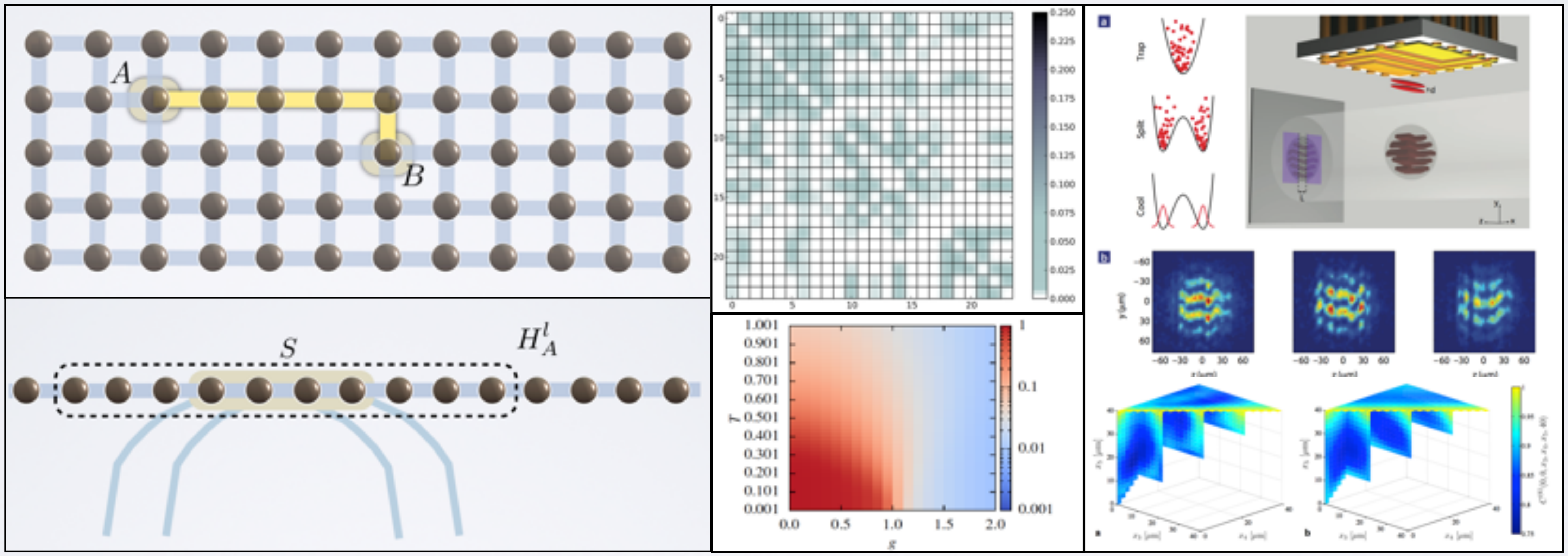
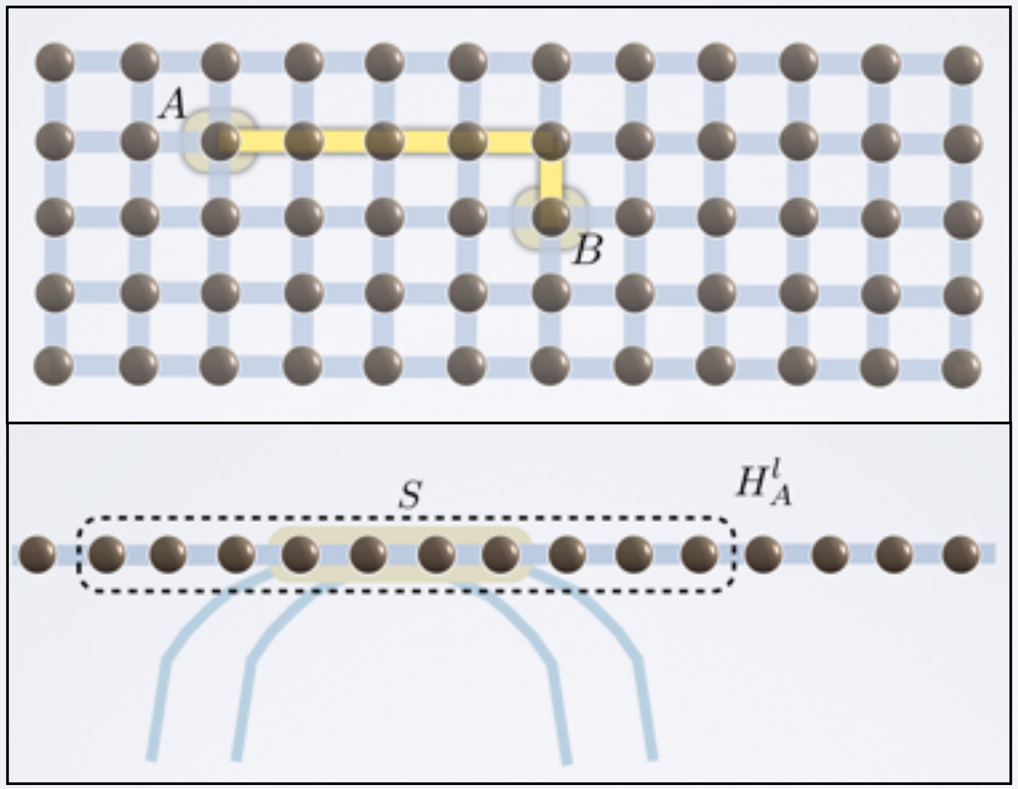
Analytical and numerical methods



for quantum many-body systems

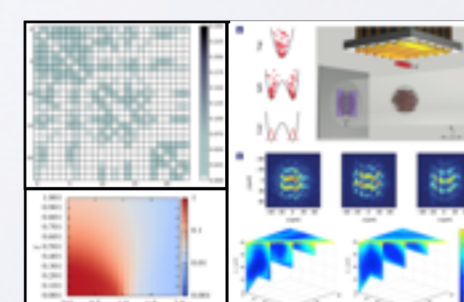
Jens Eisert, FU Berlin

Analytical methods



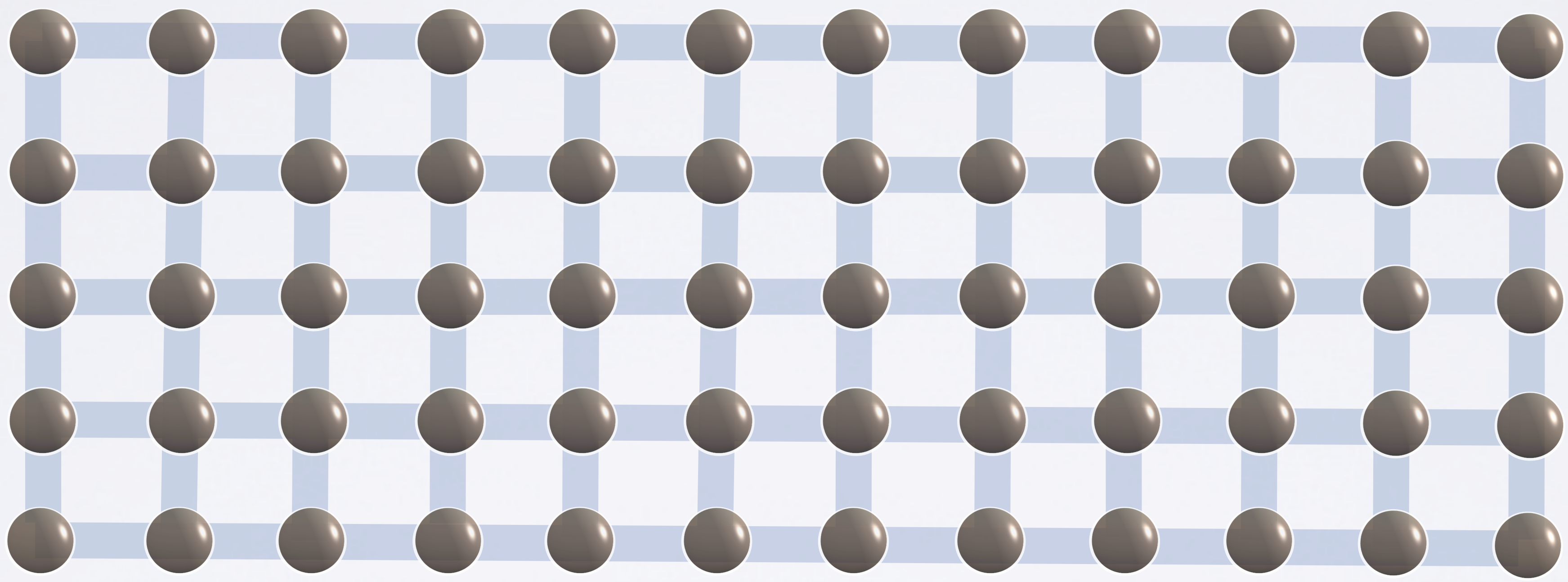
for quantum many-body systems

Jens Eisert, FU Berlin

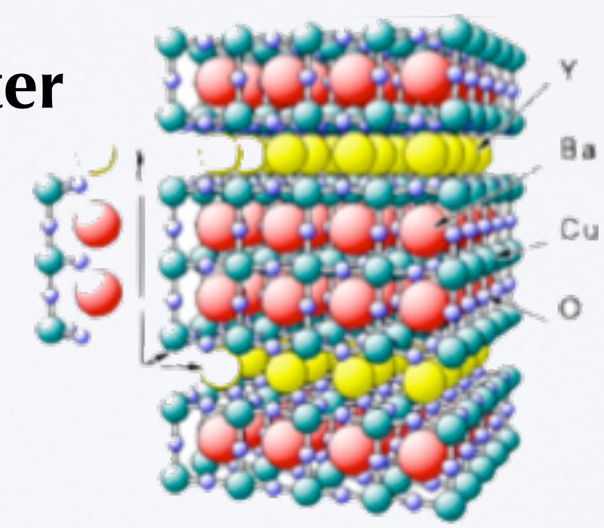


Ground states of local Hamiltonians

- Local Hamiltonians $H = \sum_j h_j$



- Models for **strongly correlated matter**



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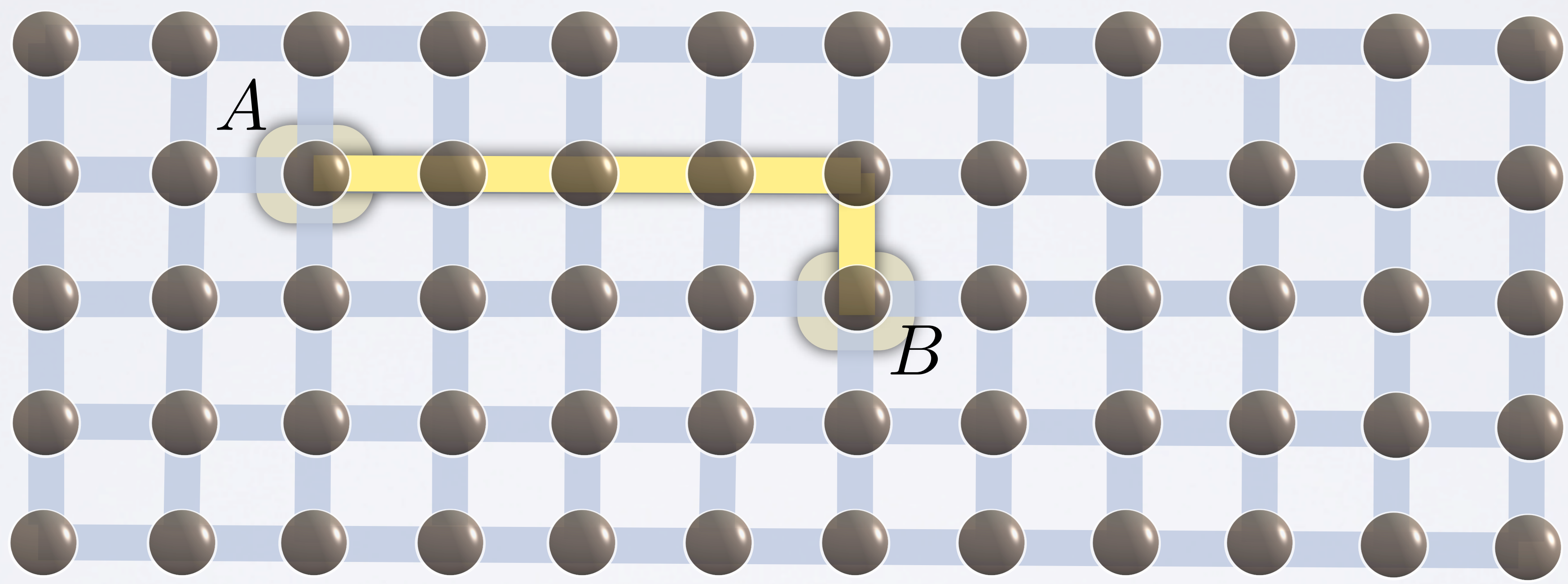


- **Energy gap** $\Delta(H) = E_1 - E_0 > 0$
- Ground states of gapped models have **exponentially decaying correlations**

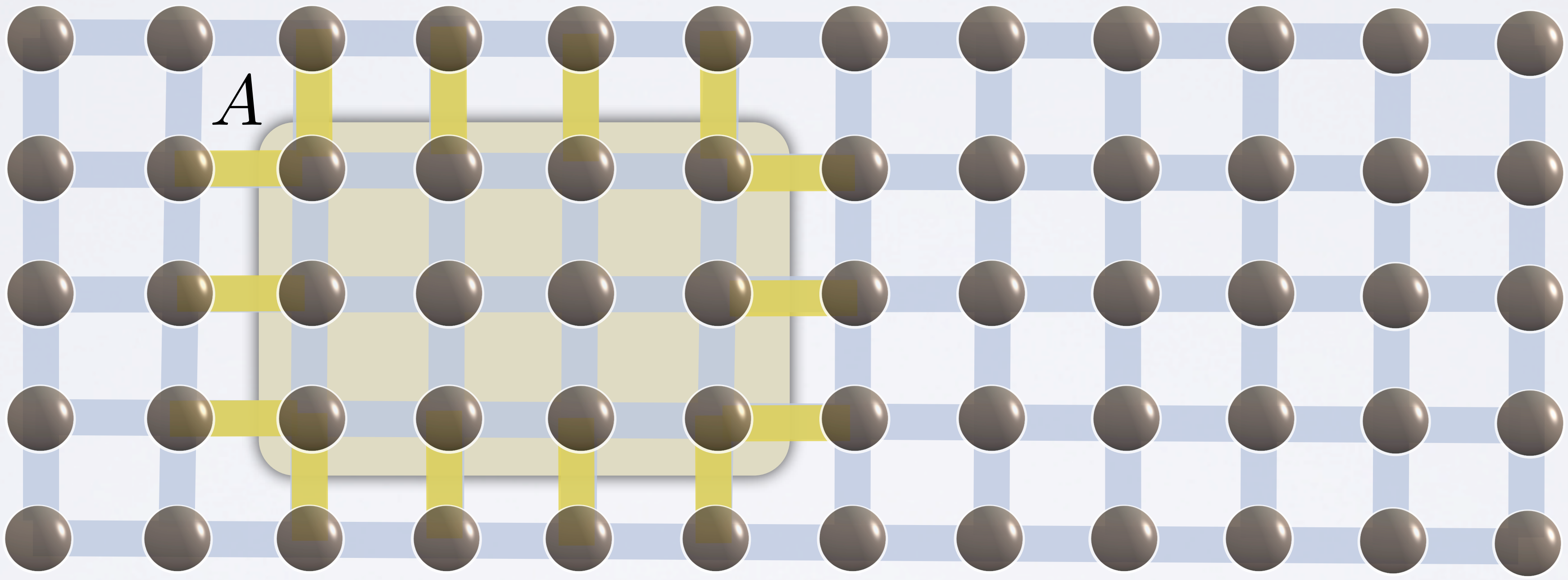
- Proof based on Lieb-Robinson bounds

  Hastings, Koma, Commun Math Phys 265, 781 (2006)
  Nachtergaele, Sims, Commun Math Phys 265, 119 (2006)

- Combinatorical proof (detectability lemma)

  Aharonov, Arad, Landau, Vazirani, arXiv:1011.3445

Area laws

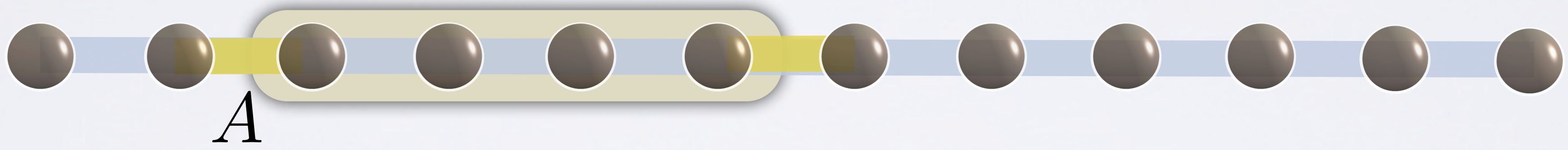


- Area laws for the **entanglement entropy** $S(\rho_A) = O(|\partial A|)$

- Proven in >1D for gapped free bosonic and fermionic systems and models in same quantum phase as one fulfilling an area law

Eisert, Cramer, Plenio, Rev Mod Phys 82, 277 (2010)
Van Acoleyen, Marien, Verstraete, Phys Rev Lett 111, 17501 (2013)
Plenio, Eisert, Dreissig, Cramer, Phys Rev Lett 94, 060503 (2005)

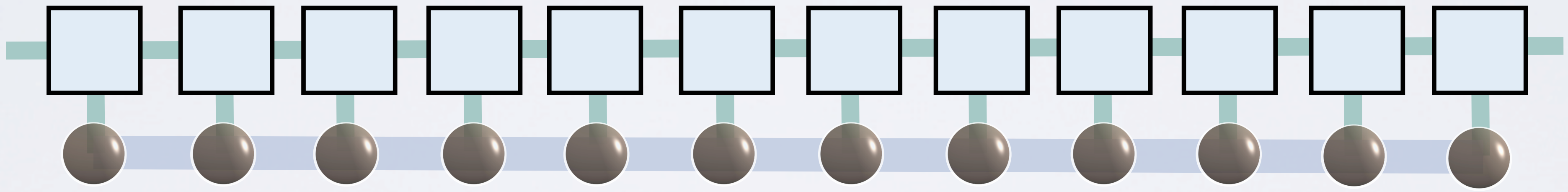
Area laws



- All gapped models in **1D** satify an area law

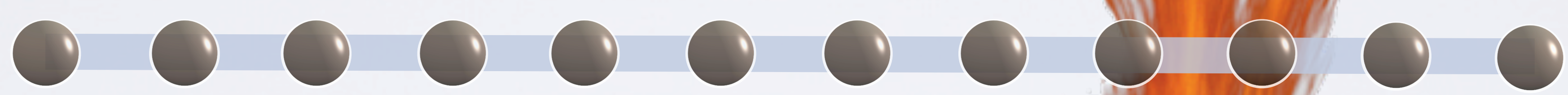
Hastings, Koma, Commun Math Phys 265, 781 (2006)
Aharonov, Arad, Landau, Vazirani, arXiv:1011.3445
Brandao, Horodecki, arXiv:1206.2947

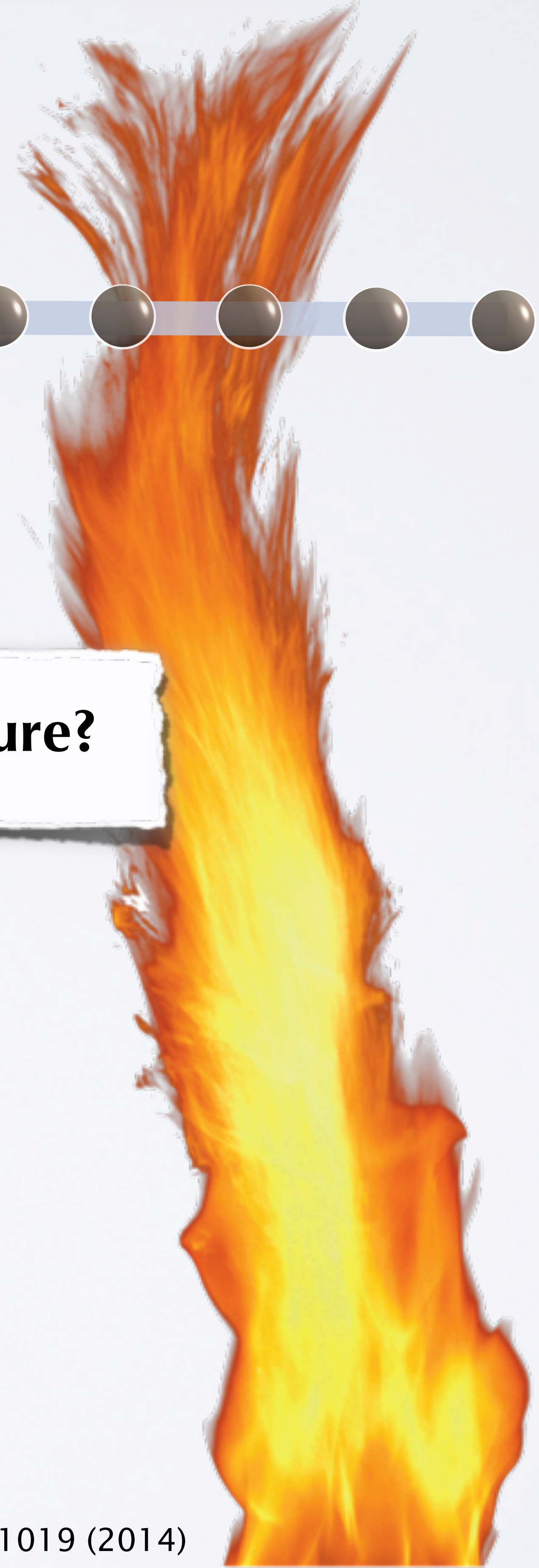
Tensor networks



- **Matrix-product states** approximate GS of gapped models well: Functioning of DMRG
- Higher-dimensional **tensor network states**

Overview over talk



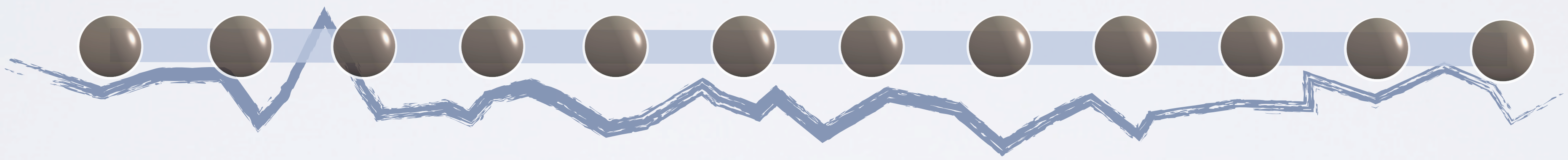


1. What happens at finite temperature?

- Locality of temperature
- Clustering of correlations
- Tensor network approximations

Kliesch, Gogolin, Kastoryano, Riera, Eisert, Phys Rev X 4, 031019 (2014)

Overview over talk

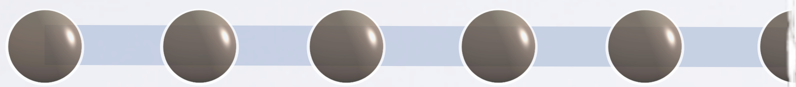


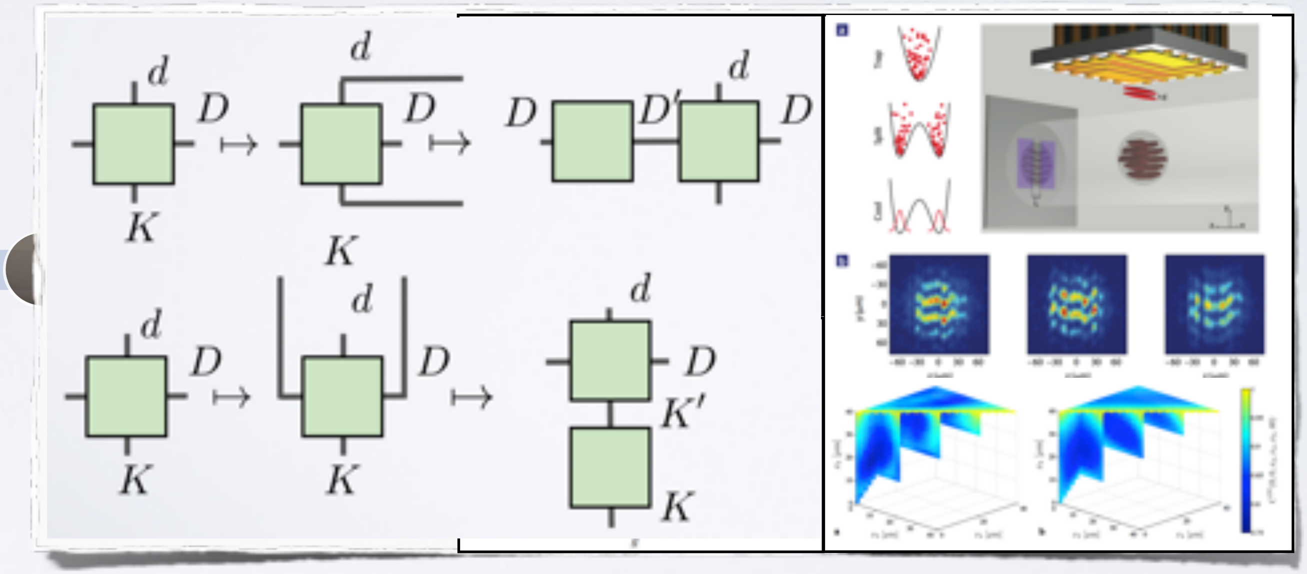
2. Many-body localisation and disordered models?

- Many complementing views on the problem
- Dynamical and static readings
- A new result on matrix-product states

Friesdorf, Werner, Scholz, Brown, Eisert, soon (2014)

Announcement of posters :)





Posters on numerical techniques for strongly correlated systems

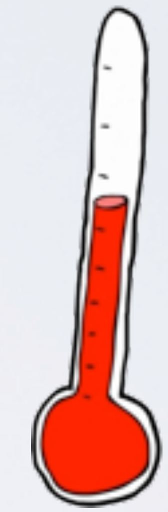
- Tensor network methods in *quantum chemistry*
- Continuous matrix-product states and *quantum field tomography*
- A positive tensor network methods for simulating *open systems*

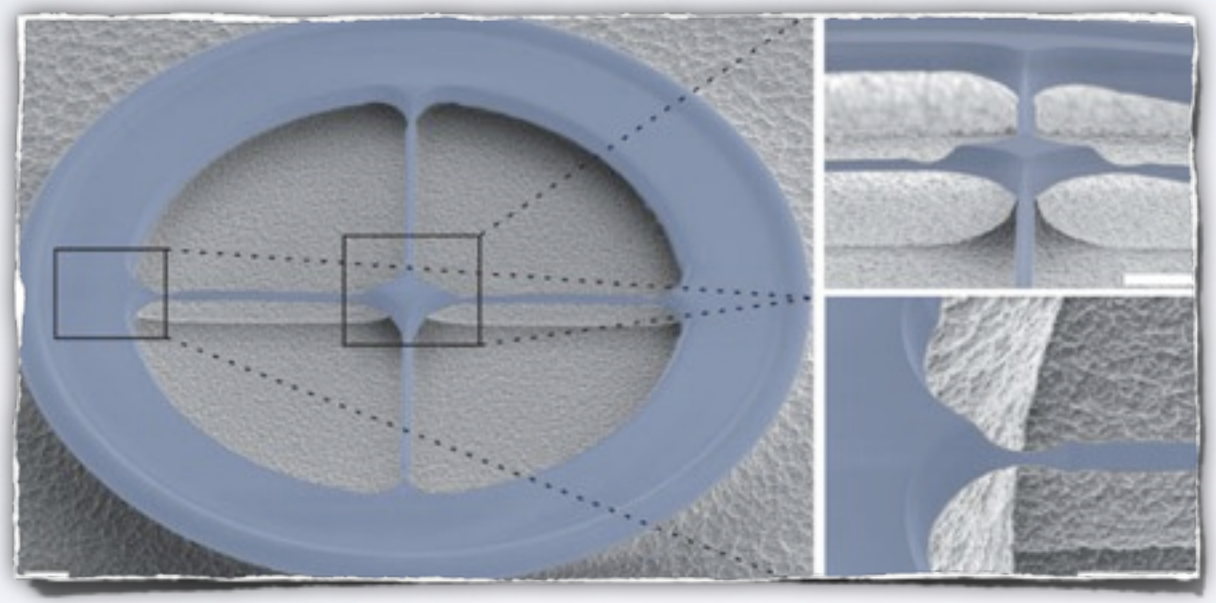
Krumnow, Legeza, Schneider, Eisert, soon (2014)
Steffens, Friesdorf, Langen, Rauer, Schweigler, Huebener, Schmiedmayer, Riofrio, Eisert, arXiv:1406.3632
Steffens, Riofrio, Huebener, Eisert, arXiv:1406.3631
Kliesch, Gross, Eisert, Phys Rev Lett 113 (2014)
Jaschke, Silvi, Calarco, Werner, Eisert, Montangero, soon (2014)

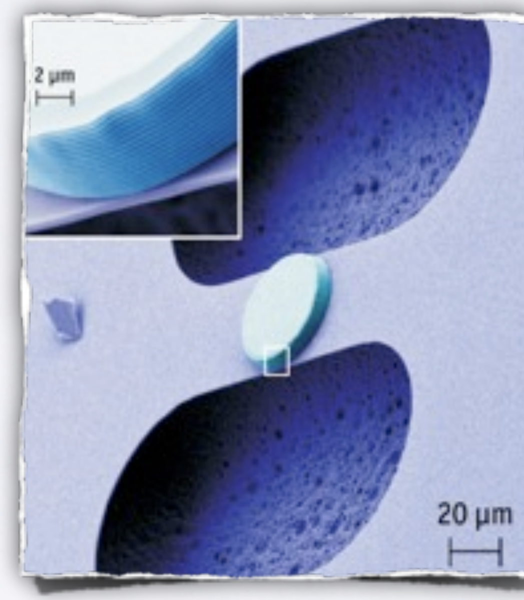
Clustering of correlations in thermal states

Locality of temperature?

- At what **length scales** is temperature well-defined?







Pothier, Gueron, Birge, Esteve, Devoret, Phys Rev Lett 79, 3490 (1997)
Peng, Su, Liu, Yu, Cheng, Bao, Nanoscale 5, 9532 (2013)
Hartmann, Mahler, Hess, Phys Rev Lett 93, 080402 (2004)
Ferraro, Garcia-Saez, Acin, Europhys Lett 98, 10009 (2012)

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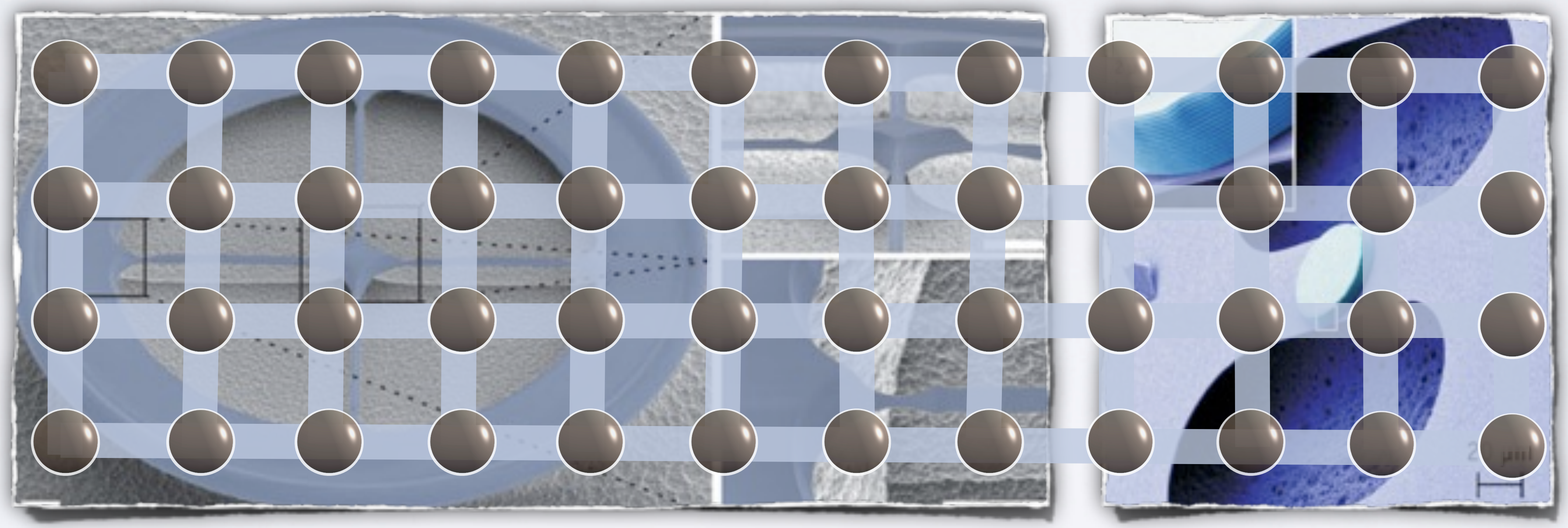

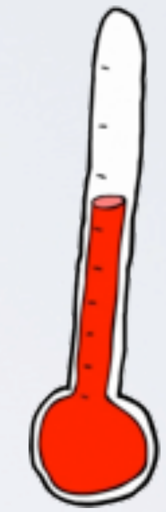

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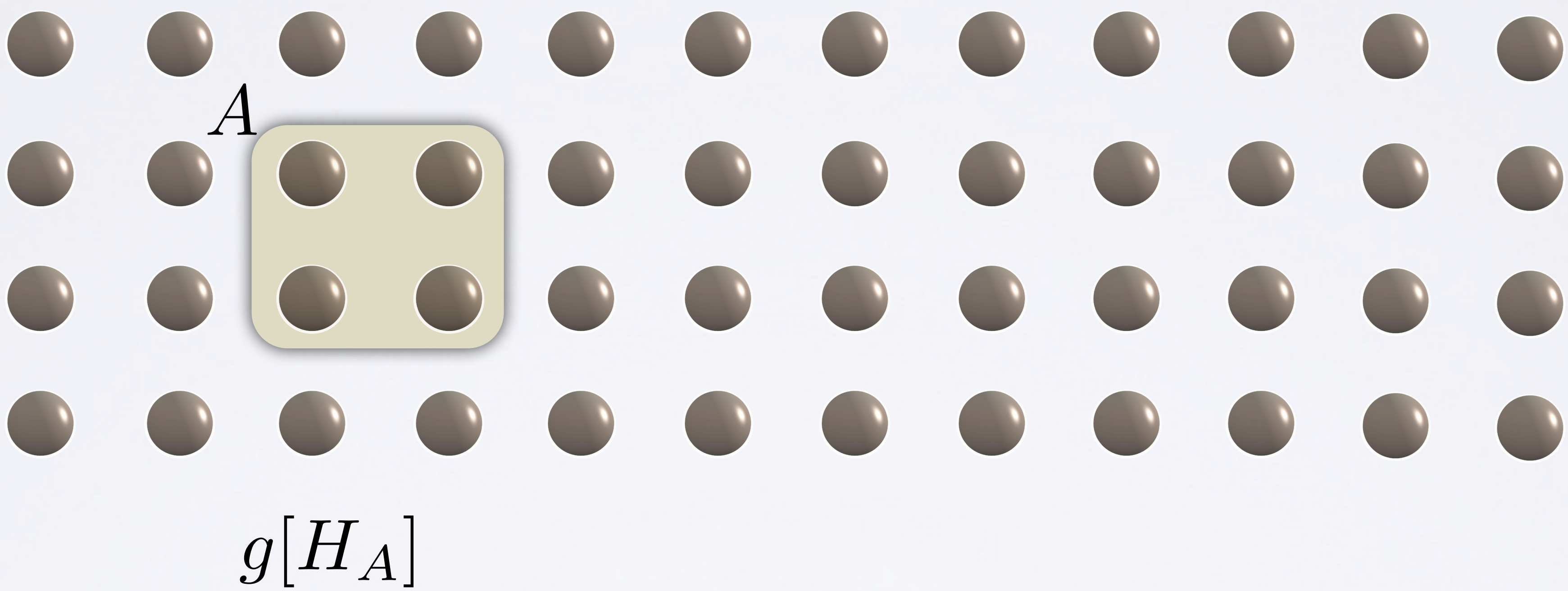

- Gibbs states $g[H] = \dfrac{e^{-\beta H}}{\mathrm{tr}(e^{-\beta H})}$

Pothier, Gueron, Birge, Esteve, Devoret, Phys Rev Lett 79, 3490 (1997)
Peng, Su, Liu, Yu, Cheng, Bao, Nanoscale 5, 9532 (2013)
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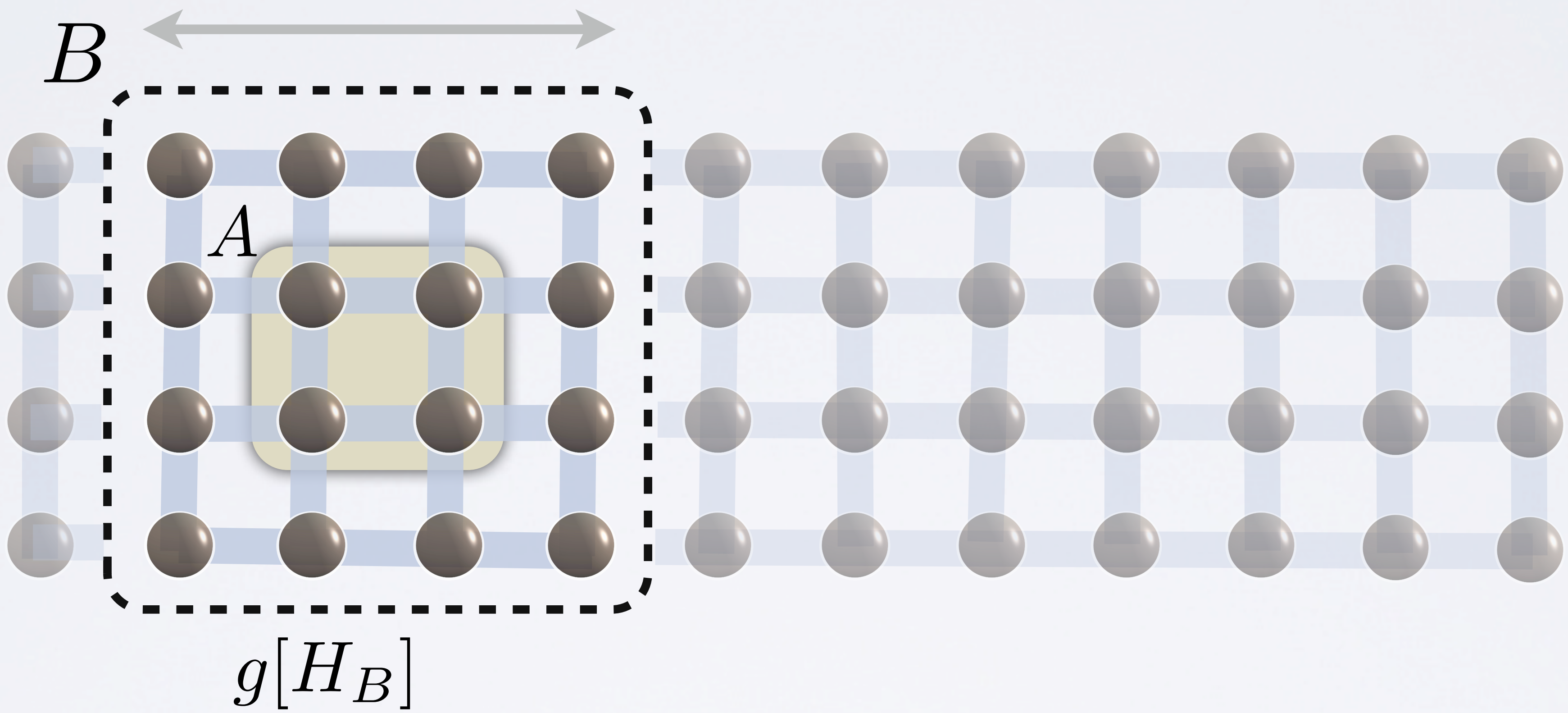

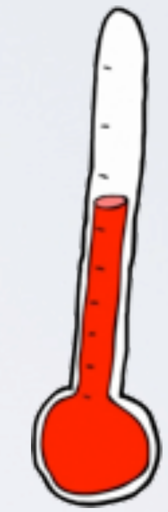

Pothier, Gueron, Birge, Esteve, Devoret, Phys Rev Lett 79, 3490 (1997)
Peng, Su, Liu, Yu, Cheng, Bao, Nanoscale 5, 9532 (2013)
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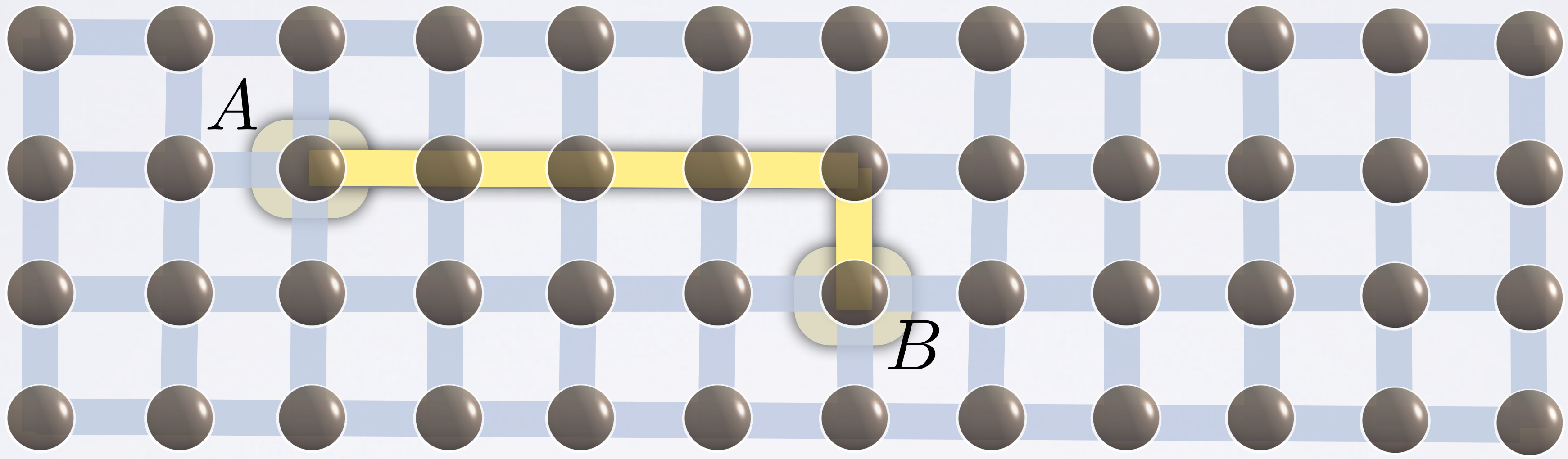
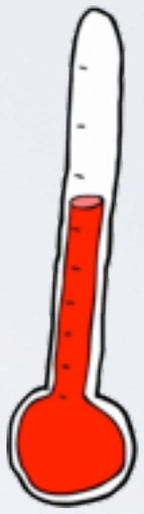
Thermal states of quantum many-body systems

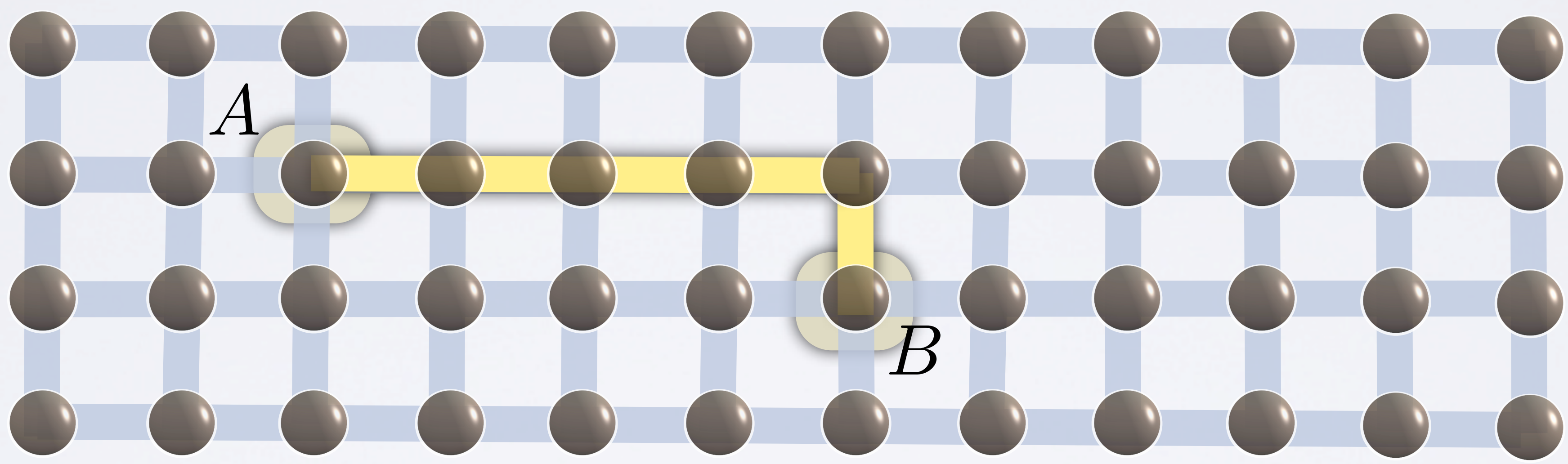


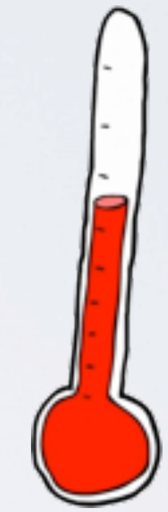


- Again, GS of gapped Hamiltonians have clustering correlations

- **Is there a thermal analogue?**

Thermal states of quantum many-body systems



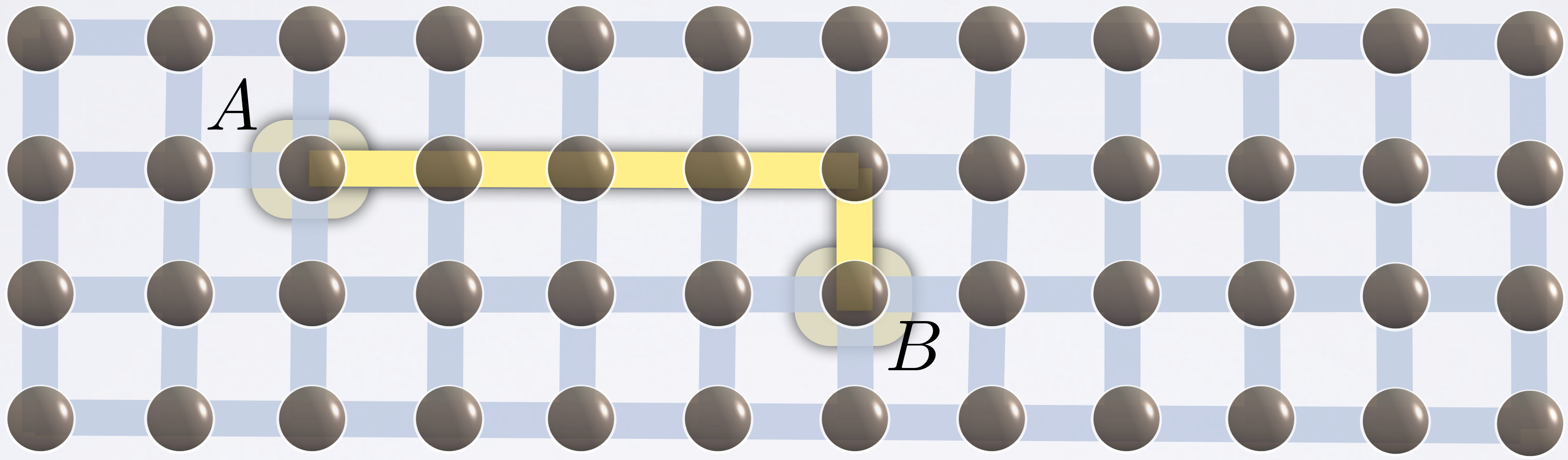


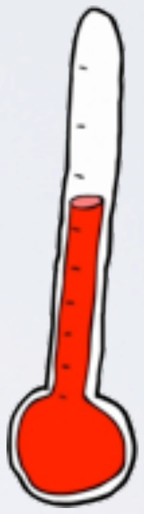
- **Critical temperature**, dependent only on crude properties of graph (+ coupling strength), above which correlations cluster?

- Long-standing **open question**, results known for **classical and continuum models**, some (few) insights into quantum lattice models

Araki, Commun Math Phys 38,1 (1974)
Ruelle, Rev Mod Phys 36, 580 (1964)
Ginibre, J Math Phys 6, 252 (1965)
Greenberg, Commun Math Phys 13, 335 (1969)
Brattelli, Robinson, Operator algebras in quantum statistical mechanics (Springer, 1981)

Thermal states of quantum many-body systems



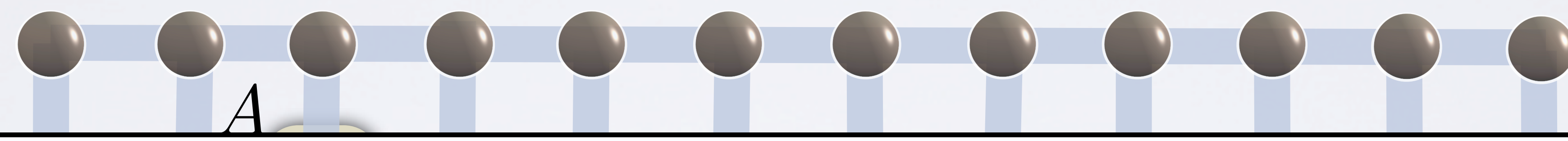


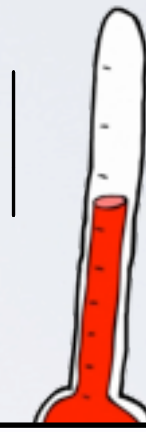
- **Yes :)**

Kliesch, Gogolin, Kastoryano, Riera, Eisert, Phys Rev X 4, 031019 (2014)

General clustering of correlations at high temperatures

$$\xi(\beta) = \left|1/\ln(\alpha e^{2|\beta|J}(e^{2|\beta|J}-1))\right|$$





- **Clustering of correlations in thermal states:** Consider local Hamiltonian on arbitrary regular lattice, $J := \max \|h_k\|$ coupling strength, then exists critical inverse temperature

$$\beta^* := \log((1+\sqrt{1+4/\alpha}/2)/(2J)$$

such that for all $\beta < \beta^*$ and $d(A,B) \geq L_0$

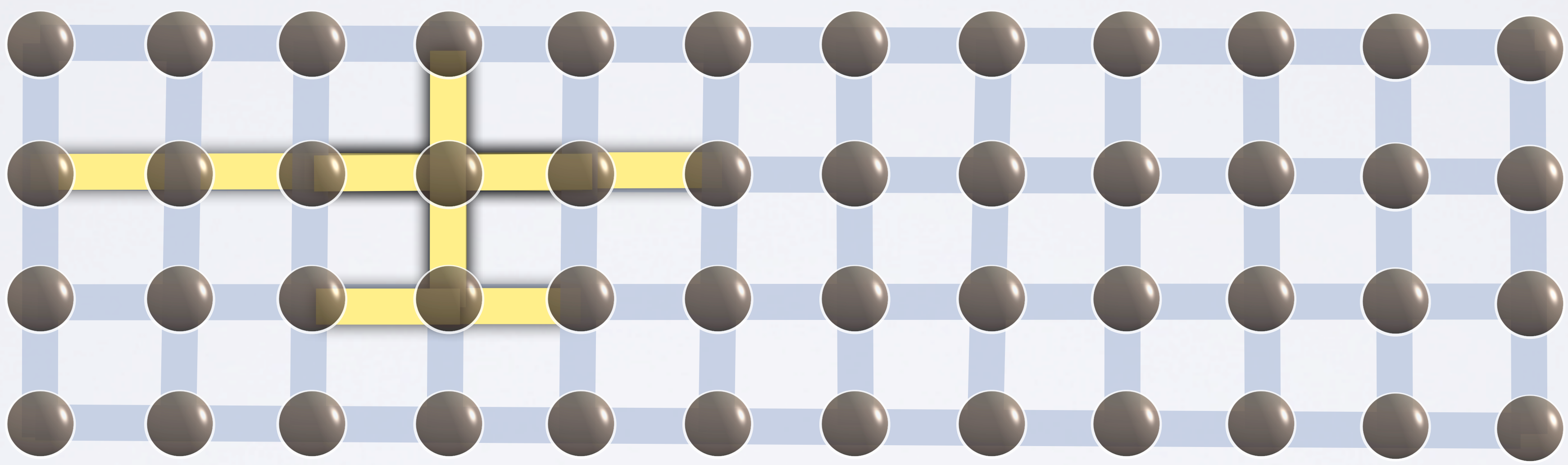
$$C_{g[H]}(A,B) \leq \frac{4\min\{|\partial A|,|\partial B|\}}{\log(3)} \frac{\|f\|\,\|g\|}{1-e^{-1/\xi(\beta)}} e^{-d(A,B)/\xi(\beta)}$$

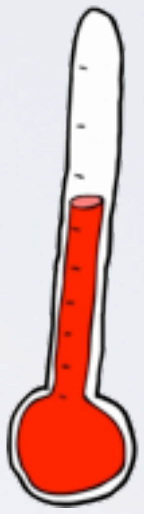
$$\xi(\beta) := \left|1/\ln(\alpha e^{2|\beta|J}(e^{2|\beta|J}-1))\right|$$

- α **lattice animal constant**
- General statement for **arbitrary lattices** and **covariances**

Kliesch, Gogolin, Kastoryano, Riera, Eisert, Phys Rev X 4, 031019 (2014)

Lattice animal constants





- Connected set of edges: **Lattice animal**
- Number a_m of lattice animals F of size $m = |F|$
- Lattice animal constant: Smallest α such that $a_m \leq \alpha^m$

Hastings, Phys Rev B 73, 085115 (2006)
Kliesch, Gogolin, Kastoryano, Riera, Eisert, Phys Rev X 4, 031019 (2014)

Flavour of proof

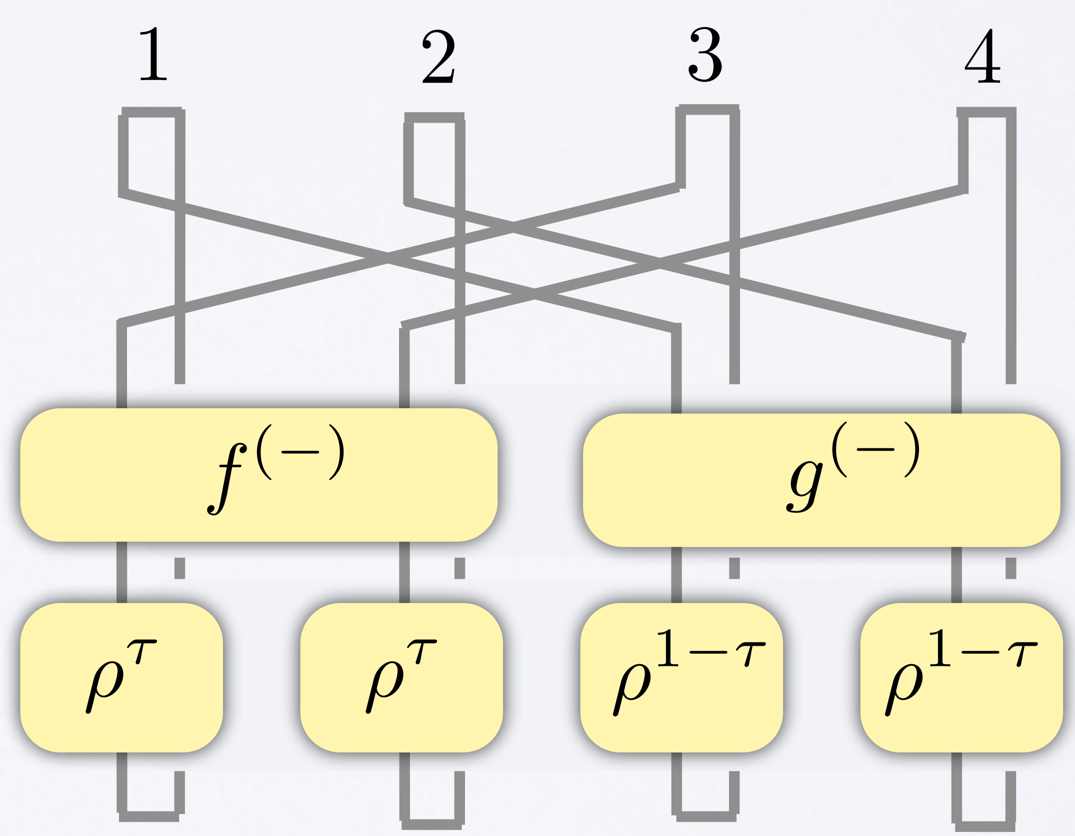
Define **generalized covariance** $\mathrm{Cov}_\rho^\tau(f,g) = \mathrm{tr}(\rho^\tau f \rho^{1-\tau} g) - \mathrm{tr}(\rho f)\mathrm{tr}(\rho g), \ \tau \in [0,1]$

Multiple "swap-trick"

Write $\mathrm{Cov}_\rho^\tau(f,g) = \frac{1}{2}\mathrm{tr}\left(\mathcal{S}^{(1,3)}\mathcal{S}^{(2,4)}(f^{(-)} \otimes g^{(-)})(\rho^\tau \otimes \rho^\tau \otimes \rho^{1-\tau} \otimes \rho^{1-\tau})\right)$

on four copies, where $f^{(-)} = f \otimes 1 - 1 \otimes f$

$$2\mathrm{Cov}_\rho^\tau(f,g) =$$



Kliesch, Gogolin, Kastoryano, Riera, Eisert, Phys Rev X 4, 031019 (2014)

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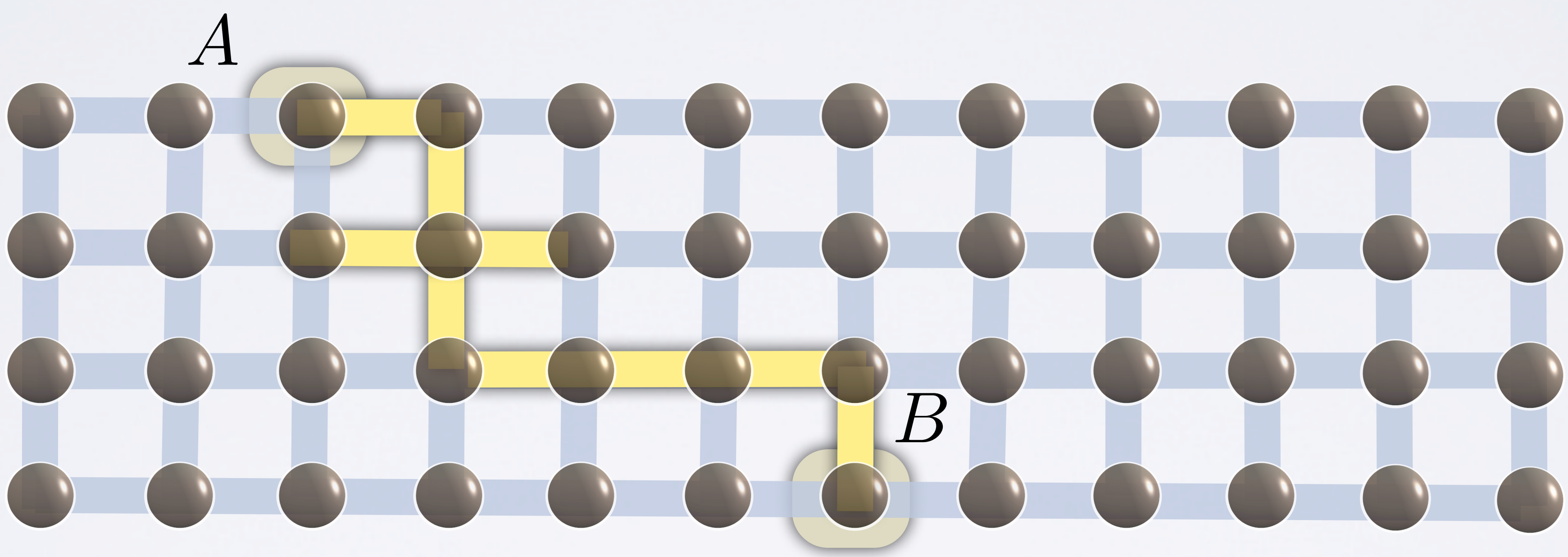
on four copies, where $f^{(-)} = f \otimes 1 - 1 \otimes f$

Cluster expansion of new Hamiltonian $\tilde{H}$

$$\frac{e^{-\beta \tilde{H}}}{\mathrm{tr}(e^{-\beta \tilde{H}})} = \rho^\tau \otimes \rho^\tau \otimes \rho^{1-\tau} \otimes \rho^{1-\tau}$$

Kliesch, Gogolin, Kastoryano, Riera, Eisert, Phys Rev X 4, 031019 (2014)

Flavour of proof



Combinatorics

Symmetry: Only clusters connecting A and B contribute

Cluster expansion of new Hamiltonian $\tilde{H}$

$$\frac{e^{-\beta \tilde{H}}}{\mathrm{tr}(e^{-\beta \tilde{H}})} = \rho^{\tau} \otimes \rho^{\tau} \otimes \rho^{1-\tau} \otimes \rho^{1-\tau}$$

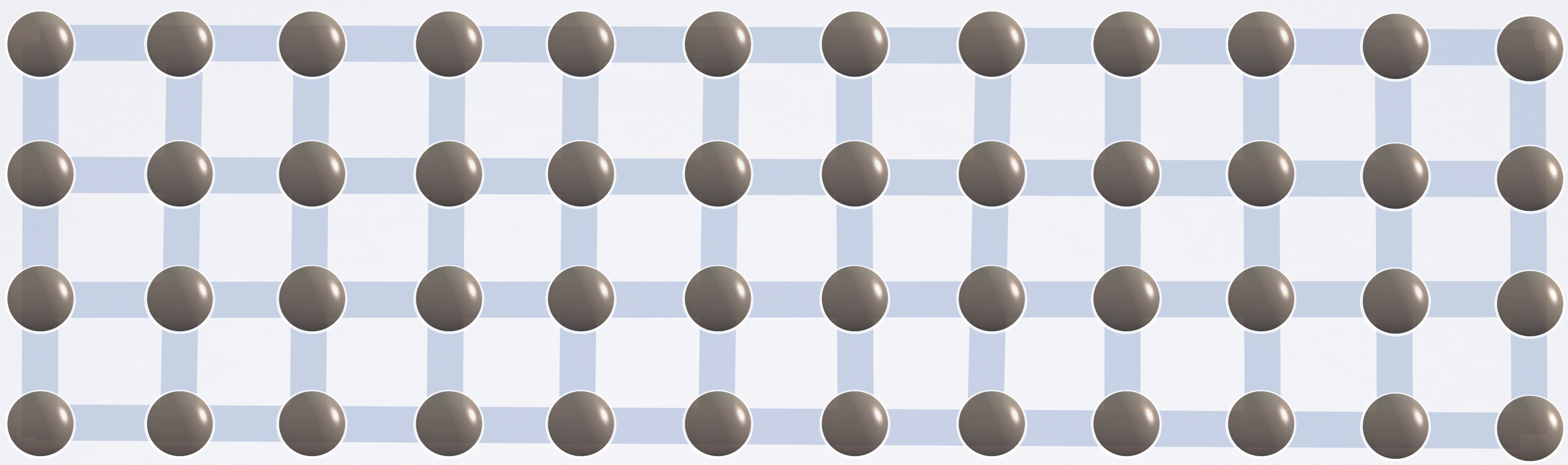
Truncated cluster expansion

$$\left\| \sum_{w \in C_{\geq L}(F)} \frac{(-\beta)^{|w|}}{|w!|} h(w) \right\|_1 \leq Z(\beta) \left(e^{|F| \frac{b(\beta)^L}{1-b(\beta)}} - 1 \right)$$

Kliesch, Gogolin, Kastoryano, Riera, Eisert, Phys Rev X 4, 031019 (2014)
Hastings, Phys Rev B 73, 085115 (2006)

Physical implications: Bounds to Curie temperatures

1. "Critical temperature" is **universal upper bound** to phase transition points

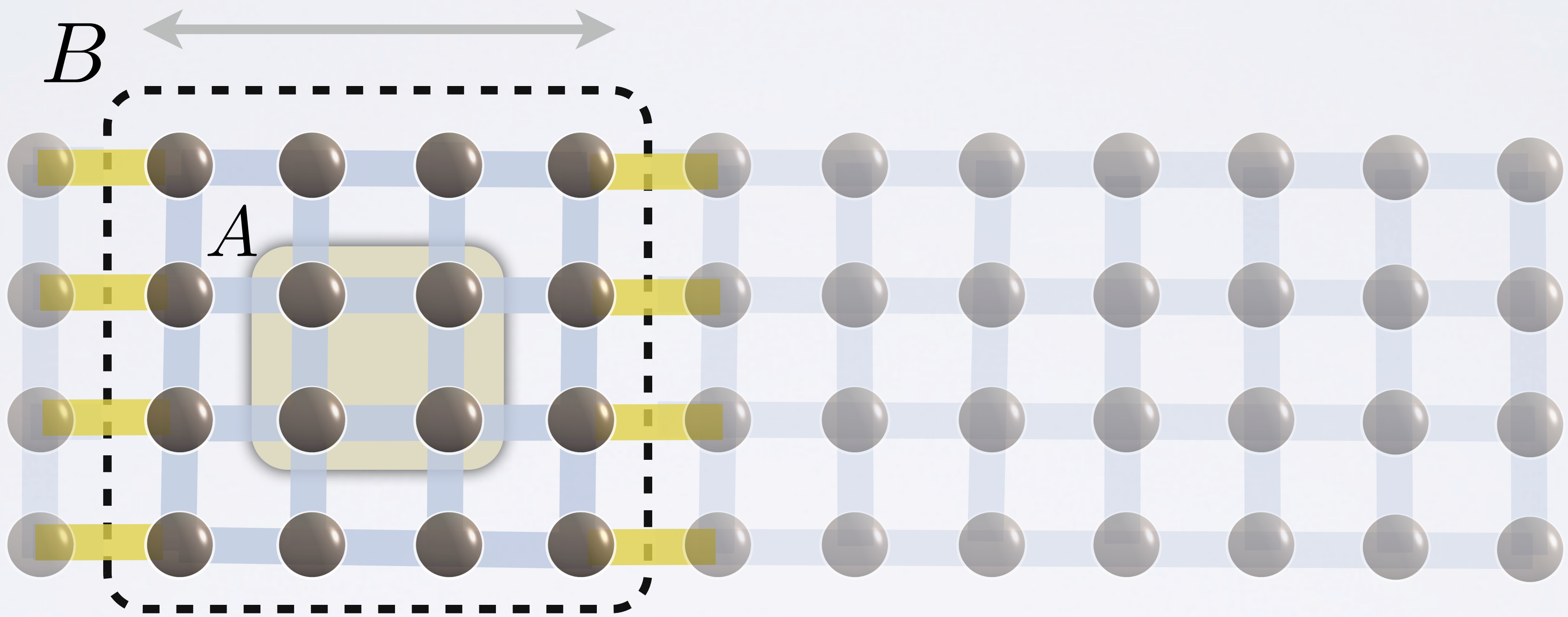


- E.g., ferromagnetic **2d isotropic Ising model** without external field, $1/(J\beta^*) = 24.58$, while phase transition known to happen at 2.27

Kliesch, Gogolin, Kastoryano, Riera, Eisert, Phys Rev X 4, 031019 (2014)

Locality of temperature

2. Length scale of temperature



$$\mathrm{tr}(Ag[H(0)]) - \mathrm{tr}(Ag[H]) = \beta \int_0^1 d\tau \int_0^1 ds \, \mathrm{Cov}^{\tau}_{g[H(s)]}(A, H_I)$$

$$H(s) = H - (1-s) H_I$$

Kliesch, Gogolin, Kastoryano, Riera, Eisert, Phys Rev X 4, 031019 (2014)

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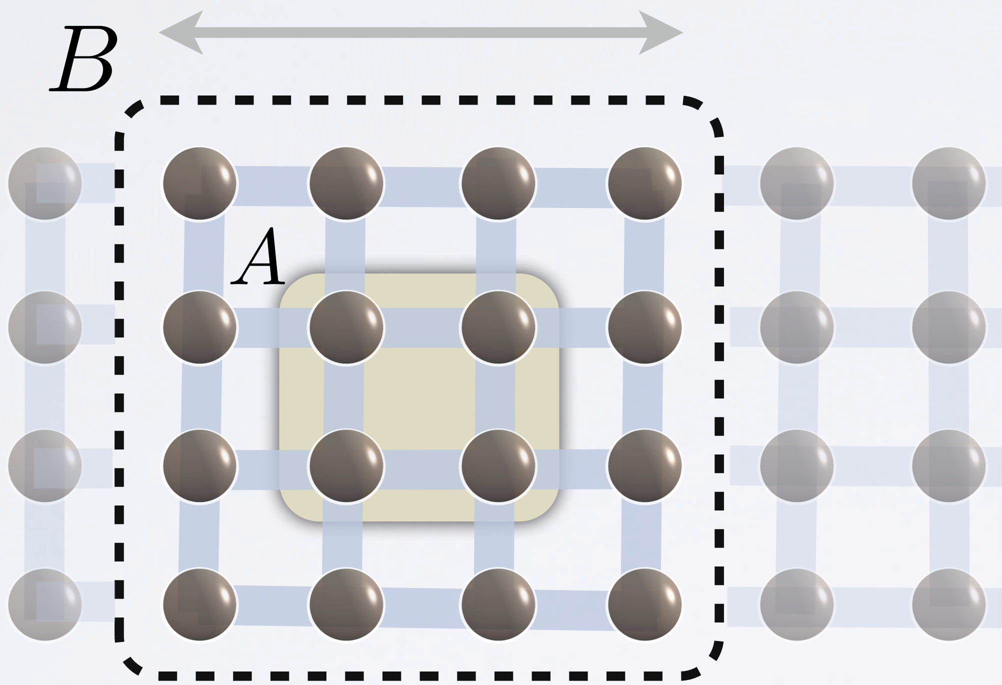
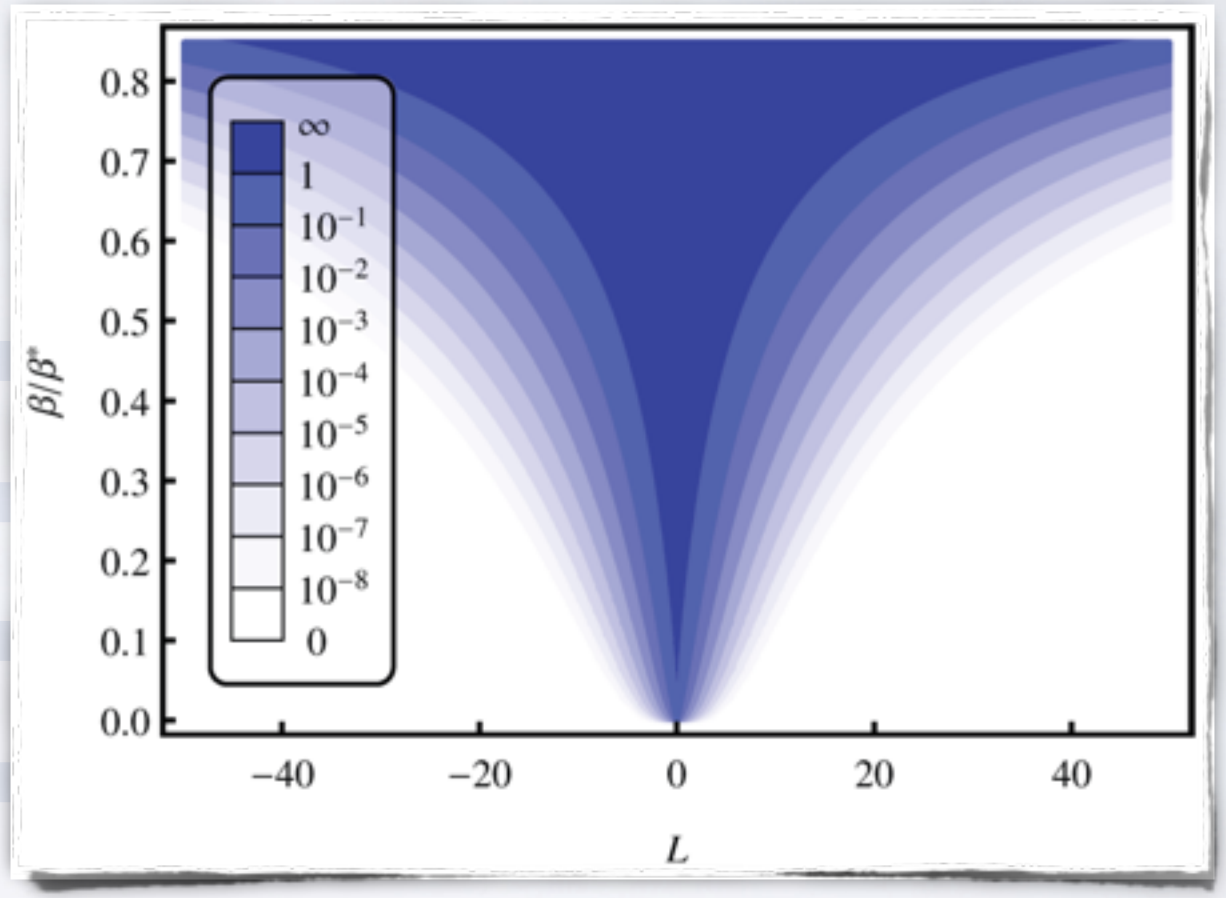


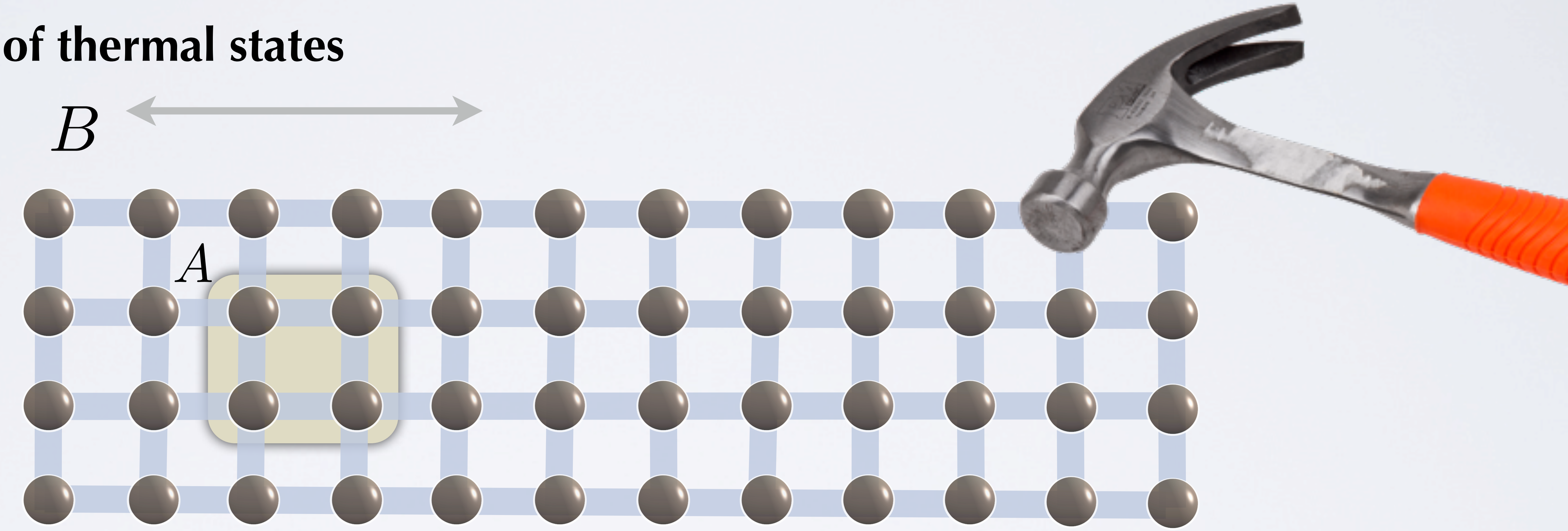


$$\|g_A[H] - g_A[H(0)]\|_1 \leq \frac{v|\beta|J}{1 - e^{-1/\xi(\beta)}} e^{-d(A,\partial A)/\xi(\beta)}$$

Kliesch, Gogolin, Kastoryano, Riera, Eisert, Phys Rev X 4, 031019 (2014)

Stability of high temperature thermal states

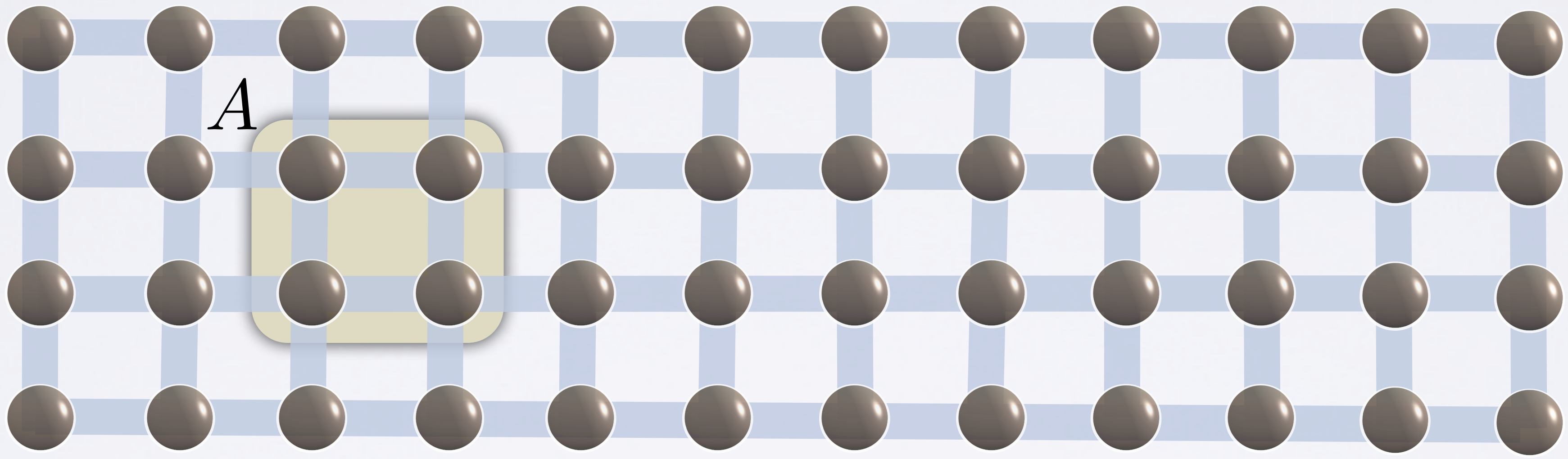
3. Stability of thermal states



Kliesch, Gogolin, Kastoryano, Riera, Eisert, Phys Rev X 4, 031019 (2014)

Efficient computation of expectation values

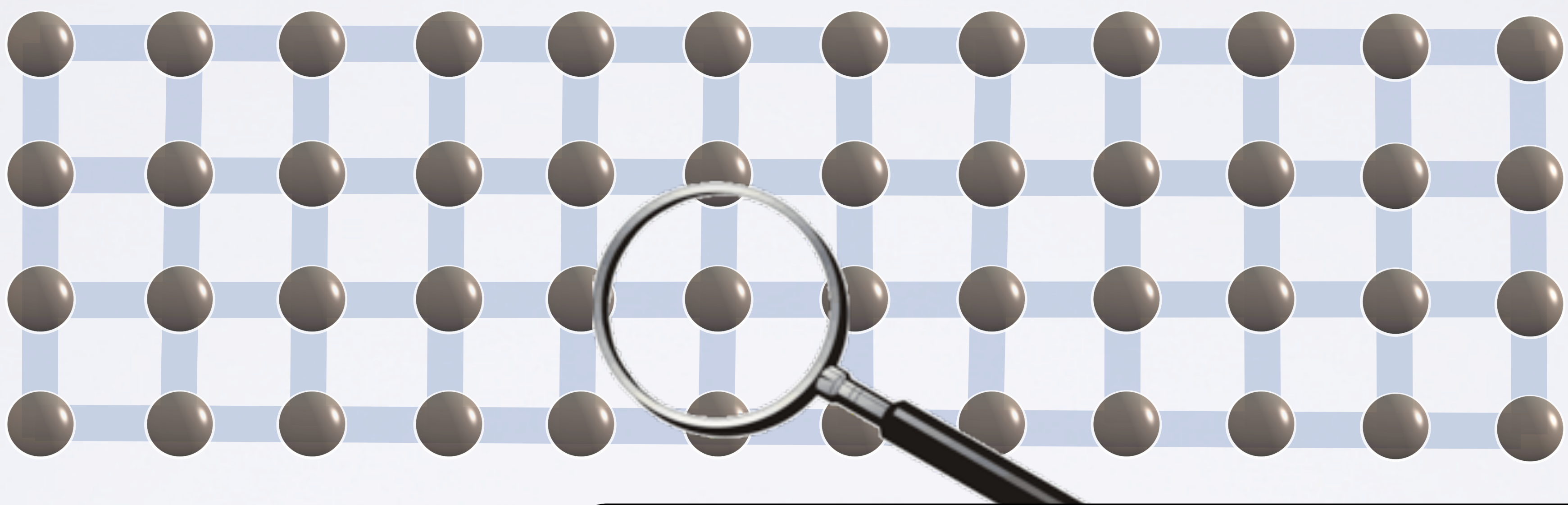
4. Local expectation can be **efficiently computed**



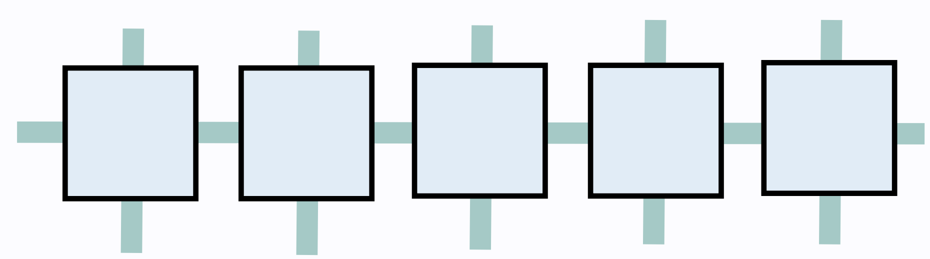
Kliesch, Gogolin, Kastoryano, Riera, Eisert, Phys Rev X 4, 031019 (2014)

Tensor network state approximations

5. Matrix-product operator approximation



PEPO approximation of sub-exponential dimension, efficient **MPO** in 1D



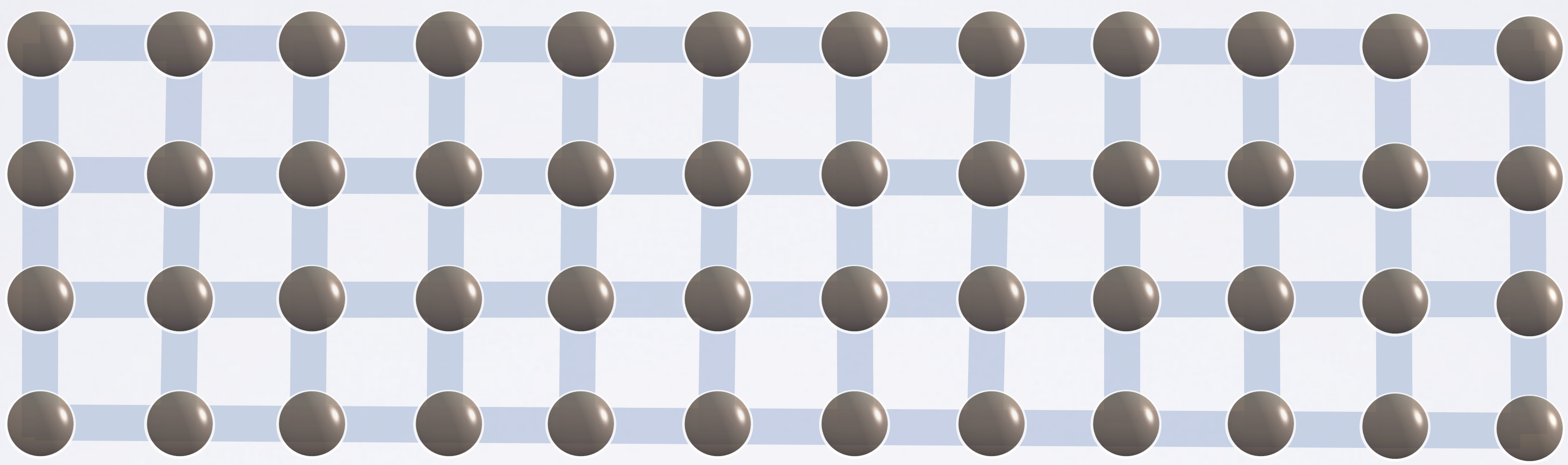
Hastings, Phys Rev B 73, 085115 (2006)
Kliesch, Gogolin, Kastoryano, Riera, Eisert, Phys Rev X 4, 031019 (2014)

- Exciting follow-up: PEPO approx for Gibbs states with bond dim $D = (N/\varepsilon)^{O(\beta)}$

Molnar, Schuch, Verstraete, Cirac, arXiv:1406.2973

Interacting fermions

6. All also true **for interacting fermions**



$$\{f_j, f_k^\dagger\} = \delta_{j,k}$$

- Generalizing earlier results on fermionic covariance matrices (second moments)

Hastings, Phys Rev Lett 93, 126402 (2004)

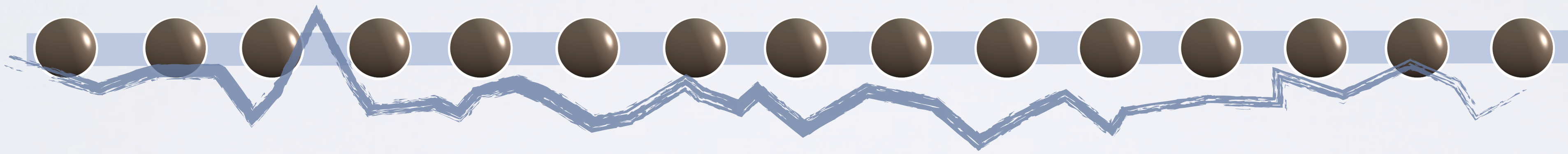
Thermal many-body systems

- **Lessons**:

- **Length scale** at which one can speak of temperature
- High temperature thermal states have **clustering correlations**
- **Tensor network** approximations

Many-body localisation and matrix-product states

Anderson localisation



- **One particle** hopping on a line for an i.i.d. disordered Hamiltonian

$$H = \sum_j (|j\rangle\langle j+1| + |j+1\rangle\langle j|) + \sum_j f_j |j\rangle\langle j|$$

(or non-interacting particles)

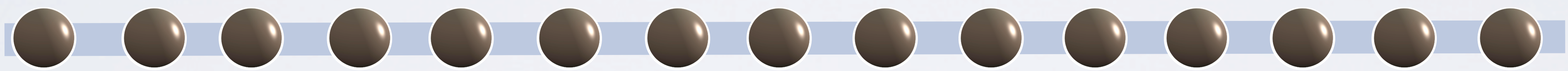
- **Static reading:** ⟷ • **Dynamical reading:**

- All eigenfunctions exponentially decaying correlations

$$\mathbb{E}(\sup_t |\langle n|e^{-itH}|m\rangle|) \leq c_1 e^{-c_2 \mathrm{dist}(n,m)}$$

Anderson, Phys Rev 109, 1492 (1958)

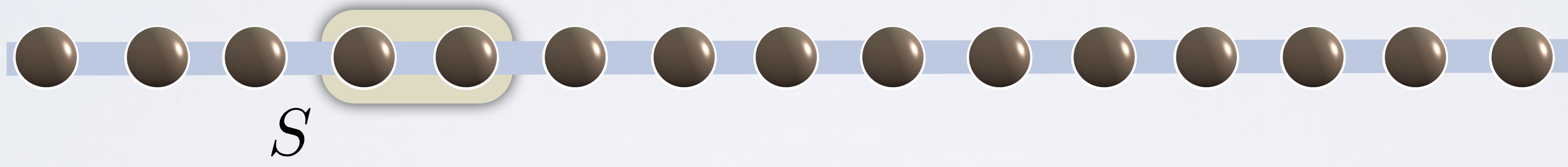
Many-body localisation



- Does Anderson localisation survive finite **interactions**?
- Yes: **Many-body localisation (MBL)**
- Far from well-understood

Anderson, Phys Rev 109, 1492 (1958)
Nandkishore, Huse, arXiv:1404.0686

Breakdown of eigenstate thermalisation



- **Eigenstate thermalisation hypothesis (ETH)**:

Srednicki, Phys Rev E 50, 888 (1994)

$$\rho = |k\rangle\langle k|$$

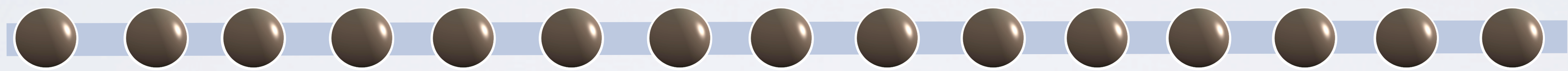
$$\rho_S = \mathrm{tr}_B|k\rangle\langle k| \sim \mathrm{tr}_B(e^{-\beta H})$$

- System exhibits MBL if ETH breaks down

Pal, Huse, Phys Rev B 82, 174411 (2010)
Ogenesyan, Huse, Phys Rev B 75, 155111 (2007)
Gogolin, Mueller, Eisert, Phys Rev Lett 106, 040401 (2011)

Anderson, Phys Rev 109, 1492 (1958)
Nandkishore, Huse, arXiv:1404.0686

Localisation in Fock space



- Anderson insulators with **perturbative interactions**

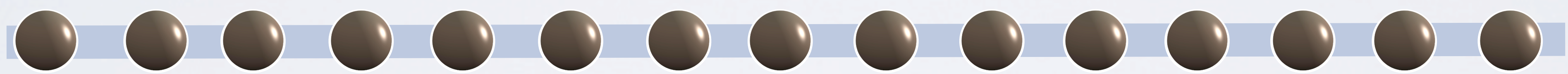
$$H = H_0 + \lambda H_{\text{int}}$$

- Solve single-particle problem, build Fock space of Slater dets
- Consider "localisation in Fock space"

Basko, Aleiner, Altshuler, Ann Phys 321, 1126 (2006)

Anderson, Phys Rev 109, 1492 (1958)
Nandkishore, Huse, arXiv:1404.0686

Static definition as MBL having MPS eigenstates



- More quantum information inspired
- MBL eigenstate ⟷ • Slater determinants

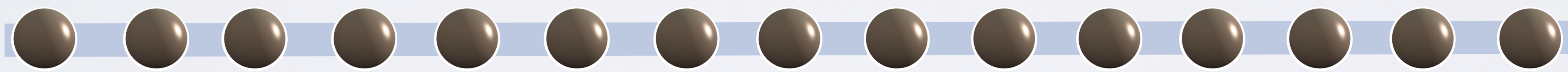
  Finite depth circuit

- Most eigenstates are **matrix-product states** of low bond dimension

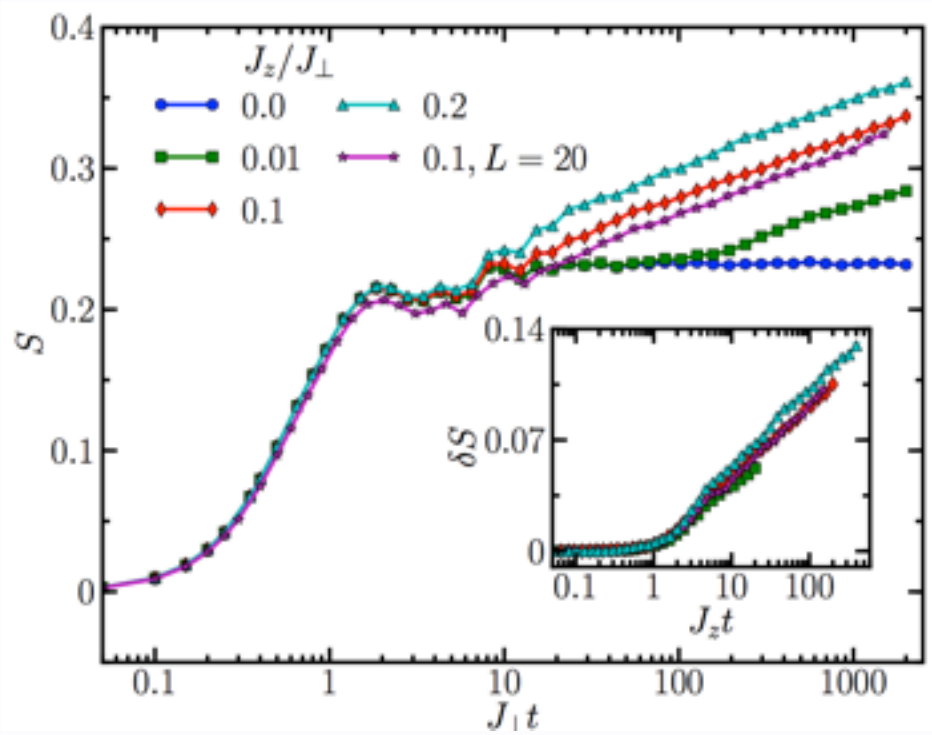
Bauer, Nayak, J Stat Mech P09005 (2013)

Anderson, Phys Rev 109, 1492 (1958)
Nandkishore, Huse, arXiv:1404.0686

Entanglement entropy growth



- Slow entanglement entropy growth following quenches

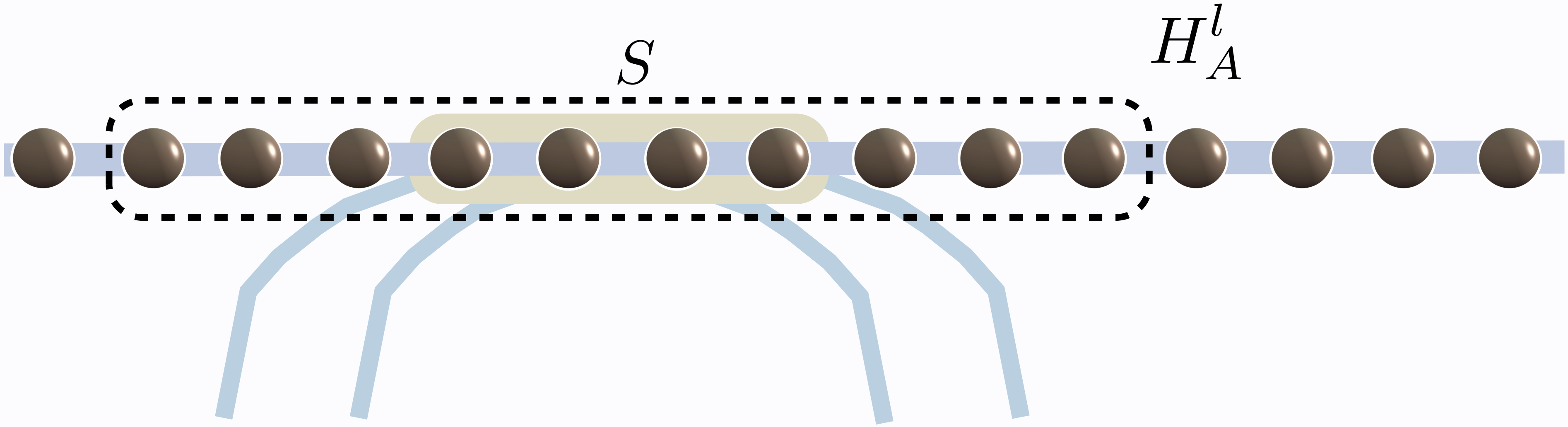


Badarson, Pollmann, Moore, Phys Rev Lett 109, 017202 (2012)

Dynamical localisation: Zero-velocity Lieb-Robinson bounds

- **Strong dynamical localisation:** All transport is blocked for arbitrary states

$$\|A(t) - e^{itH^l_A} A e^{-itH^l_A}\| \leq c_{\mathrm{loc}} e^{-\mu l}$$

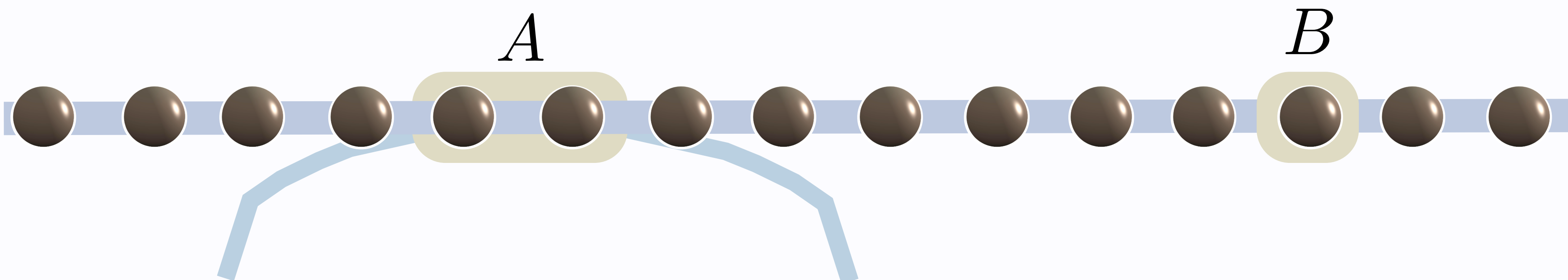


Dynamical localisation: Zero-velocity Lieb-Robinson bounds

- **Mobility edge:** Transport suppressed on the low-energy sector below E_{mob}

$$\forall \rho \in \{|l\rangle\langle k| : E_l, E_k \leq E_{\mathrm{mob}}\} :$$

$$|\mathrm{tr}(\rho[A(t), B])| \leq \min(t, 1) c_{\mathrm{mob}} e^{-\mu d(A,B)}$$



- **Excitations get stuck:** Action of local unitaries not detectable far away

$$|\psi\rangle = U|0\rangle = e^{-iG}|0\rangle$$

$$|\langle 0|A(t)|0\rangle - \langle e|e^{iG} A(t) e^{-iG}|0\rangle| \leq \min(t, 1)\|G\| C e^{-\mu d(A,U)}$$

- **Numerical** evidence, say, for this for the Heisenberg model with disorder with exact diagonalisation, by us and others, see talk by Nicolas)

Hamsa, Sims, Stolz, Commun Math Phys 315, 215 (2012)

Cleaning up?

Can the dynamical picture and the static be related?

Main result: Dynamics $\Longrightarrow$ statics

- **Theorem** (clustering of correlations of eigenvectors)

  a) If the Hamiltonian shows strong dynamical localisation then *all its eigenvectors* have exponentially clustering correlations

$$|\langle k|AB|k\rangle - \langle k|A|k\rangle\langle k|B|k\rangle| \leq 4c_{\mathrm{loc}}e^{-\mu d(A,B)/2}$$

  b) If the Hamiltonian has a mobility edge at energy, eigenstates below mob edge

$$|\langle k|AB|k\rangle - \langle k|A|k\rangle\langle k|B|k\rangle|$$
$$\leq \left(12\pi 2^N \mathcal{N}(E_k+\kappa)c_{\mathrm{mob}} + \ln\frac{\pi\mu d(A,B)e^{4+2\pi}}{\kappa^2}\right)\frac{e^{-\mu d(A,B)/2}}{2\pi}$$

  where $\mathcal{N}(E)$ is normalized integrated density of states at energy E and $\kappa > 0$

Friesdorf, Werner, Scholz, Brown, Eisert, soon (2014)

Glimpse at proof

Use of filter functions $I_f^H(A) = \int_{-\infty}^{\infty} dt\, f(t) A(t)$

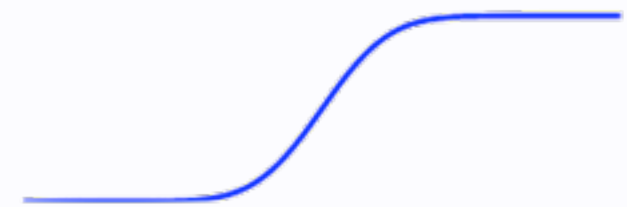
Partly diagonalizes observable in Hamiltonian basis

$$\langle k | I_f^H(A) | l \rangle = \hat{f}(E_k - E_l) \langle k | A | l \rangle$$

while still keeping some locality $\| I_f^H(A) - A_l \| \approx \int_{l/(2v)}^{\infty} dt |f(t)|$

Gaussian filter

High-pass filter



Dynamical localisation with mobility edge

Cast correlation functions into forms dependent on commutator:

Use of Gaussian filters

Decompose spectrum according to energies

$$\mathbb{I} = P + P^{\perp}$$

then use high-pass filter

Clustering of correlations

Builds upon and generalised both
Hastings, Koma, Commun Math Phys 265, 119 (2006)
Hamsa, Sims, Stolz, Commun Math Phys 315, 215 (2012)

Glimpse at proof

Use of filter functions $I_f^H(A) = \int_{-\infty}^{\infty} dt\, f(t) A(t)$

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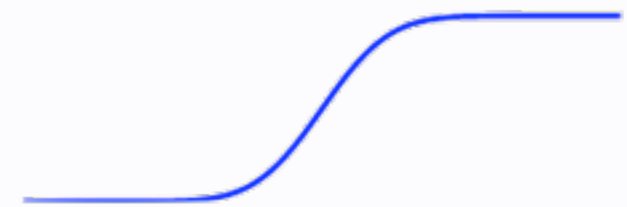

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Clustering of correlations

- All **eigenstates** below mobility edge well approximated by **MPS**

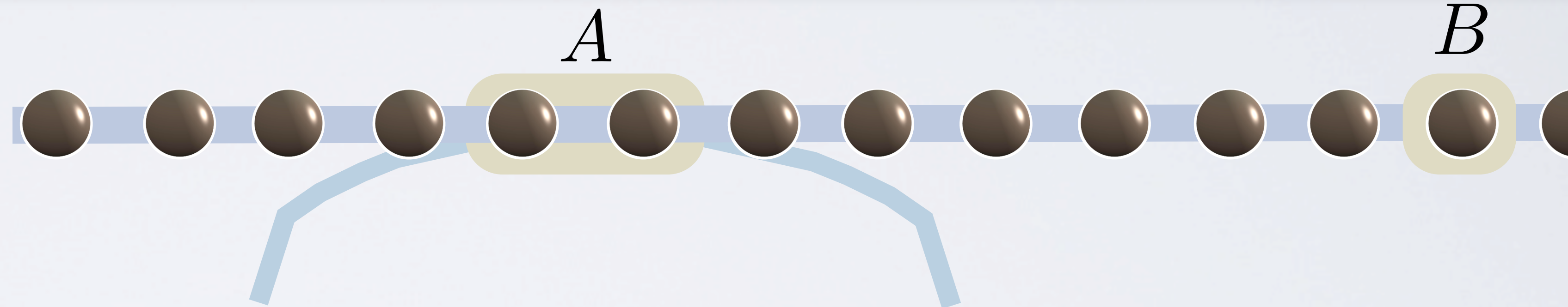
$$|\psi\rangle = \sum_{s_1,\dots,s_n} \mathrm{tr}(A_{s_1}\dots A_{s_n})|s_1,\dots,s_n\rangle\,,\ A \in \mathbb{C}^{D\times D}$$

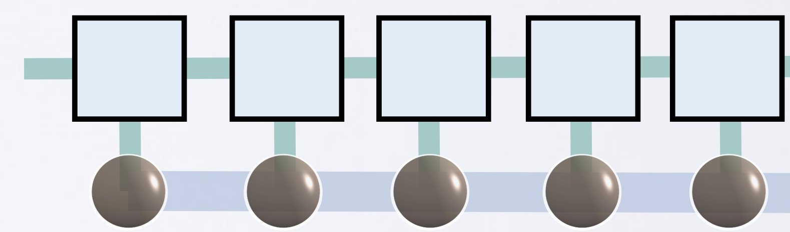
with small bond dimension D , polynomial in system size

Brandao, Horodecki, Nat Phys 9, 721 (2013)
Friesdorf, Werner, Scholz, Brown, Eisert, soon (2014)

Matrix-product states from dynamical localisation

Dynamical localisation with mobility edge





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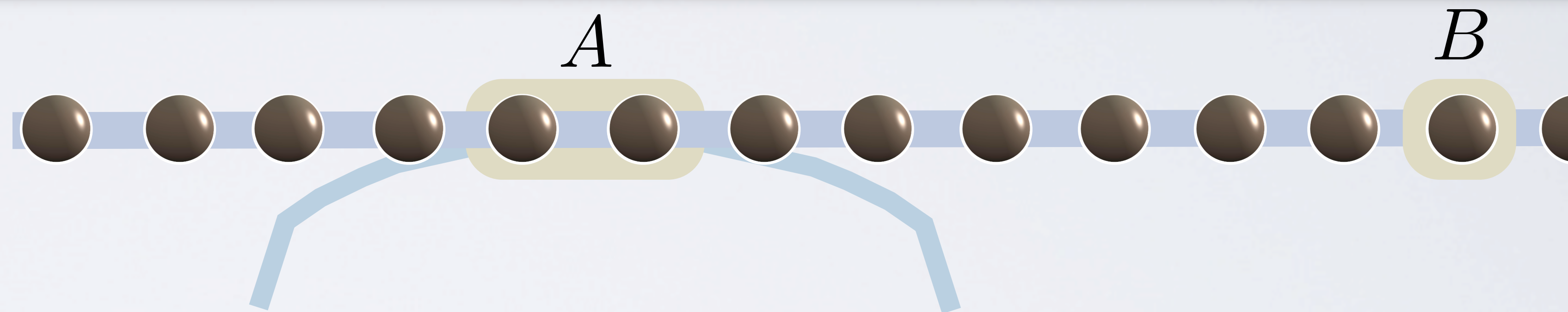
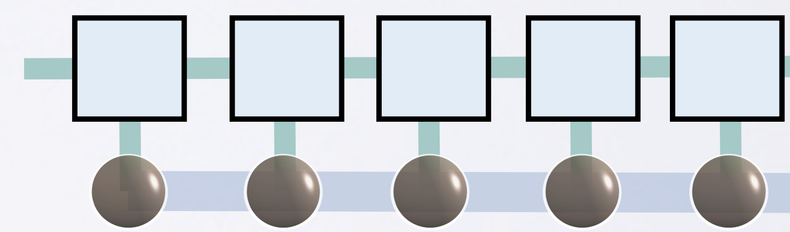
with small bond dimension D , polynomial in system size

Brandao, Horodecki, Nat Phys 9, 721 (2013)
Friesdorf, Werner, Scholz, Brown, Eisert, soon (2014)

Dynamical and static pictures



Dynamical



- **Lesson**:
- **Low energy eigenstates** (not only ground states) are **matrix-product states** of low bond dimension
- Bringing together definitions of **(many-body) localisation**

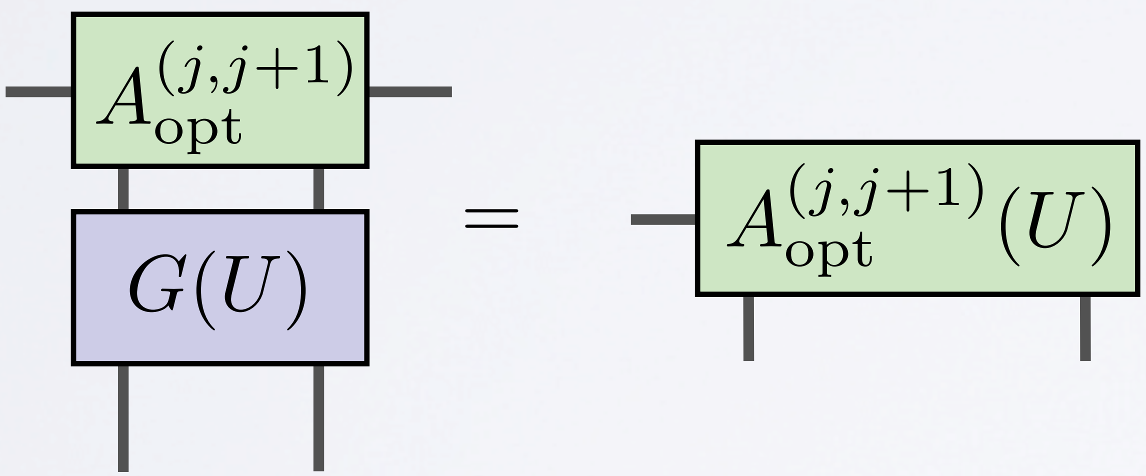
A teaser on posters

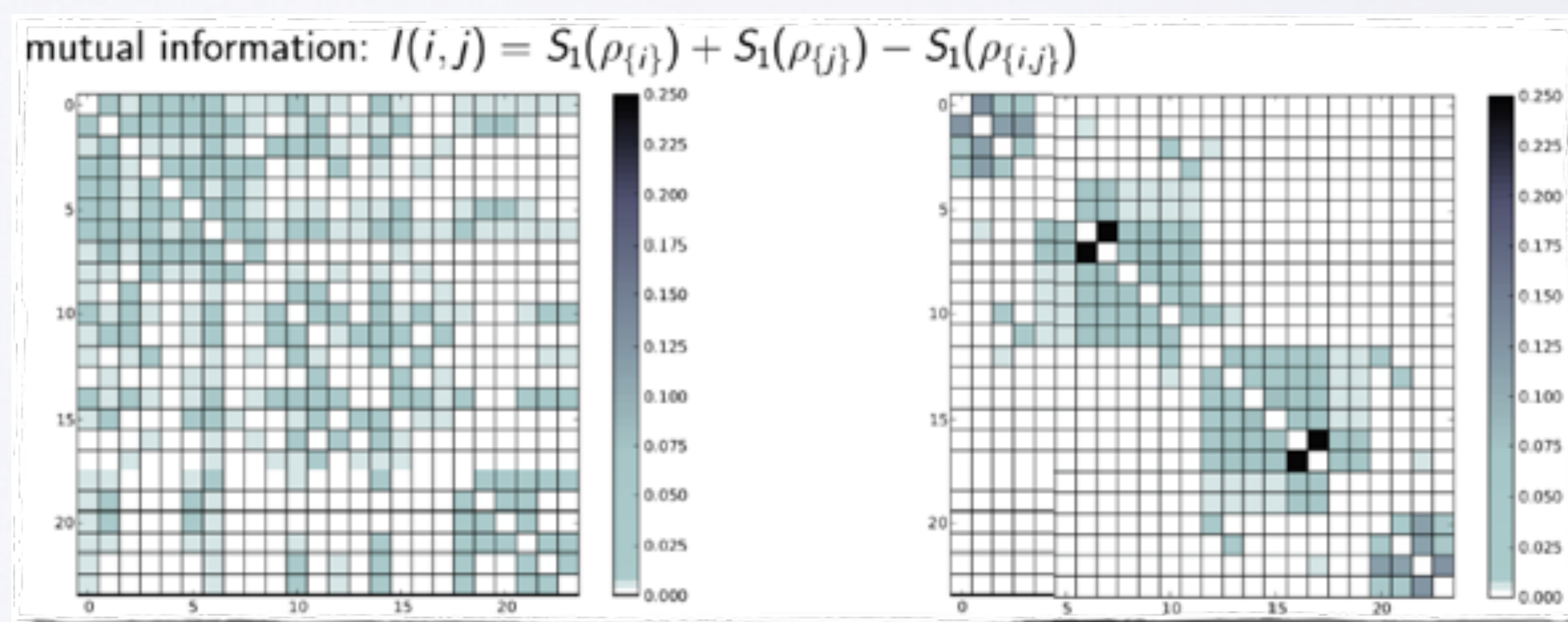
Tensor networks in quantum chemistry

- Interacting fermionic **problems in quantum chemistry**

$$H = \sum_{i,j} T_{i,j} c_i^\dagger c_j + \sum_{i,j,k,l} c_i^\dagger c_j^\dagger c_k c_l \qquad (c_1, \dots, c_n)$$

- Adaptive mode transformations: Combine MPS with local fermionic mode updates $(c_1, \dots, c_n) \mapsto (c'_1, \dots, c'_n)$



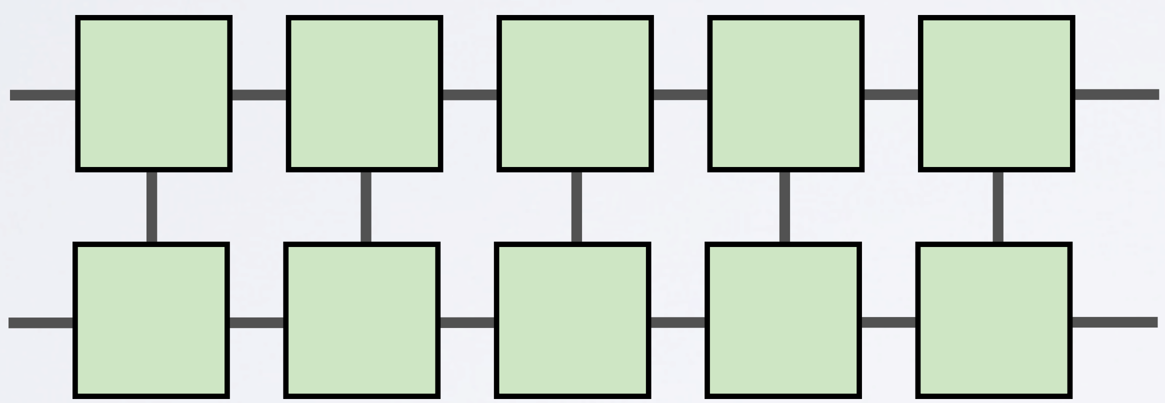


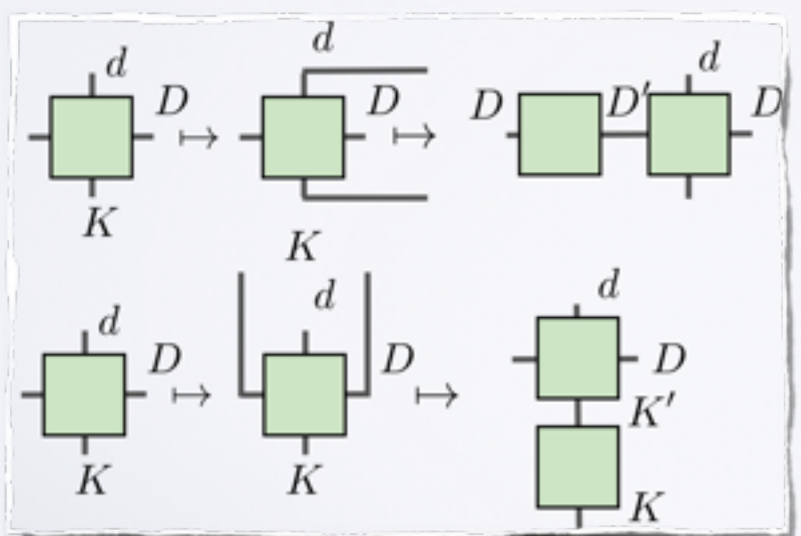
Krumnow, Legeza, Schneider, Eisert, soon (2014)

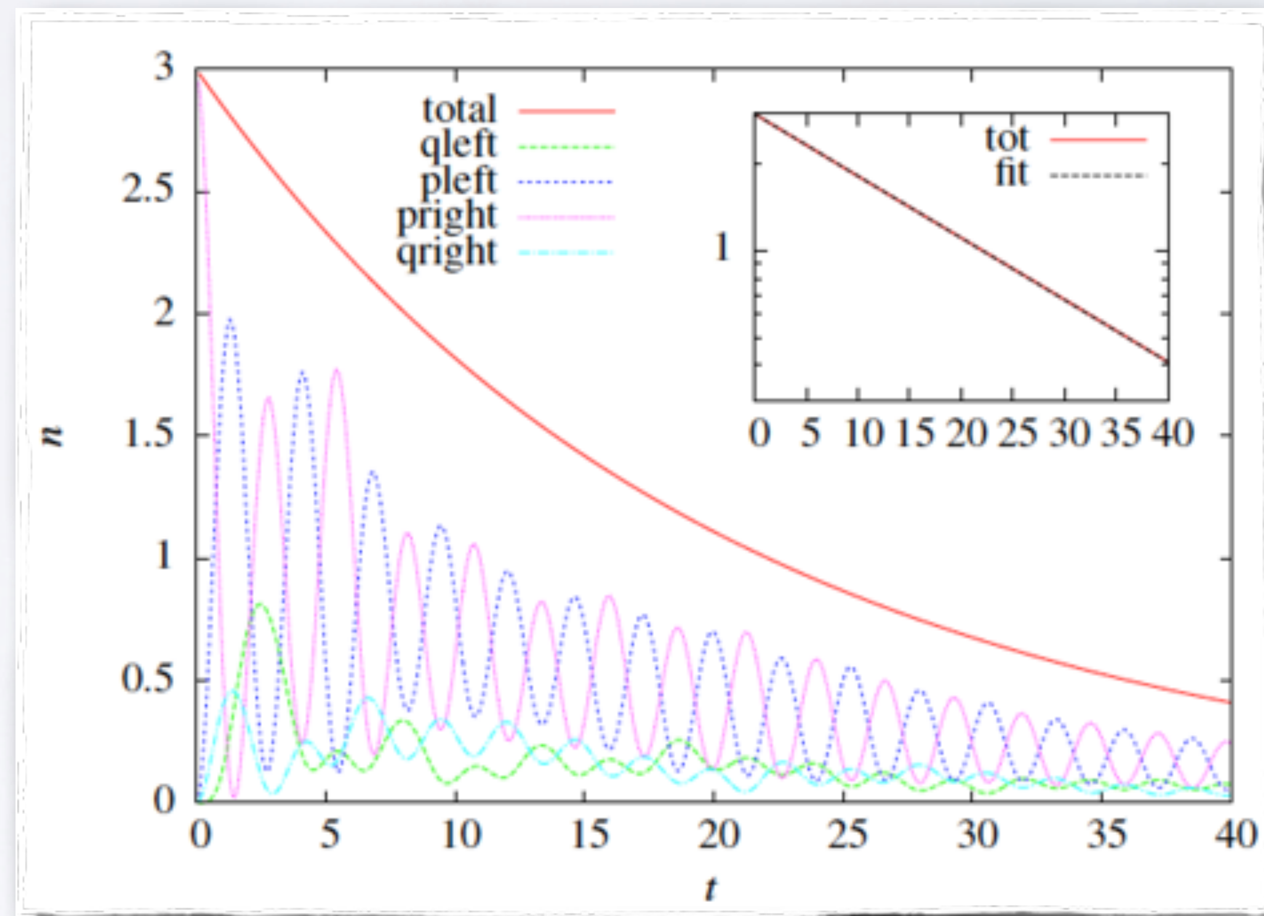
Positive tensor network approach for open quantum systems

- **Open systems simulation** with locally purified MPOs

$$\mathcal{L}(\rho) = -i\sum_j [h_j, \rho] + \sum_j \left(L_j \rho L_j^\dagger - \frac{1}{2}\{L_j^\dagger L_j, \rho\} \right)$$







Kliesch, Gross, Eisert, Phys Rev Lett 113 (2014)
Jaschke, Silvi, Calarco, Werner, Eisert, Montangero, soon (2014)

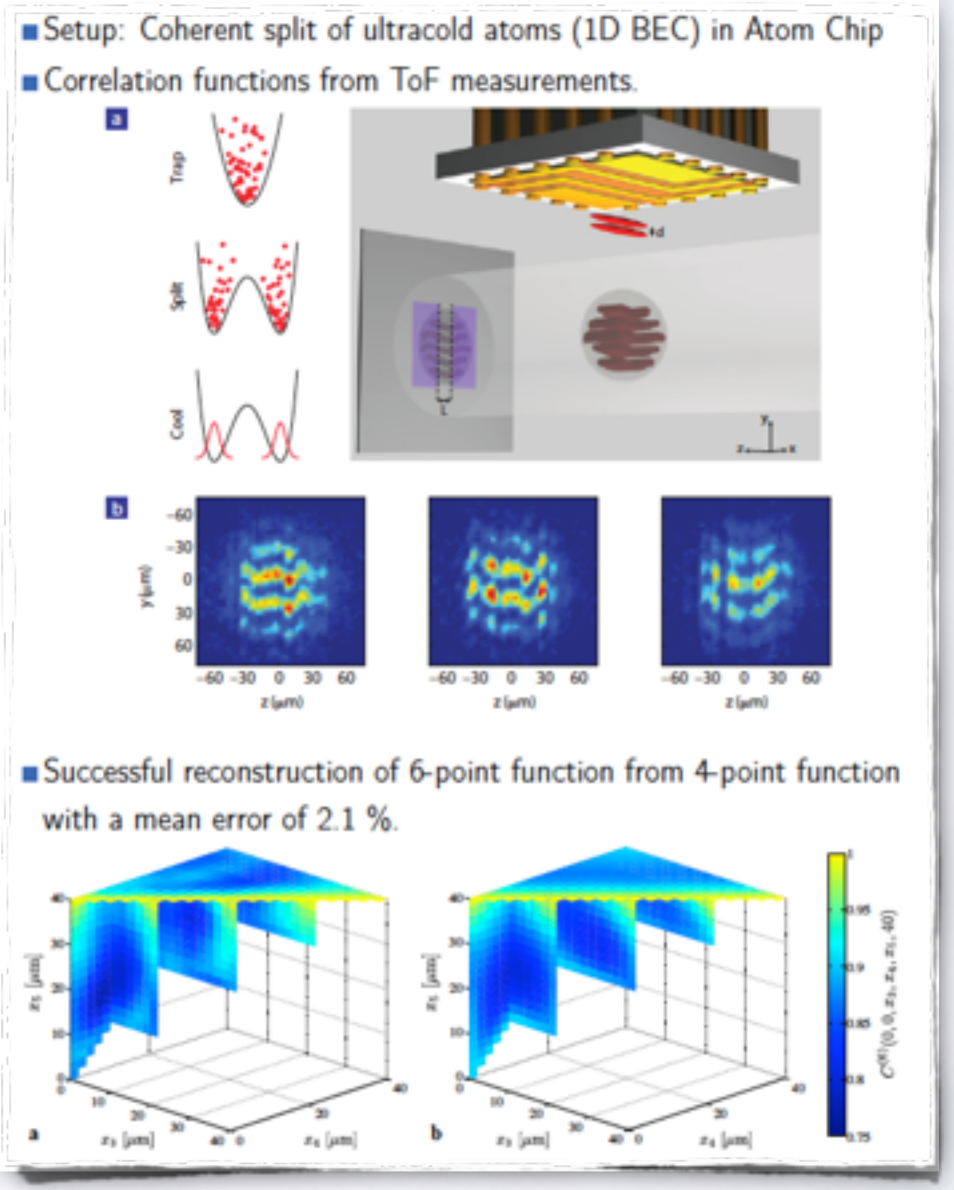
Quantum field tomography and continuous MPS

- Simulations with **continuous matrix product states**

$$|\psi\rangle = \mathrm{tr}(\mathcal{P}e^{\int_0^L dx(Q\otimes 1)+R\otimes\Psi^\dagger(x)})|\Omega\rangle \ , \quad [\Psi(y),\Psi^\dagger(x)] = \delta(x-y)$$

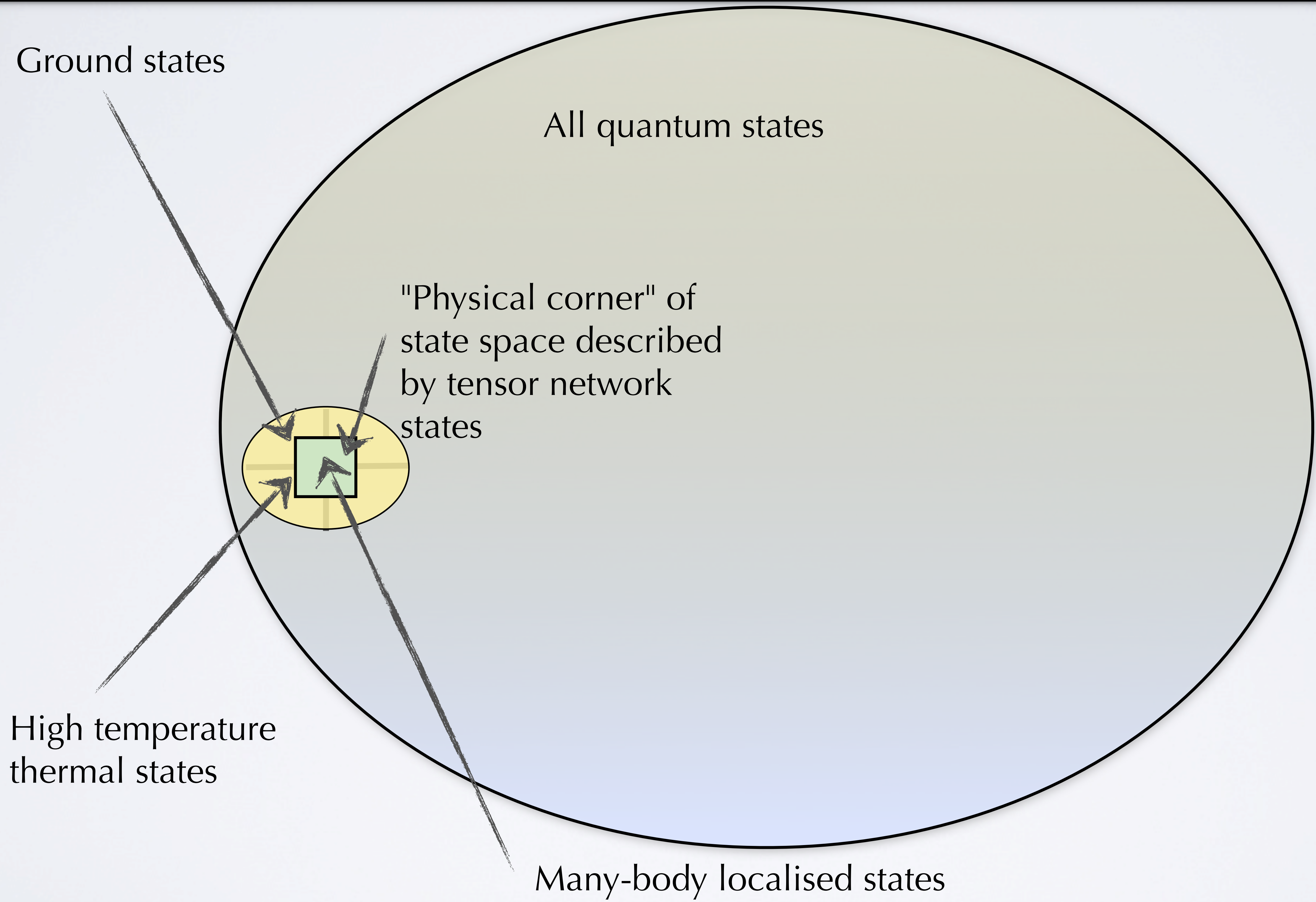
- **Quantum field tomography:** Reconstruct cMPS based on correlation functions

- Apply to **experiments** with cold atoms



Steffens, Friesdorf, Langen, Rauer, Schweigler, Huebener, Schmiedmayer, Riofrio, Eisert, arXiv:1406.3632
Steffens, Riofrio, Huebener, Eisert, arXiv:1406.3631

Summary



Thanks for your attention!