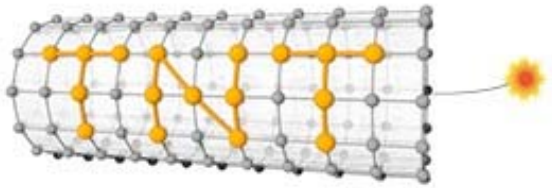

Tensor Network Theory

An introduction to DMRG and MPS methods

Quantum and Kinetic Problems: Modeling, Analysis, Numerics and Applications
IMS Singapore

Dieter Jaksch

University of Oxford

Special thanks to: Stephen Clark, University of Bristol

UNIVERSITY OF OXFORD

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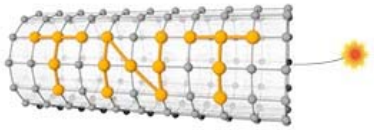


Outline of lectures

- Lecture 1

Introduction to strong correlations, many-body problem, recap on essential linear algebra we will need later.

- Lecture 2

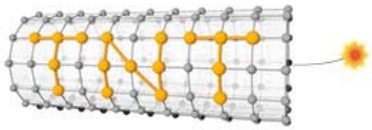
Tensors and contractions, product states and variational principle, matrix product states (MPS), and their entanglement properties.

- Lecture 3

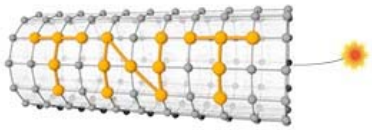
The “calculus” of MPS, algorithms for their variational optimisation, and algorithms for time-evolution of MPS.

- Lecture 4

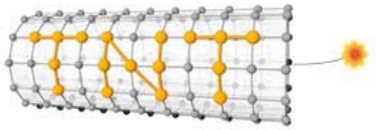
Moving to finite temperatures, renormalisation approaches to tensor networks, extension to 2D with projected entangled pairs.



Lecture 4



1: Finite temperature

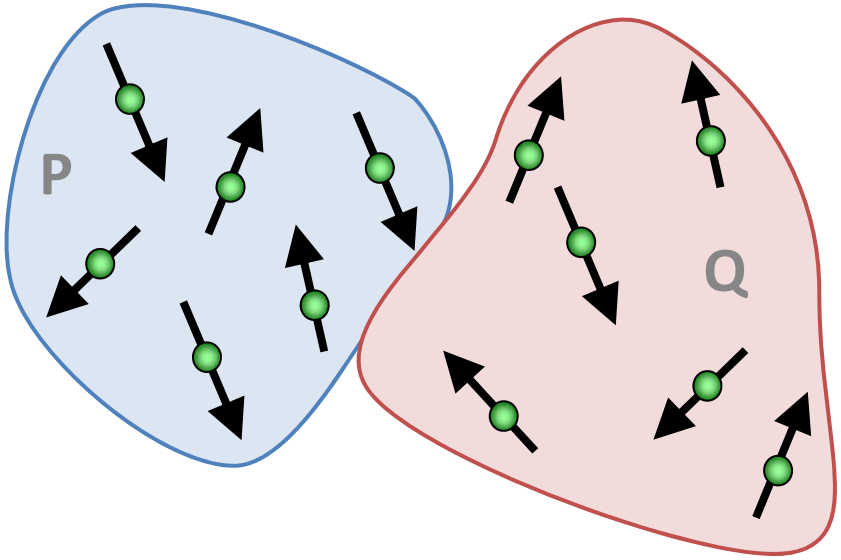


Purification of mixed states

So far we have dealt exclusively with ground states (i.e. $T = 0$). So how do we handle finite temperatures? We can use the formalism already developed by exploiting *purification*:

Suppose we have a density operator ρ describing a system **P**. By diagonalizing, this can always be written as:

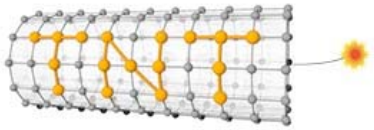
$$\rho = \sum_{a=1}^{r} p_a |a\rangle_P \langle a|_P$$



i.e. as a mixture of orthogonal states in **P**. However, by adding an identically sized ancillary system **Q** we can interpret ρ as a pure state:

$$|\psi\rangle = \sum_{a=1}^{r} \sqrt{p_a} |a\rangle_P |a\rangle_Q$$

This is just a Schmidt decomposition. Partially tracing out **Q** gives the mixed state ρ for system **P**.



Infinite temperature

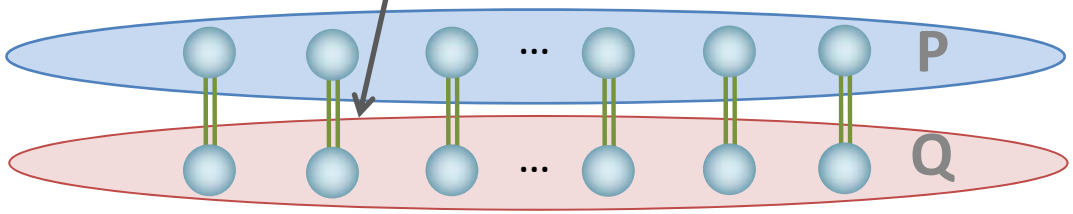
We can use this neat approach to immediately write down a purified state for infinite temperature. Recall that:

$$\rho_\beta = \frac{1}{Z(\beta)} e^{-\beta \hat{H}} \text{ with: } Z(\beta) = \mathrm{tr}(e^{-\beta \hat{H}}) \text{ and } \beta = \frac{1}{k_B T}$$

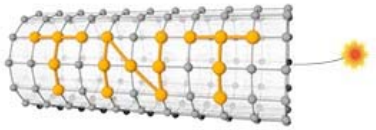
So when $\beta = 0$ we have: $\rho_0 = \frac{1}{d^L}\mathbb{1} = \left(\frac{\mathbb{1}}{d}\right)^{\otimes L}$

i.e. an equal mixture of all eigenstates. Purification of the identity operator on each site is just a maximally entangled state with one ancilla site!

$$|\psi_0\rangle = \sum_{\sigma=1}^{d} \frac{1}{\sqrt{d}} |\sigma\rangle_P |\sigma\rangle_Q \xrightarrow{L \text{ copies}} \rho_0$$



Each site in either system is otherwise unentangled.



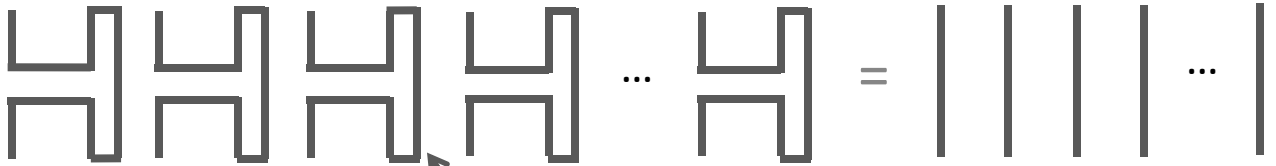
Finite temperature

Let's interleave system and ancilla sites along a chain. Graphically (ignoring factors of 1/*d*) the state has a very simple MPS form:

$|\psi_0\rangle$ =

The density operator then gives an MPO graphically as:

$\mathrm{tr}_Q(|\psi_0\rangle\langle\psi_0|)$ =

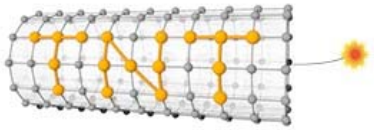


trace over **Q**

Its invariance to any local unitaries on **P** and **Q** is now obvious. Given we have infinite temperature how do we get a finite temperature? Here is a handy observation, since $\mathbb{1} = Z(0)\rho_0$ then:

$$\rho_\beta = Z(\beta)^{-1} e^{-\beta\hat{H}/2}\ \mathbb{1}\ e^{-\beta\hat{H}/2} = \frac{Z(0)}{Z(\beta)} e^{-\beta\hat{H}/2}\ \rho_0\ e^{-\beta\hat{H}/2}$$

since we have a purification for ρ_0 we then immediately get …



Finite temperature

This means that a finite temperature thermal state is given by:

$$\rho_\beta = \frac{Z(0)}{Z(\beta)} \mathrm{tr}_Q \left(e^{-\beta \hat{H}/2} |\psi_0\rangle\langle\psi_0| e^{-\beta \hat{H}/2} \right)$$

The purification of ρ_β is then simply the imaginary time-evolved infinite temperature purification:

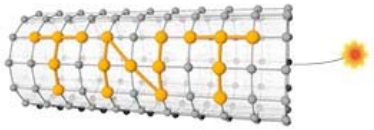
$$|\psi_\beta\rangle = e^{-\beta \hat{H}/2} |\psi_0\rangle$$

Note that $e^{-\beta \hat{H}/2}$ acts only on the system **P**, and not **Q**, so:

$$\mathrm{tr}_{PQ}(|\psi_\beta\rangle\langle\psi_\beta|) = \langle\psi_\beta|\psi_\beta\rangle = \frac{Z(\beta)}{Z(0)}$$

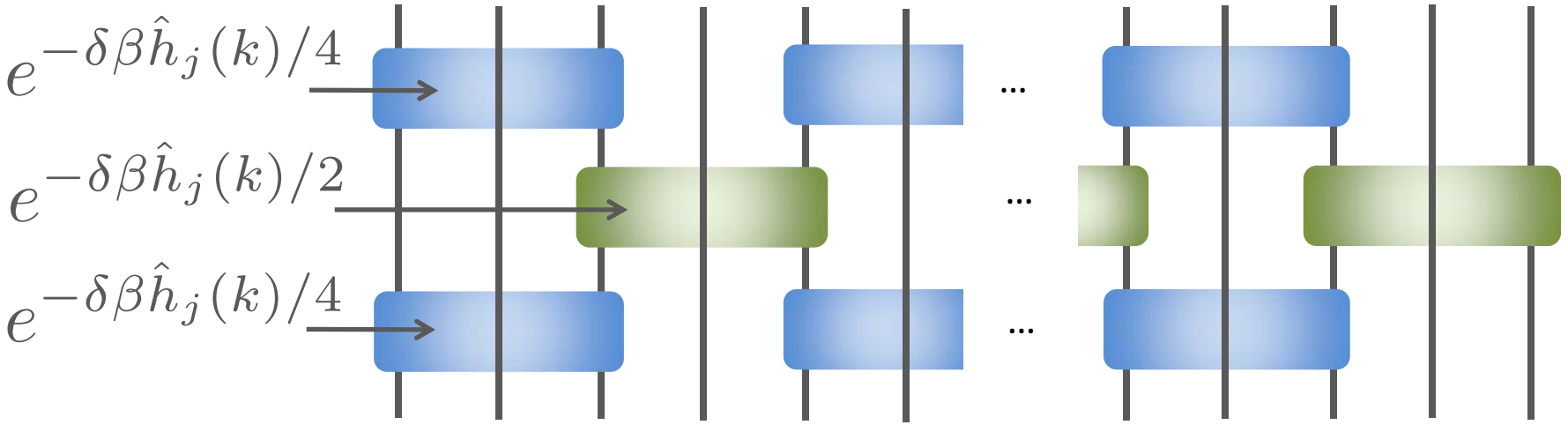
and the partition function is easy to obtain as the norm of the purified state (since $Z(0) = d^L$). Thermal expectation values are also easy:

$$\langle\hat{O}\rangle = \mathrm{tr}_P(\rho_\beta \hat{O}) = \frac{Z(0)}{Z(\beta)} \mathrm{tr}_{PQ}(|\psi_\beta\rangle\langle\psi_\beta|\hat{O}) = \frac{\langle\psi_\beta|\hat{O}|\psi_\beta\rangle}{\langle\psi_\beta|\psi_\beta\rangle}$$



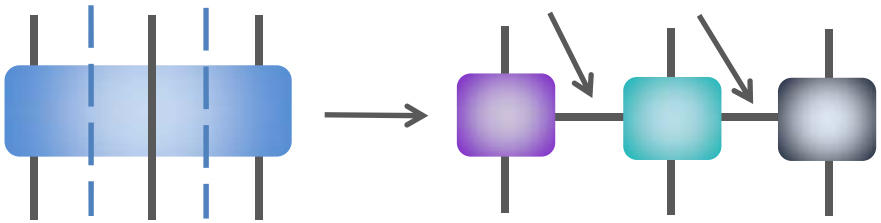
Finite temperature

We can implement imaginary time-evolution $e^{-\beta \hat{H}/2}$ as a "Trotter" MPO just like with real time-evolution earlier. The tricky part is that now the evolution only acts on every other site (i.e. just the system):

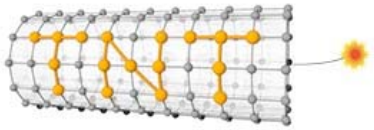


We now have to SVD twice this next-nearest neighbour "gate" to get a 3-site MPO:

dim = d^2 (at most)



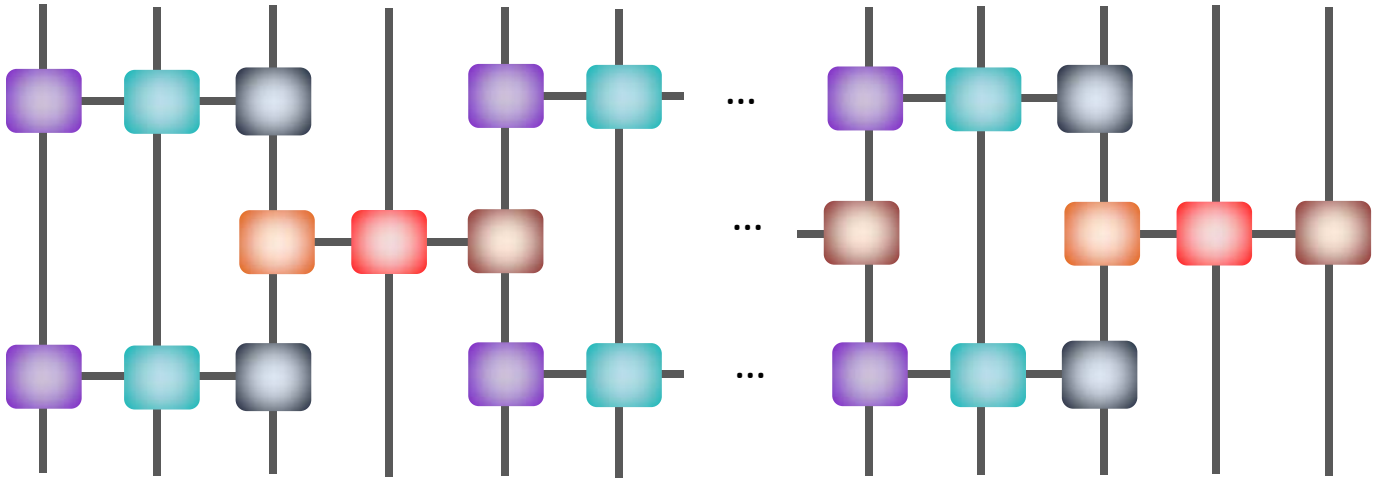
Despite the gate doing nothing to the ancilla it will have non-trivial elements in the MPO.



Finite temperature

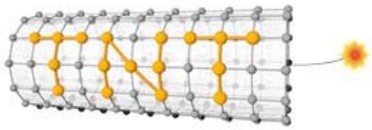
We can then construct an MPO for a complete imaginary time-evolution segment $\delta\beta$:

$$e^{-\delta\beta\hat{H}} \approx$$

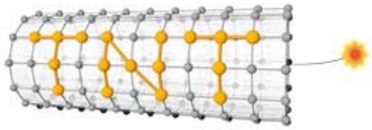


This MPO is applied repeatedly to $|\psi_0\rangle$ until the required final value of β is reached.

Once the pure state $|\psi_\beta\rangle$ is obtained real time-evolution can then be applied in an identical way giving access to dynamics at finite temperatures. Similar MPS methods also allow open quantum systems (e.g. noise) to be simulated.



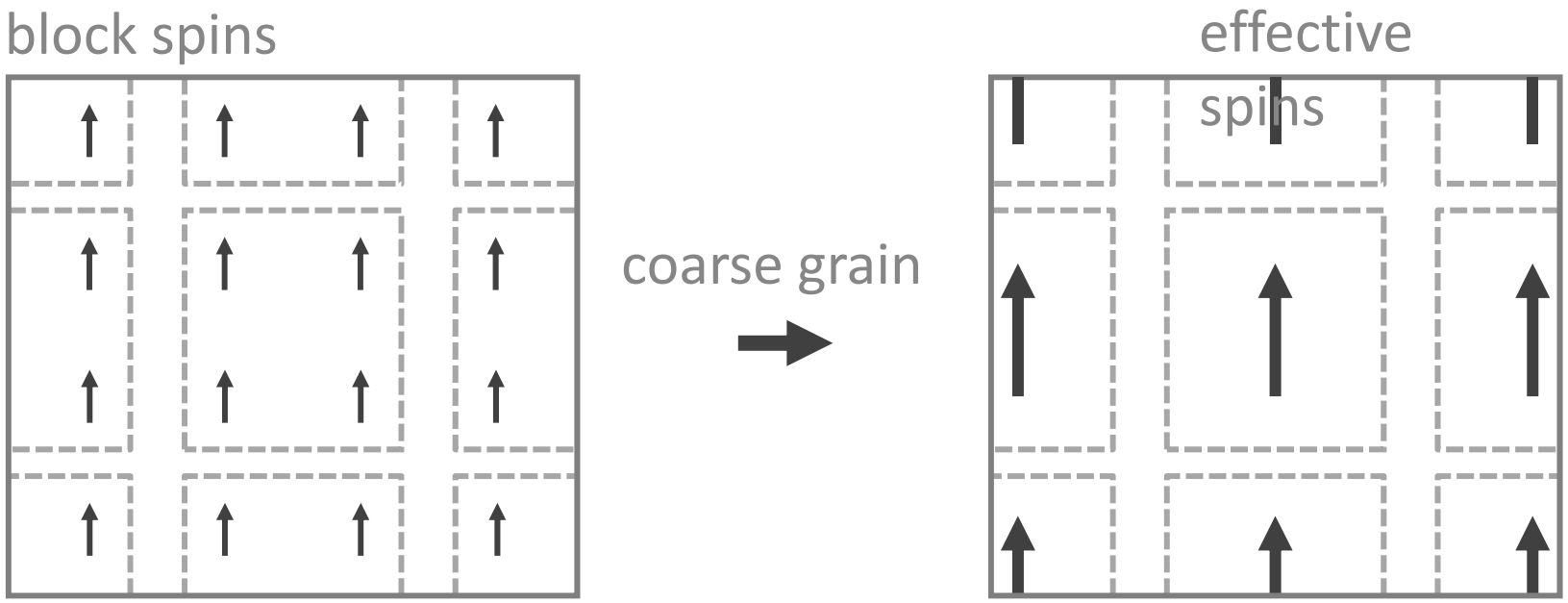
2: Renormalisation approach



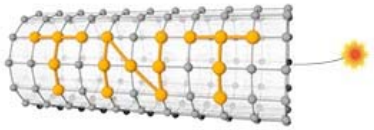
Renormalisation group

One of the first methods of handling the “curse of dimensionality” was to renormalise the system thinning the d.o.f. down successively:

Kadanoff’s spin blocking:



The leading intuition was that at criticality the system will display scale invariance and spin-blocking converges to a fixed point.



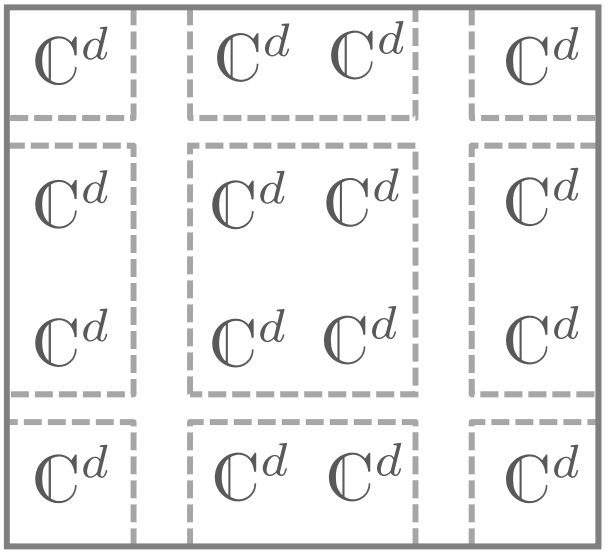
Renormalisation group

A physically sensible idea is to use the low-energy eigenstates of a block's Hamiltonian to define the coarse-graining projection:

Wilson's real-space RG:

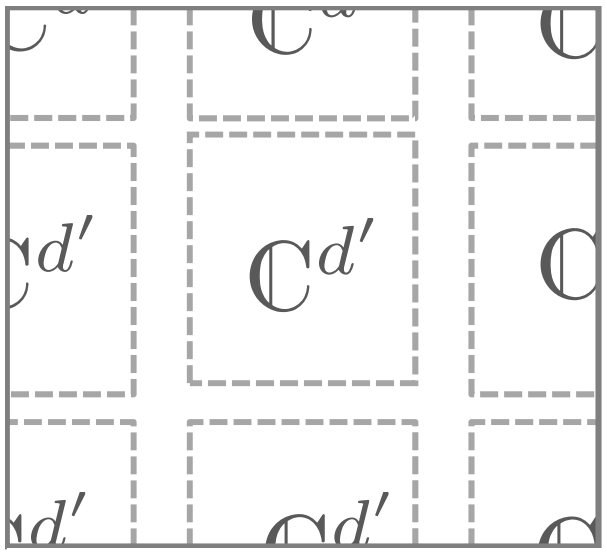
$\hat{H}_{\text{block}}$ → keep d' lowest eigenstates

block sites

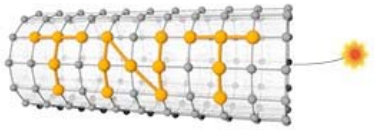


coarse grain →

effective sites



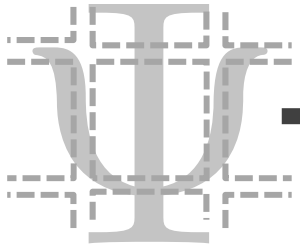
The leading intuition here is that we are searching for the ground state and so target the projection to the local low-energy sector.



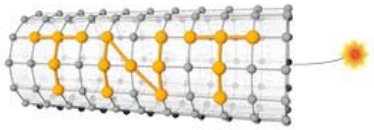
Renormalisation group

An improved scheme instead uses the eigenstates of the reduced density matrix of a block to define the coarse-graining projection:

White's density-matrix RG:

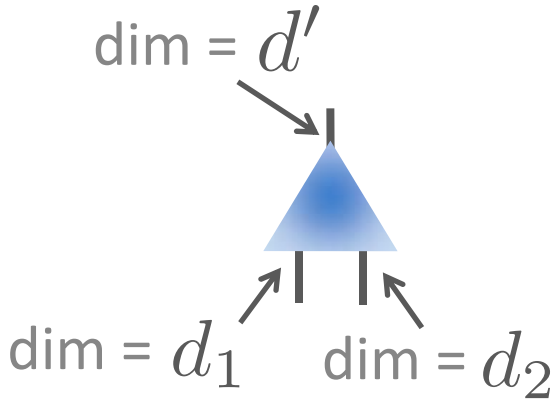


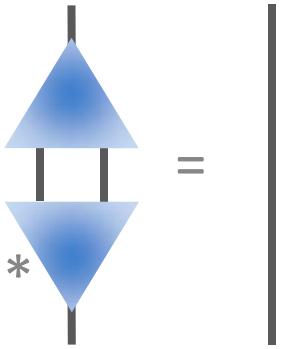
The leading intuition here is to target the local support of the global ground state (or approximation of) and so optimises state fidelity.



Renormalisation networks

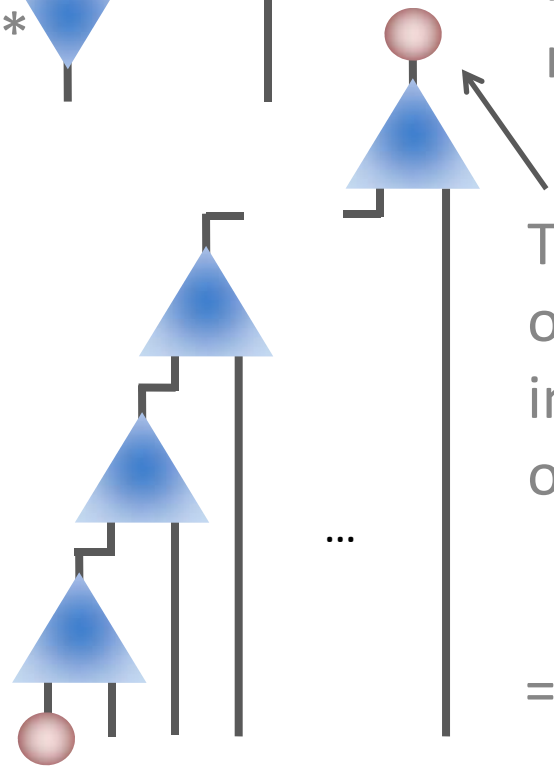
In 1D renormalisation of physical sites into an effective site is implemented by a rank-3 isometric tensor:



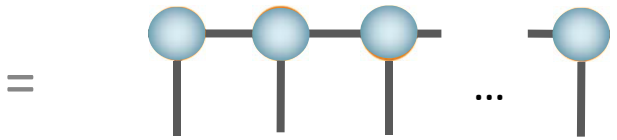


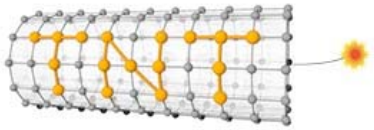
How projections are applied spatially makes a big difference to the resulting tensor network.

Suppose we renormalise an effective site with one physical site at each step. This gives MPS network since it is equivalent to sequential generation earlier.



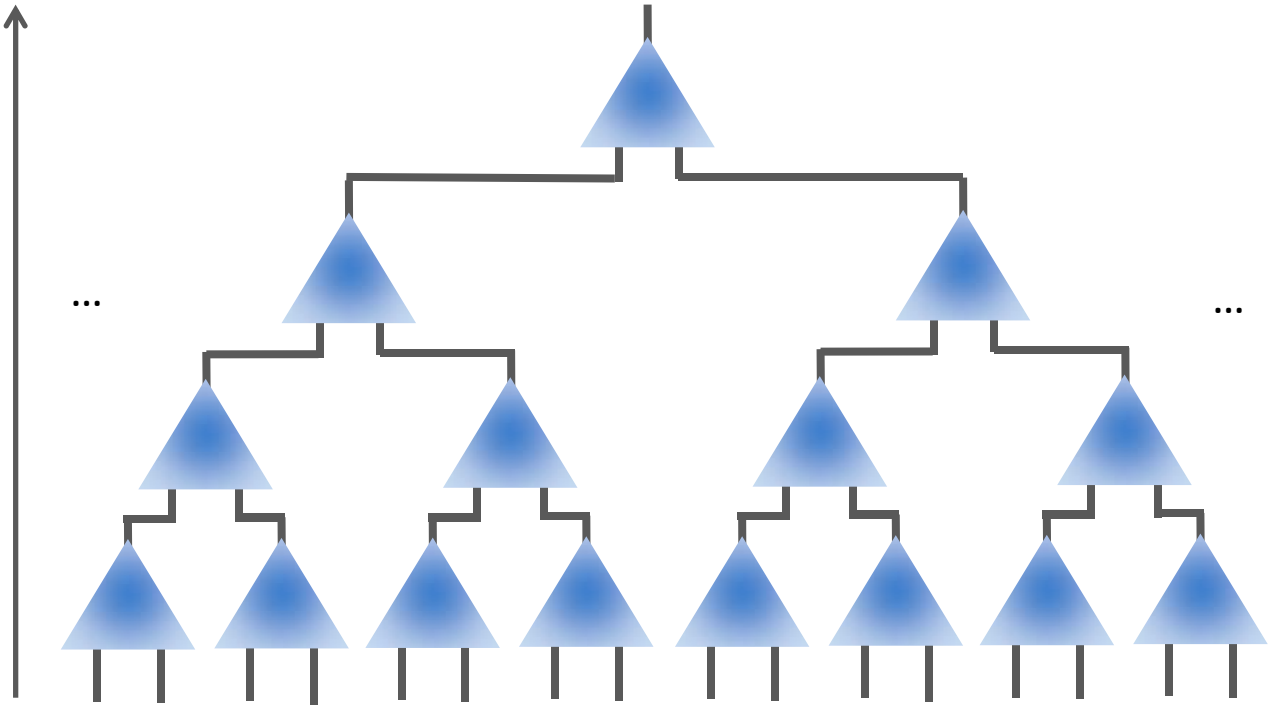
The boundary “vectors” of the MPS are the fixed input and output states of the effective sites.



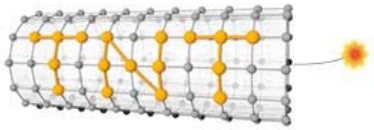


Renormalisation networks

Alternatively we could follow the Kandanoff blocking scheme and renormalise pairs of sites in parallel in each layer to get:

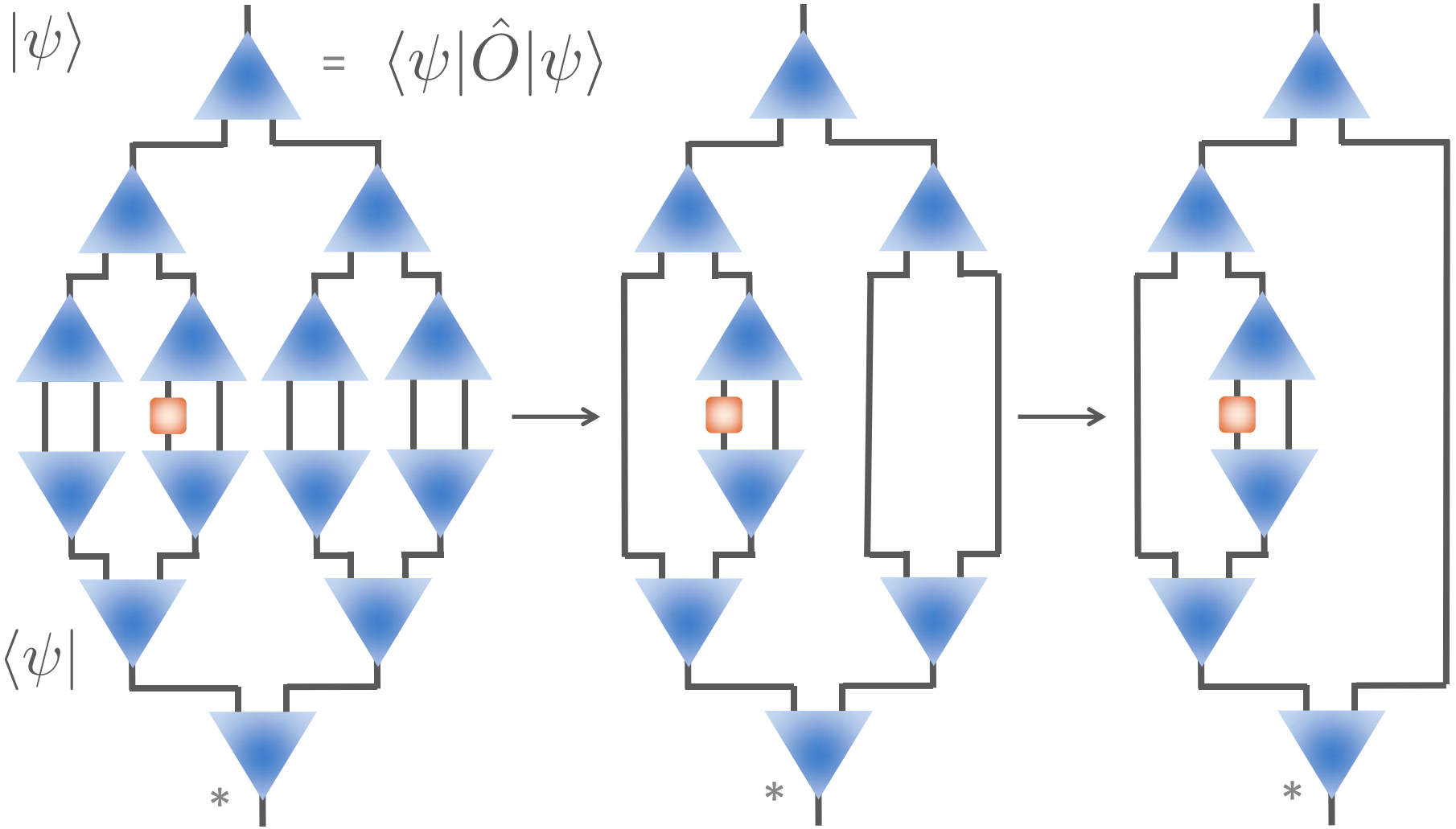


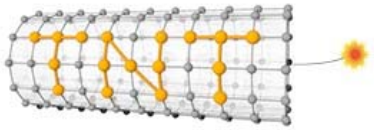
The result is a tensor tree network (TTN). This tree geometry alone ensures contraction can be done exactly and efficiently. However, it simplifies considerably for isometric tensors …



Tensor tree network

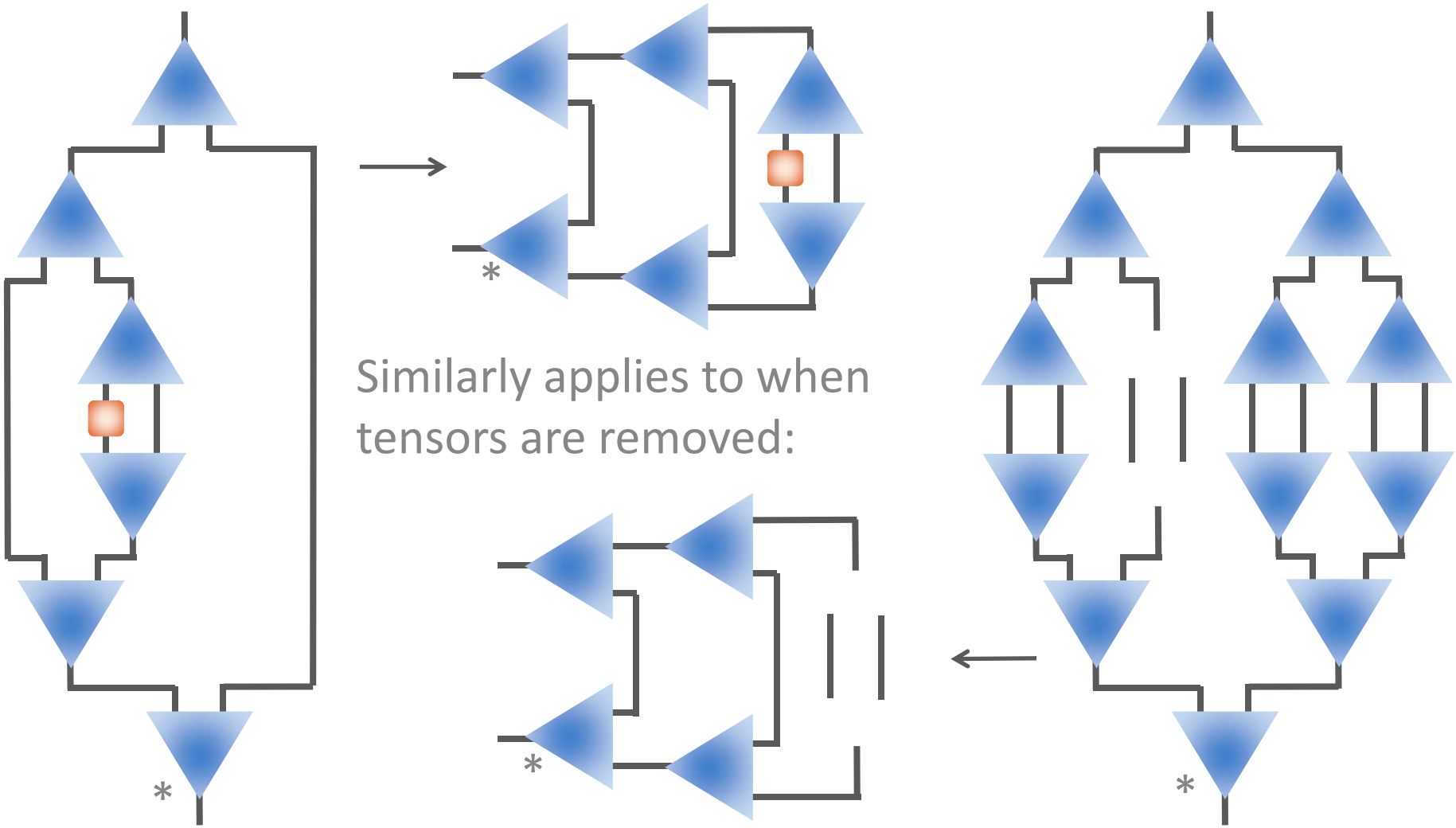
Consider the network contraction for a simple on-site expectation value after we repeatedly use the isometric property:



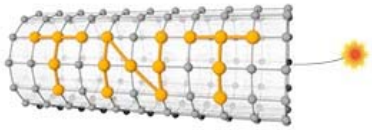


Tensor tree network

Finally we can rearrange the remaining network as a product of matrices, similar to an MPS contraction:



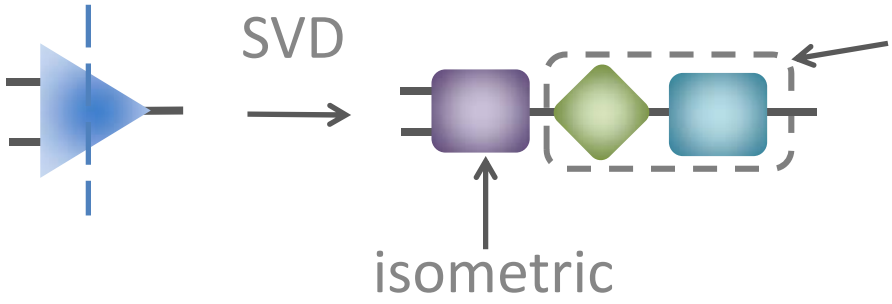
Similarly applies to when tensors are removed:



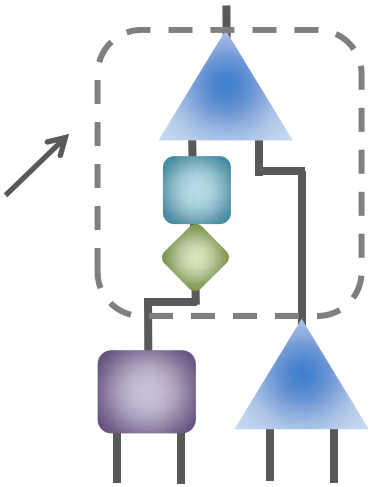
Tensor tree network

Can perform variational minimisation of the rank-3 tensors one by one as with MPS by building effective Hamiltonian and norm matrices and solving a generalised eigenvalue problem.

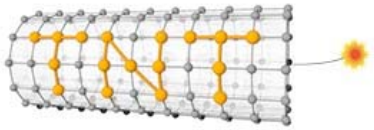
The isometric constraint on the tensors can be imposed after minimisation, if they are done layer by layer upwards, using the usual SVD and “pass on” approach:



pass remainder on to next layer up that has yet to be optimised:



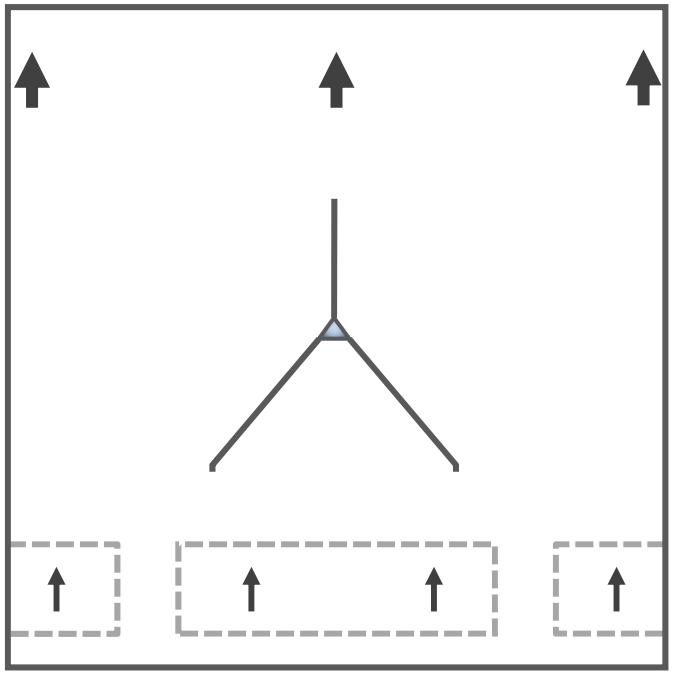
Tensor tree networks can mildly violate the boundary law. For some blocks the number of bonds connecting it to the rest scales as $\log(L)$ where L is the size of the block. This is useful for critical systems.



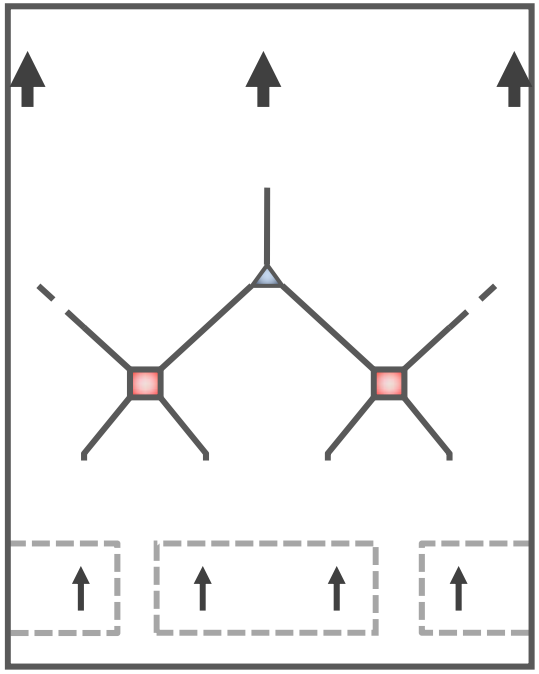
Entanglement renormalisation

An important improvement on real-space renormalisation is to account for entanglement between blocks:

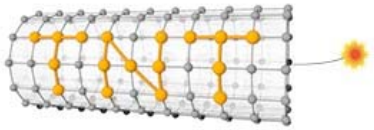
standard RG



entanglement RG

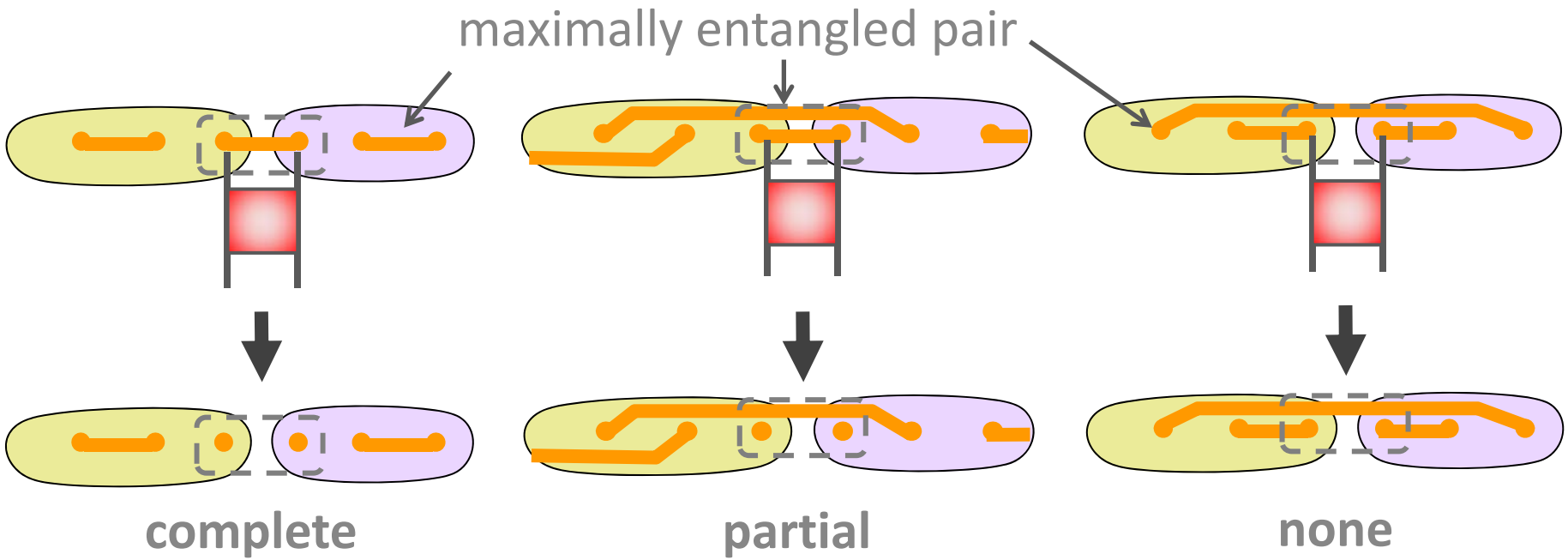


Introduce a unitary acting between the boundaries of neighbouring blocks which “disentangles” them before projection.

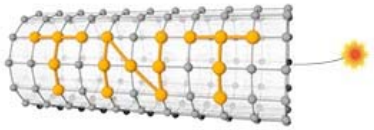


Entanglement renormalisation

We can illustrate why this might be useful by examining blocks where some sites are maximally entangled with those of other blocks:

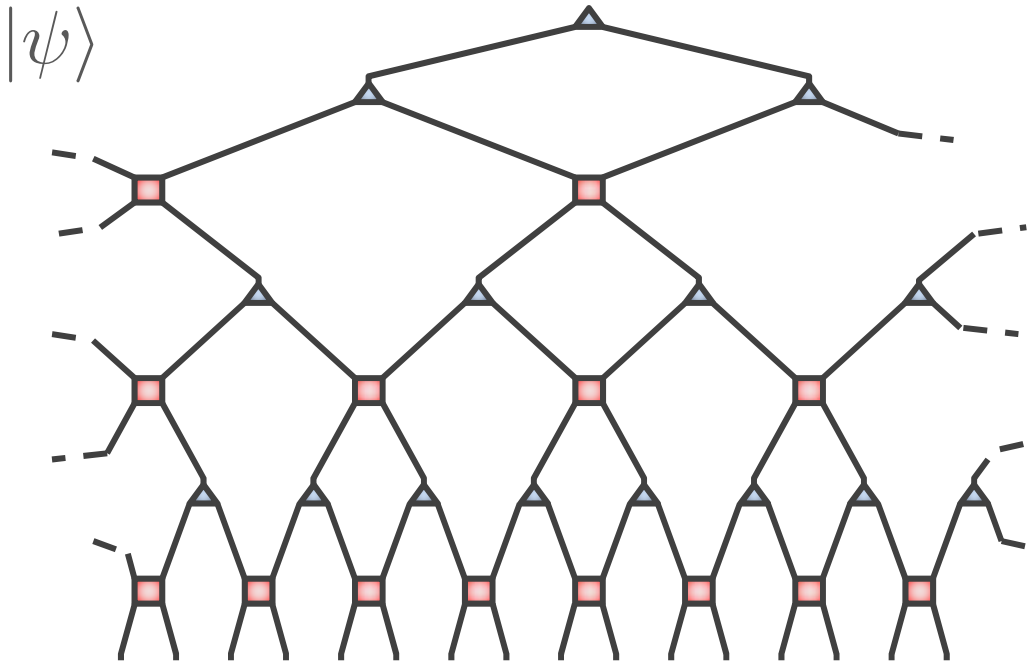


If entanglement is shared at the boundaries then then an appropriate unitary can completely disentangle the blocks (retaining/encoding this correlation) before projection. If entanglement is longer ranged then it will fail – such correlations will have to be addressed higher up.

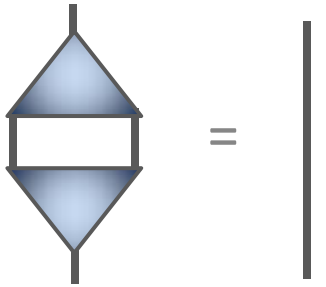


Entanglement renormalisation

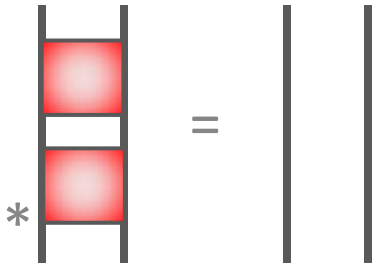
By attempting to “disentangle” as much as possible at each layer longer ranged entanglement at larger length scales will be captured. In 1D the resulting multi-scale network looks like:



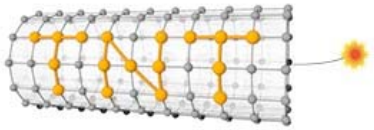
isometry for projector:



unitarity of disentangler:

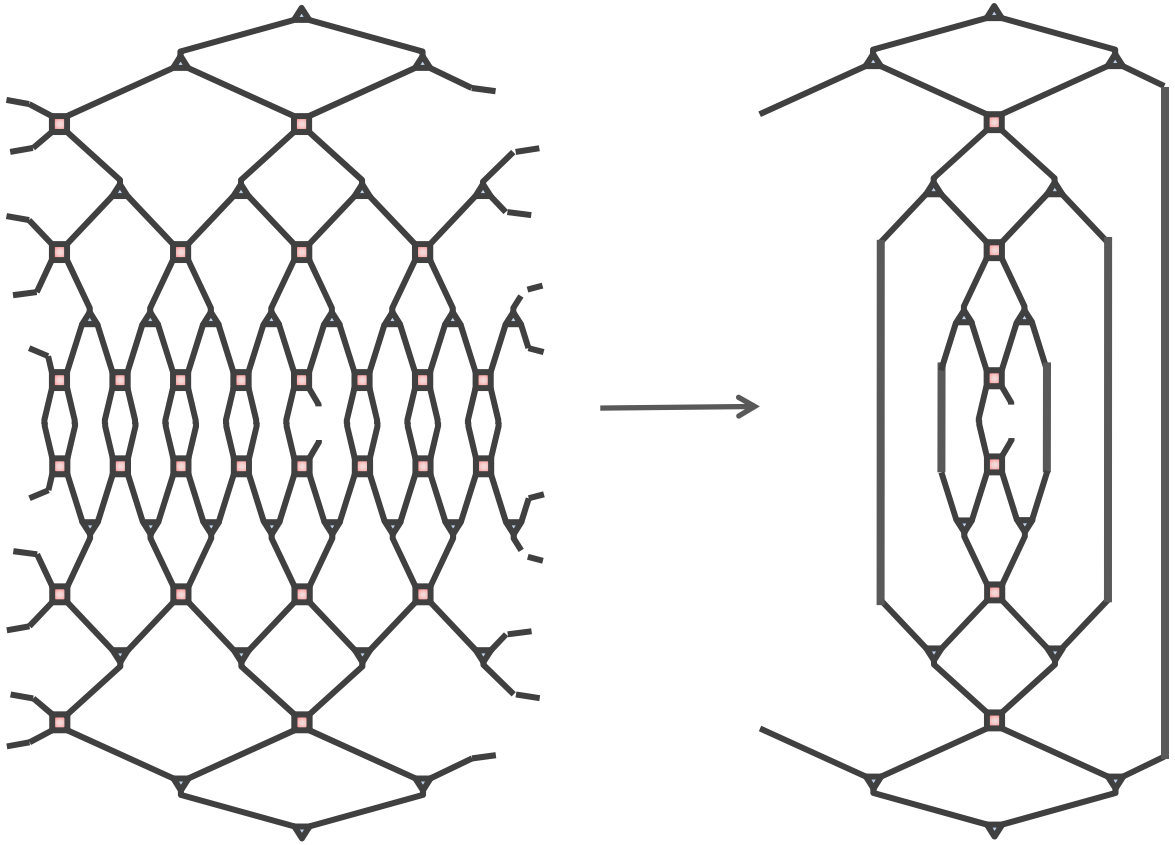


The resulting hierarchical tensor network is called the multi-scale entanglement renormalisation ansatz (MERA).



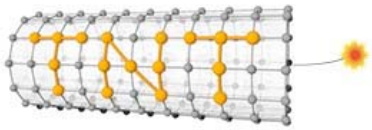
Entanglement renormalisation

The MERA ansatz also possesses exact efficient contractibility, like MPS and TTNs, due to the special properties of the tensors:

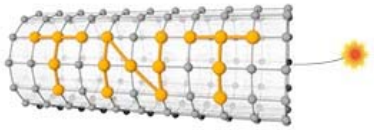


Massive cancellation. The causal cone around any site has bounded width due to the isometries.

Can similarly perform variational minimisation, but slightly more tricky now as isometric and unitarity properties **must** be preserved.



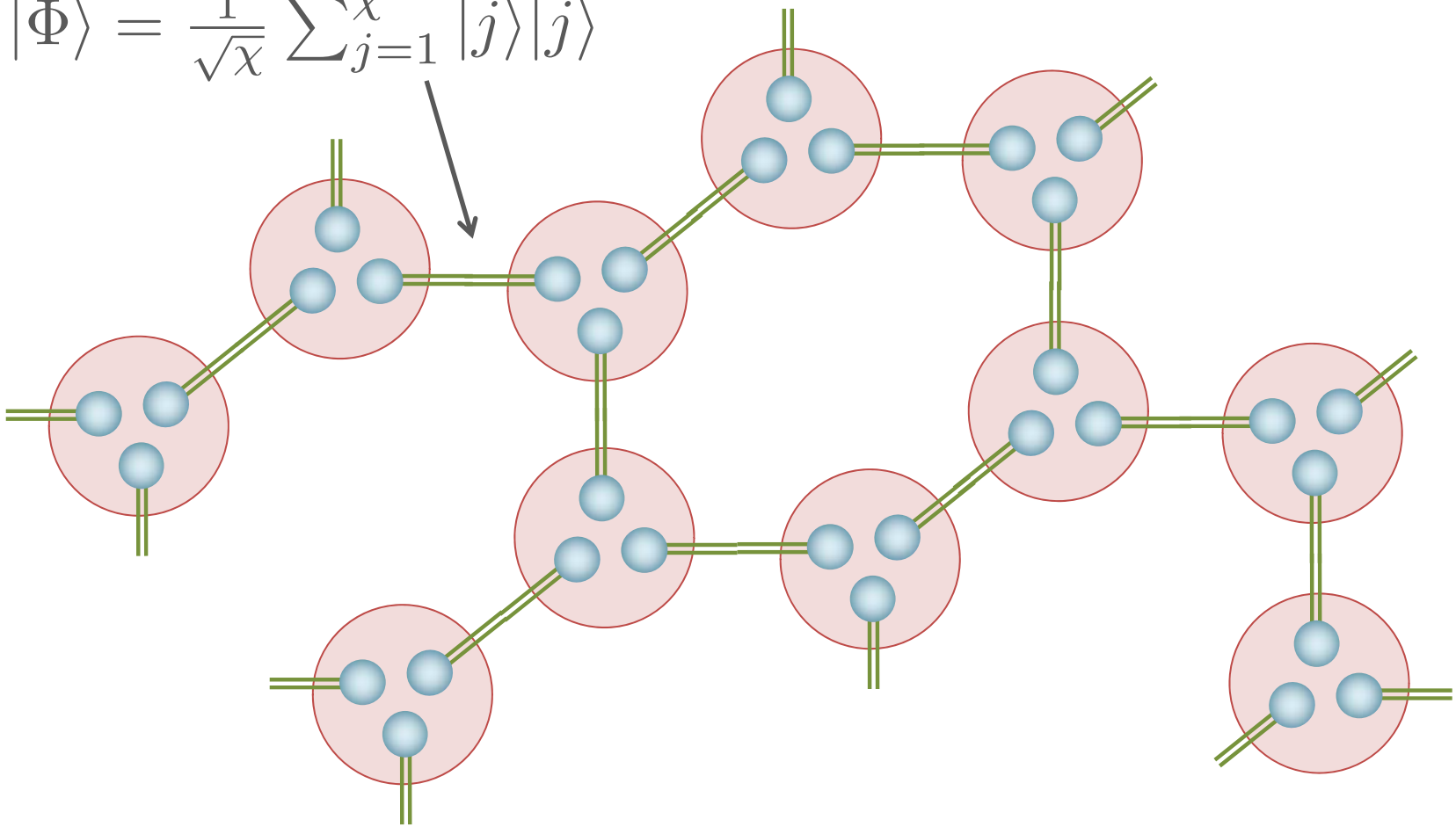
3: Extending TNT to 2D …

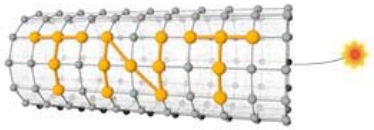


Building networks

Earlier we saw how MPS can be thought of as resulting from the projection of maximally entangled ancilla shared between neighbouring physical sites. This can be generalised to any graph:

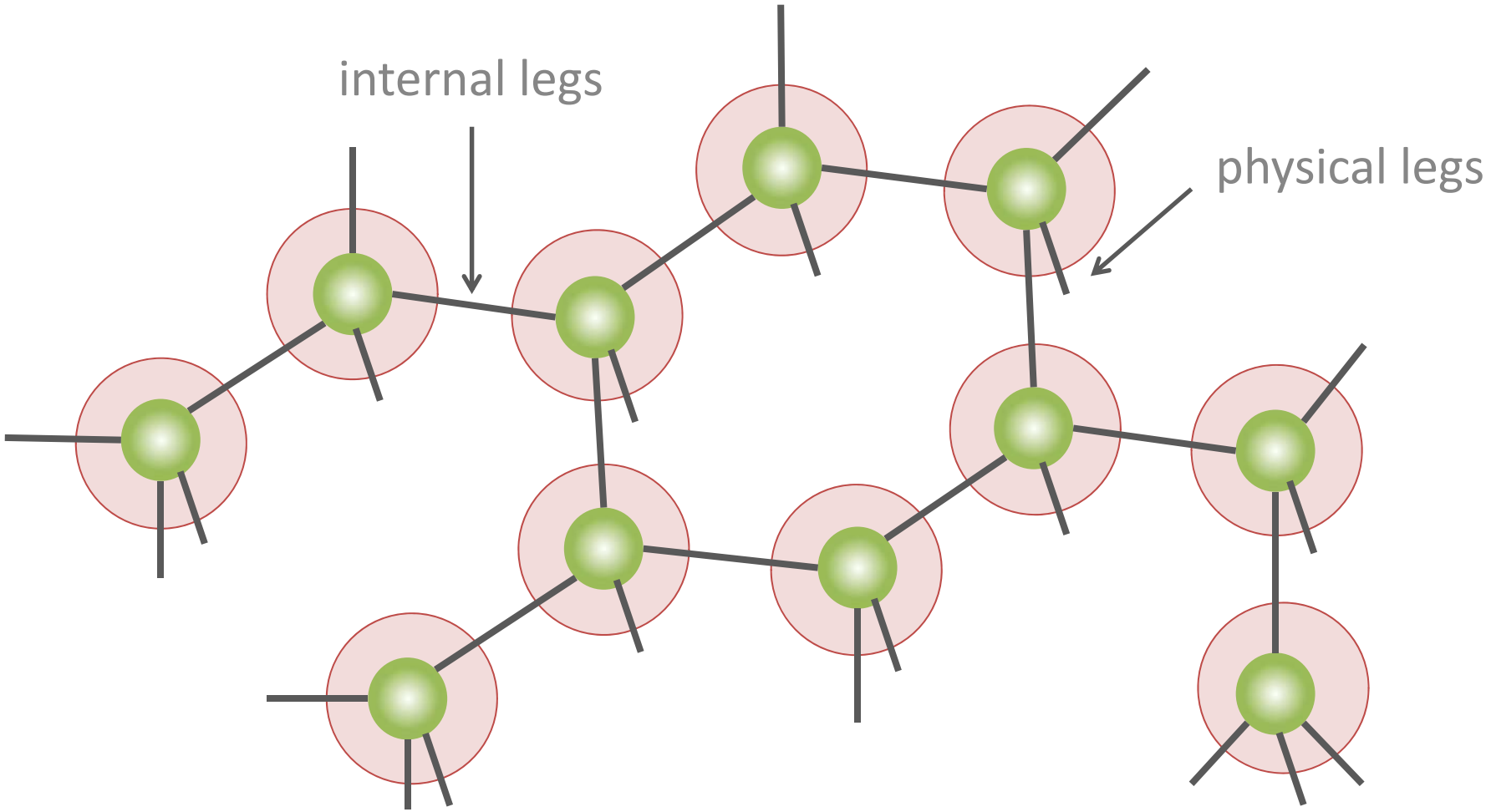
$$|\Phi\rangle = \frac{1}{\sqrt{\chi}} \sum_{j=1}^{\chi} |j\rangle|j\rangle$$

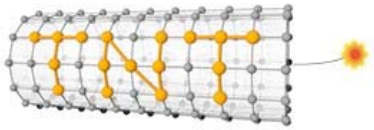




Building networks

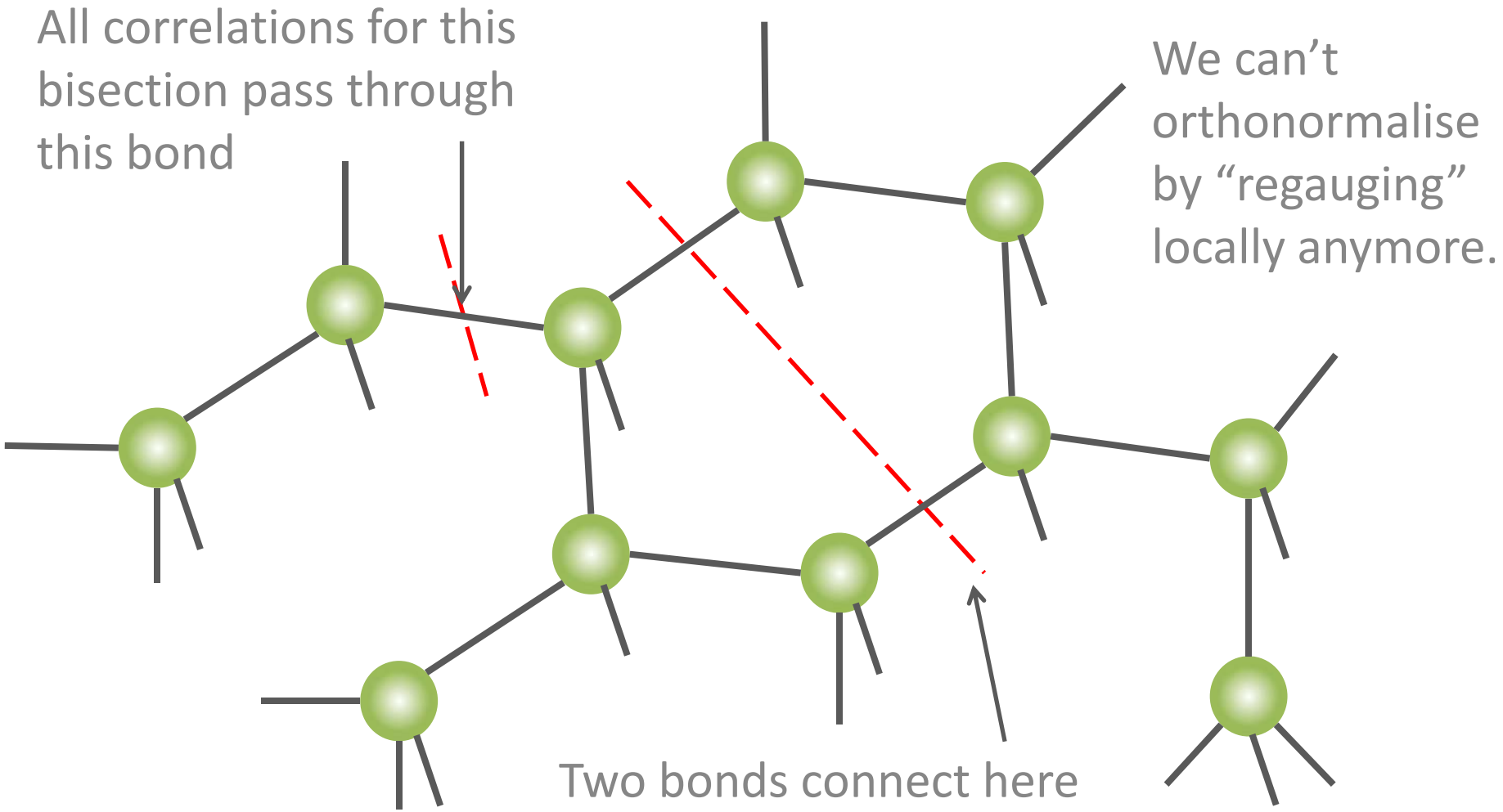
This then projects to a tensor network with tensors associated to each physical site following the geometry of the graph:

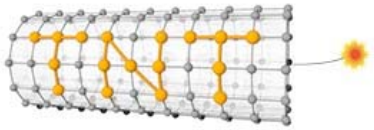




Building networks

Graphs with loops in them present difficulties. First, the association of Schmidt decompositions to internal legs only holds for trees.

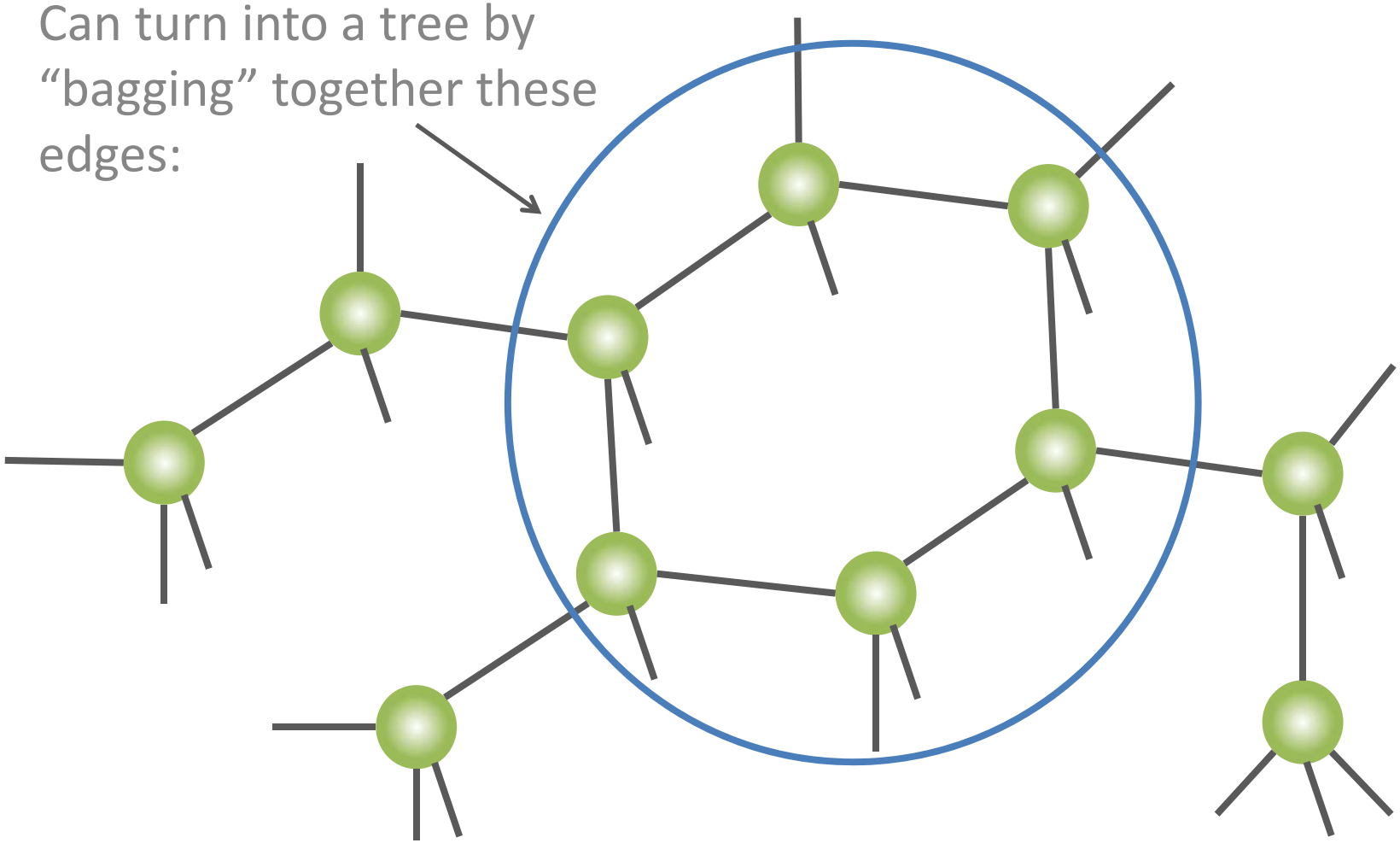


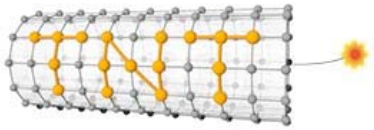


Building networks

Second, unless the graph has a bounded “tree-width”, it cannot be contracted efficiently like we had for MPS …

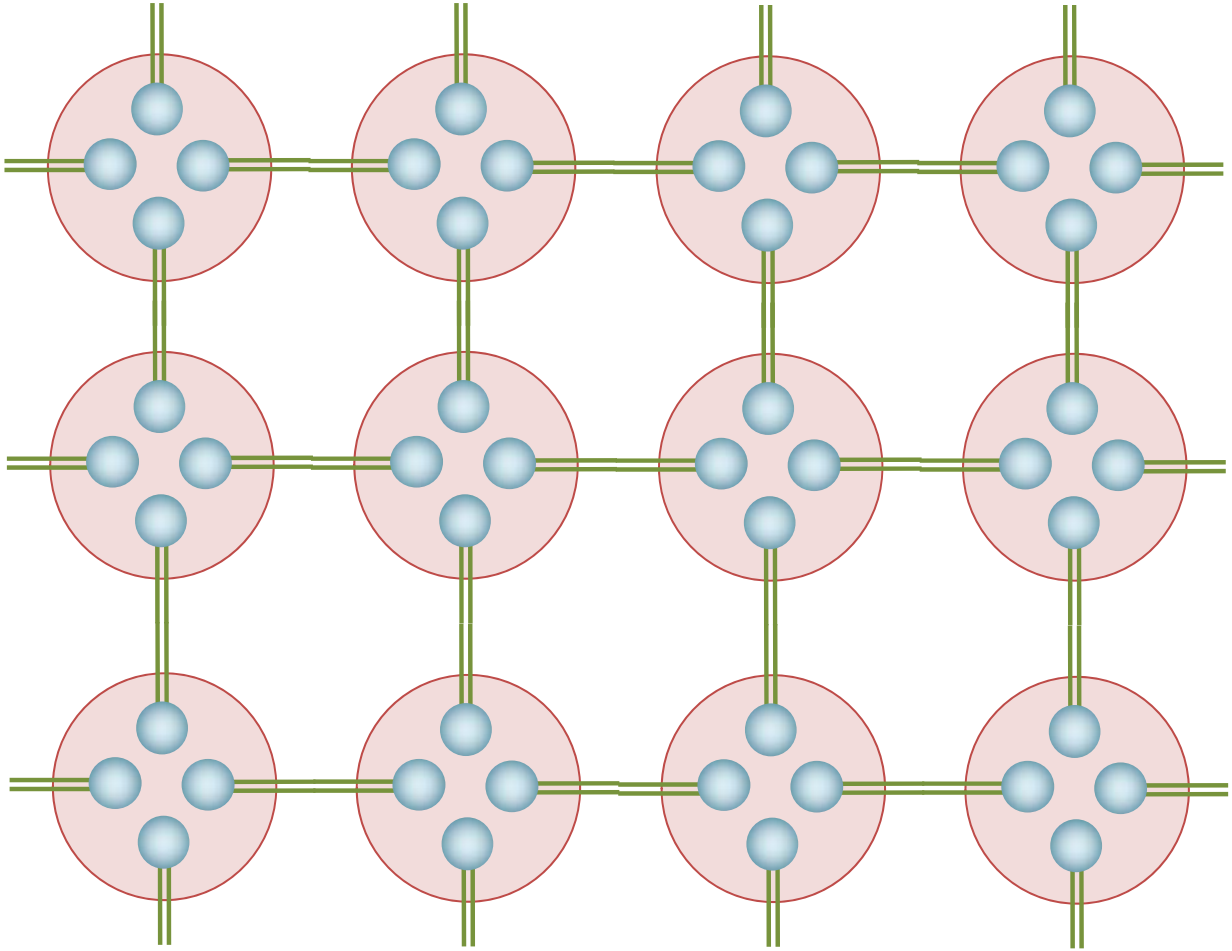
Can turn into a tree by “bagging” together these edges:

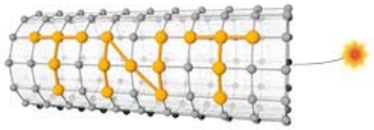




PEPS generalisation to 2D

Nonetheless this construction is worth considering for a 2D lattice (which has an infinite tree width) because it has desirable entanglement properties:

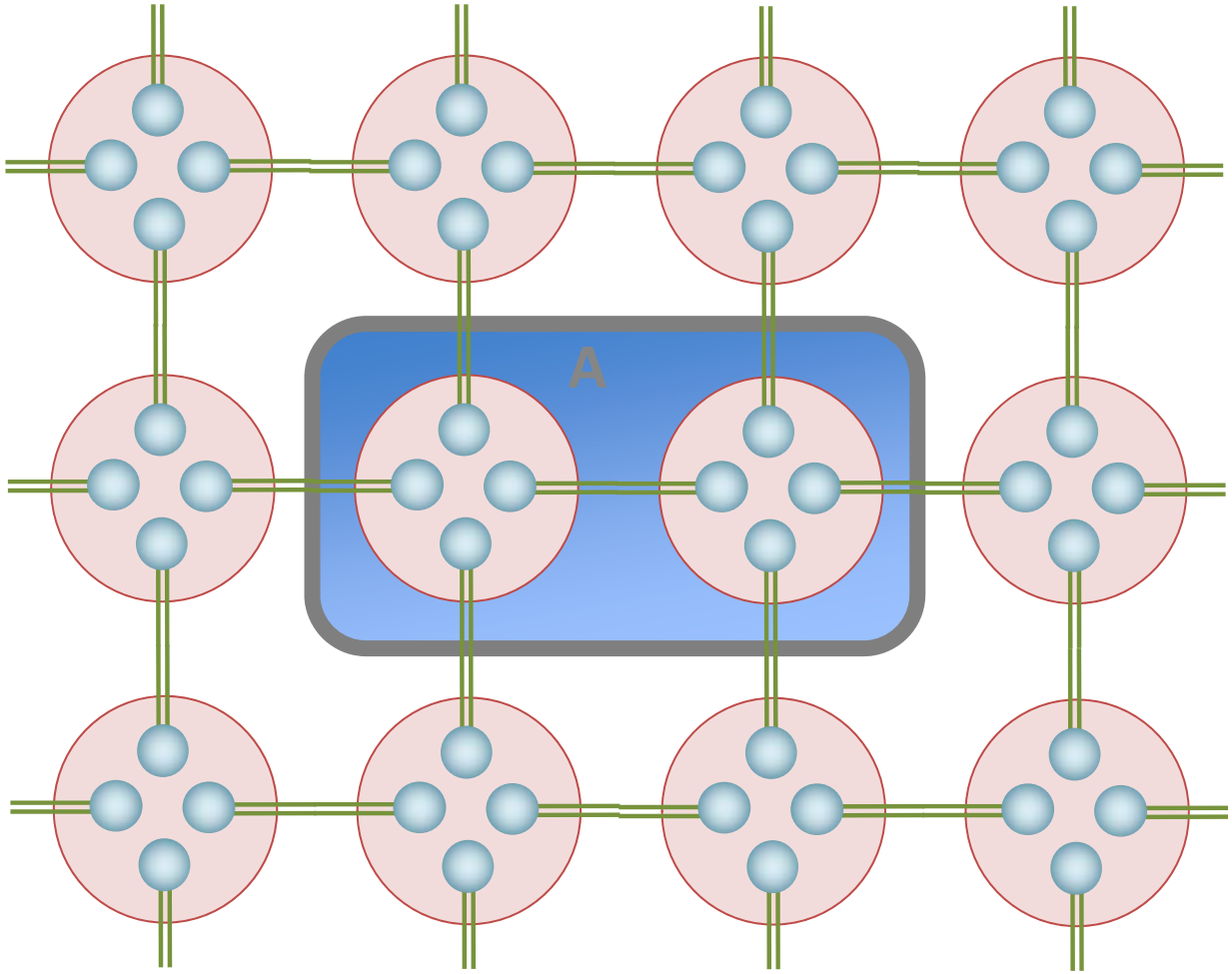




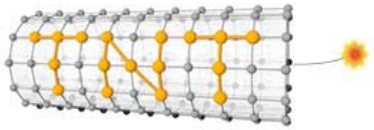
PEPS generalisation to 2D

For any contiguous region we cut through a number of entangled pairs which scales with the boundary so we automatically have:

$$S(\rho_A) \sim |\partial A|$$

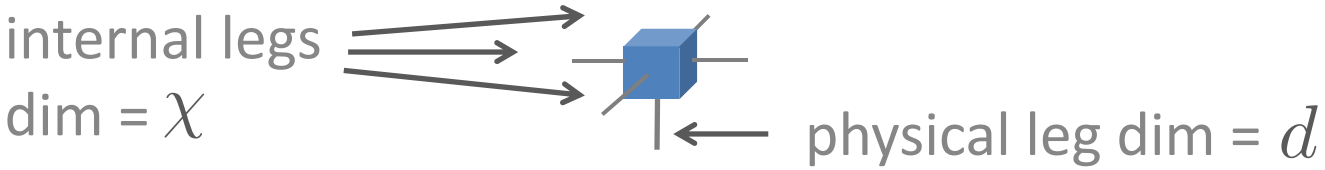


Like MPS does in 1D the PEPS construction immediately obeys the boundary-law of entanglement in 2D.

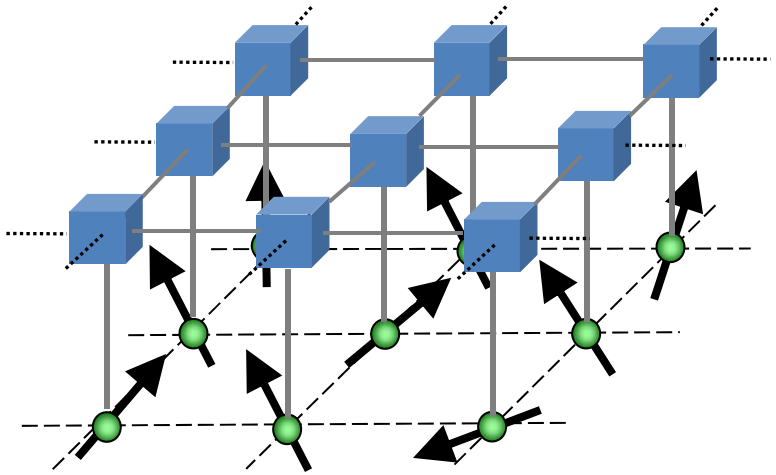


PEPS generalisation to 2D

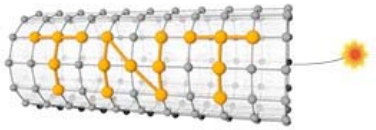
Each on-site projector now maps $\mathbb{C}^\chi \otimes \mathbb{C}^\chi \otimes \mathbb{C}^\chi \otimes \mathbb{C}^\chi \mapsto \mathbb{C}^d$
from which we identify a rank-5 **A** tensor:



Tensor network composed of a grid of these tensors contracted in a pattern mimicking the underlying lattice (i.e. shared ancilla pairs):



As “obvious” as it seems PEPS is a different beast from MPS in a number of ways …



Key PEPS example

$s_i = \pm 1$

Take a classical Ising spin model: $H(s_1, s_2, \ldots, s_N) = -J \sum_{\langle ij \rangle} s_i s_j$

Its partition function is $Z(\beta) = \sum_{s_1, s_2, \ldots, s_N} e^{-\beta H(s_1, s_2, \ldots, s_N)}$

Encode into a quantum state:

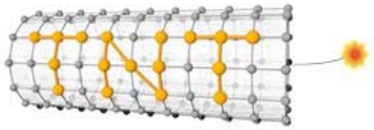
$$|\Psi\rangle = \sum_{s_1, s_2, \ldots, s_N} e^{-\frac{1}{2}\beta H(s_1, s_2, \ldots, s_N)} |s_1, s_2, \ldots, s_N\rangle$$

This state has identical *z-z* correlations as the classical model:

$$\langle \Psi | \sigma_i^z \sigma_j^z | \Psi \rangle = \sum_{s_1, s_2, \ldots, s_N} e^{-\beta H(s_1, s_2, \ldots, s_N)} s_i s_j$$

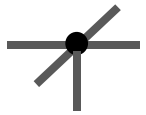
The 2D classical Ising model (solved by Onsager in the 40's) has algebraically decaying correlations at the critical temperature:

$$\beta_c = \frac{1}{2J} \log(1 + \sqrt{2})$$

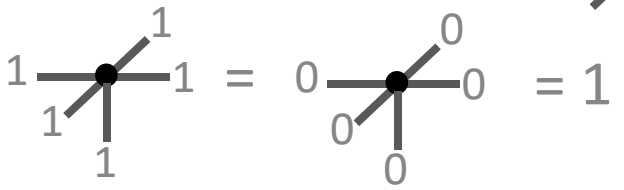


Key PEPS example

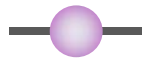
This "classical thermal" quantum state is a $\chi = 2$ PEPS. We can see this easily by using a rank-5 "copy" tensor or "diagonal" tensor:



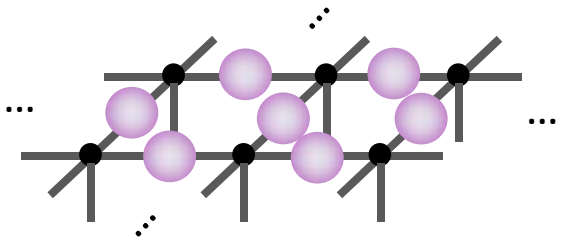
All legs identical in dimension – only non-zero when all legs have identical values:



Using the matrix $\mathbf{M} = \begin{pmatrix} e^{-J\beta/2} & e^{J\beta/2} \\ e^{J\beta/2} & e^{-J\beta/2} \end{pmatrix}$ =

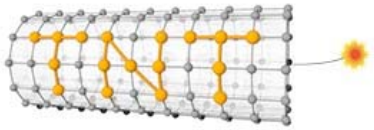


We get a PEPS network immediately by joining up copy dots with **M**:



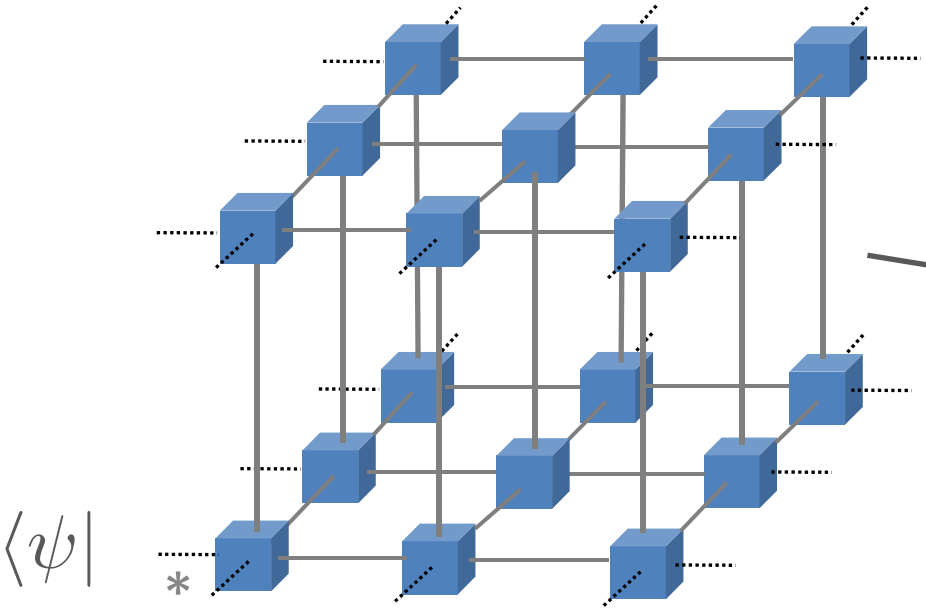
Can write down **A** tensor for this PEPS by square-rooting **M** and splitting it between sites.

So when $\beta = \beta_c$ this PEPS has algebraic correlations with at finite χ, unlike MPS which only ever has exponentially decaying correlations.

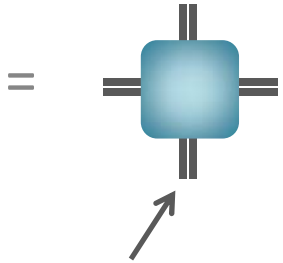


Computing expectation values

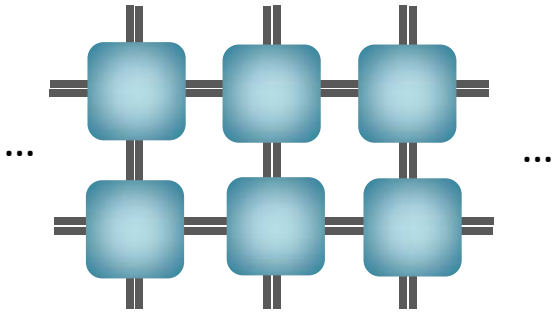
Let's consider the simplest calculation – the norm of a state:



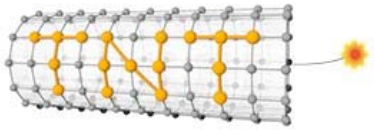
Form a transfer tensor:



We are still left with a grid tensor network of E to contract down:

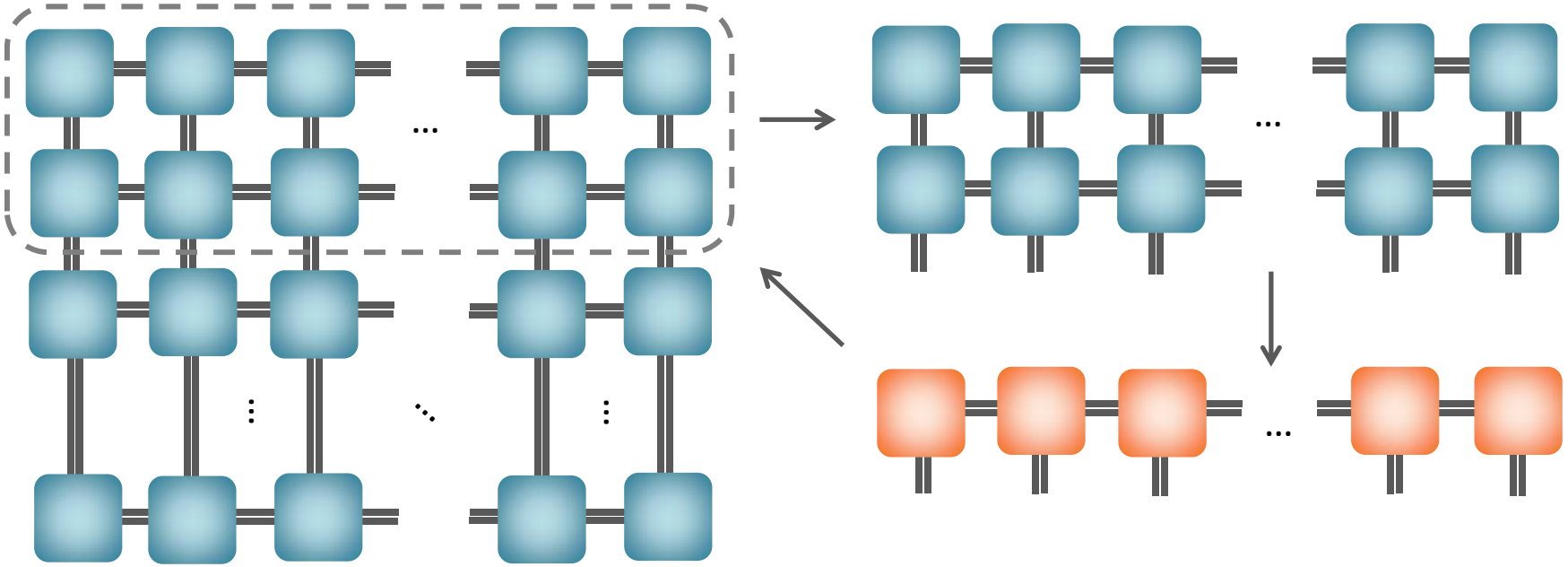


Will encounter an intermediate tensor with $\mathcal{O}(\sqrt{L})$ open legs, and is thus $(\chi^2)^{\sqrt{L}}$ = exponential in size. Exact contraction totally infeasible.



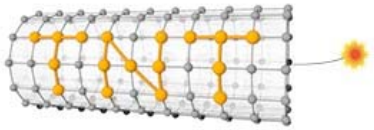
Approximate contraction

With open boundaries the contraction takes the form of a sequence of MPO x MPS calculations – can apply algorithms from earlier:



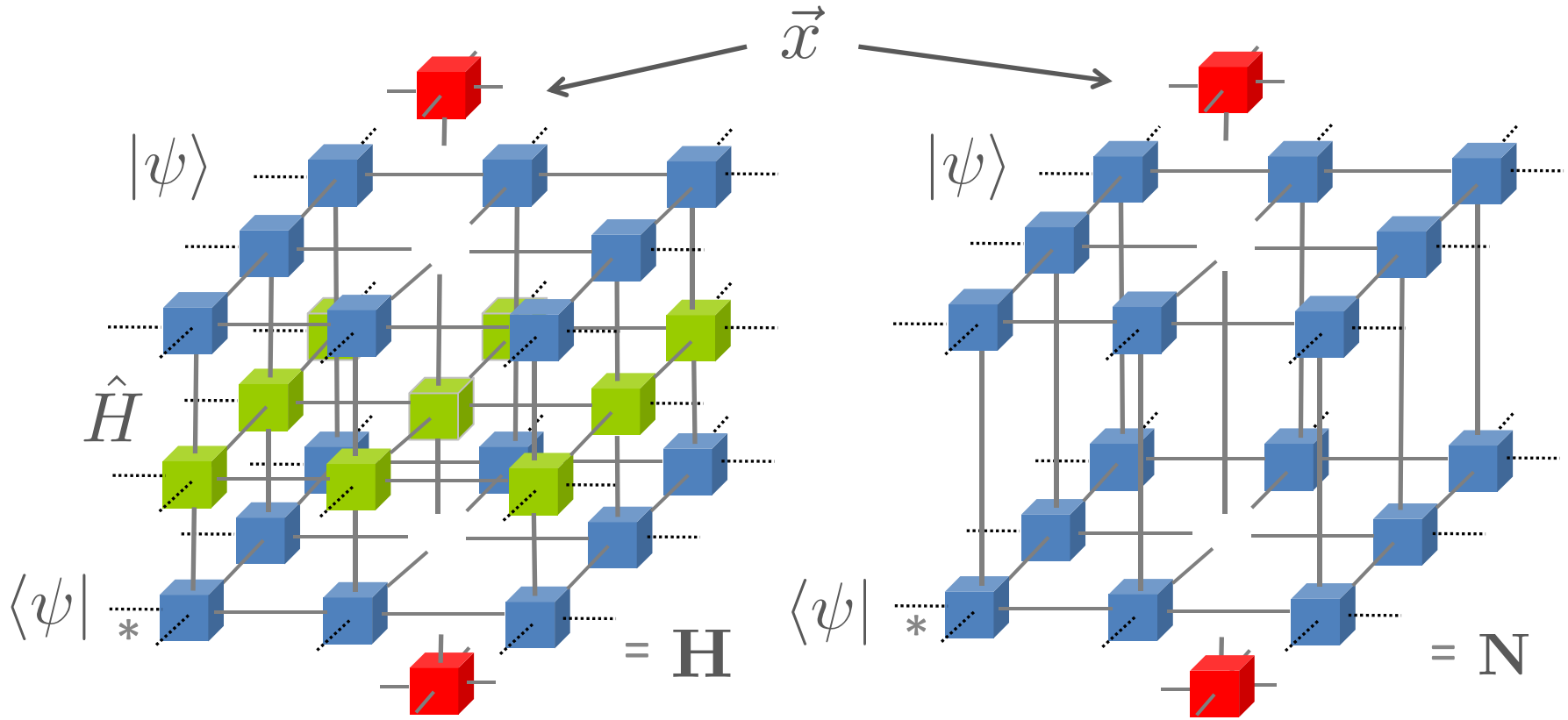
We use the truncation/compression in MPO x MPS steps to reduce the χ^4 exact MPS dimension down to χ^2, repeatedly.

Cost scales as $\mathcal{O}(\chi^8)$. Truncation error is known at each step and in practice very small. Expectation values can therefore be found.

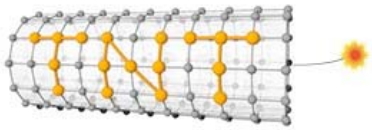


Variational minimisation

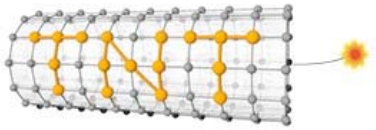
Using approximate contraction techniques we can evaluate effective Hamiltonians and norms for tensor-by-tensor variational minimisation:



We cannot avoid a generalised eigenvalue problem $\mathbf{H}\vec{x} = \mathbf{N}\vec{x}$ and so we can encounter problems if $\mathbf{N}$ is badly conditioned.



4: Conclusions



Computational physics

It is worth reflecting on what we are trying to achieve. Not long ago numerical calculations were considered distinctly 2nd rate:

Qualitative Analysis of the Cohesion in Metals[1]

EUGENE P. WIGNER AND FREDERICK SEITZ
Princeton University and the University of Illinois

I. Introduction

If one had a great calculating machine, one might apply it to the problem of solving the Schrödinger equation for each metal and obtain thereby the interesting physical quantities, such as the cohesive energy, the lattice constant, and similar parameters. It is not clear, however, that a great deal would be gained by this. Presumably the results would agree with the experimentally determined quantities and nothing vastly new would be learned from the calculation. It would be preferable instead to have a vivid picture of the behavior of the wave functions, a simple description of the essence of the factors which determine cohesion and an

LOCAL MOMENTS AND LOCALIZED STATES

Nobel Lecture, 8 December, 1977

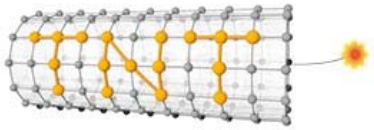
by
PHILIP W. ANDERSON
Bell Telephone Laboratories, Inc, Murray Hill, New Jersey, and Princeton University, Princeton, New Jersey, USA

⋮

Localization was a different matter: very few believed it at the time, and even fewer saw its importance; among those who failed to fully understand it at first was certainly its author. It has yet to receive adequate mathematical treatment, and one has to resort to the indignity of numerical simulations to settle even the simplest questions about it. Only now, and through primarily Sir Nevill Mott's efforts, is it beginning to gain general acceptance.

⋮

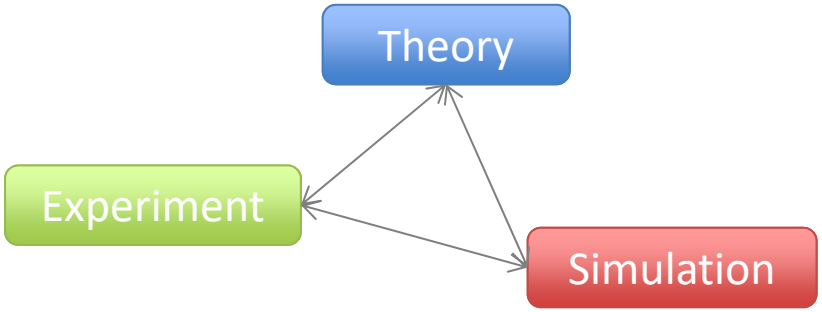
discuss. Very often such, a simplified model throws more light on the real workings of nature than any number of "ab initio" calculations of individual situations, which even where correct often contain so much detail as to conceal rather than reveal reality. It can be a disadvantage rather than an advantage to be able to compute or to measure too accurately, since often what one measures or computes is irrelevant in terms of mechanism. After all, the perfect computation simply reproduces Nature, does not explain her.



Third cornerstone of physics?

Yet, nowadays Computational Physics is considered an important branch of physics, complementary to experiment and theory:

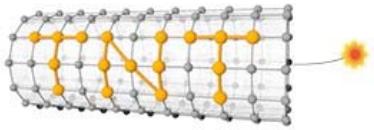
Perform “in-silica experiments on a model”



computing in SCIENCE & ENGINEERING

- Metropolis Algorithm for Monte Carlo
- Simplex Method for Linear Programming
- Krylov Subspace Iteration Methods
- The Decompositional Approach to Matrix Computations
- The Fortran Optimizing Compiler
- QR Algorithm for Computing Eigenvalues
- Quicksort Algorithm for Sorting
- Fast Fourier Transform
- Integer Relation Detection
- Fast Multipole Method

Much has been learnt about strongly correlated physics precisely by attacking/approximating the many-body problem numerically.



What have we learnt here?

- We have seen ways of encoding the physically relevant “corner” of Hilbert space using networks of tensors.

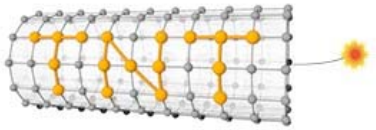
- In 1D MPS are both well motivated and possess many useful properties like being exactly and efficiently contractible.

- We formulated efficient algorithms for variationally finding ground states and computing time-evolution.

- Extensions to finite temperatures re-used these algorithms.

- We looked at generalising this success with TTN and MERA motivated from a renormalisation perspective.

- Using PEPS we constructed networks for 2D systems.



Code for doing TNT?

You could write your own, but our group is developing an open-access TNT library (in C) which does a lot of the hard work for you:

www.tensornetworktheory.org

Available:

- DMRG and td-DMRG available now.
- U(1) quantum number symmetry.

Coming soon:

- Finite-temperature calculation
- Master equation evolution.
- Quantum trajectory code.

Coming later:

- Parallelised versions of codes.
- Impurity solvers for DMFT.
- Tensor tree, PEPS and MERA.