Finite Uncostrained Tree Tensor Networks and critical systems

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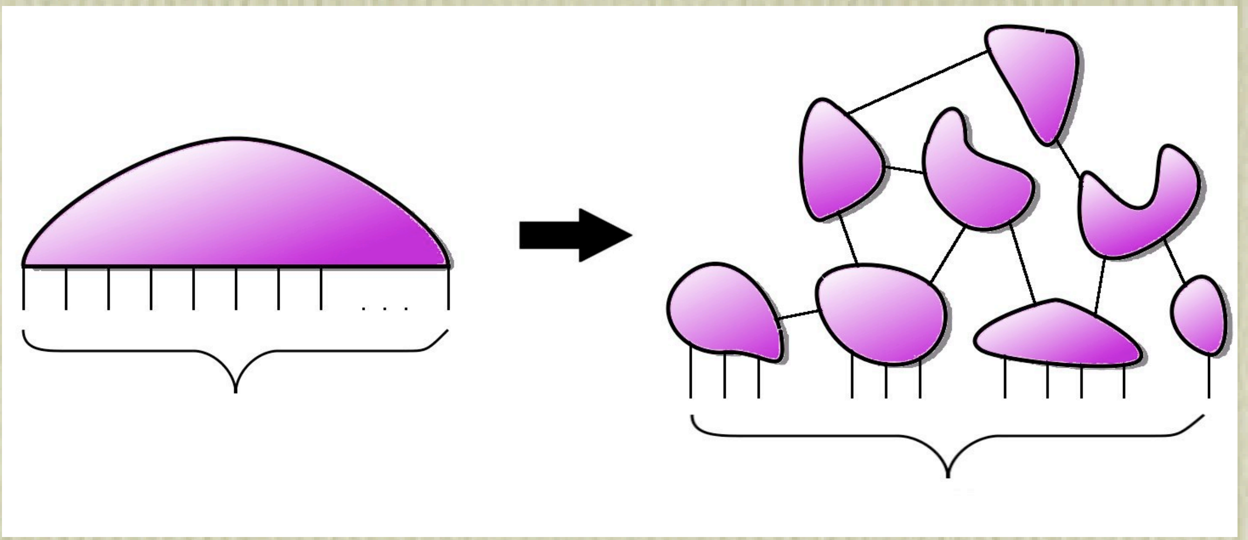
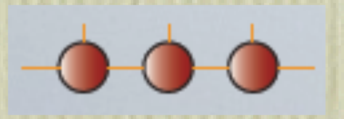
Outline

- Hierarchical Tensor Networks
- Finite Unconstrained Trees (TTN)
- Preliminary results (1D)
- Outlook

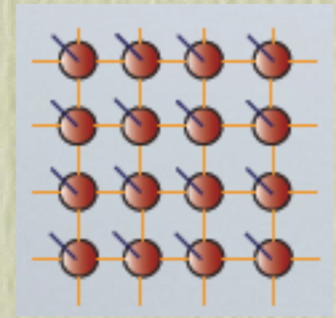
Hierarchical Tensor Networks



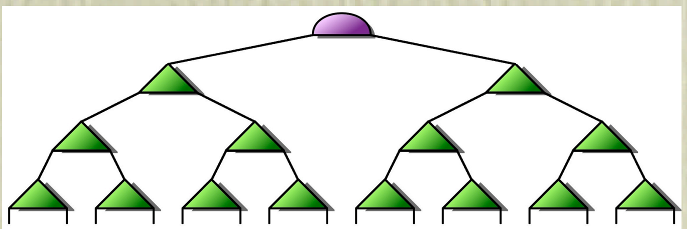
common key idea:
break down the state
into manageable structure



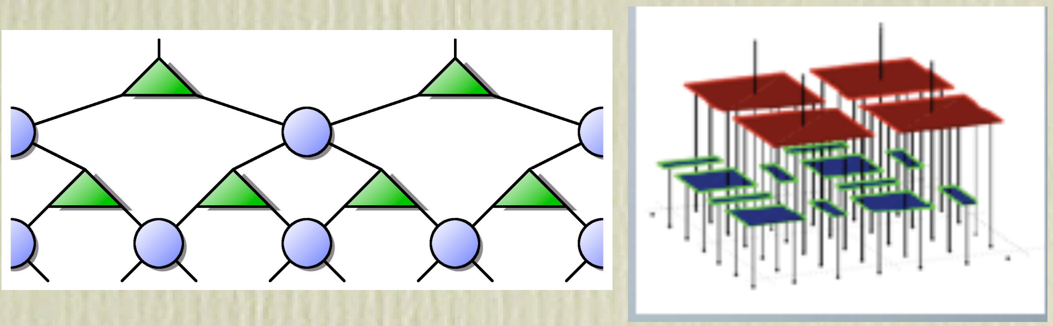
MPS



PEPS



TTN

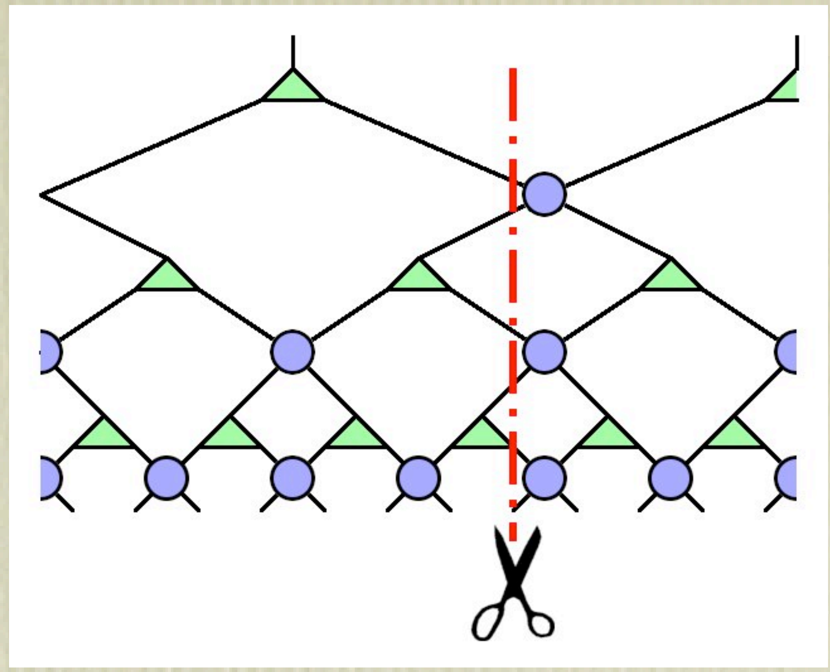


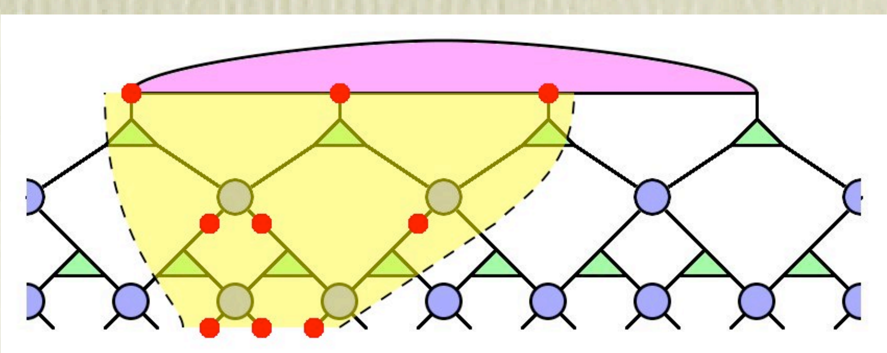
MERA

- hierarchical (TTN, MERAs) are intriguing:
  - built-in scale invariance
  - power-law correlations
  - can represent ground states of critical H

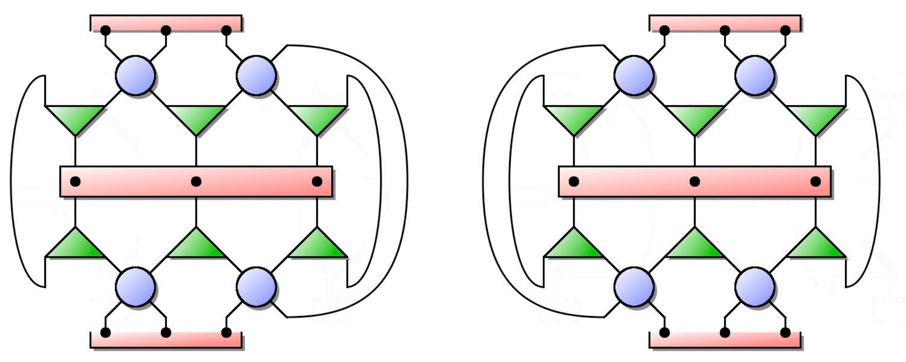
Hierarchical Tensor Networks

- good sides of MERAs:
  - nice dealing with area laws
  - causal cone structure
  - interpretation as CPT maps & computation of TL properties



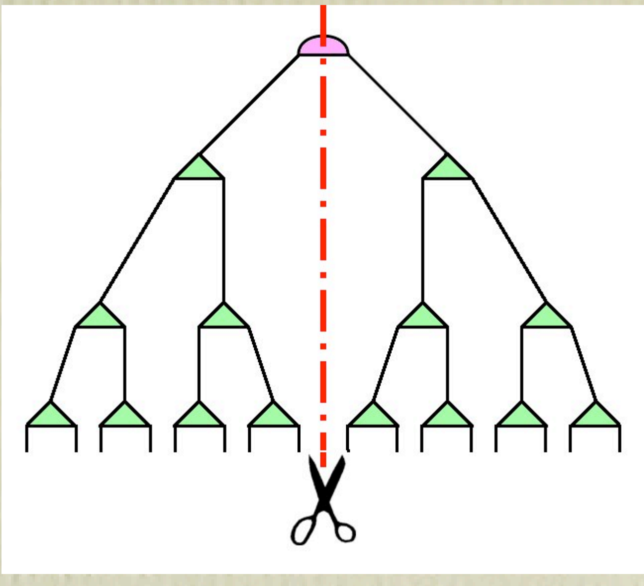


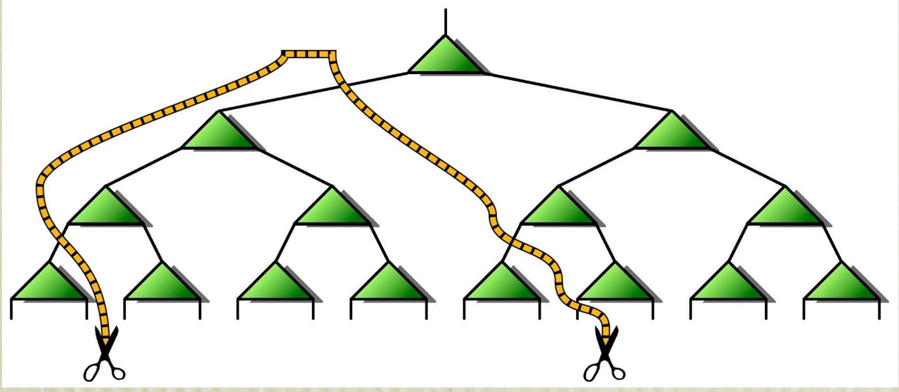
- hindrances of MERAs:
  - loopful structure
    --> high-power power law scaling
  - need for unitary constraint
    --> “complicate” minimization issues



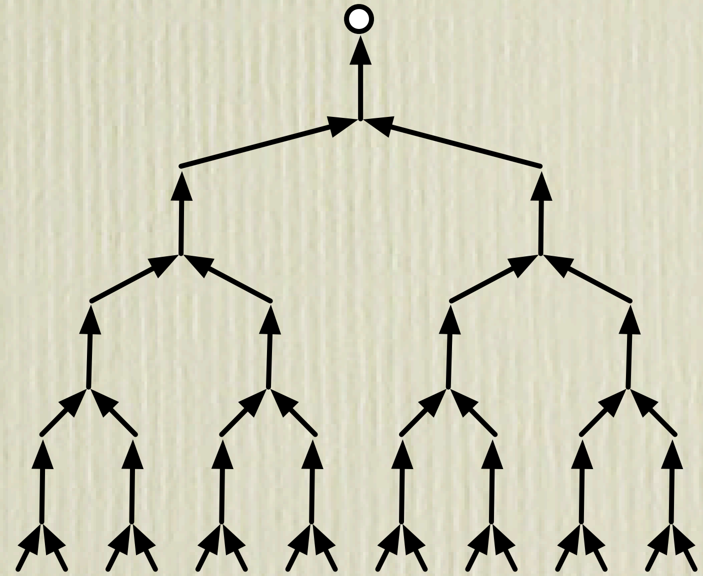
Hierarchical Tensor Networks

Loop-free structures (e.g. TTN): naive...
...BUT have good sides also:

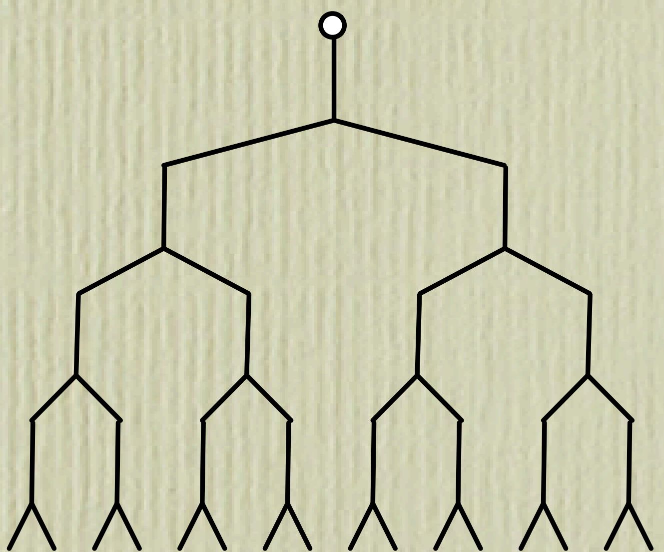




- incorporate area law on average
- allow for easier/cheaper contractions
- $\boxed{\text{allow relaxation of isometricity !}}$
  --> standard optimization methods <--
  (can be re-isometrized when needed)
- easy implementation of symmetries
- huge sizes with moderate effort



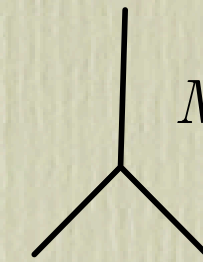
Finite Unconstrained Trees



$$N = 2^{\ell}$$

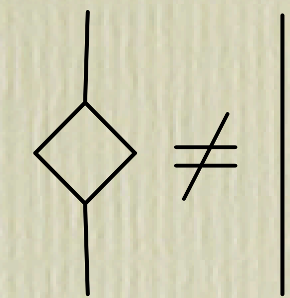
$$H = \sum_{i=1}^{N} A_i + \sum_{i=1}^{N} \sum_{\alpha} \gamma_\alpha L_i^{(\alpha)} R_{i+1}^{(\alpha)}$$

$$M(l) = \min\left(M(l+1)^2, m\right)$$



$$M(\ell) = d$$

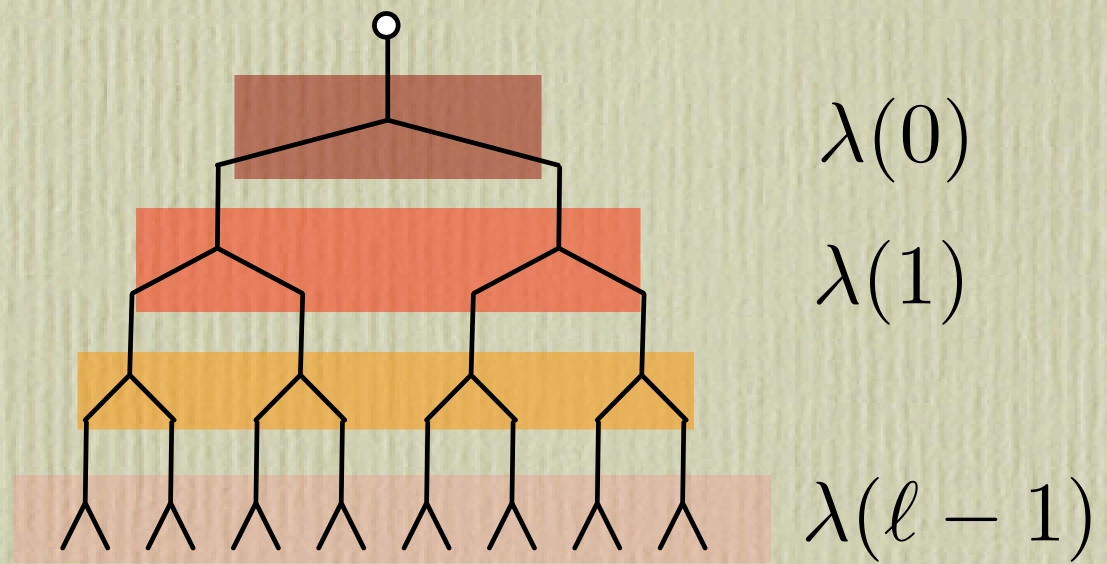
$M(l+1)$ $M(l+1)$



$$Z(\ell) = \mathbb{I}$$

$$\lambda(l)^\dagger \lambda(l) = Z(l) \neq \mathbb{I}$$

Finite Unconstrained Trees



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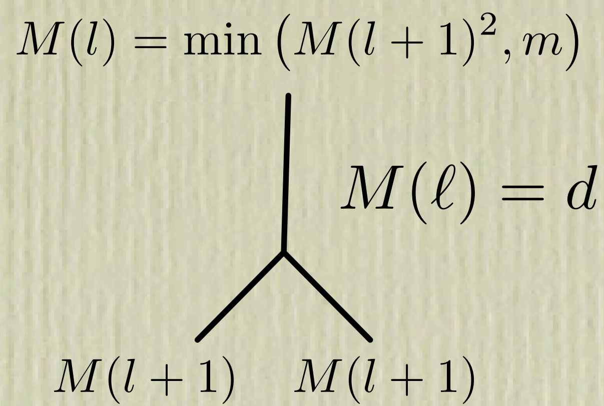
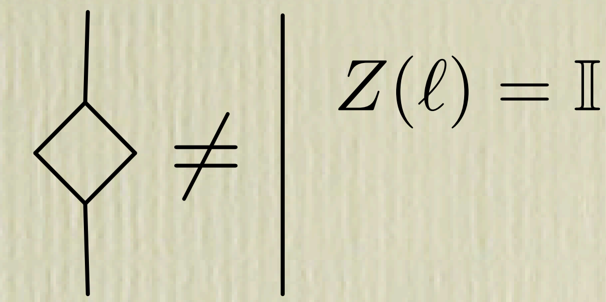


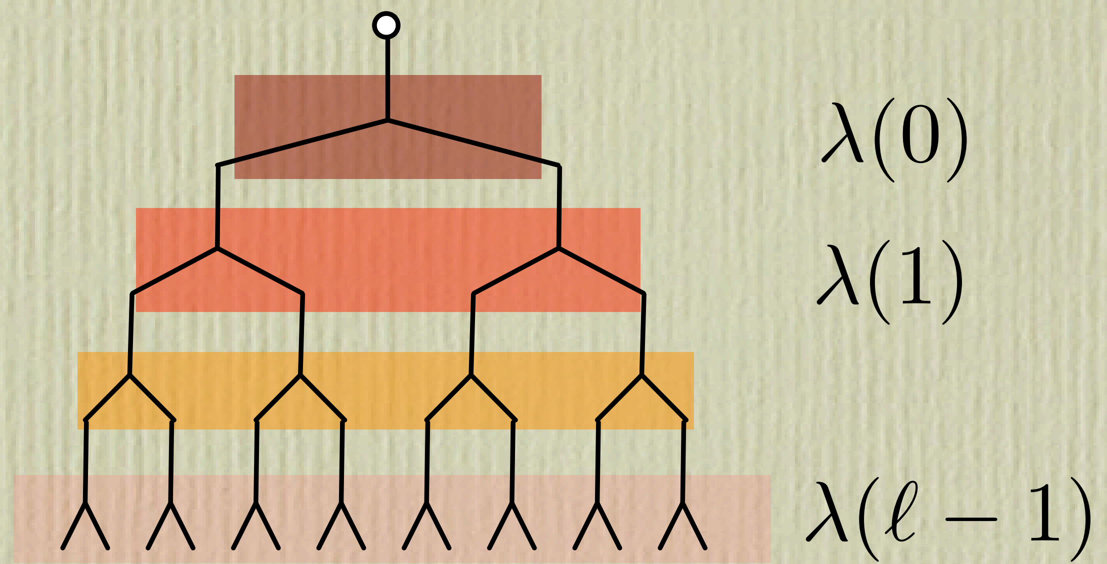


$$\lambda(l)^\dagger \lambda(l) = Z(l) \neq \mathbb{I}$$

Layer homogeneity for translational invariance

$$|\psi(l)\rangle = \left(\bigotimes^{2^{l-1}} \lambda(l-1) \right) \cdot |\psi(l-1)\rangle;$$

Finite Unconstrained Trees



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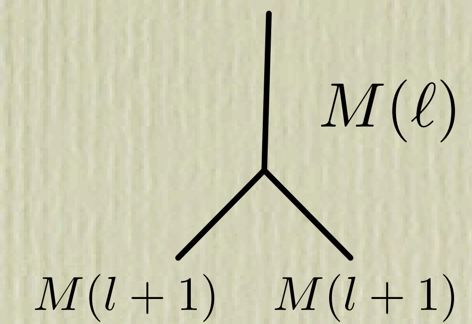

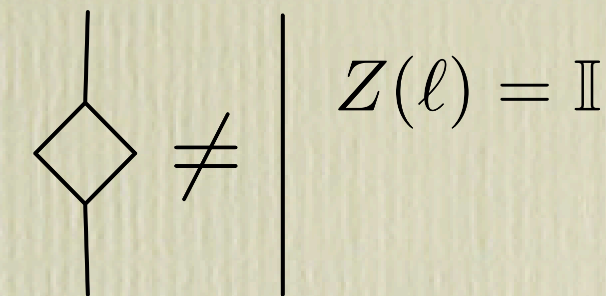

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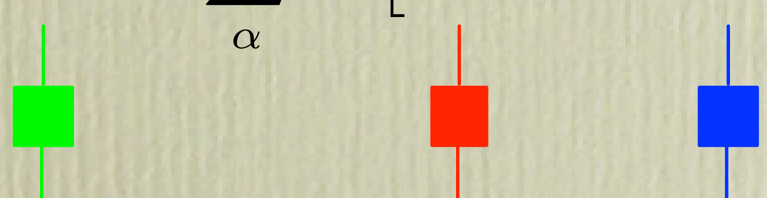
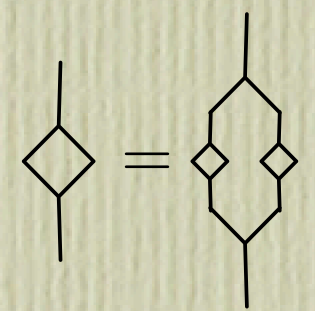
Simple form of coarse-grained Hamiltonian at each level

$$H(l) = \sum_{i=1}^{2^l} \left\{ A(l)_i + \sum_{\alpha} \gamma_\alpha \left[L^{(\alpha)}(l) \otimes R^{(\alpha)}(l) \right]_{i,i+1} \right\}$$



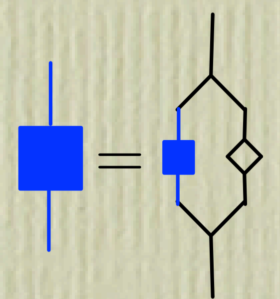
$$E = \frac{\langle \psi(l) | H(l) | \psi(l) \rangle}{\langle \psi(l) | \psi(l) \rangle} \quad \forall\, l = 0 \ldots \ell$$

Finite Unconstrained Trees

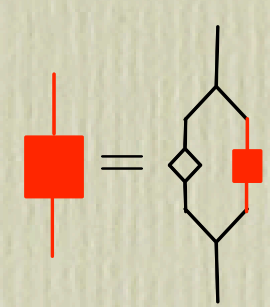


$$Z(l) = \lambda(l)^\dagger \cdot [Z(l+1) \otimes Z(l+1)] \cdot \lambda(l)$$

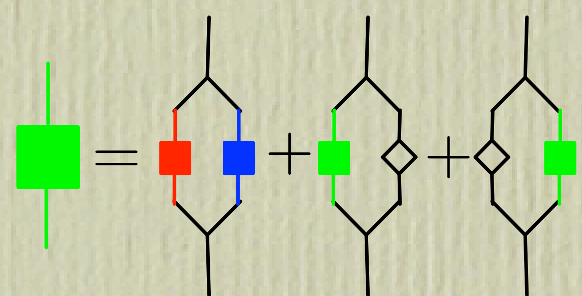
norm tensor $Z(\ell) = \mathbb{I}$



$$R'^{(\alpha)} = \lambda'^\dagger \cdot \left[R^{(\alpha)} \otimes Z\right] \cdot \lambda'$$



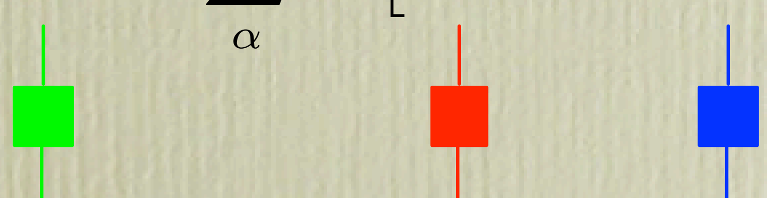
$$L'^{(\alpha)} = \lambda'^\dagger \cdot \left[Z \otimes L^{(\alpha)}\right] \cdot \lambda'$$



$$A' = \lambda'^\dagger \cdot \left[\sum_\alpha \gamma_\alpha L^{(\alpha)} \otimes R^{(\alpha)} + A \otimes Z + Z \otimes A\right] \cdot \lambda'$$

Simple form of coarse-grained Hamiltonian at each level

$$H(l) = \sum_{i=1}^{2^l} \left\{ A(l)_i + \sum_\alpha \gamma_\alpha \left[L^{(\alpha)}(l) \otimes R^{(\alpha)}(l)\right]_{i,i+1} \right\}$$



$$E = \frac{\langle\psi(l)|H(l)|\psi(l)\rangle}{\langle\psi(l)|\psi(l)\rangle} \quad \forall\, l = 0 \ldots \ell$$

Everything still doable in $O(m^4)$

Finite Unconstrained Trees

Unconstrained form of tensors

$\downarrow$

standard optimization methods can be used
(e.g. conjugate gradient)

Gradient can be computed efficiently also in $O(m^4)$

'easy' example: norm $\frac{\partial \langle \psi | \psi \rangle}{\partial \lambda^\dagger(l)} = \frac{\partial \langle \psi | \psi \rangle}{\partial Z(0)} \circ \frac{\partial Z(0)}{\partial Z(1)} \circ \ldots \circ \frac{\partial Z(l-1)}{\partial Z(l)} \circ \frac{\partial Z(l)}{\partial \lambda^\dagger(l)}$

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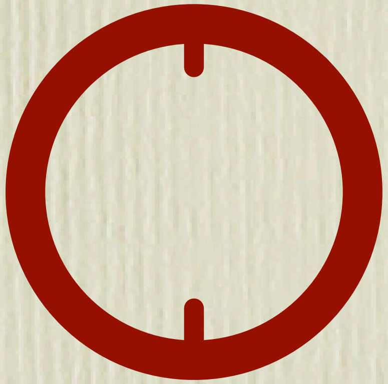
$$\frac{\partial\langle\psi|\psi\rangle}{\partial Z(0)} = \psi(0)^* \cdot \Box \cdot \psi(0)$$



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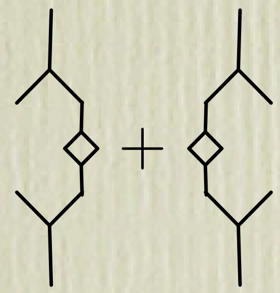
$$\frac{\partial\langle\psi|\psi\rangle}{\partial Z(0)} = \psi(0)^* \cdot \Box \cdot \psi(0)$$

$$\frac{\partial Z(l-1)}{\partial Z(l)} = \lambda(l-1)^\dagger \cdot [\Box \otimes Z(l) + Z(l) \otimes \Box] \cdot \lambda(l-1)$$



Finite Unconstrained Trees

Unconstrained form of tensors

$\Downarrow$

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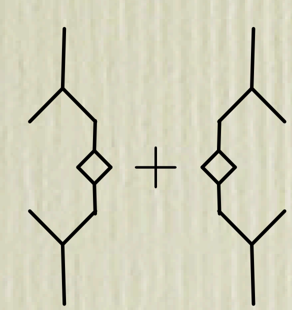
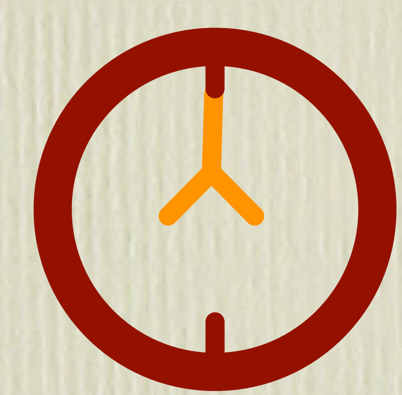
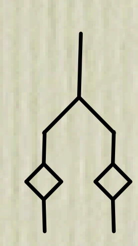
$$\frac{\partial\langle\psi|\psi\rangle}{\partial Z(0)} = \psi(0)^* \cdot \square \cdot \psi(0)$$

$$\frac{\partial Z(l-1)}{\partial Z(l)} = \lambda(l-1)^\dagger \cdot [\square \otimes Z(l) + Z(l) \otimes \square] \cdot \lambda(l-1)$$





$$\frac{\partial Z(l)}{\partial\lambda^\dagger(l)} = \square \cdot [Z(l+1) \otimes Z(l+1)] \cdot \lambda(l)$$



Finite Unconstrained Trees

Unconstrained form of tensors

$\downarrow$

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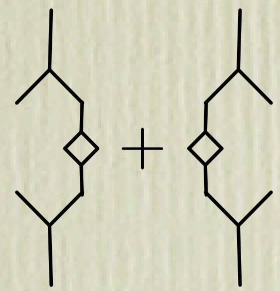
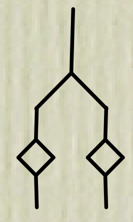
$$\frac{\partial\langle\psi|\psi\rangle}{\partial Z(0)} = \psi(0)^* \cdot \Box \cdot \psi(0)$$

$$\frac{\partial Z(l-1)}{\partial Z(l)} = \lambda(l-1)^\dagger \cdot [\Box \otimes Z(l) + Z(l) \otimes \Box] \cdot \lambda(l-1)$$

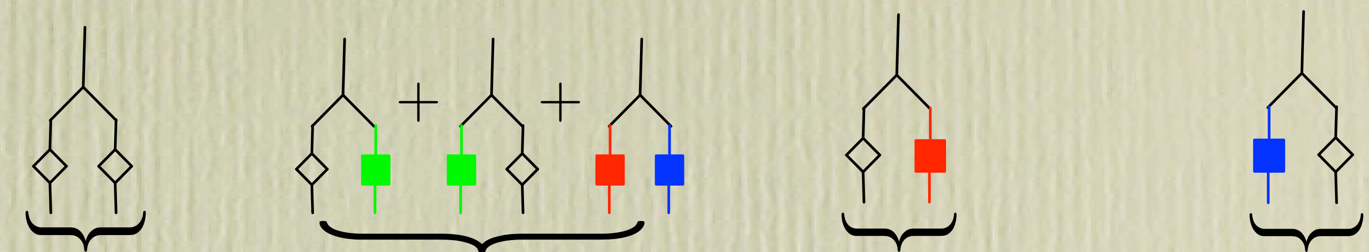


$$\frac{\partial Z(l)}{\partial\lambda^\dagger(l)} = \Box \cdot [Z(l+1) \otimes Z(l+1)] \cdot \lambda(l)$$



Finite Unconstrained Trees

energy gradient



$$\frac{\partial}{\partial \lambda^\dagger(l)} = \frac{\partial}{\partial Z(l)} \circ \frac{\partial Z(l)}{\partial \lambda^\dagger(l)} + \frac{\partial}{\partial A(l)} \circ \frac{\partial A(l)}{\partial \lambda^\dagger(l)} + \frac{\partial}{\partial L(l)} \circ \frac{\partial L(l)}{\partial \lambda^\dagger(l)} + \frac{\partial}{\partial R(l)} \circ \frac{\partial R(l)}{\partial \lambda^\dagger(l)}$$

Finite Unconstrained Trees

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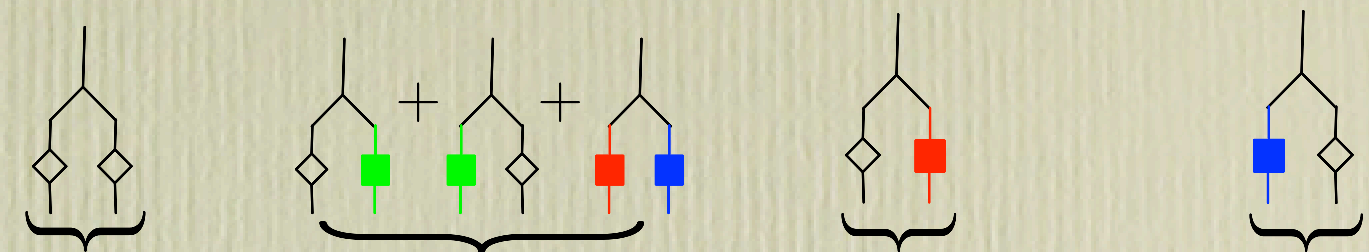

$$\frac{\partial}{\partial \lambda^\dagger(l)} = \boxed{\frac{\partial}{\partial Z(l)}} \circ \frac{\partial Z(l)}{\partial \lambda^\dagger(l)} + \frac{\partial}{\partial A(l)} \circ \frac{\partial A(l)}{\partial \lambda^\dagger(l)} + \frac{\partial}{\partial L(l)} \circ \frac{\partial L(l)}{\partial \lambda^\dagger(l)} + \frac{\partial}{\partial R(l)} \circ \frac{\partial R(l)}{\partial \lambda^\dagger(l)}$$

$$\frac{\partial}{\partial Z(l)} = \frac{\partial}{\partial Z(l-1)} \circ \frac{\partial Z(l-1)}{\partial Z(l)} + \frac{\partial}{\partial A(l-1)} \circ \frac{\partial A(l-1)}{\partial Z(l)} + \frac{\partial}{\partial L(l-1)} \circ \frac{\partial L(l-1)}{\partial Z(l)} + \frac{\partial}{\partial R(l-1)} \circ \frac{\partial R(l-1)}{\partial Z(l)}$$

Finite Unconstrained Trees

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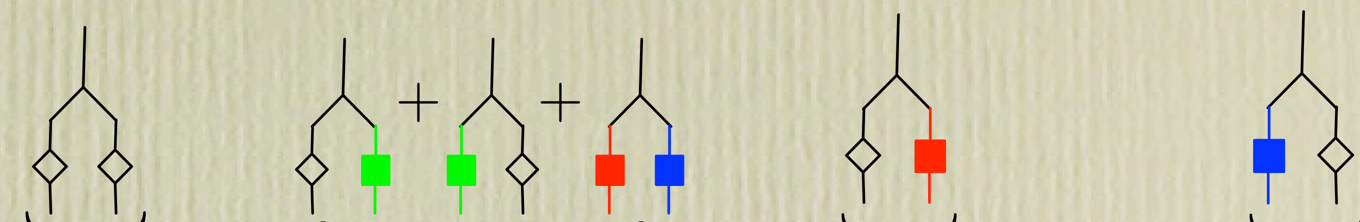

$$\frac{\partial}{\partial \lambda^\dagger(l)} = \frac{\partial}{\partial Z(l)} \circ \overbrace{\frac{\partial Z(l)}{\partial \lambda^\dagger(l)}} + \boxed{\frac{\partial}{\partial A(l)}} \circ \overbrace{\frac{\partial A(l)}{\partial \lambda^\dagger(l)}} + \frac{\partial}{\partial L(l)} \circ \overbrace{\frac{\partial L(l)}{\partial \lambda^\dagger(l)}} + \frac{\partial}{\partial R(l)} \circ \overbrace{\frac{\partial R(l)}{\partial \lambda^\dagger(l)}}$$

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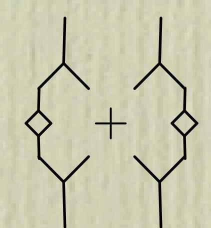
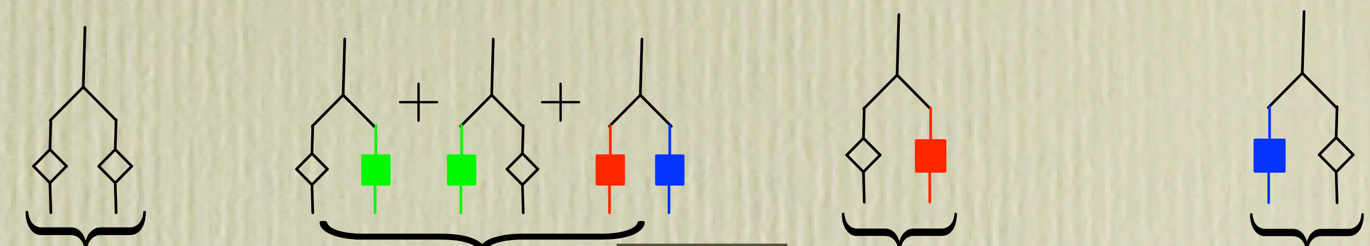


$$\frac{\partial}{\partial A(l)} = \frac{\partial}{\partial A(l-1)} \circ \overbrace{\frac{\partial A(l-1)}{\partial A(l)}} = \dots$$

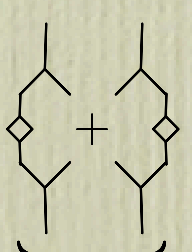
Finite Unconstrained Trees

energy gradient



$$\frac{\partial}{\partial \lambda^\dagger(l)} = \frac{\partial}{\partial Z(l)} \circ \frac{\partial Z(l)}{\partial \lambda^\dagger(l)} + \frac{\partial}{\partial A(l)} \circ \frac{\partial A(l)}{\partial \lambda^\dagger(l)} + \boxed{\frac{\partial}{\partial L(l)}} \circ \frac{\partial L(l)}{\partial \lambda^\dagger(l)} + \frac{\partial}{\partial R(l)} \circ \frac{\partial R(l)}{\partial \lambda^\dagger(l)}$$

$$\frac{\partial}{\partial Z(l)} = \frac{\partial}{\partial Z(l-1)} \circ \frac{\partial Z(l-1)}{\partial Z(l)} + \frac{\partial}{\partial A(l-1)} \circ \frac{\partial A(l-1)}{\partial Z(l)} + \frac{\partial}{\partial L(l-1)} \circ \frac{\partial L(l-1)}{\partial Z(l)} + \frac{\partial}{\partial R(l-1)} \circ \frac{\partial R(l-1)}{\partial Z(l)}$$

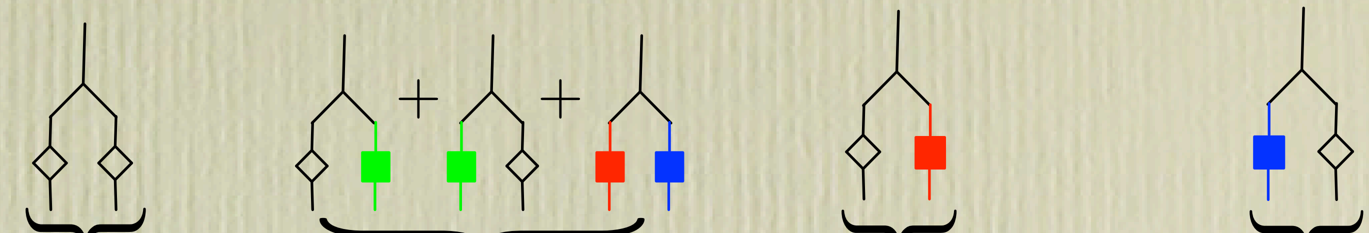


$$\frac{\partial}{\partial A(l)} = \frac{\partial}{\partial A(l-1)} \circ \frac{\partial A(l-1)}{\partial A(l)} = \dots$$

$$\frac{\partial}{\partial R(l)} = \frac{\partial}{\partial R(l-1)} \circ \frac{\partial R(l-1)}{\partial R(l)} + \frac{\partial}{\partial A(l-1)} \circ \frac{\partial A(l-1)}{\partial R(l)}$$

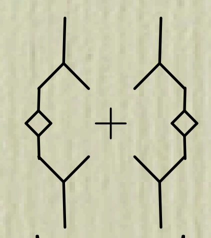
Finite Unconstrained Trees

energy gradient



$$\frac{\partial}{\partial \lambda^\dagger(l)} = \frac{\partial}{\partial Z(l)} \circ \overbrace{\frac{\partial Z(l)}{\partial \lambda^\dagger(l)}} + \frac{\partial}{\partial A(l)} \circ \overbrace{\frac{\partial A(l)}{\partial \lambda^\dagger(l)}} + \frac{\partial}{\partial L(l)} \circ \overbrace{\frac{\partial L(l)}{\partial \lambda^\dagger(l)}} + \boxed{\frac{\partial}{\partial R(l)}} \circ \overbrace{\frac{\partial R(l)}{\partial \lambda^\dagger(l)}}$$

$$\frac{\partial}{\partial Z(l)} = \frac{\partial}{\partial Z(l-1)} \circ \overbrace{\frac{\partial Z(l-1)}{\partial Z(l)}} + \frac{\partial}{\partial A(l-1)} \circ \overbrace{\frac{\partial A(l-1)}{\partial Z(l)}} + \frac{\partial}{\partial L(l-1)} \circ \overbrace{\frac{\partial L(l-1)}{\partial Z(l)}} + \frac{\partial}{\partial R(l-1)} \circ \overbrace{\frac{\partial R(l-1)}{\partial Z(l)}}$$



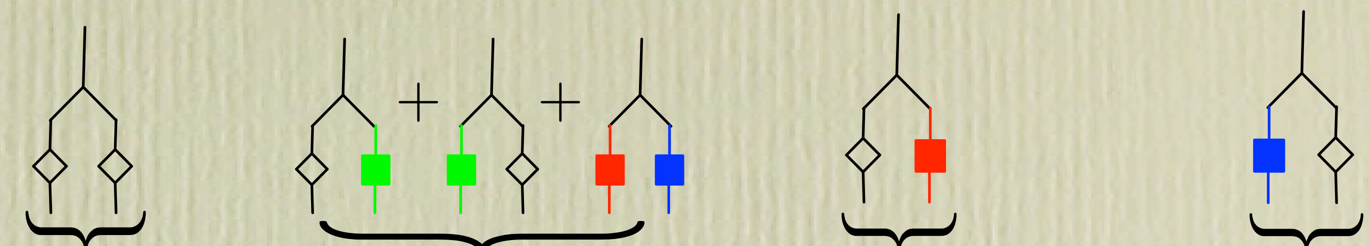
$$\frac{\partial}{\partial A(l)} = \frac{\partial}{\partial A(l-1)} \circ \overbrace{\frac{\partial A(l-1)}{\partial A(l)}} = \dots$$

$$\frac{\partial}{\partial R(l)} = \frac{\partial}{\partial R(l-1)} \circ \overbrace{\frac{\partial R(l-1)}{\partial R(l)}} + \frac{\partial}{\partial A(l-1)} \circ \overbrace{\frac{\partial A(l-1)}{\partial R(l)}}$$

$$\frac{\partial}{\partial L(l)} = \frac{\partial}{\partial L(l-1)} \circ \overbrace{\frac{\partial L(l-1)}{\partial L(l)}} + \frac{\partial}{\partial A(l-1)} \circ \overbrace{\frac{\partial A(l-1)}{\partial L(l)}}$$

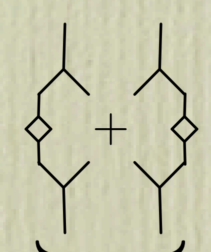
Finite Unconstrained Trees

energy gradient



$$\frac{\partial}{\partial \lambda^\dagger(l)} = \frac{\partial}{\partial Z(l)} \circ \frac{\partial Z(l)}{\partial \lambda^\dagger(l)} + \frac{\partial}{\partial A(l)} \circ \frac{\partial A(l)}{\partial \lambda^\dagger(l)} + \frac{\partial}{\partial L(l)} \circ \frac{\partial L(l)}{\partial \lambda^\dagger(l)} + \frac{\partial}{\partial R(l)} \circ \frac{\partial R(l)}{\partial \lambda^\dagger(l)}$$

$$\frac{\partial}{\partial Z(l)} = \frac{\partial}{\partial Z(l-1)} \circ \frac{\partial Z(l-1)}{\partial Z(l)} + \frac{\partial}{\partial A(l-1)} \circ \frac{\partial A(l-1)}{\partial Z(l)} + \frac{\partial}{\partial L(l-1)} \circ \frac{\partial L(l-1)}{\partial Z(l)} + \frac{\partial}{\partial R(l-1)} \circ \frac{\partial R(l-1)}{\partial Z(l)}$$



$$\frac{\partial}{\partial A(l)} = \frac{\partial}{\partial A(l-1)} \circ \frac{\partial A(l-1)}{\partial A(l)} = \dots$$

only few kinds of contractions per every layer !

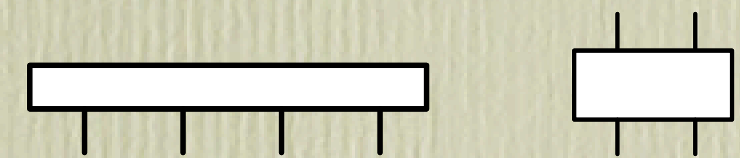
$$\frac{\partial}{\partial R(l)} = \frac{\partial}{\partial R(l-1)} \circ \frac{\partial R(l-1)}{\partial R(l)} + \frac{\partial}{\partial A(l-1)} \circ \frac{\partial A(l-1)}{\partial R(l)}$$

$$\frac{\partial}{\partial L(l)} = \frac{\partial}{\partial L(l-1)} \circ \frac{\partial L(l-1)}{\partial L(l)} + \frac{\partial}{\partial A(l-1)} \circ \frac{\partial A(l-1)}{\partial L(l)}$$

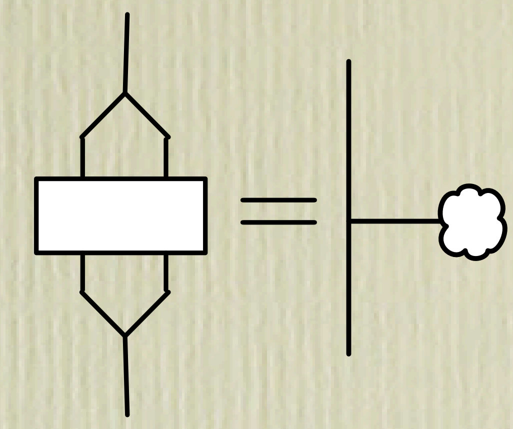
Finite Unconstrained Trees

TTN initialization à la DMRG:

Hamiltonian
on 4 (effective) sites



ground wavefunction
and 2-sites density matrix



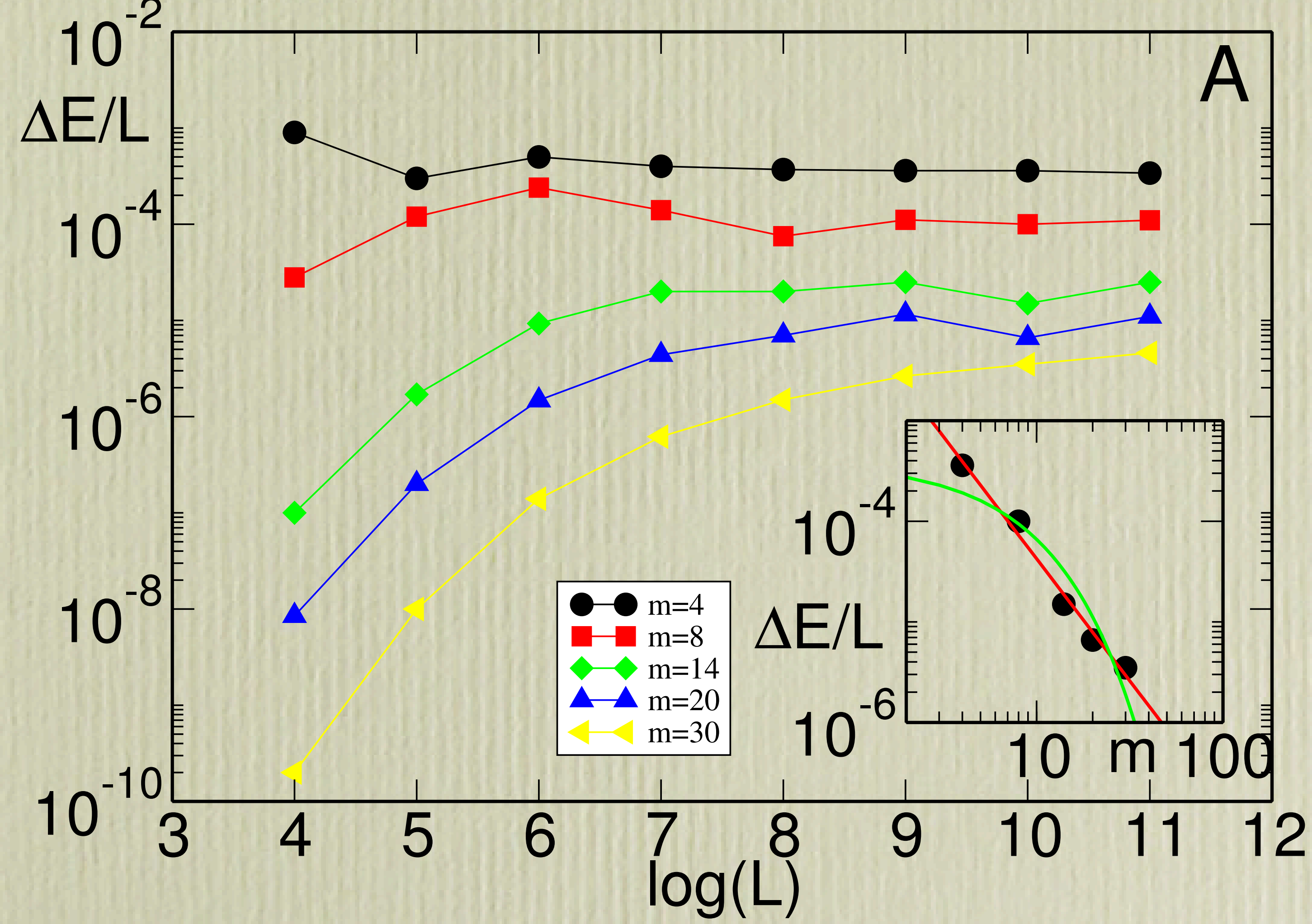
truncation isometry
defines the tensors

- naive, not so correlated as it should... :(
- avoids long paths due to random start
  (already 2-3 digits of energy in critical cases) :)
- helps to guess symmetry multiplets :)
- is feasible only up to m=16-20 :(

Larger m's started by 'enlarging' ansätze with smaller bonds:
add extra random elements to tensors

Preliminary results (1D)

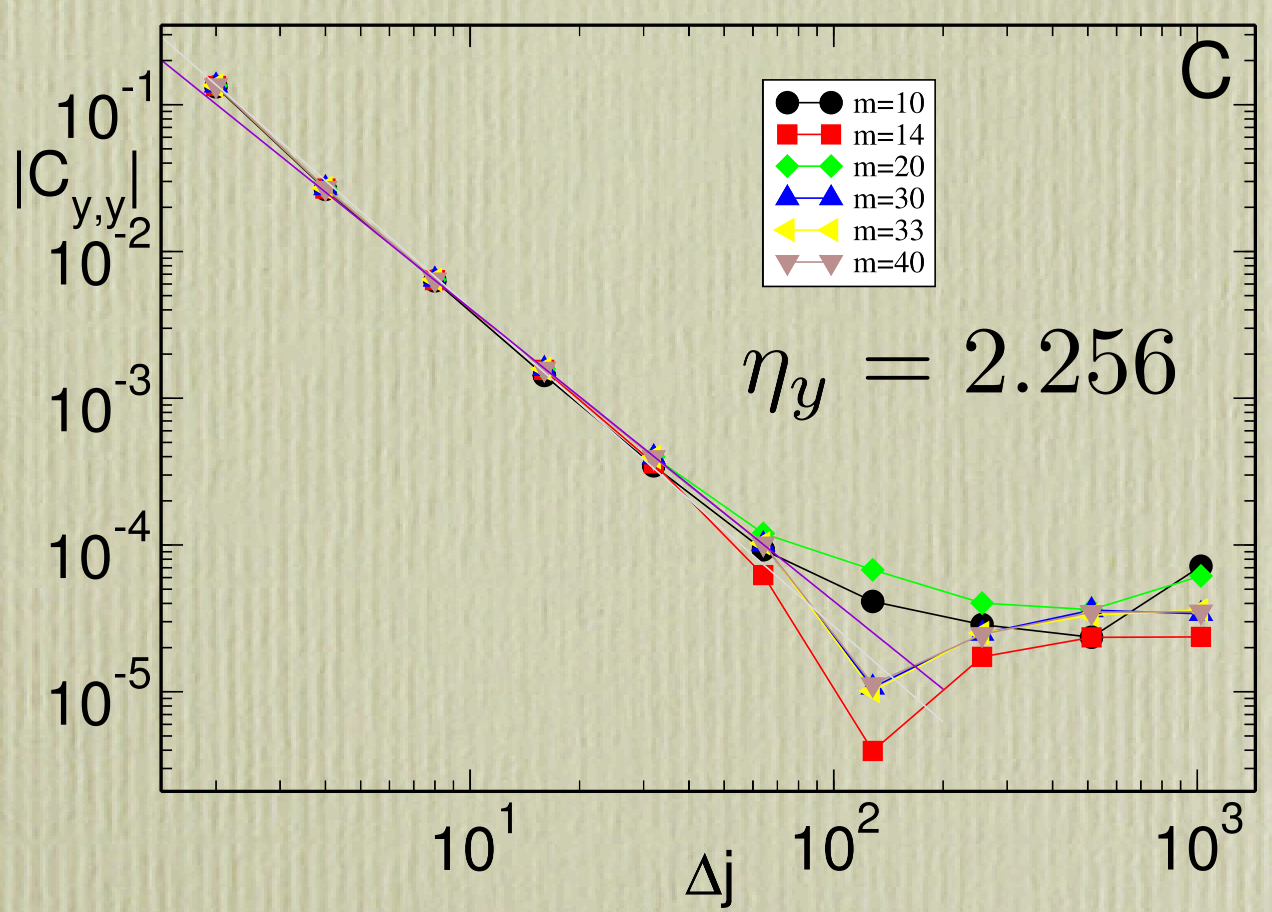
Critical Ising model $$H = \sum_j \sigma_j^x \sigma_{j+1}^x + \sigma_j^z$$

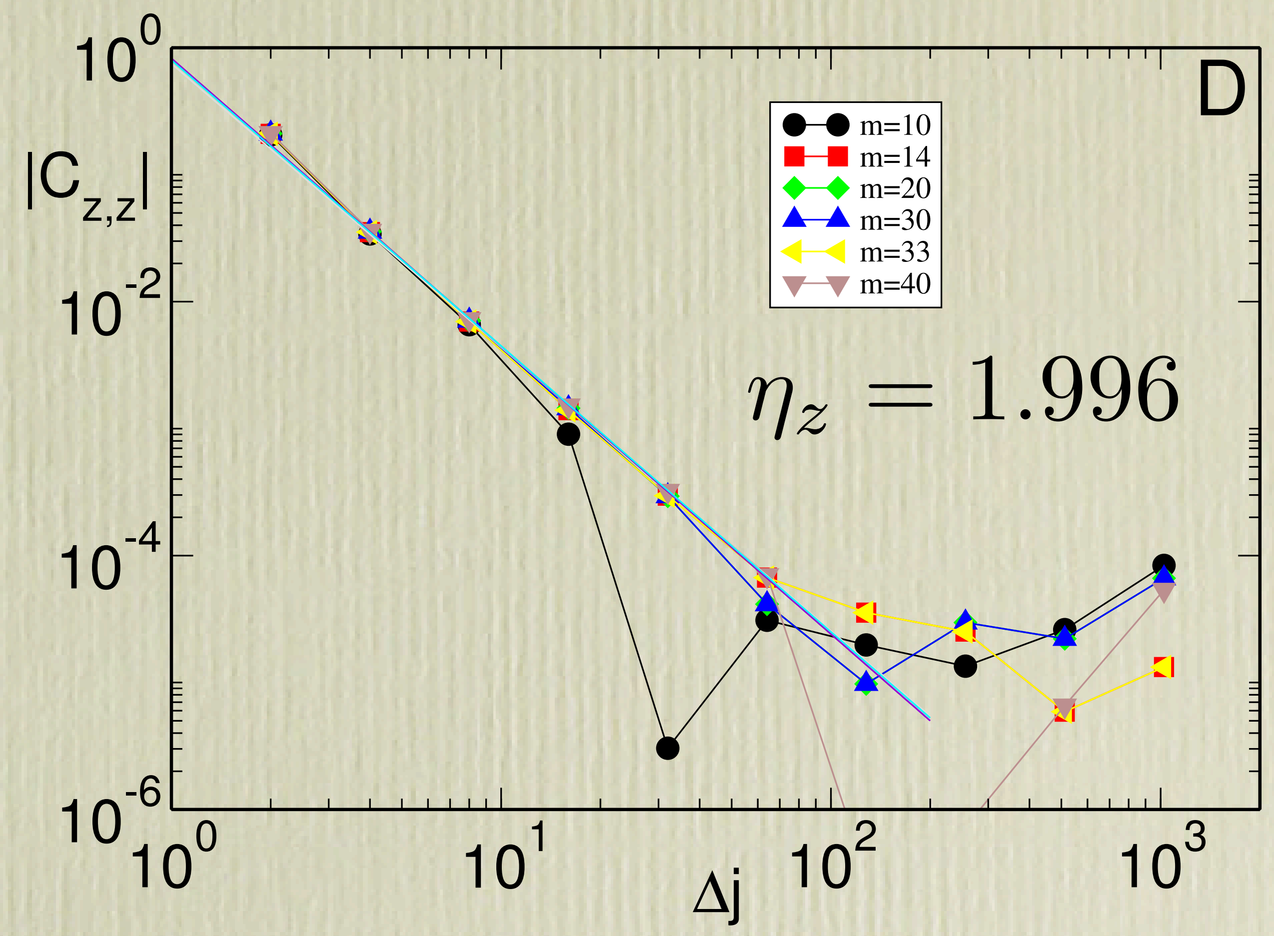


- ~ size independent precision on E (as for MERA)
- quite precise local observables (4 digits at m=20)
- tiny dimerization < $10^{-4 \div 5}$ despite binary structure

Preliminary results (1D)

Critical Ising model $\quad H = \sum_j \sigma_j^x \sigma_{j+1}^x + \sigma_j^z$

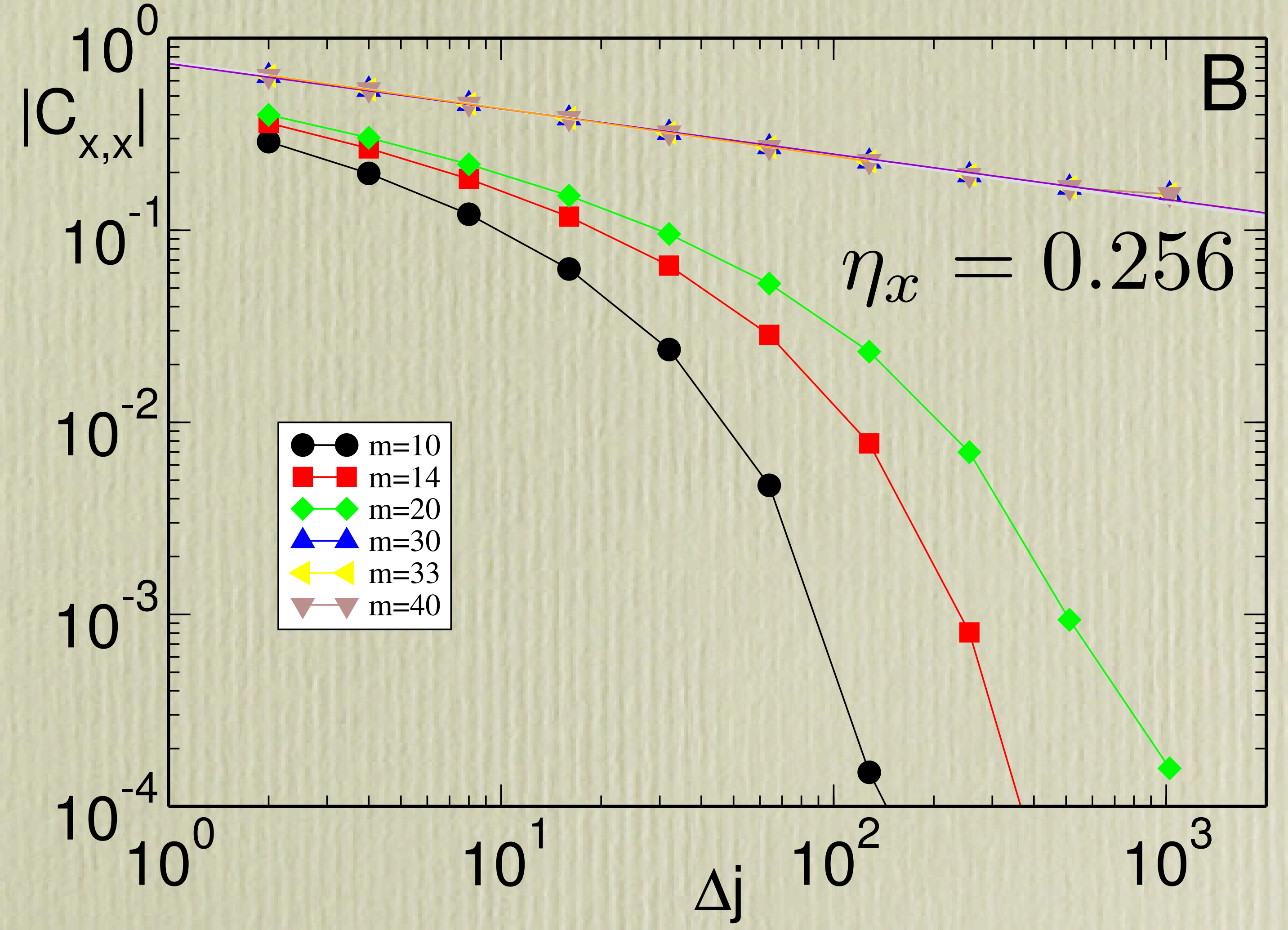




- fast decaying correlations captured well at m~10
- good precision on critical exponents (large N helps)

Preliminary results (1D)

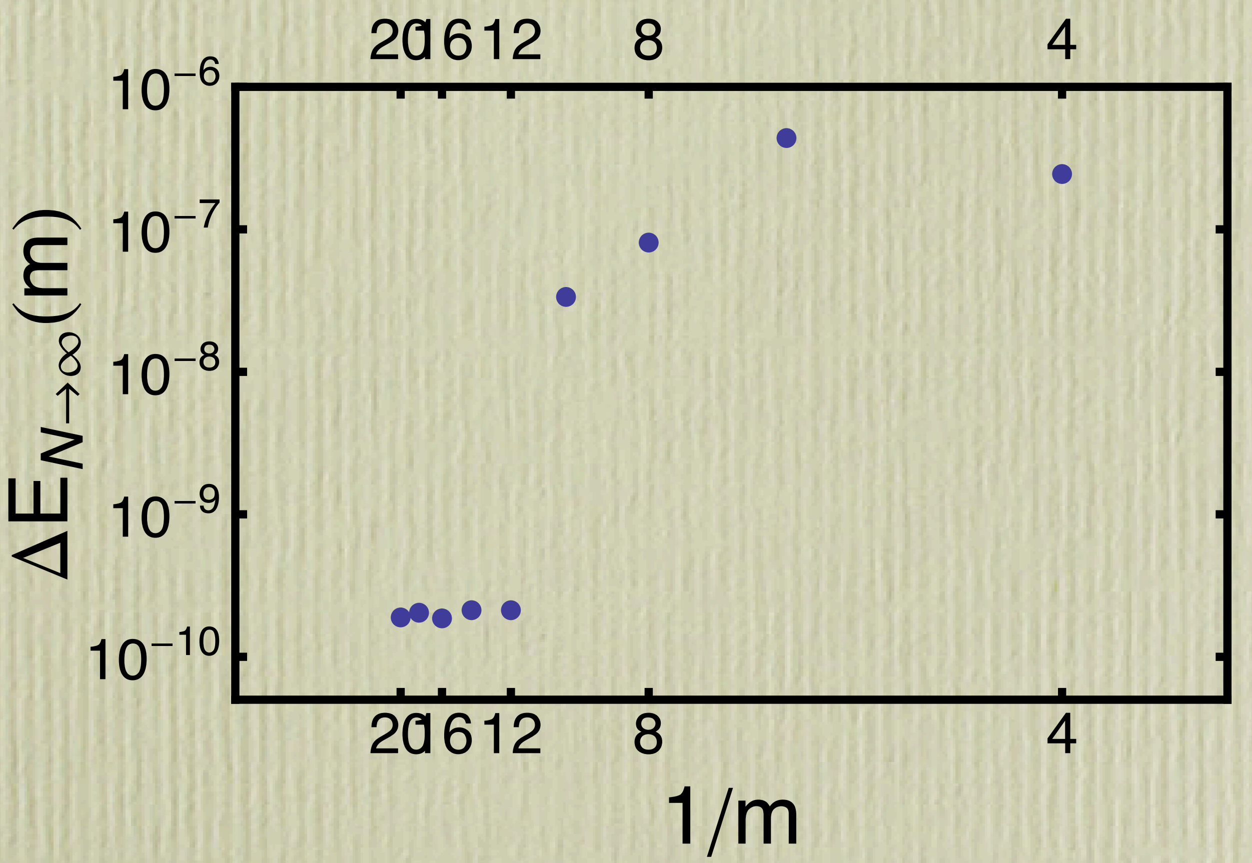
Critical Ising model $H = \sum_j \sigma_j^x \sigma_{j+1}^x + \sigma_j^z$

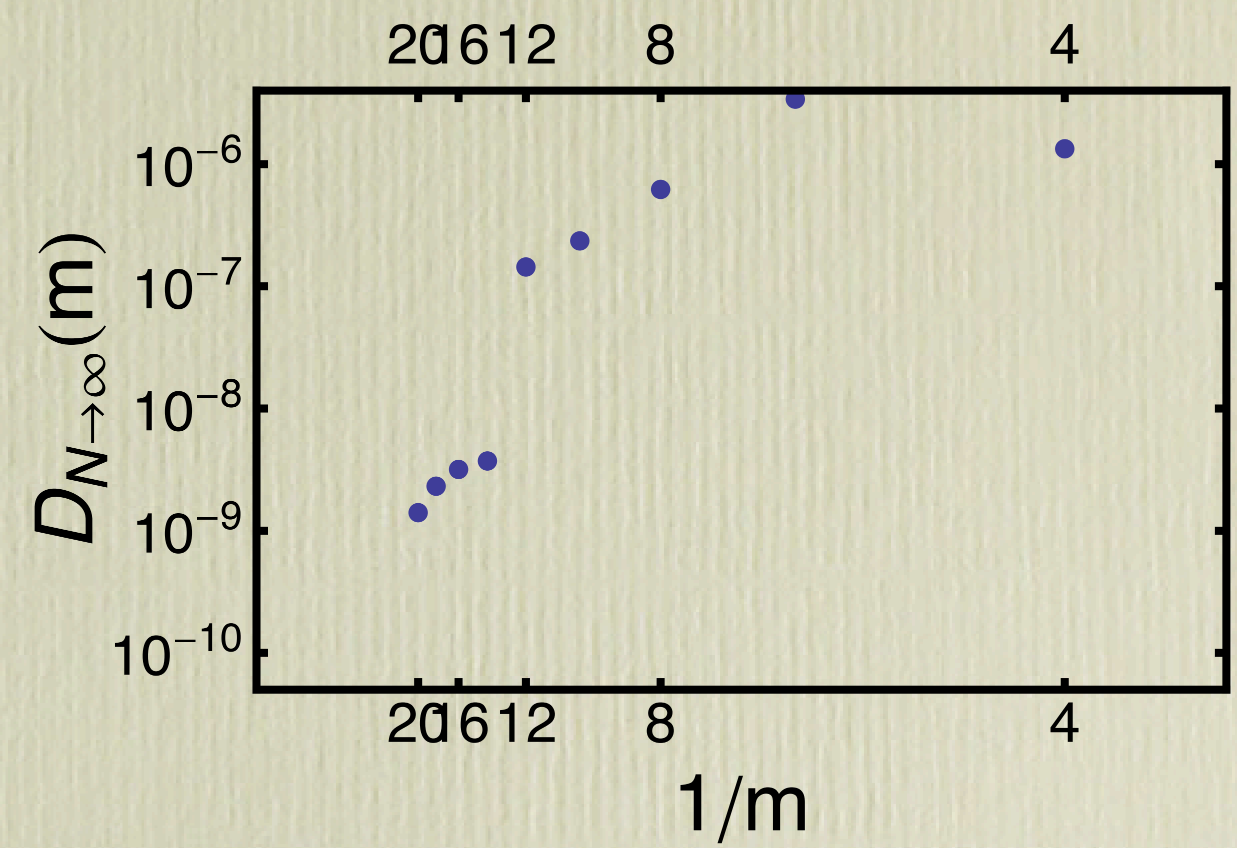


- super-slow correlations need a large m~30 but, over it, very precise on dx~1000 !!!

Preliminary results (1D)

Non-critical Ising model $\quad H = \sum_j \sigma_j^x \sigma_{j+1}^x + \frac{1}{2}\sigma_j^z$



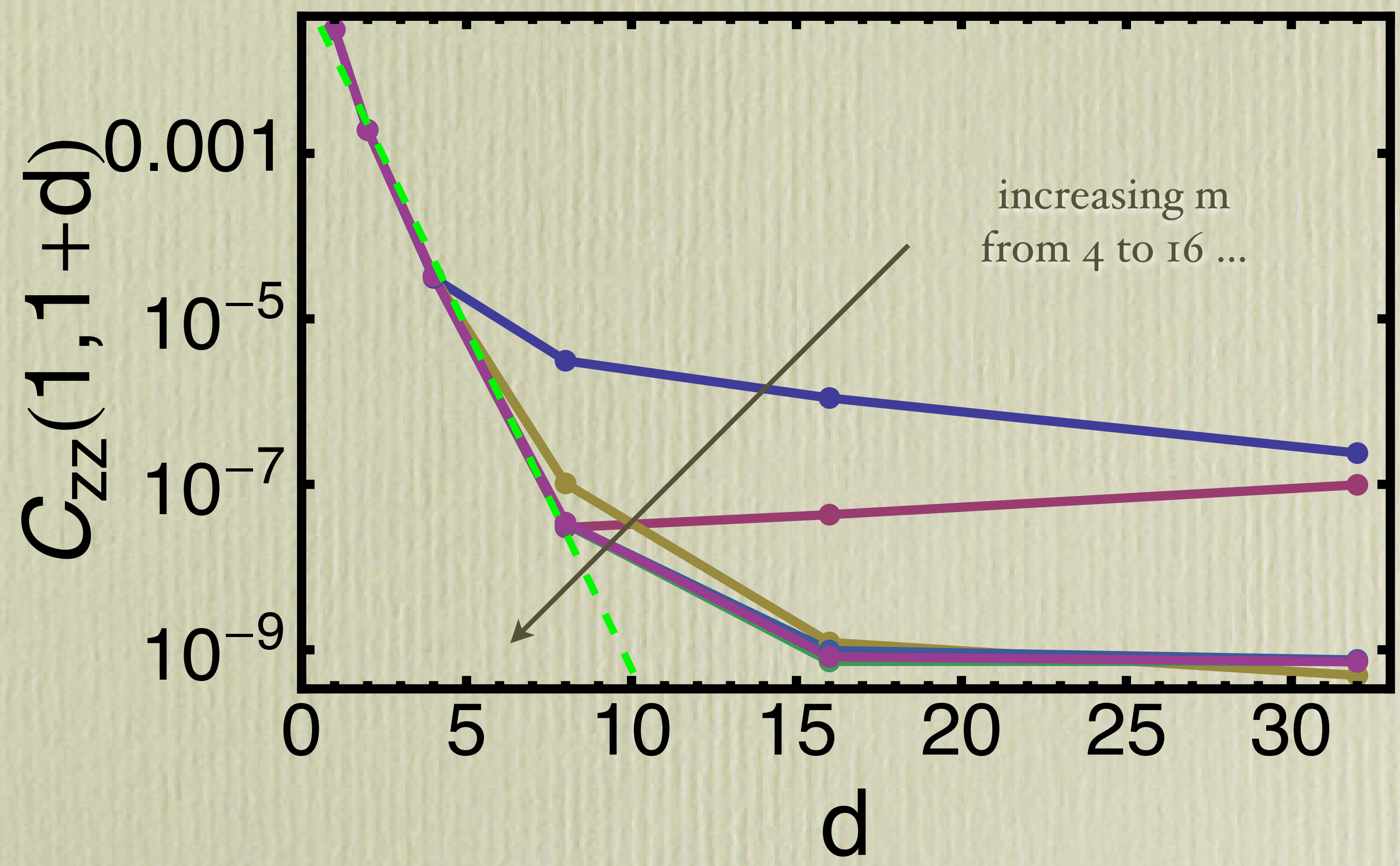


- accurate energy
- vanishing dimerization
- m-12 captures almost everything

expected from a nearly product state :)

Preliminary results (1D)

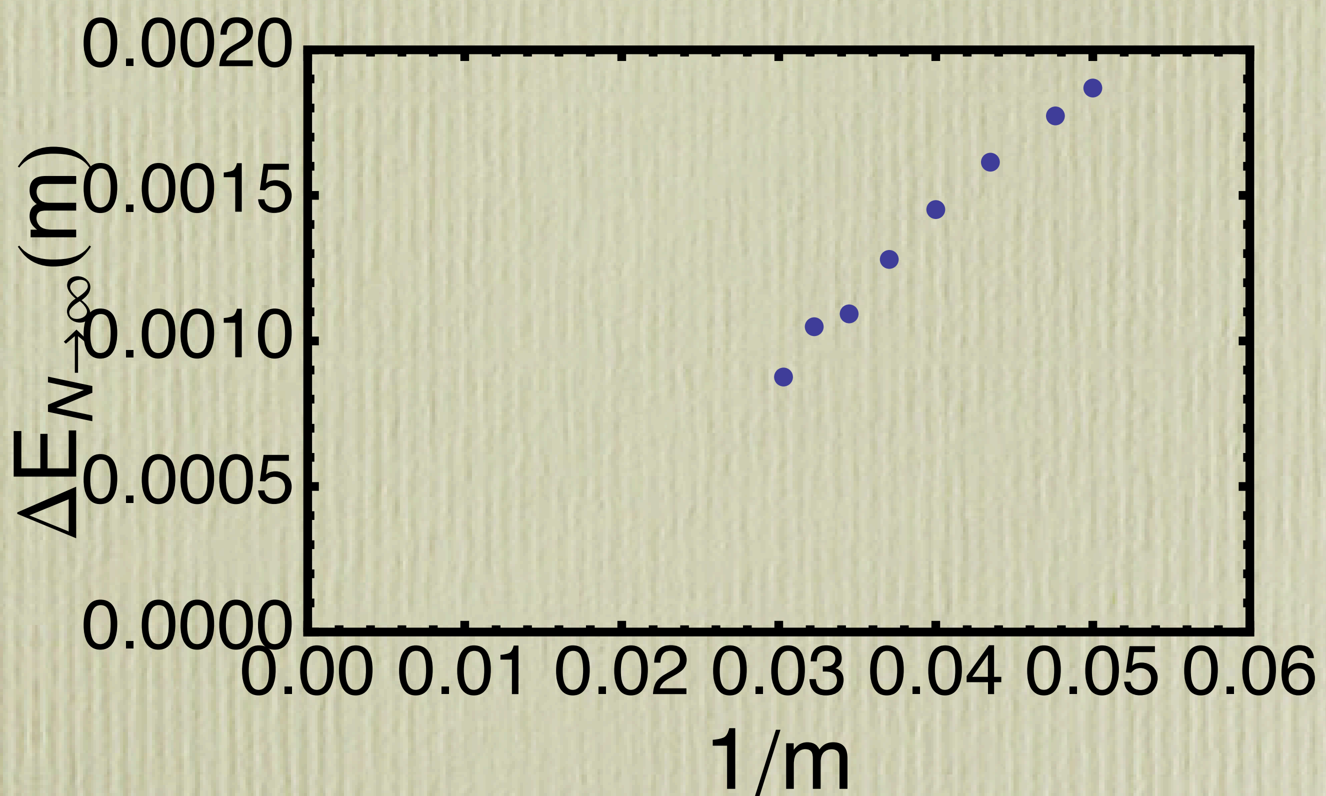
Non-critical Ising model $\quad H = \sum_j \sigma^x_j \sigma^x_{j+1} + \frac{1}{2}\sigma^z_j$

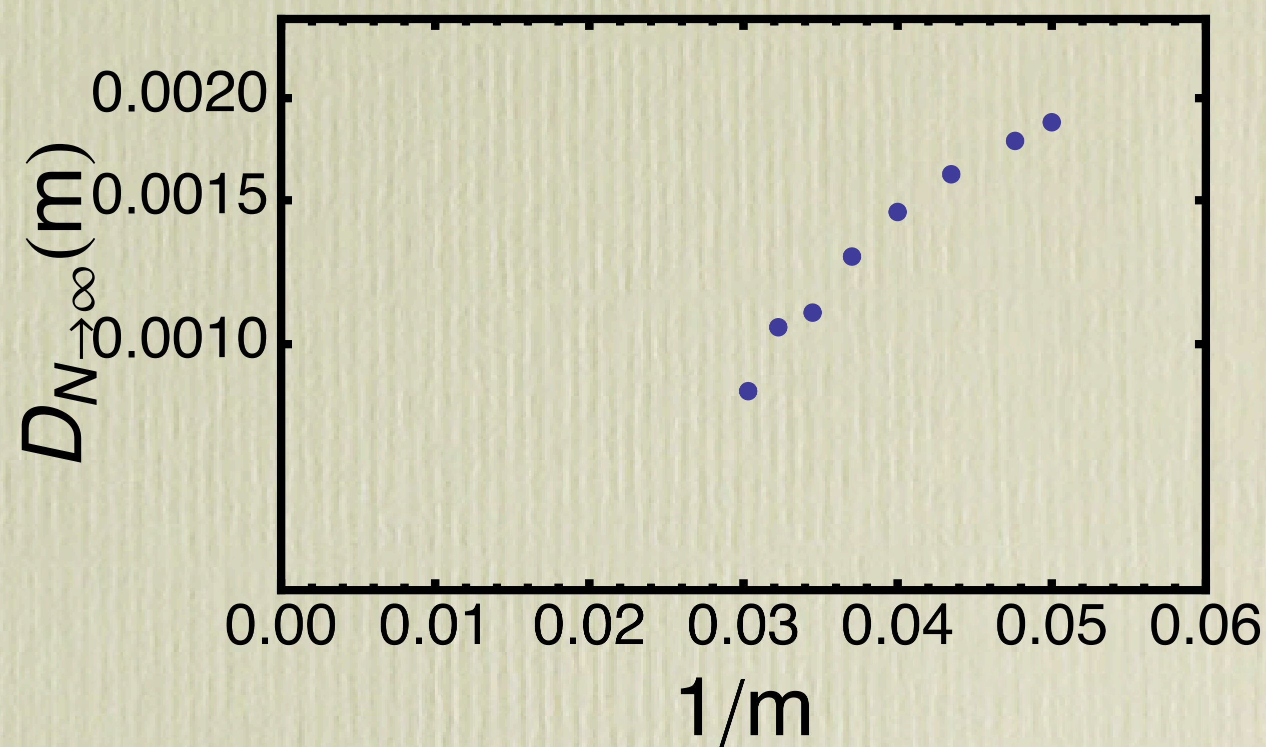


- curiously, correlations approximated 'from above' as if TTN is summing power-laws to cancel their effect !?

Preliminary results (1D)

AF Heisenberg spin 1 $\quad H = \sum_j \vec{\sigma}_j \cdot \vec{\sigma}_{j+1}$

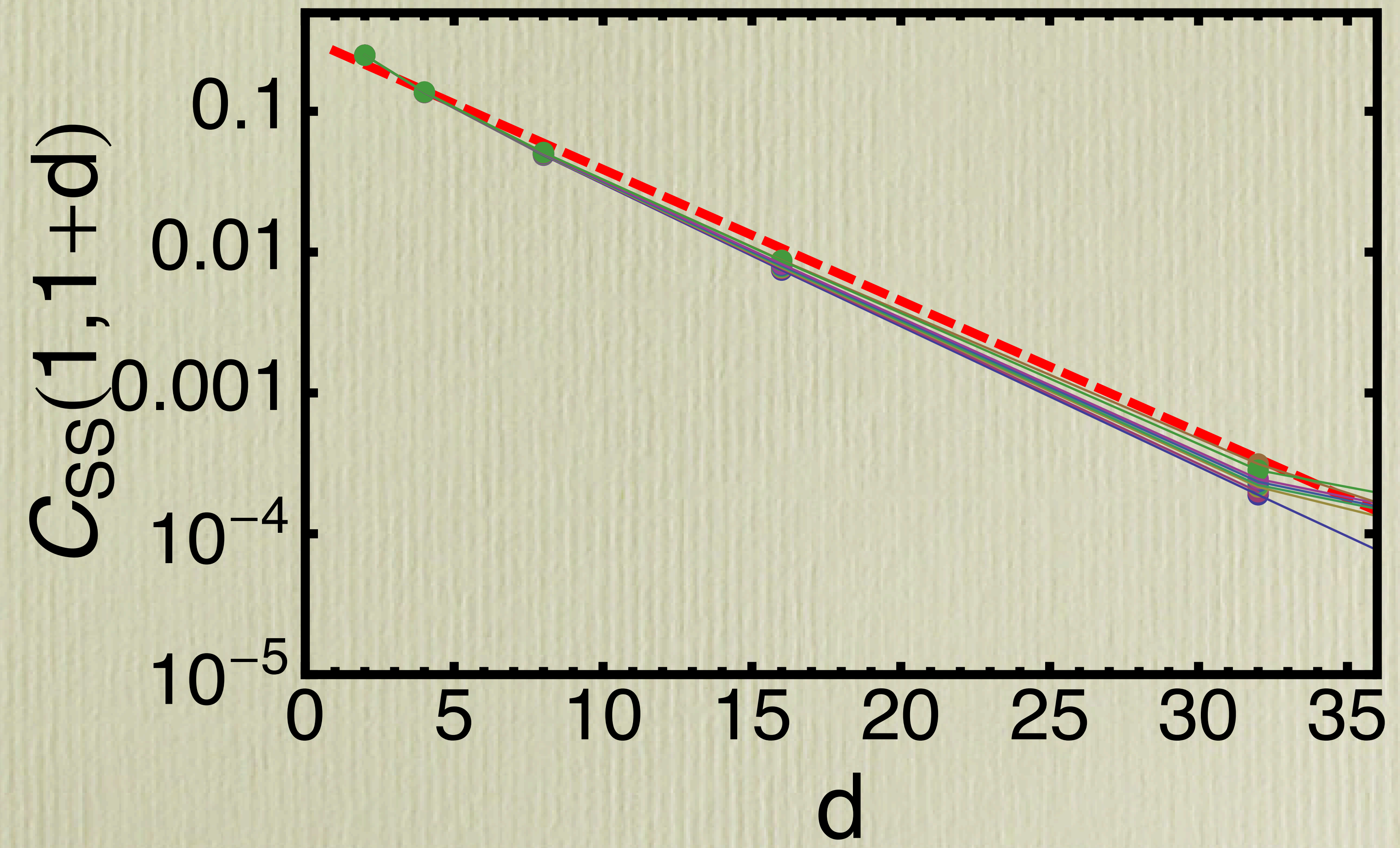




- despite non-critical, precision lacking even for m~30 (reference energy from White's DMRG'93)
- does it depend on local dim? or on symmetries?

Preliminary results (1D)

AF Heisenberg spin 1 $\quad H = \sum_j \vec{\sigma}_j \cdot \vec{\sigma}_{j+1}$

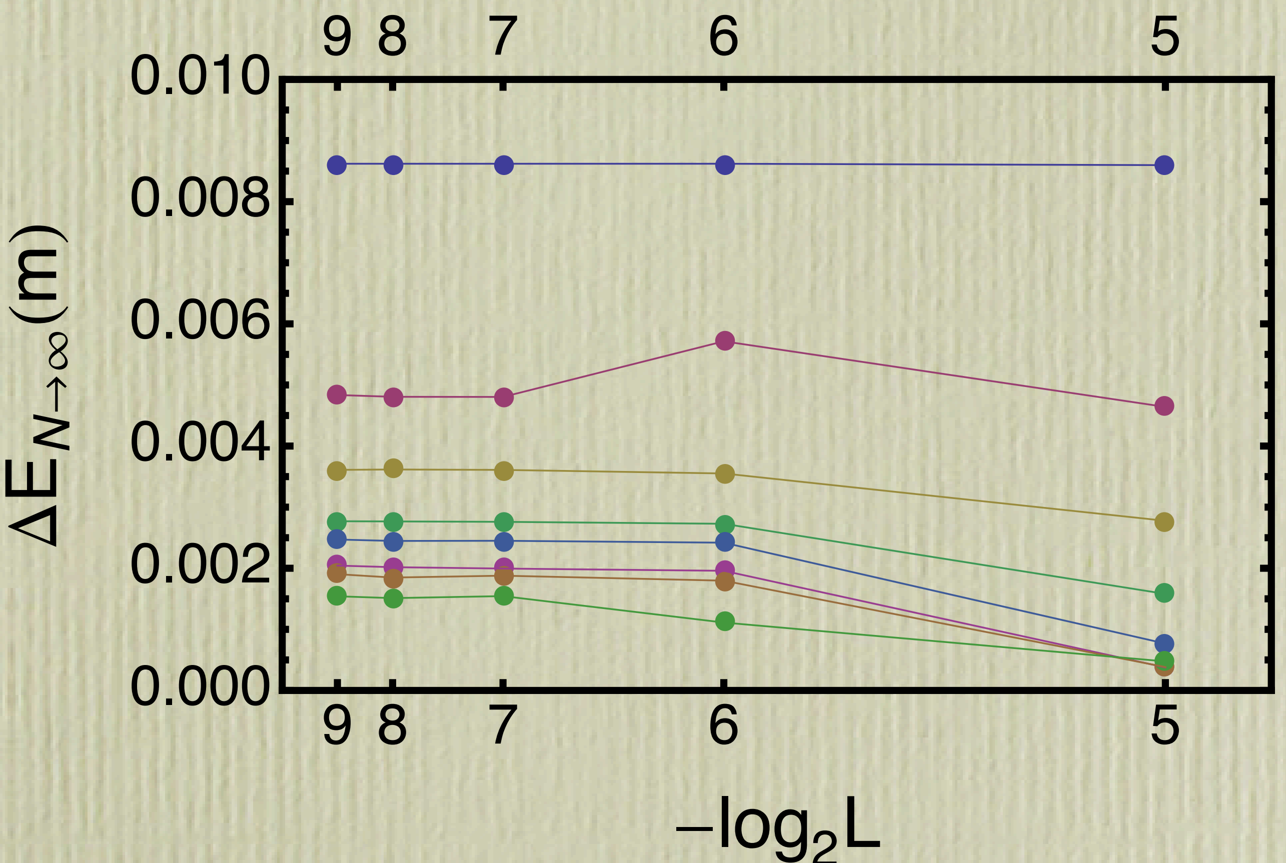


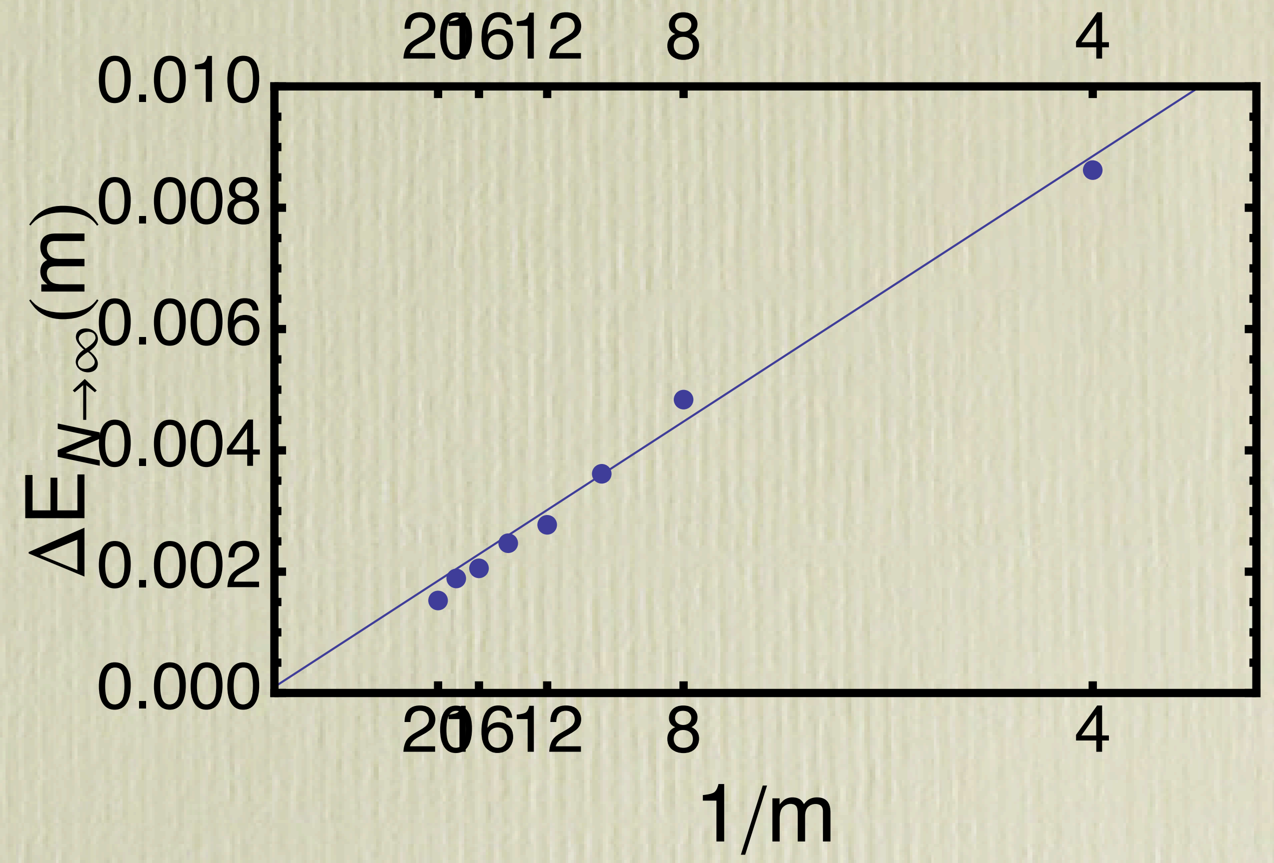
- correlations consistent with $C \simeq \dfrac{e^{-d/5.6}}{d^{1/3}}$

  but the corrections (exp+pow) make it tricky

Preliminary results (1D)

AF Heisenberg spin 1/2 $\quad H = \sum_j \vec{\sigma}_j \cdot \vec{\sigma}_{j+1}$



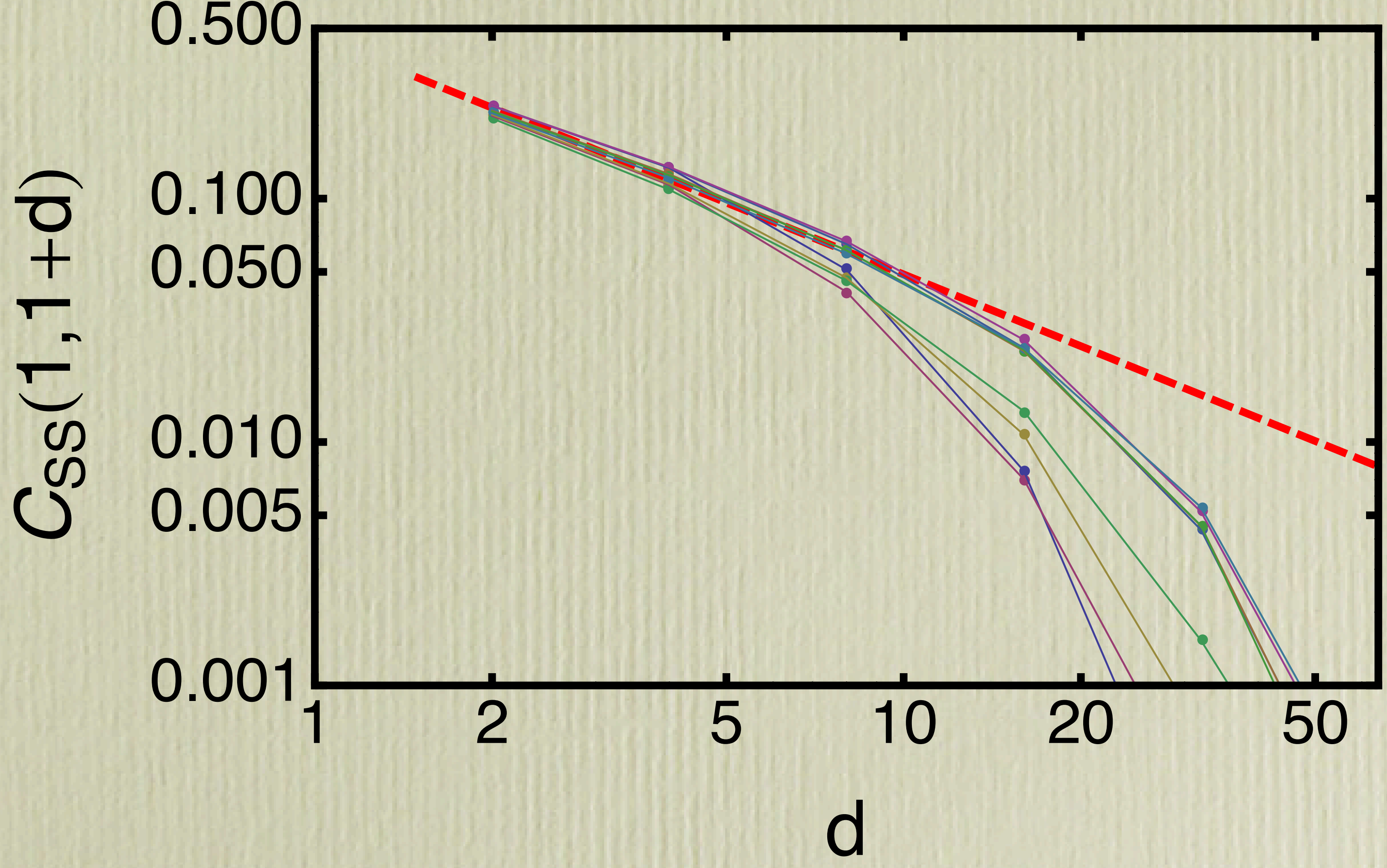


- constant precision in m at big sizes :)
- energy less precise than Ising :(
- quite 'brutal' dimerization ~$10^{-1\div 2}$:(

$\boxed{\text{! symmetry !}}$

Preliminary results (1D)

AF Heisenberg spin 1/2 $\quad H = \sum_j \vec{\sigma}_j \cdot \vec{\sigma}_{j+1}$

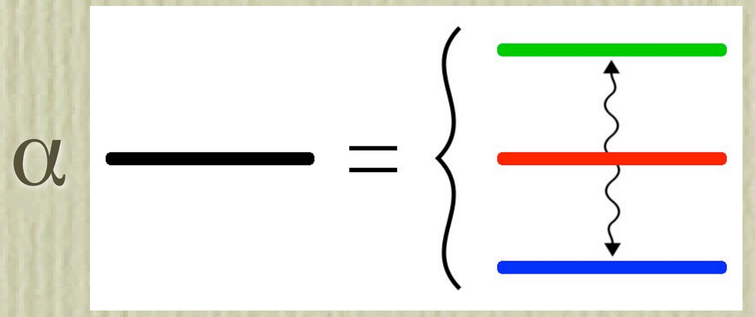


- nonetheless, at short enough d, decay d^{-1} :)
  need for larger m's as in critical Ising C_{xx} ...

Outlook: symmetries

3-legs structure ease the symmetry preservation

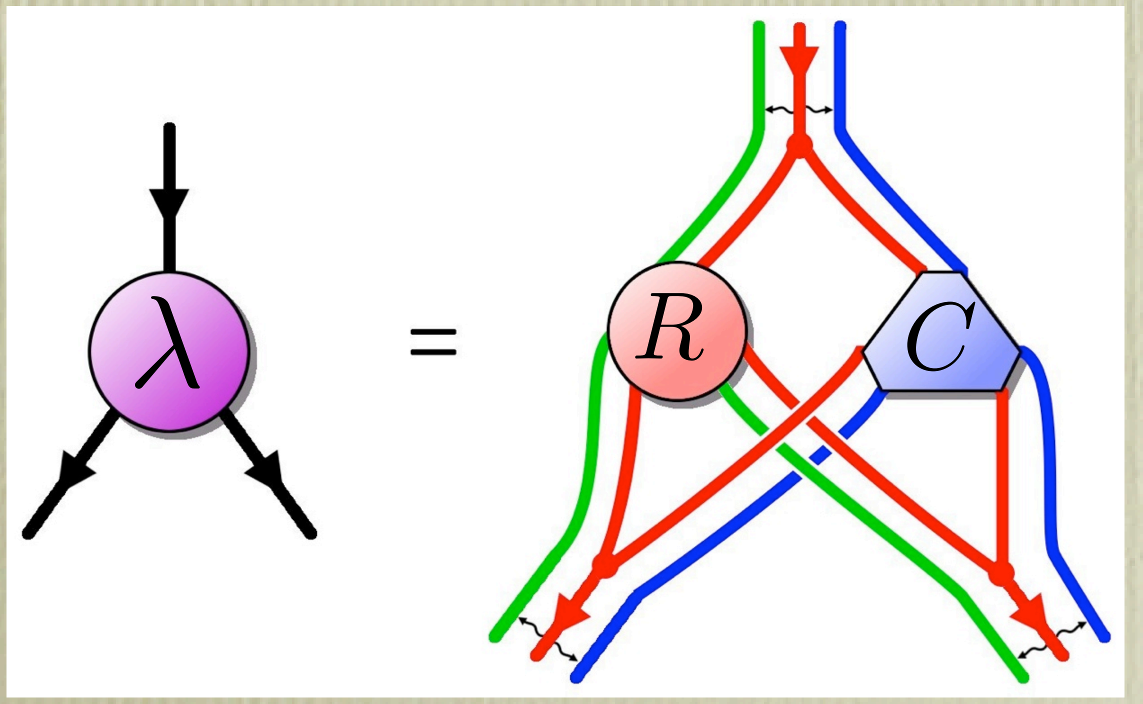
(work in progress in our code)



a = degeneracy index

j = irreducible representation index

m = internal index of irred.rep.



C = structure tensor

(e.g. δ in U(1), CG in SU(2),...)

R = variational tensor

(few free parameters)

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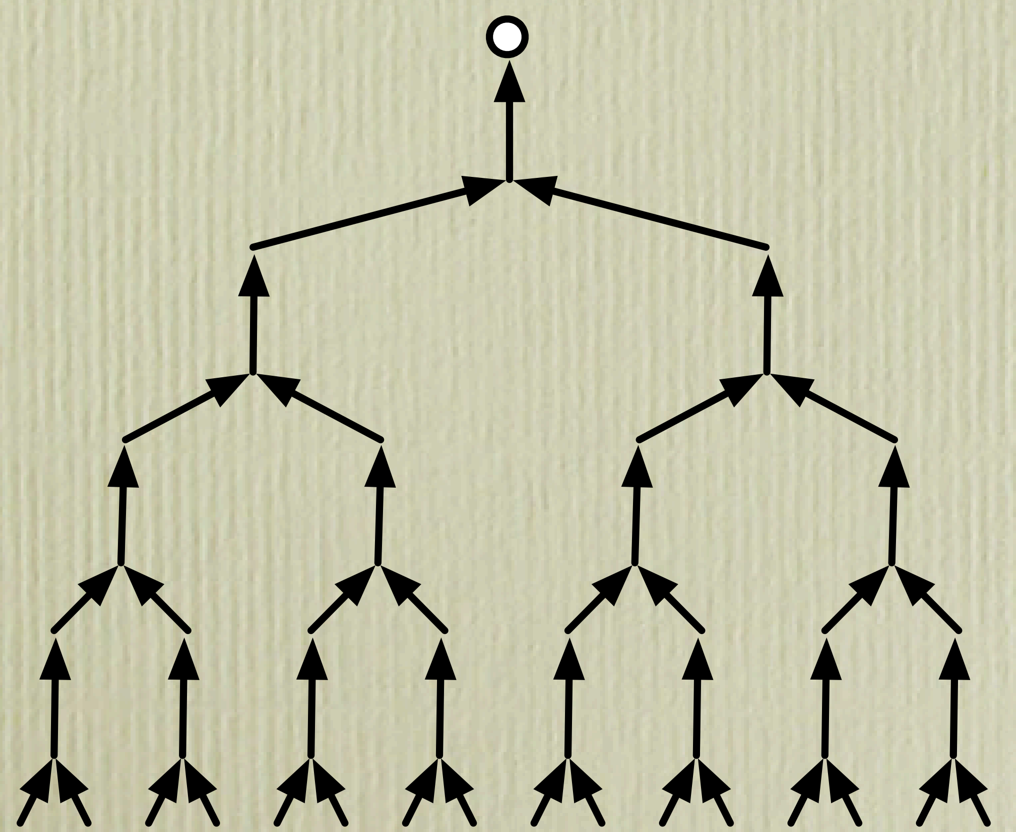
isometric gauge condition redirectionable at will

(also useful for CPT map interpretation)



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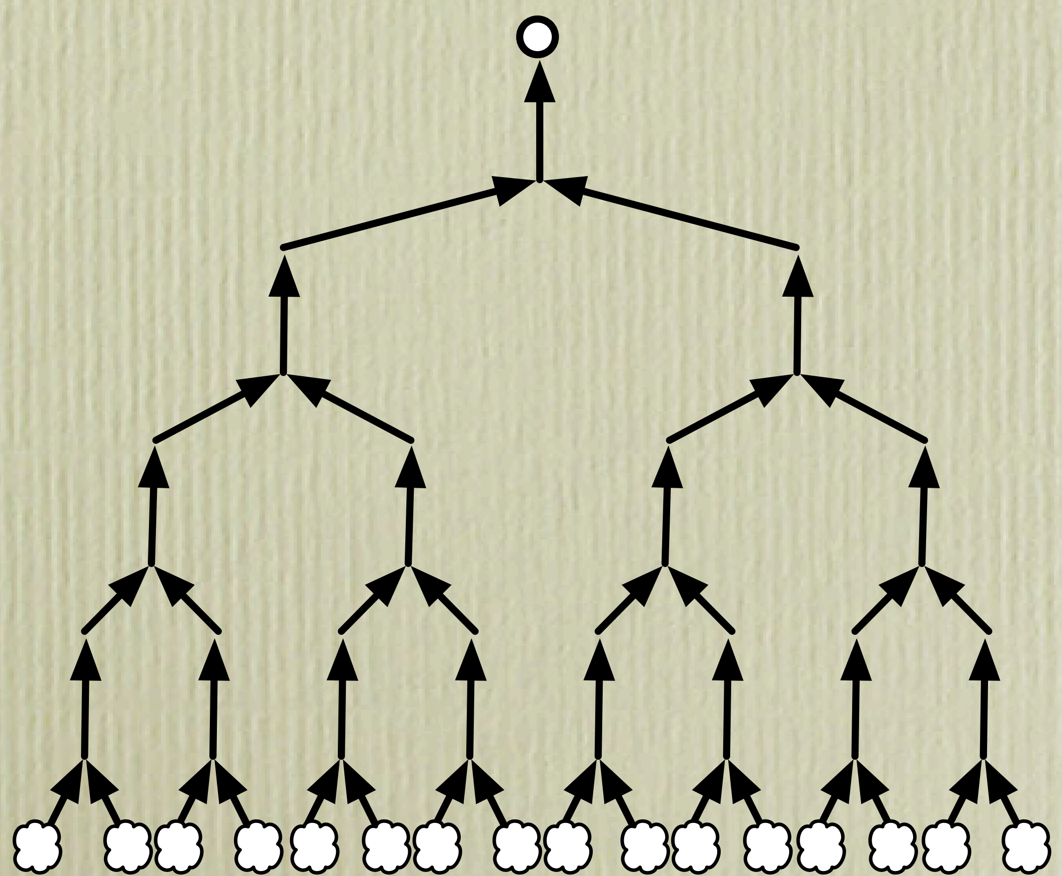

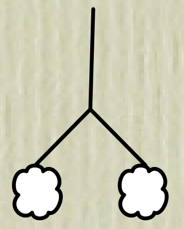

$$[\phi(l+1) \otimes \phi(l+1)] \cdot \lambda(l)$$

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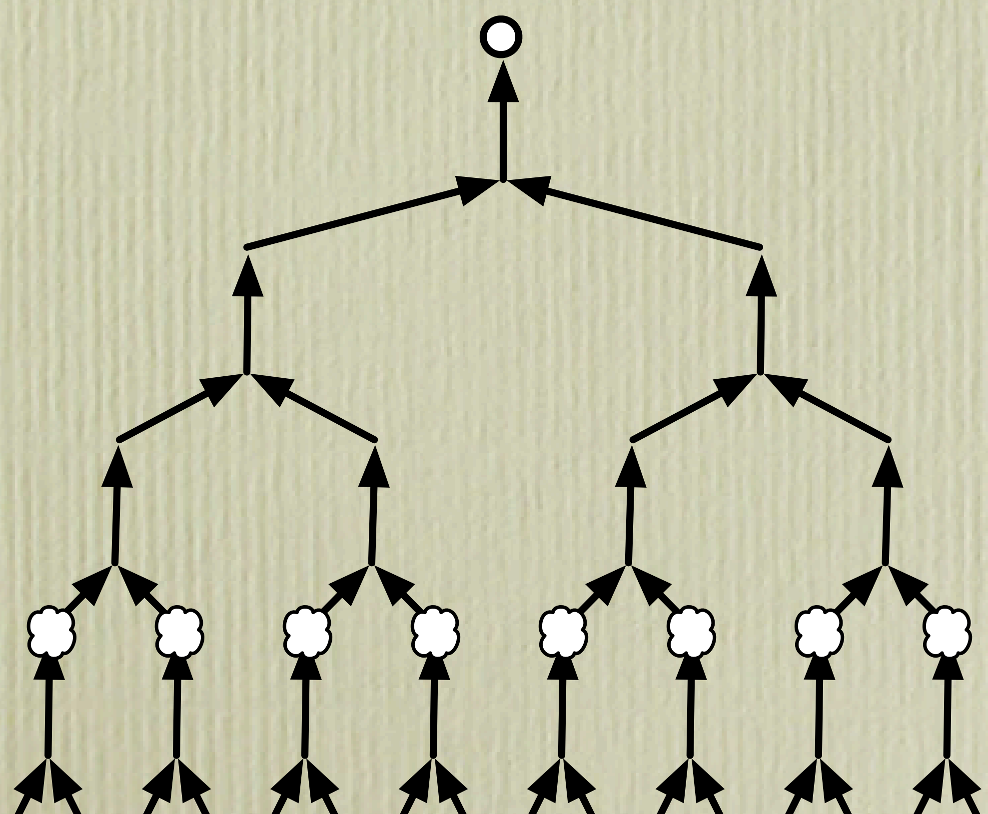

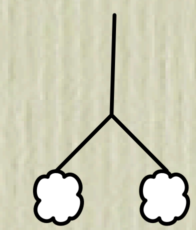

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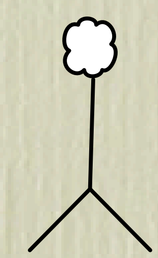
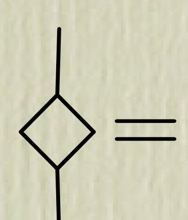


$$\overline{\lambda}(l) \cdot \phi(l)$$



$$\overline{\lambda}(l)^\dagger \cdot \overline{\lambda}(l) = \mathbb{I}$$

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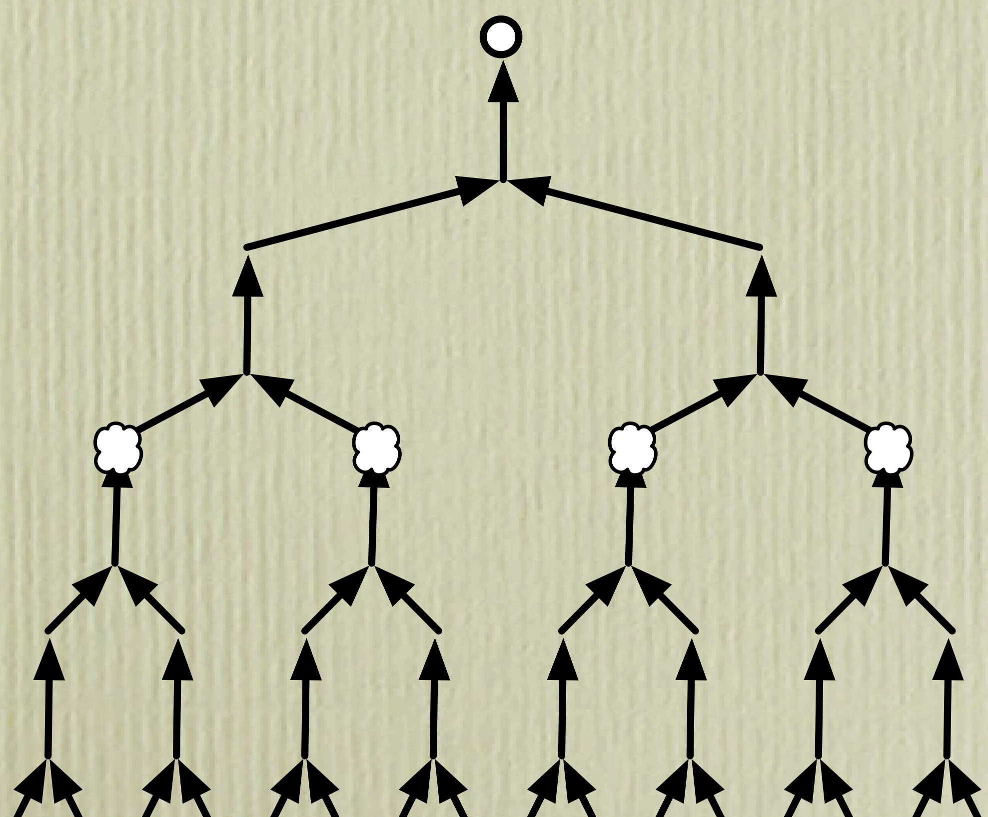

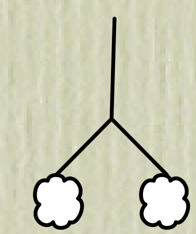

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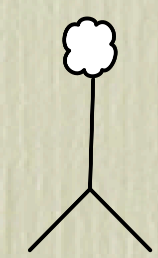

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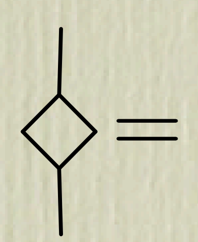

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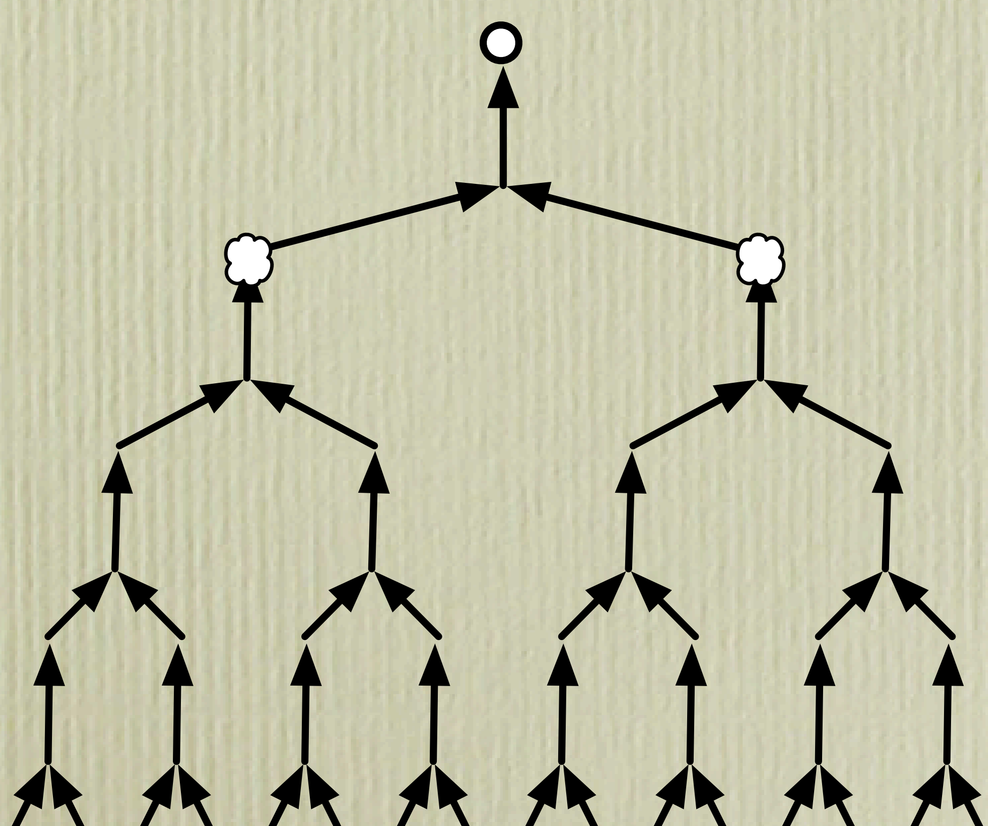
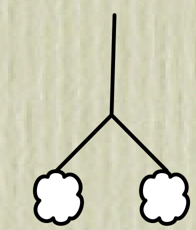
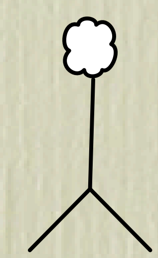
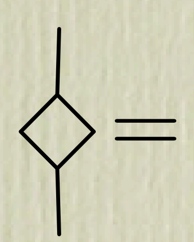




$[\phi(l+1) \otimes \phi(l+1)] \cdot \lambda(l)$



$\overline{\lambda}(l) \cdot \phi(l)$



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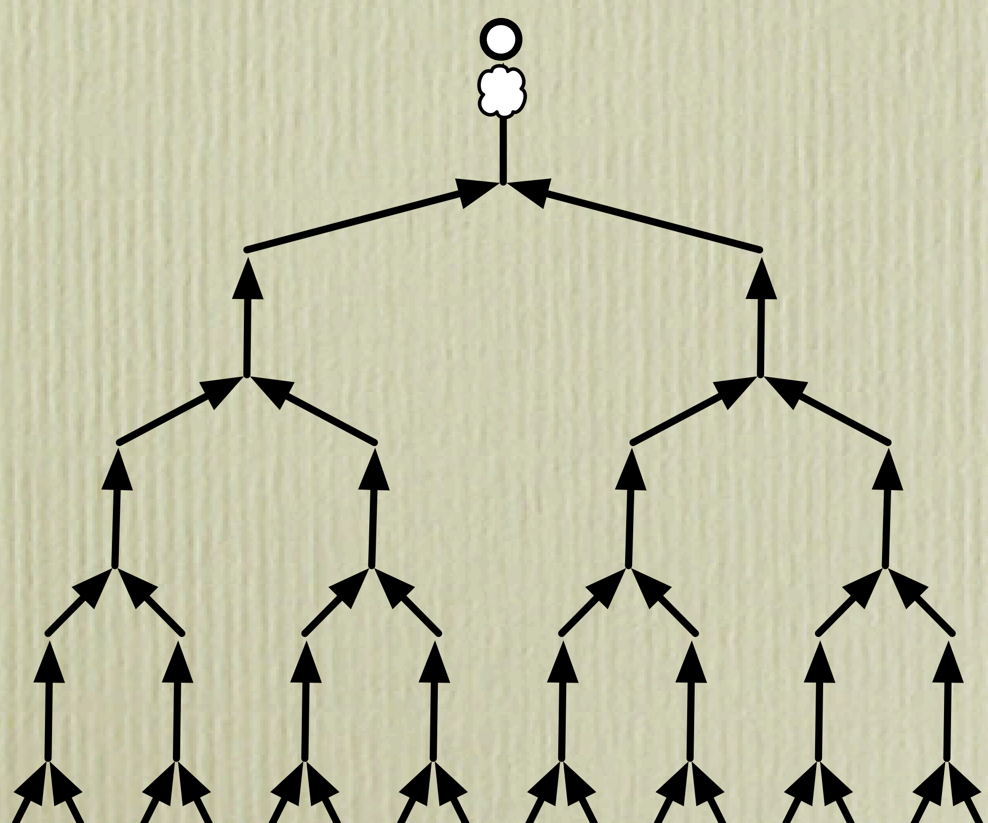
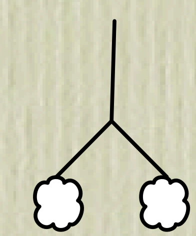
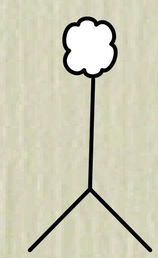




$$[\phi(l+1) \otimes \phi(l+1)] \cdot \lambda(l)$$



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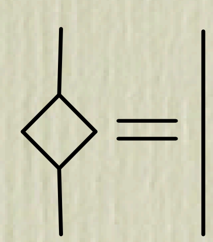

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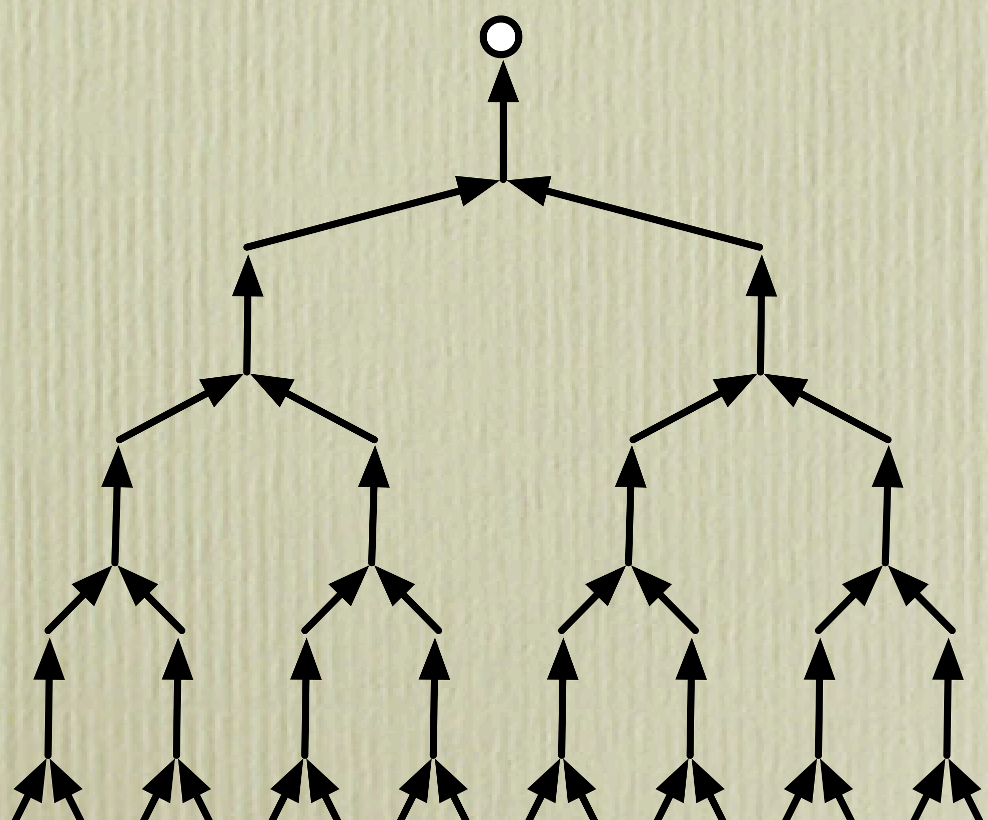

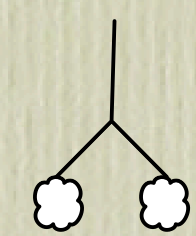

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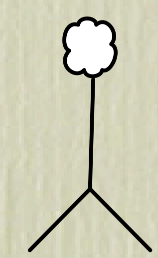

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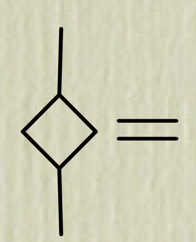

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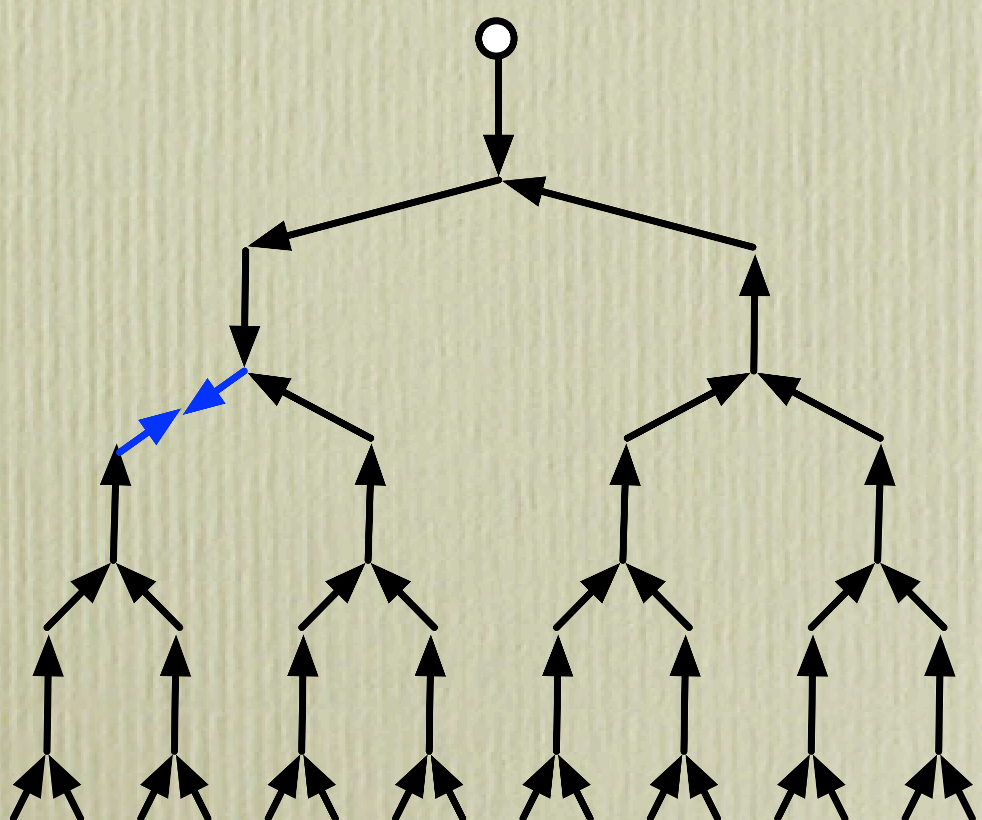

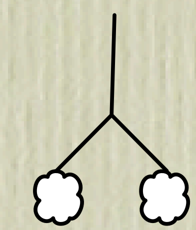

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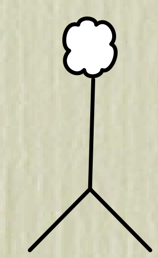

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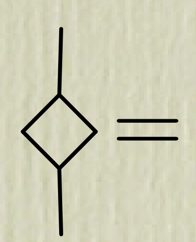

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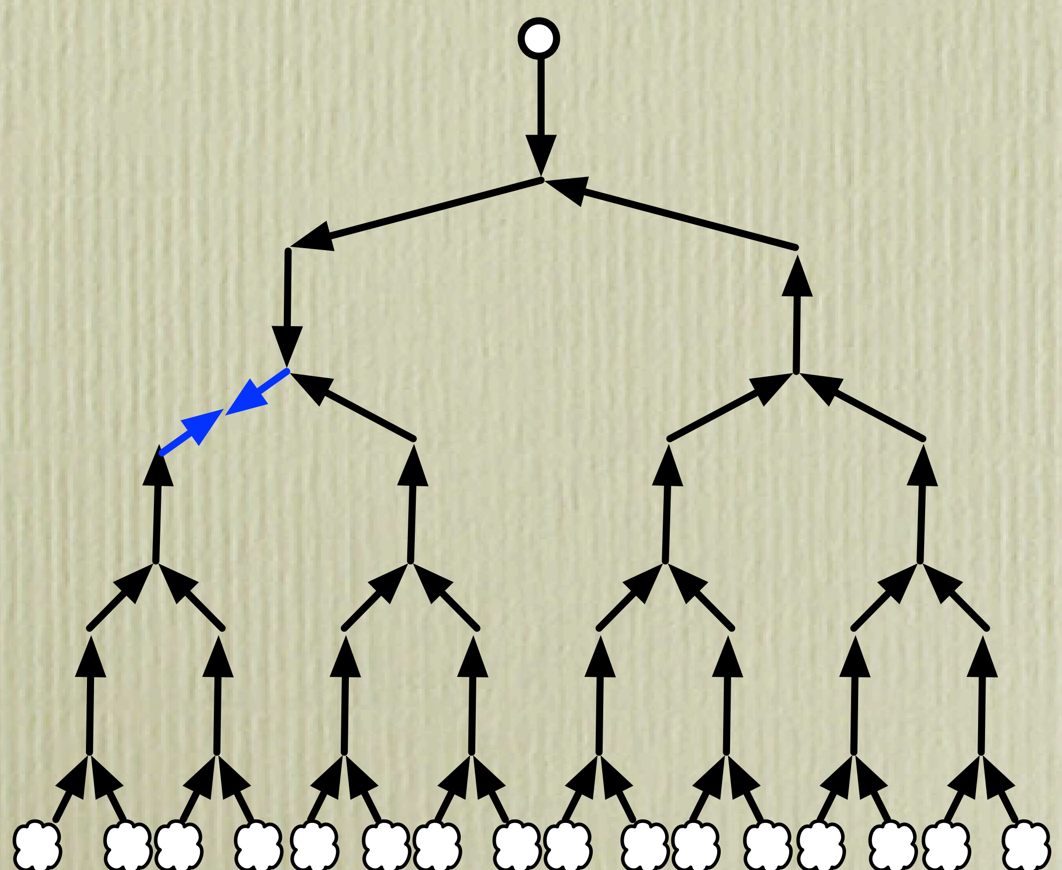

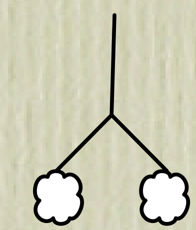

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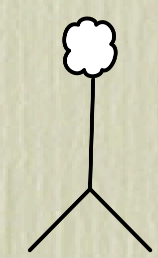
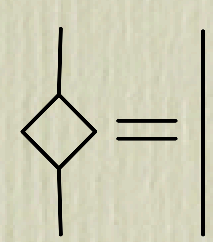


$$\overline{\lambda}(l) \cdot \phi(l)$$



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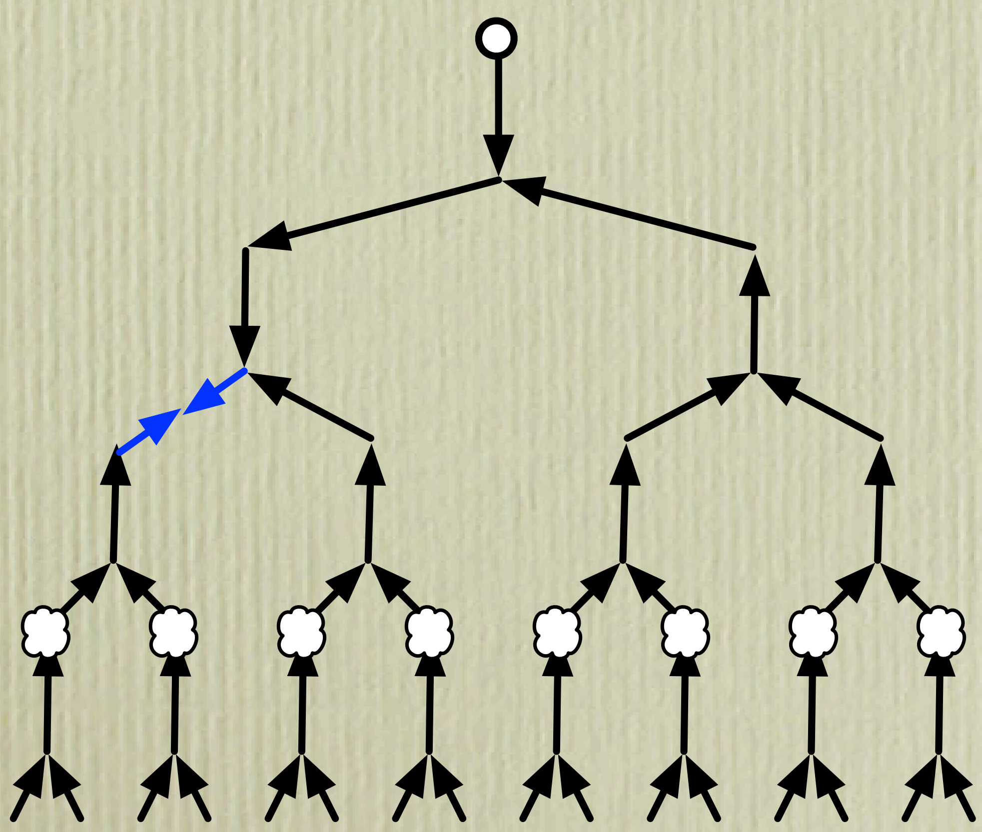
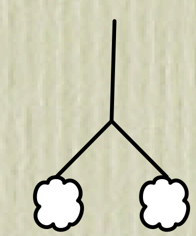
3-legs structure ease the symmetry preservation

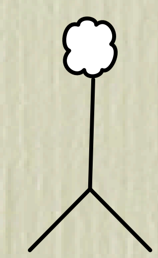
(work in progress in our code)

isometric gauge condition redirectionable at will
(also useful for CPT map interpretation)





$$[\phi(l+1) \otimes \phi(l+1)] \cdot \lambda(l)$$



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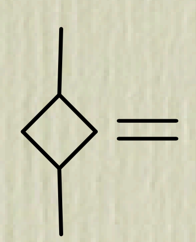

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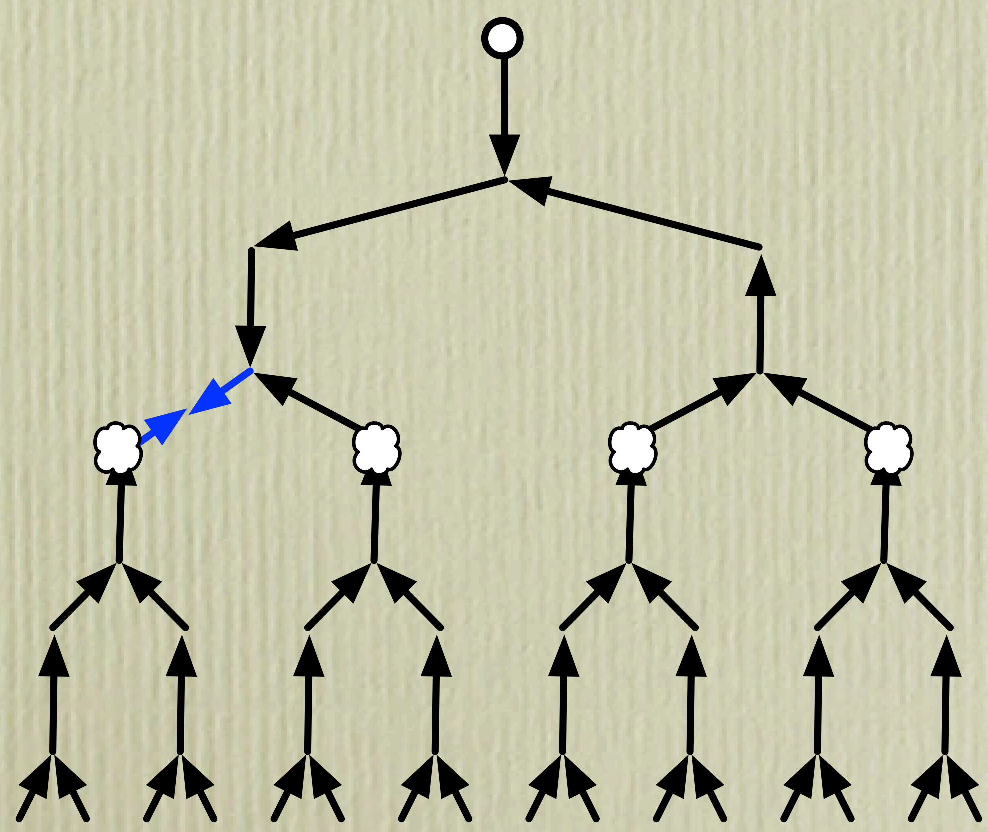

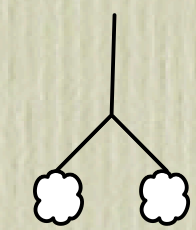

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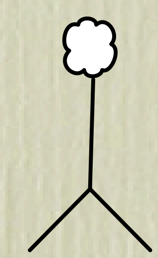

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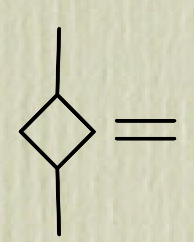

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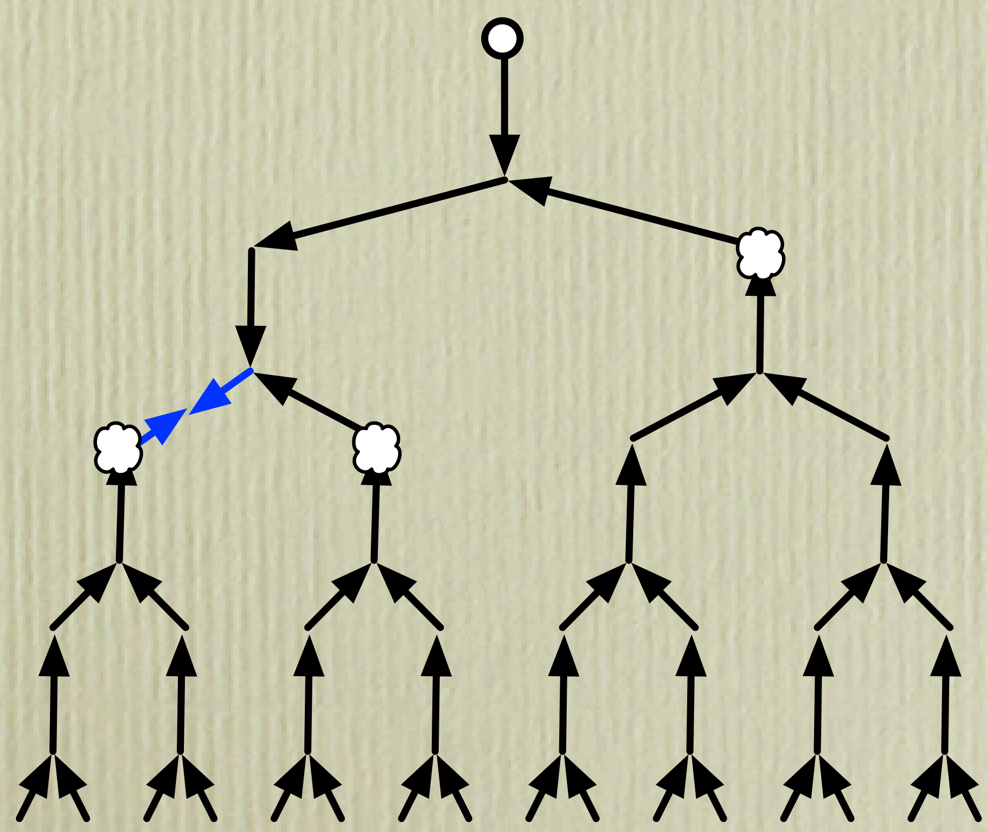

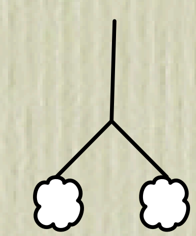

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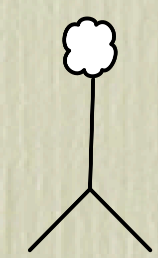

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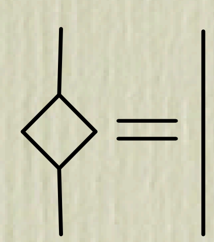

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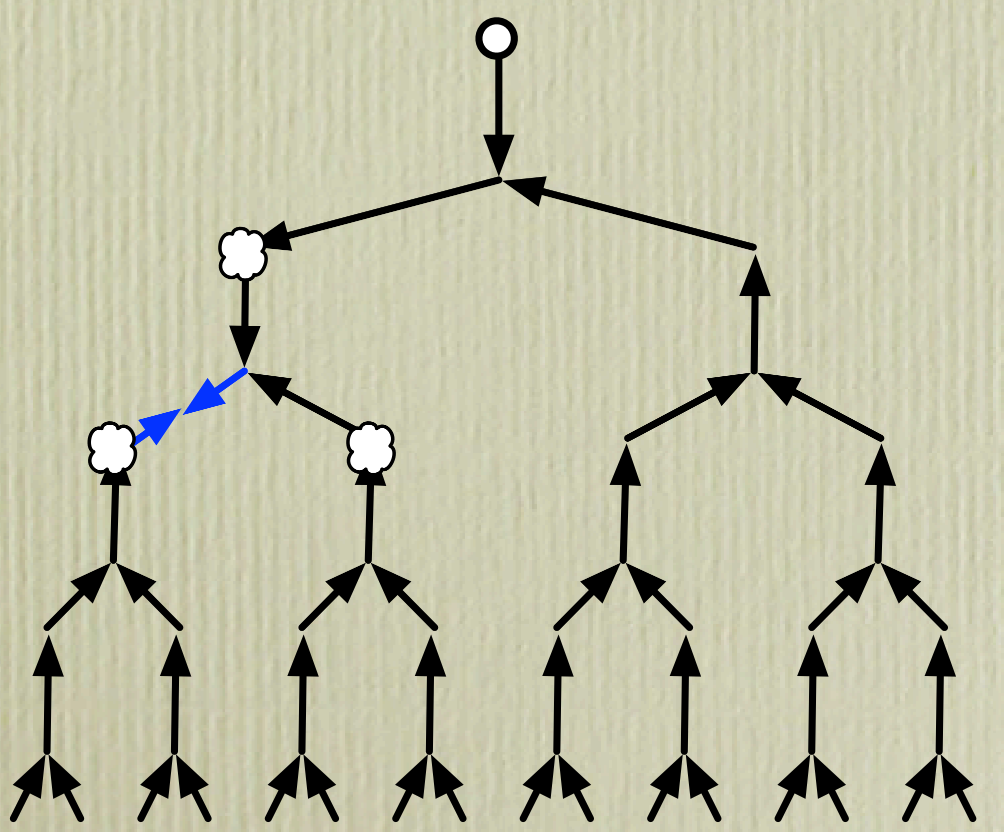

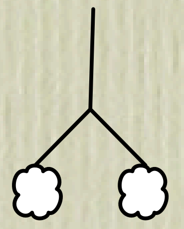

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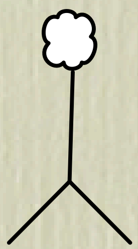

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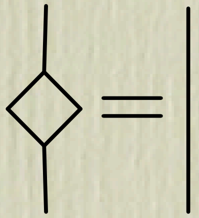

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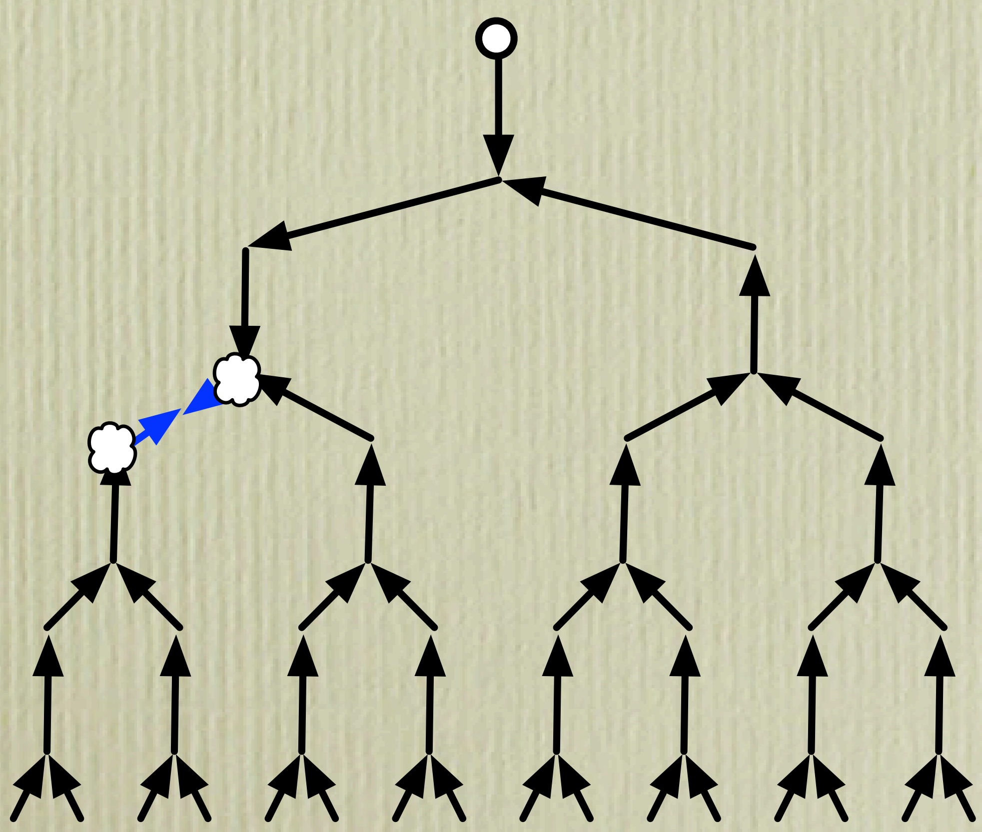

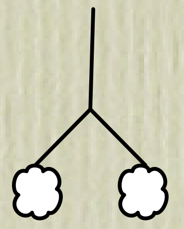

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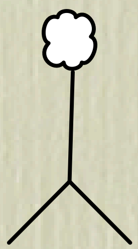

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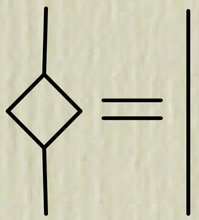
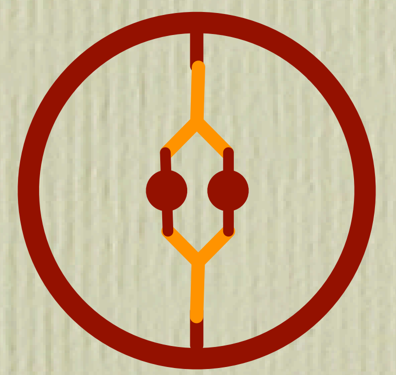


$\overline{\lambda}(l)^{\dagger} \cdot \overline{\lambda}(l) = \mathbb{I}$

Outlook: local optimization

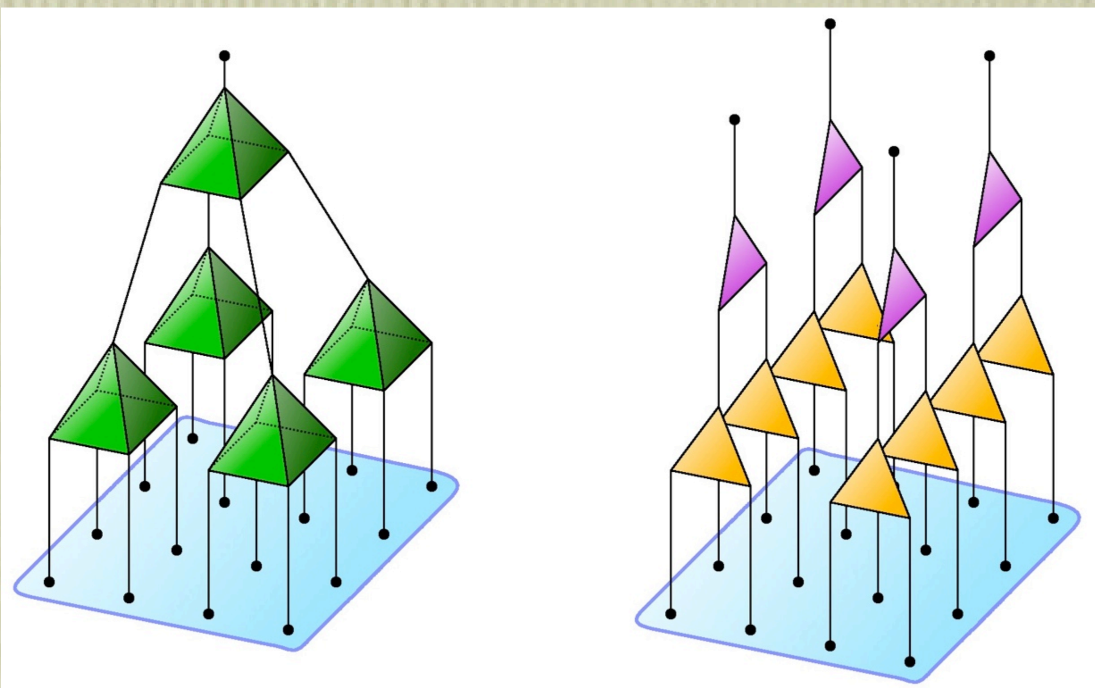
Loop-free and non-unitary nature of tensors
permits to deal with non-translational invariant networks
via generalized eigen-problems à la MPS



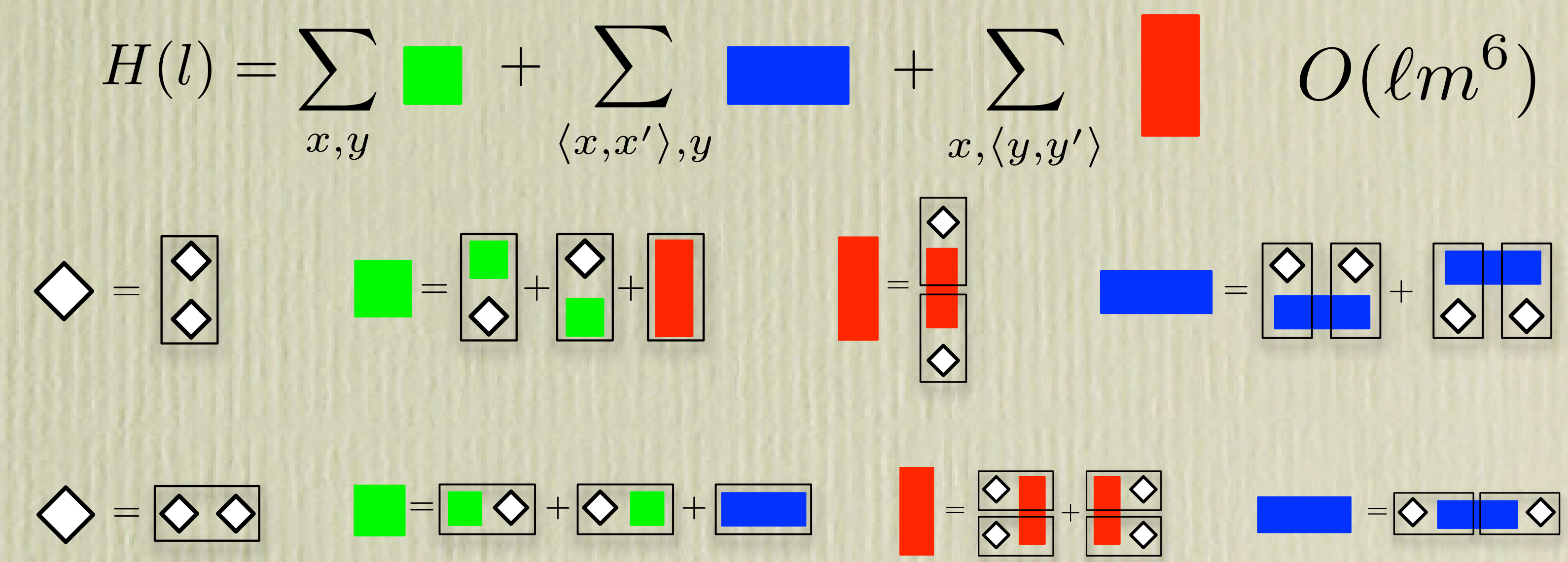
Same contraction as for gradients
(i.e. $O(m^4)$ operations)

Might these additional freedom help
towards better results?
(in progress)

Outlook: use in 2D ?



site-by-site H is not invariant $O(Lm^4)$ but...



might the use of 2D-TTNs be revived ?

- low contraction costs
- uncostrained optimization
- ‘simplicity’ of programming

make them appealing even if probably not optimal

Thanks

- Simone Montangero (Ulm)
- Pietro Silvi (Ulm)
- Vittorio Giovannetti (SNS-Pisa)
- Rosario Fazio (SNS-Pisa)
- Ignacio Cirac (MPQ)

Outlook

- Hierarchical Tensor Networks
- Finite Unconstrained Trees
    - standard optimization / small cost
- Preliminary results (1D)
    - size-indep. precision at fixed bond
    - ~same precision on Energy/Observables
- future(?) directions:
    - need for symmetries !
    - revive the use in 2D?