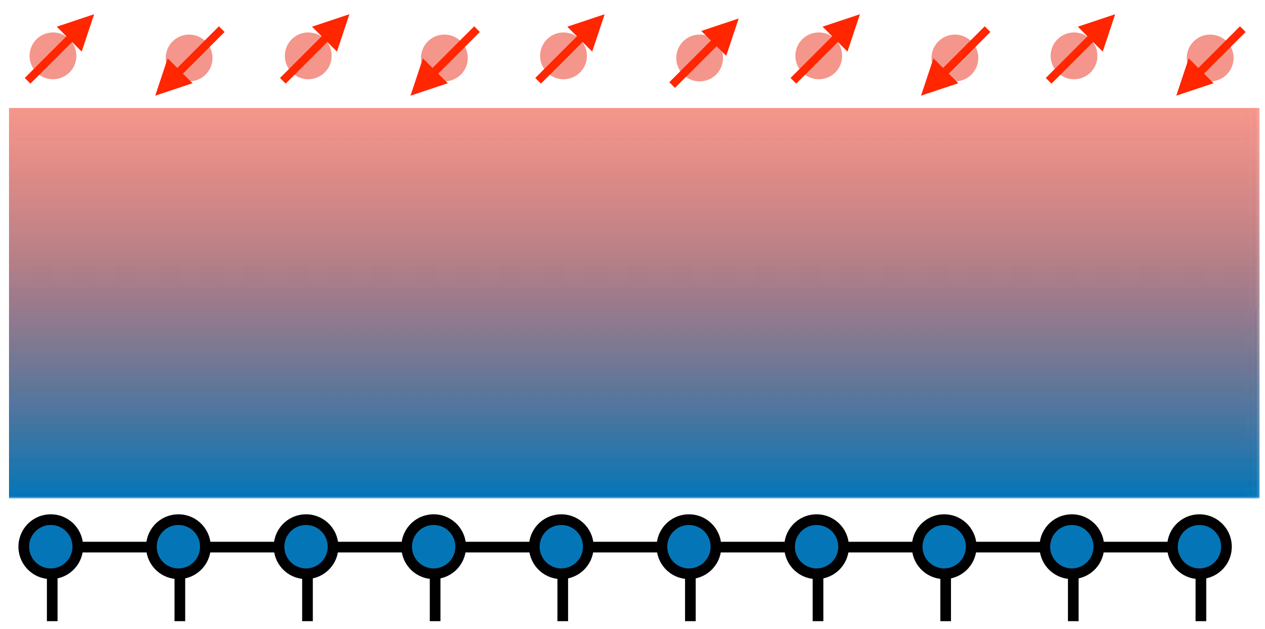
Introduction and Perspective on Tensor Network Methods for Quantum Many-Body Physics



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Jun 2021 - Collège de France

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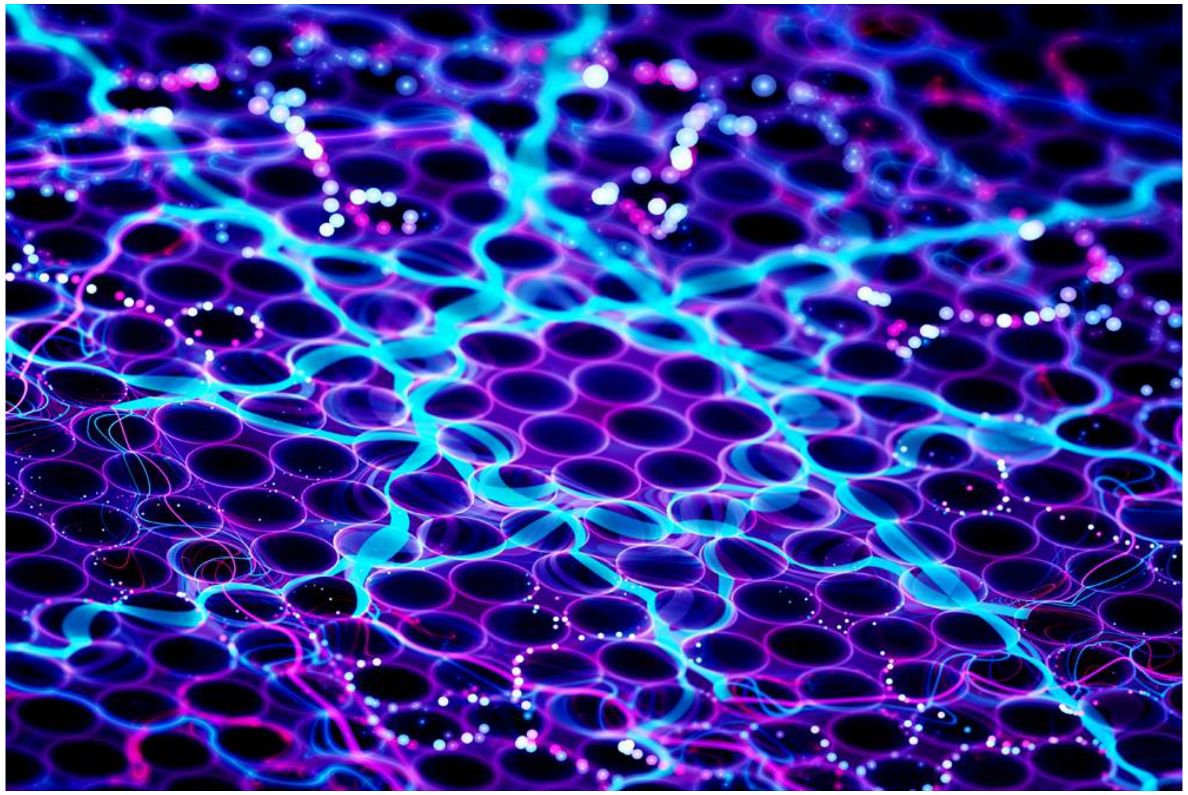
Major progress in last 30 years:
understanding structure of *quantum wavefunctions*
(or quantum "states")



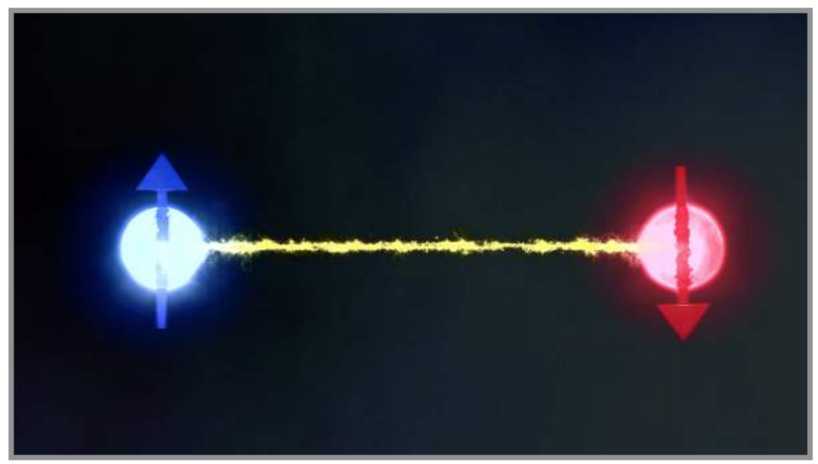
Mathematical description of a quantum state is unimaginably vast

$$\Psi =$$

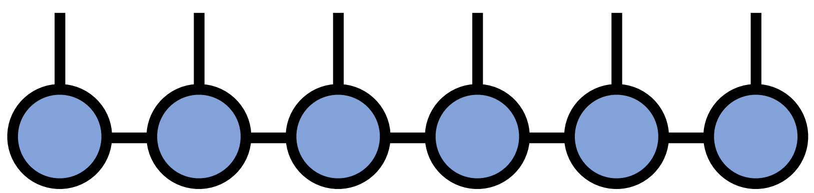
```
0.4838 -0.1254 0.4480 0.1293 0.4253 0.3043 0.1415 -0.3943 -0.1237 -0.3411 0.3707 0.4697
-0.3150 -0.0219 0.2702 0.4844 -0.0639 0.4380 -0.0305 -0.0179 -0.3312 0.4734 -0.1749
0.4126 -0.4746 -0.3346 0.4457 0.1062 0.0350 -0.4284 -0.4392 0.3516 -0.0667 -0.2332
0.4516 -0.0228 -0.4497 -0.4137 -0.2730 0.1811 -0.2679 -0.1046 0.4408 0.3211 -0.1506
0.3923 0.2490 0.3931 -0.2902 -0.4754 -0.0290 -0.1136 0.3742 -0.2364 -0.3652 -0.1279
0.4175 0.1493 0.2413 0.3722 -0.1782 0.3172 -0.4666 -0.4873 -0.3202 -0.2749 0.4662
0.4086 0.1137 -0.3144 -0.0653 0.4328 -0.4703 -0.1076 0.3656 -0.1982 0.3134 -0.0689
-0.3617 0.0295 -0.2461 -0.0194 -0.2068 -0.0643 0.3705 -0.2612 0.0619 -0.1382 0.4018
-0.2481 -0.4666 0.1091 -0.0434 -0.2705 0.3034 -0.4285 0.2276 0.4733 -0.1143 -0.0688
0.3667 0.2244 -0.1190 0.0759 -0.4259 -0.0432 0.0211 0.2320 0.4673 0.1837 0.4889 -0.2433
0.0421 -0.0932 -0.2526 0.2174 -0.1993 -0.1698 0.1183 0.2083 0.4662 0.1054 -0.1427
-0.3739 -0.4851 0.1276 0.4294 -0.4959 0.1514 0.4410 0.1387 -0.4891 -0.0989 0.1523
0.4141 0.0229 -0.2018 -0.1047 0.3957 -0.4772 0.2328 0.2119 -0.1617 0.0295 0.2459
0.3378 -0.0844 0.0926 0.0403 0.0868 -0.4895 -0.1887 0.3829 -0.3239 -0.3538 0.3549
-0.3763 0.1980 0.0334 -0.0676 -0.4214 -0.2405 -0.0068 -0.3043 0.3768 -0.3903 0.3625
0.2141 0.4840 -0.1668 -0.0682 -0.3314 -0.3117 -0.2942 0.0529 0.2541 -0.4427 -0.3690
0.3095 -0.3536 0.1424 -0.0545 0.3577 0.4979 0.4581 0.3492 0.4247 -0.0024 -0.3346 0.3823
0.4916 0.4125 -0.0565 -0.4466 -0.0765 -0.4172 -0.1200 0.1712 -0.1814 0.1211 -0.0305
0.2731 -0.4123 0.3410 0.0112 -0.0343 0.1853 0.4424 -0.1157 0.2665 -0.1759 -0.1797
0.4186 0.4012 0.3687 -0.2233 -0.4976 -0.2052 -0.1462 -0.1230 -0.3735 -0.4492 0.2621
-0.0322 0.4011 0.3472 0.1471 0.2549 -0.0751 0.0165 -0.4245 -0.0242 -0.4596 -0.3528
0.1781 0.0606 0.3207 0.4076 0.1446 -0.0485 0.4185 0.2485 -0.3112 -0.3895 0.0222 0.4948
-0.2362 0.2558 0.3032 0.1868 0.0001 -0.3667 -0.4846 0.4612 0.1831 -0.0334 -0.1691
-0.2108 0.0022 0.1082 -0.0410 -0.1681 0.1058 0.1304 -0.0272 -0.3245 -0.4714 -0.1954
-0.0692 -0.2680 -0.2022 0.1401 -0.1510 0.0543 0.4548 0.3042 -0.4270 -0.1932 -0.4843
0.2404 -0.1085 0.3345 0.4777 -0.2789 -0.3552 -0.4433 0.0247 -0.1857 -0.2978 -0.4323
-0.4655 0.2010 0.1385 -0.0723 -0.2033 0.0867 0.1511 0.2401 -0.4549 0.1013 -0.4637
0.4546 0.0035 0.4291 0.3540 -0.3975 -0.2342 0.1500 -0.2810 -0.3555 0.4292 -0.1696
0.2019 -0.1906 0.1590 0.3959 0.1673 0.3019 -0.3597 0.0368 0.0498 -0.4730 -0.2287
0.2351 -0.2074 0.1402 0.3312 -0.2531 -0.4642 0.0112 0.2991 0.3106 0.2700 -0.0499
-0.3839 0.2488 0.3712 -0.3905 -0.1389 -0.0298 0.2599 -0.3162 0.0886 0.2221 0.0130
0.0871 0.4659 -0.1590 0.3191 0.0405 -0.2341 0.0233 -0.2214 0.2174 -0.3168 -0.4215
-0.4656 -0.0940 0.0622 0.1237 0.1804 -0.2926 0.3411 0.4340 0.3854 -0.2560 -0.1148
0.4037 0.1308 0.3851 0.2471 -0.2636 -0.4579 -0.4432 -0.0018 -0.1018 0.0554 0.2119
-0.3493 -0.4723 0.0298 0.1595 0.1991 0.0992 0.3845 -0.2337 -0.1724 0.2335 -0.3664
-0.3796 0.1485 -0.0156 0.3551 0.0977 0.0092 0.1835 0.1115 -0.4520 -0.1859 0.1761 0.0439
-0.1694 0.0667 -0.4222 -0.1027 -0.2947 -0.0826 -0.4814 0.1997 -0.1338 -0.3859 0.2407
0.2463 -0.1803 -0.3503 -0.0361 -0.1122 -0.2970 -0.0012 -0.2580 0.1485 0.2910 0.2312
-0.3264 0.0934 -0.3536 -0.2796 -0.0026 -0.2784 -0.0991 0.2217 -0.2769 -0.2569 0.3027
0.1259 -0.2038 0.3351 0.0750 0.4359 -0.0046 0.3199 -0.1125 -0.3213 0.2834 0.2758 0.1714
0.3764 -0.2559 -0.1267 0.3182 -0.3546 0.4768 0.0421 -0.3999 0.0642 0.1276 0.1372
-0.0899 0.1679 0.2201 0.4092 -0.2378 -0.2499 0.4386 -0.4194 0.1641 -0.0386 0.2397
-0.1474 -0.2185 0.4699 -0.0174 0.4122 -0.1422 0.0562 -0.1193 -0.0231 -0.3941 0.4766
-0.1175 0.0928 -0.4447 0.1936 -0.3190 0.1430 -0.2636 -0.4486 0.2344 0.3896 0.0362
0.2708 0.1189 -0.4562 -0.2521 -0.0699 -0.1683 0.4022 -0.0158 -0.0392 -0.2438 0.1960
0.1763 0.2857 -0.4274 -0.2628 -0.1526 0.0773 -0.0641 -0.1773 -0.4086 0.2405 0.4295
0.3396 0.0119 -0.2425 -0.4298 -0.3472 0.2623 0.1254 0.3346 -0.1334 -0.4701 0.3356
```

Describing state of just 140 quantum particles requires more numbers than atoms in the universe

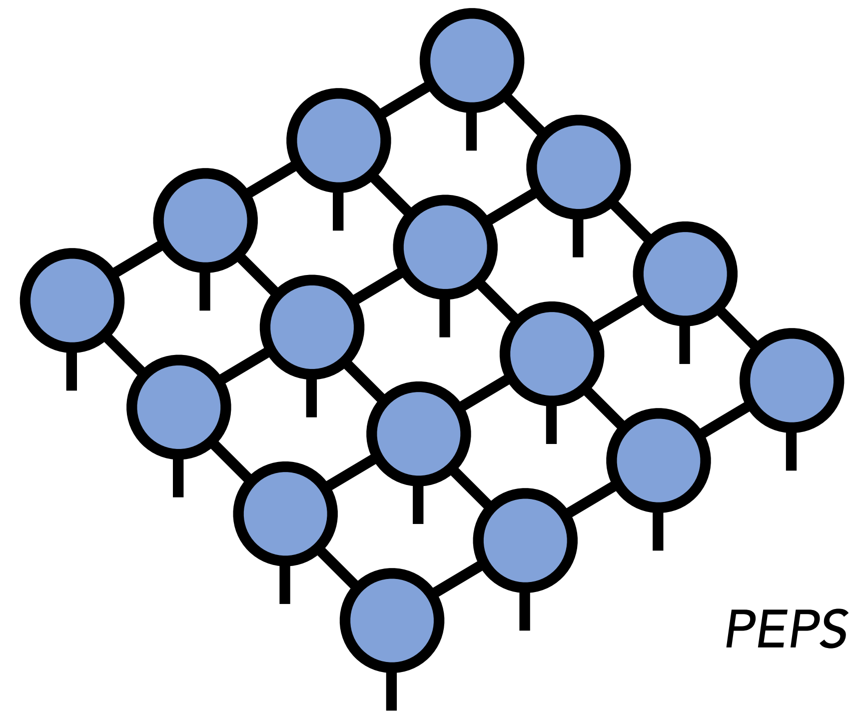
But the wavefunction harbors patterns
of *quantum entanglement* between particles



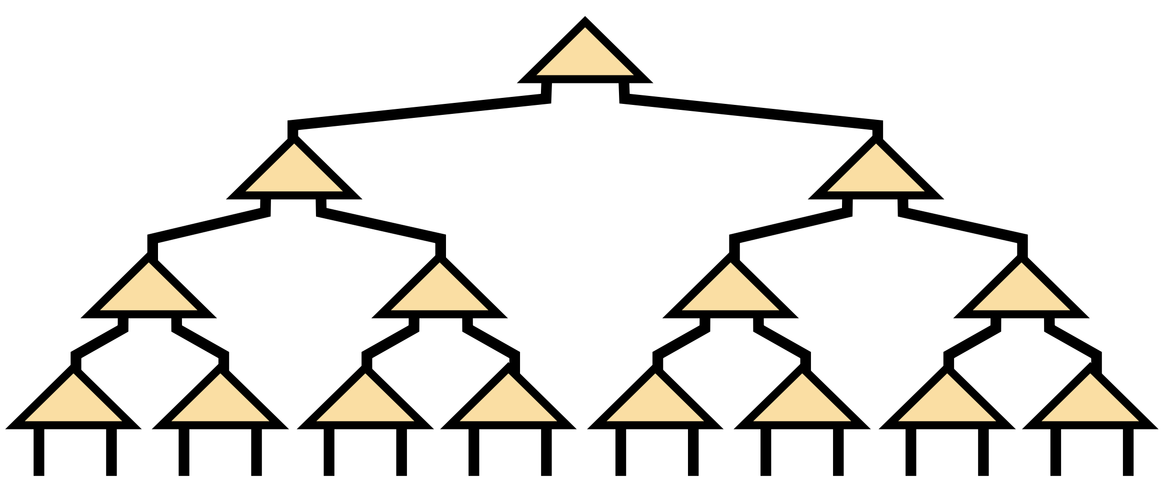
Entanglement patterns impart *internal structure* to the wavefunction



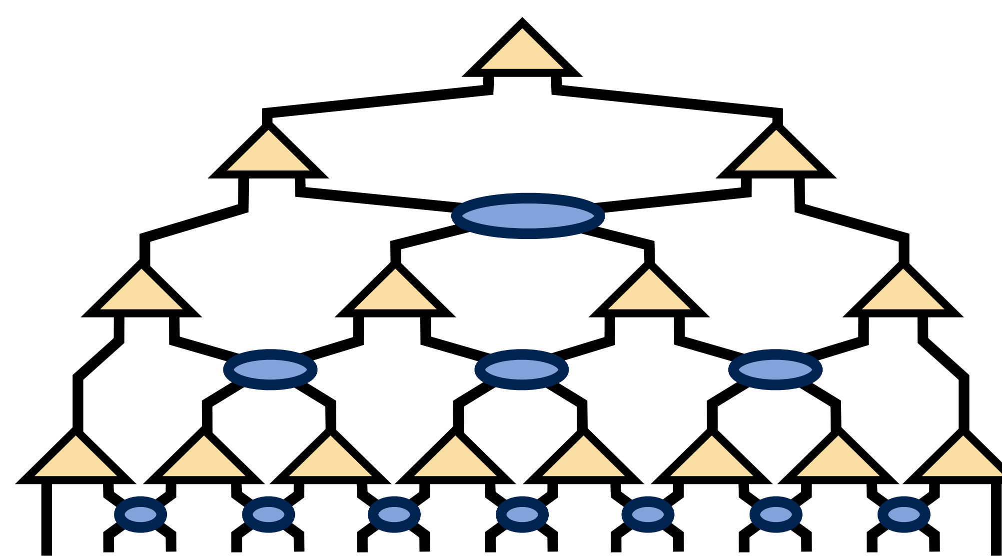
matrix product state



PEPS network



tree tensor network

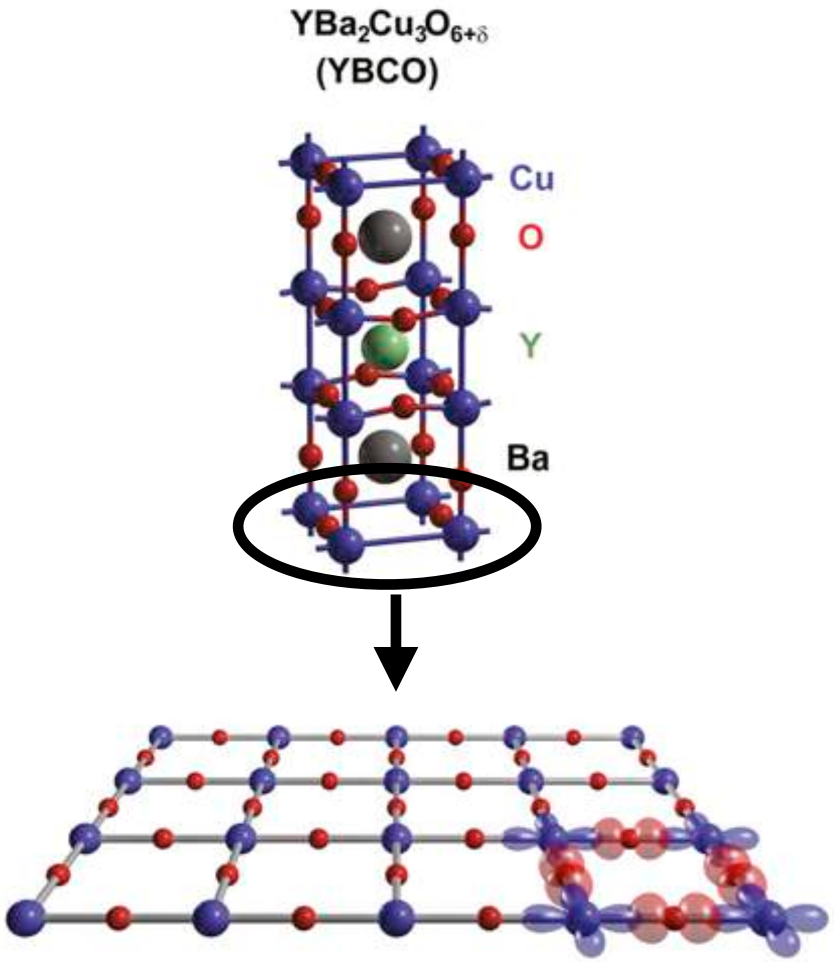


MERA network

The Quantum Many-Body Problem

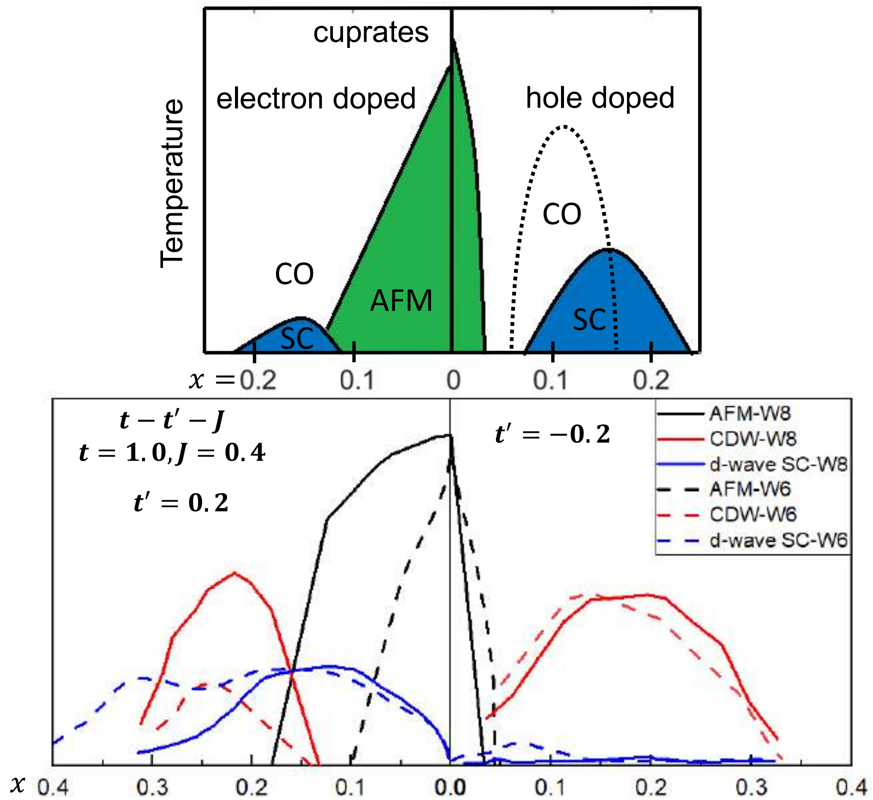
Accurate calculations of many-fermion systems are central to condensed matter physics

High-temperature superconductor



Barisic, Chan, Li, PNAS 2013

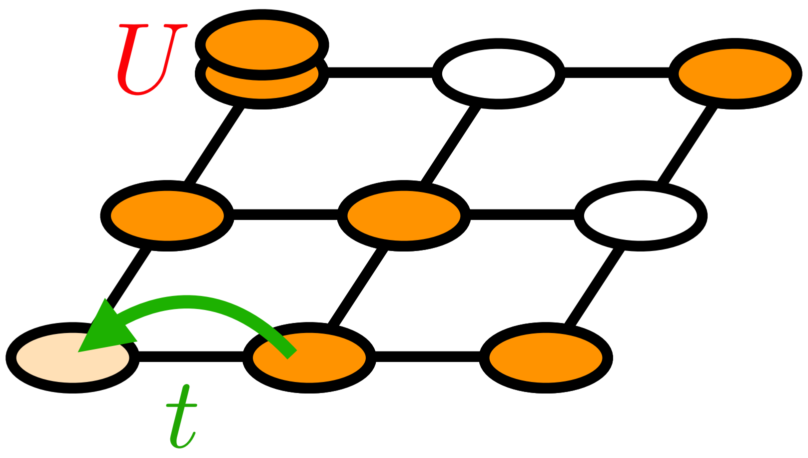
Copper-oxygen plane



Jiang, Scalapino, White, 2104.10149

Numerical study of t-t'-J model

Often simplified to minimal model:
the **Hubbard** model



$$\hat{H} = -\,t\sum_{ij}(\hat{c}_i^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_j) + U\sum_j \hat{n}_{j\uparrow}\hat{n}_{j\downarrow}$$

Quantum physics "simple" mathematically speaking
Given Hamiltonian $\hat{H}$

All we must do is find lowest eigenvector (zero temperature):

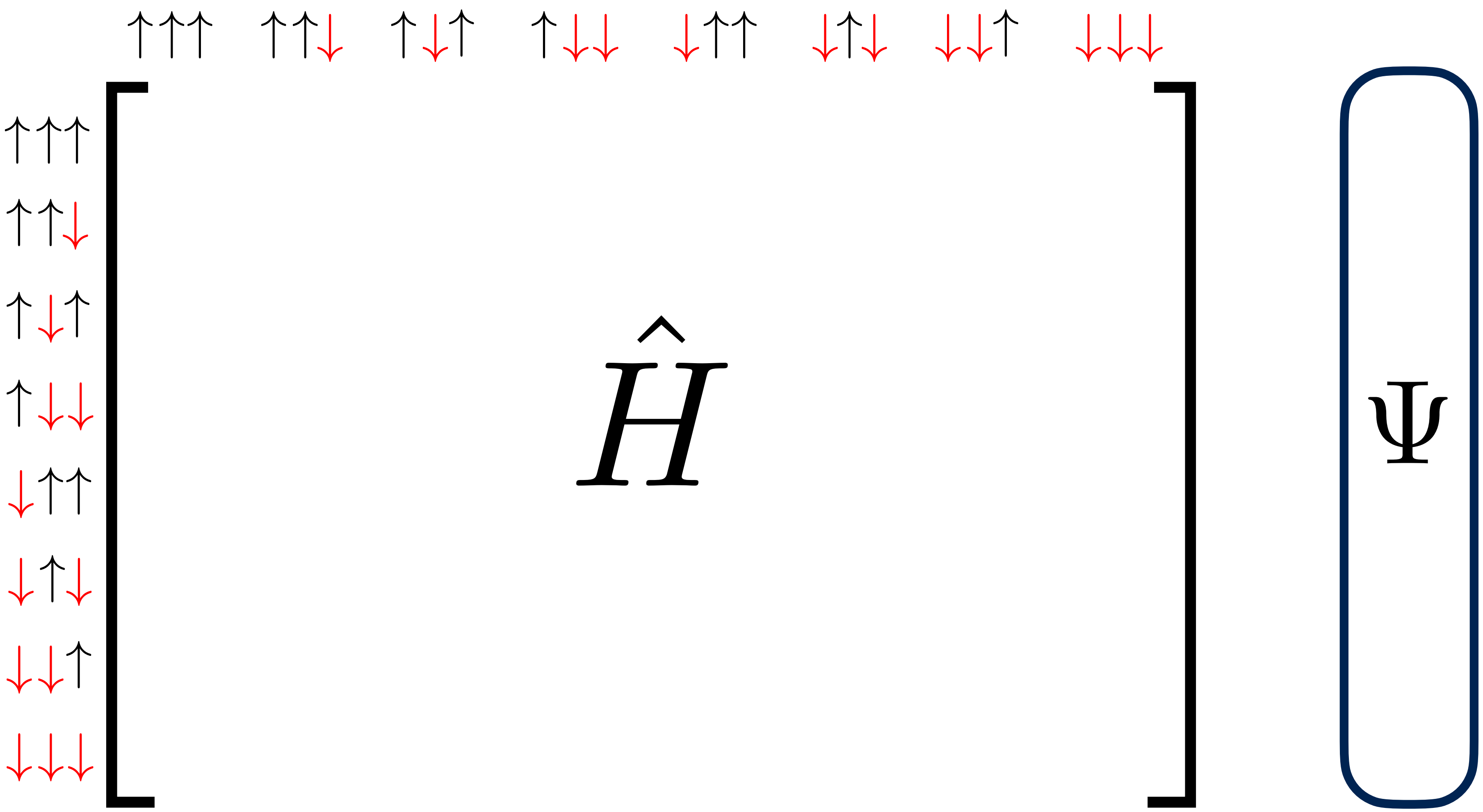
$$\hat{H}\Psi = E\Psi$$

Or exponentiate (finite temperature):

$$\rho = e^{-\hat{H}/T}$$

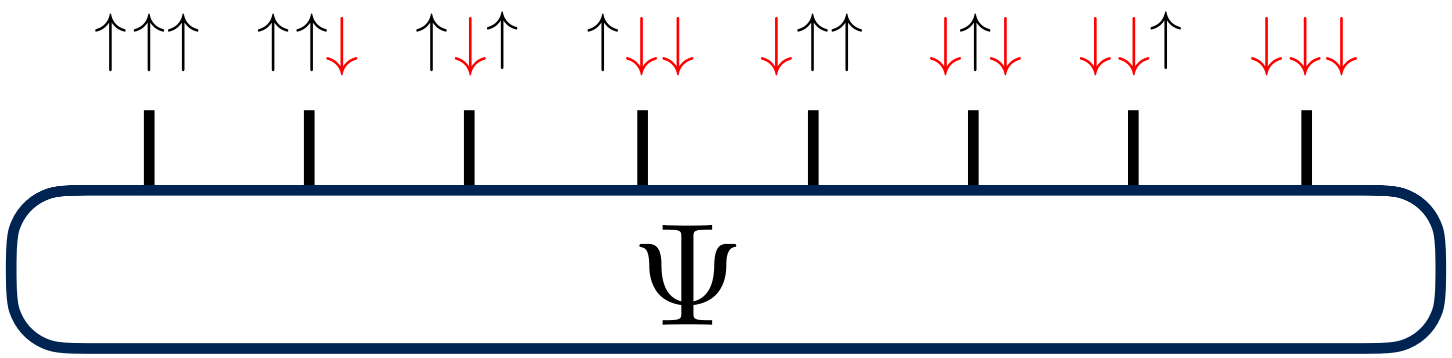
What is the problem?

Hamiltonian acts in space of <u>all</u> configurations (4^N x 4^N matrix)



Ψ also defined for all configurations

Many-body wavefunction lives in 4^N dimensional space

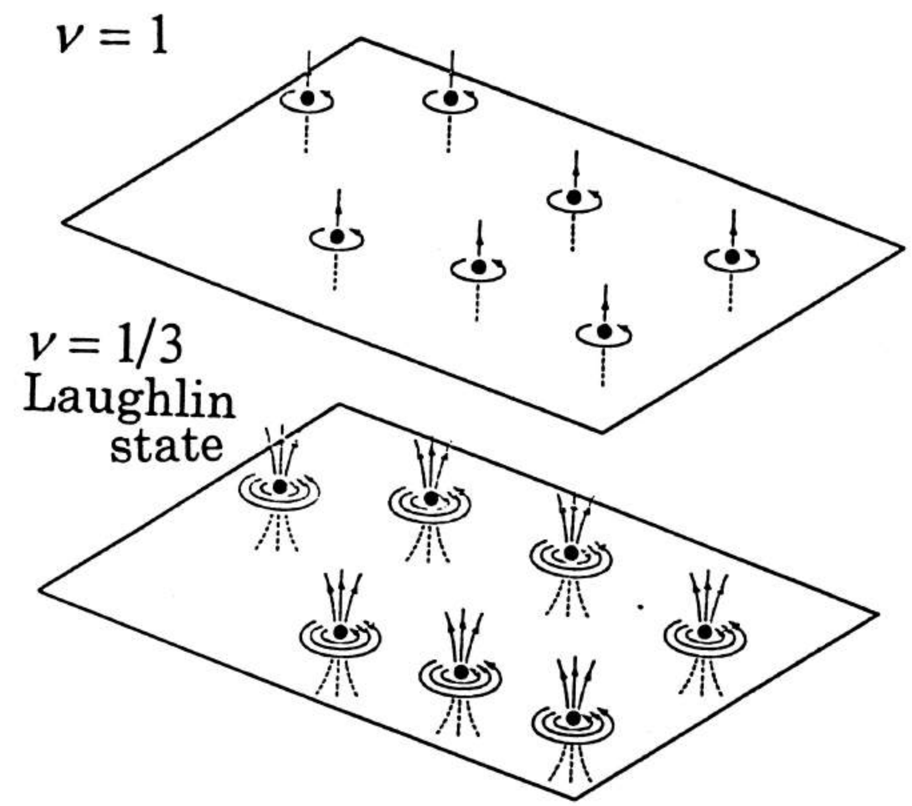


Wavefunction Ψ seemingly *intractable*

Can we get around this <u>many-body</u> problem?

1. Guess the Wavefunction

Can sometimes work!



Famously, Laughlin guessed wavefunctions qualitatively explaining the fractional quantum Hall effect

$$\psi=\left\{\prod_{j<k} f(z_j - z_k)\right\}\exp\left(-\tfrac{1}{4}\sum_l |z_l|^2\right)$$

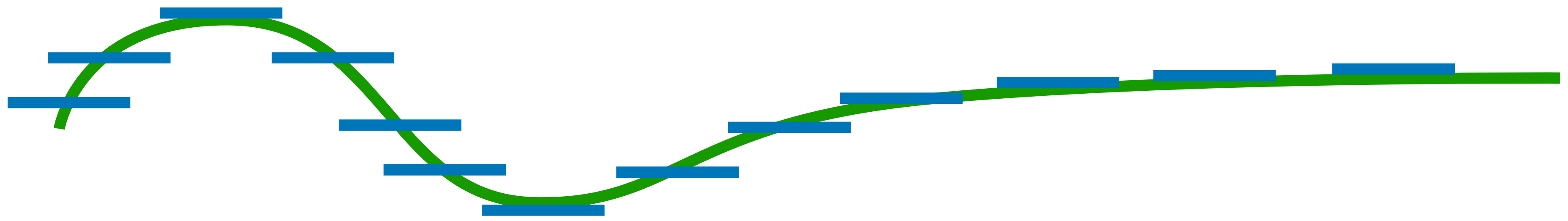
Laughlin, Phys. Rev. Lett. 50, 1395 (1983)

2. Avoid the Wavefunction

In the 70's, Kohn, Hohenberg, and Sham developed *density functional theory*

Proved <u>*all*</u> T=0 properties determined by electron density

Local density approximation:



Energy sum of *interacting uniform gas* energies pinned to each density value

Workhorse of realistic materials calculations

3. Sum Simpler Wavefunctions

Take non-interacting problem (solvable)

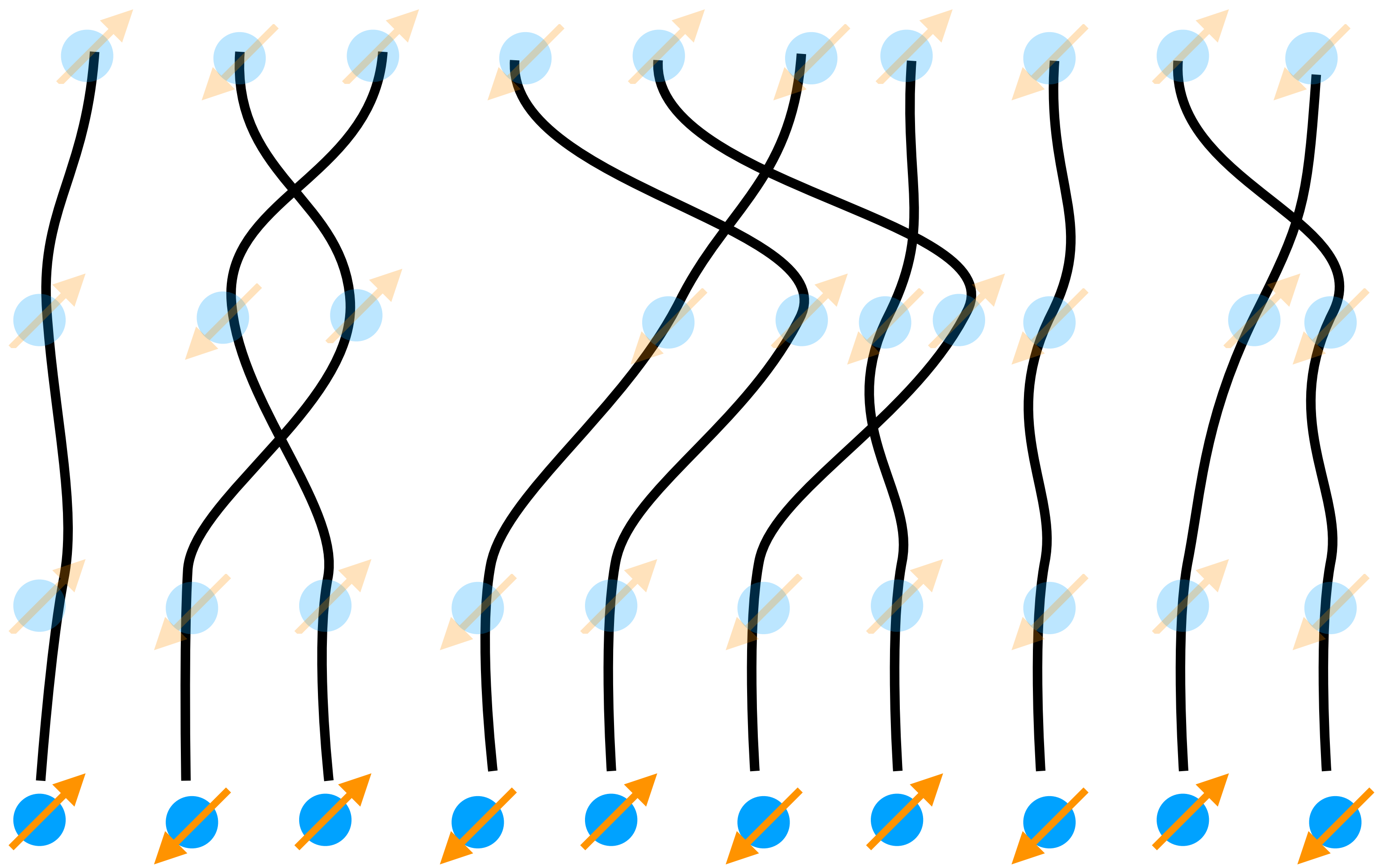
$$|\Psi_0\rangle = \hat{\phi}_1^\dagger \hat{\phi}_2^\dagger \cdots \hat{\phi}_N^\dagger |0\rangle$$

Interacting wavefunction by summing non-interacting wavefunctions:

$$\begin{aligned}|\Psi\rangle = {} & a_1 \ \hat{\phi}_1^{(1)\dagger} \hat{\phi}_2^{(1)\dagger} \cdots \hat{\phi}_N^{(1)\dagger} |0\rangle \\ & + a_2 \ \hat{\phi}_1^{(2)\dagger} \hat{\phi}_2^{(2)\dagger} \cdots \hat{\phi}_N^{(2)\dagger} |0\rangle \\ & + a_3 \ \hat{\phi}_1^{(3)\dagger} \hat{\phi}_2^{(3)\dagger} \cdots \hat{\phi}_N^{(3)\dagger} |0\rangle \\ & + \ldots\end{aligned}$$

4. Sample the Wavefunction (quantum Monte Carlo)

Can rewrite as paths in *imaginary time (= path integral)*



Now a <u>classical</u> problem – sample with Monte Carlo

But all these methods encounter some trouble...

Summing wavefunctions:

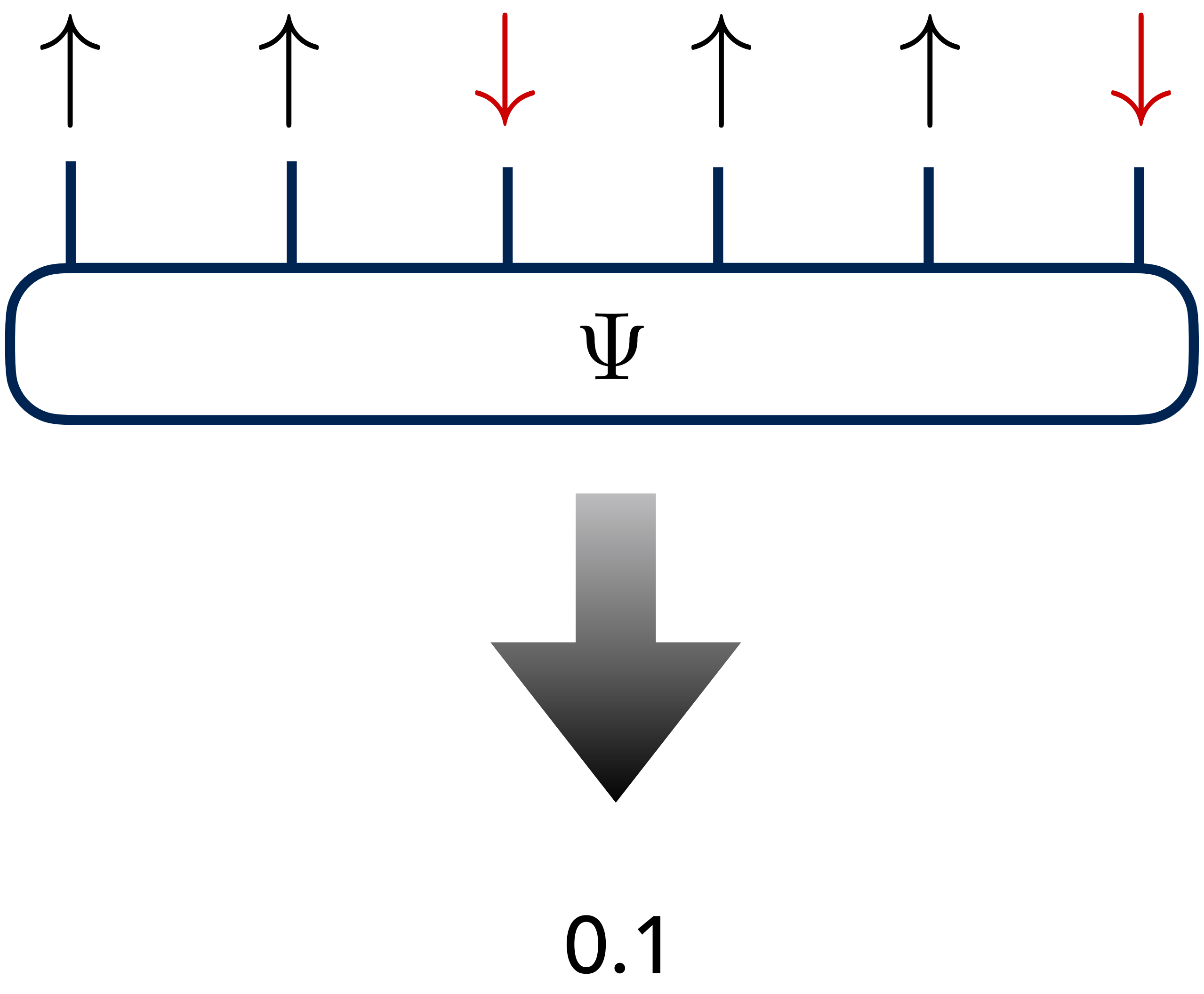
exponentially many terms needed for large U

Sampling / quantum Monte Carlo:

exponentially many samples for low temperature T

Possibly to work with wavefunction directly?

What is a wavefunction? Map of configurations to numbers



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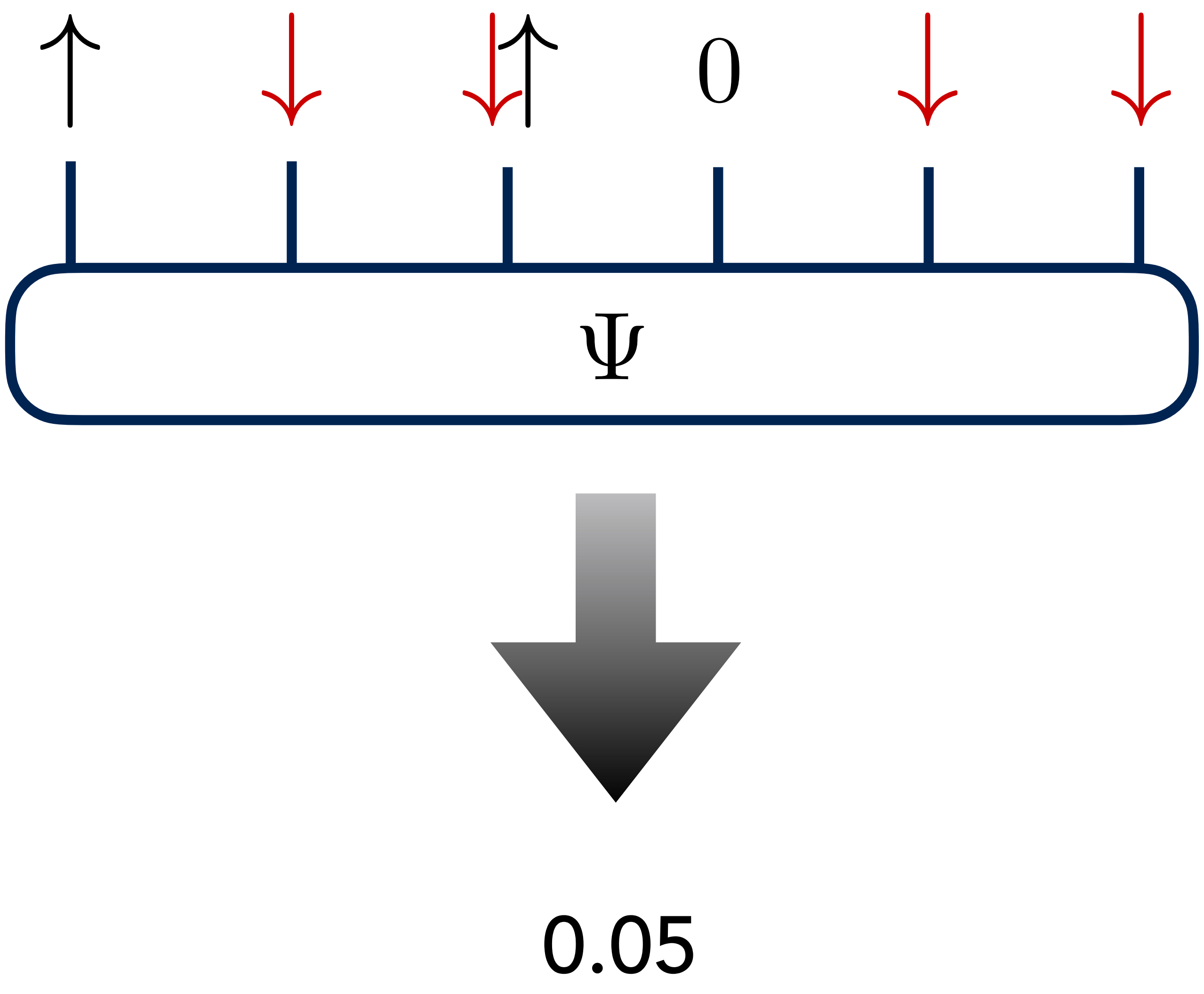
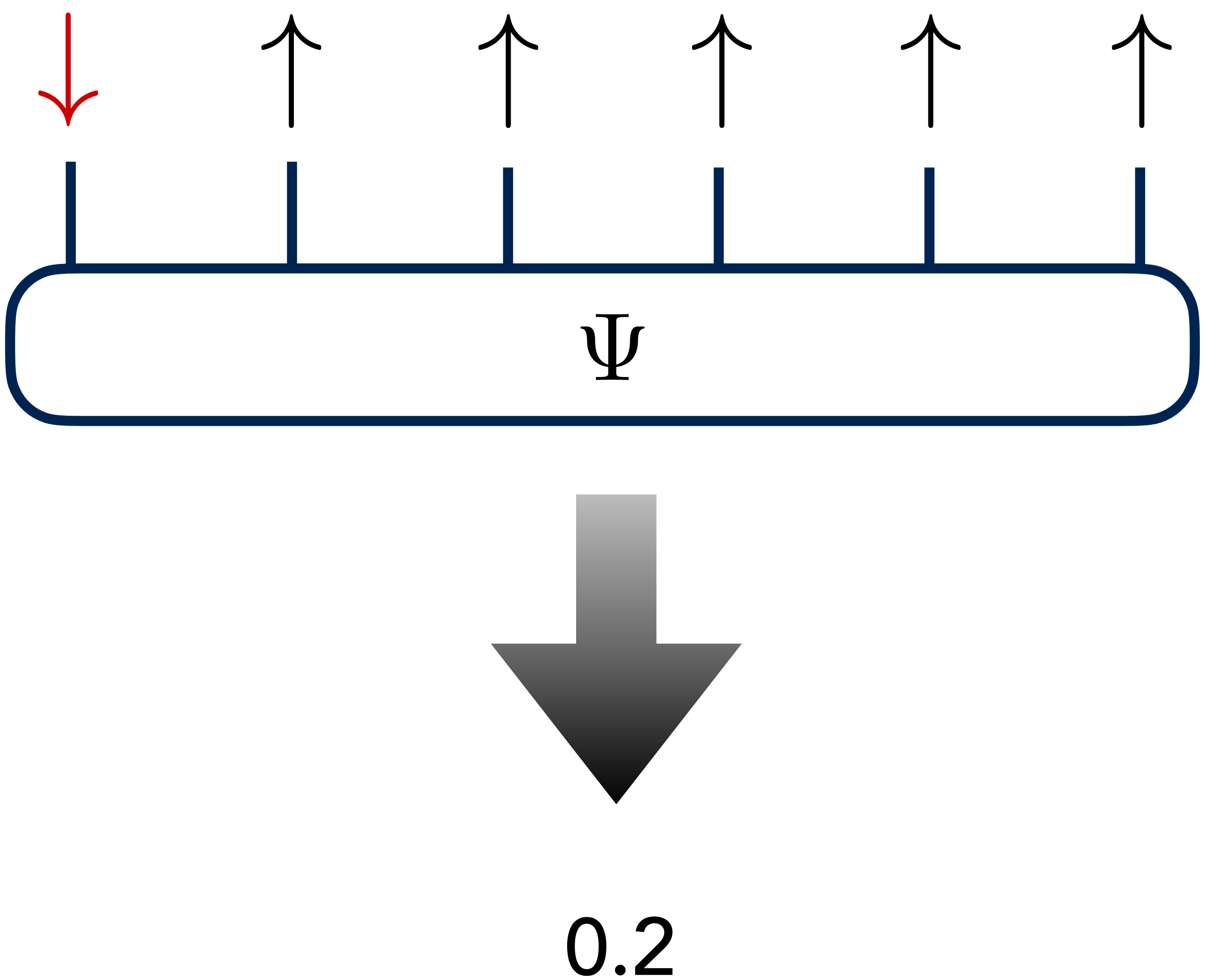
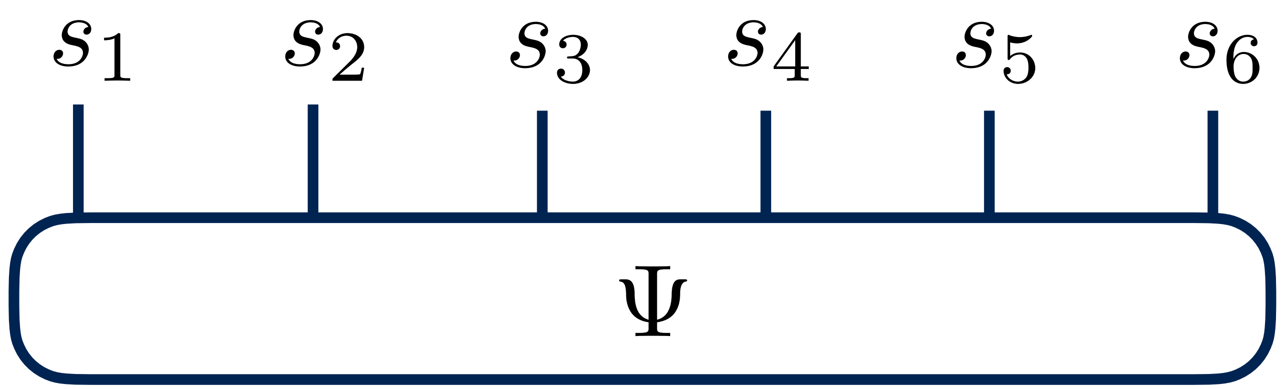


What is a wavefunction? Map of configurations to numbers



Formally a *tensor* with N indices

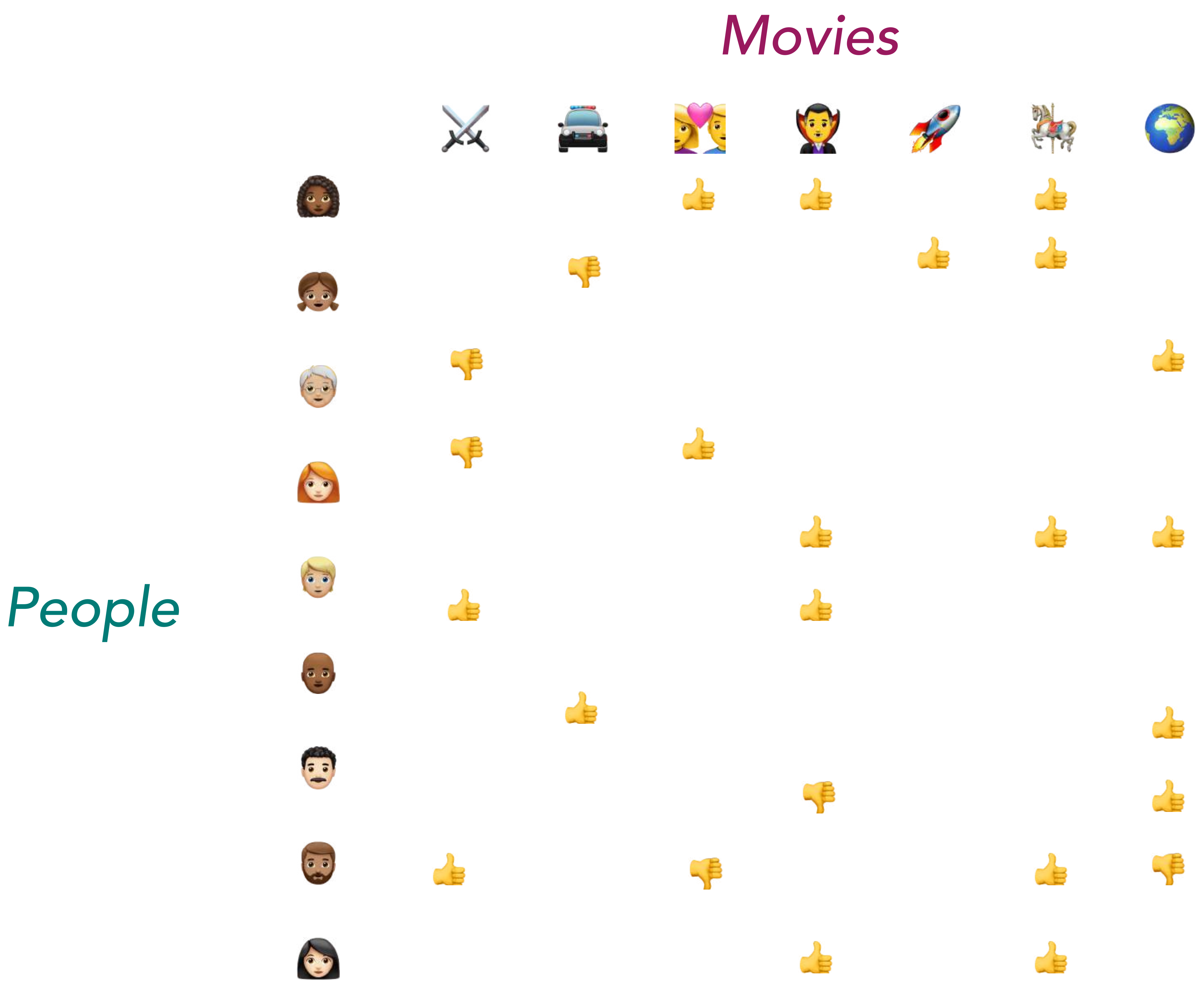
$$\Psi^{s_1 s_2 s_3 s_4 s_5 s_6} =$$



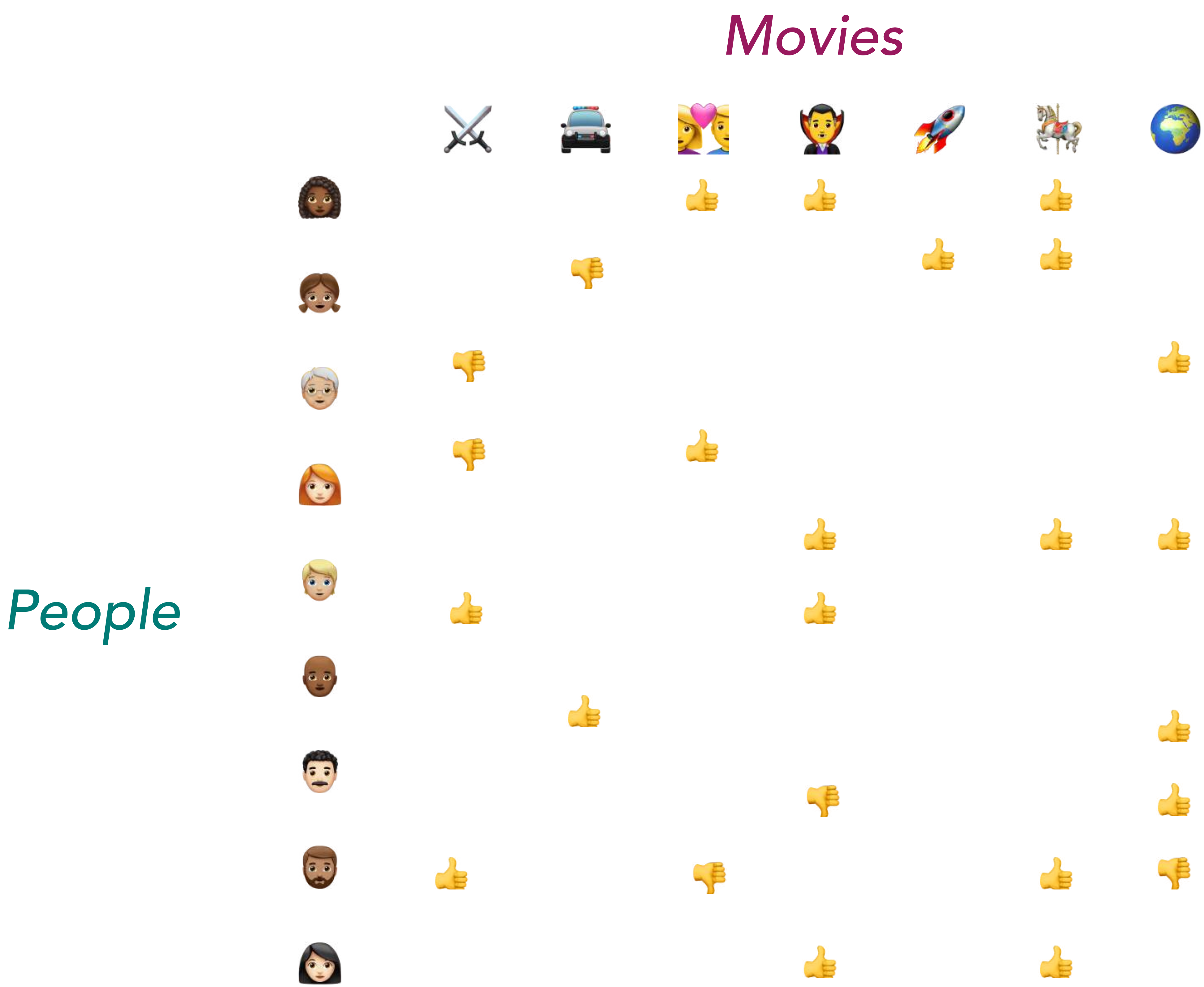
A tensor with N indices of dimension 4 $(0, \uparrow, \downarrow, \downarrow\uparrow)$
has 4^N different parameters

Can parameters be truly unrelated?

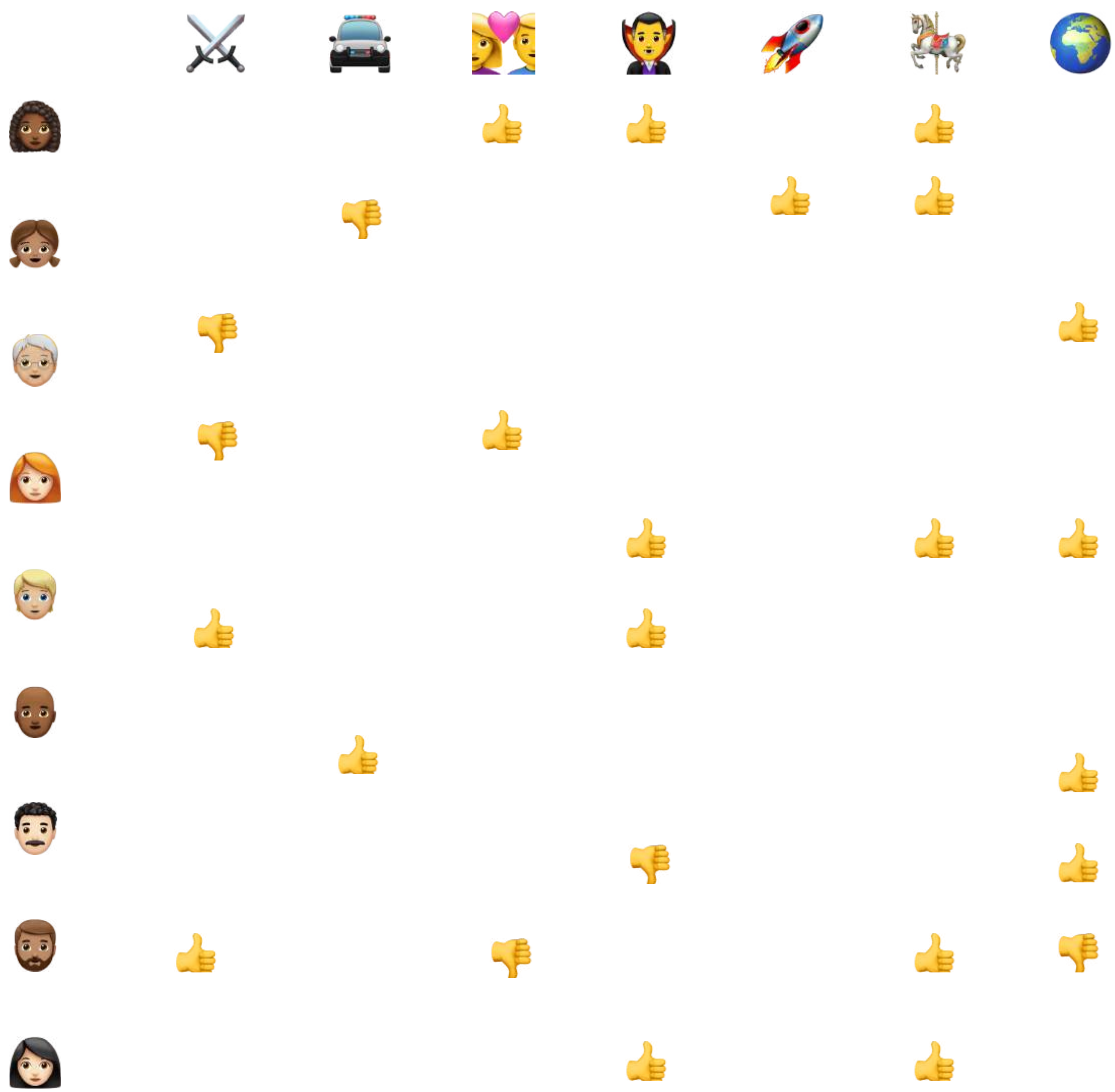
Take inspiration from Netflix (!)



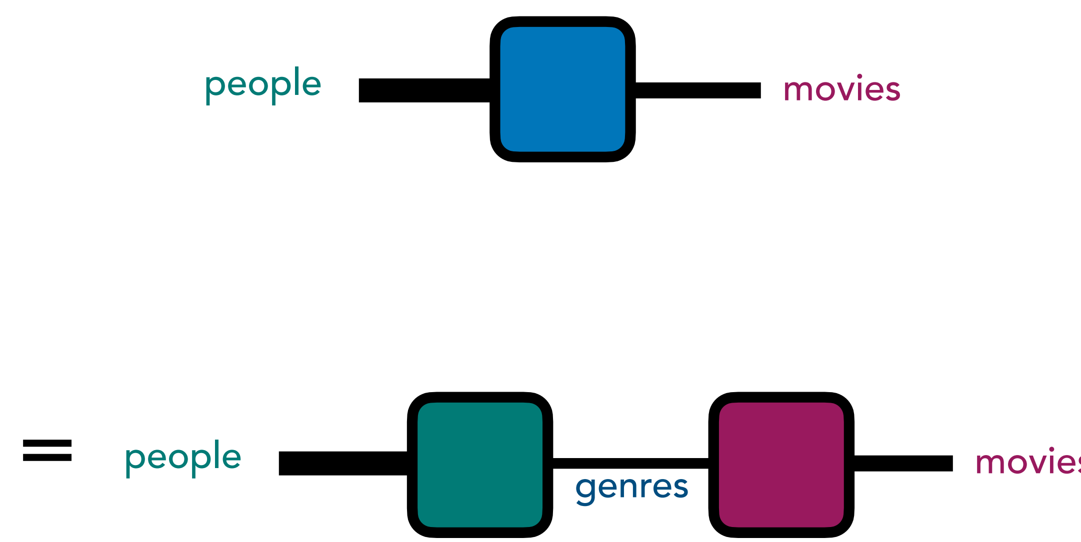
Millions of people, but can not be millions of unique tastes / genres



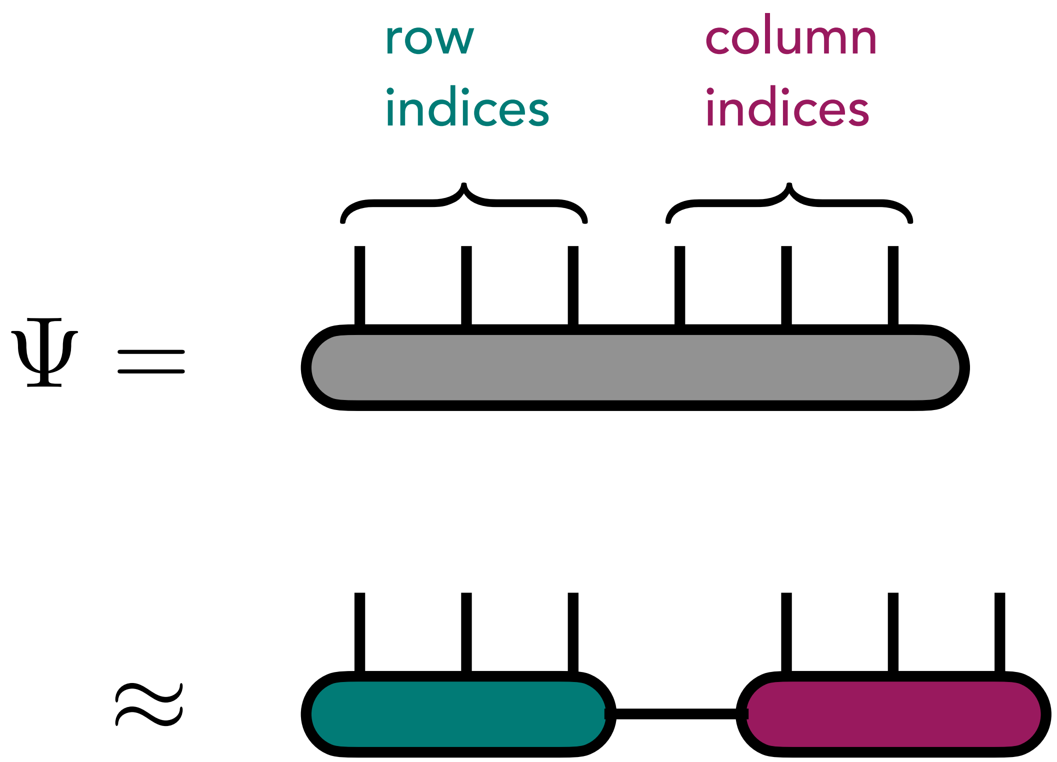
Can not be millions of unique tastes / genres ...



Rating matrix must be *low rank*



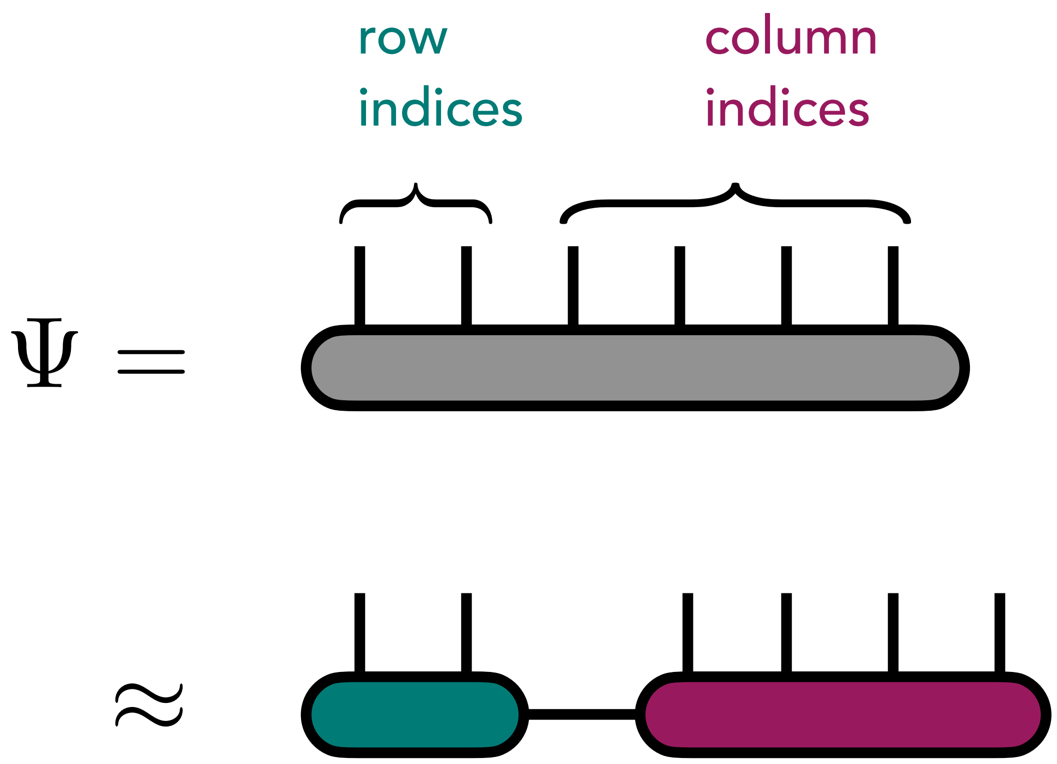
In similar fashion, ground state wavefunction is low rank



Properties of one electron can not really depend on 4^{N-1} states of other electrons

Electrons mostly correlate with others nearby to them

Nothing special about center bipartition



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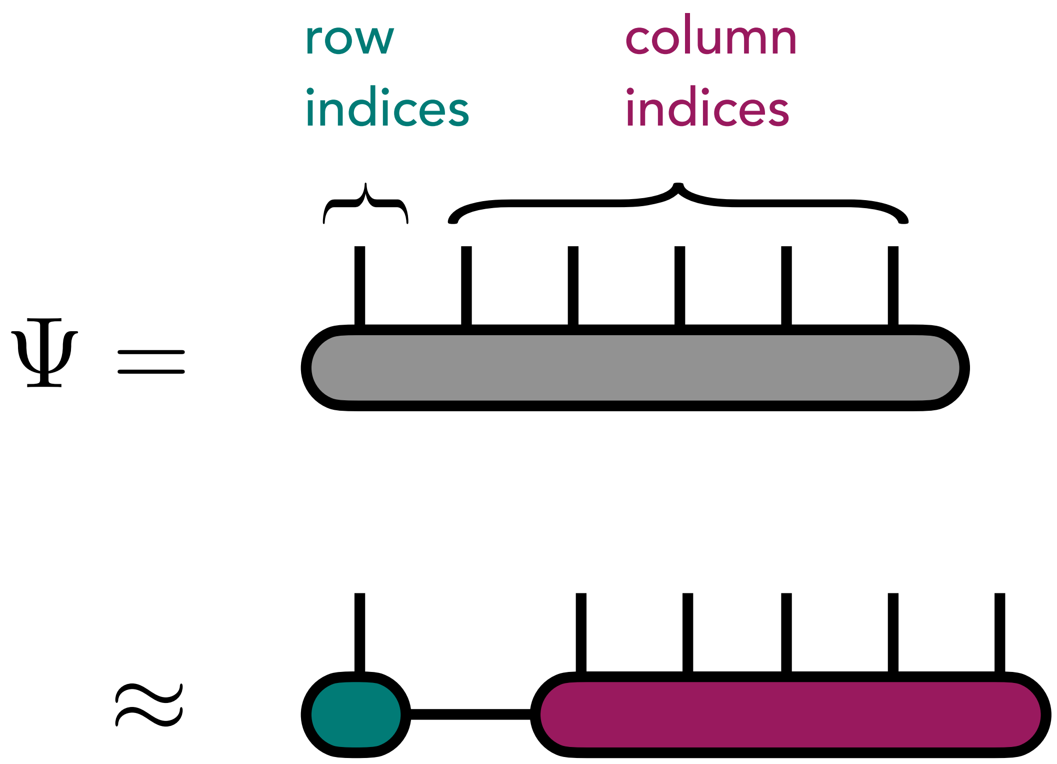


Motivates following decomposition

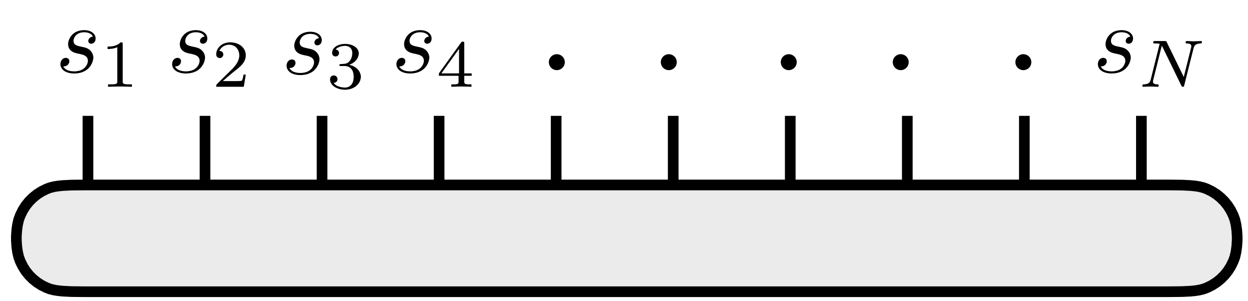
Low-rank factorization across all 1D bipartitions

Tensor Diagram Notation

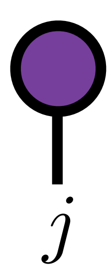
Convenient for notating large tensors

N-index tensor = shape with N lines

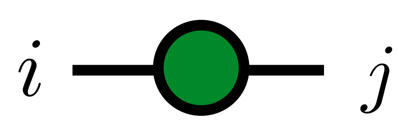
$$T^{s_1 s_2 s_3 \cdots s_N} =$$



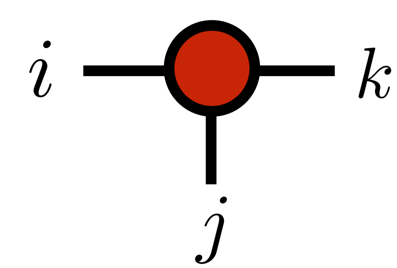
Low-order tensor examples:



v_j



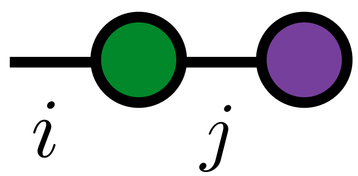
M_{ij}



T_{ijk}

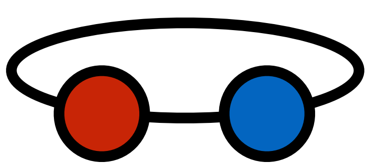
Tensor Diagram Notation

Joined lines are contracted, can omit names



↔

$$\sum_j M_{ij} v_j$$

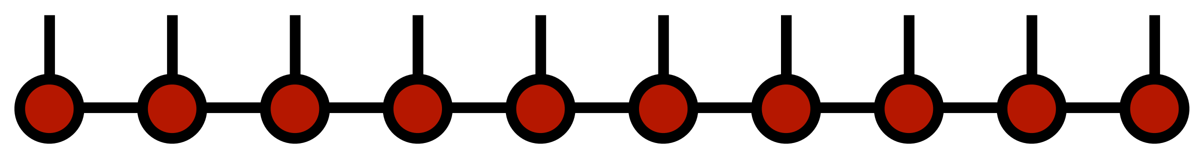


↔

$$A_{ij} B_{ji} \quad = \mathrm{Tr}[AB]$$

Notation – Tensor Diagrams

Compare to traditional notation



$$T^{n_1 n_2 n_3 n_4 n_5 n_6} = \sum_{\mathbf{a}} A^{n_1}_{a_1} A^{n_2}_{a_1 a_2} A^{n_3}_{a_2 a_3} A^{n_4}_{a_3 a_4} A^{n_5}_{a_4 a_5} A^{n_6}_{a_5 a_6} A^{n_7}_{a_6}$$

hard to write and interpret, many index names...

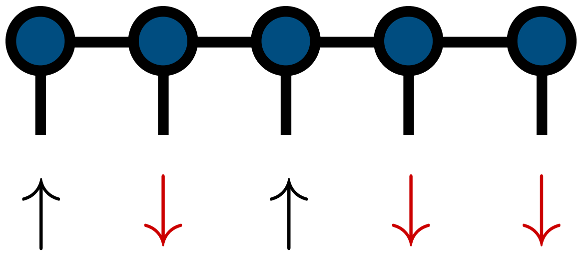
Following decomposition known as *matrix product state* (MPS) [1,2]

Simplest example of a *tensor network*

[1] Östlund, Rommer, PRL 75, 3537 (1995)

[2] Vidal, PRL 91, 147902 (2003)

Name matrix product state refers to retrieving elements:



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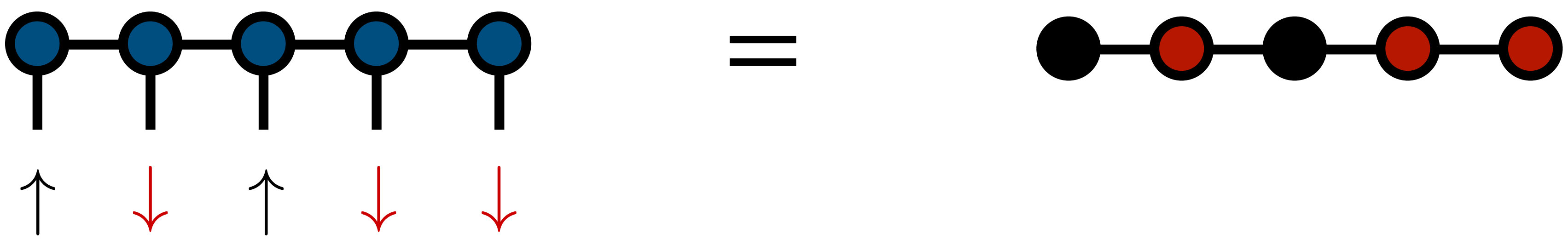

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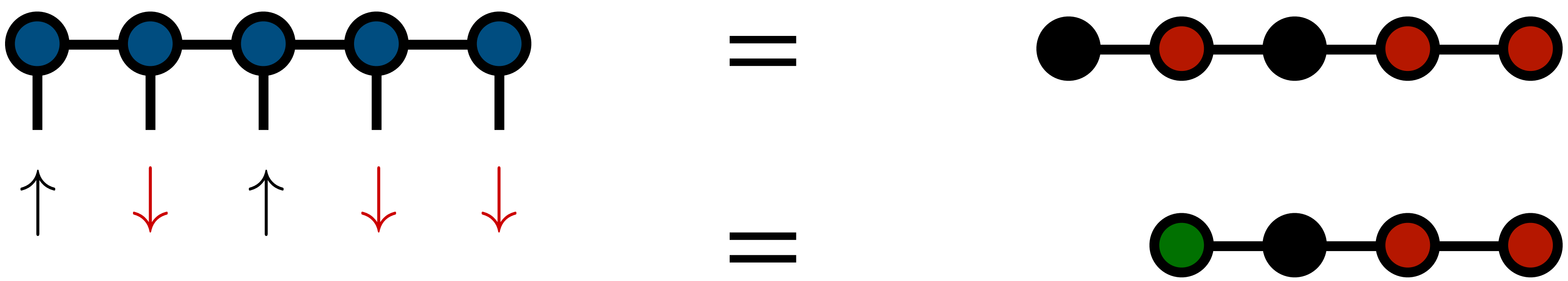

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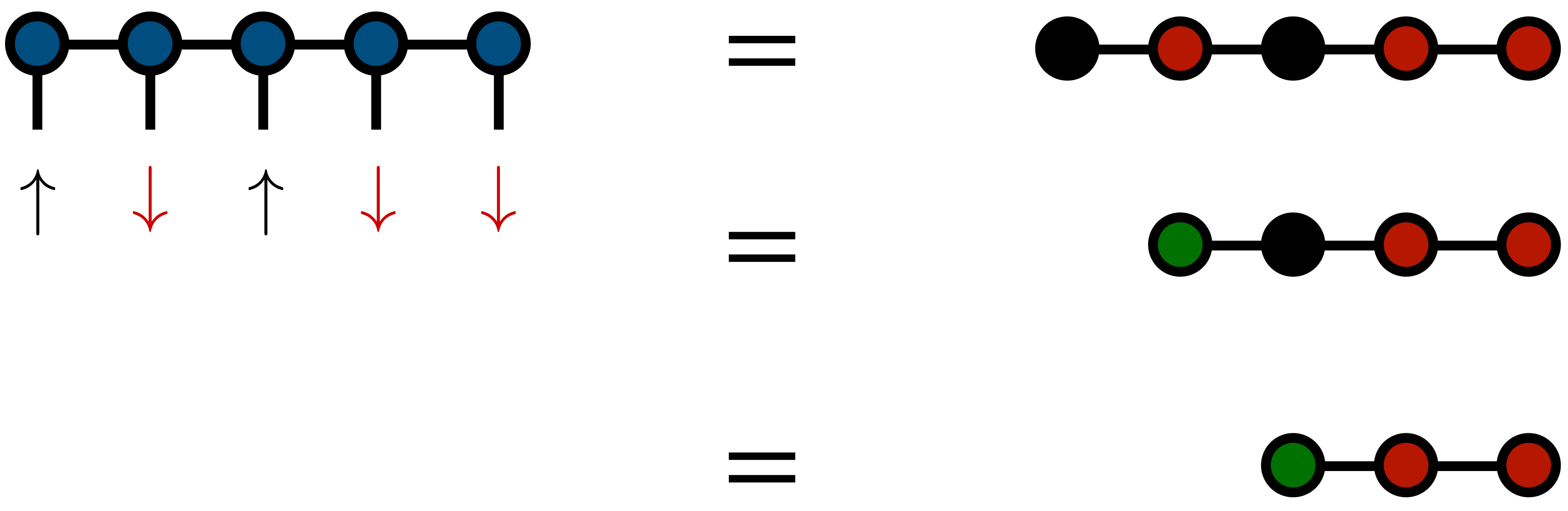

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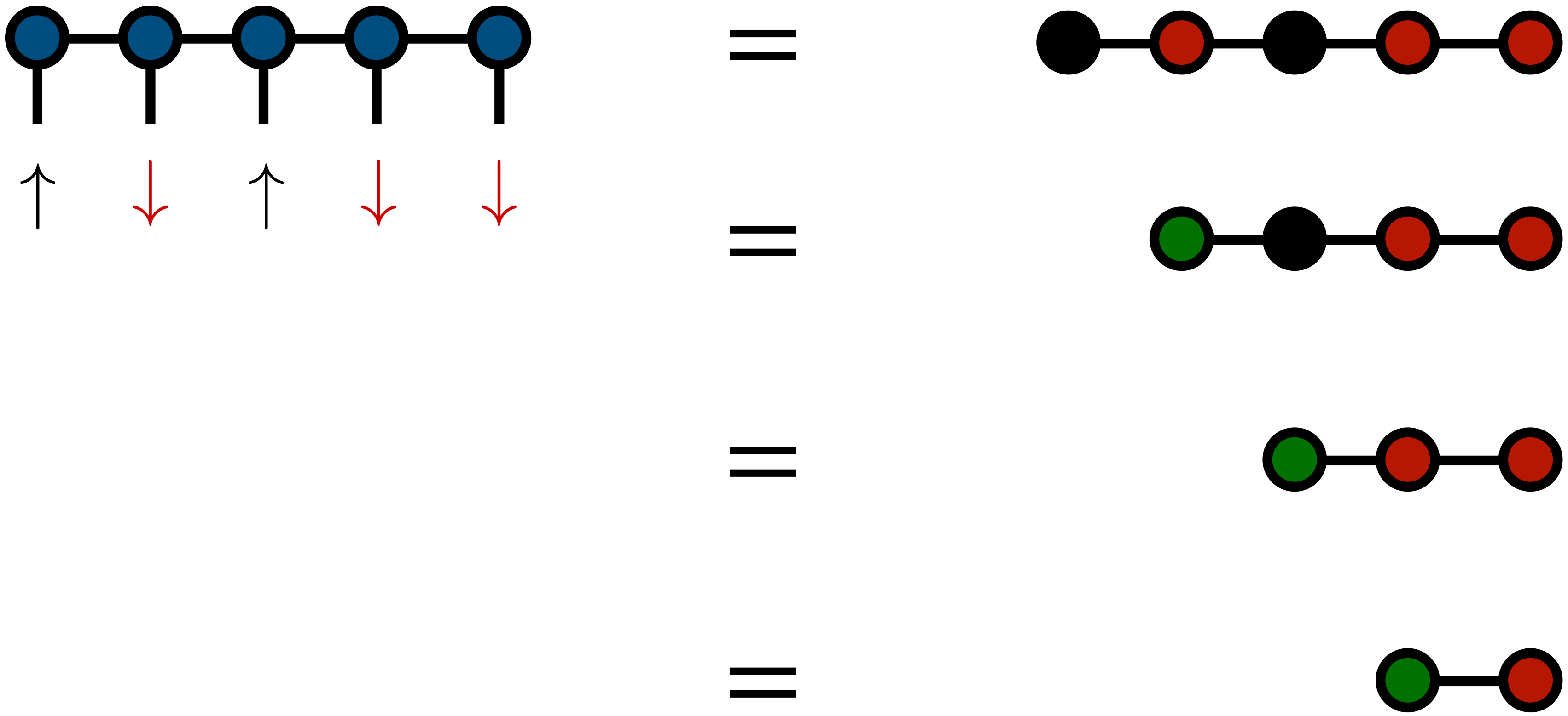

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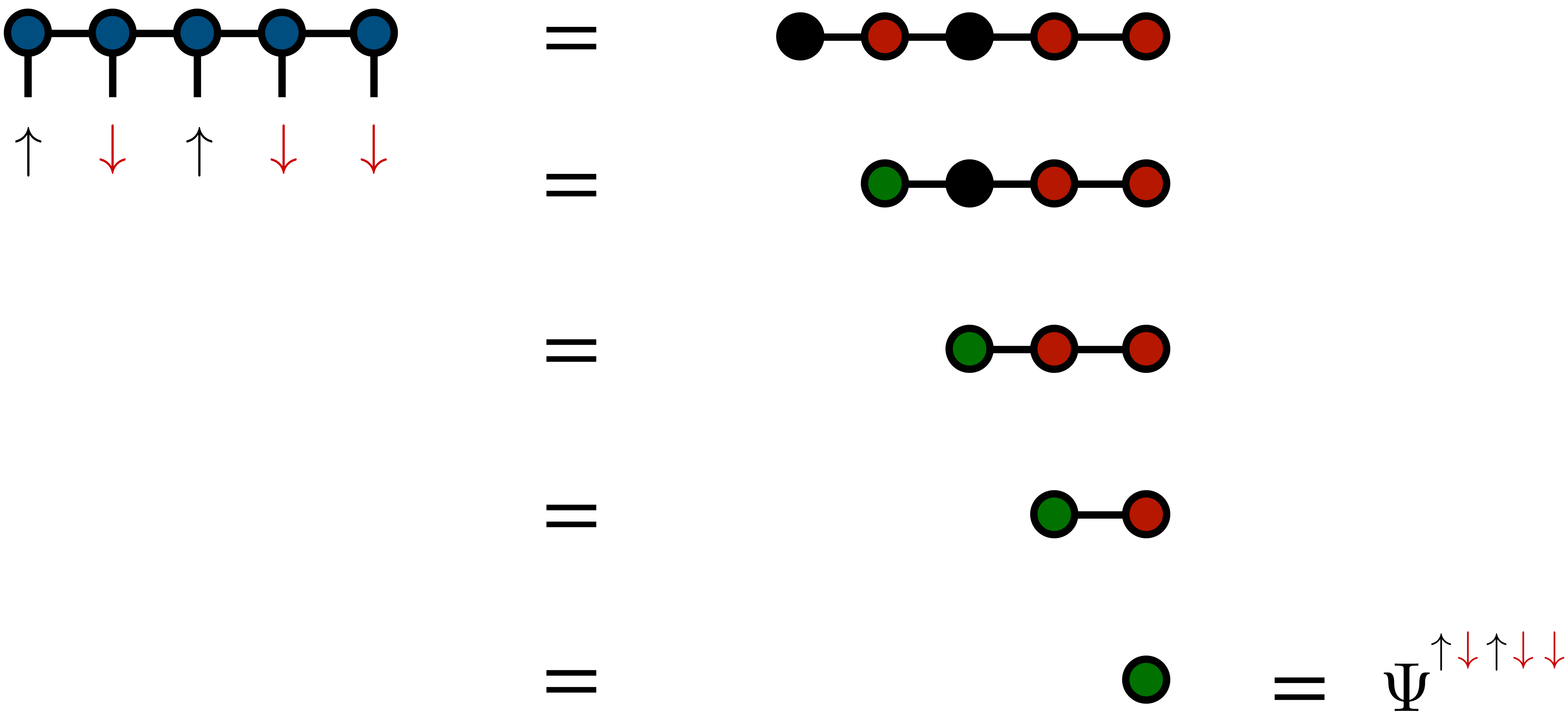
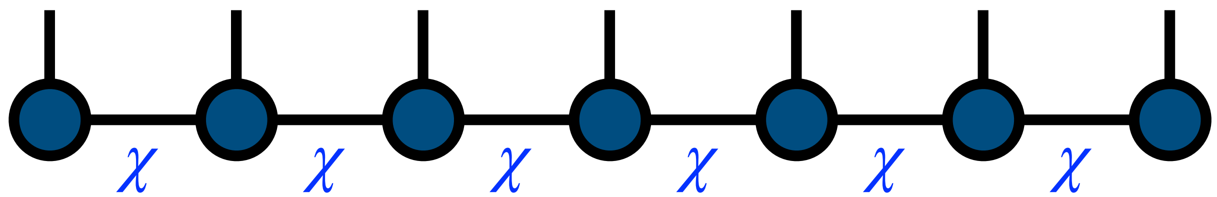


Size of Matrix Product States (MPS)

Main control parameter is bond dimension χ

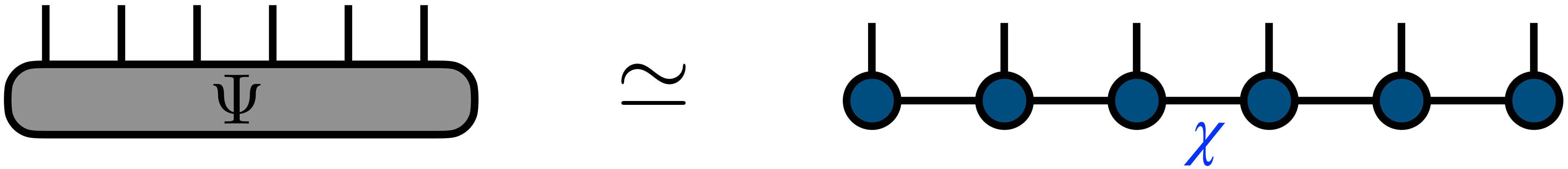


MPS tensors have $4\chi^2$ entries

Reduces memory needed from $4^N \longrightarrow 4N\chi^2$

For $\chi = 4^{N/2}$, can represent any state

When can MPS be used?

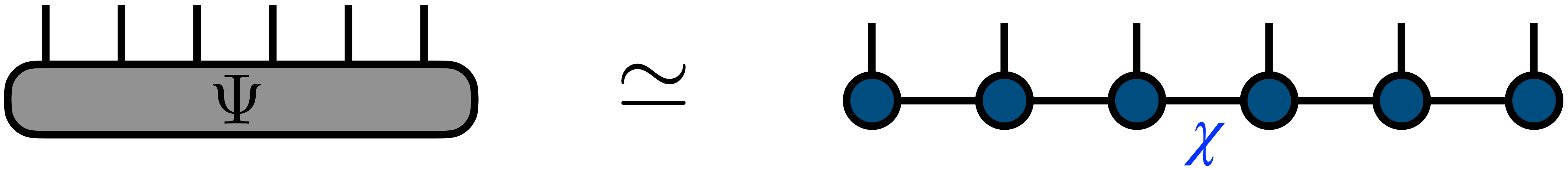


Bond dimension χ bounds *quantum entanglement* S between halves of system as

$$S \leq \ln \chi$$

Tensor network $\Longrightarrow$ low-entanglement state

When can MPS be used?



Has been proven[1] that

- ground states of
- finite-range 1D Hamiltonians with
- gap to first excited state

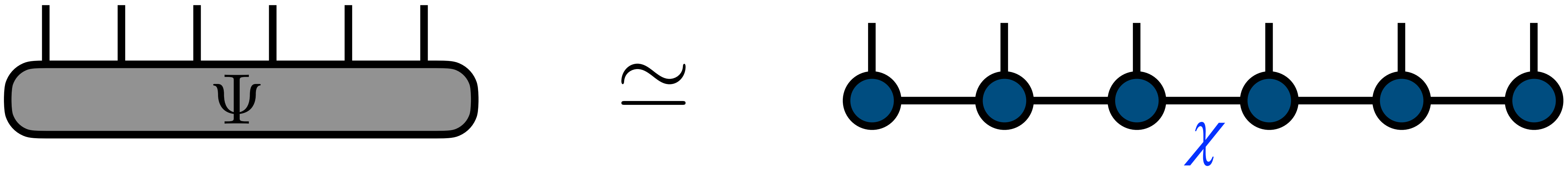
are low-entangled states

They are tensor networks!

Can refine further: area law, entanglement scaling[2]

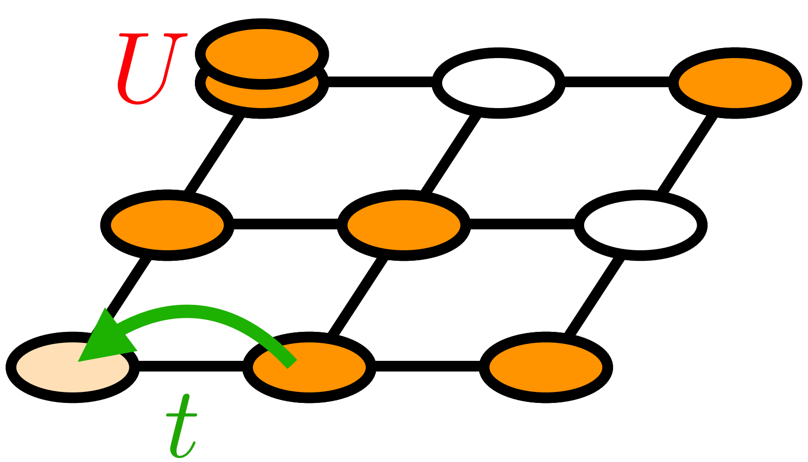
[1] Hastings, J. Stat. Mech, P08024 (2007)
[2] Evenbly, Vidal, J. Stat. Phys. 145 (2011)

When can MPS be used?



For the electronic Hubbard model:

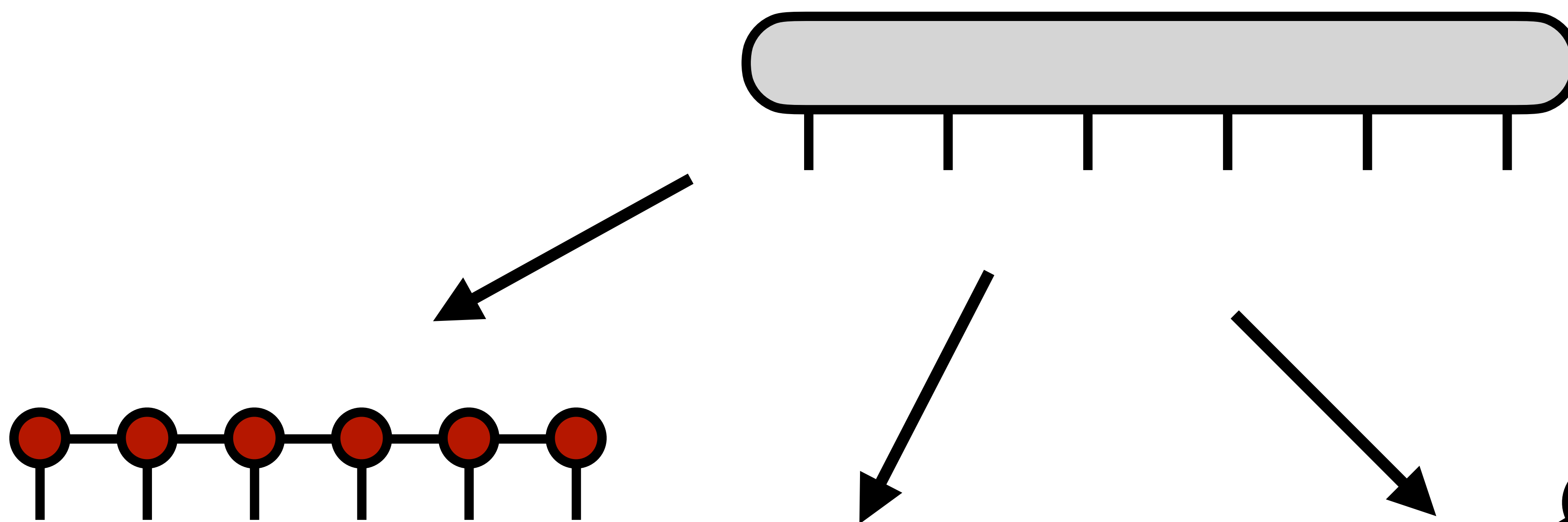
- works for all U (best for large U!)
- can be applied at high or low temperature T
- challenges remain to handle large 2D systems



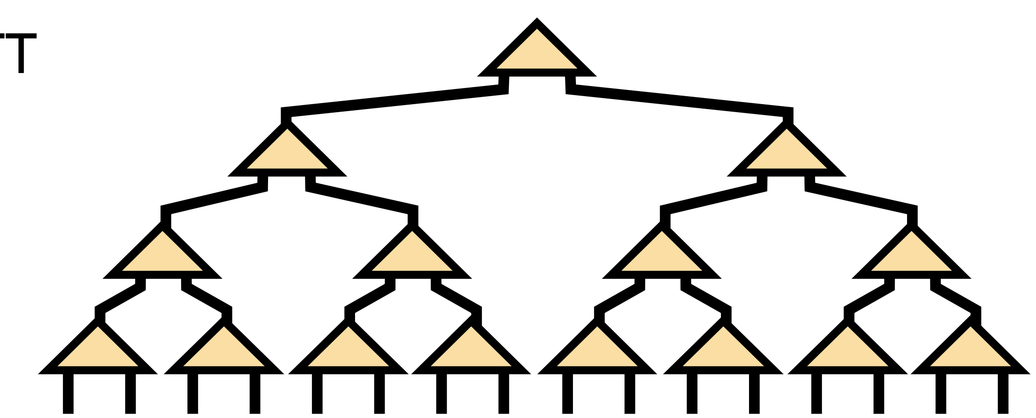
Tensor Networks

Many other tensor network formats

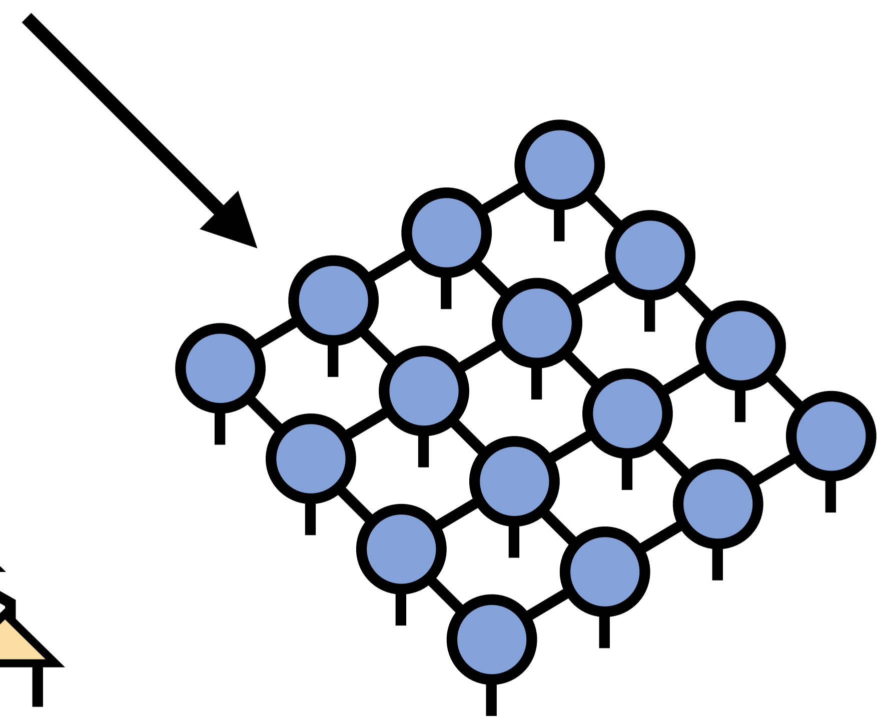
Varying expressiveness, algorithms, and research questions



MPS / TT



tree tensor network
/ hierarchical Tucker



PEPS / tensor grid

Optimizing Tensor Networks at Zero Temperature

How to determine parameters of a tensor network?

Simplest scheme: imaginary time evolution

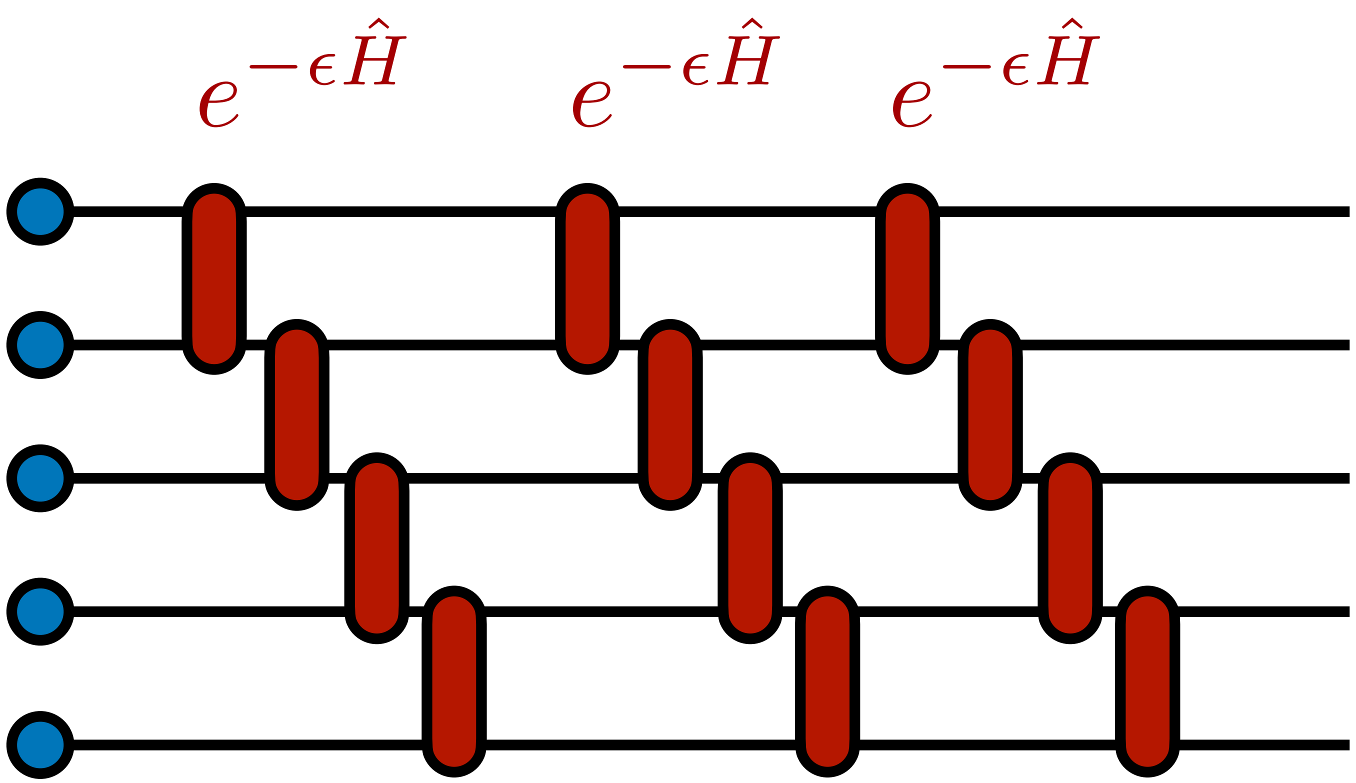
Compute: $e^{-\tau \hat{H}}|\psi_0\rangle \rightarrow |\psi_\tau\rangle$

For large $\tau \rightarrow \infty$, $\hat{H}|\psi_\infty\rangle = E|\psi_\infty\rangle$ (becomes ground state)

How to determine parameters of a tensor network?

Simplest scheme: imaginary time evolution

Compute: $e^{-\tau \hat{H}} |\psi_0\rangle$ $\qquad \tau \to \infty$



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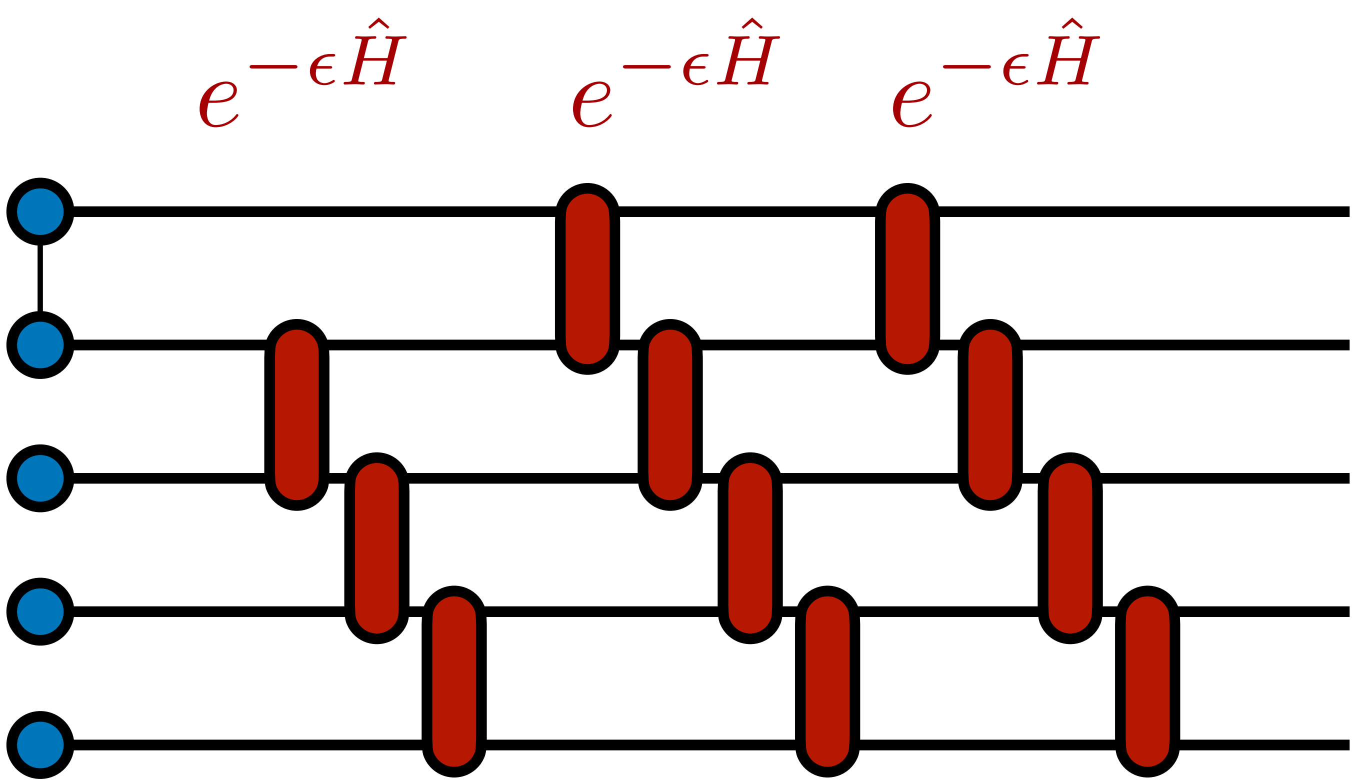

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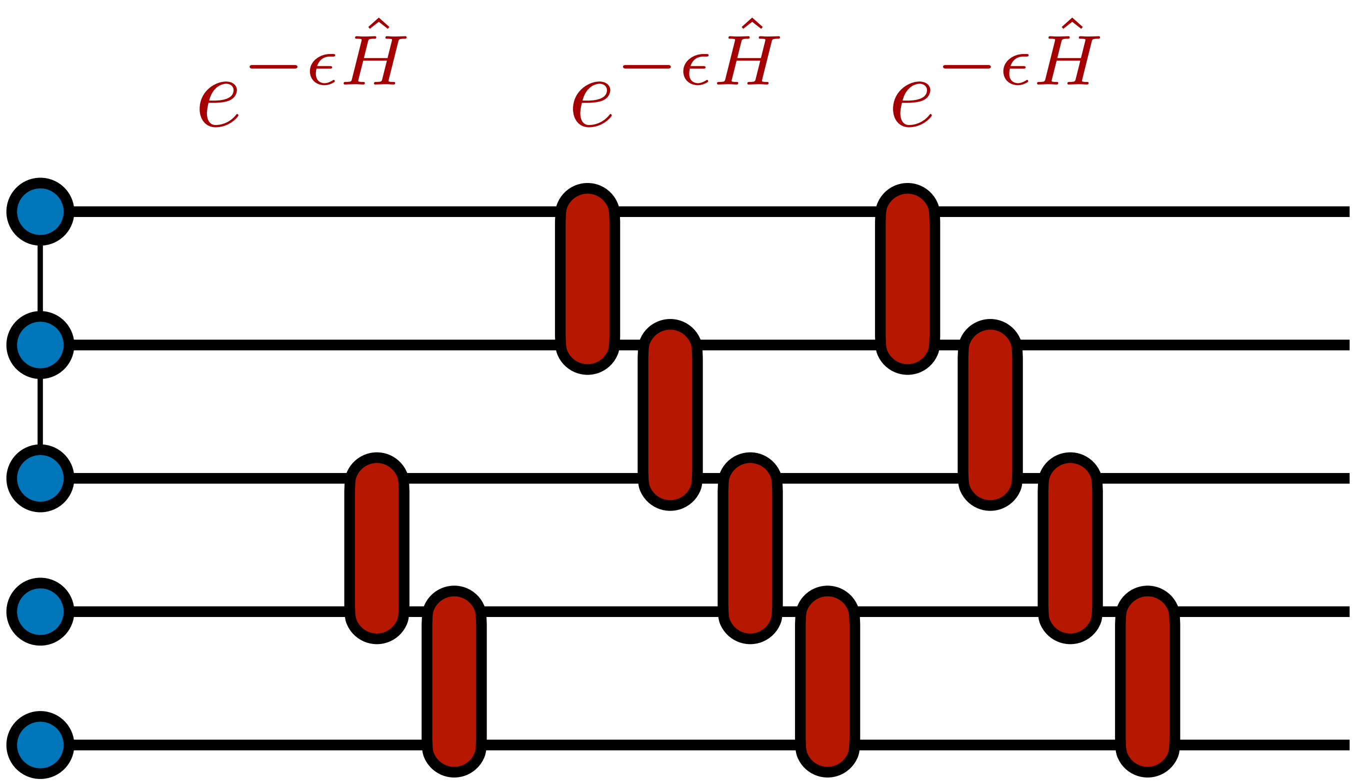

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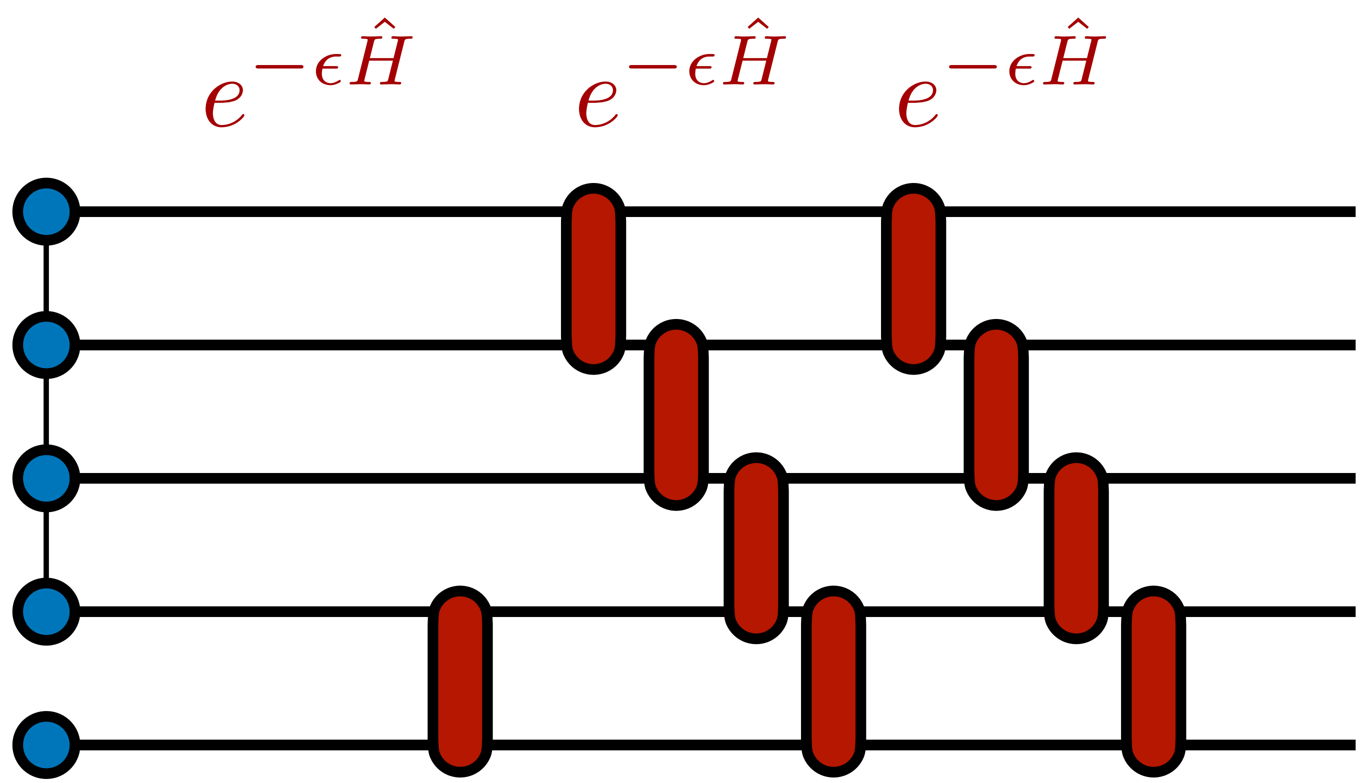

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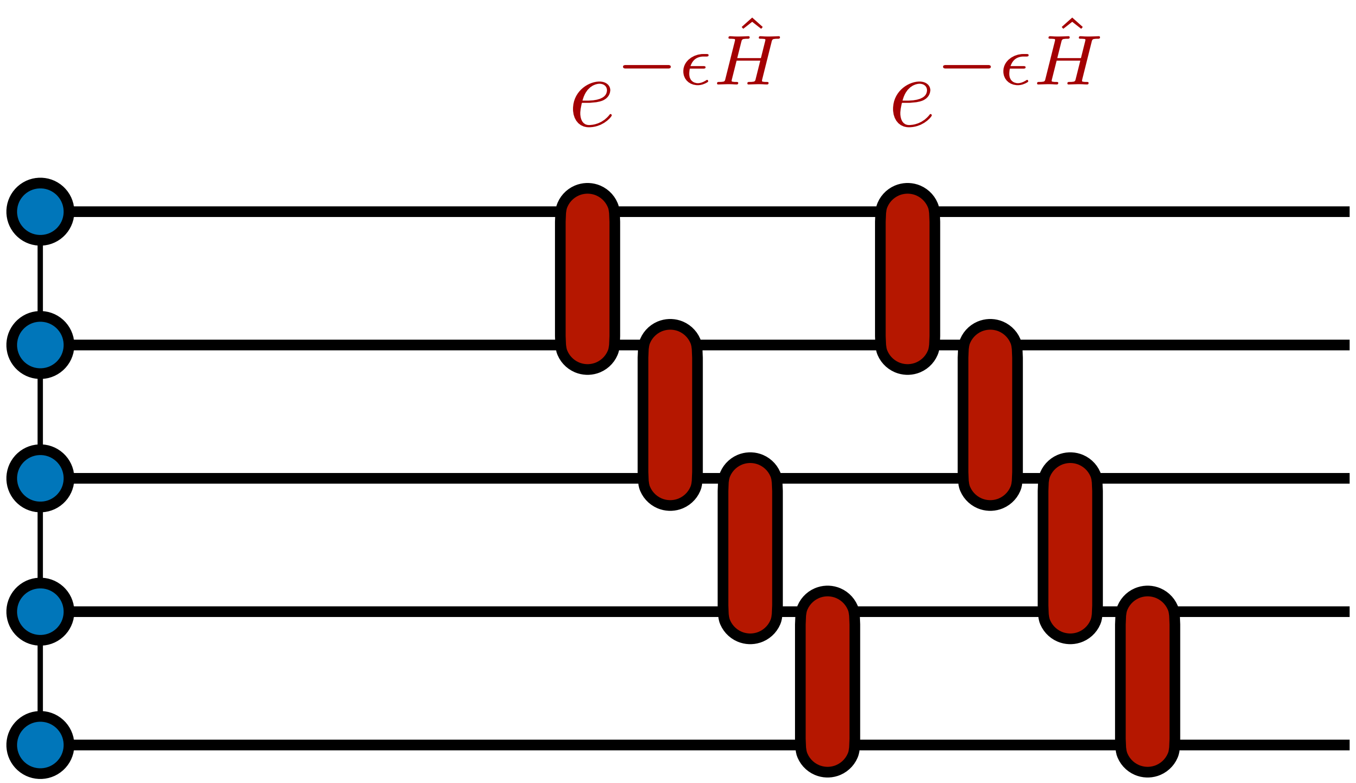

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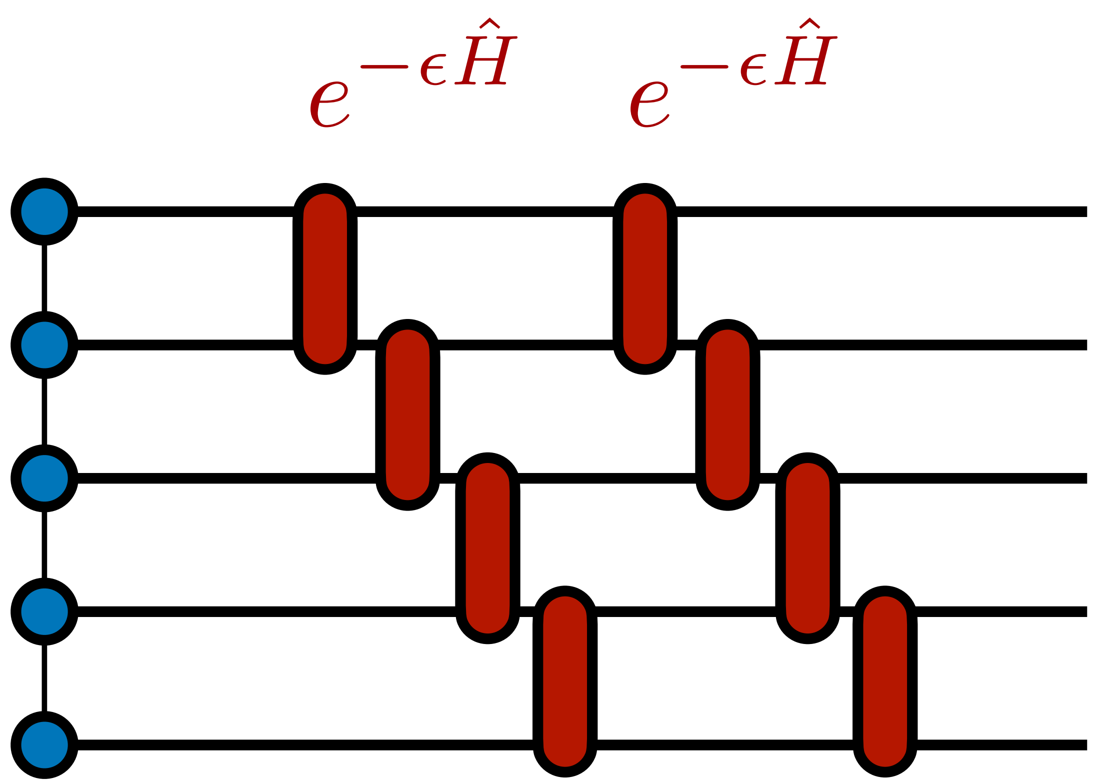
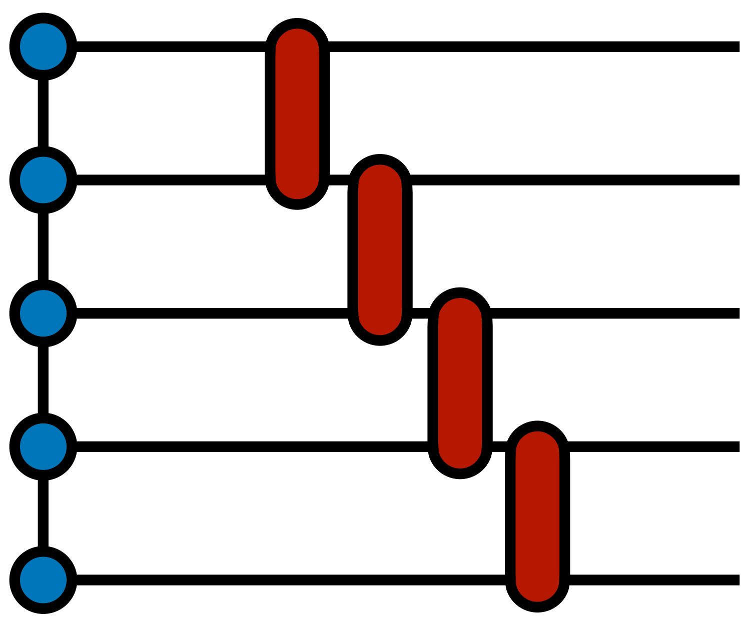


How to determine parameters of a tensor network?

Simplest scheme: imaginary time evolution

Compute: $e^{-\tau \hat{H}} |\psi_0\rangle$ $\tau \to \infty$

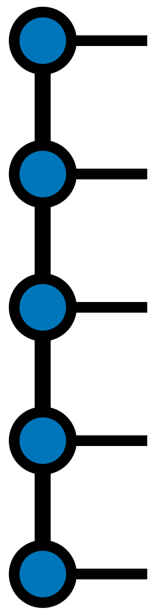
$$e^{-\epsilon \hat{H}}$$



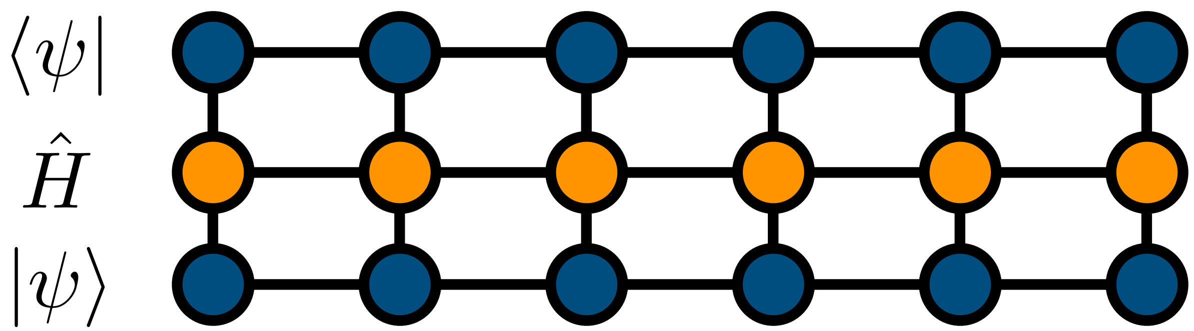
How to determine parameters of a tensor network?

Simplest scheme: imaginary time evolution

$$|\psi_\infty\rangle =$$



Even better scheme: density matrix renormalization group (DMRG) algorithm[1,2]

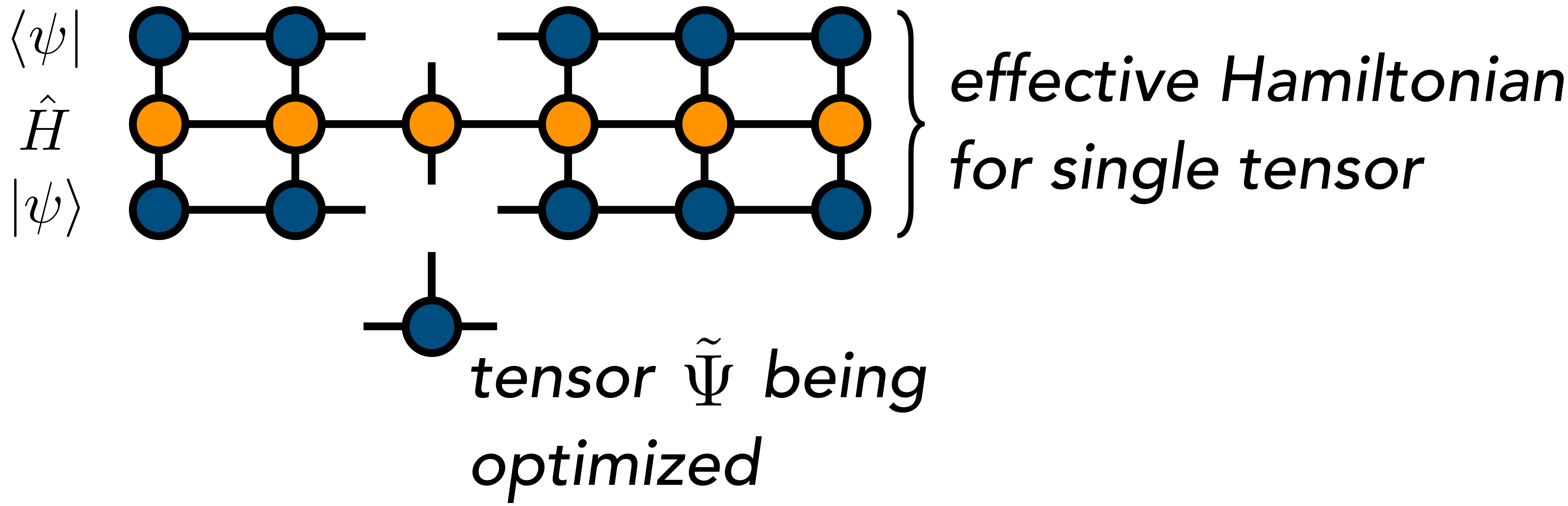


$$= \langle\psi|\hat{H}|\psi\rangle$$

want to minimize

[1] White, PRL 69 (1992)
[2] Schollwöck, Ann. Phys. 326 (2011)

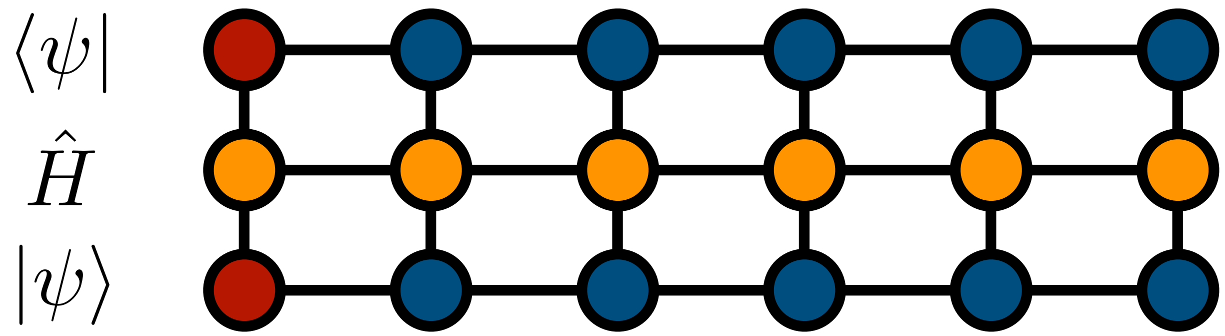
Strategy: improve one tensor at a time



Solve $\hat{H}_{\text{eff}}\tilde{\Psi} = E\tilde{\Psi}$ for just this one tensor

Strategy: improve one tensor at a time

"Sweep" back and forth over all the tensors



Strategy: improve one tensor at a time

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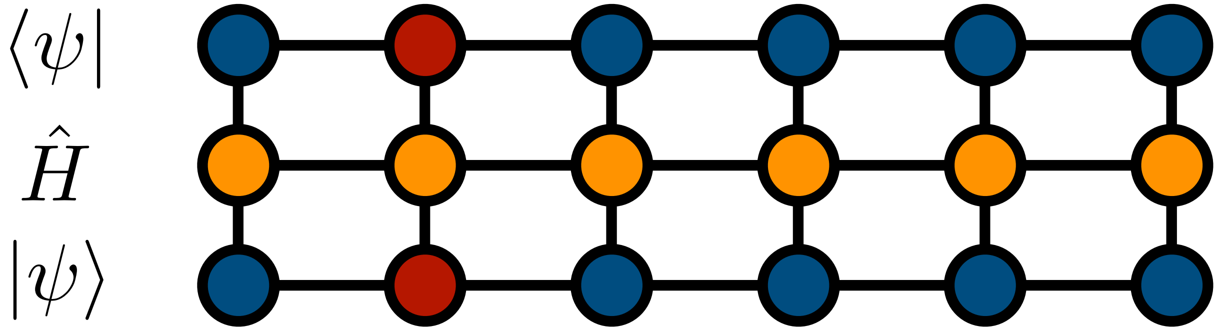
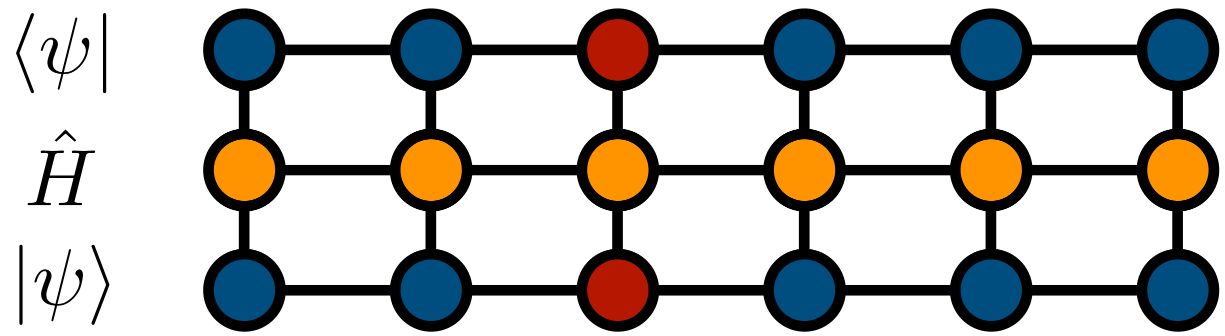


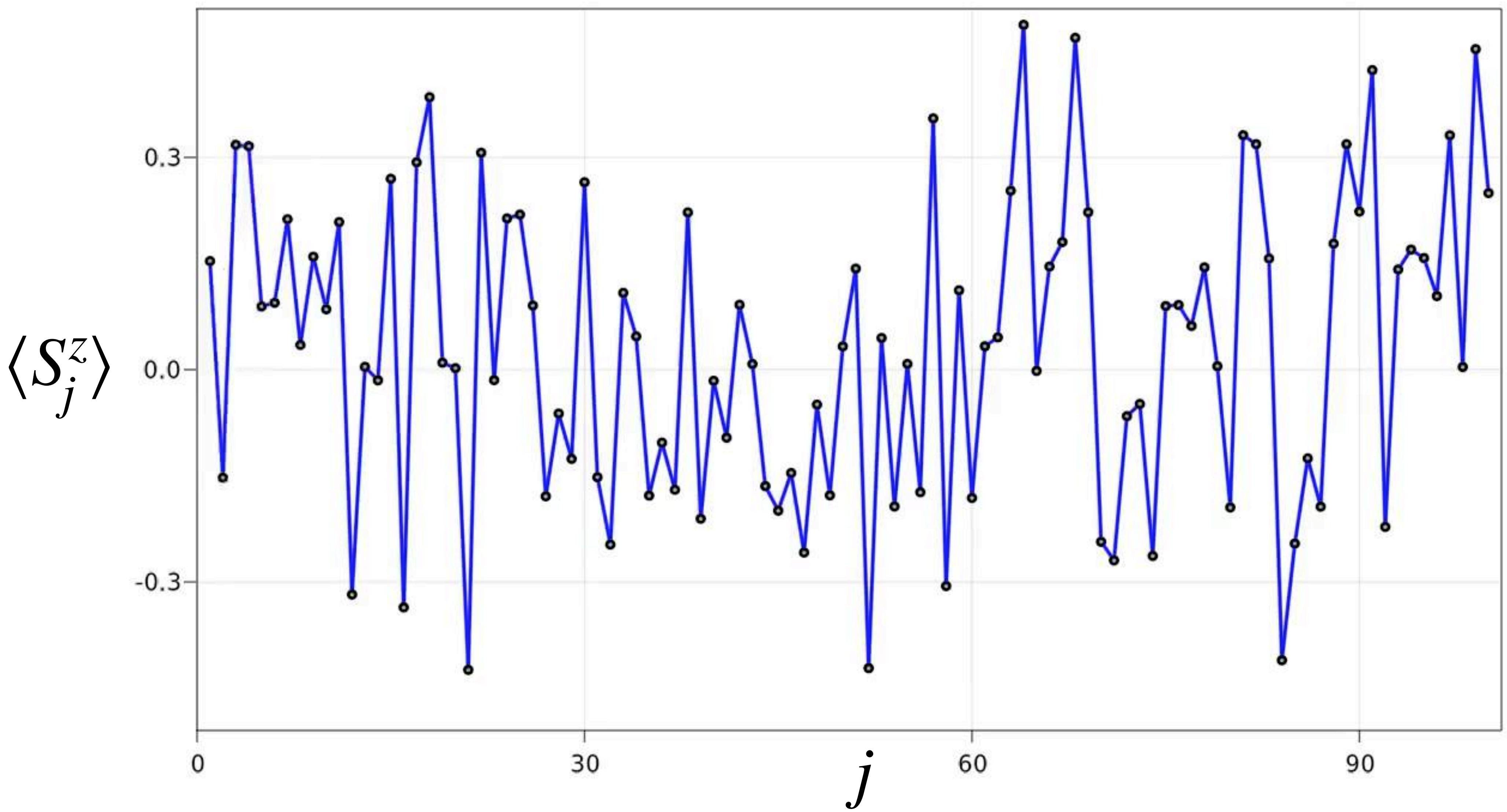
Strategy: improve one tensor at a time

"Sweep" back and forth over all the tensors



Example of DMRG in action

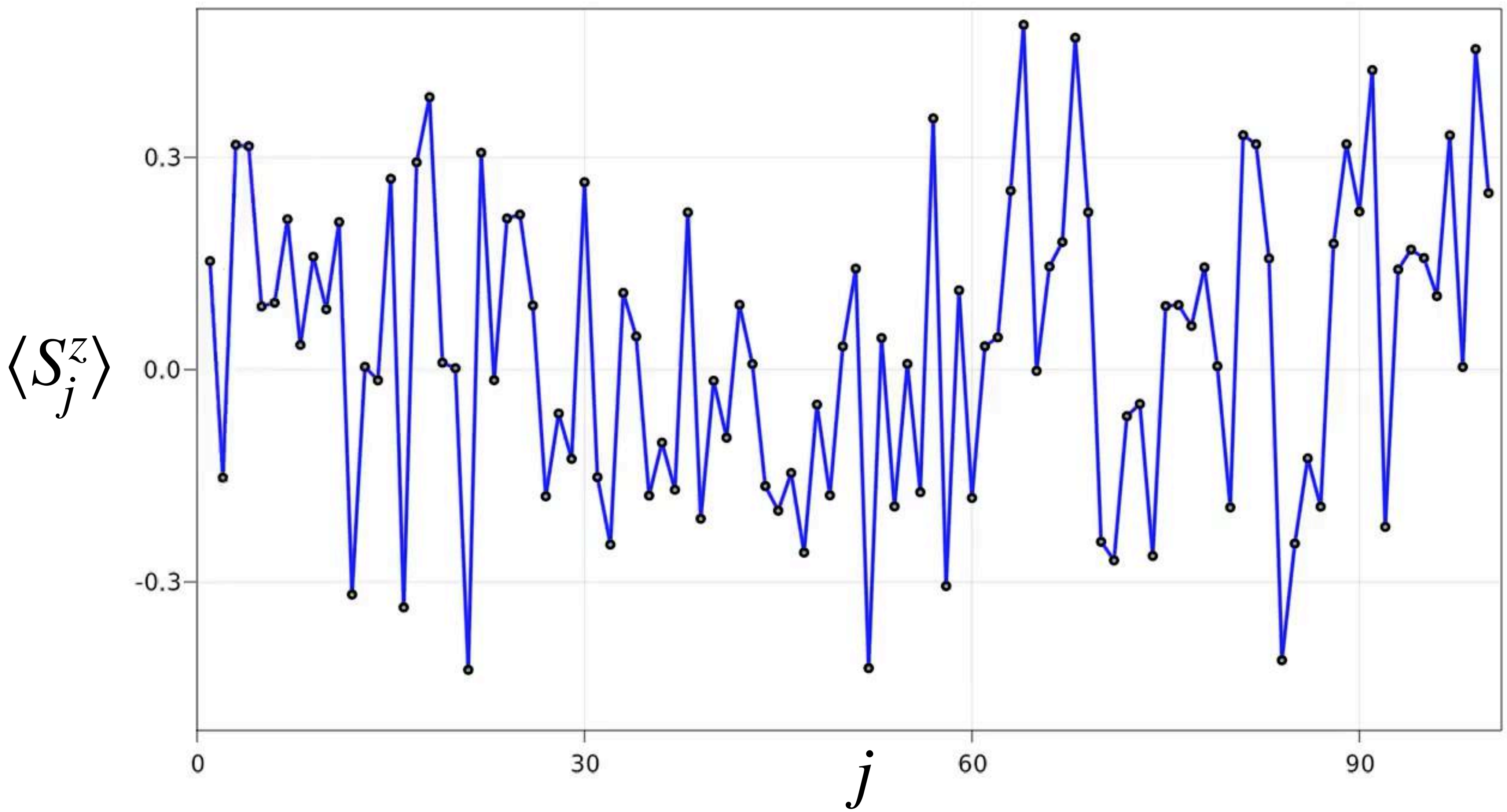
1D Heisenberg model $\hat{H} = \sum_j \vec{S}_j \cdot \vec{S}_{j+1}$



Heisenberg model is $U/t \to \infty$ limit of Hubbard model

Example of DMRG in action

1D Heisenberg model $\hat{H} = \sum_j \vec{S}_j \cdot \vec{S}_{j+1}$



Heisenberg model is $U/t \to \infty$ limit of Hubbard model

Finite Temperature
Tensor Networks

Finite Temperature Quantum

Textbook prescription: "just" obtain all eigenstates

$$\hat{H}|\epsilon_n\rangle = \epsilon_n|\epsilon_n\rangle$$

Then finite T density matrix is nicely diagonal

$$e^{-\hat{H}/T} = \sum_n e^{-\epsilon_n/T}|\epsilon_n\rangle\langle\epsilon_n|$$

Finite Temperature Quantum

Textbook prescription: "just" obtain all eigenstates

$$\hat{H}|\epsilon_n\rangle = \epsilon_n|\epsilon_n\rangle$$

Thermal averages given by

$$\langle\hat{A}\rangle = \frac{1}{Z}\sum_n e^{-\epsilon_n/T}\langle\epsilon_n|\hat{A}|\epsilon_n\rangle$$

But eigenstates terrible numerically! $\hat{H}|\epsilon_n\rangle = \epsilon_n|\epsilon_n\rangle$

- Exponentially small energy spacing
- Non-classical even at high T
- Very *high entanglement*

↓

No chance for tensor networks!

Need a different way...

First write density matrix symmetrically

$$e^{-\beta \hat{H}} = e^{-\frac{\beta}{2}\hat{H}} e^{-\frac{\beta}{2}\hat{H}} \qquad \beta = \frac{1}{T}$$

Insert complete set of states

$$e^{-\beta \hat{H}} = \sum_i \underbrace{e^{-\frac{\beta}{2}\hat{H}}|i\rangle}\langle i|e^{-\frac{\beta}{2}\hat{H}} \propto \sum_i |\phi_i\rangle\langle\phi_i|$$

Freedom to choose these $|\phi_i\rangle \propto e^{-\frac{\beta}{2}\hat{H}}|i\rangle$

By decomposing finite T state

$$e^{-\beta \hat{H}} = \sum_i e^{-\frac{\beta}{2}\hat{H}} |i\rangle\langle i| e^{-\frac{\beta}{2}\hat{H}} \propto \sum_i |\phi_i\rangle\langle\phi_i|$$

Obtain observables as

$$\langle\hat{A}\rangle = \frac{1}{\mathcal{Z}}\mathrm{Tr}\left[e^{-\beta\hat{H}}\hat{A}\right] = \frac{1}{\mathcal{Z}}\sum_i P_i \ \langle\phi_i|\hat{A}|\phi_i\rangle$$

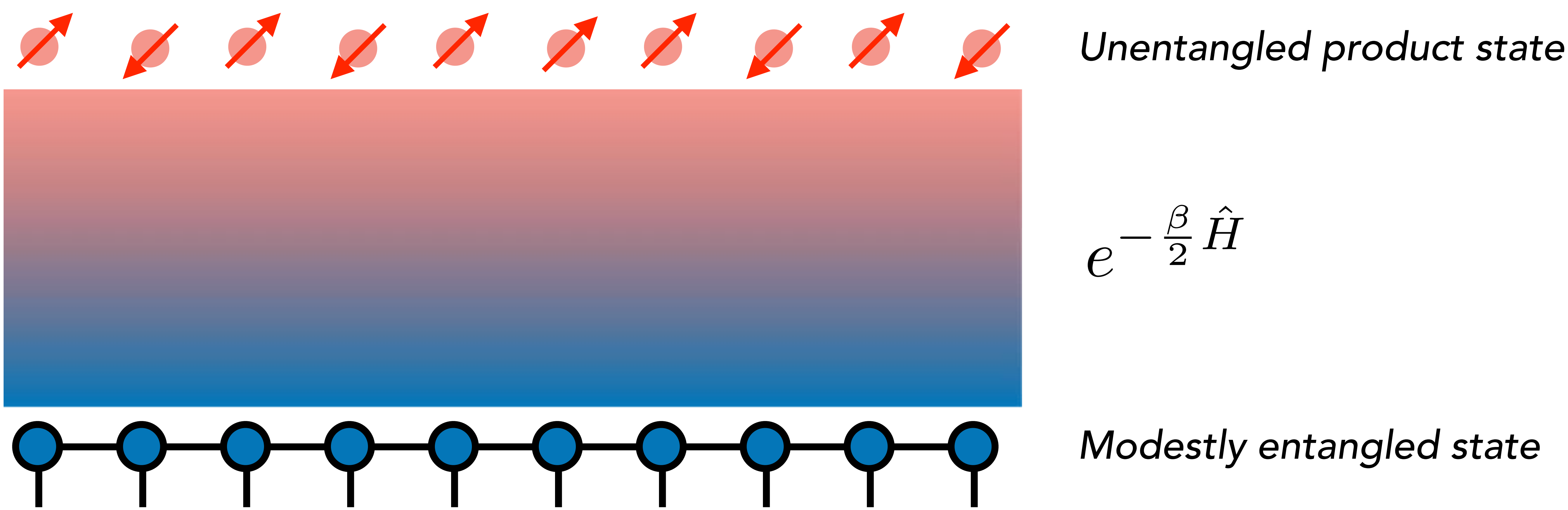
an average over pure states

Expanding $e^{-\beta \hat{H}} \propto \sum_i |\phi_i\rangle\langle\phi_i|$

To give tensor networks their best chance

choose $|\phi_i\rangle \propto e^{-\frac{\beta}{2}\hat{H}}|i\rangle$ to "descend" from

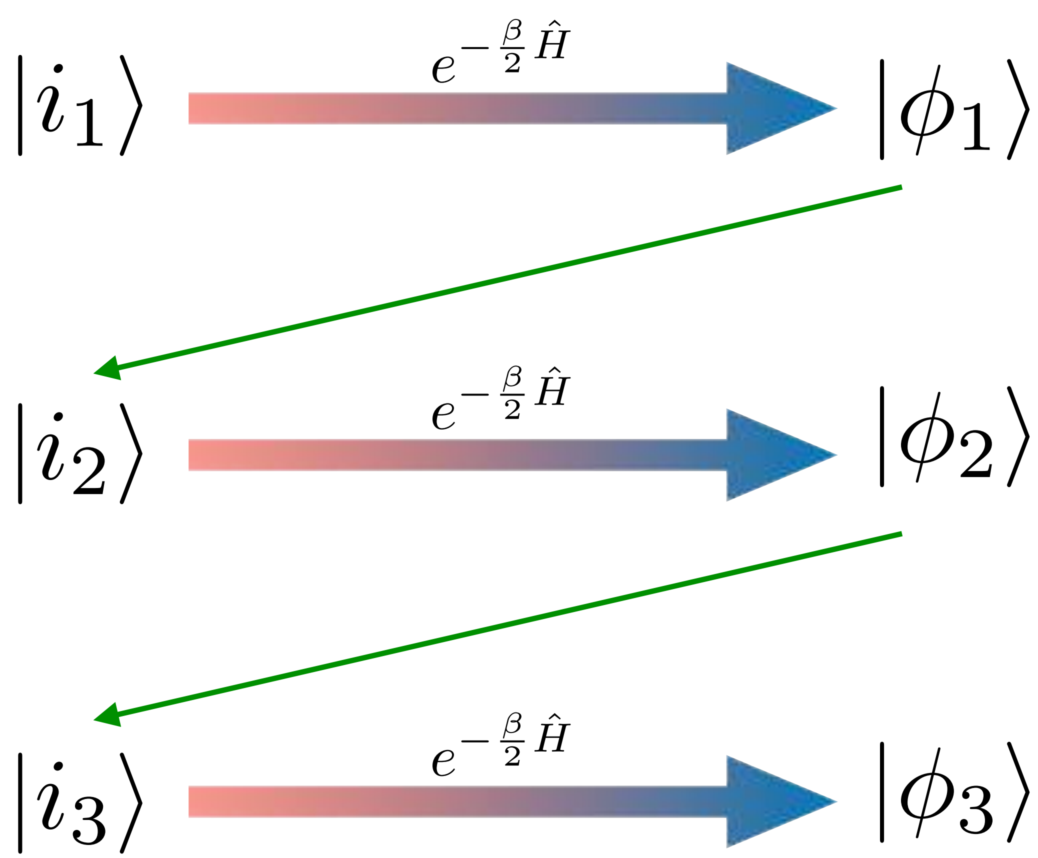
untentangled (zero-entanglement) states



☑ Solved problem of representing $|\phi_i\rangle \propto e^{-\frac{\beta}{2}\hat{H}}|i\rangle$
(choose $|i\rangle$ as product states)

One more problem: too many states –
there are exponentially many $|i\rangle$ and thus $|\phi_i\rangle$

☑ Solution: sample over the $|i\rangle$



$$p(\phi_1 \to i_2) = |\langle i_2|\phi_1\rangle|^2$$

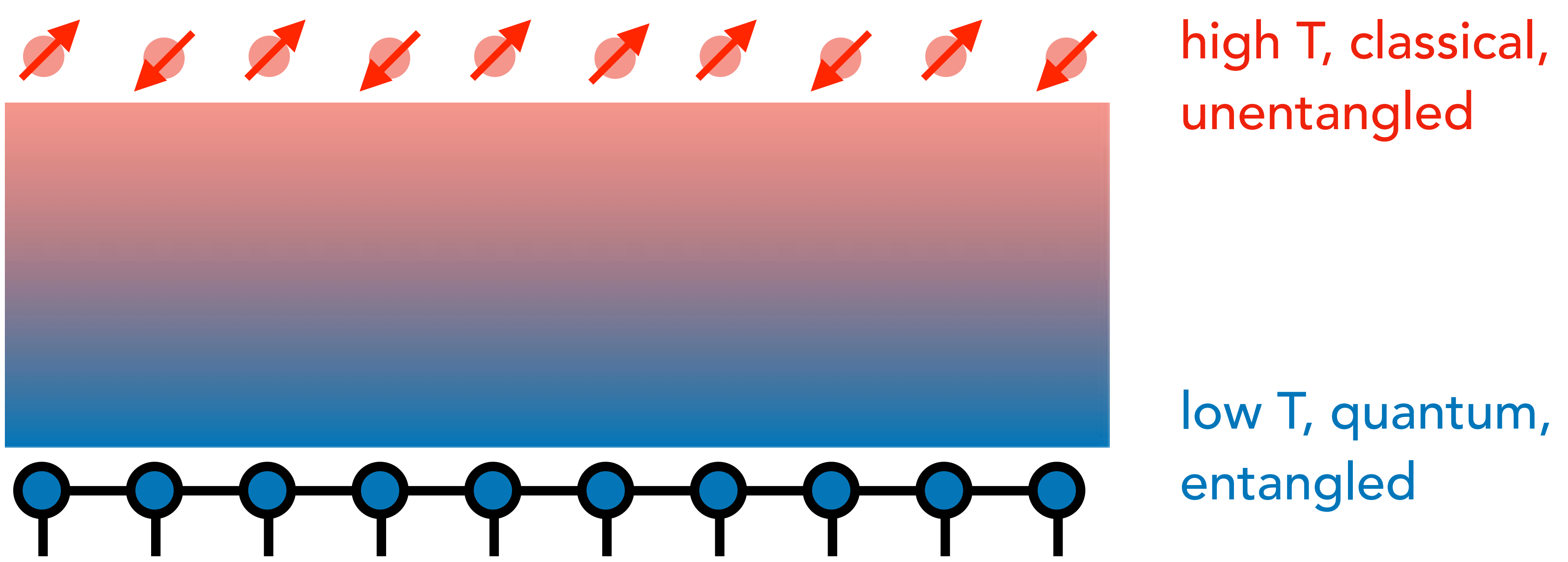
$$p(\phi_2 \to i_3) = |\langle i_3|\phi_2\rangle|^2$$

Algorithm just described named
minimally entangled typical thermal states (**METTS**)[1,2]

$$|\phi_i\rangle \propto e^{-\frac{\beta}{2}\hat{H}}|i\rangle$$ METTS wavefunction

Quantum Monte Carlo where samples are
entangled wavefunctions, not classical configurations

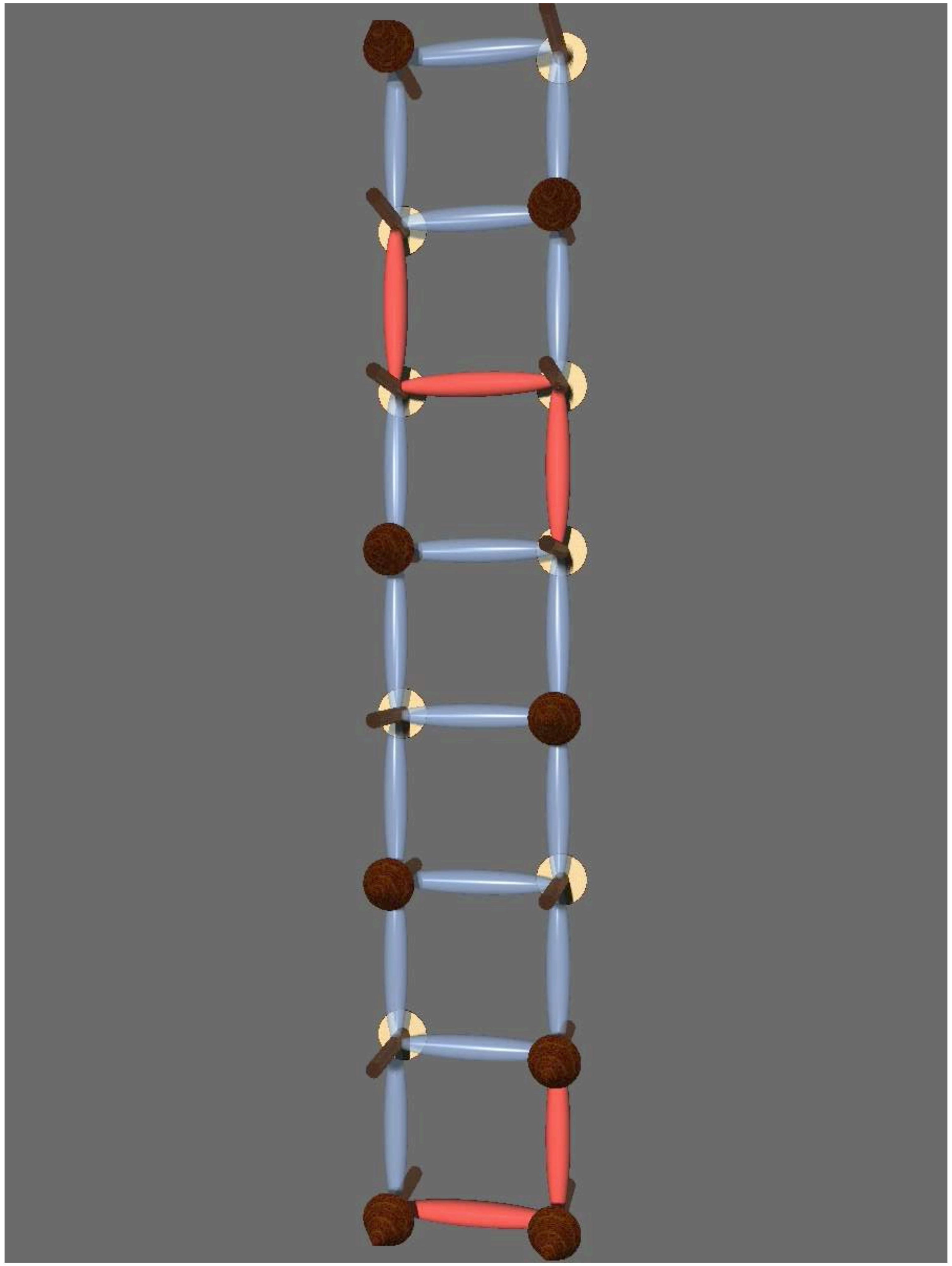
Classicality of METTS depend on T



[1] S.R. White, PRL (2009)
[2] Stoudenmire, White, NJP (2010)

Minimally Entangled Typical Thermal States

Movie of METTS algorithm (S=1/2 Heisenberg ladder, $\beta = 5$)



$$e^{-\frac{\beta}{2}\hat{H}}|i_1\rangle$$

Minimally Entangled Typical Thermal States

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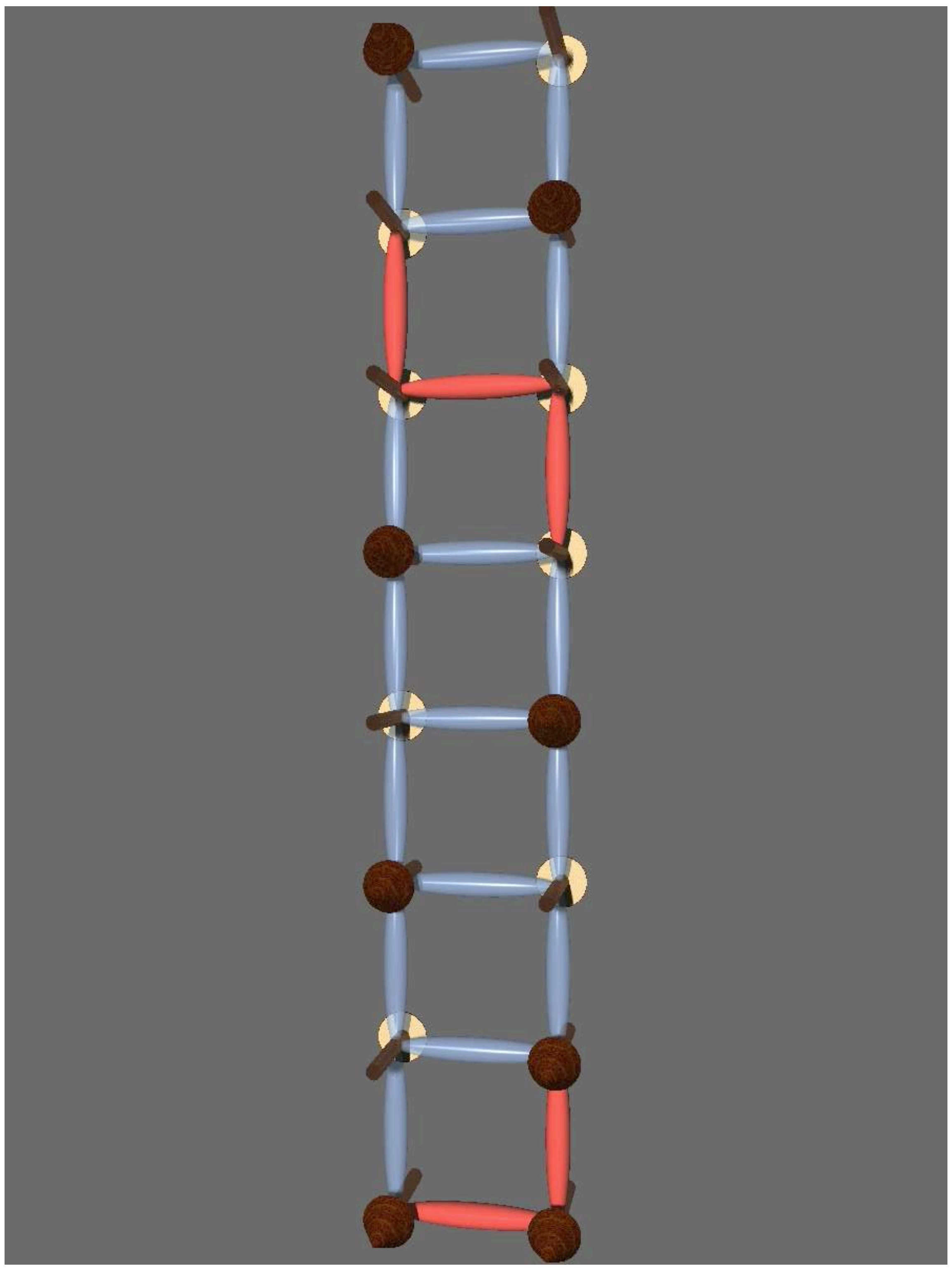

$$e^{-\frac{\beta}{2}\hat{H}}|i_1\rangle \longrightarrow |\phi_1\rangle$$

Minimally Entangled Typical Thermal States

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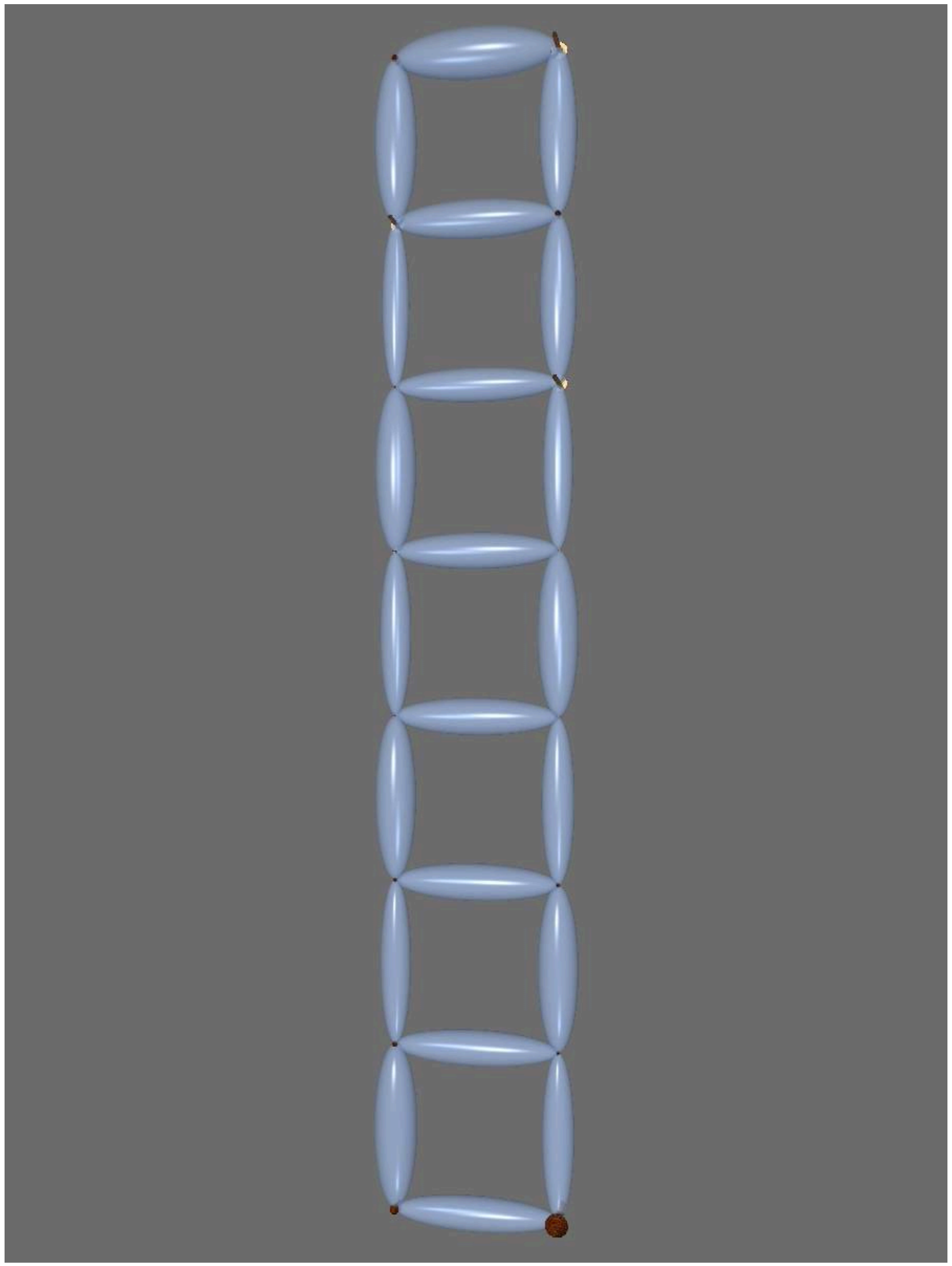

$$e^{-\frac{\beta}{2}\hat{H}}|i_1\rangle \rightarrow |\phi_1\rangle$$

$$e^{-\frac{\beta}{2}\hat{H}}|i_2\rangle$$

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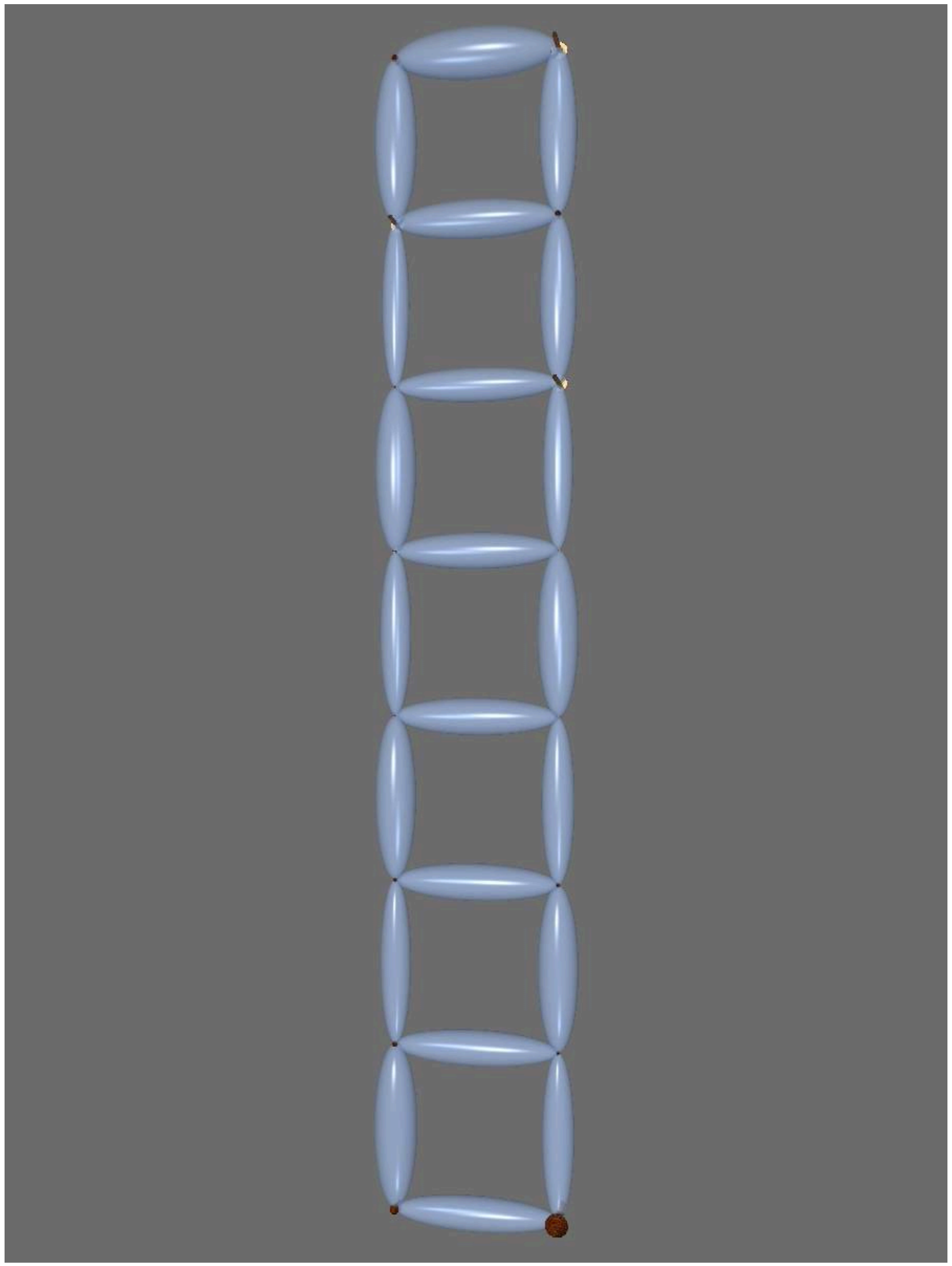

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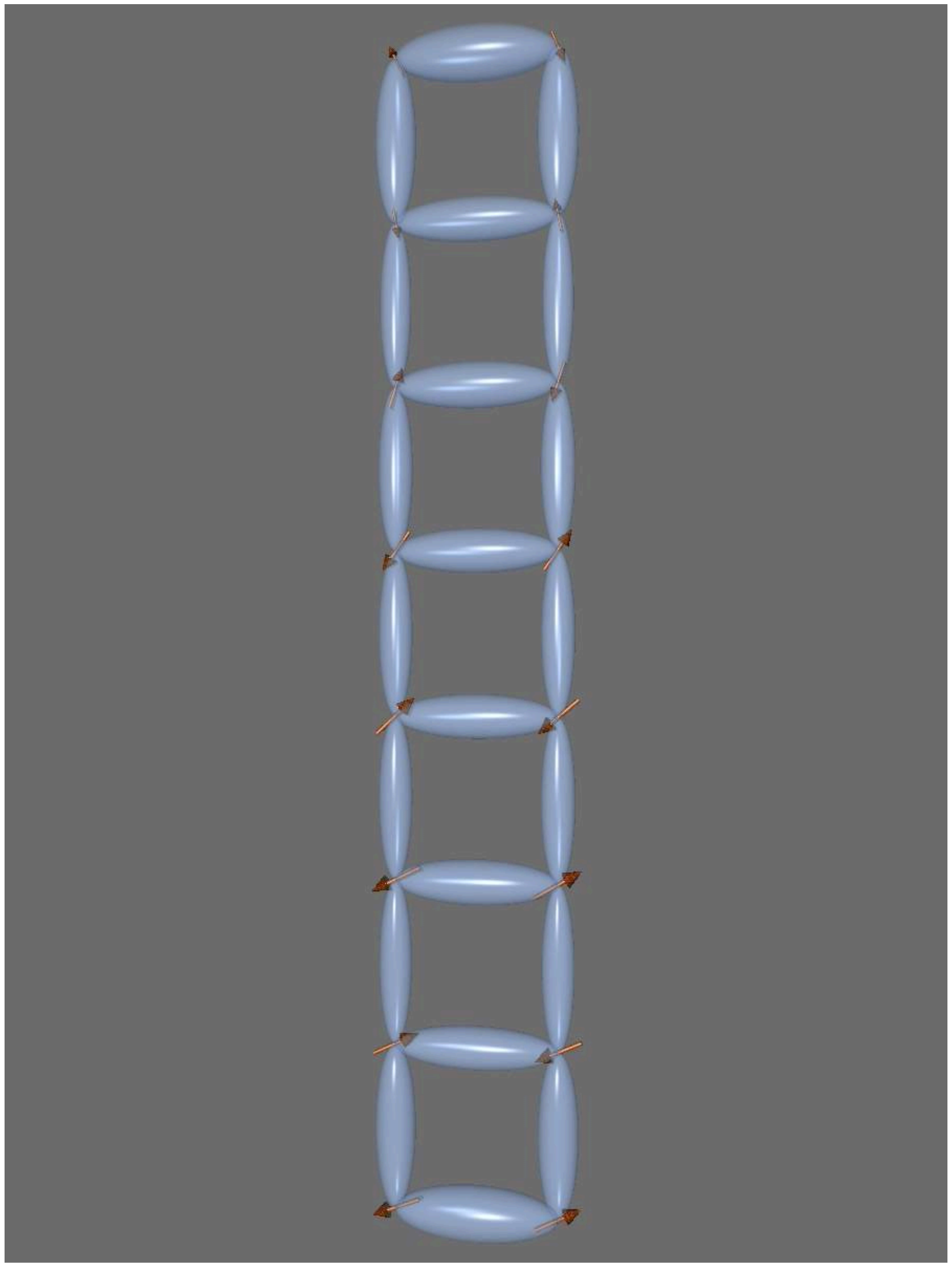

$$e^{-\frac{\beta}{2}\hat{H}}|i_1\rangle \rightarrow |\phi_1\rangle$$

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$$e^{-\frac{\beta}{2}\hat{H}}|i_3\rangle$$

Minimally Entangled Typical Thermal States

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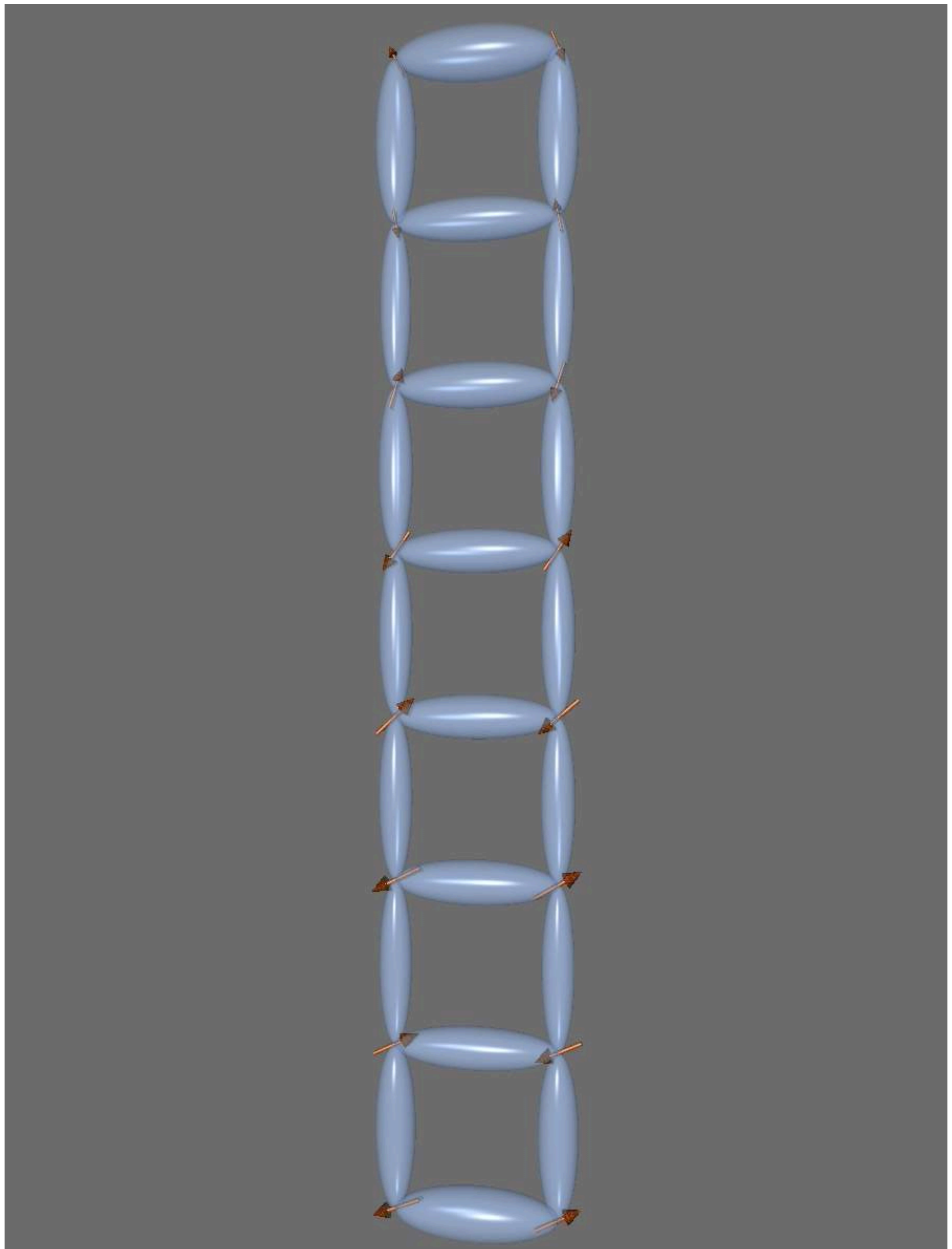

$$e^{-\frac{\beta}{2}\hat{H}}|i_1\rangle \rightarrow |\phi_1\rangle$$

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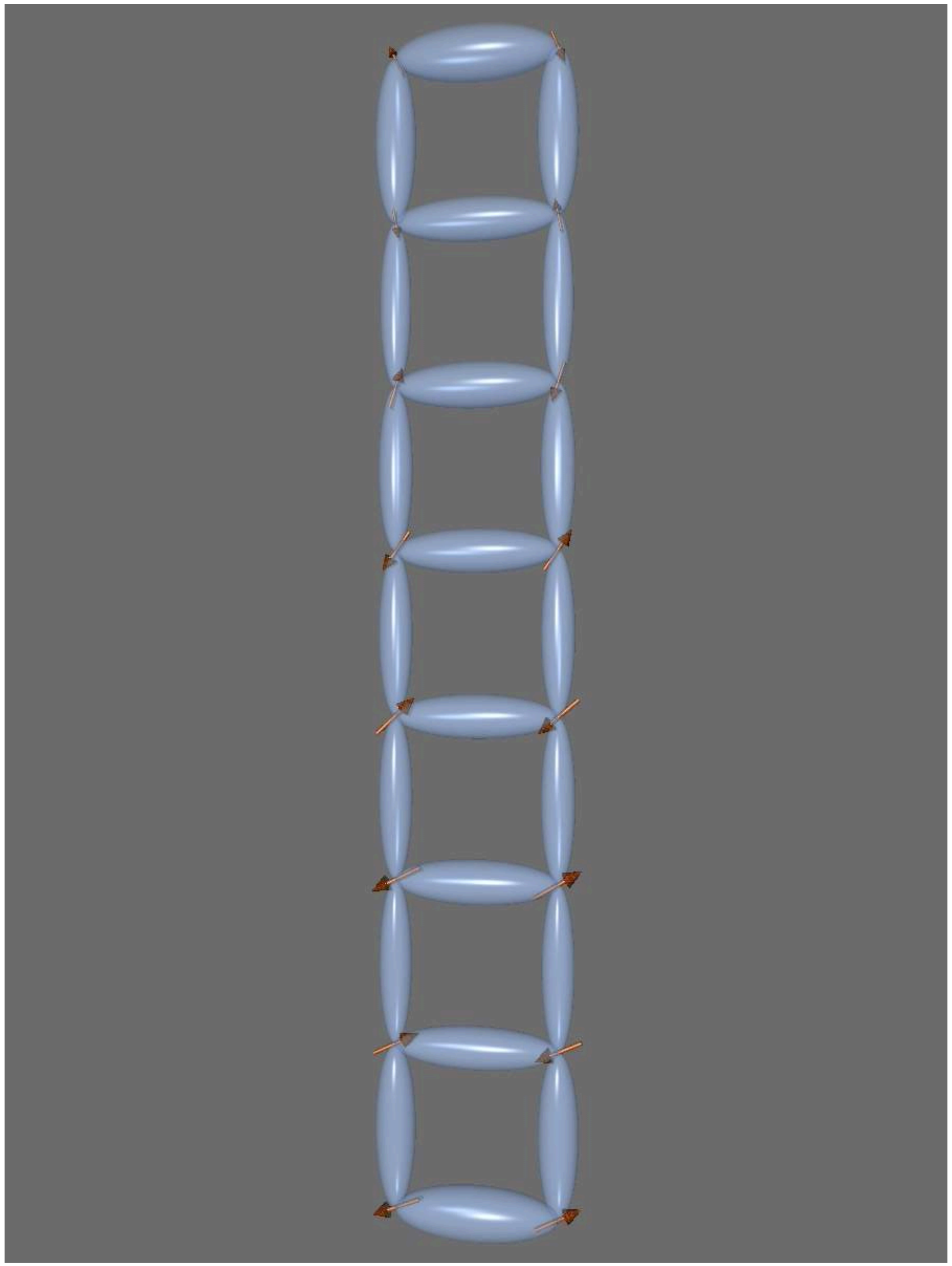

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$$e^{-\frac{\beta}{2}\hat{H}}|i_3\rangle \rightarrow |\phi_3\rangle$$

Summary and Future Directions

Summary

Tensor networks, such as matrix product states, succeed because of low entanglement in quantum states

Can avoid exponential costs of other methods, at least for low dimensional systems

Finite temperature treatable by avoiding eigenstates, working with "typical" states instead

Future Directions

Frontier for tensor networks are two– and three–dimensional systems

Zero-temperature methods working well in 2D now, time is ripe for finite temperature approaches *(see next talk: Alex Wietek)*

Goal of coherent, unified understanding of Hubbard model and strongly-correlated electron systems