THE ROUGH GUIDE to

Quantum many-body systems

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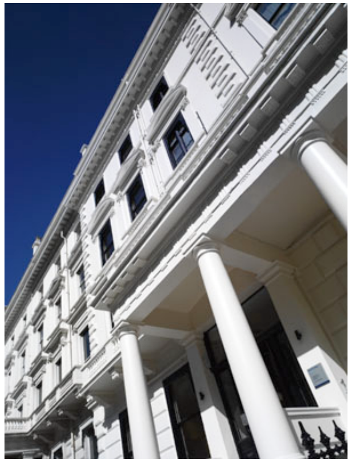
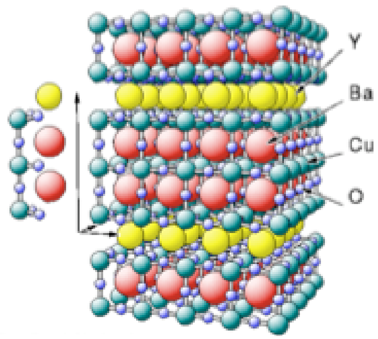


Mention joint work with
M. Cramer, C. Dawson, T.J. Osborne, M.B. Plenio, F. Verstraete
+ lots of tutorial material

See also Frank’s talk just afterwards

• Introduction

• Quantum many-body systems on a lattice:



x

Hilbert space: $\mathcal{H} = \bigotimes_{x \in L} \mathcal{H}_x$

Quantum degree of freedom per lattice site

Hamiltonian: $\hat{H} = \sum_{x \in L} (\hat{h}_x + \hat{k}_x)$

Spin degree of freedom: $\mathbb{C}^2$ or bosonic/fermionic/...

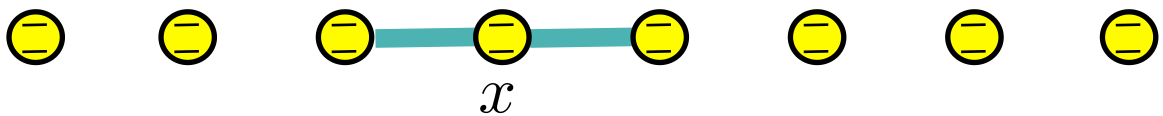
On-site interaction

Finite-ranged interaction to neighbors

Metric: $d(.,.)$

• Introduction

• Quantum many-body systems on a lattice:



Spin chains: XY model, Heisenberg model

$$\hat{H}_{XY} = -\sum_{\alpha\in\mathbb{Z}} \left[\frac{1+\gamma}{2} \hat{\sigma}^x_\alpha \hat{\sigma}^x_{\alpha+1} + \frac{1-\gamma}{2} \hat{\sigma}^y_\alpha \hat{\sigma}^y_{\alpha+1} + \lambda \hat{\sigma}^z_\alpha \right]$$

Bose/Fermi-Hubbard-type models

$$\hat{H} = -J \sum_{\alpha\in\mathbb{Z}} \left[\hat{a}^\dagger_{\alpha+1} \hat{a}_\alpha + \hat{a}^\dagger_\alpha \hat{a}_{\alpha+1} \right] + U \sum_{\alpha\in\mathbb{Z}} \hat{n}_\alpha (\hat{n}_\alpha - 1) - \mu \sum_{\alpha\in\mathbb{Z}} \hat{n}_\alpha$$

Quasi-free bosonic or fermionic systems

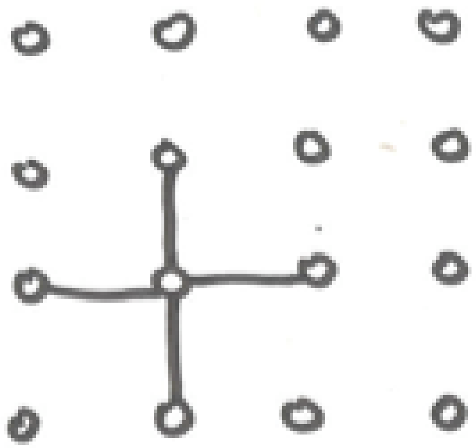
$$\hat{H} = \frac{1}{2} \left[\sum_{\alpha\in\mathbb{Z}} \hat{p}^2_\alpha + \sum_{\alpha,\beta\in\mathbb{Z}} \hat{x}_\alpha V \hat{x}_\beta \right]$$

• **Introduction**

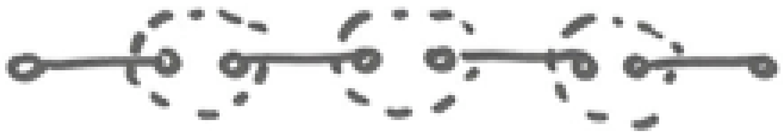
• **Quantum many-body systems on a lattice:**

• Introduction

• Outline of the talk:

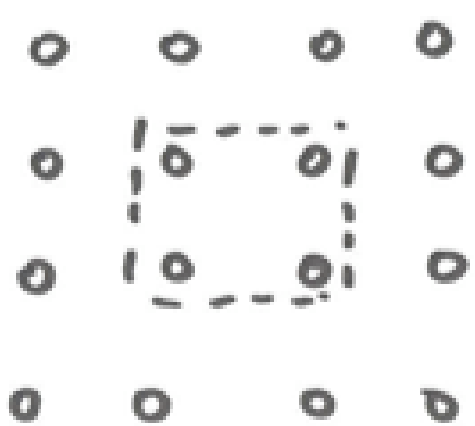


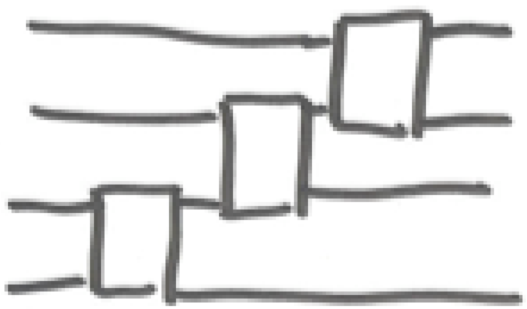
1. Locality in quantum many-body systems



3. Matrix-product states and unitary networks

2. Area laws

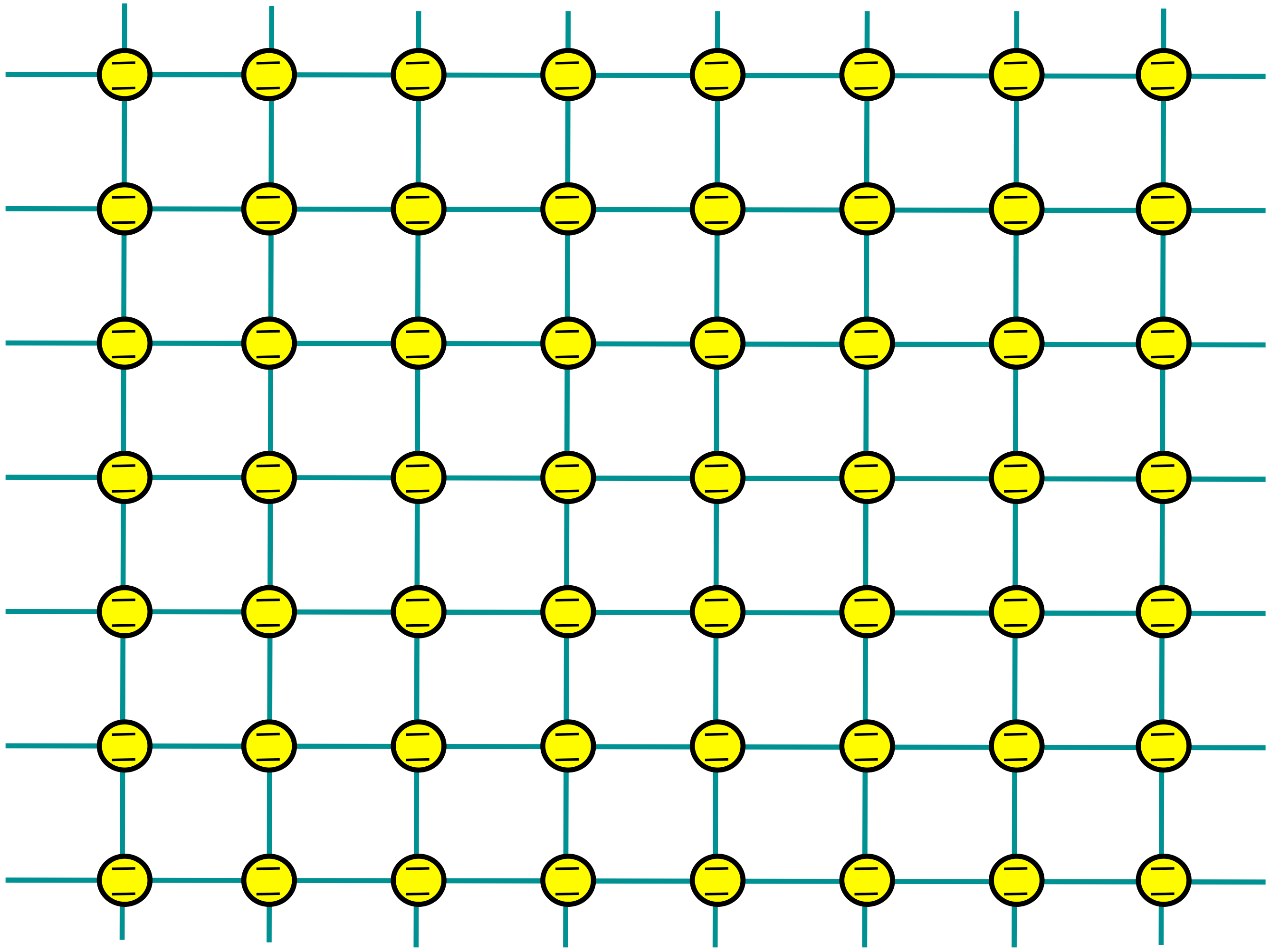




4. Flow

• Locality in quantum many-body systems

- Simple to **describe** (Hamiltonian), typically difficult to **find** (ground/Gibbs state) **properties**



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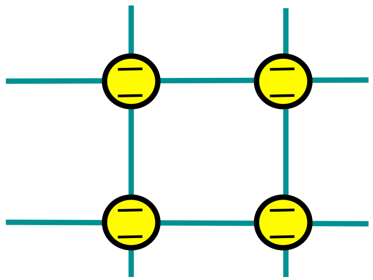

- Hilbert space dimension for spin model: 16

• Locality in quantum many-body systems

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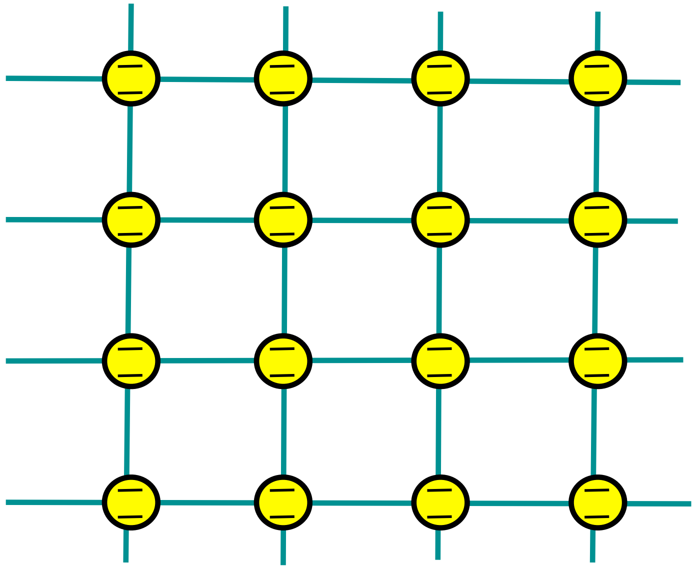
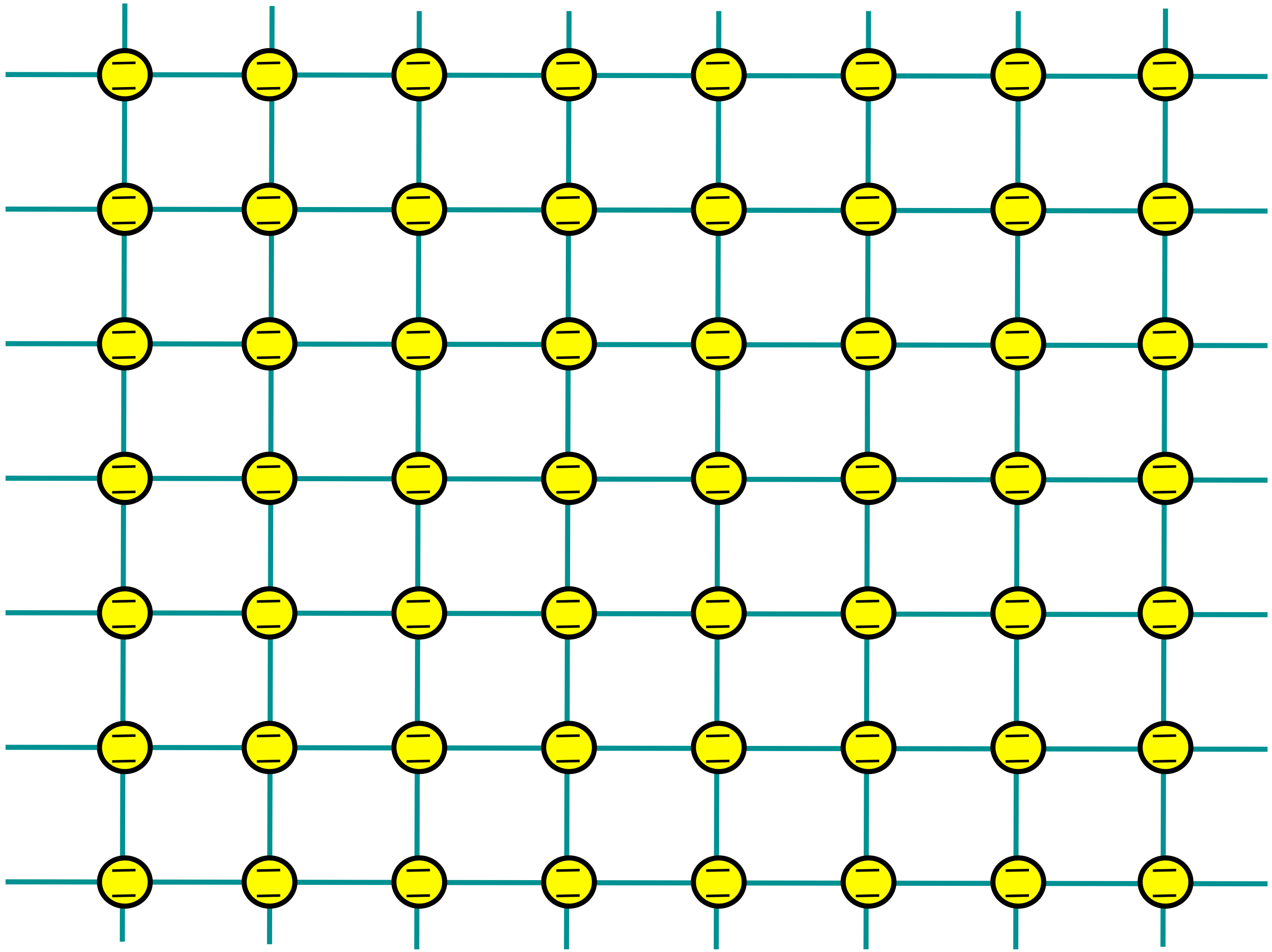


- Hilbert space dimension for spin model: 65.536

• Locality in quantum many-body systems

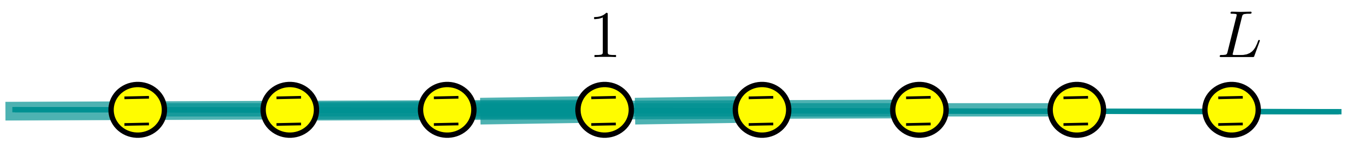
- Simple to **describe** (Hamiltonian), typically difficult to **find** (ground/Gibbs state) **properties**



- Hilbert space dimension for spin model: 72.057.594.037.927.936

• Locality in quantum many-body systems

- **Insight:** to faithfully describe ground states of local Hamiltonians, no need to consider exponentially large Hilbert space



- Finite interaction length,

  - exponentially decaying correlations (non-critical), or $\xi^{-1} = \lim_{L\to\infty} \frac{1}{L} \log C_{1,L}$

  - algebraically decaying **correlation functions**

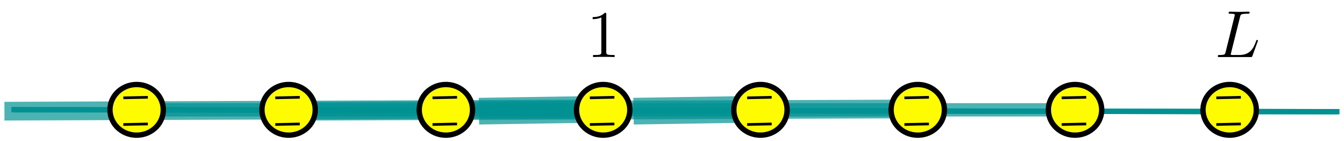
$$C_{a,L} = \langle \hat{o}_1 \hat{o}_L \rangle - \langle \hat{o}_1 \rangle \langle \hat{o}_L \rangle$$

- Systems with spectral gap $\Delta E > 0$ are non-critical (from *Lieb-Robinson bounds*)

Hastings, Koma (2005)

• Locality in quantum many-body systems

- **Insight:** to faithfully describe ground states of local Hamiltonians, no need to consider exponentially large Hilbert space

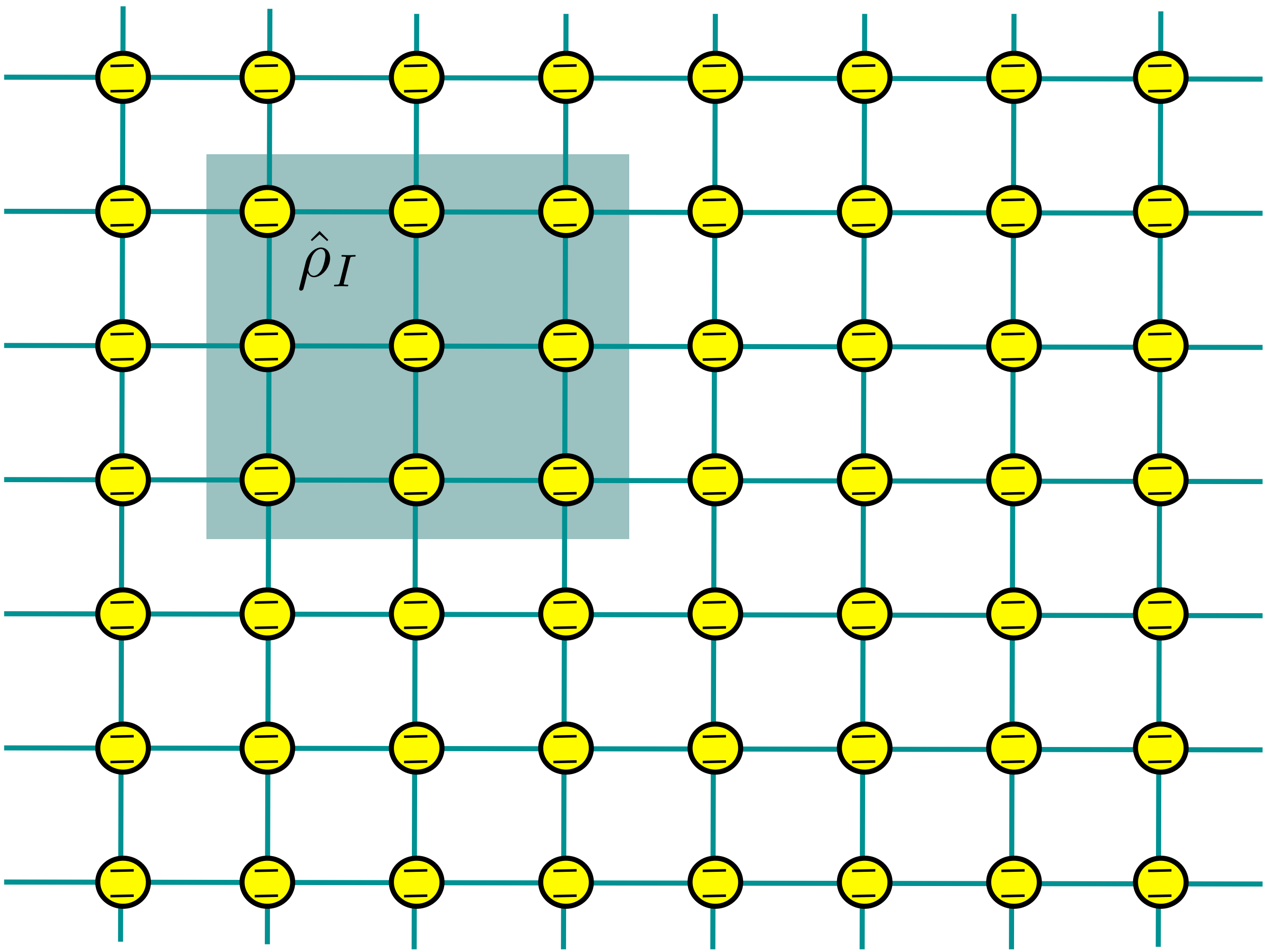


  - Is this locality inherited by **quantum correlations + entanglement**?
  - What does this mean for **classical simulatability**?

2. Area laws

• Area laws

- **Scaling** of geometric entropy/**entanglement entropy?**



$$S(\hat{\rho}_I) = -\mathrm{tr}[\hat{\rho}_I \log \hat{\rho}_I]$$

Area laws

- **"History of the problem"**

  - *Black hole context*: Geometric entropy satisfies area law?

    Bombelli, Koul, Lee, Sorkin (1986)
    Srednicki (1993)
    Holzhey, Larsen, Wilczek (1994)

- **Quantum information interest:**

  - Relationship between **entanglement scaling and criticality**
  - **Locality** of interactions inherited by entanglement?

    Audenaert, Eisert, Plenio, Werner (2002)
    Vidal, Latorre, Kitaev, Rico (2003)
    Its, Jin, Korepin (2005)
    Calabrese, Cardy (2004)

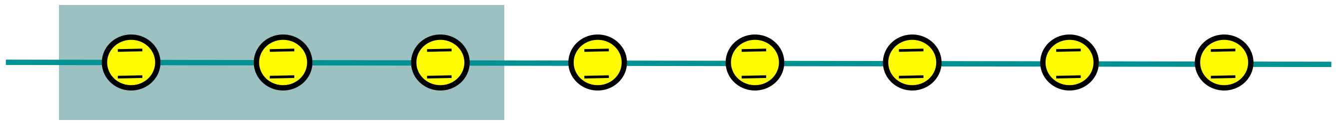
  - Question of **simulatability** (effective degrees of freedom)

    Verstraete, Cirac (2006)
    Peres-Garcia, Verstraete, Wolf, Cirac (2006)

- Let's have look at problem where the **higher-dim case** can be tackled

  Plenio, Eisert, Dreissig, Cramer (2005)
  Cramer, Eisert (2006)

- Here: **Bosonic and fermionic systems on a lattice, D>1**



$$\hat{H} = \sum_{j,k\in L} \left(\hat{a}_j^\dagger A_{j,k} \hat{a}_k + \hat{a}_j A'_{j,k} \hat{a}_k^\dagger + \hat{a}_j B_{j,k} \hat{a}_k + \hat{a}_j^\dagger B'_{j,k} \hat{a}_k^\dagger \right)$$

$$= \hat{a}^T \left[\begin{array}{cc} B & A' \\ A & B' \end{array} \right] \hat{a}, \;\; \hat{a} = (\hat{a}_1, \ldots, \hat{a}_{|L|}, \hat{a}_1^\dagger, \ldots, \hat{a}_{|L|}^\dagger)^T$$

$\hat{b} = \Omega \hat{r}$ "Canonical coordinates"

$$\hat{H} = \hat{r}^T \left[\begin{array}{cc} A+B & 0 \\ 0 & A-B \end{array} \right] \hat{r}$$

$$(i[\hat{r}_j, \hat{r}_k]) = \left[\begin{array}{cc} 0 & -\mathbb{1} \\ \mathbb{1} & 0 \end{array} \right]$$

- Bosons

$\hat{f} = \Omega \hat{m}$ "Majorana fermions"

$$\hat{H} = i\hat{m}^T \left[\begin{array}{cc} 0 & A+B \\ B-A & 0 \end{array} \right] \hat{m}$$

$$\{\hat{m}_j, \hat{m}_k\} = \delta_{j,k}$$

- Fermions

- **Technical difficulty:** Problem no longer has symmetry of Hamiltonian

- **Idea 1:** Bound to entropy from correlation functions

$$S(\hat\rho_I) \leq 4\lambda_{\max}((A-B)^{-1}) \times \sum_{j\in I,k\in O} |((A+B)^{-1})_{j,k}|$$

- Ideas: Bound via logarithmic negativity, use l_1 norm

- Bosons

Cramer, Eisert (2006)
Plenio, Eisert, Dreissig, Cramer (2005)

$$S(\hat\rho_I) \leq 2 \sum_{j\in I,k\in O} |\langle \hat f_j^\dagger \hat f_k\rangle + \langle \hat f_j \hat f_k\rangle|$$

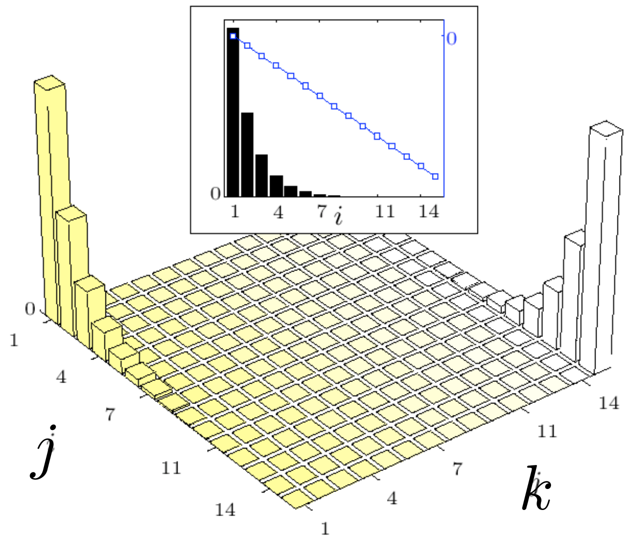
- ... or use quadratic bounds

- Fermions

Wolf (2006)
Cramer, Eisert, Plenio (2007)

- **Idea 2:** Exponential decay in matrix functions:

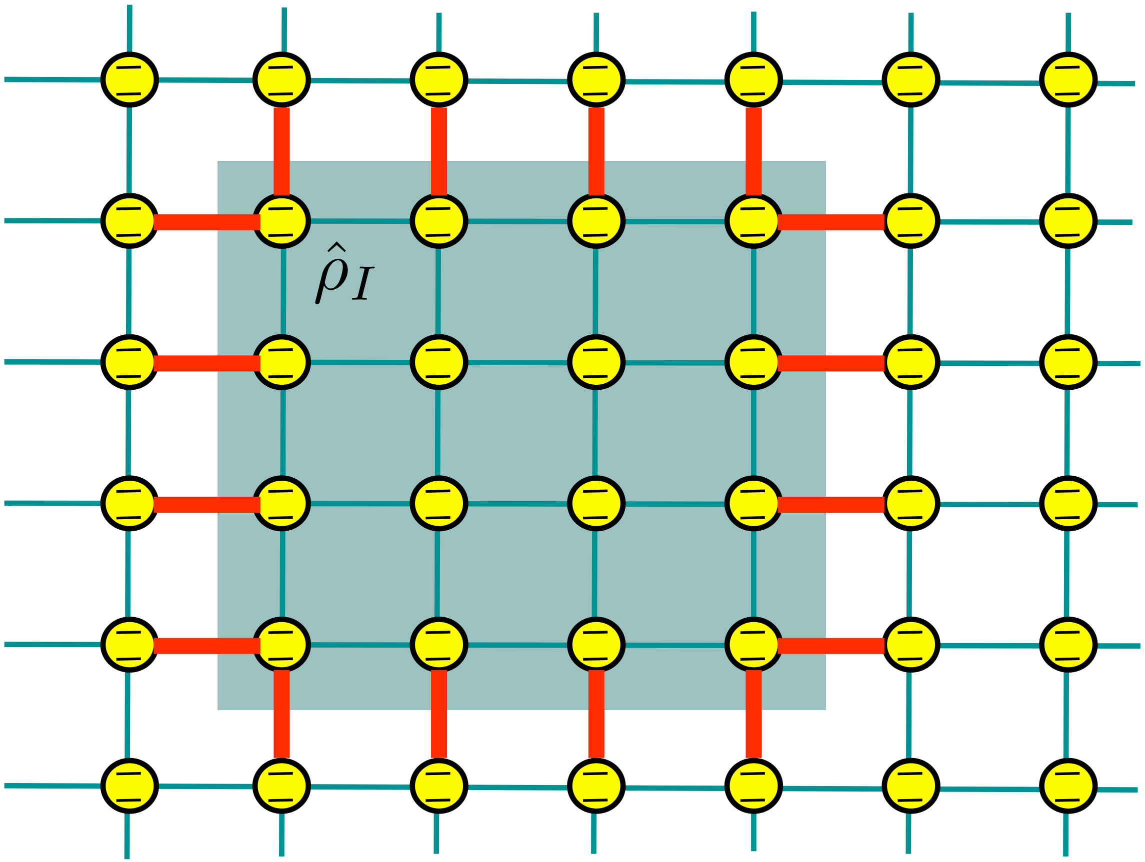
$$|[f(M)]_{j,k}| \leq K\, e^{-d(j,k)/\xi}$$



- Bosons

Benzi, Golub (1999)
Cramer, Eisert (2006), general graphs

- **And ... it does give an area law**



- Gapped quasi-free, local *bosonic* systems:

$$S(\hat{\rho}_I) \leq K s(I)$$

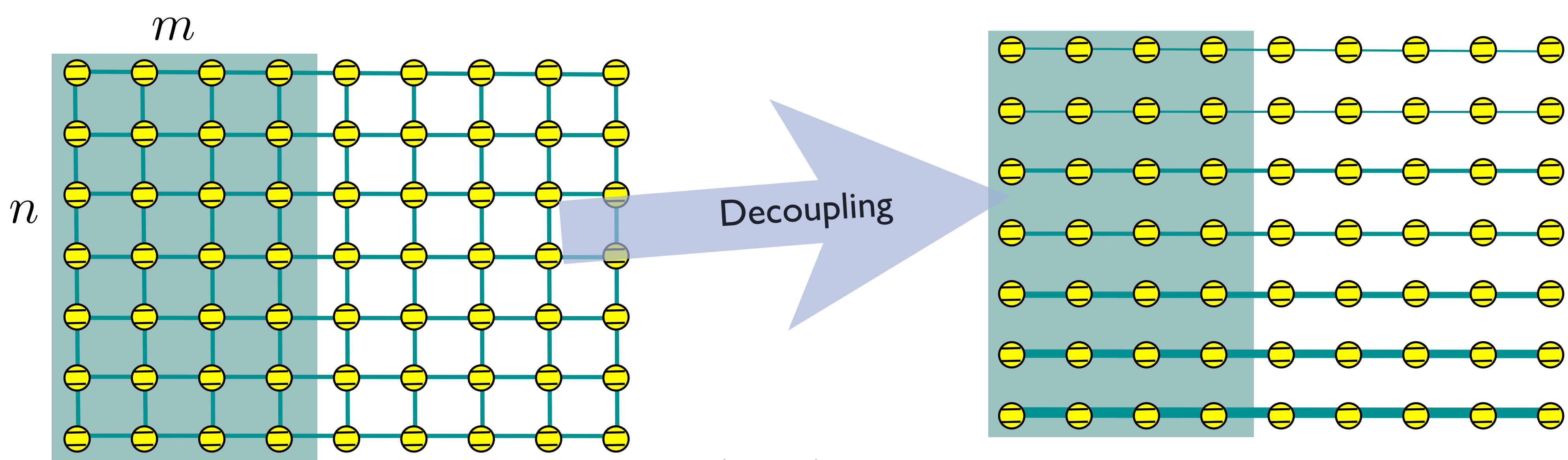
- Bosons

Cramer, Eisert (2006)
Plenio, Eisert, Dreissig, Cramer (2005)

- Ok, this is gapped, how about **critical** systems, with no length scale of correlations?

• Area laws

- Critical bosons and fermions in half spaces:

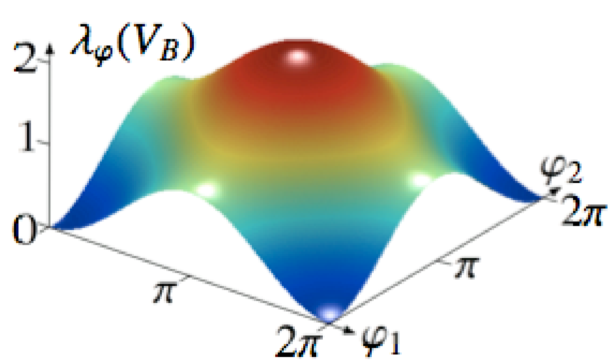


$$L = [1, \ldots, m] \times [1, \ldots, n]^{\times (D-1)}$$

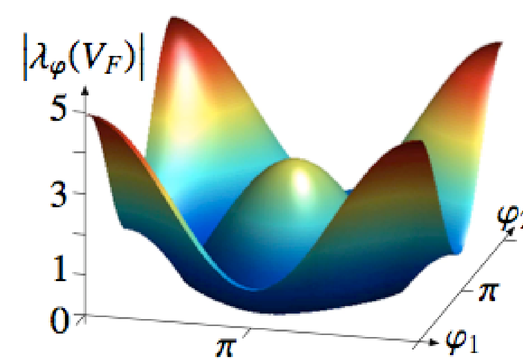
$$\hat{H} = \sum_j \hat{h}_j$$

- **Ideas:** Upper bound from negativity for half-chains, using flip symmetry

- **Ideas:** Bounds using Fisher-Hartwig methods for Toeplitz determinants



- Bosons



- Fermions

• Area laws

- Critical bosons and fermions in half spaces:

$$S(\hat{\rho}_I) = O(n^{D-1})$$

- **Area law**, despite being critical!

$$S(\hat{\rho}_I) = O(n^{D-1}\log n)$$

- **Violation** of area law

- here with *known prefactor*, dependent on topology of Fermi surface

- Can hence depend on statistics whether area law is violated or not

- Bosons

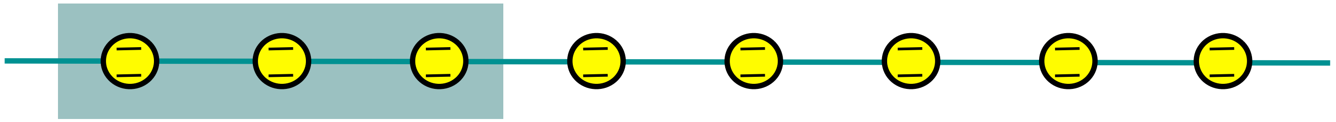
Cramer, Eisert, Plenio (2006)

- Fermions

Wolf (2006)
Gioev, Klich (2006)
Cramer, Eisert, Plenio (2006)

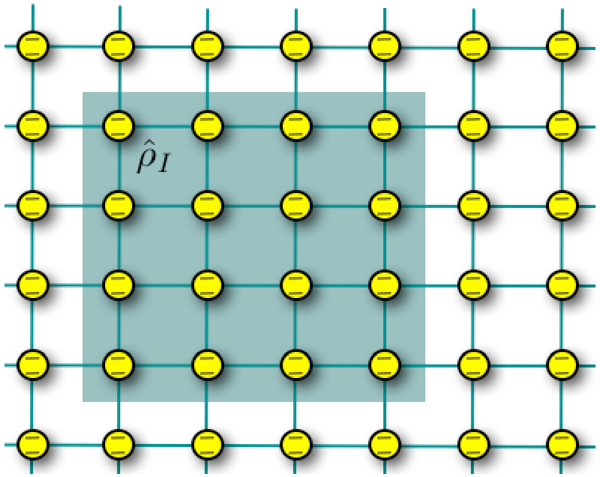
• Area laws

- **1D:** In the meantime: Full proof of area laws for local gapped models



Hastings (2007)

- >1D: For the **quantum mutual information** as correlation measure for *thermal states*: Area law for general local interactions



$$I(I:O) = S(\rho_I) + S(\rho_O) - S(\rho)$$

Wolf, Verstraete, Hastings, Cirac (2007)

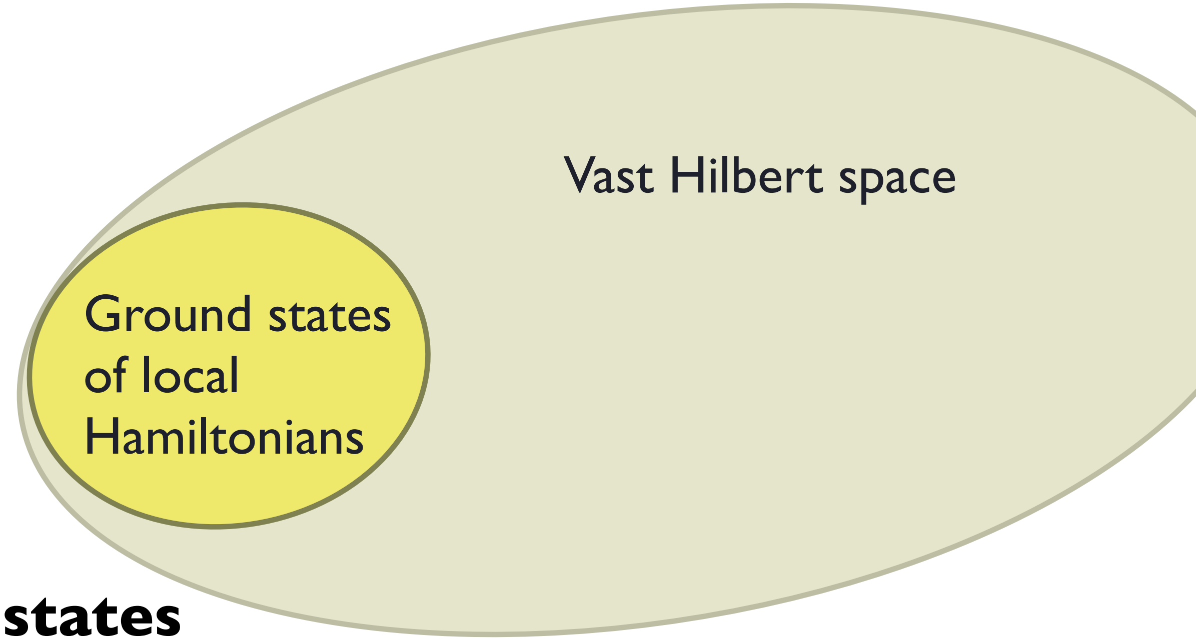
- Lesson: There is **much less** entanglement typically than could be (volume)!

3. Matrix-product states, MERA, and the zoo of unitary networks

- **Insight, again:** To faithfully describe ground states of local Hamiltonians, one does not need to consider exponentially large Hilbert space

- Look at much smaller (poly-sized) **subspaces** that grasp ground state properties

- Such that one can **efficiently compute** $\langle\psi|\hat{A}|\psi\rangle$ for local (supp on finite number of sites) observables $\hat{A}$

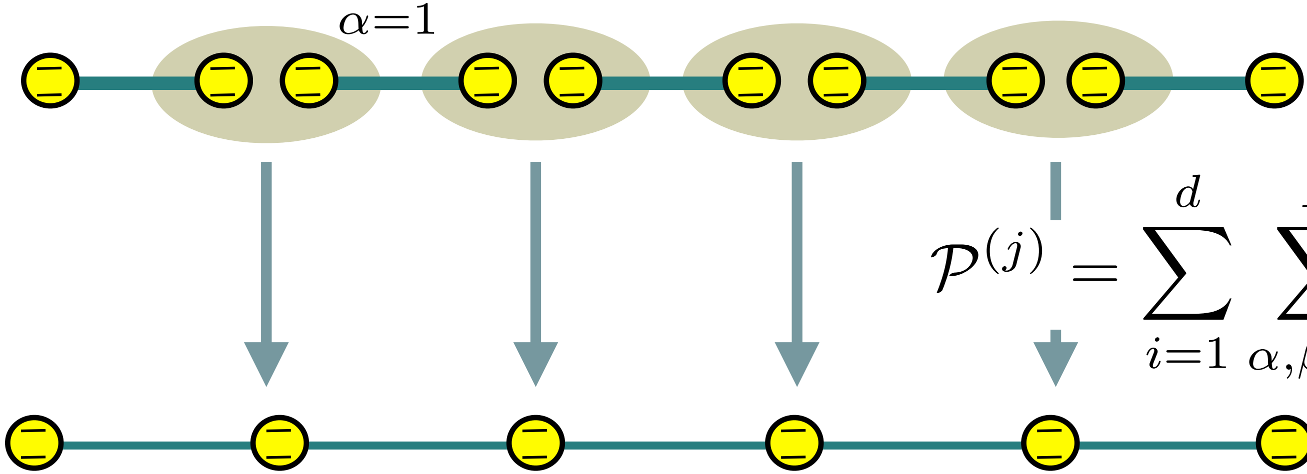


- Will have look at such **classes of states**

• Matrix-product states, MERA, and the zoo of unitary networks

- Valence bond picture of **matrix product states**:

$$|I\rangle = \sum_{\alpha=1}^{D} |\alpha, \alpha\rangle$$



$$\mathcal{P}^{(j)} = \sum_{i=1}^{d} \sum_{\alpha,\beta=1}^{D} A^{(j)}_{i_j,\alpha,\beta} |i\rangle\langle\alpha, \beta|$$

$$|\psi\rangle = \sum_{i_1,\ldots,i_N} \mathrm{tr}[A^{(1)}_{i_1} A^{(2)}_{i_2} \ldots A^{(N)}_{i_N}] |i_1, i_2, \ldots, i_N\rangle$$

• Matrix-product states, MERA, and the zoo of unitary networks

- **Matrix product states (MPS)**:
- Characterized by matrices $\{A_1^{(j)}, \dots, A_d^{(j)}\}$ per site
- DMRG - *workhorse of simulation in 1D* - is essentially variation over MPS better and better approximating the true ground state
- DMRG works *well in practice*
- **Area law** (for Renyi entropies) satisfied: ex. efficient MPS approximation of ground state

Peschel (2001)
Schuch, Wolf, Verstraete, Cirac (2007)

(Strictly speaking not certifiable: Variations over MPS can be NP-hard

Eisert (2006)

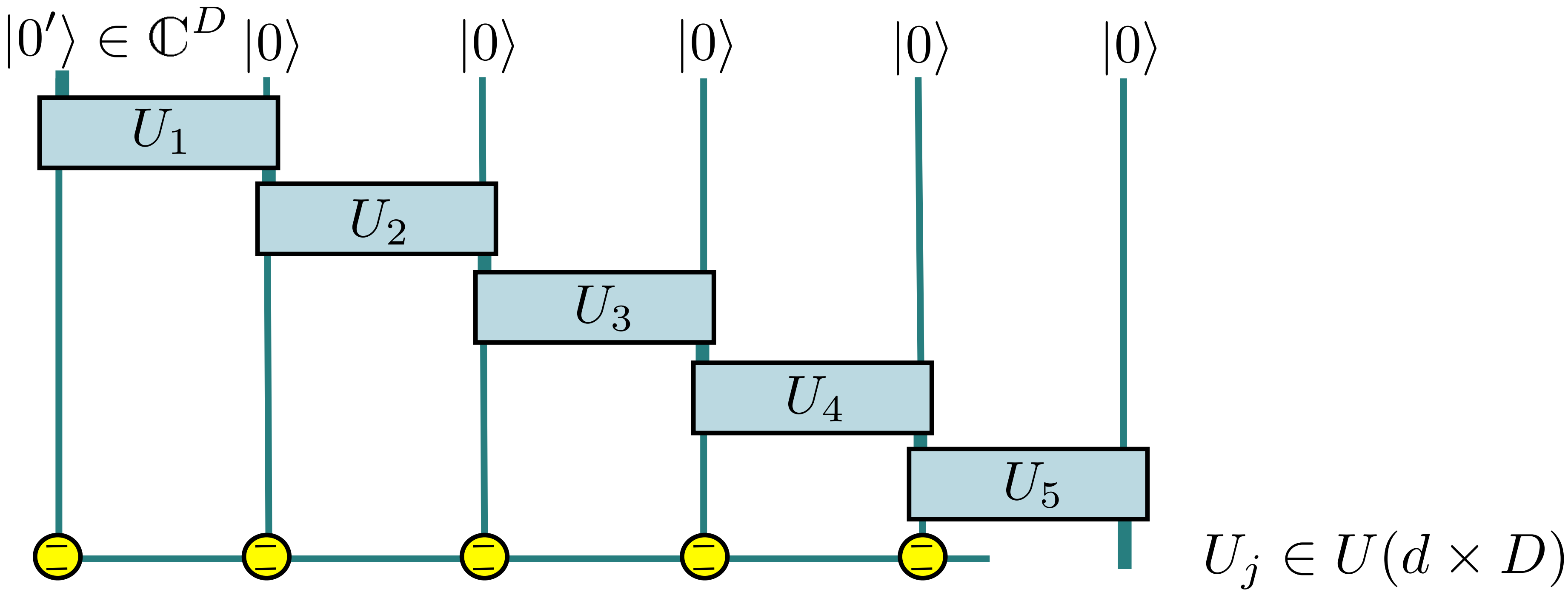
Gapped models with MPS as ground states; to find it is NP-hard)

Schuch, Cirac, Verstraete, in preparation

$$|\psi\rangle = \sum_{i_1,\dots,i_N} \mathrm{tr}[A_{i_1}^{(1)} A_{i_2}^{(2)} \dots A_{i_N}^{(N)}] |i_1, i_2, \dots, i_N\rangle$$

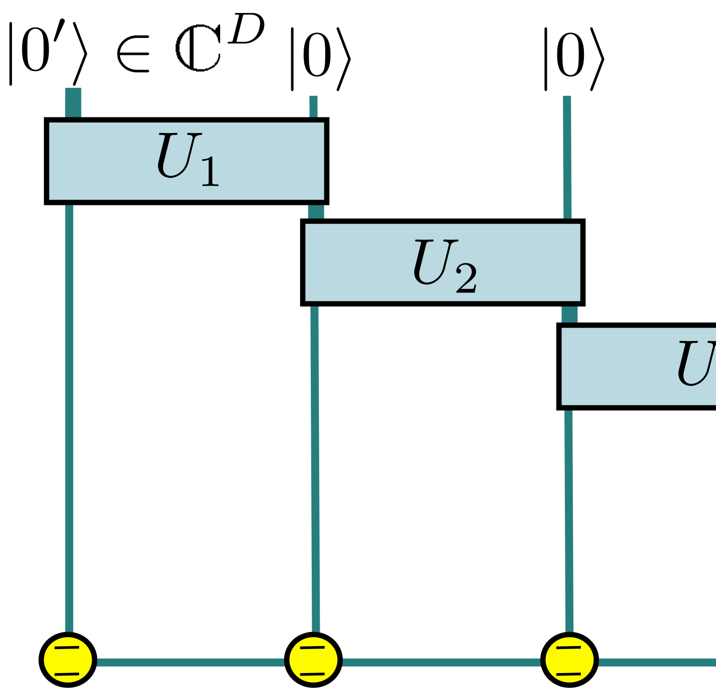
• Matrix-product states, MERA, and the zoo of unitary networks

- Unitary network preparation of MPS: **Staircase circuit**

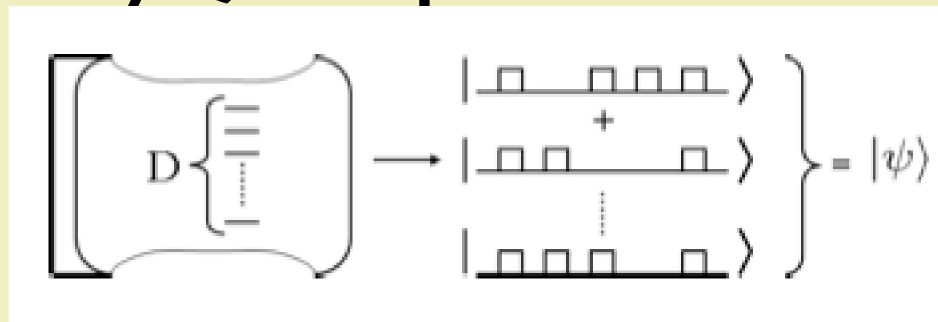


Fannes, Naechtergaele, Werner (1992)
Schoen, Hammerer, Wolf, Cirac, Solano (2006)
Schoen, Solano, Verstraete, Cirac, Wolf (2005)
Dawson, Eisert, Osborne (2007)

- Unitary network preparation of MPS: **Staircase circuit**



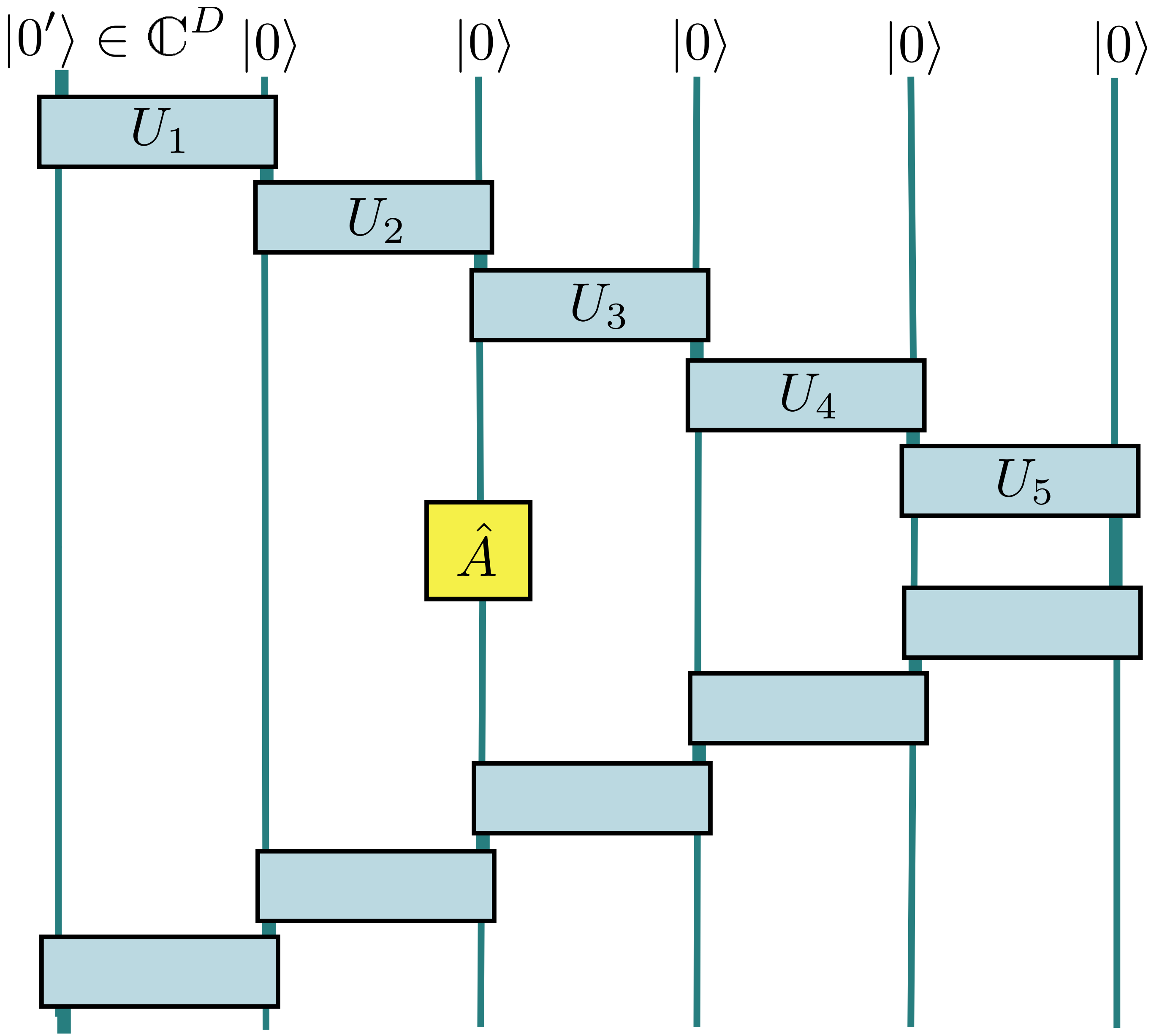
- **Cavity-QED implementation:**



- Trapped D-level atom coupled to time-bin qubits of optical cavity field mode

Schoen, Hammerer, Wolf, Cirac, Solano (2006)
Schoen, Solano, Verstraete, Cirac, Wolf (2005)

- Contraction: Compute $\langle\psi|A|\psi\rangle$, in a way that we will use later



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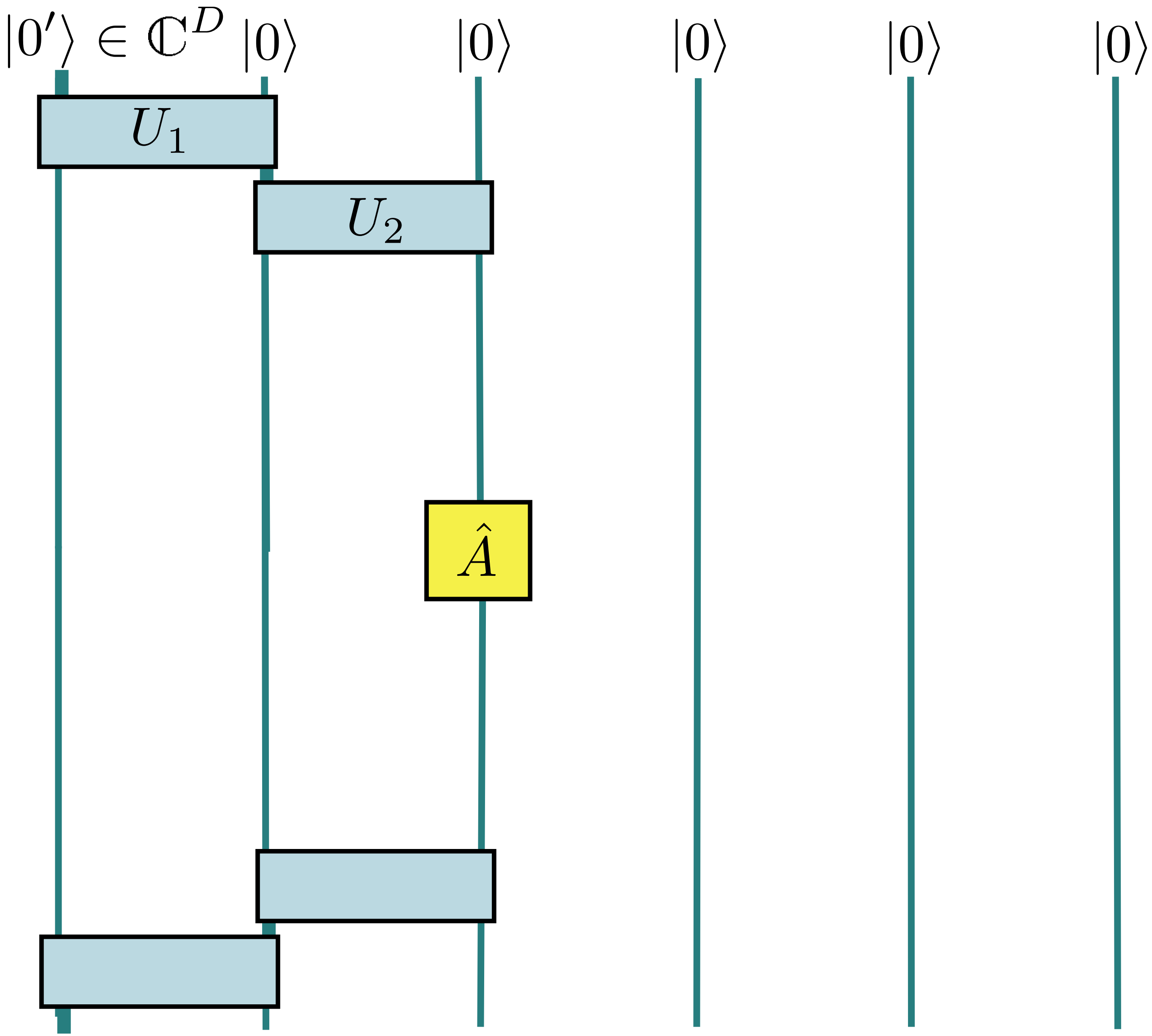
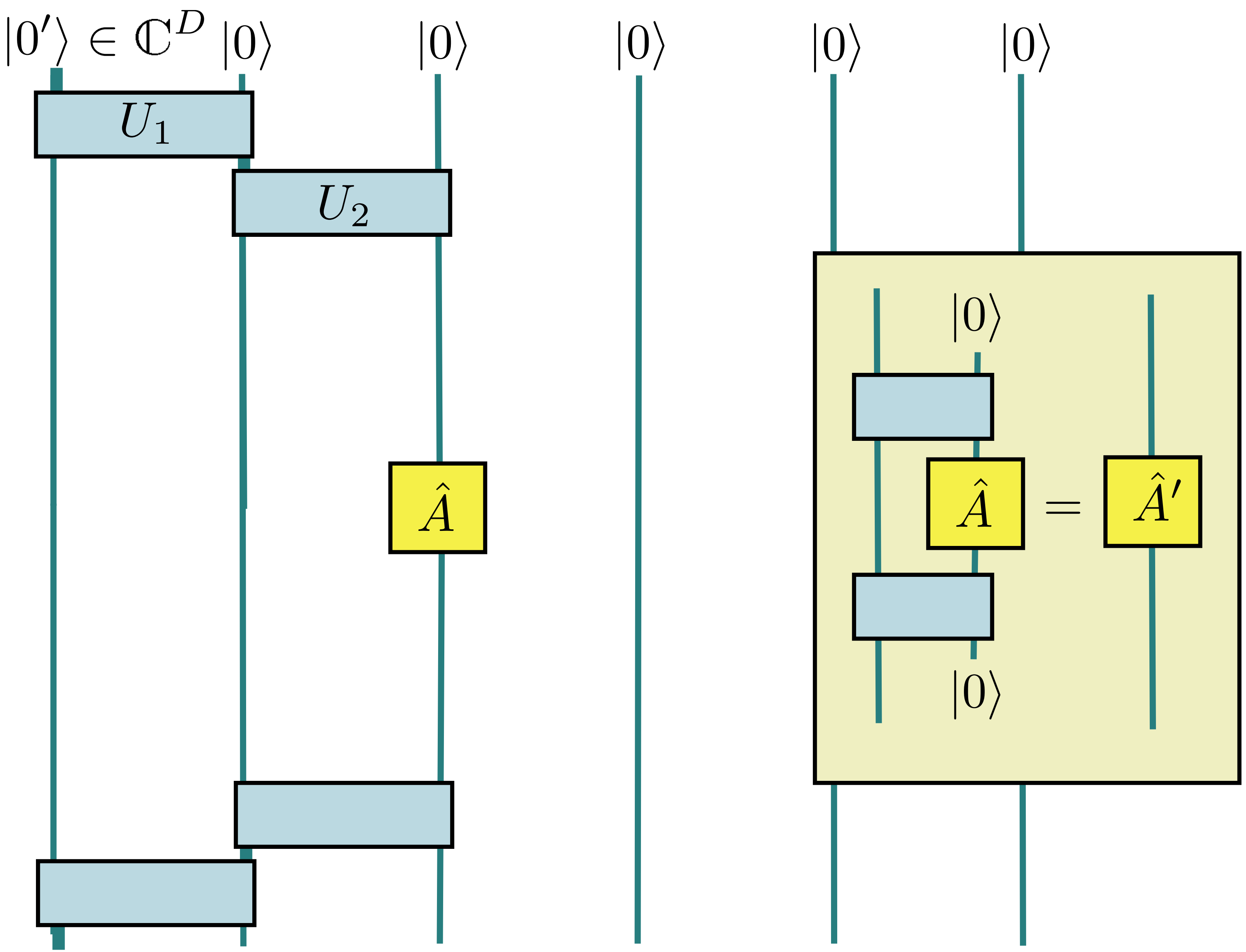


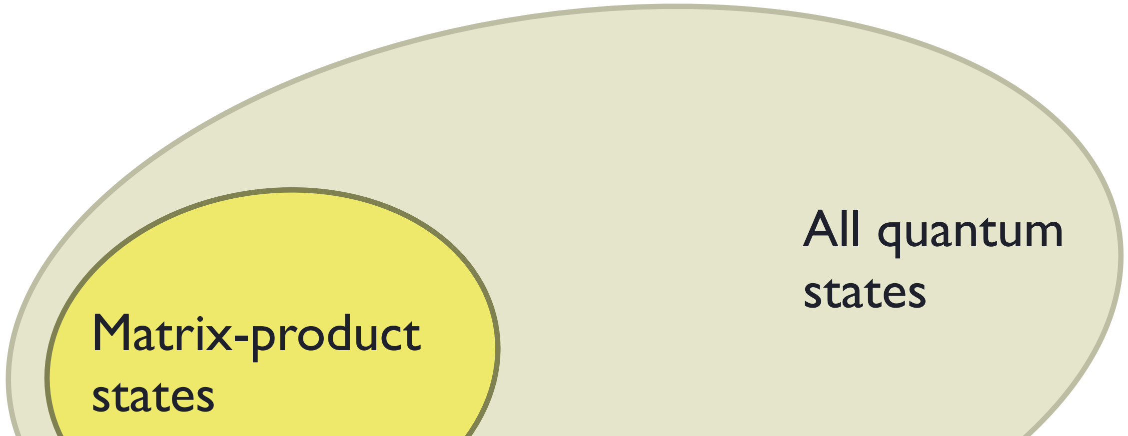
- Contraction: Efficiently computable!



• Matrix-product states, MERA, and the zoo of unitary networks

- Interestingly, more generally: **MPS + "weighted graphs"**

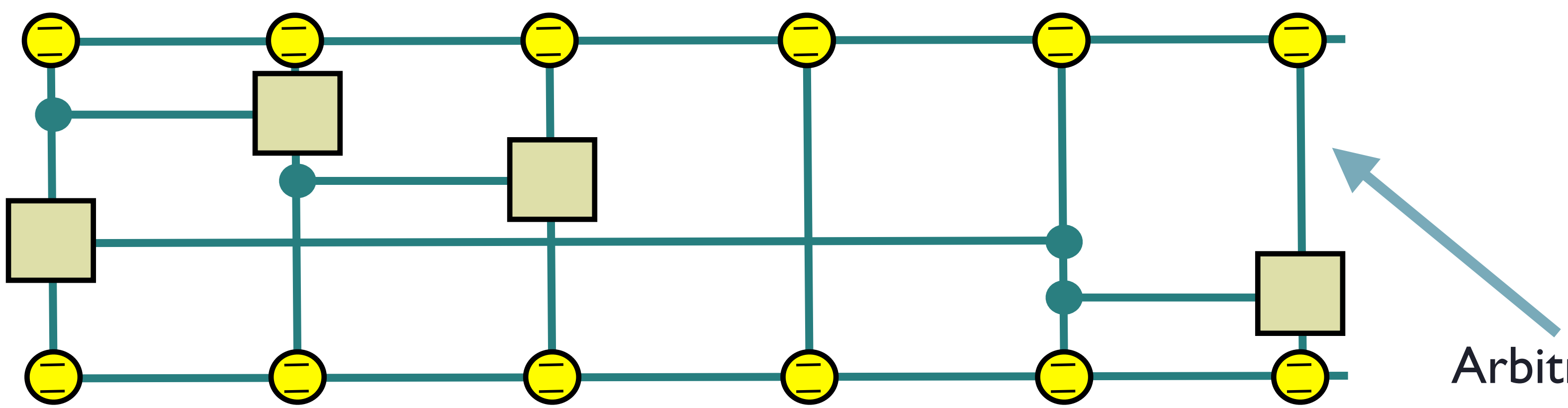
$$|\psi\rangle = \sum_{i_1,\ldots,i_N} \mathrm{tr}[A^{(1)}_{i_1} A^{(2)}_{i_2} \ldots A^{(N)}_{i_N}] |i_1, i_2, \ldots, i_N\rangle$$



Eisert, Plenio, Verstraete, in prep
Anders, ..., Briegel, in prep

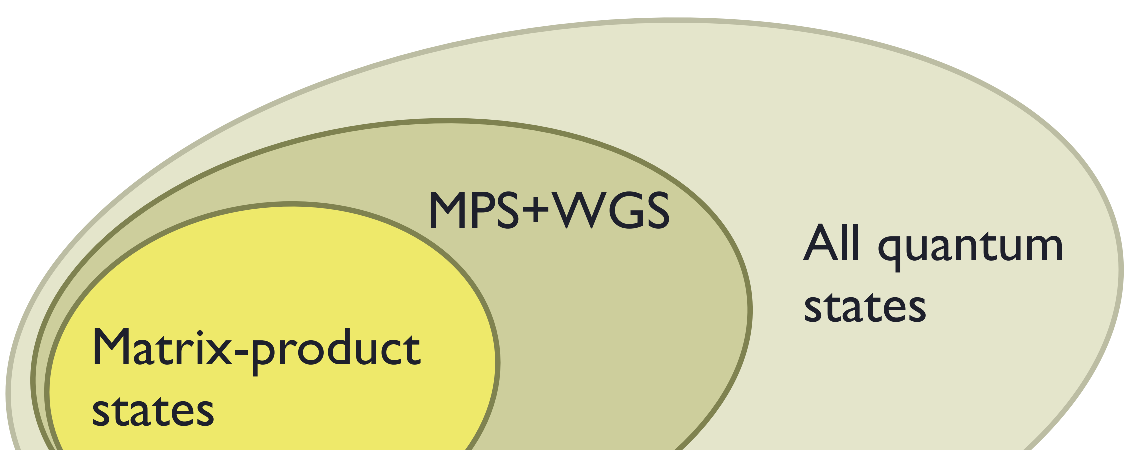
• Interestingly, more generally: **MPS + "weighted graphs"**

$$|\psi\rangle = \prod_k U_k \sum_{i_1,\ldots,i_N} \mathrm{tr}[A^{(1)}_{i_1} A^{(2)}_{i_2} \ldots A^{(N)}_{i_N}]|i_1, i_2, \ldots, i_N\rangle$$



Arbitrary phase gates between arbitrary constituents

• Can **still contract** and compute local expectation values

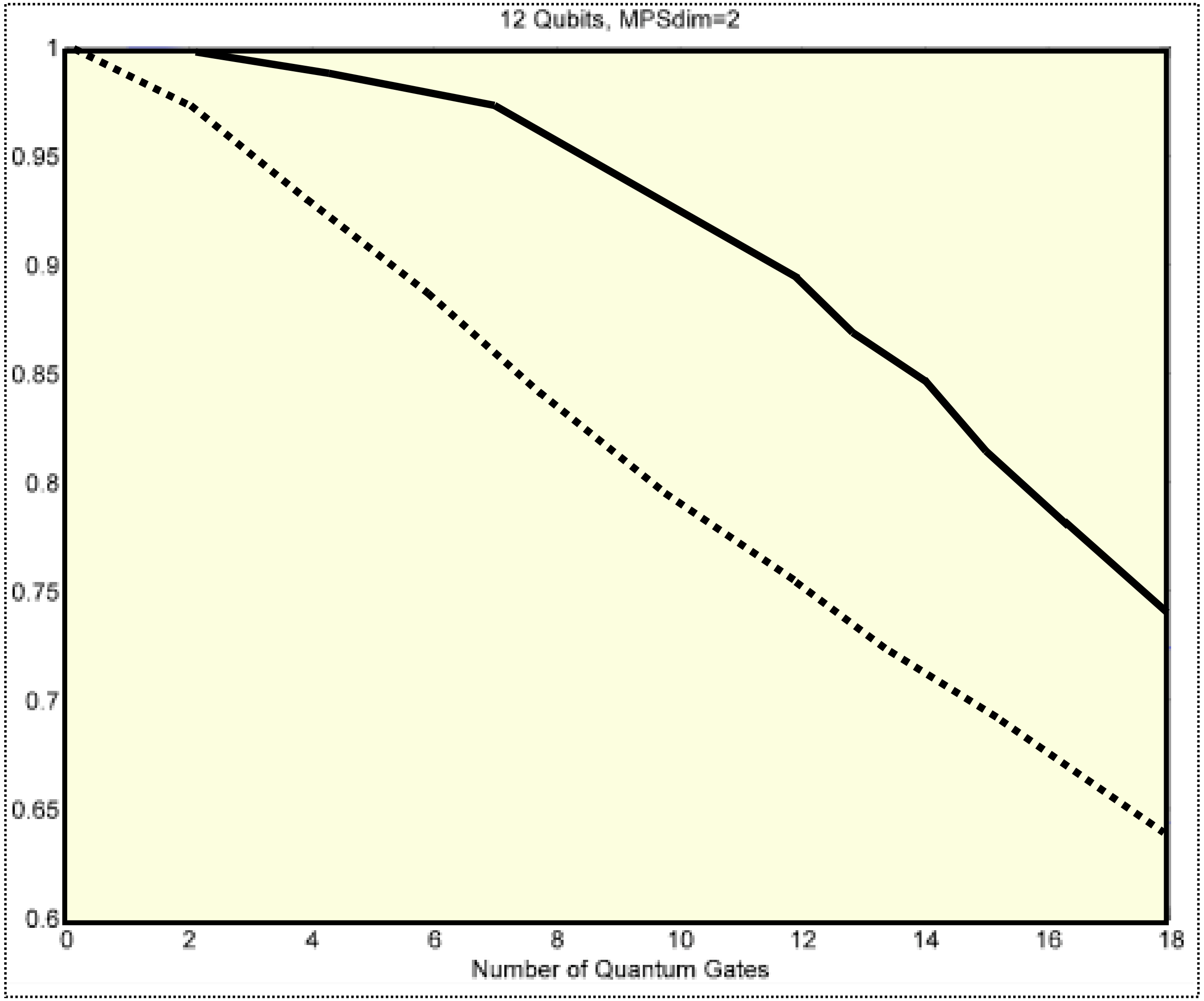


Eisert, Plenio, Verstraete, in prep
Anders, ..., Briegel, in prep

- Interestingly, more generally: **MPS + "weighted graphs"**
- E.g., use networks to simulate **random quantum circuits** in quantum computing

Fidelity

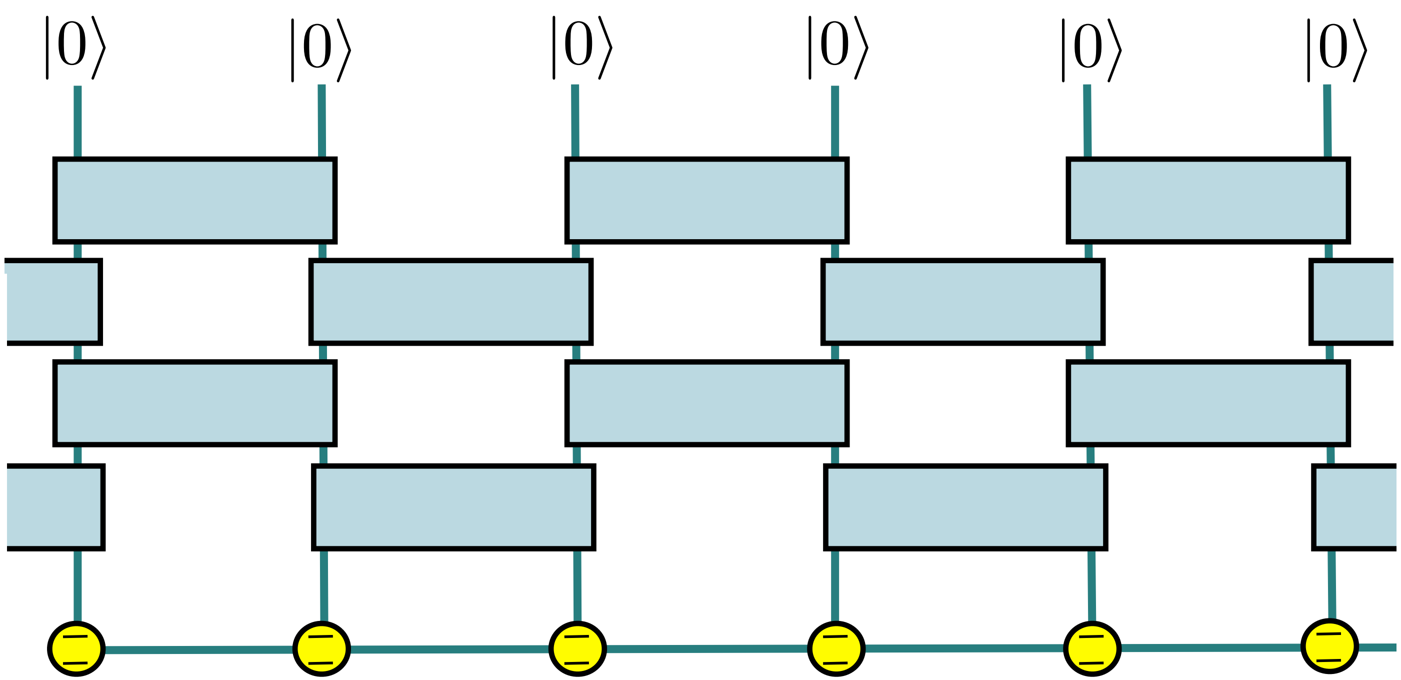
$$F = |\langle\psi'|U|\psi\rangle|$$



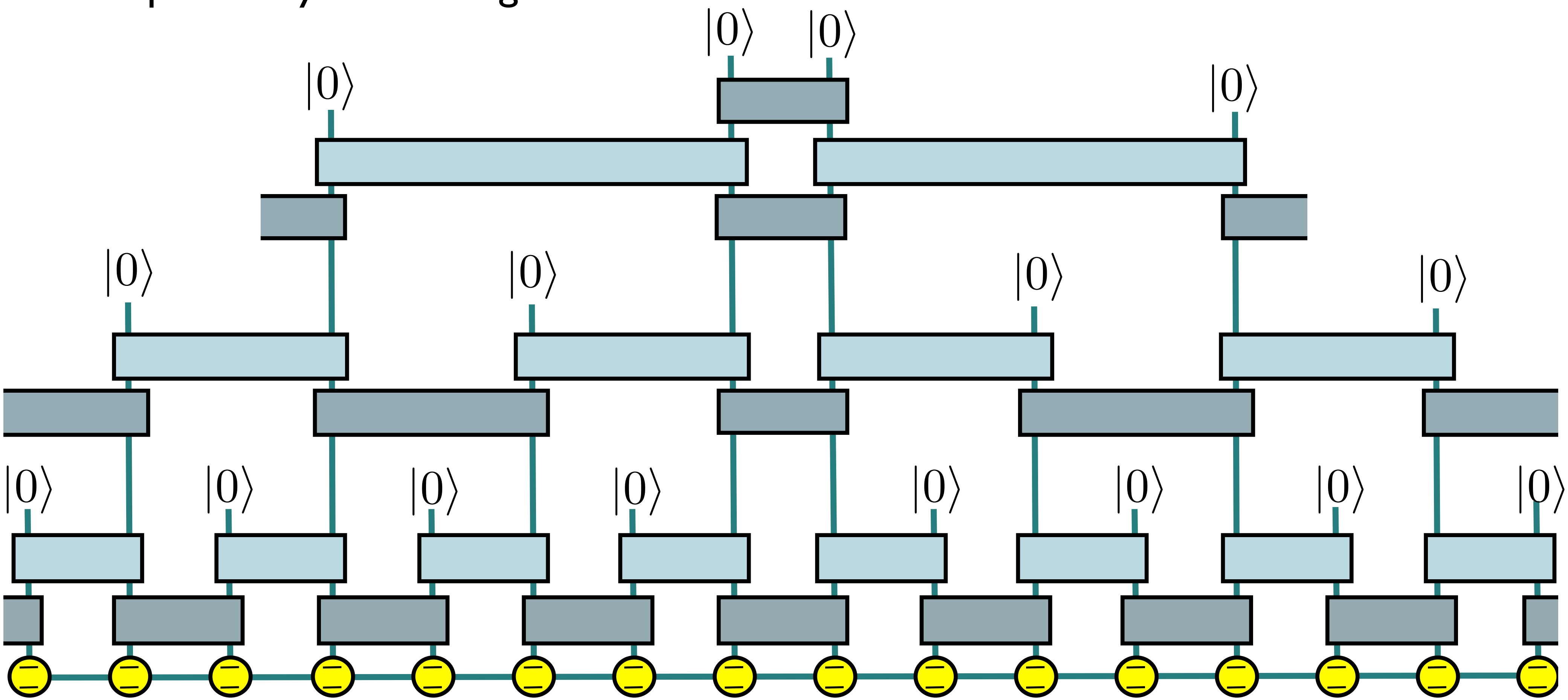
(Starting from product state, random phase gates and local gates, 12 qubits, 100 realizations)

- **Other classes of states:**

Margolus partitioning of **quantum cellular automata** of fixed depth:

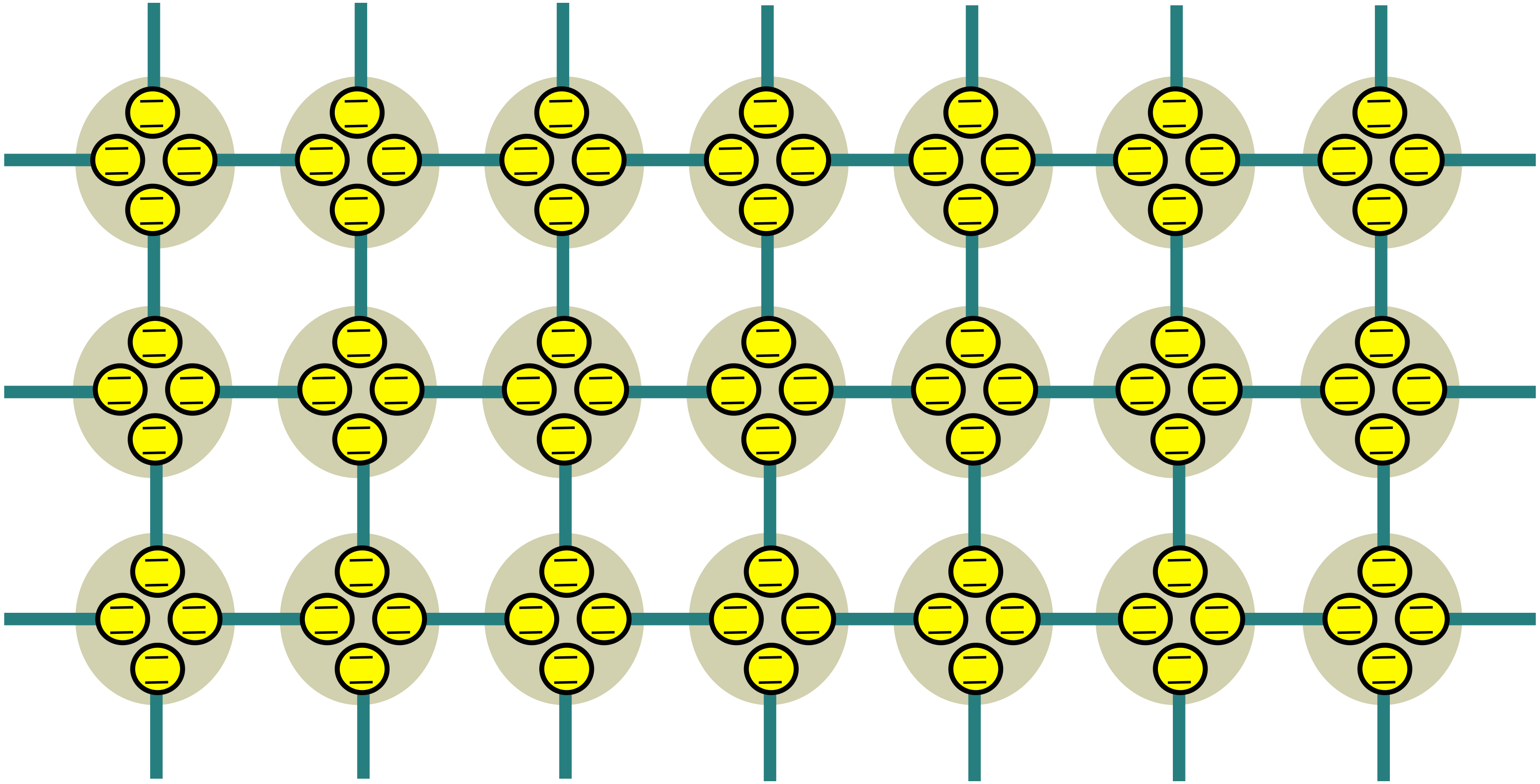


- Unitary network of **MERA** (multiscale entanglement renormalization):
- "Disentanglers" and "isometries", scale invariant
- $\log(n)$ layers, contraction $O(n)$ effort
- Idea specifically interesting in 2D



Vidal (2006)
Morningstar, Weinstein (1996)

- PEPS, **projected entangled pair states**, higher-dimensional MPS, see Frank's talk



- **Lesson:** Approximate **ground states of quantum many-body systems** by tensor networks that can be efficiently contracted

4. Flow and optimal control approach to simulating quantum many-body systems

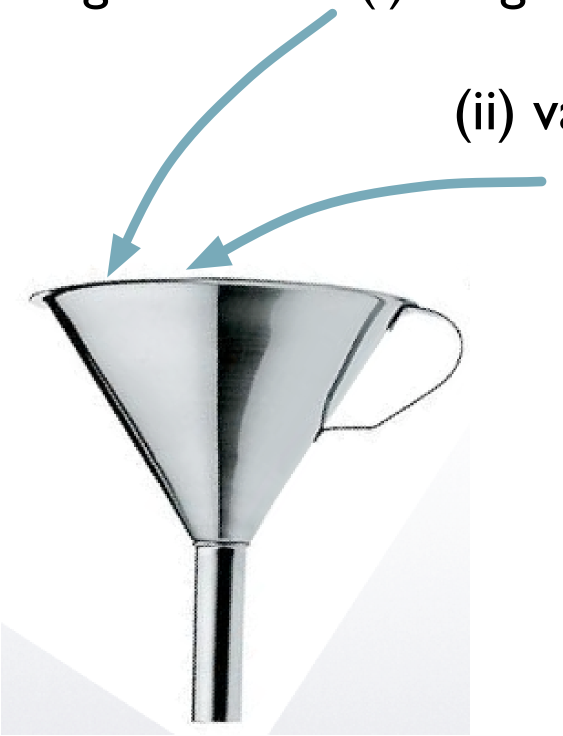
(in progress!)

• Flow and optimal control approach to simulation

- How to **optimize** over such unitary networks?

- Approach: Bring ideas of (i) Wegner-flow, optimal control together with

  (ii) variational principles



- **Starting point:** Write variational set again as **unitary network**

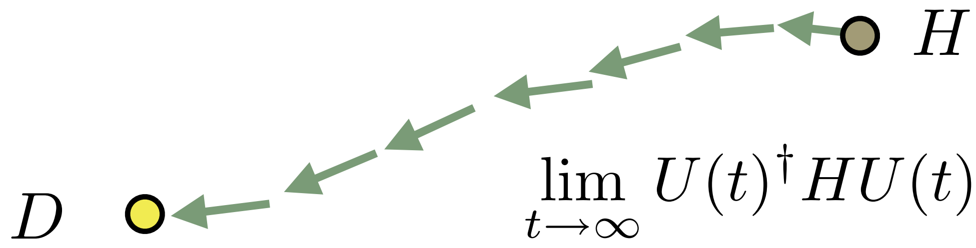
$$\mathcal{S}_D = \{U|\mathbf{0}\rangle : U \in U_D\} \quad U = \prod_j U_j$$

such that local properties computable

Dawson, Eisert, Osborne (2007)

Flow and optimal control approach to simulation

- **Flow ideas:** “Diagonalize the Hamiltonian with infinitesimal unitaries”



$$\lim_{t\to\infty} U(t)^\dagger H U(t) = D$$

- In terms of **generator**: $U(t) = \mathcal{T} \exp\left(-i \int_0^t ds G(s) ds\right)$

- Consider **figure of merit**: $E(t) = \langle \mathbf{0} | U(t)^\dagger H U(t) | \mathbf{0} \rangle$

> **Lemma:** $\displaystyle \min_{\mathrm{tr}[G(t)^\dagger G(t)]=\varepsilon} \frac{dE(t)}{dt}$
>
> for “bracket” generator $G(t) \sim [|\mathbf{0}\rangle\langle\mathbf{0}|, U(t)^\dagger H U(t)]$

Brockett (1972)
Schulte-Herbrueggen, Spoerl, Khaneja, Glaser (2005)

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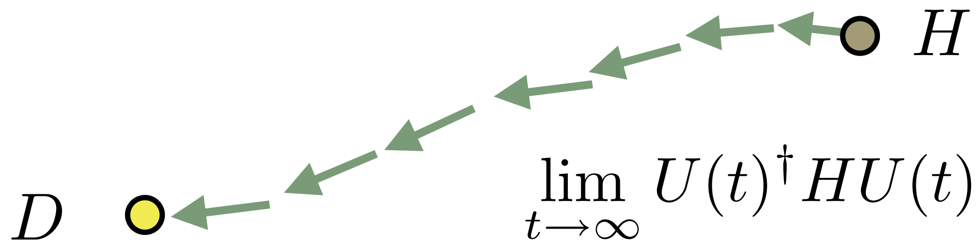
- **Flow ideas:** "Diagonalize the Hamiltonian with infinitesimal unitaries"



$$\lim_{t \to \infty} U(t)^\dagger H U(t) = D$$

- Of course, this **cannot** be done over the **unitary group** $U(d^n)$
- **Wegner's flow renormalization:** *Expansions* in a parameter, truncate
- **Way out in the following:**

> - Use flow ideas to take it as a **method** to vary over unitary networks describing "data sets" in the Heisenberg picture

Wegner (1994)
Glazek, Wilson (1994)
Dawson, Osborne, Eisert (2007)

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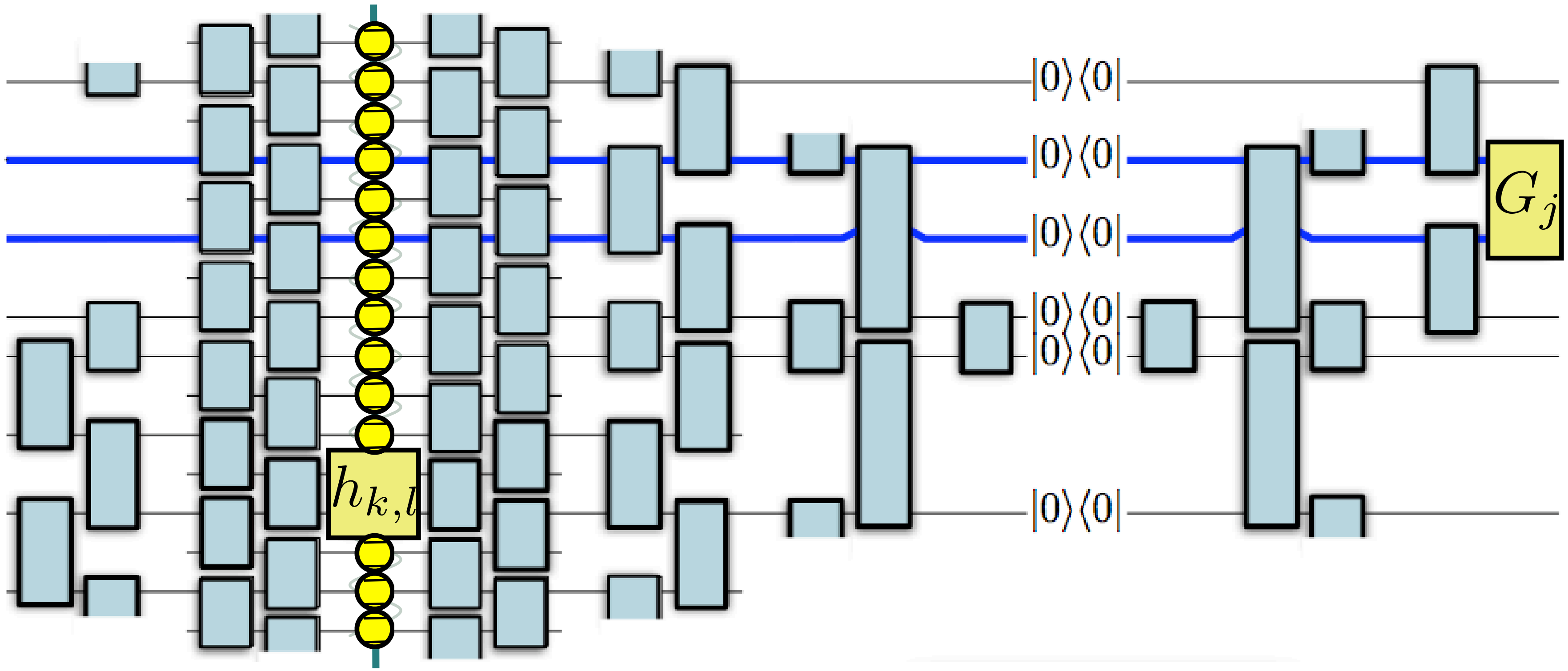
- For
$$\partial_t E = \langle \mathbf{0} | \partial_t U^\dagger H U + U^\dagger H \partial_t U | \mathbf{0} \rangle$$
$$U(t) = \prod_{j=1}^{M} U_j(t)$$
$$\partial_t U = -i \sum_{j=1}^{M} \Big(\prod_{k=j+1}^{M} U_k \Big) G_j \Big(\prod_{k=1}^{j} U_k \Big).$$

- **Lemma:** Optimal generator $G_j \sim F_j + F_j^\dagger$
$$F_j = \mathrm{tr}_{R_j} \left[(\prod_{k=1}^{j} U_k) | \mathbf{0} \rangle \langle \mathbf{0} | U^\dagger H (\prod_{k=j+1}^{M} U_k) \right]$$

Dawson, Osborne, Eisert (2007)

• Flow and optimal control approach to simulation

- For example, for **MERA:** Hamiltonian and generator causal cone:



Dawson, Osborne, Eisert (2007)

• Flow and optimal control approach to simulation

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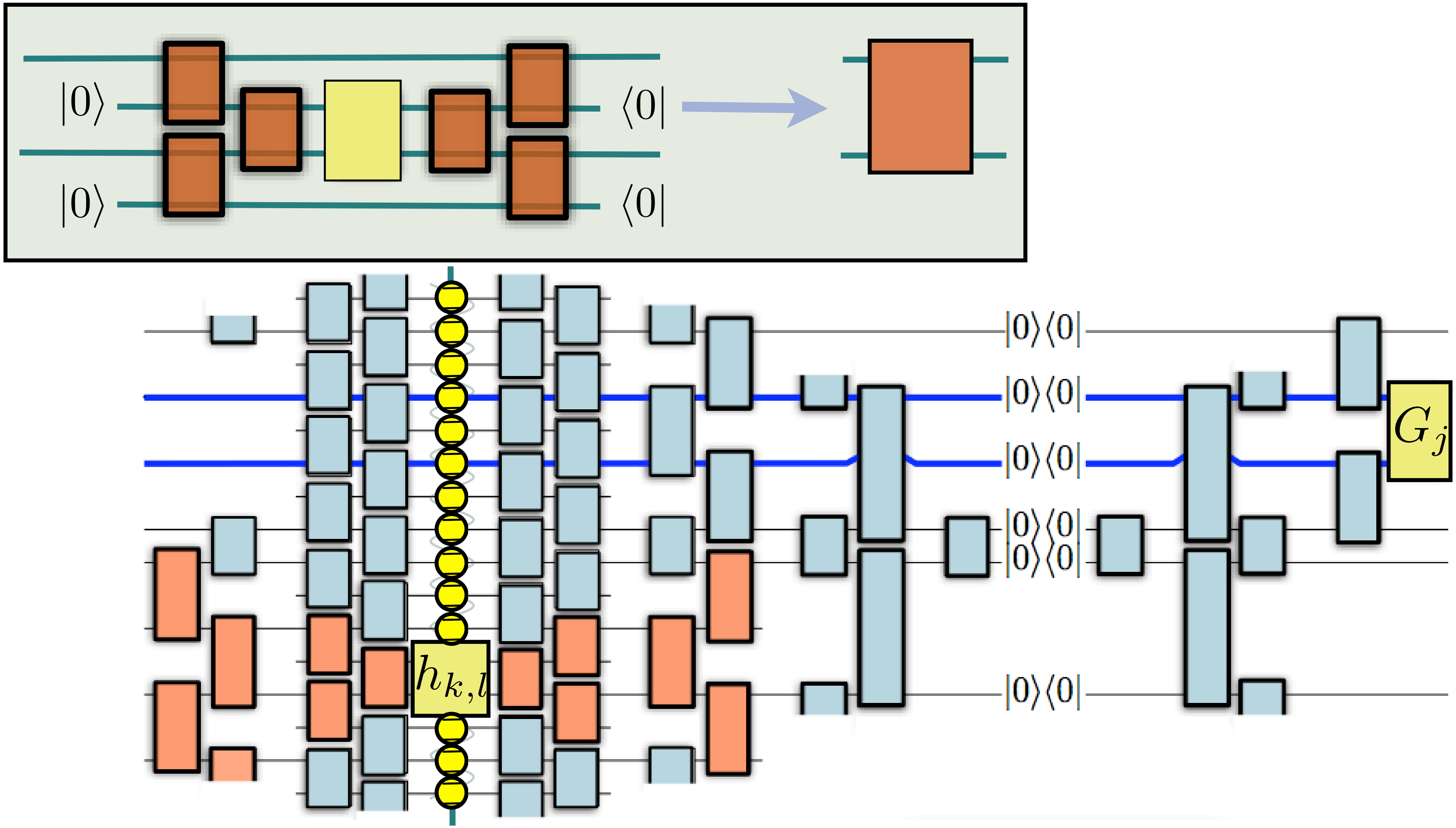
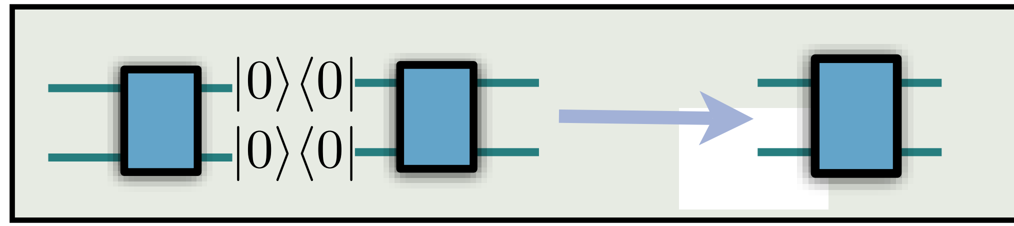
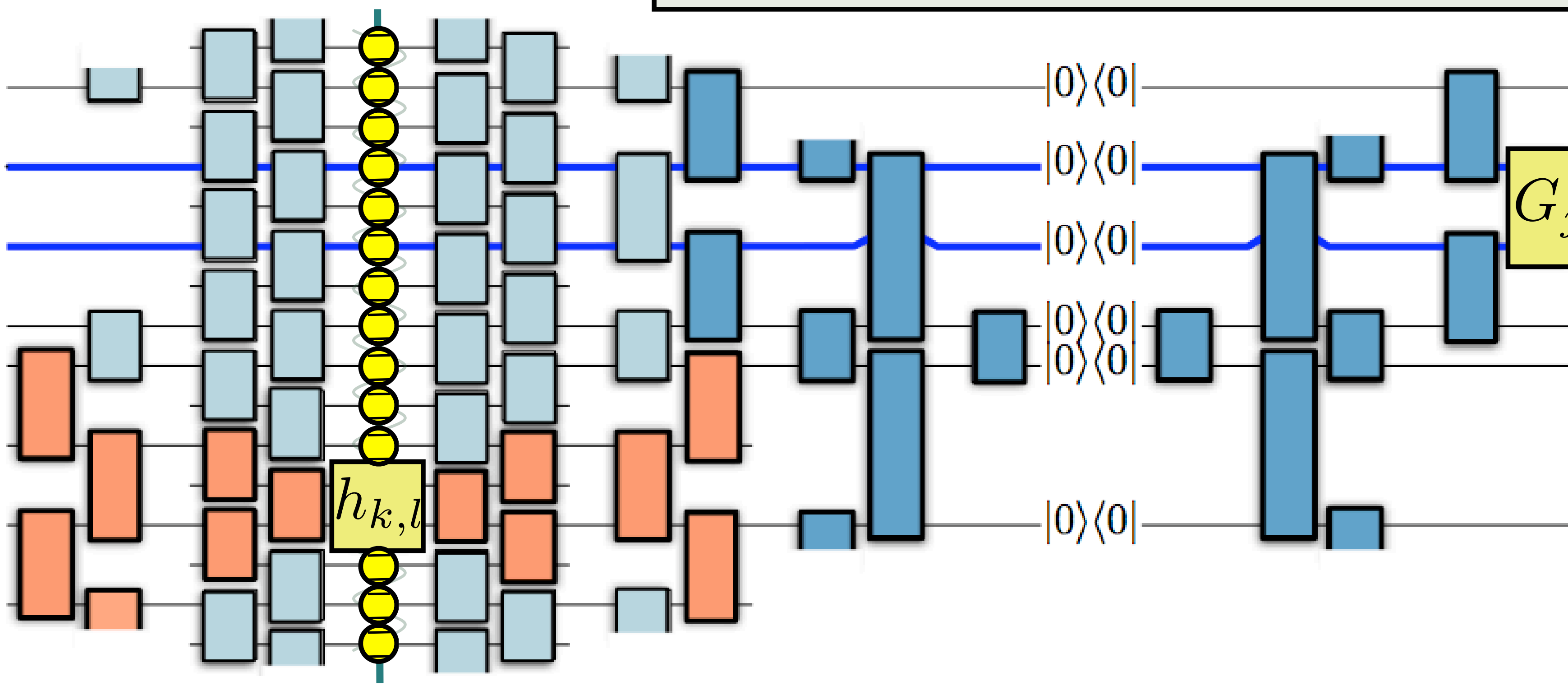


Dawson, Osborne, Eisert (2007)

- For example, for **MERA:** Hamiltonian and generator causal cone:
- Optimal generator can be found with effort $O(n\log(n))$ for MERA, and $O(nD^3)$ for staircase





Dawson, Osborne, Eisert (2007)

- Comparison with benchmark of DMRG, *Heisenberg-chain* of 28 spins
- *Staircase circuit*

$$H = -\frac{1}{2}\sum_{j=1}^{n}\left(J\sum_{k=1}^{3}\sigma_j^k\sigma_{j+1}^k\right)$$

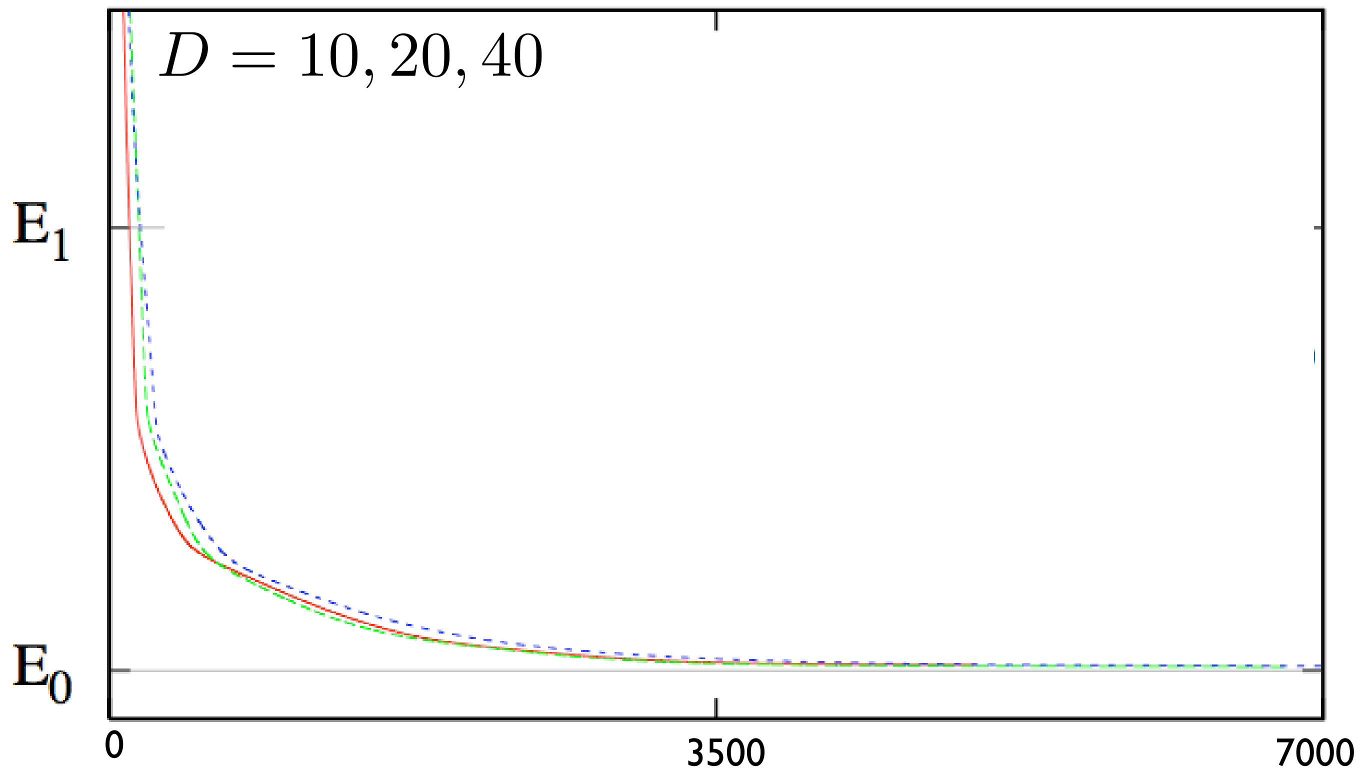
- Compared with ALPS

Exact: $E_0 = -52.44542$

$\Delta E = -0.49962$

ALPS DMRG/flow:

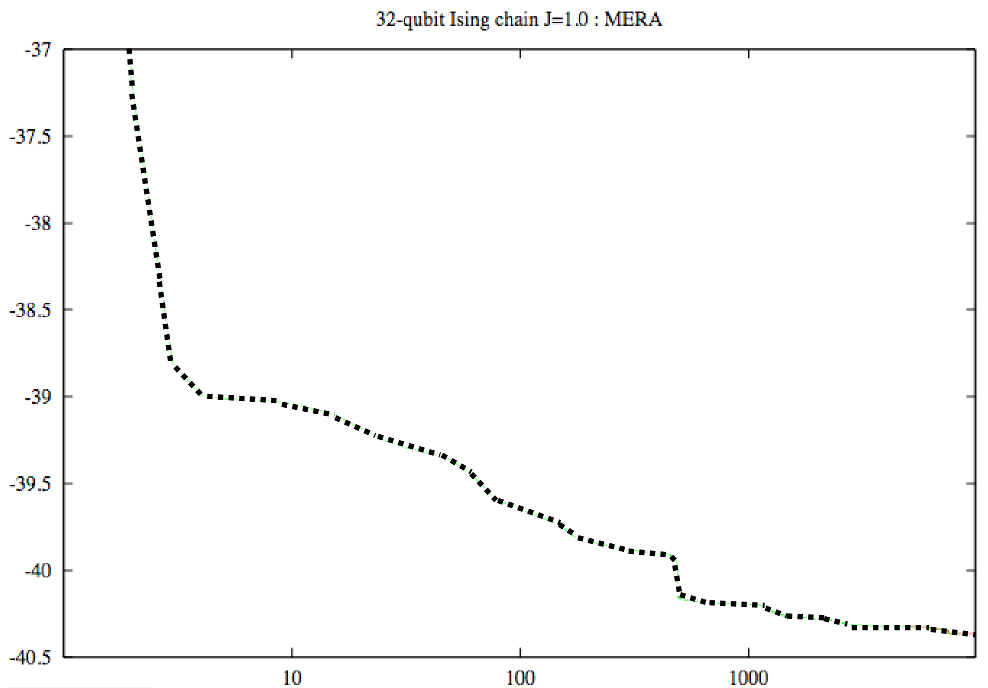
$E_0(20) = -52.44100$



- Does not get stuck in local minima

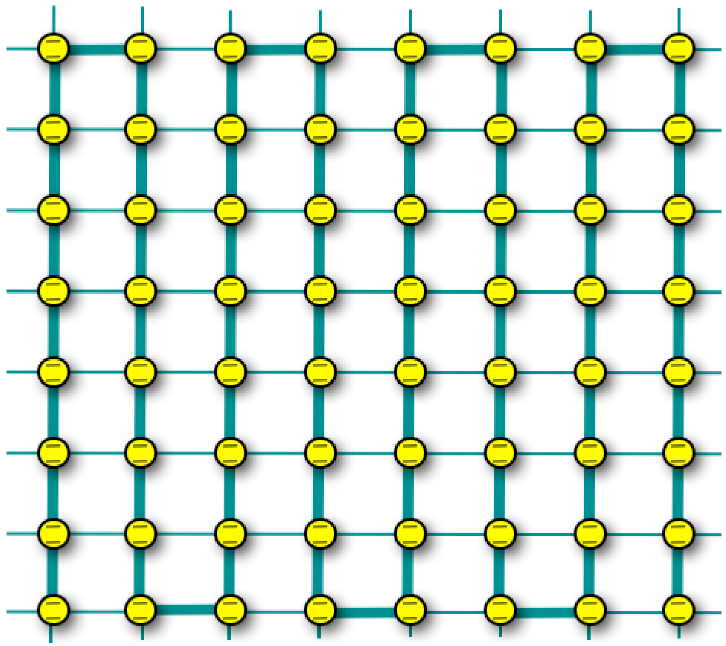
• Flow and optimal control approach to simulation

- MERA: Surprisingly, just as well as staircase (DMRG) for $D = 30$ open boundary condition *Ising chain* with $N = 32$



- **Flow and optimal control approach to simulation**

- Funny enough: If one (just for fun) makes use of a "snake", as historically done in DMRG to simulate 2D-Ising systems, MERA performs not so badly

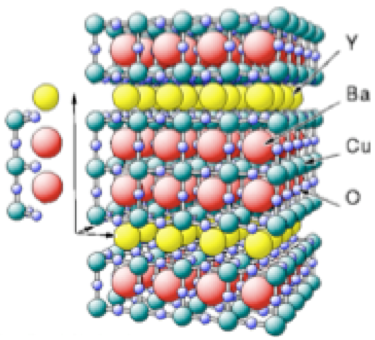


- Run of last night: Ising 8x8, $E = -133.052$ (compared to $E = -112.124$ DMRG, $D = 30$)

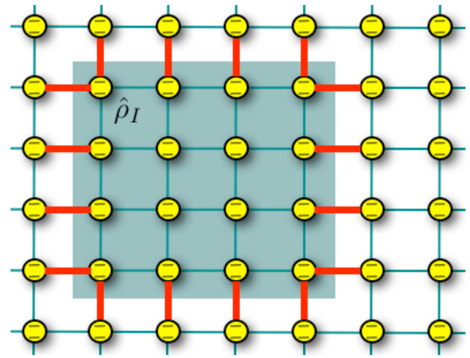
  - But, needless to say, actual promise is in proper 2D MERA, ...

• Point of tutorial in a nutshell

- **Summary:**

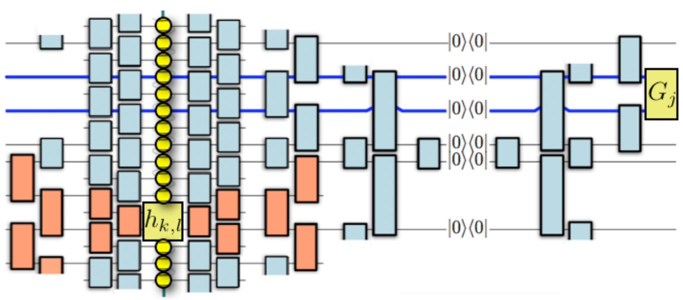


Many-body systems
interesting challenge



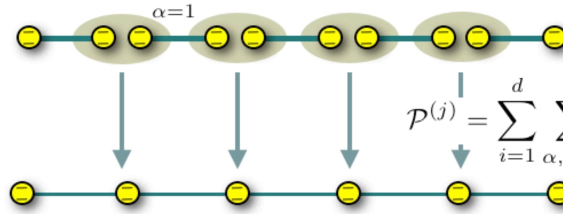
Locality of interactions inherited by scaling of **entanglement: area laws**

Unwise/impossible to vary over all states: Look for smart much **smaller sets of variational states**



Flow approaches may bring together optimal control ideas and simulation

$$|I\rangle = \sum_{\alpha=1}^{D} |\alpha,\alpha\rangle$$



$$\mathcal{P}^{(j)} = \sum_{i=1}^{d} \sum_{\alpha,\beta=1}^{D} A^{(j)}_{i_j,\alpha,\beta} |i\rangle\langle\alpha,\beta|$$

$$|\psi\rangle = \sum_{i_1,\dots,i_N} \mathrm{tr}[A^{(1)}_{i_1} A^{(2)}_{i_2} \dots A^{(N)}_{i_N}] |i_1, i_2, \dots, i_N\rangle$$

Matrix-product states as in DMRG satisfy area laws, MERA and MPS+WGS ... can also efficiently be contracted

Thanks for your attention!