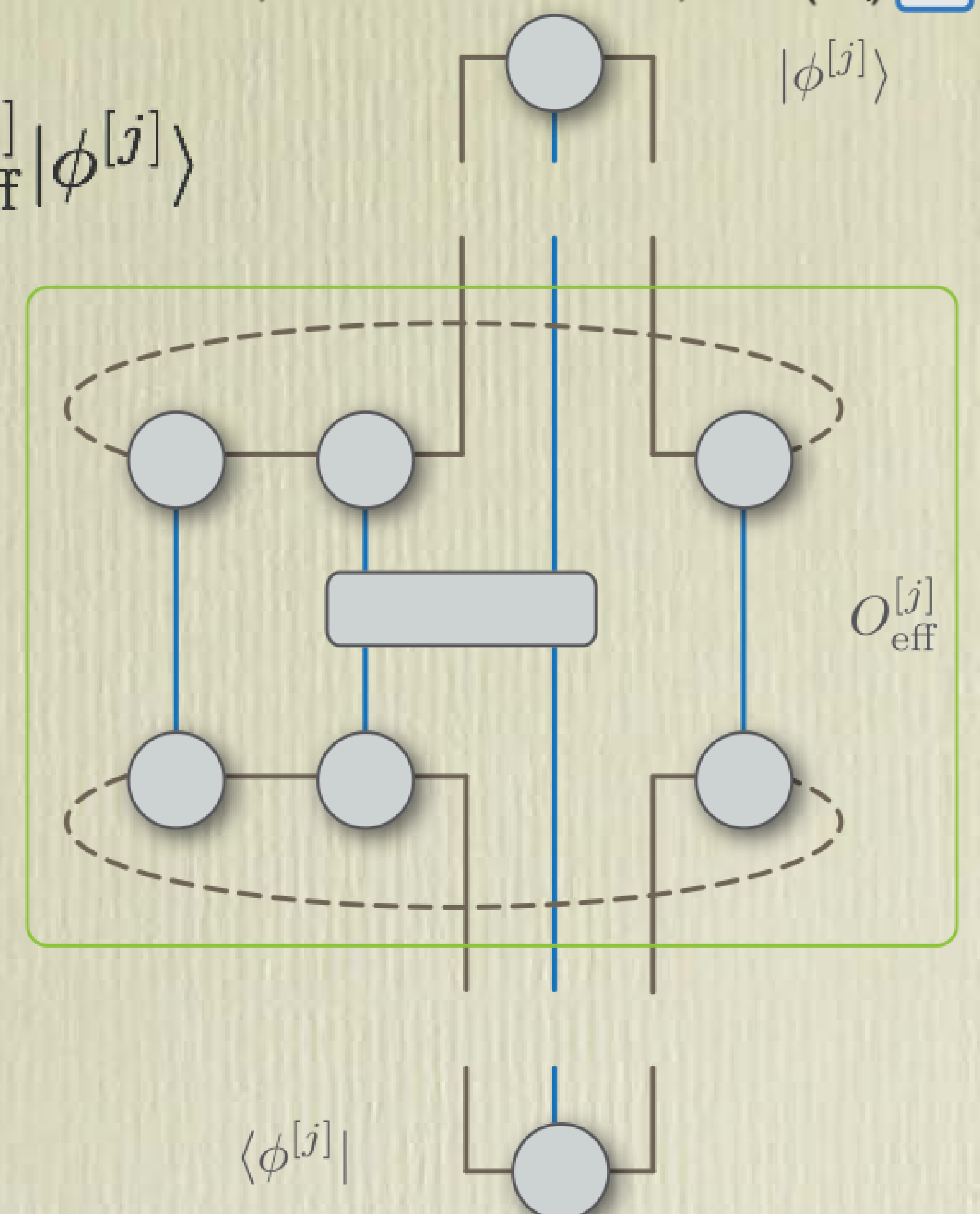
Find such matrices A[j] that the energy is minimal

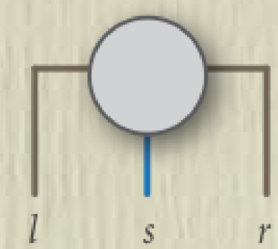
Variational approach

F Verstraete, D Porras & JI Cirac, PRL (04)

$$\langle\Psi|O|\Psi\rangle = \langle\phi^{[j]}|O^{[j]}_{\rm eff}|\phi^{[j]}\rangle$$





$A^{[j]\,s}_{l,r} =$ 

All tensor elements of $A^{[j]}$ contained in $|\phi^{[j]}\rangle$

$$H = \sum_\nu H_\nu \rightarrow H^{[j]}_{\rm eff} = \sum_\nu H^{[j]}_{\nu;{\rm eff}}$$

Variational optimization

F Verstraete, D Porras & JI Cirac, PRL (04)

1. Choose a fixed site j

2. Find tensor $A_{l,r}^{[j]\,s}$ that minimizes the energy

$$E = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \frac{\langle \phi^{[j]} | H_{\text{eff}}^{[j]} | \phi^{[j]} \rangle}{\langle \phi^{[j]} | N_{\text{eff}}^{[j]} | \phi^{[j]} \rangle}$$

Quadratic form in tensor elements!

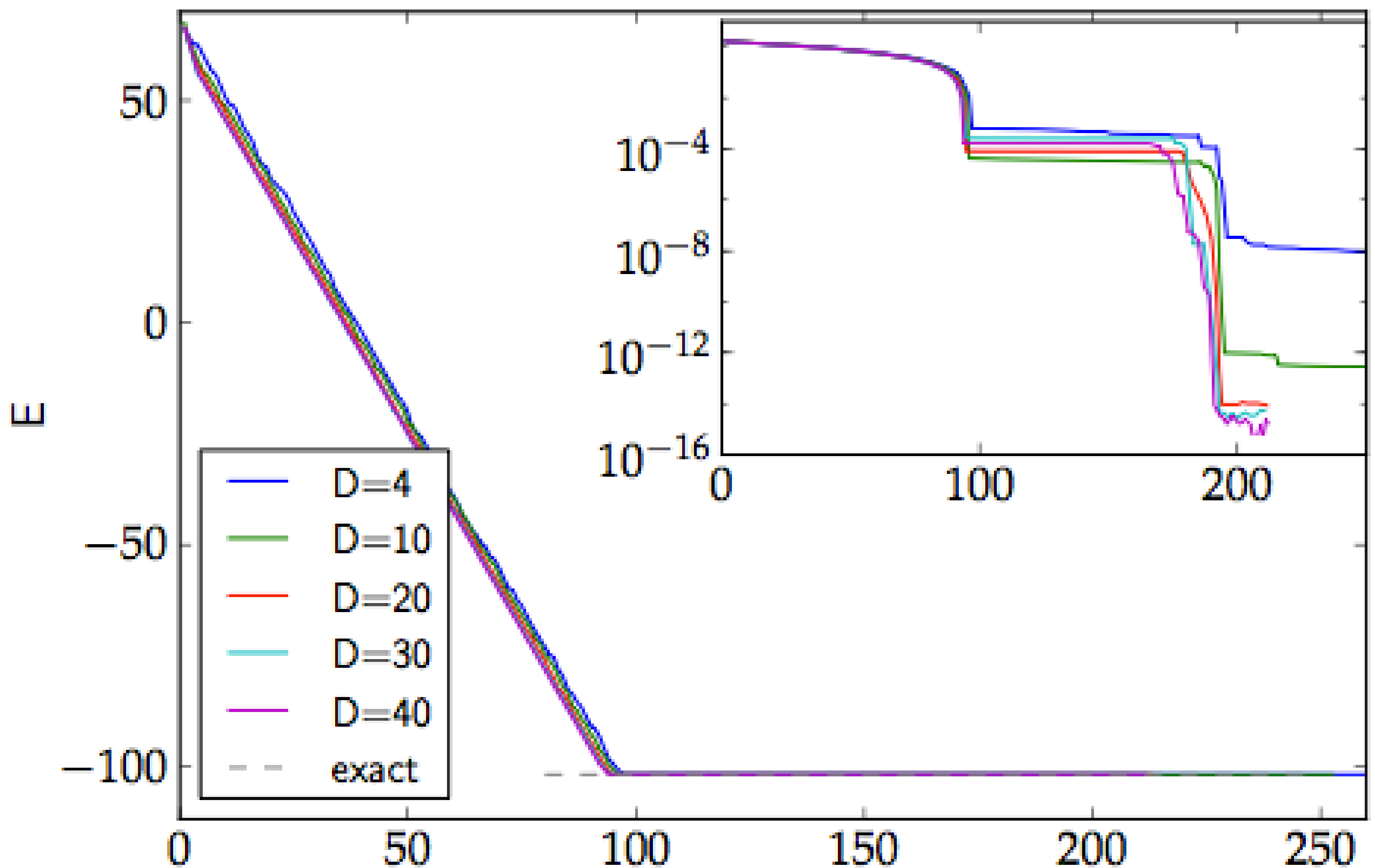
3. Move to the next site

Technical details:
Re-gauge the MPS such that Neff = I and solve an eigenvalue problem H x = E x

4. Repeat 2-3 until convergence reached

Variational optimization

$$H = \sum_{j=1}^{n-1} \left(\frac{1+\gamma}{2} \sigma_j^{x} \sigma_{j+1}^{x} + \frac{1-\gamma}{2} \sigma_j^{y} \sigma_{j+1}^{y} \right) + \sum_{j=1}^{n} h \sigma_j^{z}$$

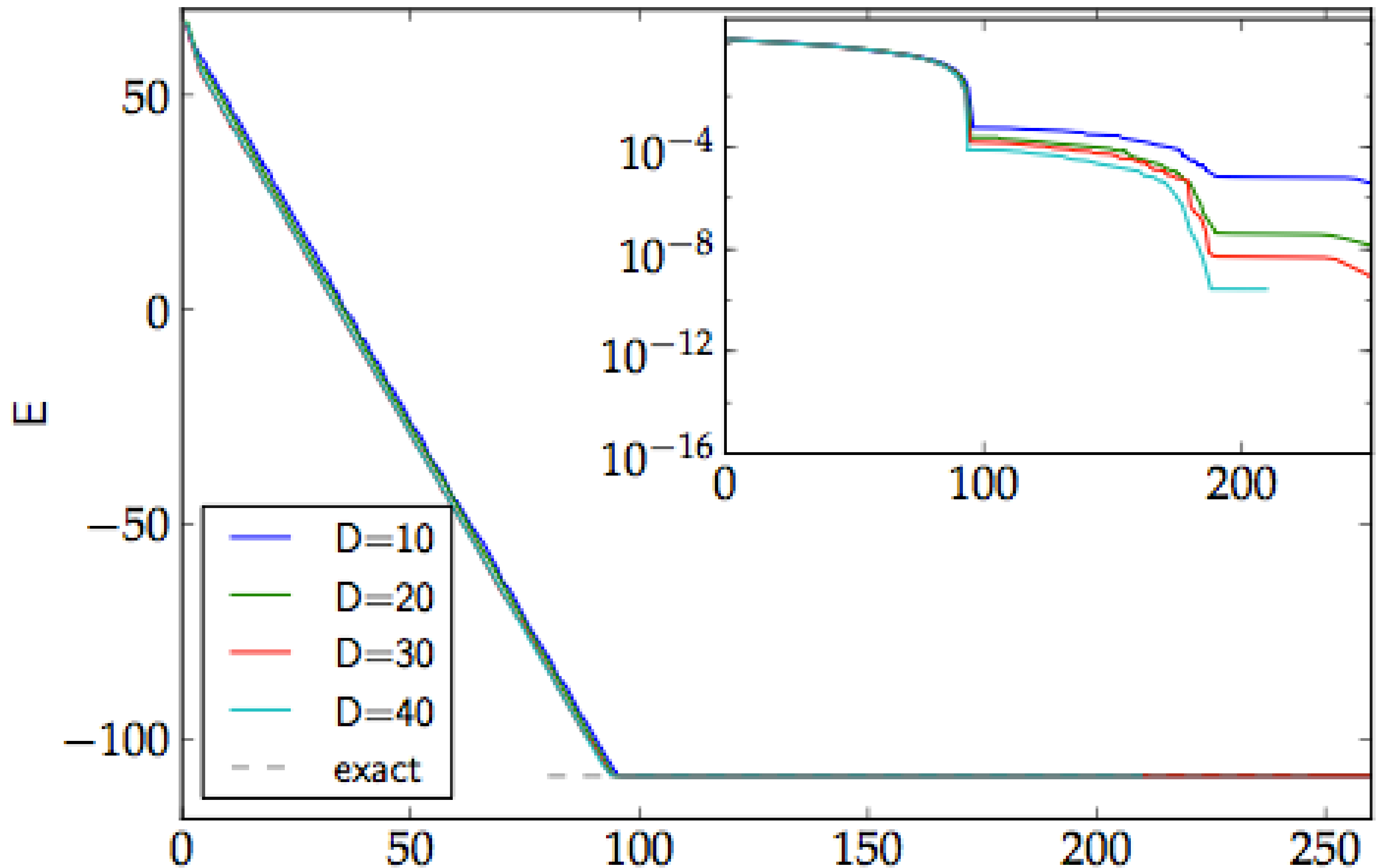


n=100

$\gamma = 0.5, h = 0.9$

Variational optimization

$$H = \sum_{j=1}^{n-1} \left(\frac{1+\gamma}{2} \sigma_j^x \sigma_{j+1}^x + \frac{1-\gamma}{2} \sigma_j^y \sigma_{j+1}^y \right) + \sum_{j=1}^{n} h \sigma_j^z$$



n=100

$\gamma = 0.5, h = 1$

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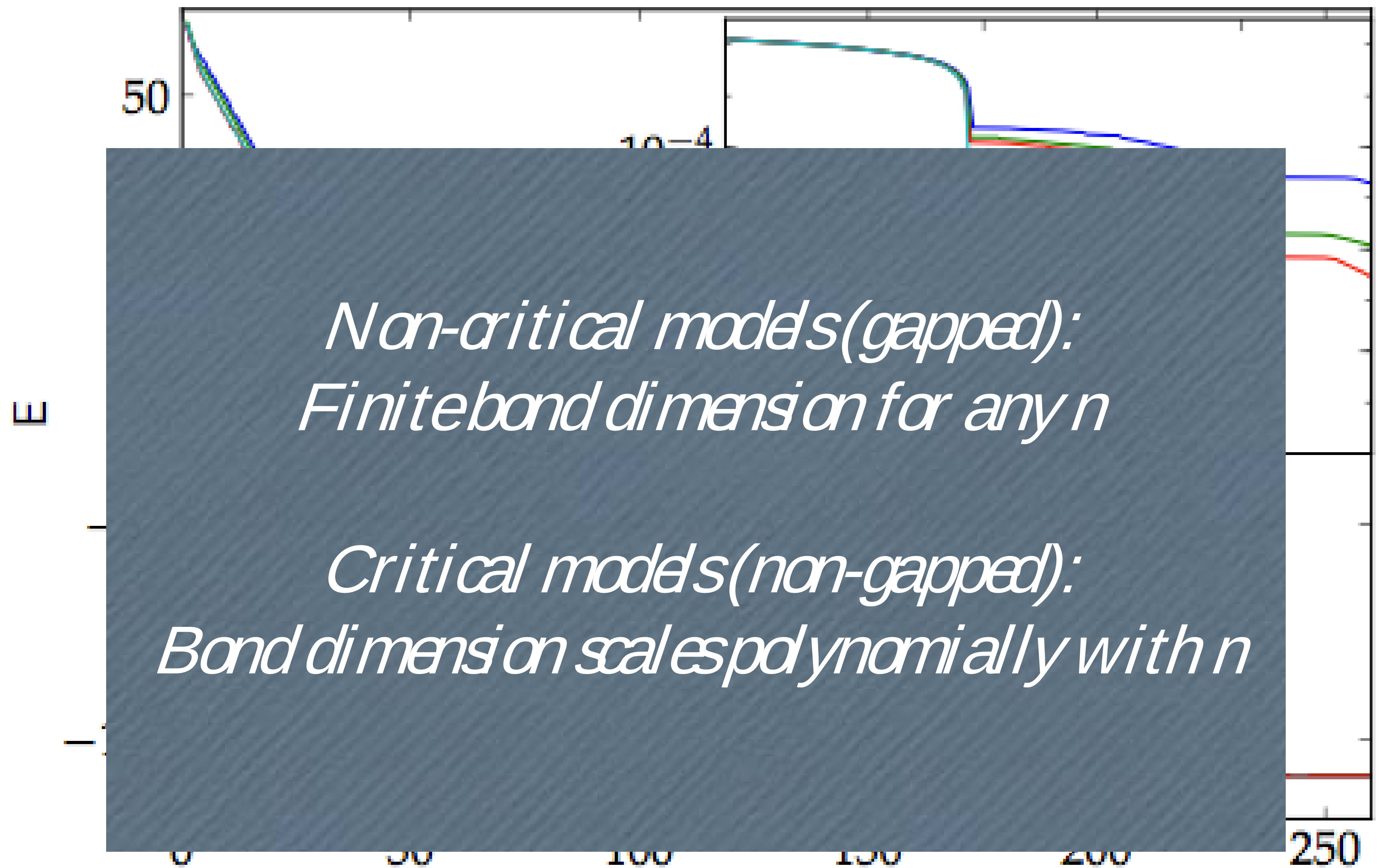
Variational optimization

$$H = \sum_{j=1}^{n-1} \left(\frac{1+\gamma}{2} \sigma_j^{\mathrm{x}} \sigma_{j+1}^{\mathrm{x}} + \frac{1-\gamma}{2} \sigma_j^{\mathrm{y}} \sigma_{j+1}^{\mathrm{y}} \right) + \sum_{j=1}^{n} h \sigma_j^{\mathrm{z}}$$



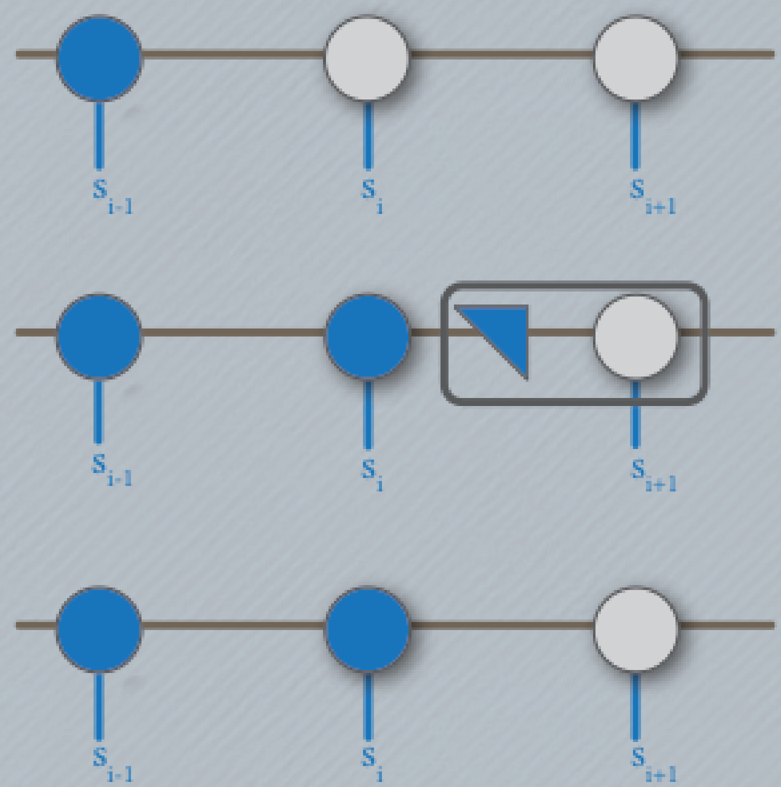
Non-critical models (gapped):
Finite bond dimension for any n

Critical models (non-gapped):
Bond dimension scales polynomially with n

n=100

$\gamma = 0.5, h = 1$

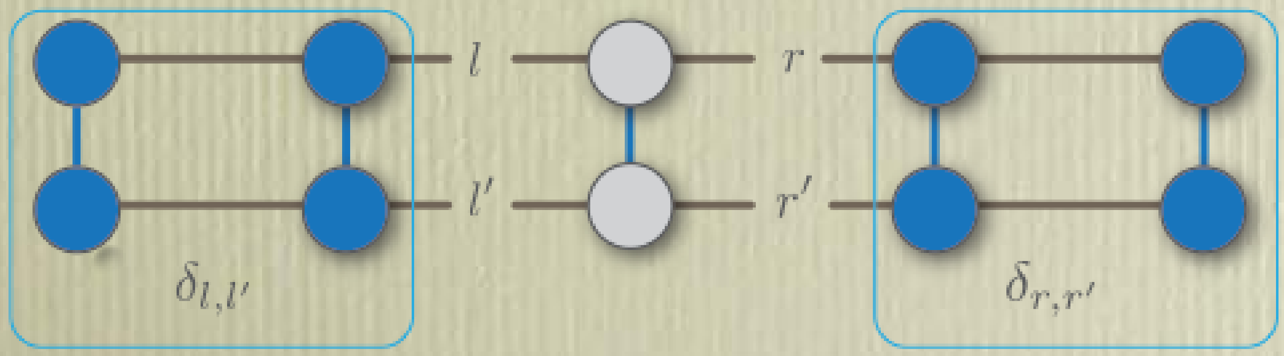
Gauge transformations



$$\mathbf{Q}^{[j-1]s_{j-1}}\mathbf{A}^{[j]s_j}\mathbf{A}^{[j+1]s_{j+1}}$$

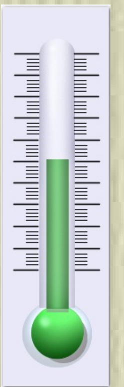
$$\mathbf{Q}^{[j-1]s_{j-1}}\mathbf{Q}^{[j]s_j}\mathbf{R}\mathbf{A}^{[j+1]s_{j+1}}$$

$$\mathbf{Q}^{[j-1]s_{j-1}}\mathbf{Q}^{[j]s_j}\tilde{\mathbf{A}}^{[j+1]s_{j+1}}$$



$$\mathbf{N}_{\text{eff}}^{[i]} = \mathbf{I} \qquad E = \frac{\langle \phi | H_{\text{eff}}^{[i]} | \phi \rangle}{\langle \phi | \phi \rangle}$$

Imaginary time evolution



G Vidal, PRL (03)

$$|\Psi_{\mathrm{GS}}\rangle = \lim_{t\to -i\infty} \mathrm{e}^{-itH}|\Psi\rangle \quad \longrightarrow \quad \lim_{\beta\to\infty} \mathrm{e}^{-\beta H}|\Psi\rangle$$

Evolve in small time steps

$$\mathrm{e}^{-itH} = \underbrace{\mathrm{e}^{-i\delta t H}\mathrm{e}^{-i\delta t H}\cdots\mathrm{e}^{-i\delta t}}_{k} \qquad \delta t = t/k$$

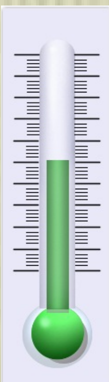
$\mathrm{e}^{-it\delta H}$ how to decompose into local time steps?

Suzuki-Trotter decomposition

$$\mathrm{e}^{z(A+B)} = \mathrm{e}^{zA/2}\mathrm{e}^{B}\mathrm{e}^{zA/2} + O(z^3)$$

All we need is a smart decomposition of H

Imaginary time evolution



G Vidal, PRL (03)

$$|\Psi_{\mathrm{GS}}\rangle = \lim_{t\to -i\infty} \mathrm{e}^{-itH}|\Psi\rangle \quad \longrightarrow \quad \lim_{\beta\to\infty} \mathrm{e}^{-\beta H}|\Psi\rangle$$

$$H = \sum_j \left(\sigma_j^{\mathrm{x}}\sigma_{j+1}^{\mathrm{x}} + h\sigma_j^z\right)$$

$$H_{i,i+1} = \sigma_i^{\mathrm{x}}\sigma_{i+1}^{\mathrm{x}} + (h/2)(\sigma_j^{\mathrm{z}} + \sigma_{j+1}^{\mathrm{z}})$$

$$H = \left(H_{1,2} + H_{3,4} + \ldots\right) + \left(H_{2,3} + H_{4,5} + \ldots\right)$$

$$\mathrm{e}^{z(H_{1,2}+H_{3,4}+\cdots)} = \mathrm{e}^{zH_{1,2}}\mathrm{e}^{zH_{3,4}}\ldots$$

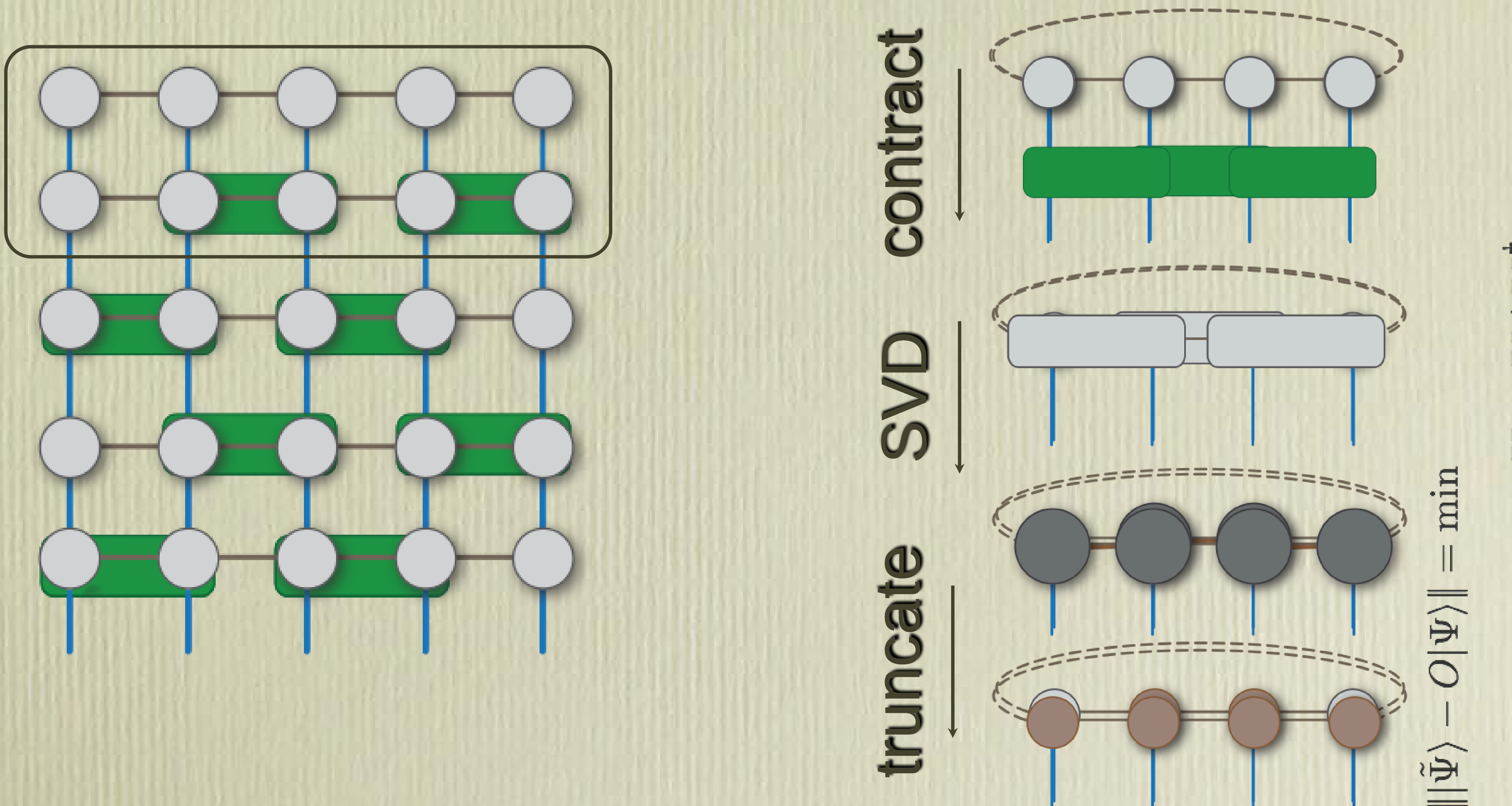
Suzuki-Trotter decomposition

$$\mathrm{e}^{z(A+B)} = \mathrm{e}^{zA/2}\mathrm{e}^{zB}\mathrm{e}^{zA/2} + O(z^3)$$

$$|\tilde{\Psi}\rangle = \mathrm{e}^{-i\delta t H_{i,i+1}}|\Psi\rangle$$

MPS time evolution

$$|\Psi(\beta+\delta\beta)\rangle \approx \mathrm{e}^{-(\delta\beta/2)(H_{2,3}+H_{4,5})}\mathrm{e}^{-\delta\beta(H_{1,2}+H_{3,4})}\mathrm{e}^{-(\delta\beta/2)(H_{2,3}+H_{4,5})}|\Psi(\beta)\rangle$$



Sufficiently long time yields the ground state...

Real time evolution

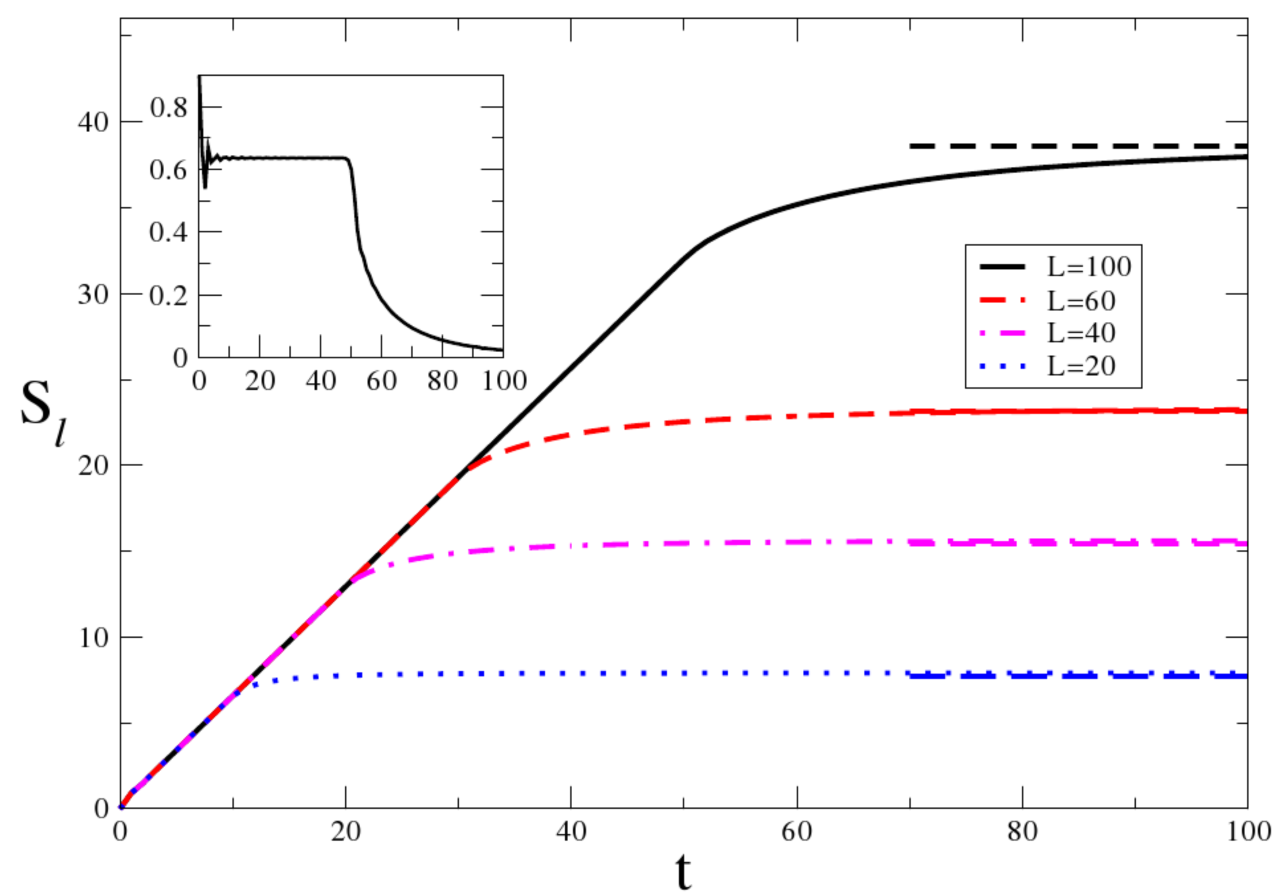
$$|\Psi(t)\rangle = \mathrm{e}^{-itH}|\Psi_0\rangle$$

A state gets entangled and bond dimension explodes!

$$S(t) \sim t$$

$$\Longrightarrow D(t) \sim \mathrm{e}^t$$

P Calabrese & J Cardy, JSM (05)



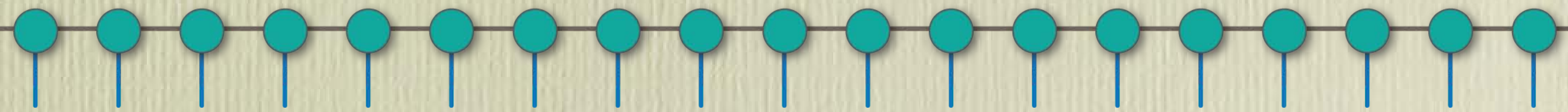
Efficient in very limited cases....

$$|\Psi_0\rangle = \sigma^{\mathrm{x}}_{n/2}|\Psi_{\mathrm{GS}}\rangle$$

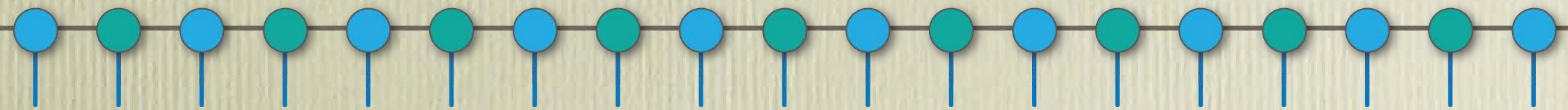
Infinite chains

G Vidal, PRL (07)

Assumption:
invariance under shifts by (1,2,...) sites



$$|\Psi\rangle = \sum_{s_1,s_2,\ldots} \mathrm{Tr}\Big(\mathbf{A}^{s_1}\mathbf{A}^{s_2}\cdots\Big)|s_1,s_2,\ldots\rangle \qquad H = \sum_j H_j$$

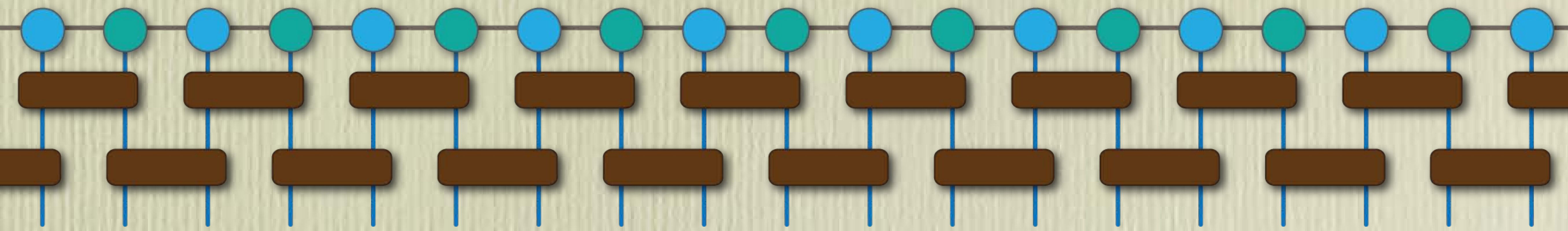


$$|\Psi\rangle = \sum_{s_1,s_2,\ldots} \mathrm{Tr}\Big(\mathbf{A}^{s_1}\mathbf{B}^{s_2}\mathbf{A}^{s_3}\mathbf{B}^{s_4}\cdots\Big)|s_1,s_2,\ldots\rangle \qquad H = \sum_j (H_j + W_{j,j+1})$$

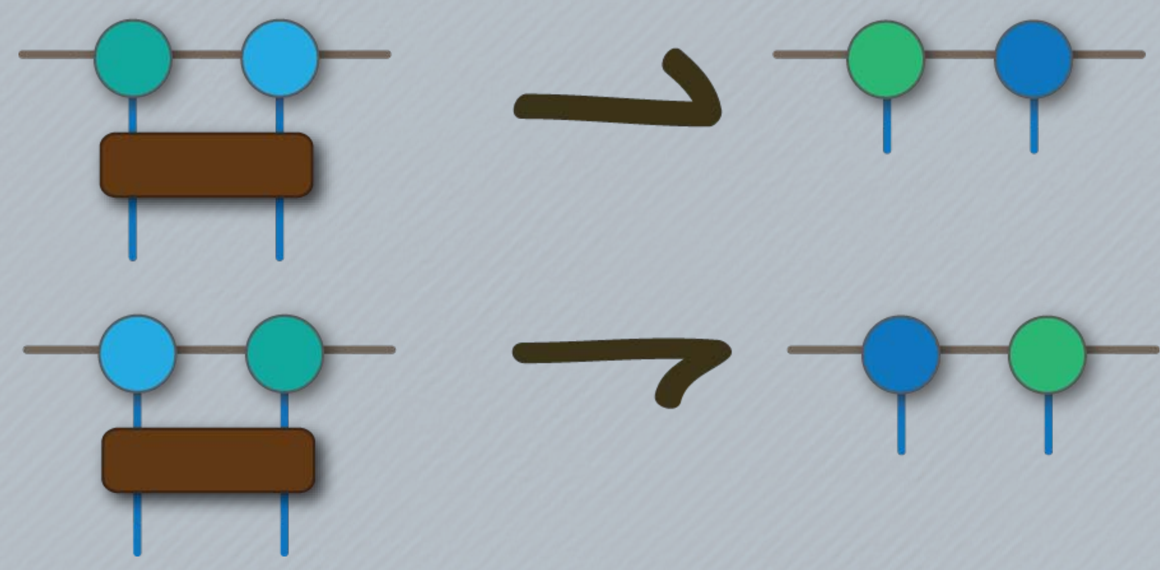
Much fewer parameters!

iMPS simulation

$$H = H_{\mathrm{AB}} + H_{\mathrm{BA}} \qquad |\Psi_{\mathrm{GS}}\rangle = \left(\mathrm{e}^{-\delta\beta H_{\mathrm{AB}}/2}\mathrm{e}^{-\delta\beta H_{\mathrm{BA}}}\mathrm{e}^{-\delta\beta H_{\mathrm{AB}}/2}\right)^{\infty}|\Psi_0\rangle$$



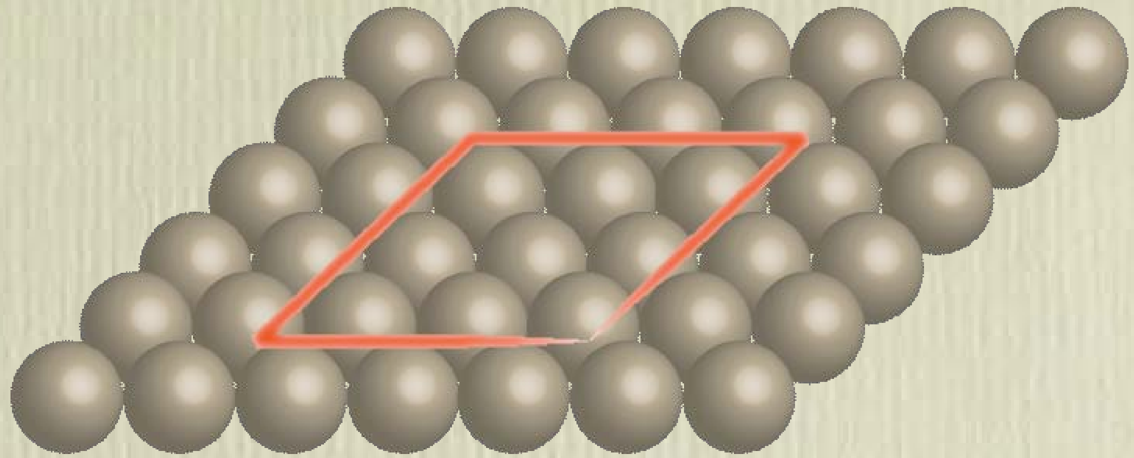
Basic elements



Only local tensor updates required!

Projected entangled pair states (PEPS)

- Generalization of matrix product states to two spatial dimensions
- Entangled pairs between neighboring sites
- Success not entirely guaranteed by the area law
- More costly than MPS

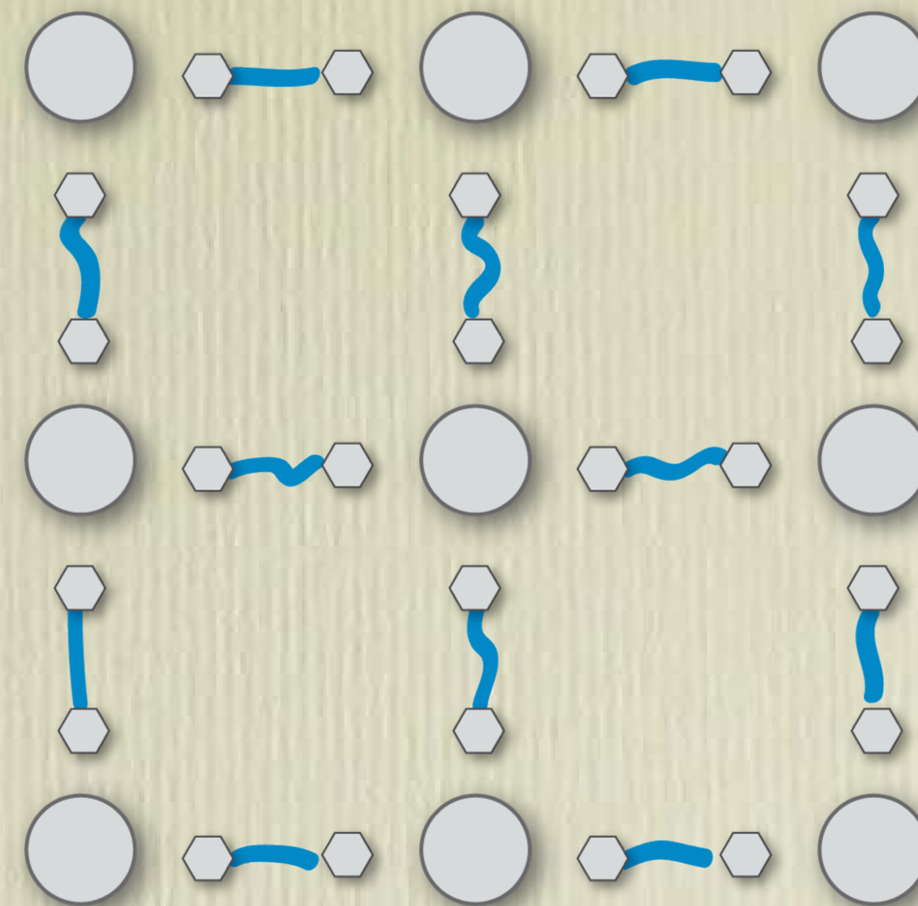


$$S_{\max} \propto L$$

$$S_{\max}/\text{bond} \sim 1$$

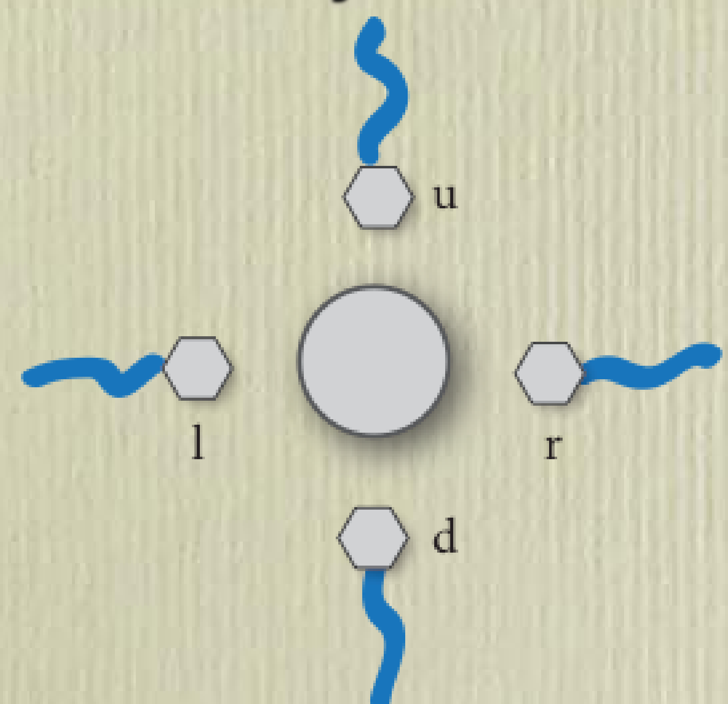
PEPS Ansatz

F Verstraete, JI Cirac (unpublished)

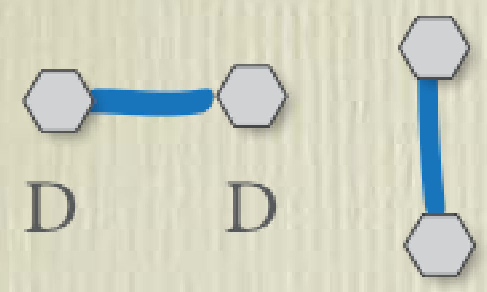


$$|\Psi\rangle = Q_{1,1} \cdots Q_{m,n} \prod_{\nu \in \{\text{ent.pairs}\}} |\phi_\nu\rangle$$

Projector



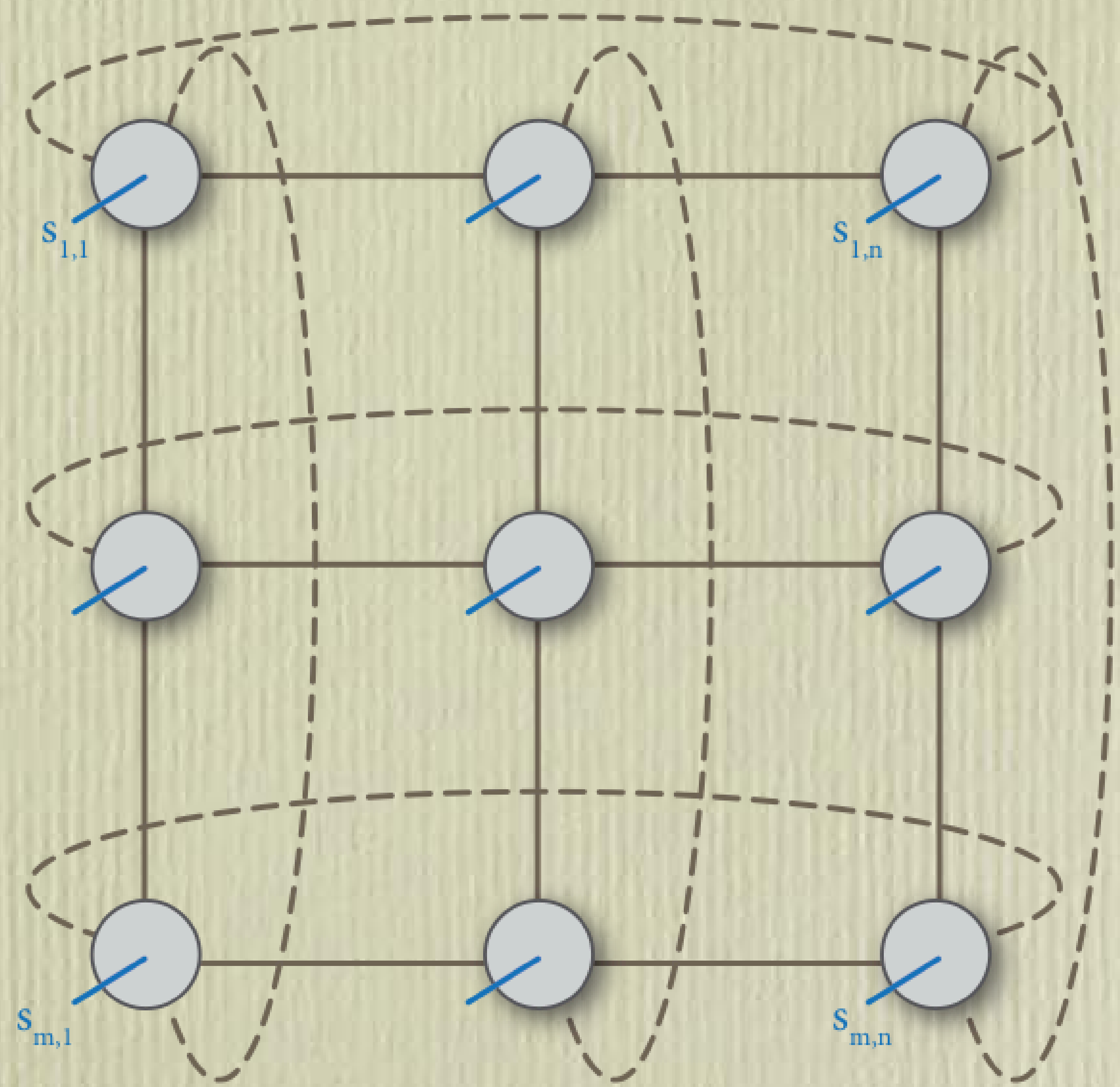
Entangled pair



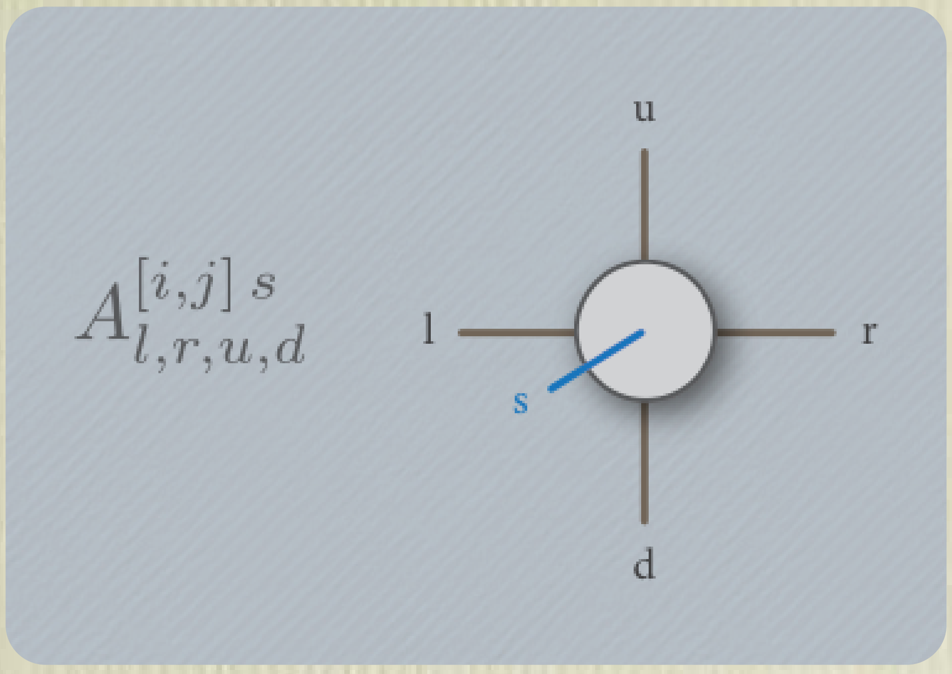
$$Q_{i,j} = \sum_{lruds} A^{[i,j]s}_{lrud} |s\rangle\langle l|\langle r|\langle u|\langle d|$$

$$|\phi\rangle = \sum_{i=1}^{D} |i\rangle|i\rangle$$

PEPS: Tensor Network



5-leg tensors



$2D^4$ parameters/site

$$|\Psi\rangle = \sum_{s_{i,j}} \mathrm{Tr}\left[\mathbf{A}^{[1,1]s_{1,1}} \ldots \mathbf{A}^{[1,n]s_{1,n}} \ldots \mathbf{A}^{[m,n]s_{m,n}}\right] |s_{1,1}\rangle \cdots |s_{1,n}\rangle \cdots |s_{m,n}\rangle$$

4-leg tensors

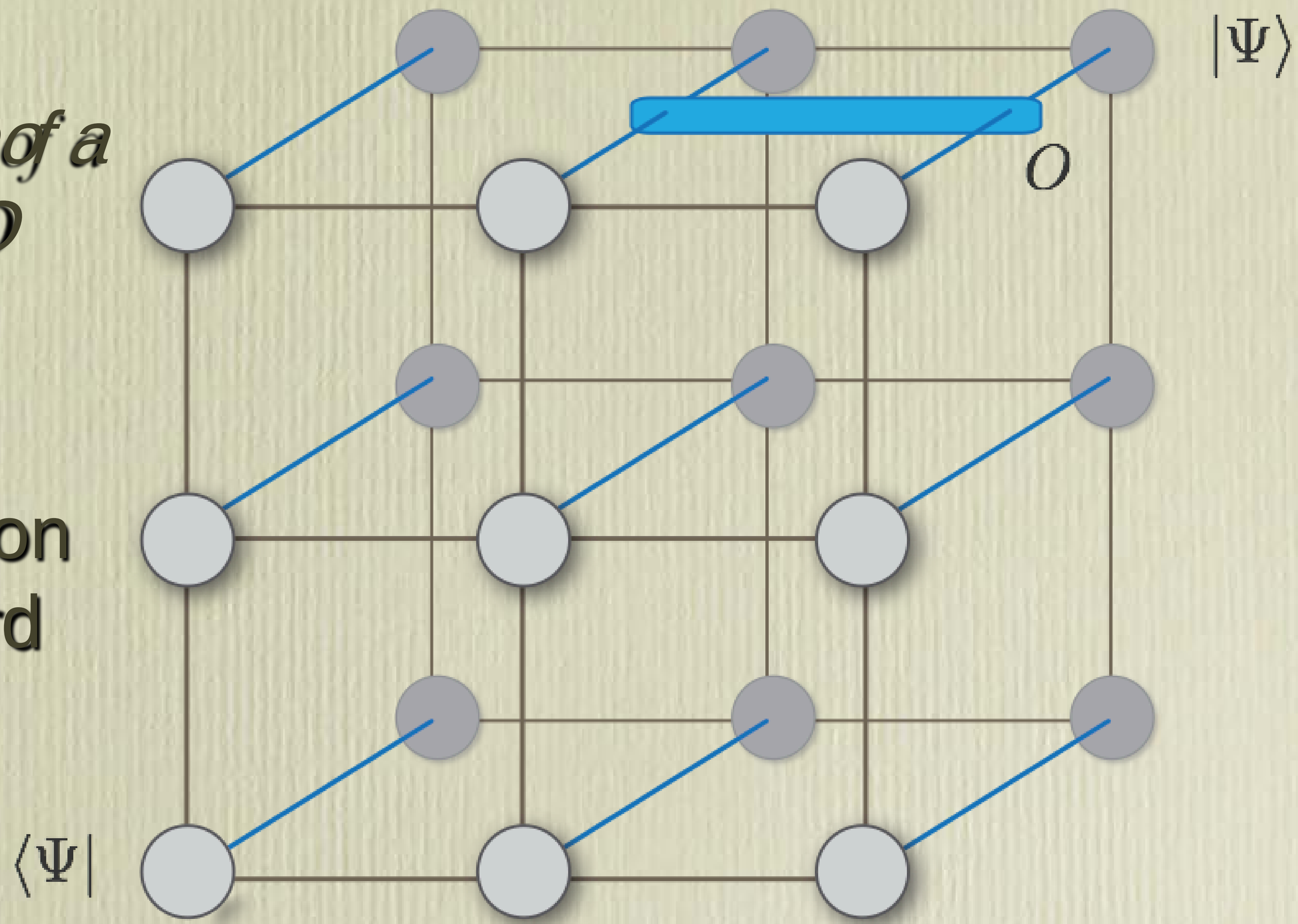
Tr = “Tr”

Observables and PEPS

Expectation value of a local operator O

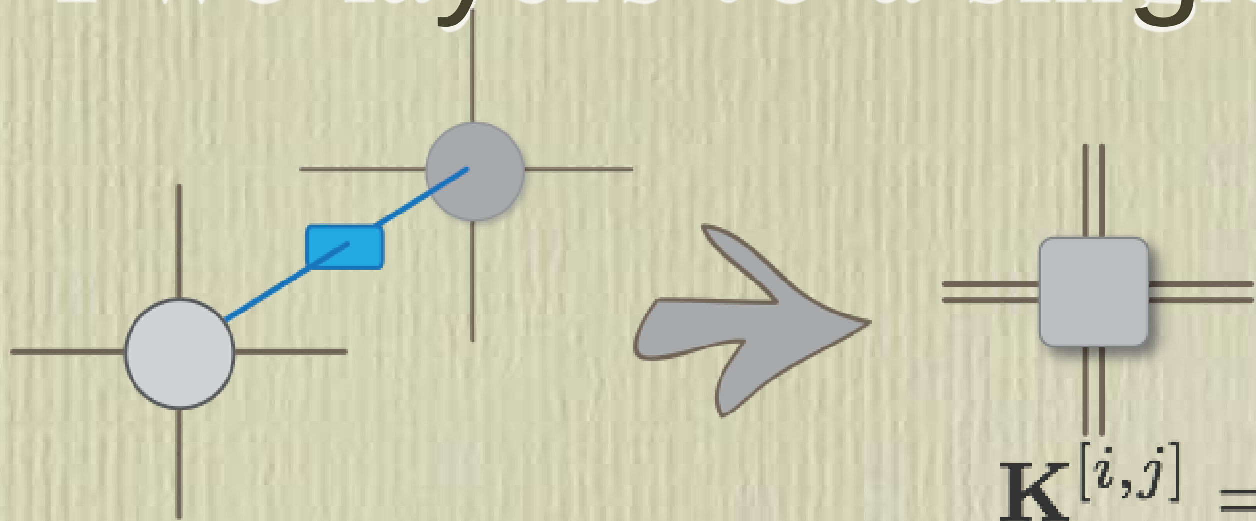
$\langle\Psi|O|\Psi\rangle$

Exact contraction straight forward but costly!



$$\langle\Psi|O|\Psi\rangle = \sum_{s_1,s_2,\ldots,s'_1,s'_2,\ldots} O_{s'_1,s'_2,\ldots,s_1,s_2,\ldots} \mathrm{Tr}\left(\mathbf{A}^{[1,1]s'_{1,1}*}\ldots\mathbf{A}^{[m,n]s'_{m,n}*}\otimes\mathbf{A}^{[1,1]s_{1,1}}\ldots\mathbf{A}^{[m,n]s_{m,n}}\right)$$

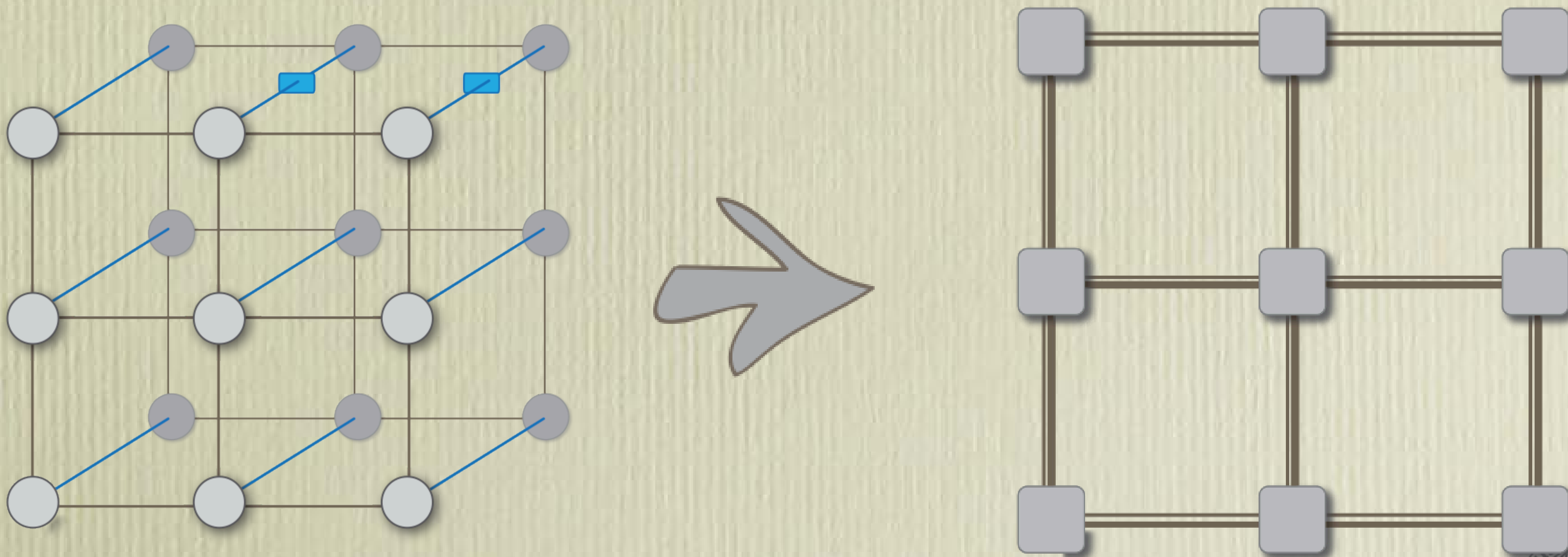
Two layers to a single double layer



Bond dimension D^2

$$\mathbf{K}^{[i,j]} = \sum_{s,s'} O^{[i,j]}_{s',s} \mathbf{A}^{[i,j]s} \otimes \mathbf{A}^{[i,j]\,s'*}$$

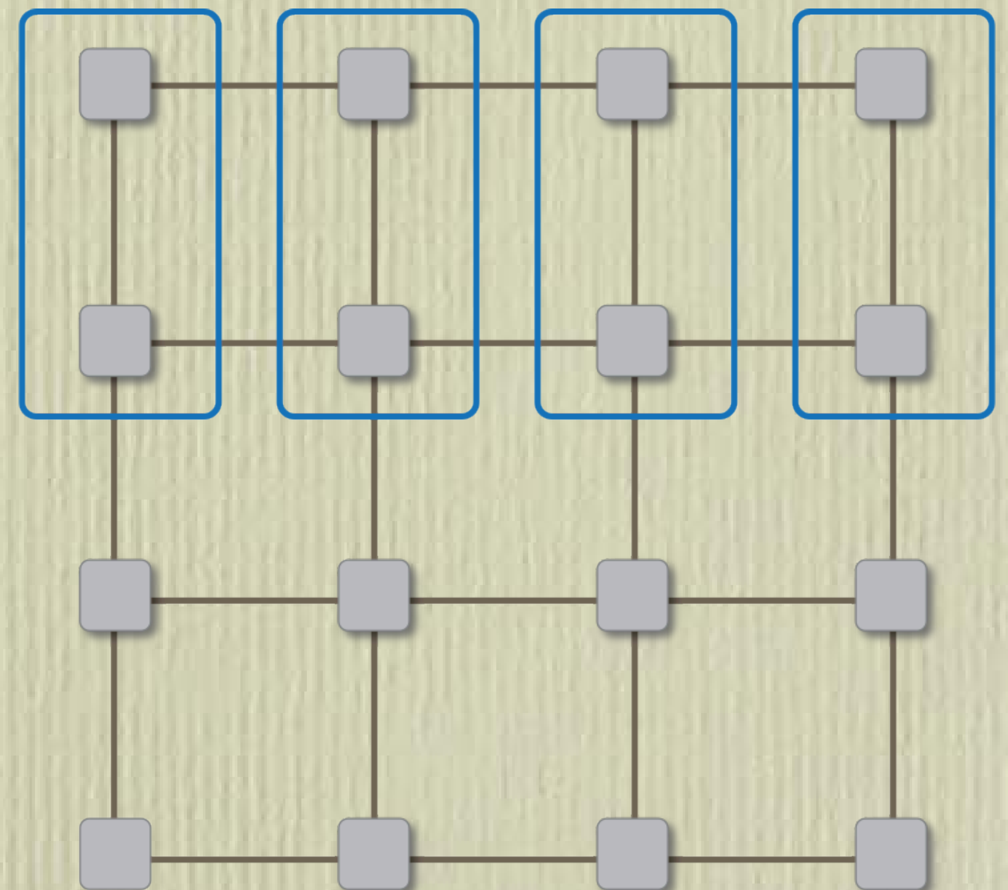
$$K^{[i,j]}_{l',l,r',r} = \sum_{s,s'} O^{[i,j]}_{s',s} A^{[i,j]s}_{l,r} A^{[i,j]s'*}$$

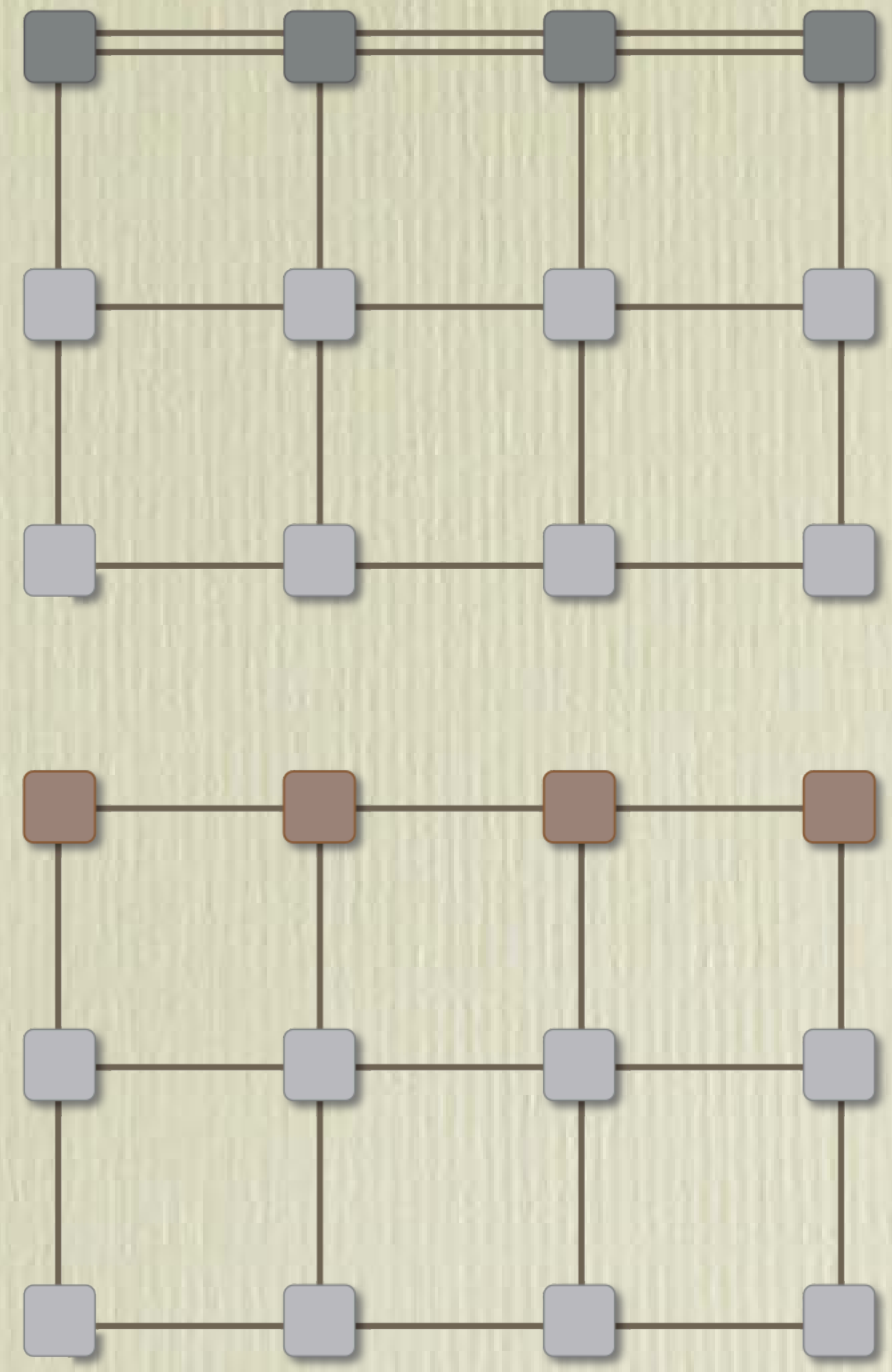


$$\langle\Psi|O|\Psi\rangle = \mathrm{tr}\Big(\mathbf{K}^{[1,1]}\mathbf{K}^{[1,2]}\dots\mathbf{K}^{[m,n]}\Big)$$

Efficient contraction of PEPS

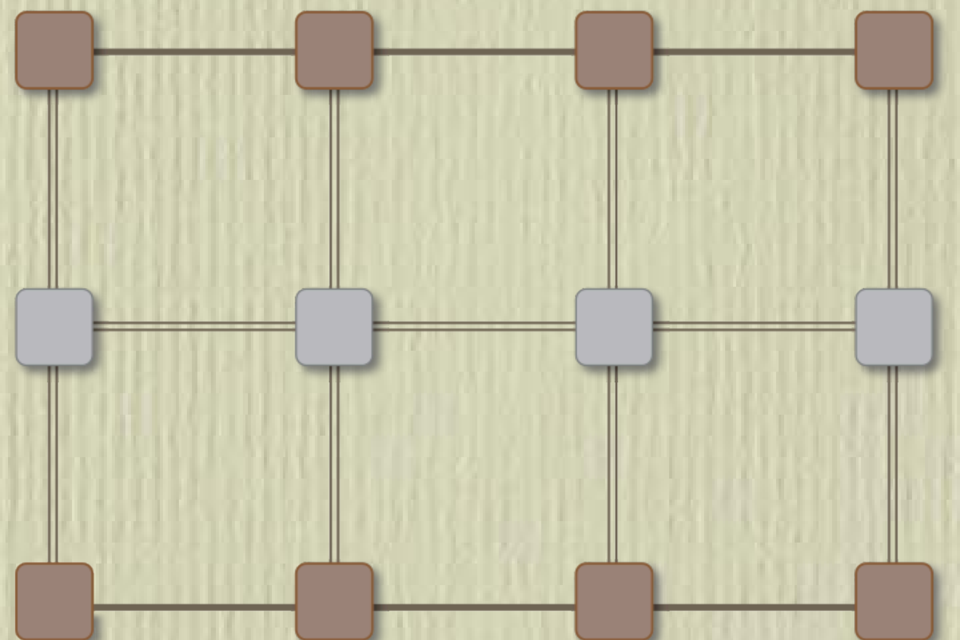
F Verstraete & JI Cirac (unpublished)

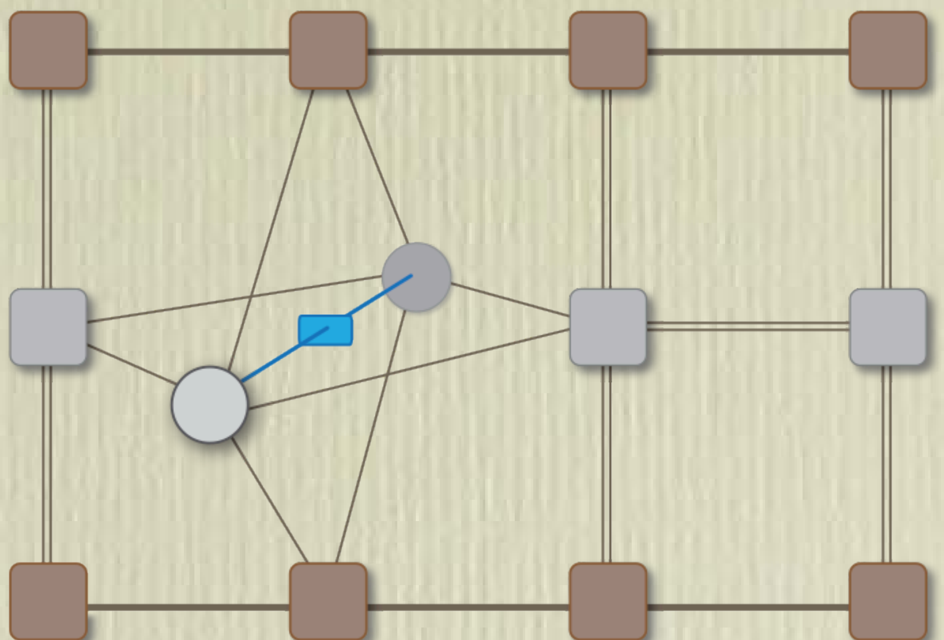




1. Merge two rows together
2. Truncate $D^4 \to \tilde{D}$
3. Replace the two rows

Variational minimization





$$E = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{\langle\phi^{[i,j]}|H_{\text{eff}}^{[i,j]}|\phi^{[i,j]}\rangle}{\langle\phi^{[i,j]}|N_{\text{eff}}^{[i,j]}|\phi^{[i,j]}\rangle}$$

$$A_{lrud}^{[i,j]s} \rightarrow \left[\phi^{[i,j]}\right]_{(lruds)}$$

How to minimize energy?

Solve a generalized eigenvalue problem

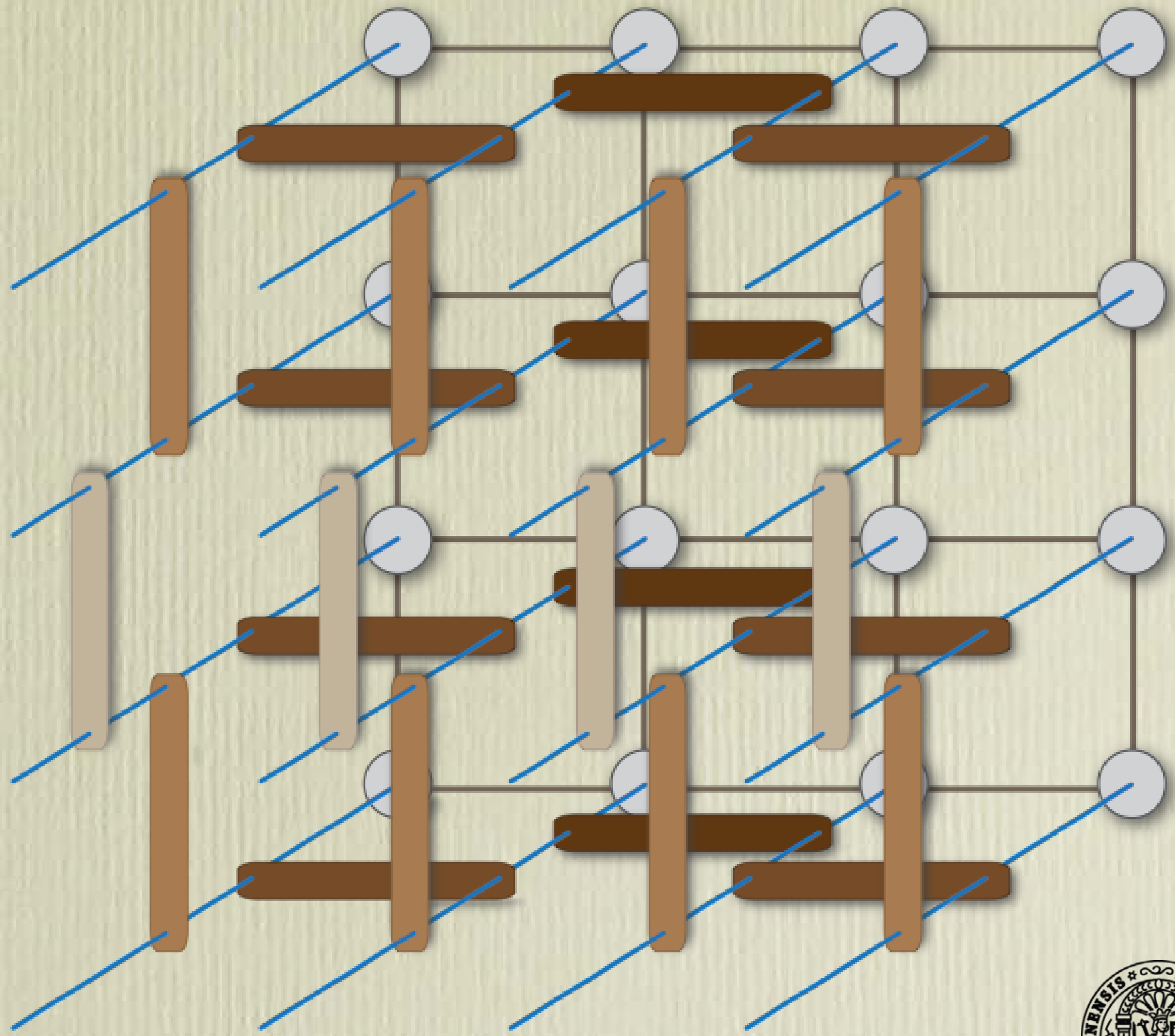
$$\mathbf{H}\phi = \lambda\mathbf{N}\phi$$

and move to the next site...

(Imaginary) time evolution

Finite-site PEPS:
Time evolution very costly

i-PEPS:
Imaginary time evolution the way to go!



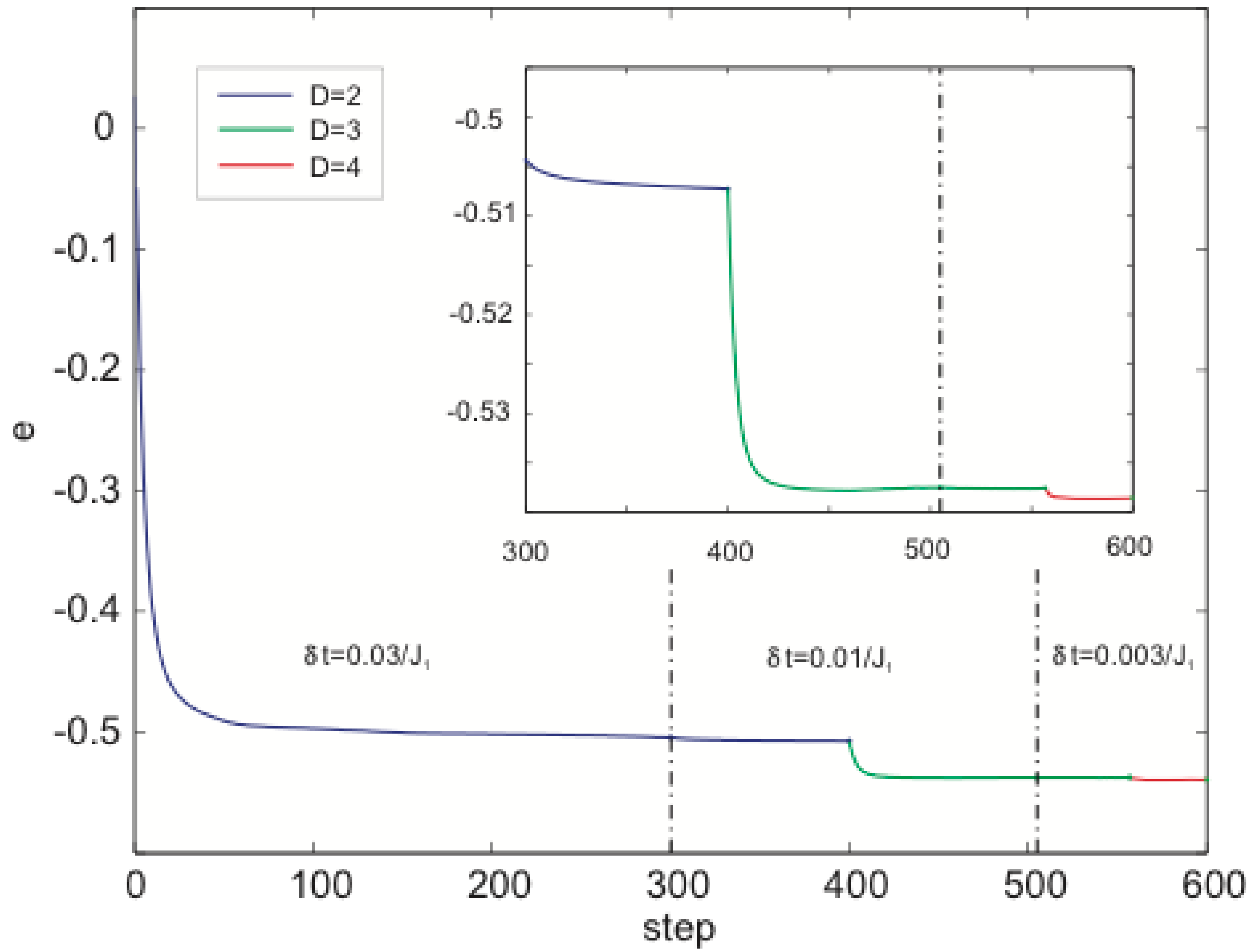
(Imaginary) time evolution

V Murg, F Verstraete & JI Cirac, PRB (09)

Fini
Tim
ver

i-PE
Ima
evo
way

$$H = J_1 \sum_{\langle ij \rangle} \mathbf{s}_i \cdot \mathbf{s}_j + J_3 \sum_{\langle\langle\langle ij \rangle\rangle\rangle} \mathbf{s}_i \cdot \mathbf{s}_j$$



10×10

$J_3/J_1 = 0.5$

There's more...

- infinite PEPS (iPEPS)

J Jordan, R Orus, G Vidal, F Verstraete, & JI Cirac, PRL (08)

- multiscale entanglement renormalization (MERA)

G Vidal, PRL (07)

- quantum monte carlo + tensor networks

N Schuch, MM Wolf, F Verstraete & JI Cirac, PRL (08)
A Sandvik & G Vidal, PRL (07)

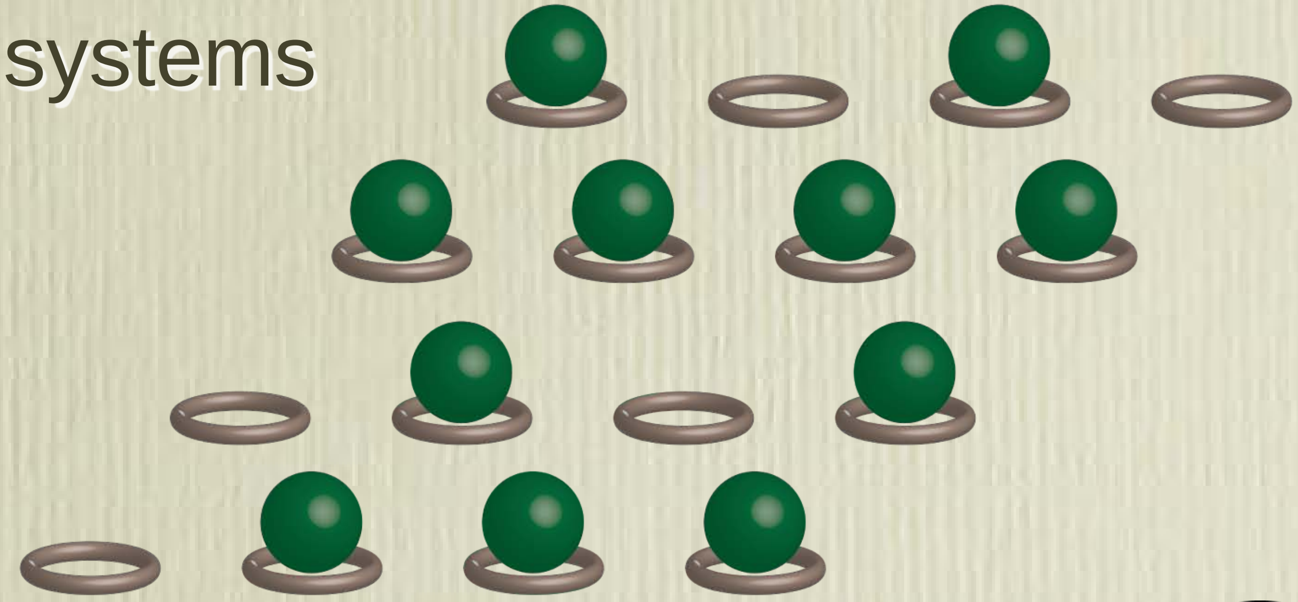
- tensor renormalization

HH Zhao et al, PRB (10)

Fermionic systems

- 1-dimensional fermionic systems
  - Jordan-Wigner transformation

- 2-dimensional fermionic systems
  - fermionic PEPS



Fermionic 1-D systems

$$\sum_j \left[(c_j c_{j+1}^\dagger - c_j^\dagger c_{j+1}) + \mu c_j^\dagger c_j\right]$$

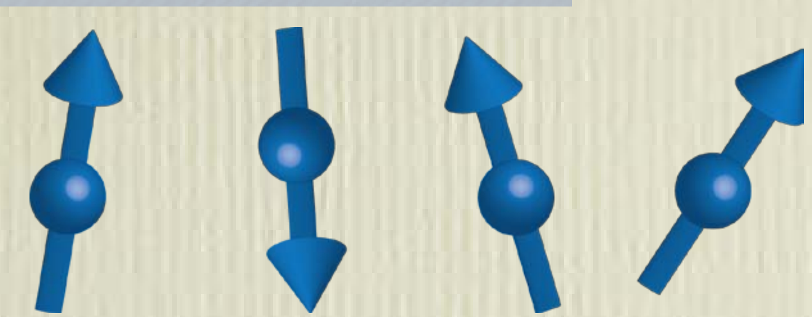
Jordan-Wigner Transformation

$$c_j^\dagger \to (1/2)\Big(\prod_{j'<j} \sigma_j^{\mathrm{z}}\Big)\sigma_j^+$$

$$c_j \to (1/2)\Big(\prod_{j'<j} \sigma_j^{\mathrm{z}}\Big)\sigma_j^-$$

$$\sigma_j^\pm = \sigma_j^{\mathrm{x}} \pm i\sigma_j^{\mathrm{y}}$$

$$\sum_j \left[(\sigma_j^- \sigma_{j+1}^+ + \sigma_j^+ \sigma_{j+1}^-)/4 + (\mu/2)(1+\sigma_j^{\mathrm{z}})\right]$$



Locality of interactions is preserved!

PEPS and fermions

1. Fermionic (contraction) order is important

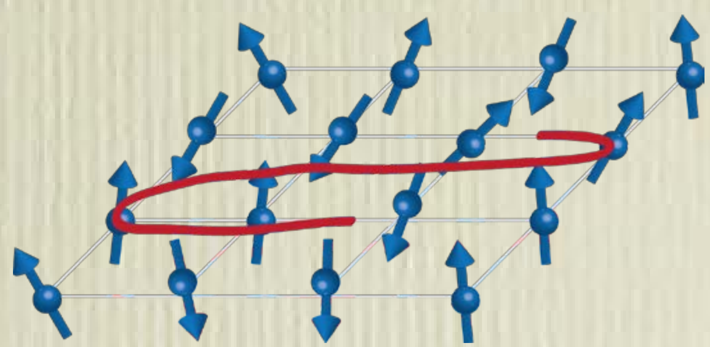
$$\{c_i, c_j^\dagger\} = \delta_{ij} \qquad \{c_i, c_j\} = 0$$

$$(c_1^\dagger)^{k_1}(c_2^\dagger)^{k_2} = (-1)^{k_1 k_2}(c_2^\dagger)^{k_2}(c_1^\dagger)^{k_1}$$

2. Fock space

$$|\Psi\rangle = \sum_{k_1,\ldots,k_n} C_{k_1,\ldots,k_n} c_1^{\dagger\, k_1} \cdots c_n^{\dagger\, k_n} |0\rangle$$

3. Jordan-Wigner transformation
   destroys locality



4. Parity preservation

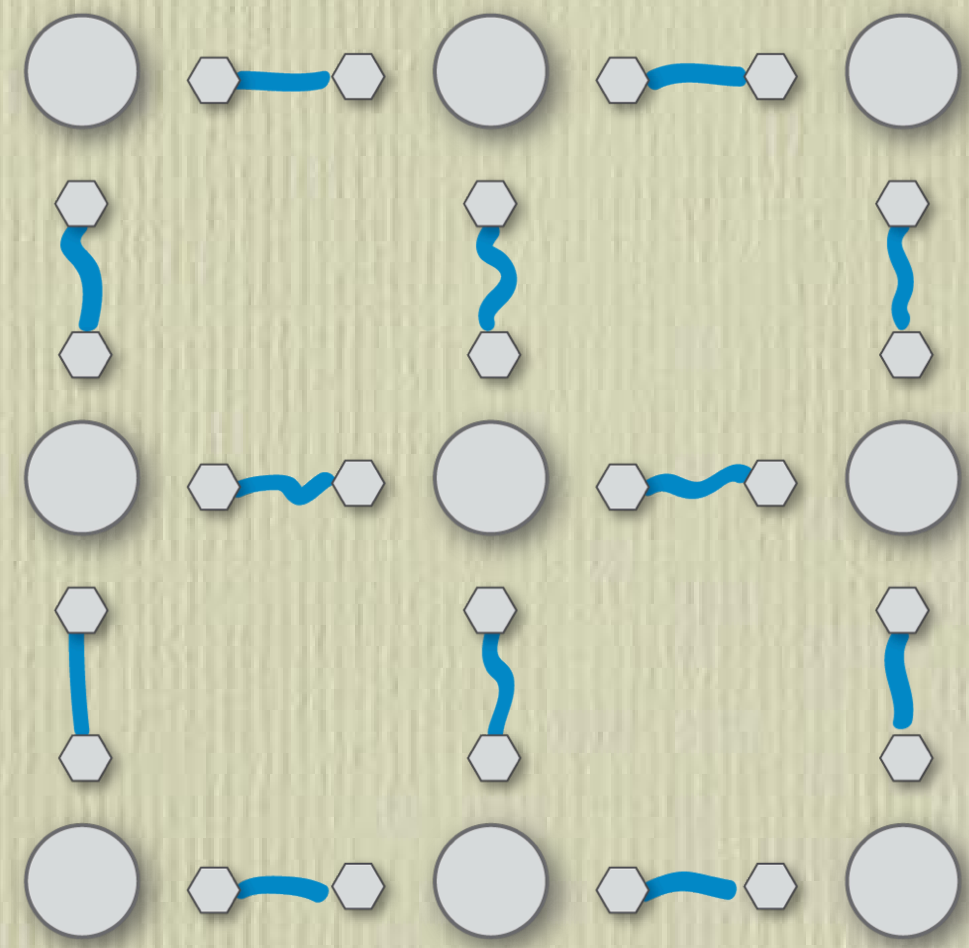
$$\langle\Psi|c_j|\Psi\rangle = 0$$

$$H = \sum_j (c_j + c_j^\dagger)$$

fPEPS = PEPS + parity + contraction order

fPEPS

CV Kraus, N Schuch, F Verstraete & JI Cirac PRA (10)



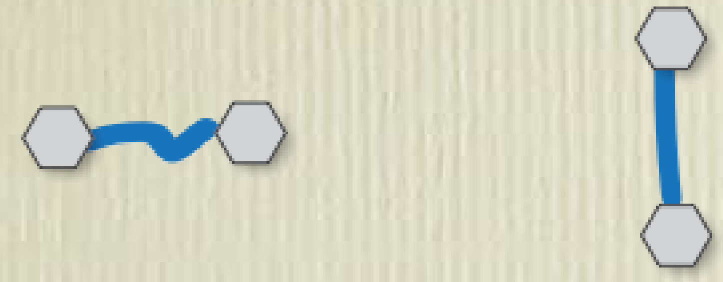
$$Q_{i,j} \equiv \sum_{lrudk} A^{[i,j]k}_{lrud} c^{\dagger\, k}_{i,j} \alpha^l_{i,j} \beta^r_{i,j} \gamma^u_{i,j} \delta^d_{i,j}$$

$$\text{parity}(Q_{i,j}) = P_{i,j}$$

$$H_{(i,j)\to(i,j+1)} \equiv (1 + \beta^\dagger_{i,j} \alpha^\dagger_{i,j+1})$$

$$V_{(i,j)\to(i+1,j)} \equiv (1 + \delta^\dagger_{i,j} \gamma^\dagger_{i+1,j})$$

Entangled pair



Q's (anti-)commute   H's and V's commute

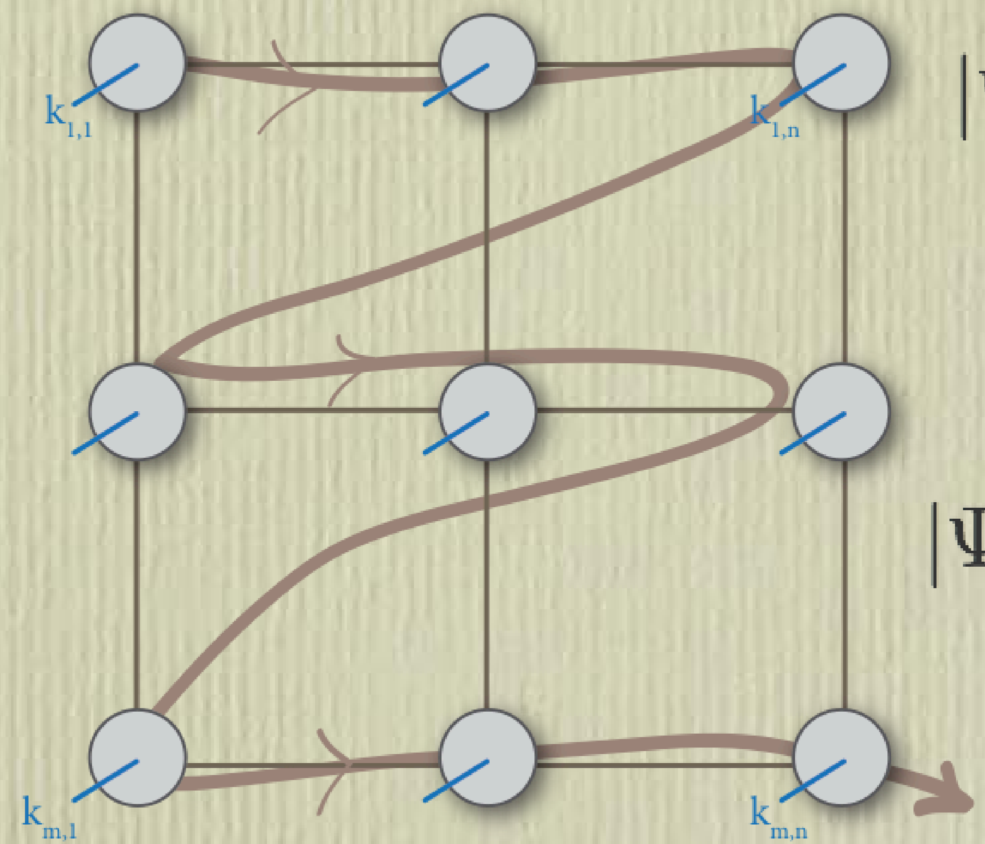
$$|\Psi\rangle = \langle Q_{1,1} \cdots Q_{m,n} \prod_\nu H_\nu \prod_\mu V_\mu \rangle_{\text{aux}} |0\rangle$$

How to get a tensor network from this mess?

f-Contraction order

IP & F Verstraete PRB (10)

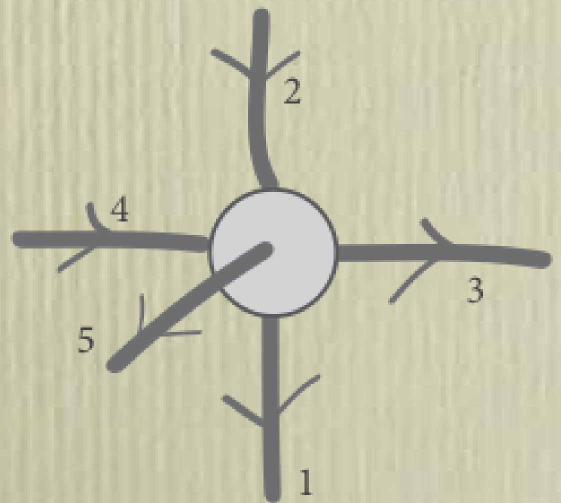
Choose a contraction order



$$|\Psi\rangle = \langle Q_{1,1} \cdots Q_{m,n} \prod_{\nu} H_\nu \prod_{\mu} V_\mu \rangle_{\text{aux}} |0\rangle$$

$$A_{i,j} = Q_{i,j} H_{i,j} V_{i,j}$$

$$|\Psi\rangle = \langle A_{m,n} \cdots A_{m,1} \cdots A_{2,1} A_{1,n} \cdots A_{1,1} \rangle_{\text{aux}} |0\rangle$$

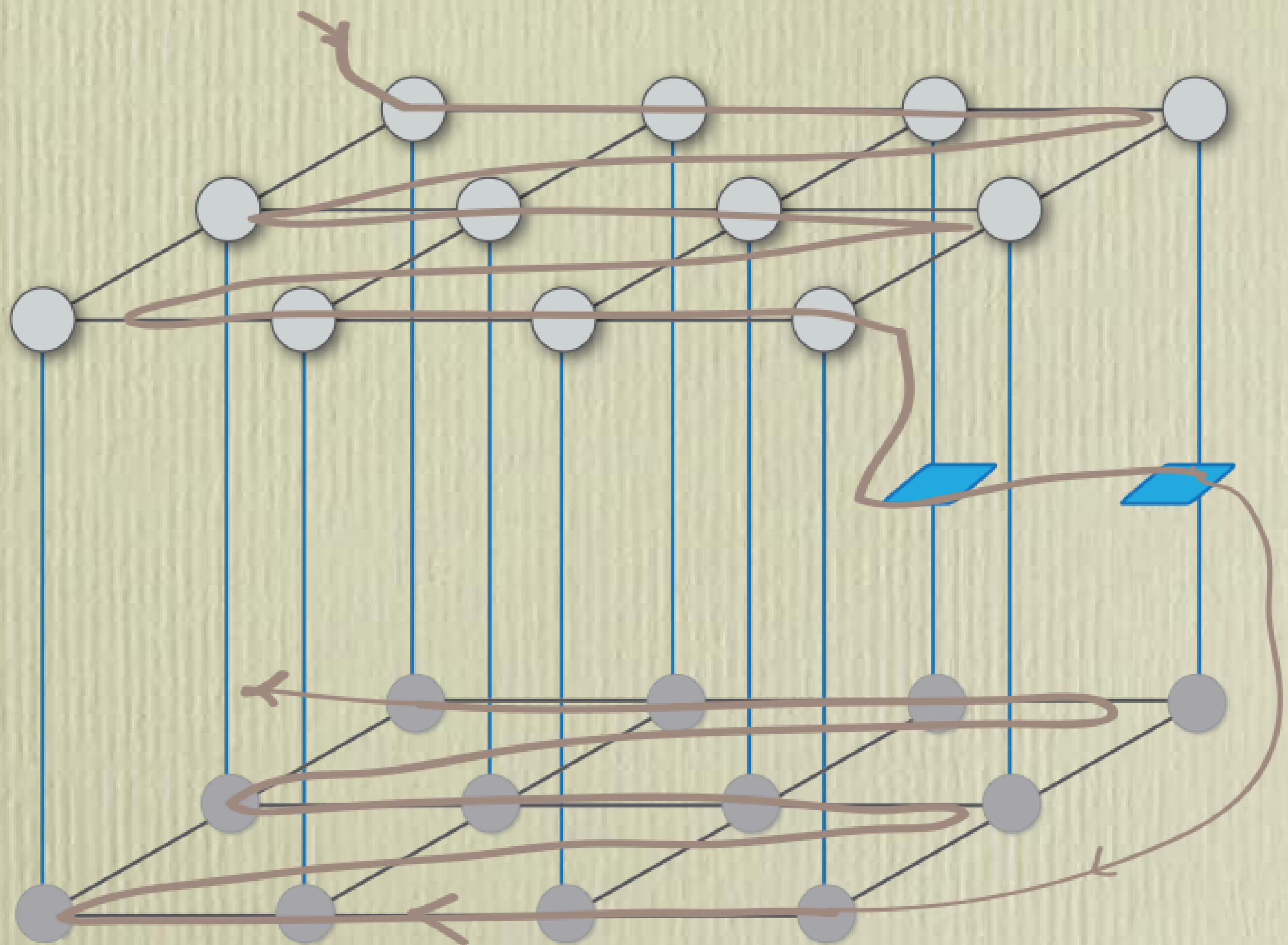


$$A_{i,j} = \sum_{lrudk} A^{[i,j]k}_{lrud} c^{\dagger\, k}_{i,j} \alpha^{l}_{i,j} \alpha^{\dagger\, r}_{i,j+1} \gamma^{u}_{i,j} \gamma^{\dagger\, d}_{i+1,j}$$

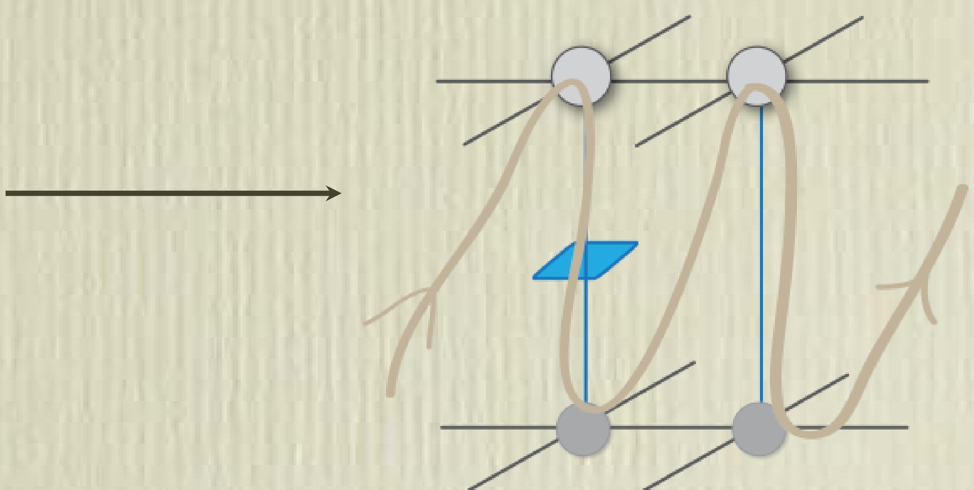
Further changes to the contraction order produce signs

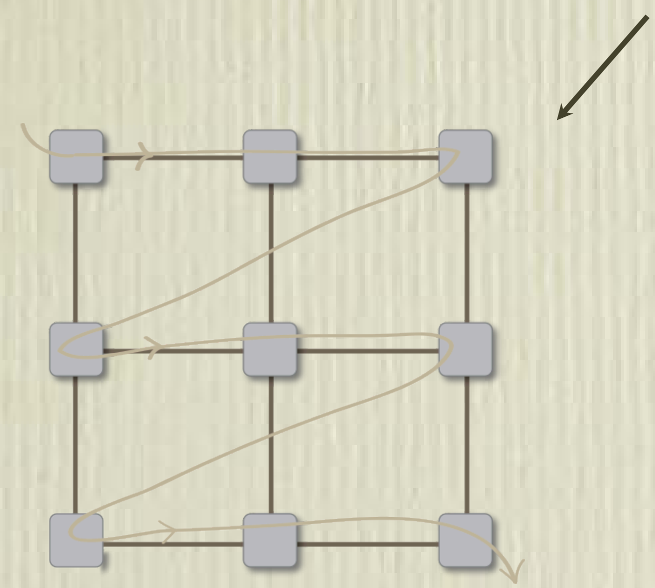
f-Observables

$$\langle\Psi|O|\Psi\rangle = \langle 0|A'^{\dagger}_{1,1}\cdots A'^{\dagger}_{m,n}O_{m,n}\cdots O_{1,1}A_{m,n}\cdots A_{1,1}|0\rangle$$



$$A'^{\dagger}_{1,1}A'^{\dagger}_{1,2} = \tilde{A}'_{1,2}\tilde{A}'_{1,1}$$



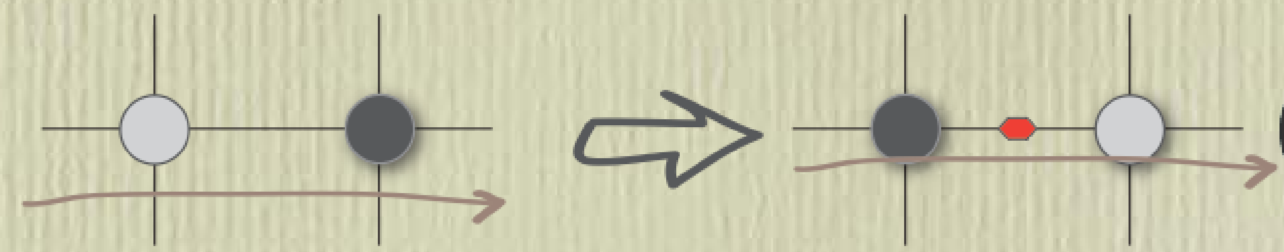


$$A'^{\dagger}_{1,1} = \sum_{\ldots,r'}\cdots\alpha'^{r'}_{1,2}$$

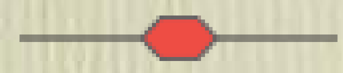
$$A'^{\dagger}_{1,2} = \sum_{\ldots,l'}\cdots\alpha'^{l'\dagger}_{1,2}$$

Fermionic swap rule

P Corboz et al (09)
T Barthel, C Pineda & J Eisert (10)
IP & F Verstraete (10)
....



$$(-1)^{p_A p_B}$$



$$\sigma(s,s') = \delta_{s,s'}(-1)^s$$

Example

$$A = 2c_1 c_2 c_3^\dagger + 3c_1^\dagger \qquad \tilde{A} = 2c_1 c_2^\dagger c_3^\dagger + 3c_1^\dagger$$

$$B = 4c_2^\dagger c_4 + 5c_4^\dagger c_5^\dagger \qquad \tilde{B} = -4c_2 c_4 + 5c_4^\dagger c_5^\dagger$$

$$\langle AB \rangle_{c_2} = \langle \tilde{B}\tilde{A} \rangle_{c_2}$$

but

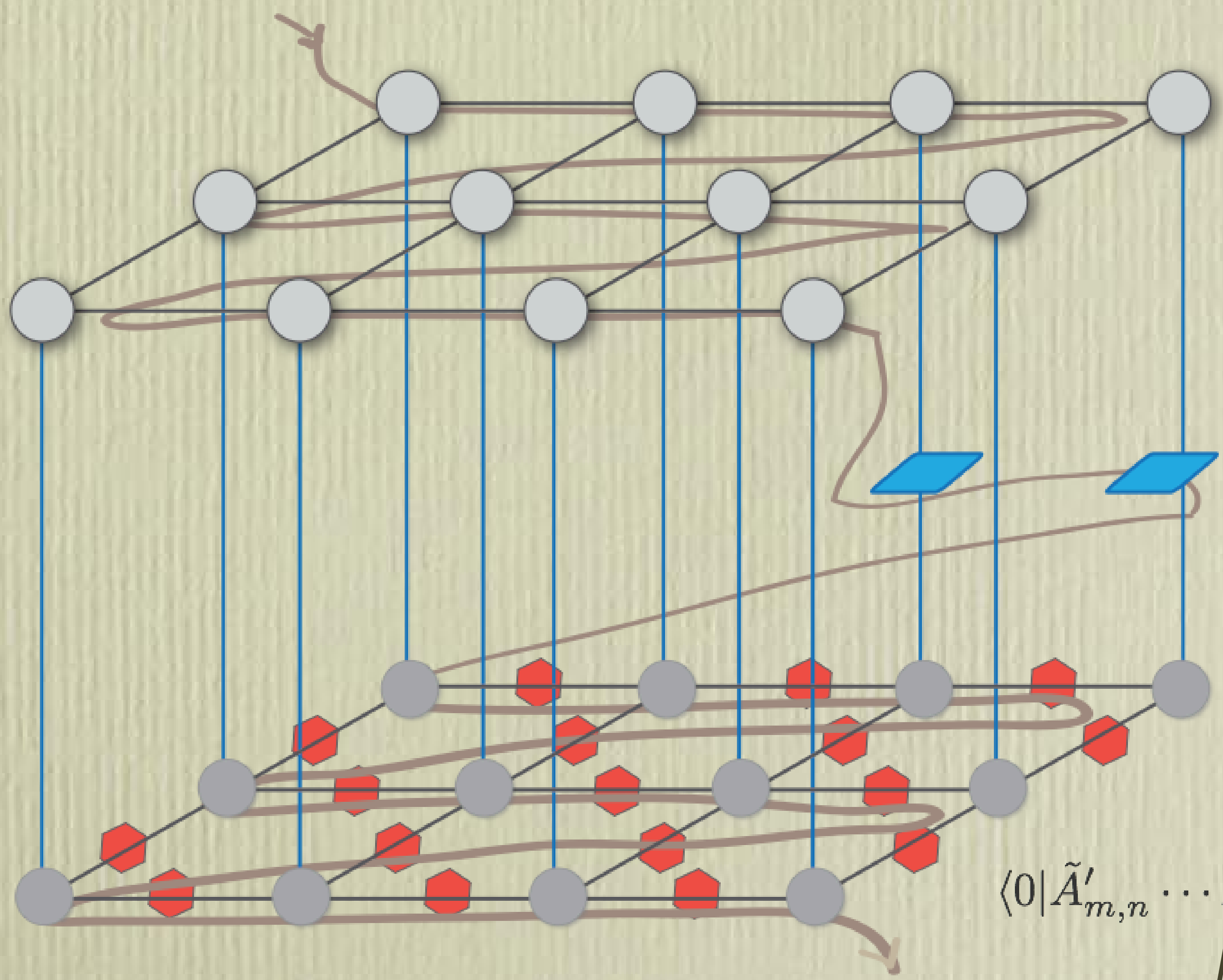
$$AB \neq \tilde{B}\tilde{A}$$

$$A'^\dagger_{1,1} \cdots A'^\dagger_{m,n} \to \tilde{A}'_{m,n} \cdots \tilde{A}'_{1,1}$$

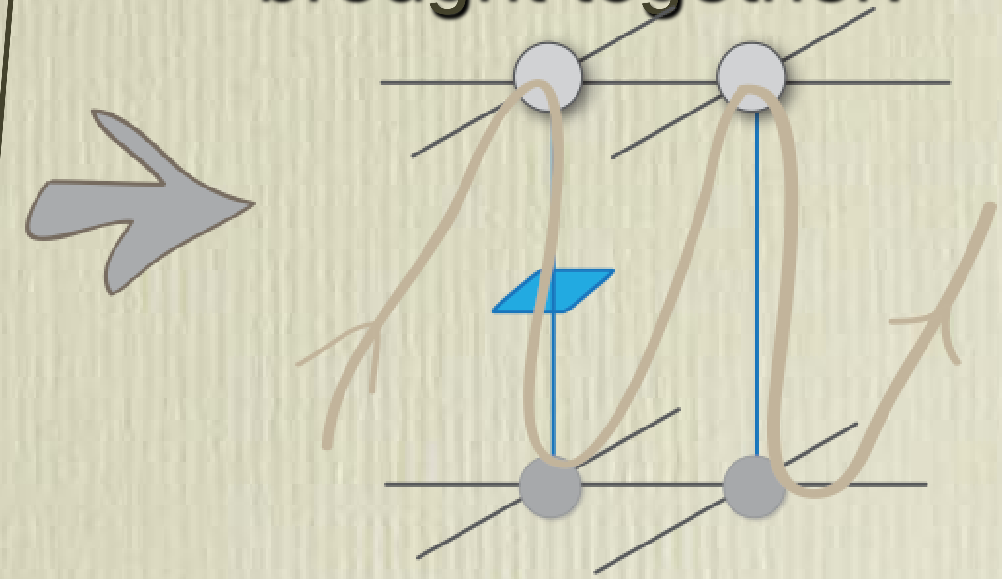
f-Observables

IP & F Verstraete PRB (10)

$$\langle\Psi|O|\Psi\rangle = \langle 0|\tilde{A}'_{m,n}\cdots\tilde{A}'_{1,1}O_{m,n}\cdots O_{1,1}A_{m,n}\cdots A_{1,1}|0\rangle$$



Physical sites in <bra| and |ket> can now be brought together!



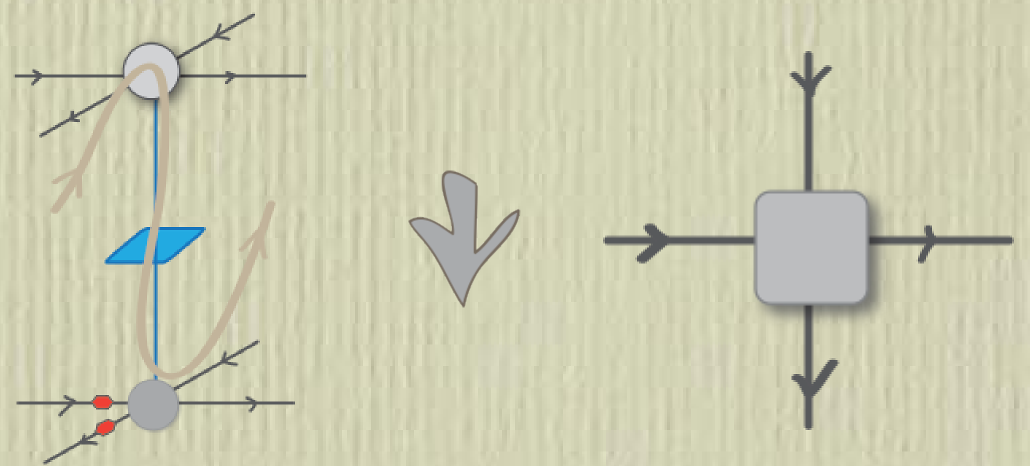
$$\langle 0|\tilde{A}'_{m,n}\cdots\tilde{A}'_{1,2}O_{m,n}\cdots O_{1,2}A_{m,n}\cdots A_{1,2}\tilde{A}'_{1,1}O_{1,1}A_{1,1}|0\rangle$$

$$\langle\Psi|O|\Psi\rangle = \langle 0|\tilde{A}'_{m,n}O_{m,n}A_{m,n}\cdots\tilde{A}'_{1,1}O_{1,1}A_{1,1}|0\rangle$$

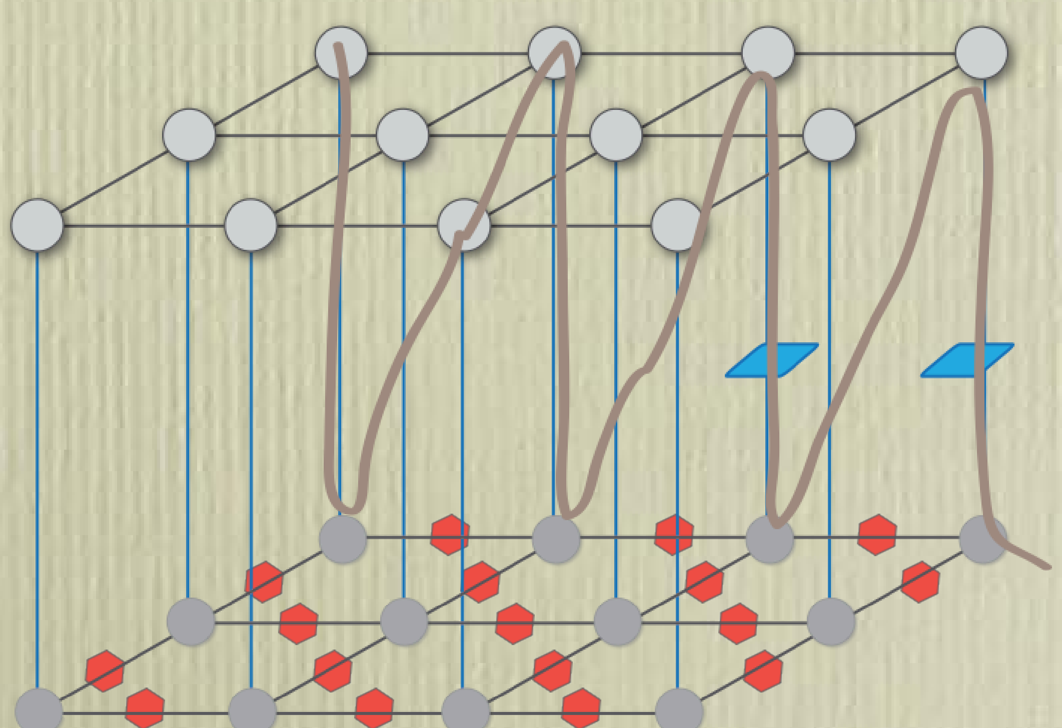
f-Observables: double-layer

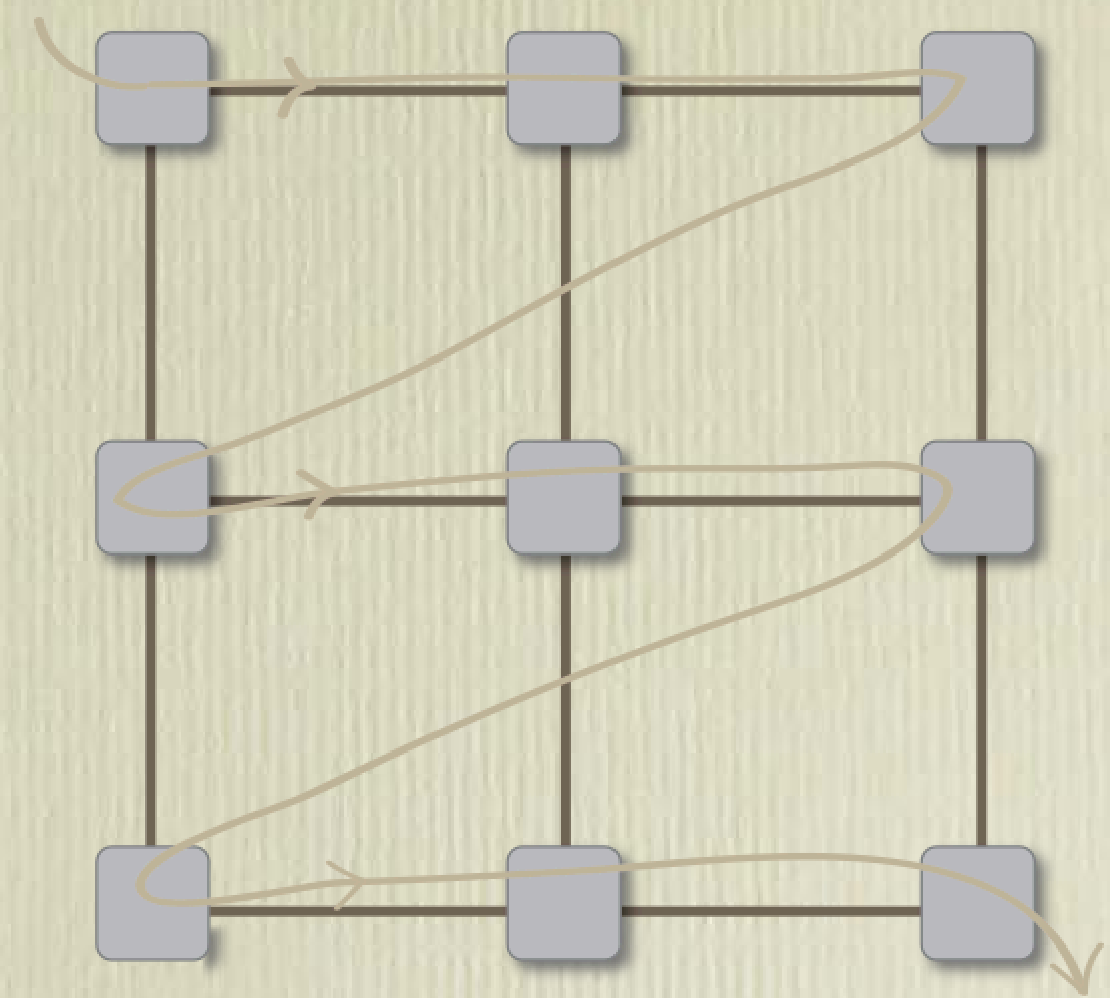
IP & F Verstraete PRB (10)

$$\langle \Psi | O | \Psi \rangle = \langle 0 | K_{m,n} \cdots K_{1,2} K_{1,1} | 0 \rangle$$



$$\langle \tilde{A}'_{i,j} O_{i,j} A_{i,j} \rangle_{\text{phys}} \equiv K_{i,j}$$





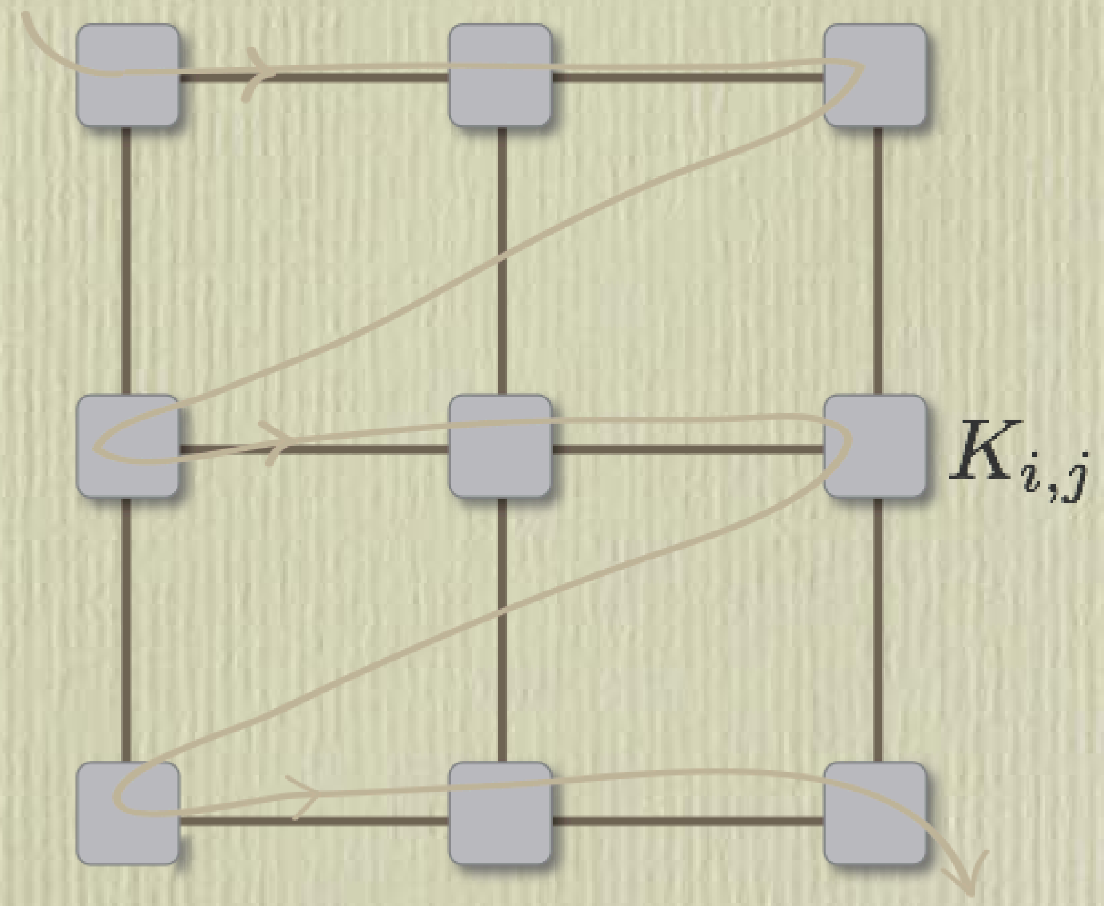
$$\alpha^{\underline{l}}_{i,j} \equiv \alpha^{l}_{i,j} {\alpha'}^{l'}_{i,j}$$

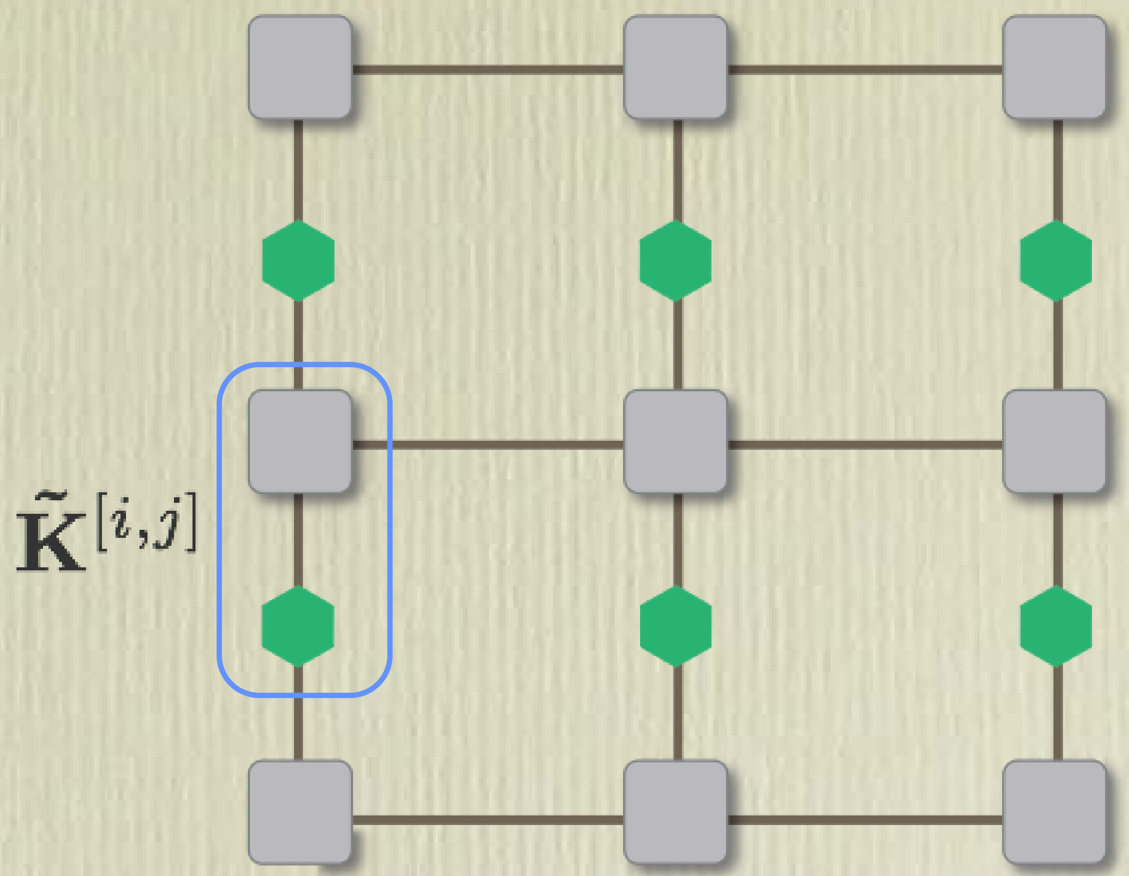
$$K_{i,j} = \sum_{\underline{l},\underline{r},\underline{u},\underline{d}} K^{[i,j]}_{\underline{l},\underline{r},\underline{u},\underline{d}} \alpha^{\dagger\,\underline{r}}_{i,j+1} \gamma^{\dagger\,\underline{d}}_{i+1,j} \alpha^{\underline{l}}_{i,j} \gamma^{\underline{u}}_{i,j}$$

$$K^{[i,j]}_{\underline{lrud}} = f_{\text{K}}(\underline{l},\underline{r},\underline{u},\underline{d}) \sum A^{[i,j]\,k}_{lrud} O_{k',k} A^{[i,j]\,k\,*}_{l'r'u'd'}$$

Conversion to sign-free TN

IP & F Verstraete PRB (10)





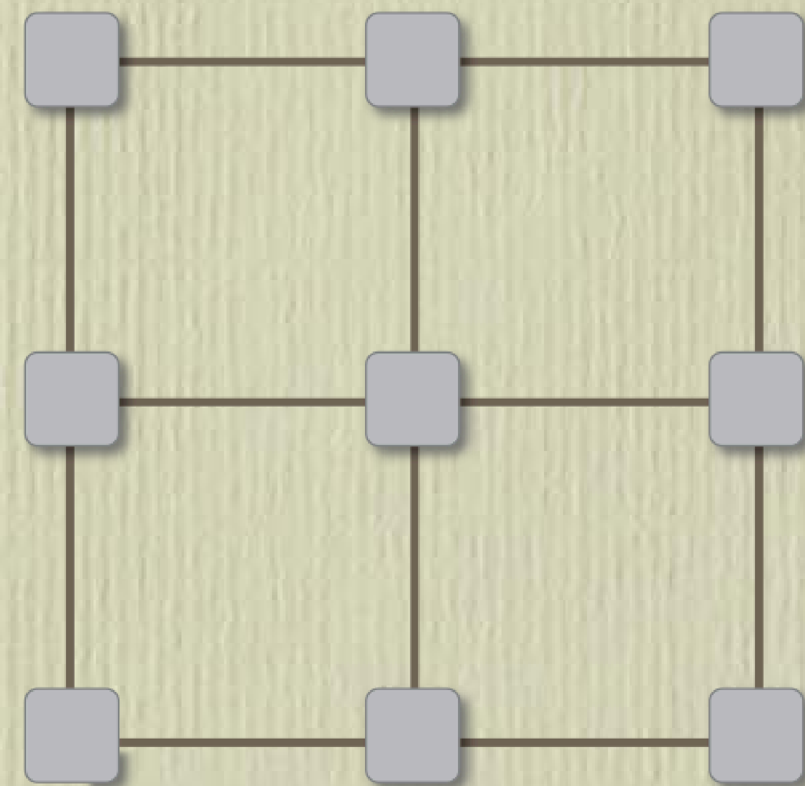
$$\langle 0|K_{m,n}\cdots K_{1,1}|0\rangle \to \mathrm{Tr}\left(\tilde{\mathbf{K}}^{[1,1]}\ldots\tilde{\mathbf{K}}^{[m,n]}\right)$$

site&product operator dependent sign factors (globally determined)

$$\sigma_{(i,j)\to(i+1,j)}(v,v') = \delta_{v,v'}(-1)^{v(\sum_{j'<j} p_{i+1,j'})}$$

Sign-free contraction of fPEPS

IP & F Verstraete PRB (10)



All fermionic signs are accounted for locally!

$$\langle\Psi|O|\Psi\rangle = \mathrm{Tr}\left(\tilde{\mathbf{K}}^{[1,1]}\dots\tilde{\mathbf{K}}^{[m,n]}\right)$$

Technical details

$$K^{[i,j]}_{\underline{lrud}} = f_{\mathrm{K}}(\underline{l},\underline{r},\underline{u},\underline{d})\, g_{i,j}(\underline{d},\underline{p}) \sum_{k,k'} A^{[i,j]\,k}_{lrud}\, O^{[i,j]}_{k',k}\, A^{[i,j]\,k\,*}_{l'r'u'd'}$$

$$f_{\mathrm{K}}(\underline{l},\underline{r},\underline{u},\underline{d}) = (-1)^{u'+l'+(l+l')(u+u')+l'l+(l+l')(r+u+d)+(r+r')(u'+d')+d(u+u')+u'u}$$

$$g_{i,j}(\underline{d},\underline{p}) = (-1)^{(d+d')\sum_{j'<j} p_{i+1,j}}$$

It's not very pretty - but it's local!

fPEPS algorithm

1. Choose a site (i,j) and calculate effective operators

$$H = \sum_{\mu \in \mathrm{loc.prod.op.}} H^{[\mu]} \quad \Rightarrow \quad H_{\mathrm{eff}} = \sum_{\mu} H^{[\mu]}_{\mathrm{eff}}$$

2. Find A[i,j] minimizing the total energy

$$E = \frac{\mathbf{A}^{[i,j]} \cdot \mathbf{H}^{[i,j]}_{\mathrm{eff}} \mathbf{A}^{[i,j]}}{\mathbf{A}^{[i,j]} \cdot \mathbf{N}^{[i,j]}_{\mathrm{eff}} \mathbf{A}^{[i,j]}} \qquad O^{[i,j]}_{\mathrm{eff}} = O^{[i,j]}_{\mathrm{even-even}} \oplus O^{[i,j]}_{\mathrm{odd-odd}}$$

3. Move to the next site and repeat

Once we've obtained a sign-free tensor network, all intermediate steps are well known.

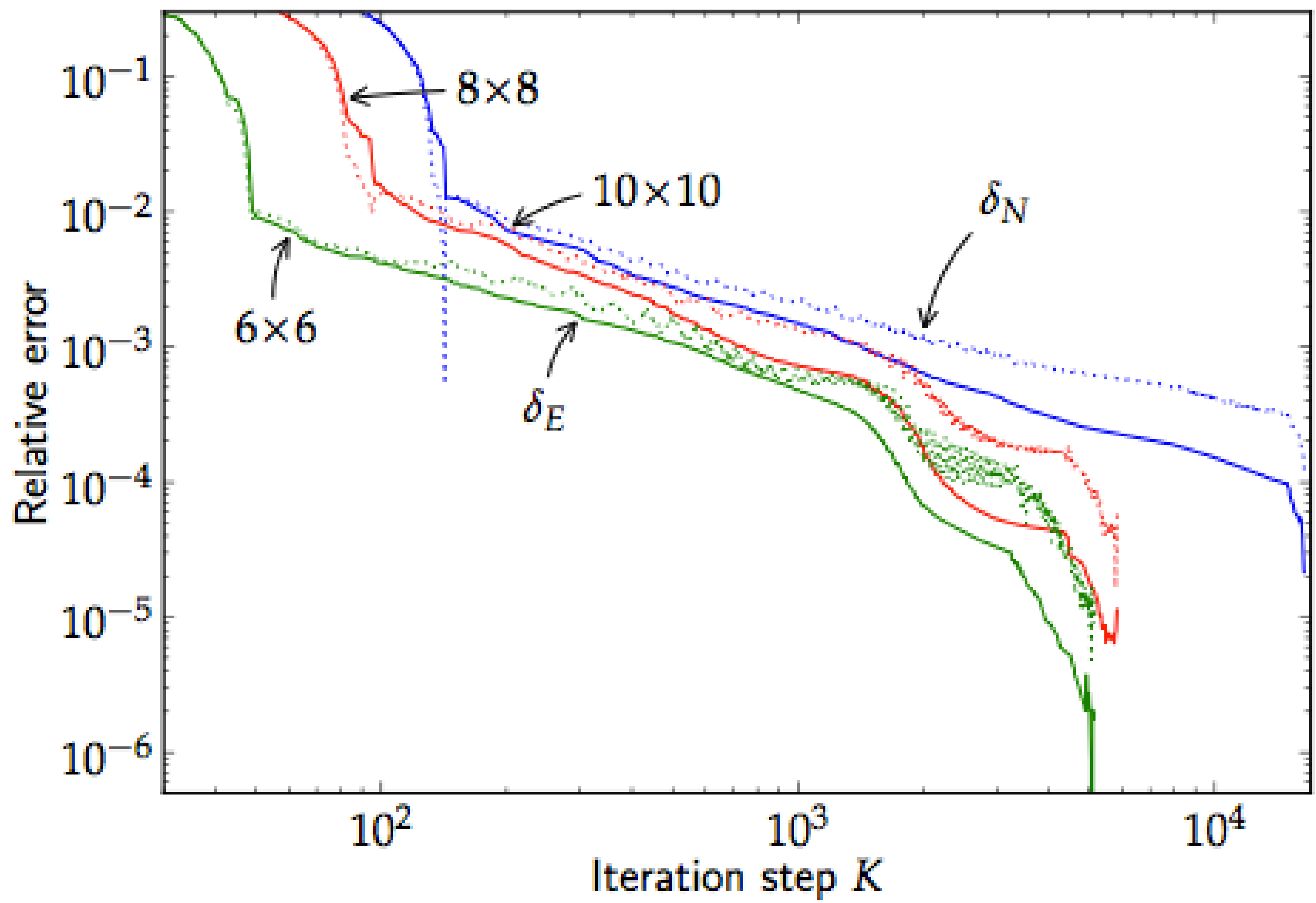
fPEPS algorithm

IP & F Verstraete PRB (10)

1.

$$H = \sum_{\langle \mu\nu \rangle} \left[c_\mu^\dagger (c_\nu - \gamma c_\nu^\dagger) + \text{h.c.} \right] - 2 \sum_\nu \lambda c_\nu^\dagger c_\nu$$

2.



$D = 4$

3.

$\gamma = 1$

$\lambda = 3$

fPEPS algorithm

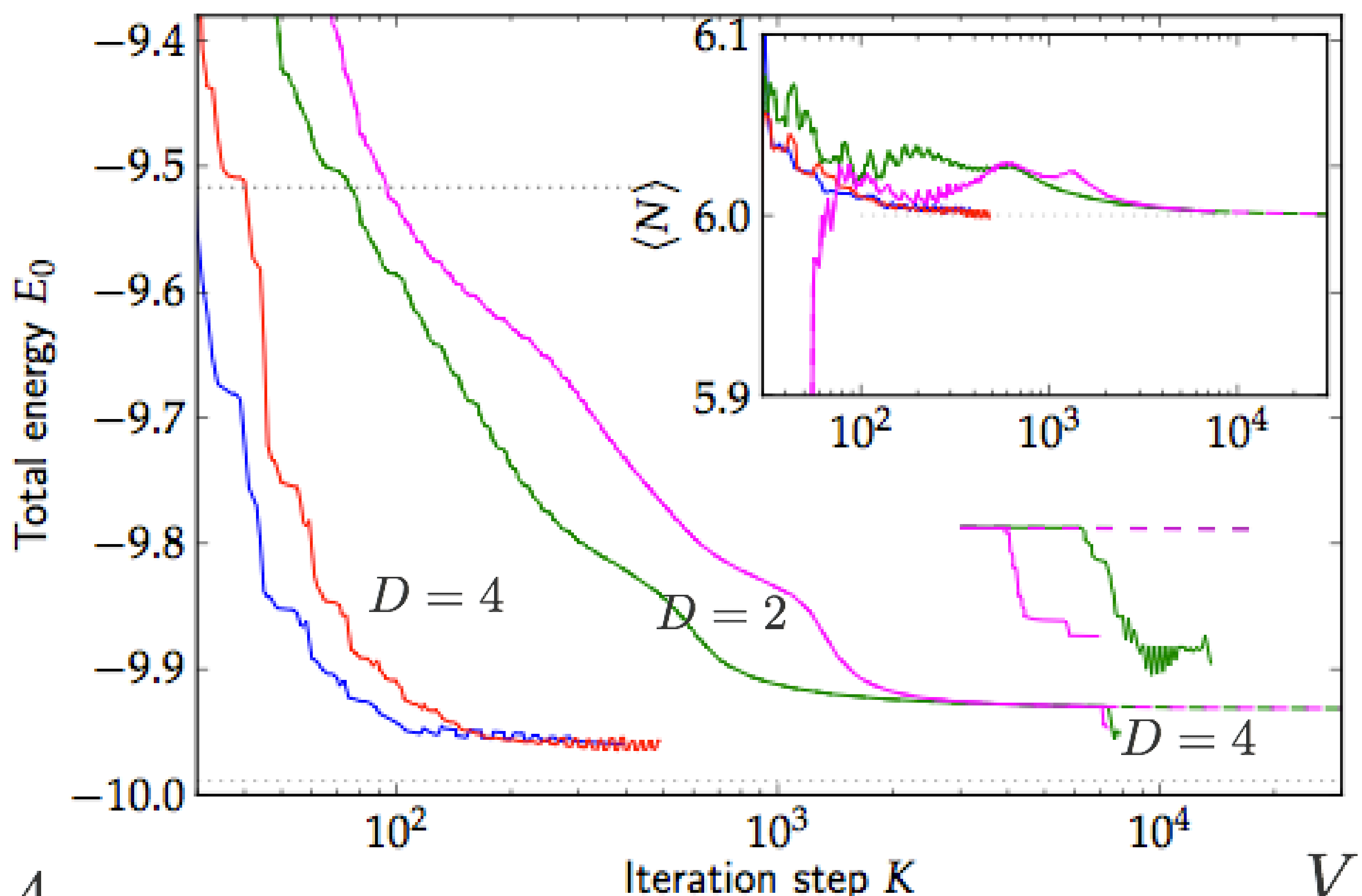
IP & F Verstraete PRB (10)

1.

2.

3.

$$H = -\sum_{\langle \nu\mu \rangle} \left[c_\nu^\dagger c_\mu + \text{h.c.} \right] + V \sum_{\langle \nu\mu \rangle} n_\nu n_\mu$$



4×4

$V = 0.5$

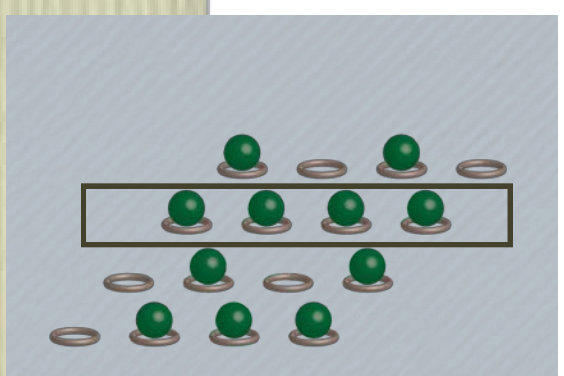
fPEPS algorithm

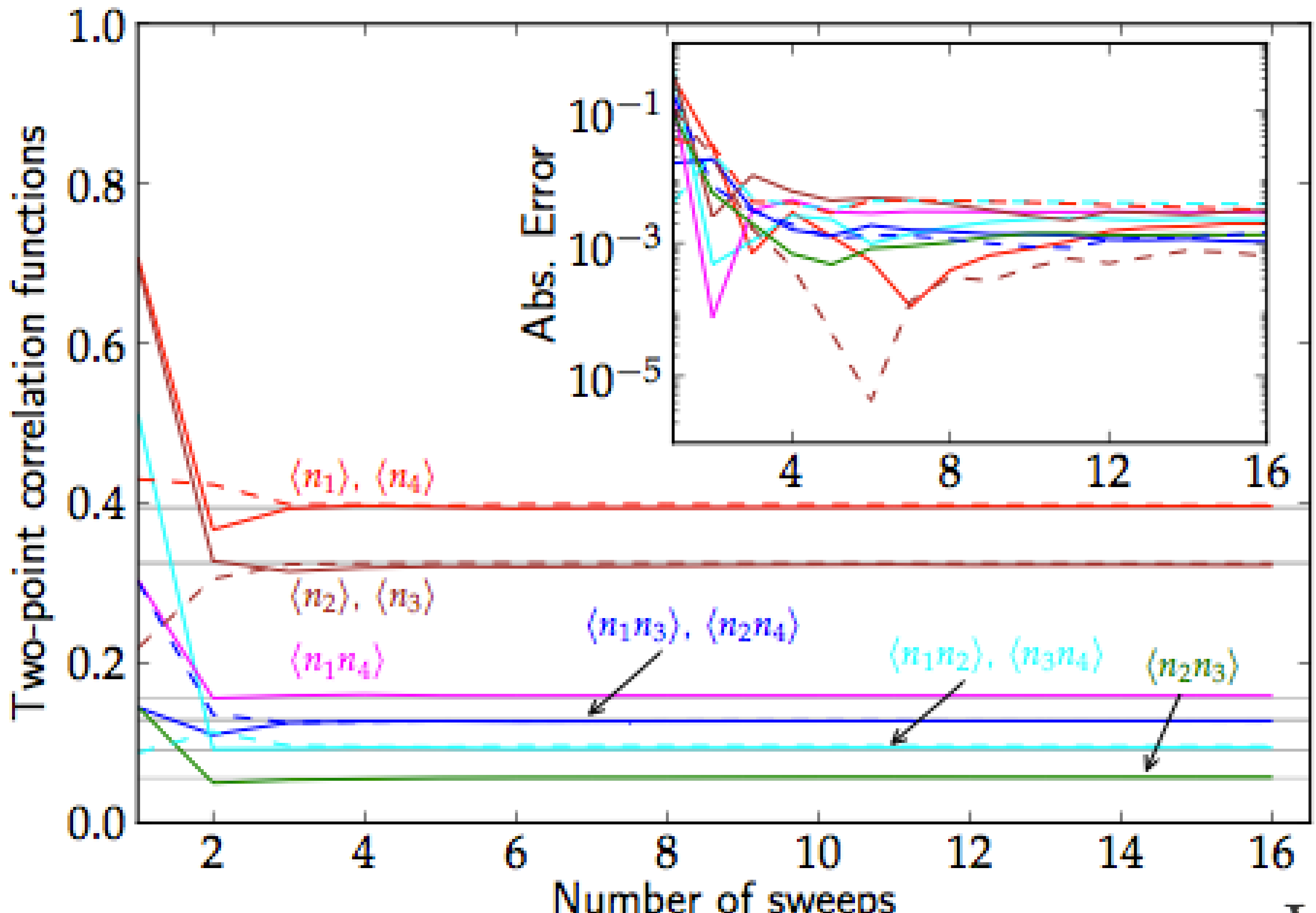
IP & F Verstraete PRB (10)

1.

$$H = -\sum_{\langle \nu\mu \rangle} [c_\nu^\dagger c_\mu + \mathrm{h.c.}] + V \sum_{\langle \nu\mu \rangle} n_\nu n_\mu$$

2.





4×4

$V = 0.5$

PEPS & fPEPS

- fPEPS basically same complexity as PEPS
- no “sign problem” (quantum monte carlo feature) with
  - fermionic systems
  - frustrated spin systems
- relatively small bond dimensions accessible presently (D~8)

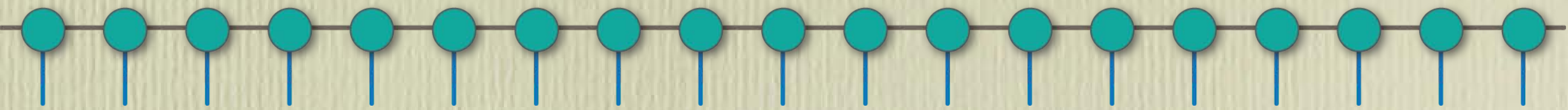
Other tensor networks

- Tree tensor networks
  - Quantum chemistry
  - Momentum space
- MERA
- String states
- Continuous matrix product states

III: Time evolution & Mixed states

- Time evolution of matrix product states:
  - a projected evolution approach
- Mixed states and time evolution
  - Systems in a thermal equilibrium
  - Systems far from the equilibrium
  - Time evolution in Heisenberg picture

Projected dynamics



$$\mathcal{T}|s_1, s_2, \ldots, s_n\rangle = |s_2, s_3, \ldots, s_n, s_1\rangle$$

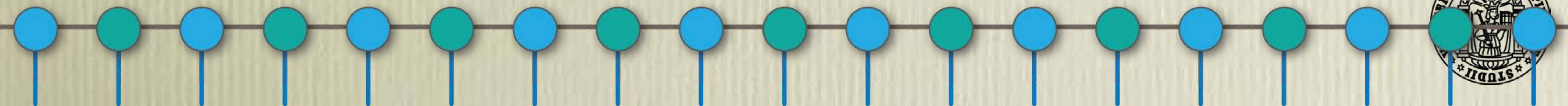
$$[H, \mathcal{T}] = 0 \qquad \mathcal{T}|\Phi_p\rangle = \mathrm{e}^{i\phi_p}|\Phi_p\rangle \qquad \phi_p \in \{0, \frac{1}{2\pi n}, \frac{2}{2\pi n}, \ldots, \frac{n-1}{2\pi n}\}$$

$$H = \sum_j \left(\sigma_j^{\mathrm{x}}\sigma_{j+1}^{\mathrm{z}} + h\sigma_j^{\mathrm{z}}\right) \Longrightarrow H = \sum_j \left(\sigma_j^{\mathrm{x}}\sigma_{j+1}^{\mathrm{z}} + (h/2)(\sigma_j^{\mathrm{z}} + \sigma_{j+1}^{\mathrm{z}})\right)$$

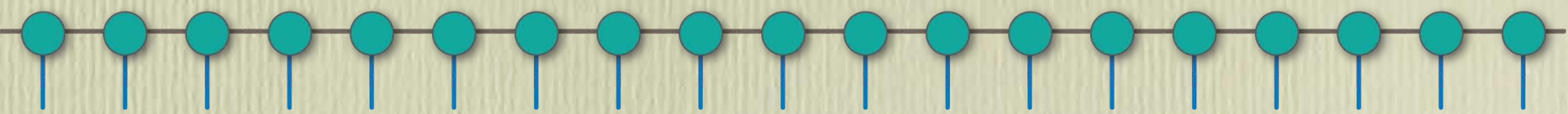
Time evolution

$$\mathcal{T}|\Psi_0\rangle = \mathrm{e}^{i\phi}|\Psi_0\rangle \quad \Longrightarrow \quad \mathcal{T}|\Psi(t)\rangle = \mathrm{e}^{i\phi}|\Psi(t)\rangle$$

But translation invariant MPS breaks the T-invariance!



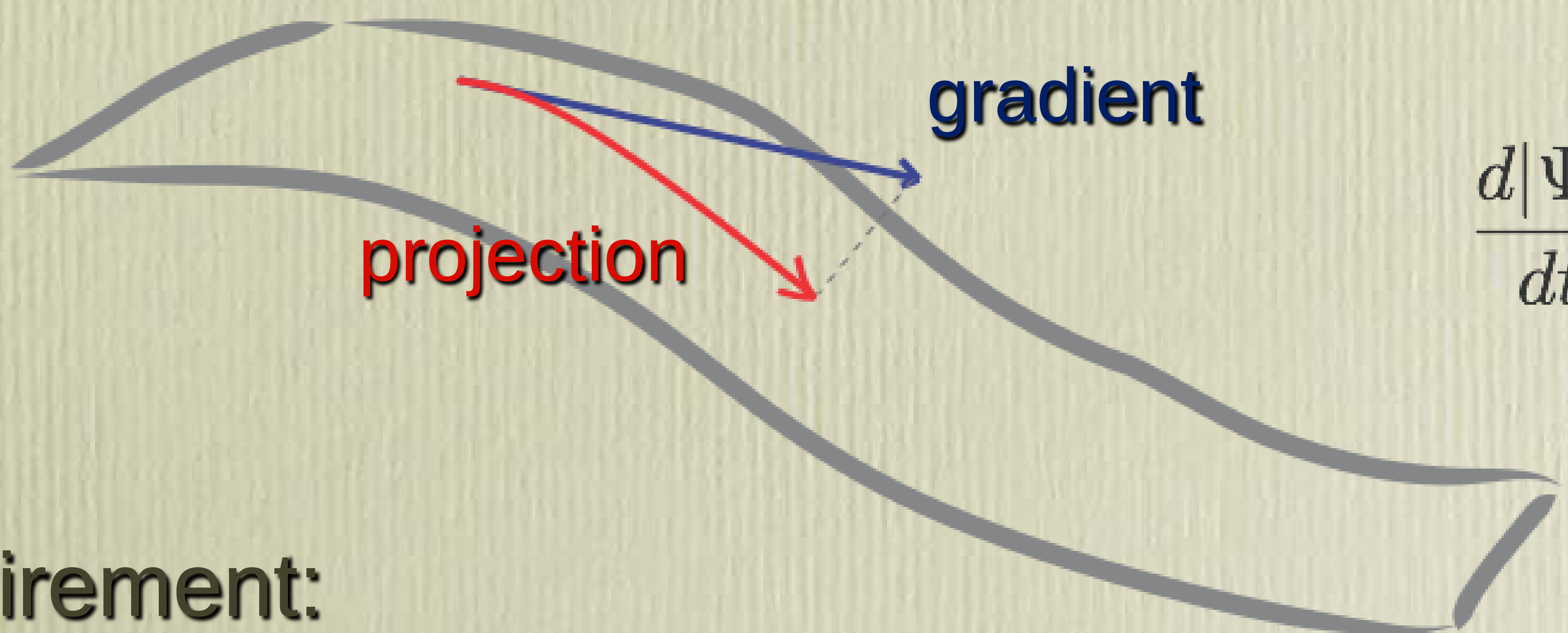
Projected dynamics



Let's choose $\phi = 0$ $\quad \mathcal{T}|\Psi\rangle = |\Psi\rangle$

quite often
$\mathcal{T}|\Psi_{\mathrm{GS}}\rangle = |\Psi_{\mathrm{GS}}\rangle$
$\mathcal{T}|\Psi_{\mathrm{GS}}\rangle = -|\Psi_{\mathrm{GS}}\rangle$

$$|\Psi\rangle = \sum_{s_1, s_2, \ldots} \mathrm{Tr}\big(\mathbf{A}^{s_1}\mathbf{A}^{s_2}\cdots\mathbf{A}^{s_n}\big)|s_1, s_2, \ldots, s_n\rangle$$



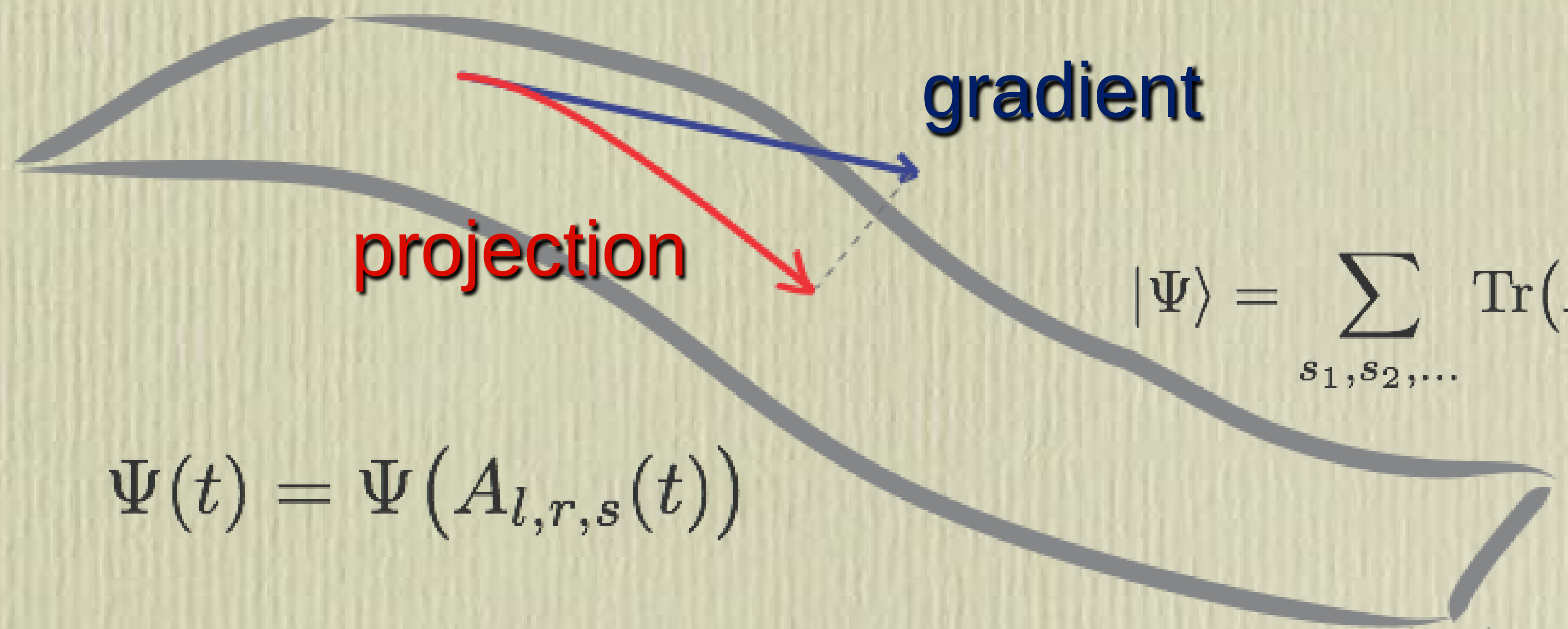
$$\frac{d|\Psi\rangle}{dt} = -iH|\Psi\rangle$$

Requirement:

$|\Psi(t)\rangle = \mathrm{e}^{-itH}|\Psi_0\rangle$ must stay in the same T-class

Projected dynamics

IP, TJ Osborne, K Temme & F Verstraete (in prep)



$$|\Psi\rangle = \sum_{s_1,s_2,\ldots} \mathrm{Tr}\left(\mathbf{A}^{s_1}\mathbf{A}^{s_2}\cdots\mathbf{A}^{s_n}\right)|s_1,s_2,\ldots,s_n\rangle$$

$$\Psi(t) = \Psi\left(A_{l,r,s}(t)\right)$$

$$\frac{d|\Psi\rangle}{dt} = -iH|\Psi\rangle \quad \Rightarrow \quad \frac{d|\Psi\rangle}{dt} = \sum_{l,r,s} \frac{\partial|\Psi\rangle}{\partial A_{lrs}} \frac{dA_{lrs}}{dt}$$

$$|\Psi_{(l,r,s)}\rangle \equiv \frac{\partial|\Psi\rangle}{\partial A_{lrs}}$$

$$H|\Psi\rangle \approx \sum_{l,r,s} x_{lrs}|\Psi_{(l,r,s)}\rangle$$

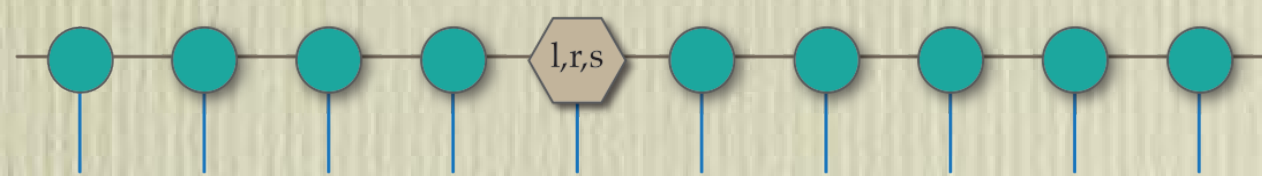
$$\boxed{\frac{dA_{lrs}}{dt} = -ix_{lrs}}$$

Infinite translation-invariant chains

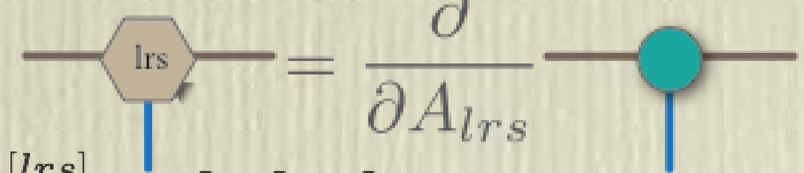
IP, TJ Osborne, K Temme & F Verstraete (in prep)

$$|\Psi_{(lrs)}\rangle \equiv \frac{\partial|\Psi\rangle}{\partial A_{lrs}}$$

$$|\Psi_{(lrs)}\rangle = \sum_{j=0}^{\infty} \mathcal{T}^j \Big($$



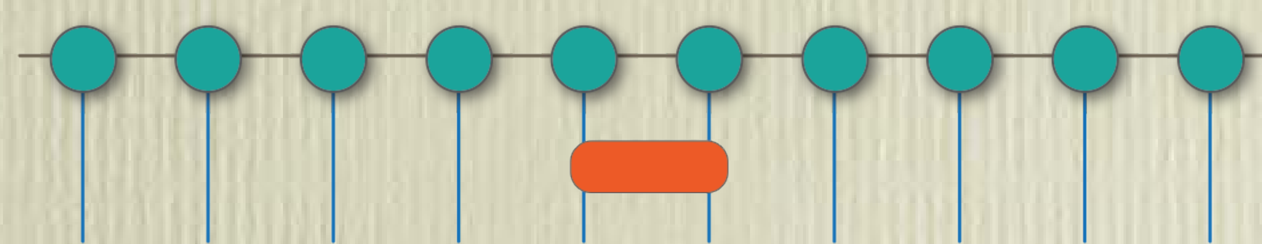
$\Big)$



$$K^{[lrs]}_{l'r's'} = \delta_{ll'}\delta_{rr'}\delta_{ss'}$$

$$H = \sum_{j=0}^{\infty} H_{j,j+1}$$

$$H|\Psi\rangle = \sum_{j=0}^{\infty} \mathcal{T}^j \Big($$



$\Big)$

$$H|\Psi\rangle \approx \sum_{lrs} x_{lrs}|\Psi_{(lrs)}\rangle \qquad \left|\left| H|\Psi\rangle - \sum_{lrs} x_{lrs}|\Psi_{(lrs)}\rangle \right|\right| = \min$$

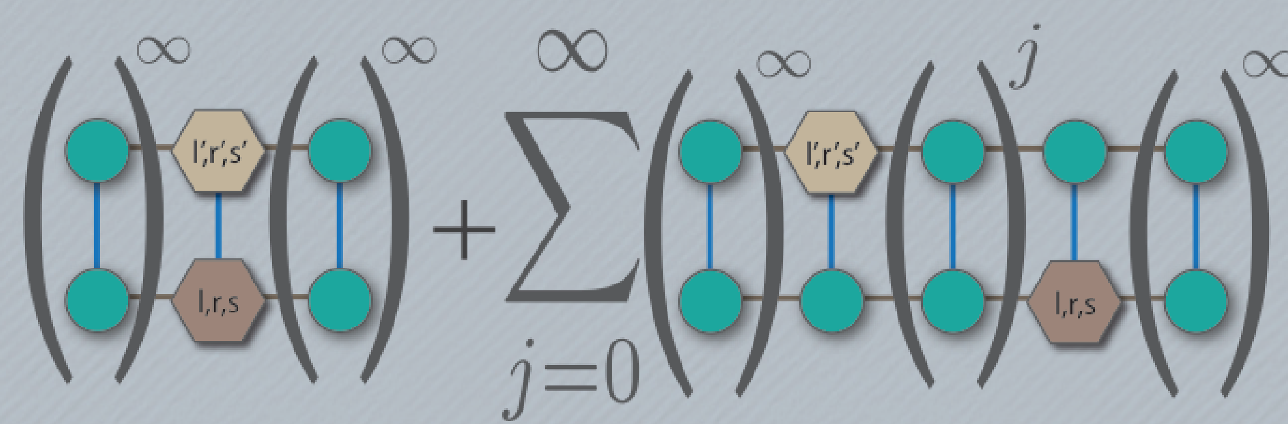
Infinite translation-invariant chains

IP, TJ Osborne, K Temme & F Verstraete (in prep)

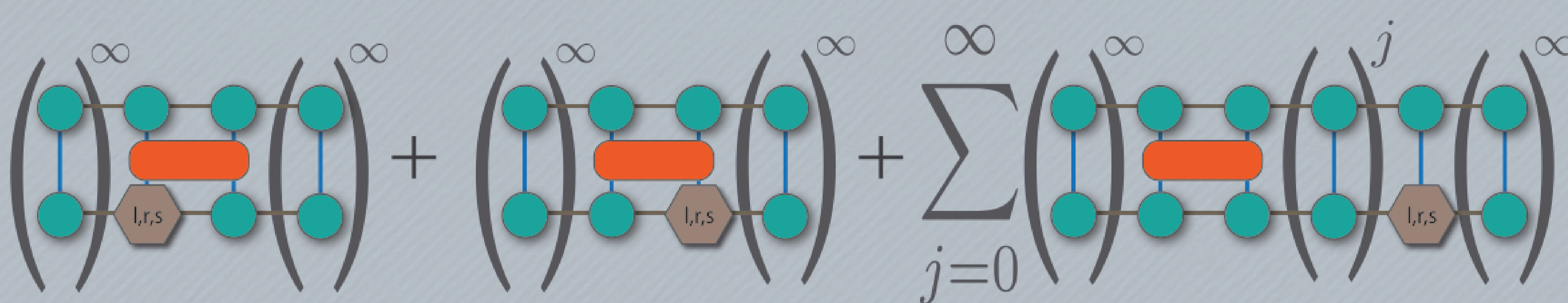
$$\left|\left|H|\Psi\rangle - \sum_{lrs} x_{lrs}|\Psi_{(lrs)}\rangle\right|\right| = \min$$

$$\underbrace{\langle\Psi_{(lrs)}|\Psi_{(l'r's')}\rangle}_{\mathbf{G}} x_{l'r's'} = \underbrace{\langle\Psi_{(lrs)}|H|\Psi\rangle}_{\mathbf{h}}$$

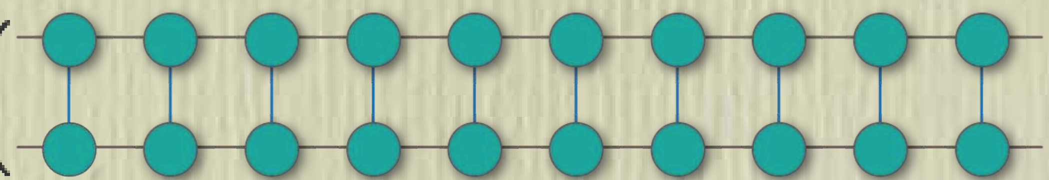
$G_{(lrs),(l'r's')} =$

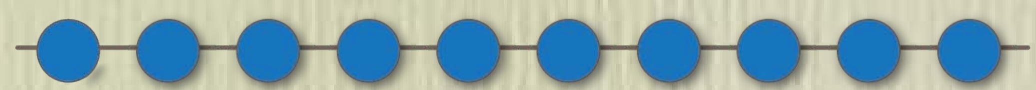


$h_{lrs} =$



Essentials of iMPS

$\langle\Psi|\Psi\rangle = \mathrm{Tr}\Big($  $\Big)$

$\langle\Psi|\Psi\rangle = \mathrm{Tr}\Big($  $\Big)$

$\langle\Psi|\Psi\rangle = \mathrm{Tr}\Big($  $\Big)$ $\qquad \langle\Psi|\Psi\rangle = \mathrm{tr}(\mathbf{E}^\infty)$

$$\mathbf{E} = \sum_s \mathbf{A}^s \otimes \mathbf{A}^{s\,*}$$

Leading eigenvectors only!

$$\mathbf{E}^\infty = |r_{\max}\rangle E_{\max}^\infty \langle l_{\max}|$$

$$\mathbf{E}|r_j\rangle = E_j|r_j\rangle$$

$$\langle l_j|\mathbf{E} = \langle l_j|E_j$$

$$\langle l_j|r_{j'}\rangle = \delta_{j,j'}$$

$$\mathbf{E} = \sum_j |r_j\rangle E_j \langle l_j|$$

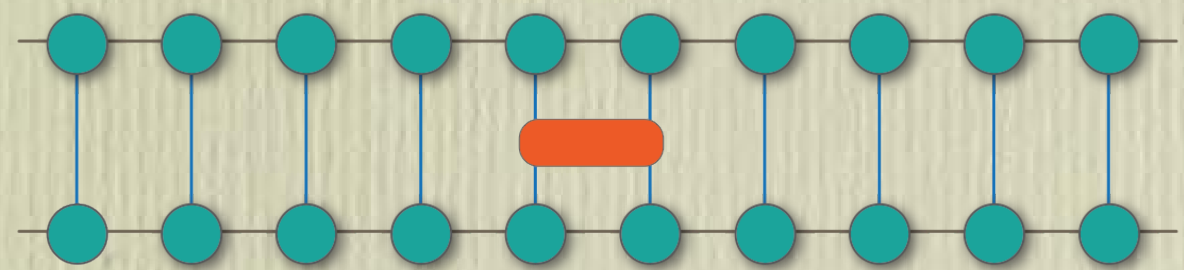
$$\langle\Psi|\Psi\rangle = \langle l_{\max}|r_{\max}\rangle E_{\max}^\infty$$

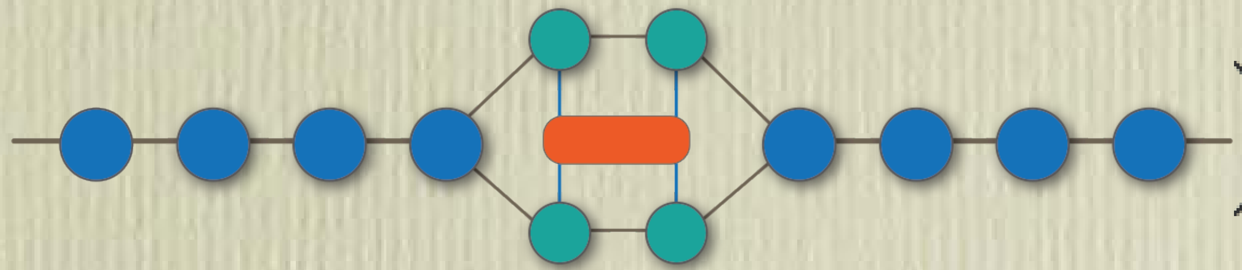
Scale A such that $E_{\max} = 1$

$$\langle\Psi|\Psi\rangle = 1$$

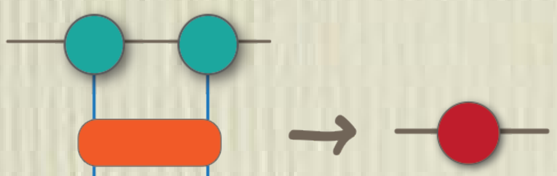
Essentials of iMPS

$$\langle\Psi|H|\Psi\rangle = \sum_{j=0}^{\infty}\langle\Psi|H_{j,j+1}|\Psi\rangle = \infty\langle\Psi|H_{j,j+1}|\Psi\rangle$$

$$\langle\Psi|H_{j,j+1}|\Psi\rangle = \mathrm{Tr}\Big($$  $$\Big)$$

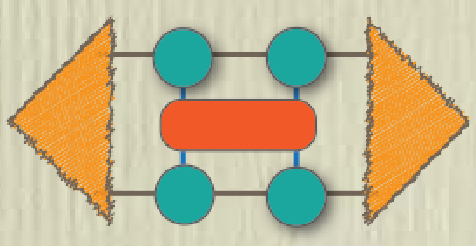
$$\langle\Psi|H_{j,j+1}|\Psi\rangle = \mathrm{Tr}\Big($$  $$\Big)$$

$$\langle\Psi|H_{j,j+1}|\Psi\rangle = \mathrm{Tr}(\mathbf{E}^{\infty}\mathbf{G}\mathbf{E}^{\infty})$$



$\mathbf{G}$

$$\langle\Psi|H_{j,j+1}|\Psi\rangle = \langle l_{\max}|\mathbf{G}|r_{\max}\rangle$$



$$E_{\text{per particle}} = \langle\Psi|H_{j,j+1}|\Psi\rangle$$

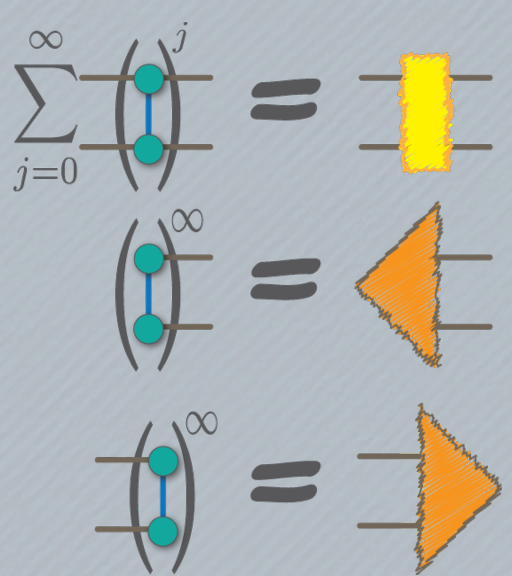
Infinite translation-invariant chains

IP, TJ Osborne, K Temme & F Verstraete (in prep)

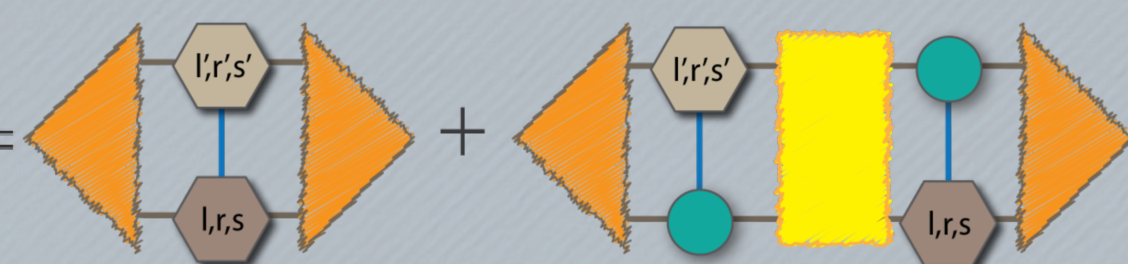
$$\left|\left|H|\Psi\rangle - \sum_{lrs} x_{lrs}|\Psi_{(lrs)}\rangle\right|\right| = \min$$

$$\underbrace{\langle\Psi_{(lrs)}|\Psi_{(l'r's')}\rangle}_{\mathbf{G}} x_{l'r's'} = \underbrace{\langle\Psi_{(lrs)}|H|\Psi\rangle}_{\mathbf{h}}$$

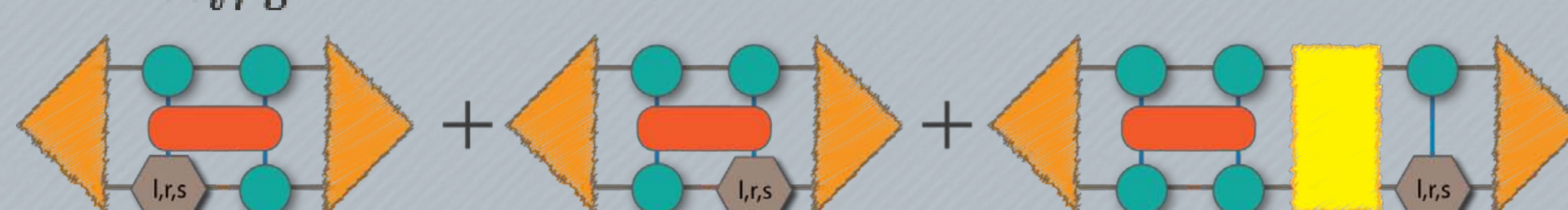
$$\sum_{j=0}^{\infty} E^j = (1-E)^{-1}$$



$$G_{(lrs),(l'r's')} =$$



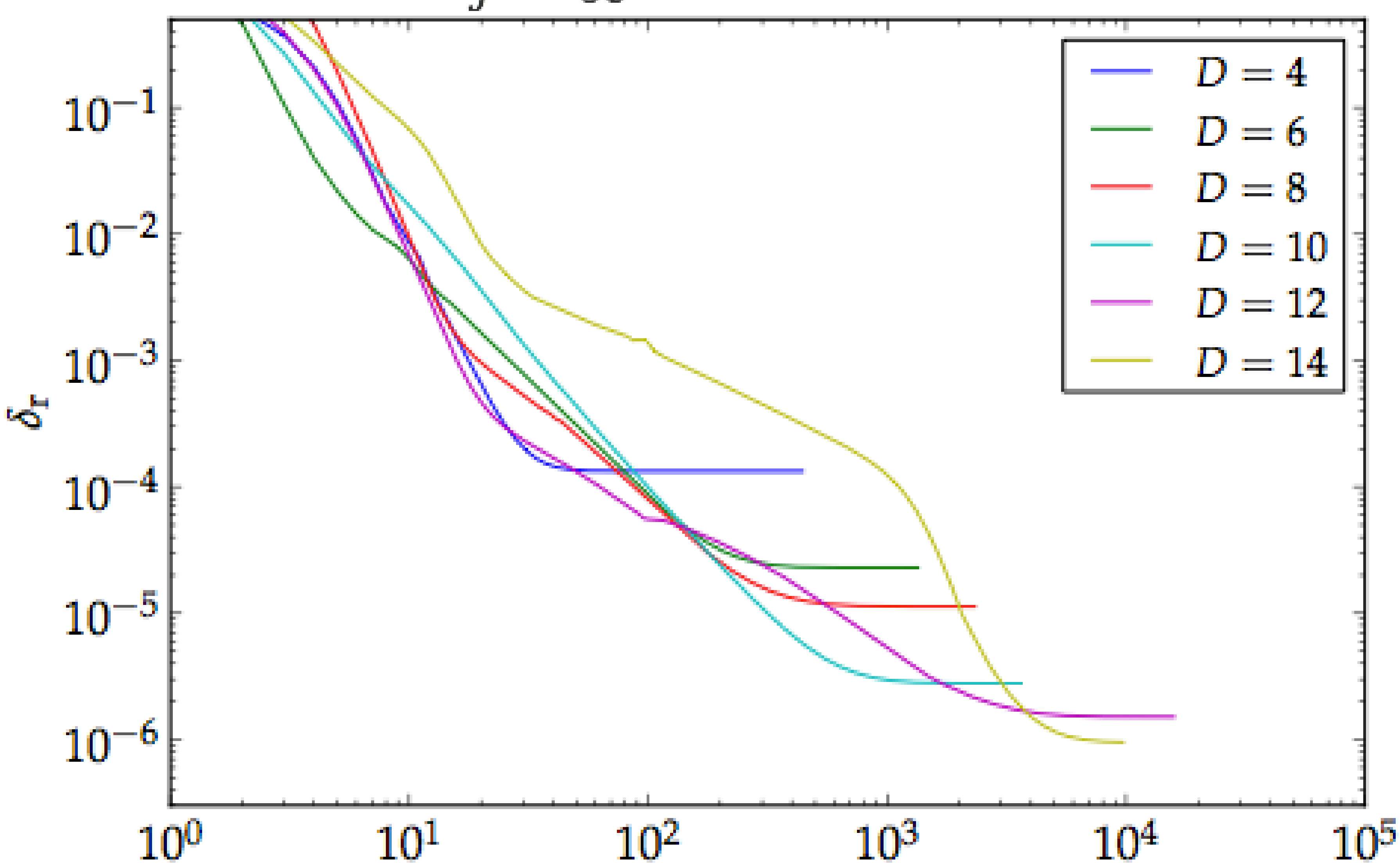
$$h_{lrs} =$$



Infinite translation-invariant chains

IP, TJ Osborne, K Temme & F Verstraete (in prep)

$$H = \sum_{j=-\infty}^{\infty} \left(\sigma_j^{\mathrm{x}} \sigma_{j+1}^{\mathrm{x}} + \sigma_j^{\mathrm{z}}\right)$$

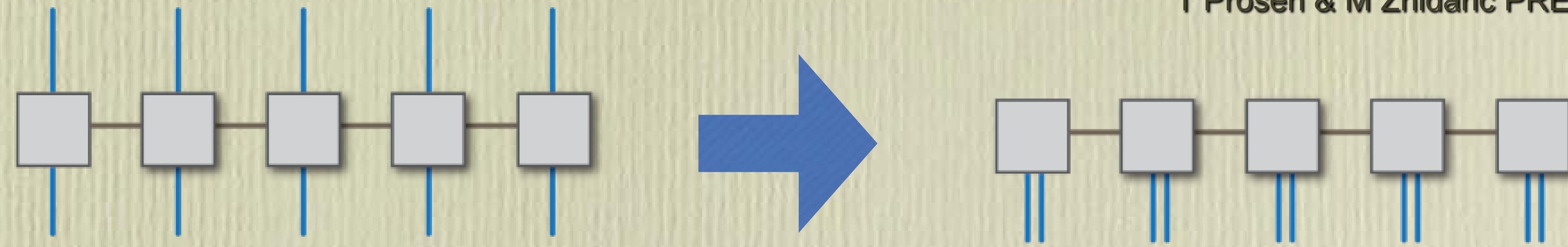


Projected dynamics

- Preserves the translation invariance properties
- Infinite & finite systems
- Imaginary time evolution (fast & easy)
- Real time evolution (ODE solvers)
- Slower than the usual MPS time evolution
- Continuous Matrix Product States (cMPS): the way to go!

Matrix product operators

F Verstraete, JJ Garcia-Ripoll & JI Cirac, PRL (04)
T Prosen & M Znidaric PRE (07)



$$O = \sum_{s_1,s_1',s_2,s_2'\dots} \mathrm{Tr}\left(\mathbf{M}^{[1]s_1,s_1'}\mathbf{M}^{[2]s_2,s_2'}\dots\right)|s_1'\rangle\langle s_1| \otimes |s_2\rangle\langle s_2'|\cdots$$

$$O = \sum_{\alpha_1,\alpha_2,\dots} \mathrm{Tr}\left(\mathbf{B}^{[1]\alpha_1}\mathbf{B}^{[2]\alpha_2}\dots\right)\sigma_1^{\alpha_1}\sigma_2^{\alpha_2}\cdots$$

$$\sigma^0 \equiv \mathbf{1}$$
$$\sigma^{1,2,3} \equiv \sigma^{\mathrm{x,y,z}}$$

Any operator can be written in this form
(if D is sufficiently large)

Why operators?

A system can be in a mixed state

$$\rho = \sum_j p_j |\Psi_j\rangle\langle\Psi_j|$$

Thermal equilibrium

$$\rho = \frac{\mathrm{e}^{-\beta H}}{\mathrm{Tr}(\mathrm{e}^{-\beta H})} \qquad \beta = (k_\mathrm{B} T)^{-1}$$

$$\rho(T=0) = |\Psi_\mathrm{GS}\rangle\langle\Psi_\mathrm{GS}|$$

Far from the equilibrium

$$\frac{d}{dt}\rho_\mathrm{NESS} = 0$$

Can tensor networks be used for these systems?

Systems in a thermal equilibrium

Zero temperature | **Infinite temperature**

$\rho = |\Psi_{\mathrm{GS}}\rangle\langle\Psi_{\mathrm{GS}}|$ $\qquad \rho = Z^{-1}\mathrm{e}^{-\beta H} \qquad$ $\rho = 2^{-n}\mathbf{1}$

$$A = \sum_{\alpha_1,\alpha_2,\ldots,\alpha_n} a_{\alpha_1,\alpha_2,\ldots,\alpha_n} \sigma^{\alpha_1} \otimes \sigma^{\alpha_2} \otimes \cdots \otimes \sigma^{\alpha_n}$$

$$\alpha_j \in \{0, \mathrm{x}, \mathrm{y}, \mathrm{z}\}$$

$$|A\rangle = \sum_{\alpha_1,\alpha_2,\ldots,\alpha_n} a_{\alpha_1,\alpha_2,\ldots,\alpha_n} |\alpha_1\rangle|\alpha_2\rangle\cdots|\alpha_n\rangle$$

An operator is just a “state” in the operator space

$$|\rho(T=\infty)\rangle = 2^{-n}|0\rangle|0\rangle\cdots|0\rangle$$

$$|\rho(T)\rangle = \sum_{\alpha_1,\alpha_2,\ldots,\alpha_n} \rho_{\alpha_1,\alpha_2,\ldots,\alpha_n} |\alpha_1\rangle|\alpha_2\rangle\cdots|\alpha_n\rangle$$

On operator space

T Prosen & IP, PRA (07)

$$\langle A|B\rangle \equiv 2^{-n}\mathrm{tr}(A^\dagger B)$$

$$\mathrm{tr}(\rho) = 2^n\langle \mathbf{1}|\rho\rangle$$
$$\mathrm{tr}(O\rho) = 2^n\langle O|\rho\rangle$$

$$|\mathbf{1}\rangle \equiv |0\rangle|0\rangle\cdots|0\rangle$$

How can we get $|\rho(\beta)\rangle$

$$\rho \propto \mathrm{e}^{-\beta H} \Longrightarrow |\rho(\beta)\rangle \propto |\mathrm{e}^{-\beta H}\rangle$$

$$|HA\rangle = \hat{\chi}|A\rangle \Longrightarrow |\mathrm{e}^{-\beta H}\rangle = \mathrm{e}^{-\beta\hat{\chi}}|\mathbf{1}\rangle$$

Simple time evolution!

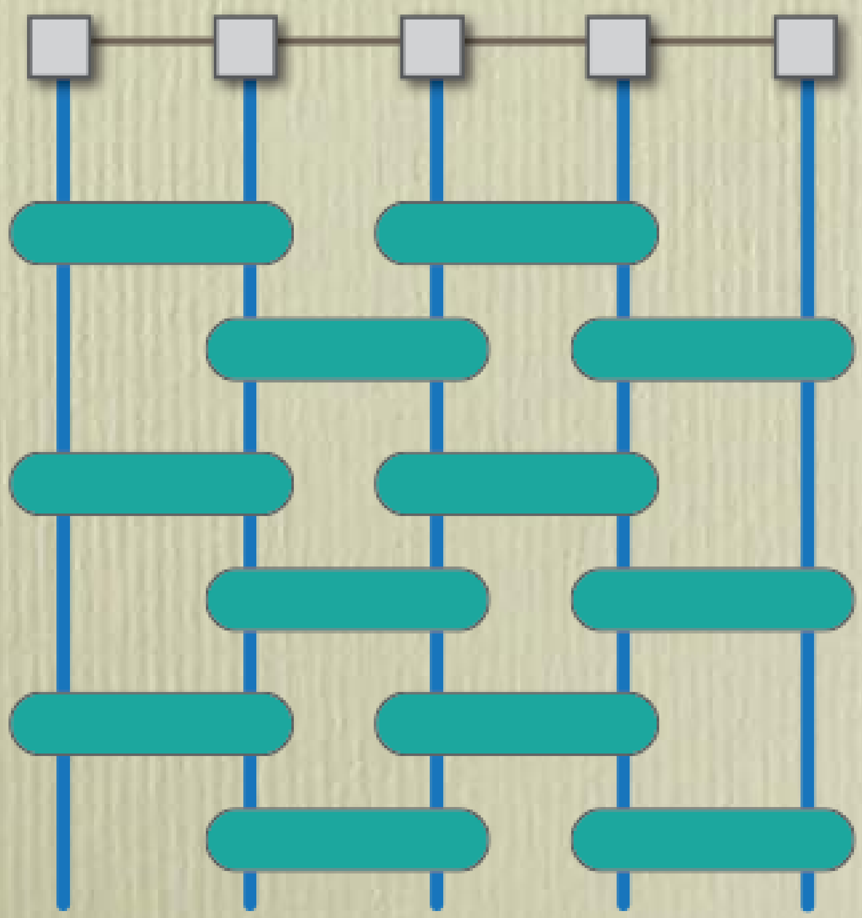
$$|\rho(\beta)\rangle = \mathrm{e}^{-\beta\hat{\chi}}|\rho(0)\rangle$$

Example

$$H = \sum_j \left(\sigma_j^1 \sigma_{j+1}^1 + h\sigma_j^3\right) \Longrightarrow \hat{\chi} = \sum_j \left(\hat{\Sigma}_j^1 \hat{\Sigma}_{j+1}^1 + h\hat{\Sigma}_j^3\right)$$

$$\hat{\Sigma}^k \equiv |\sigma^k\rangle\langle 1| + |1\rangle\langle\sigma^k| - i\epsilon^{ijk}|\sigma^j\rangle\langle\sigma^k|$$

$$\hat{\Sigma}^3 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$



1. start with a product state |1>
2. evolve MPS in “time”

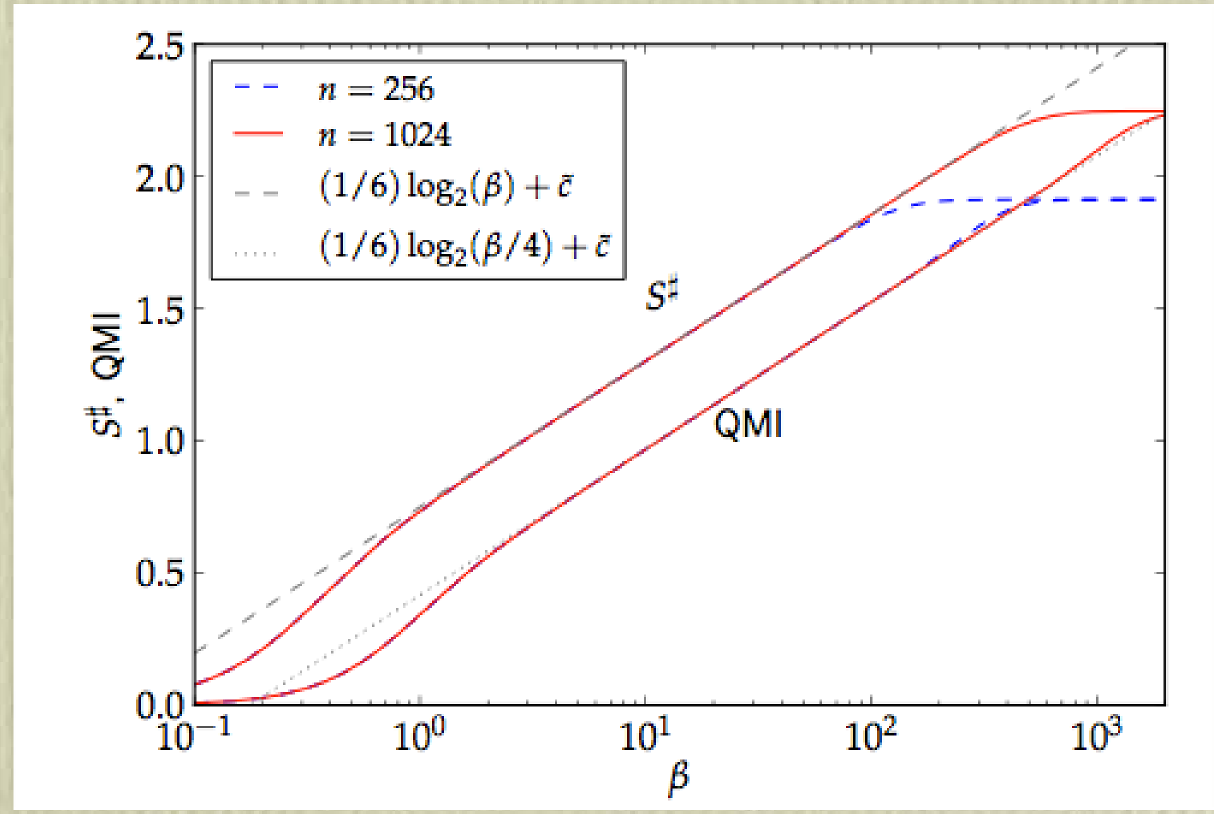
$$|\mathrm{e}^{-\beta H}\rangle = \mathrm{e}^{-\delta\beta\hat{\chi}}\mathrm{e}^{-\delta\beta\hat{\chi}}\cdots\mathrm{e}^{-\delta\beta\hat{\chi}}|\mathbf{1}\rangle$$

$$|\rho(\beta)\rangle = \frac{2^{-n}}{\langle 1|\mathrm{e}^{-\beta H}\rangle}|\mathrm{e}^{-\beta H}\rangle$$

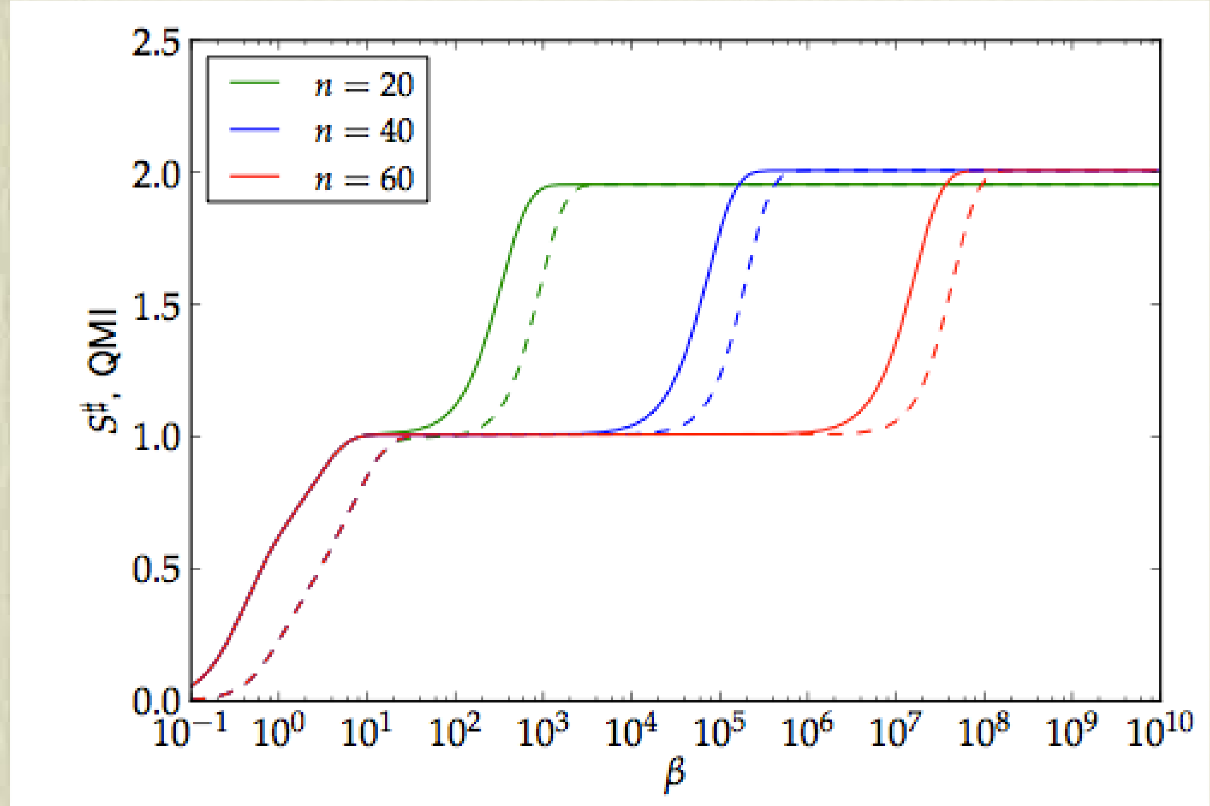
Is it efficient?

M Znidaric, T Prosen & IP, PRA (08)

Quantum mutual information $I_{A:B} = S(\rho_A) + S(\rho_B) - S(\rho)$



critical



non-critical

(1/6) comes from the central charge in CFT

Same behavior as for the ground states!

Dynamics of mixed states

$$\frac{d}{dt}|\Psi\rangle = -iH|\Psi\rangle \quad \Longrightarrow \quad \frac{d}{dt}\rho = \mathcal{L}(\rho) \qquad \rho = \sum_j p_j |\Psi_j\rangle\langle\Psi_j|$$

Schrödinger equation | Liouville equation

Isolated systems

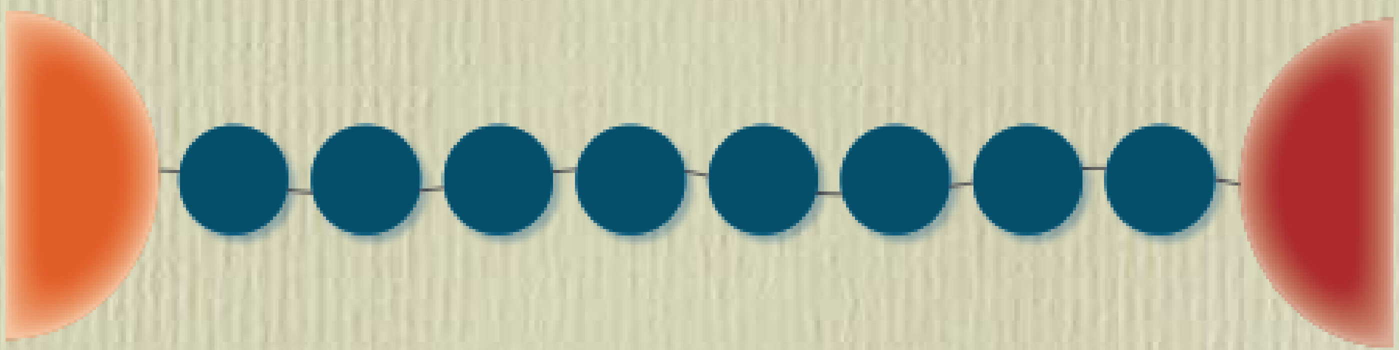
$$\mathcal{L}(\rho) = i[\rho, H]$$

Liouvillian operator is a linear operator

$$\mathcal{L}(\rho) \Longrightarrow \hat{\mathcal{L}}|\rho\rangle \qquad |\rho(t)\rangle = \mathrm{e}^{\hat{\mathcal{L}}t}|\rho_0\rangle$$

Again: time evolution (in operator space)

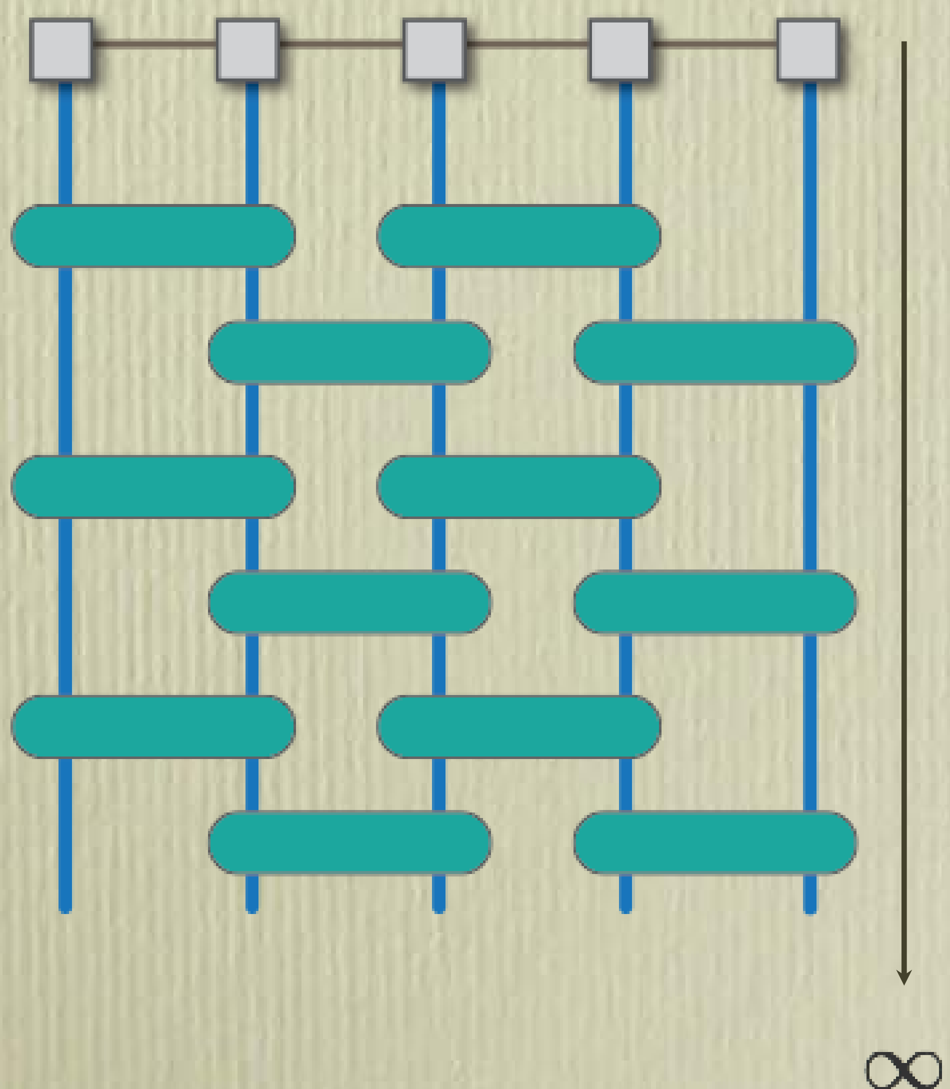
Open systems



$$\mathcal{L}(\rho) = i[\rho, H] + \mathcal{L}_{\text{diss}}(\rho)$$

$$\frac{d}{dt}|\rho\rangle = \hat{\mathcal{L}}|\rho\rangle$$

Lindblad master equation



Non-equilibrium steady state

$$|\rho_{\text{ness}}\rangle = |\rho(t \to \infty)\rangle \qquad \frac{d}{dt}\rho_{\text{ness}} = 0$$

$$\hat{\mathcal{L}}|\rho_{\text{ness}}\rangle = 0$$

NESS shouldn't be too correlated!

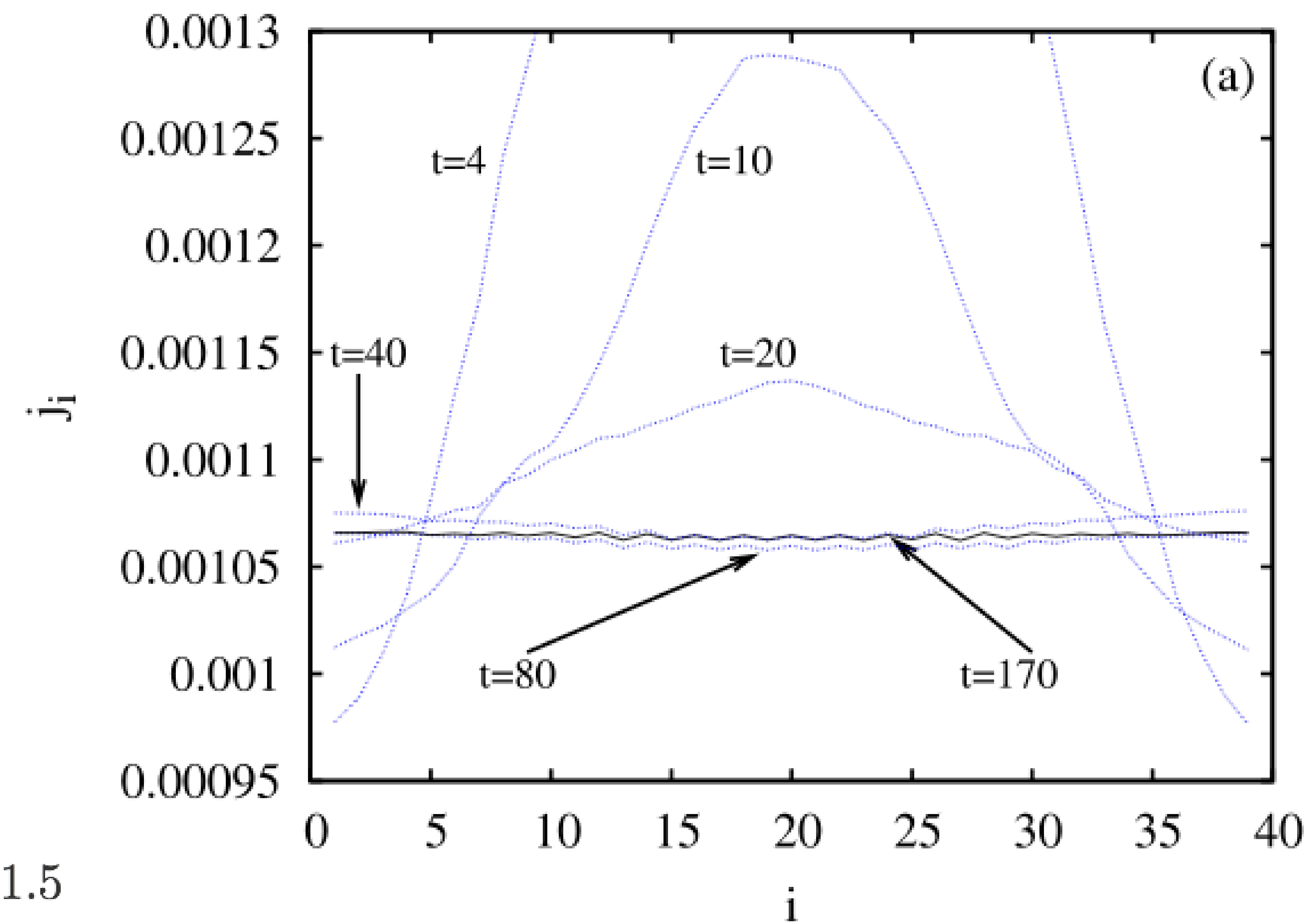
T Prosen & IP, PRL (08)

But it is sometimes.

Open systems

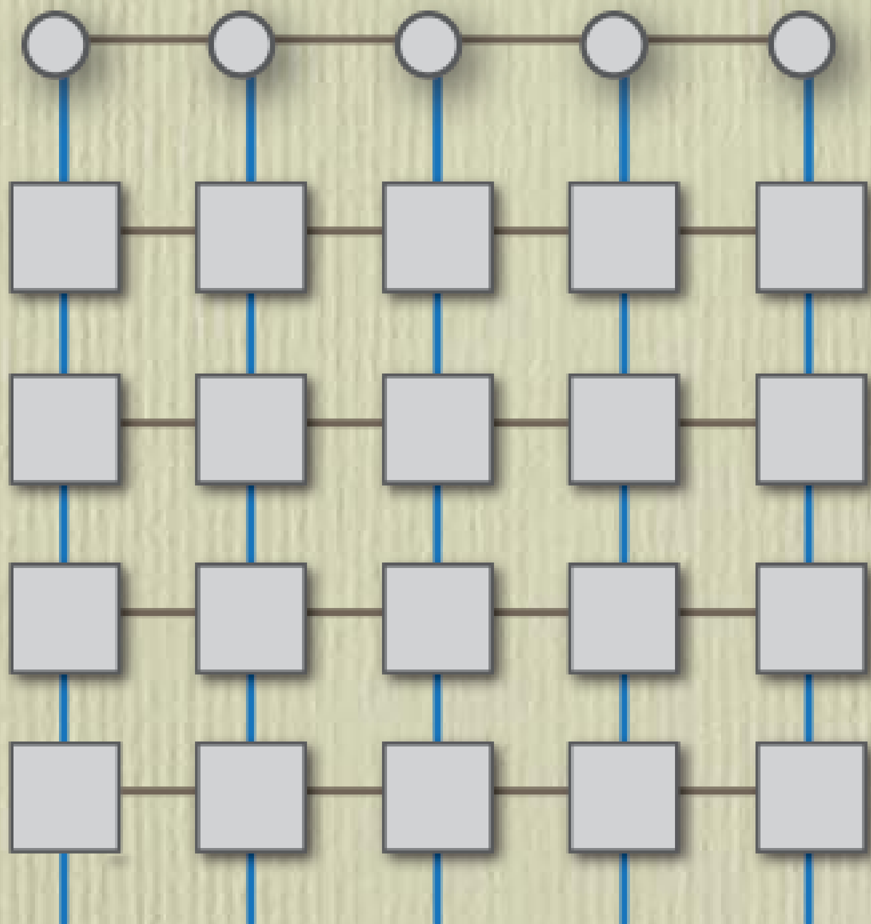
Convergence, spin current, XXZ

T Prosen & M Znidaric, JSM (09)

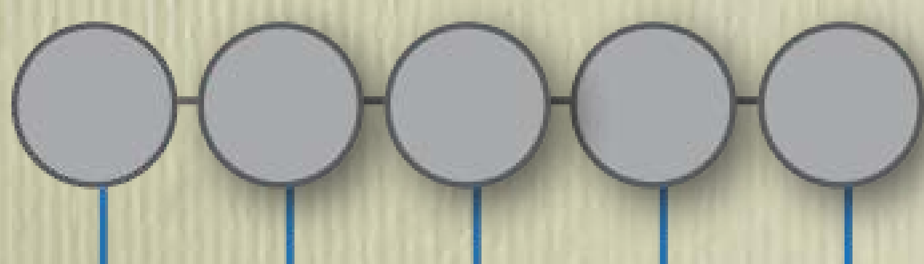


$\Delta = 1.5$

Heisenberg picture

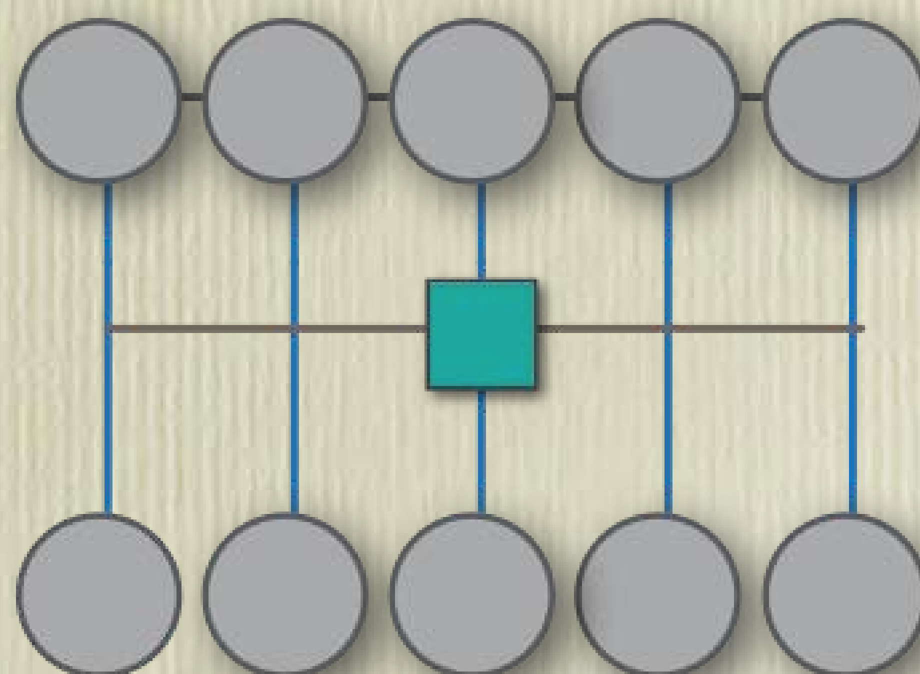


$$|\Psi(t)\rangle = \mathrm{e}^{-itH}|\Psi_0\rangle$$

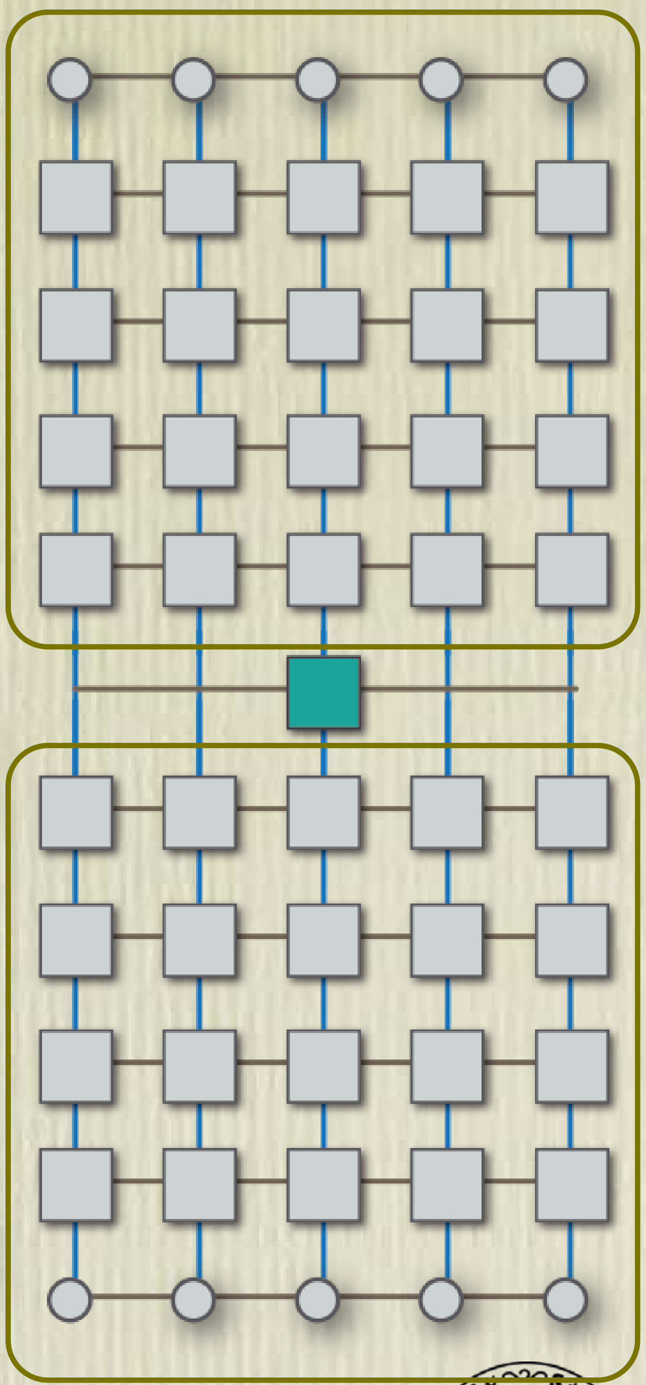


$$\sigma_j^{\mathrm{z}}(t)$$
$$\sigma_j^{\mathrm{z}}\sigma_{j+1}^{\mathrm{z}}(t)$$
$$\sigma_j^{\mathrm{x}}\sigma_{j+1}^{\mathrm{x}}(t)$$

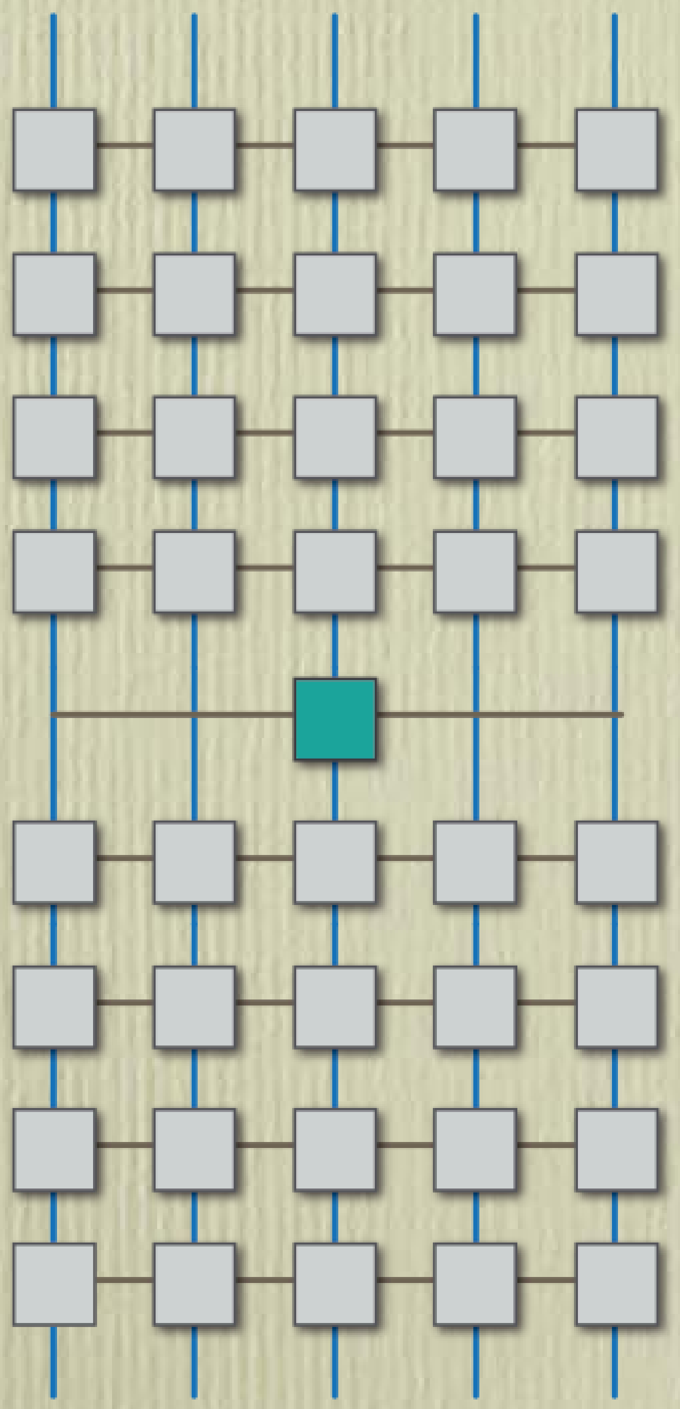
$$\langle\Psi(t)|O|\Psi(t)\rangle$$



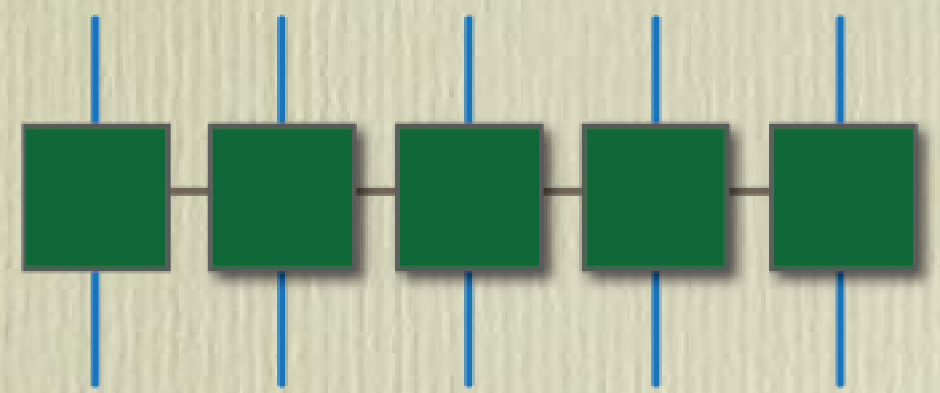
$$\langle\Psi_0|\mathrm{e}^{itH}O\mathrm{e}^{-itH}|\Psi_0\rangle$$



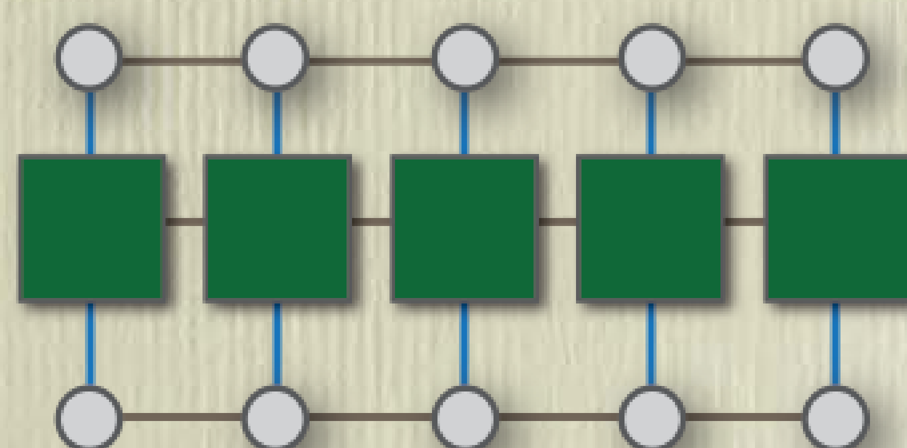
Heisenberg picture



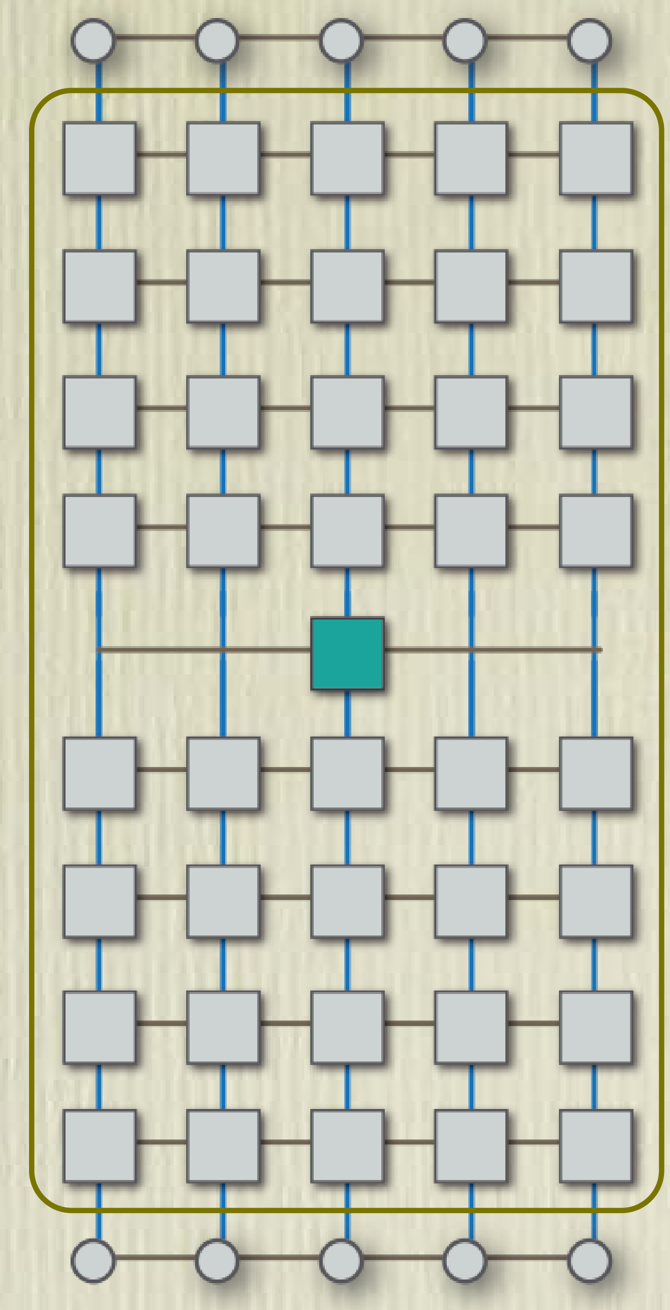
$$O(t) = \mathrm{e}^{itH} O \mathrm{e}^{-itH}$$



$$\langle \Psi_0 | O(t) | \Psi_0 \rangle$$



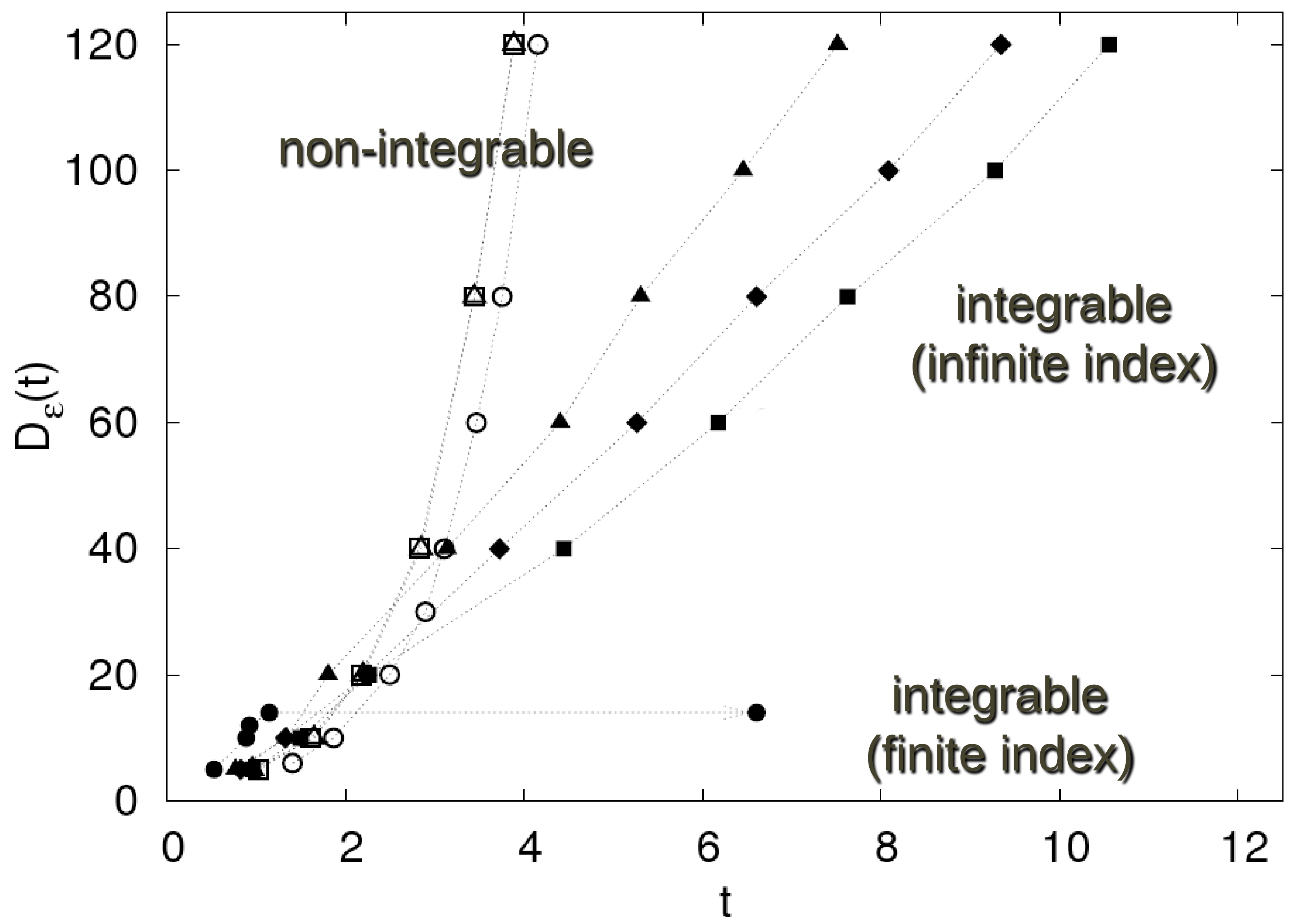
$$\langle \Psi_0 | \mathrm{e}^{itH} O \mathrm{e}^{-itH} | \Psi_0 \rangle$$



Heisenberg picture

T Prosen & M Znidaric, PRE (07)

Growth of effective MPO-bond dimension

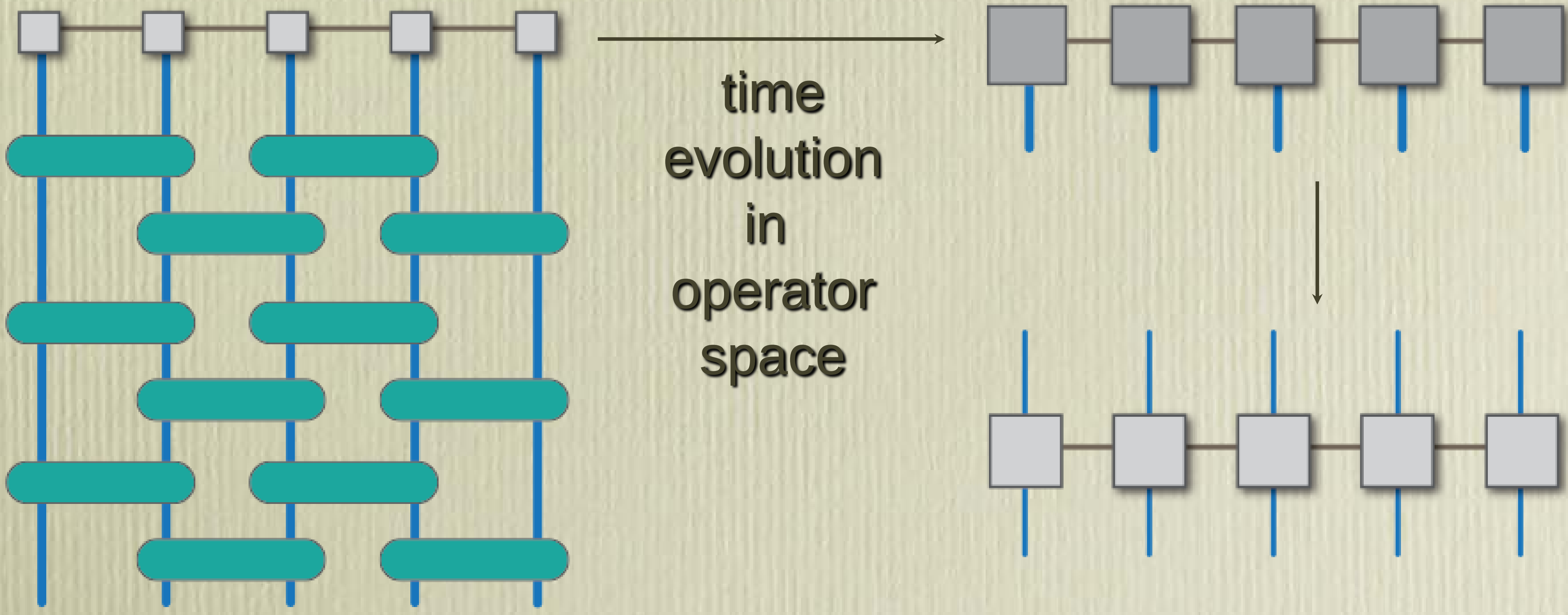


Heisenberg picture

T Prosen & IP, PRA (07)

$$(d/dt)O = -i[O,H] \quad \Rightarrow \quad (d/dt)|O\rangle = -i\hat{H}|O\rangle$$

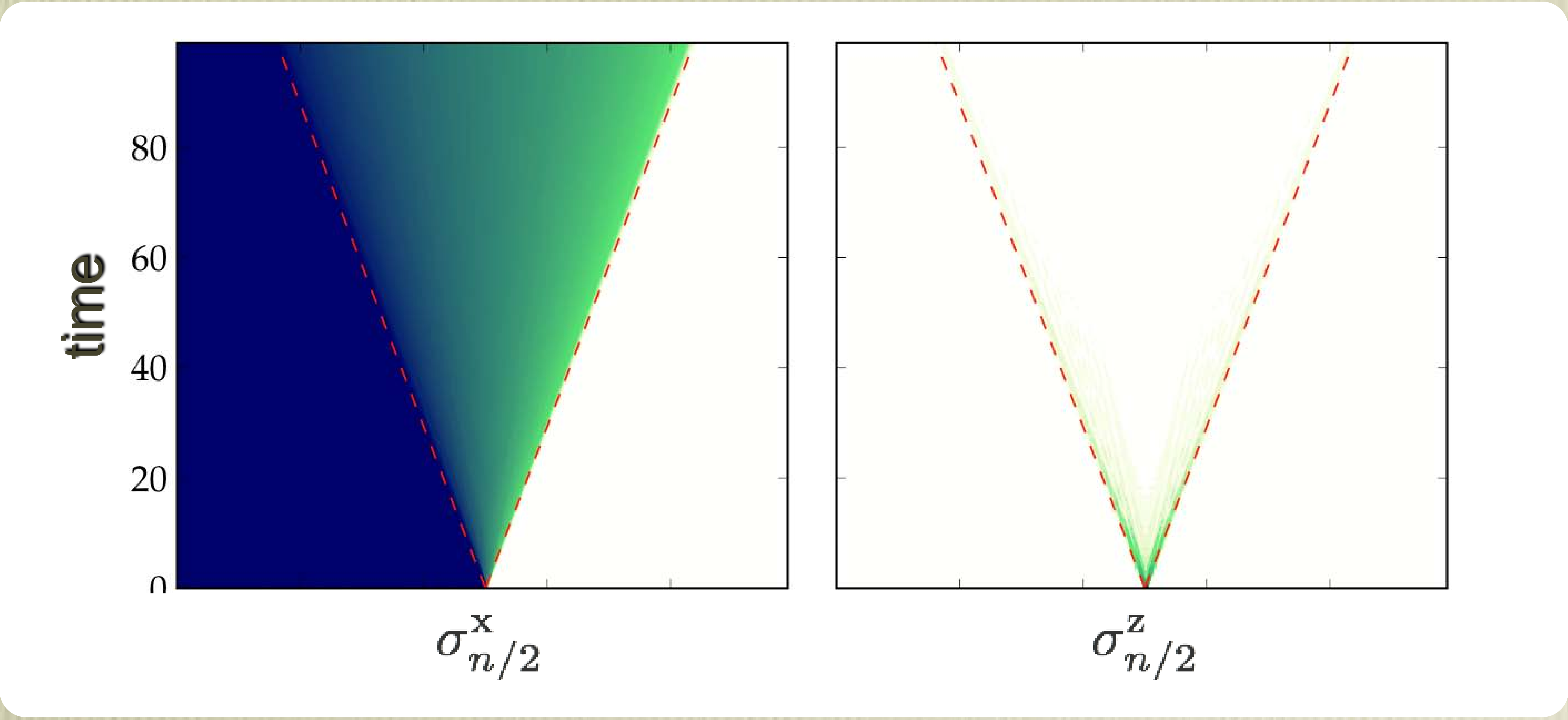
$$O(t) = \mathrm{e}^{itH} O \mathrm{e}^{-itH} \quad \Rightarrow \quad |O(t)\rangle = \mathrm{e}^{-it\hat{H}}|O\rangle$$



Why?

T Prosen & IP, PRA (07)
IP & T Prosen, PRB (09)

Local operators are very simple!



Still, it only works in integrable models!