A Hierarchy of Spectral Gap Certificates based on Semidefinite Programs

K. Sneh rai, I. Kull, P. Emonts, J. Tura, N. Schuch, F. Baccari

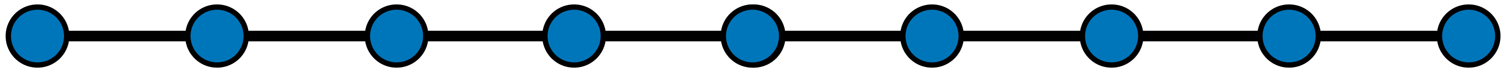
arXiv:2411.?????

What is the problem?

THE 1D SPECTRAL GAP PROBLEM

$$H = \sum_{i=1}^{N} h_{i,i+1}$$

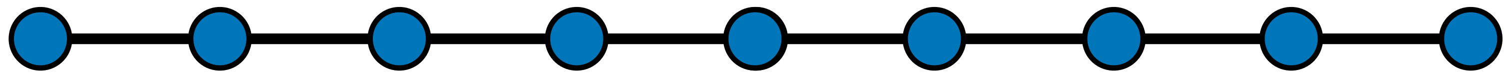
Translationally-invariant



THE 1D SPECTRAL GAP PROBLEM

$$H = \sum_{i=1}^{N} h_{i,i+1}$$

Translationally-invariant

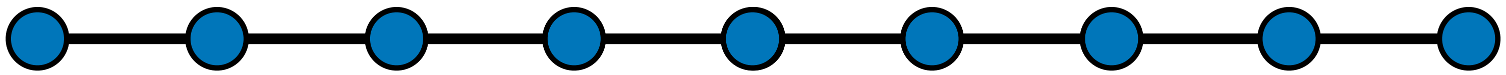


$$H = \sum_{k} E_k \left|\psi_k\right\rangle\left\langle\psi_k\right|$$

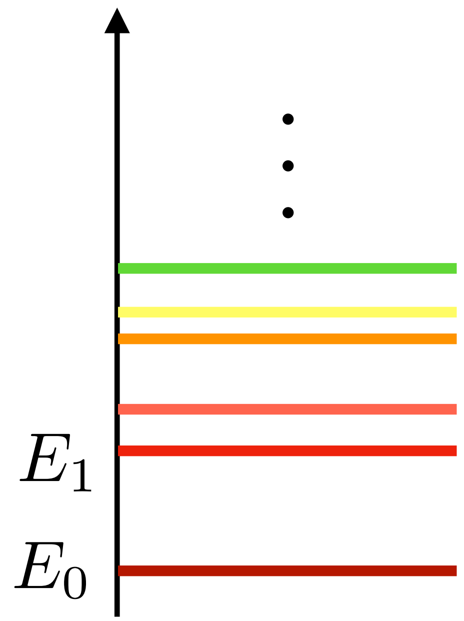
THE 1D SPECTRAL GAP PROBLEM

$$H = \sum_{i=1}^{N} h_{i,i+1}$$

Translationally-invariant



$$H = \sum_k E_k \, |\psi_k\rangle\langle\psi_k|$$

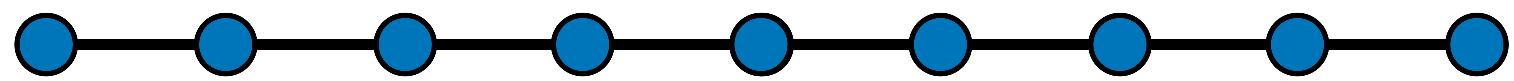


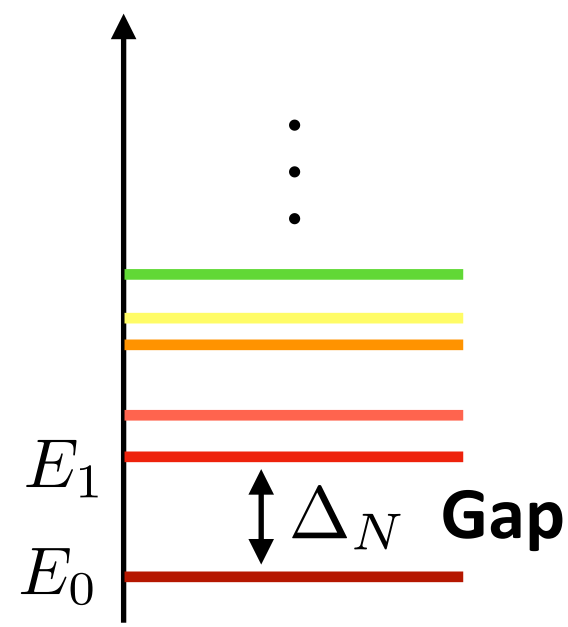
THE 1D SPECTRAL GAP PROBLEM

$$H = \sum_{i=1}^{N} h_{i,i+1}$$

$$H = \sum_{k} E_k \, |\psi_k\rangle\langle\psi_k|$$

Translationally-invariant

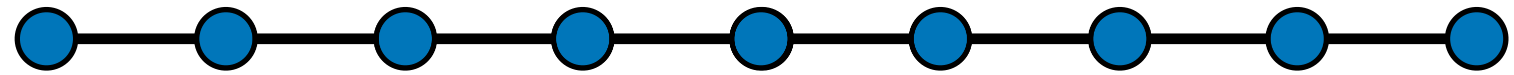




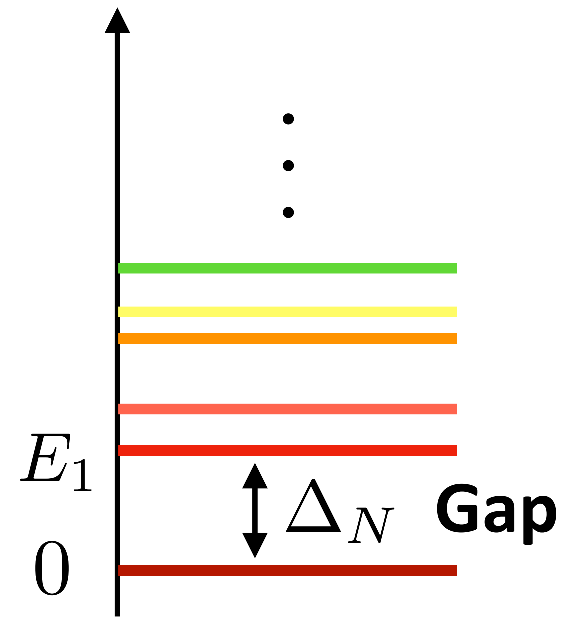
THE 1D SPECTRAL GAP PROBLEM

$$H = \sum_{i=1}^{N} h_{i,i+1}$$

Translationally-invariant



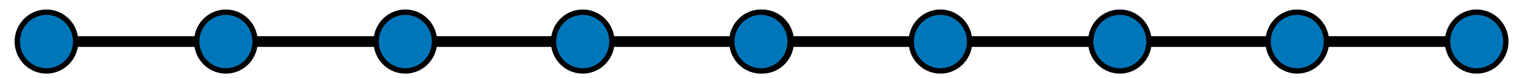
$$H = \sum_k E_k \, |\psi_k\rangle\langle\psi_k|$$



Frustration-Free $\quad E_0 = 0 \quad h_{i,i+1}\,|\psi_0\rangle = 0$

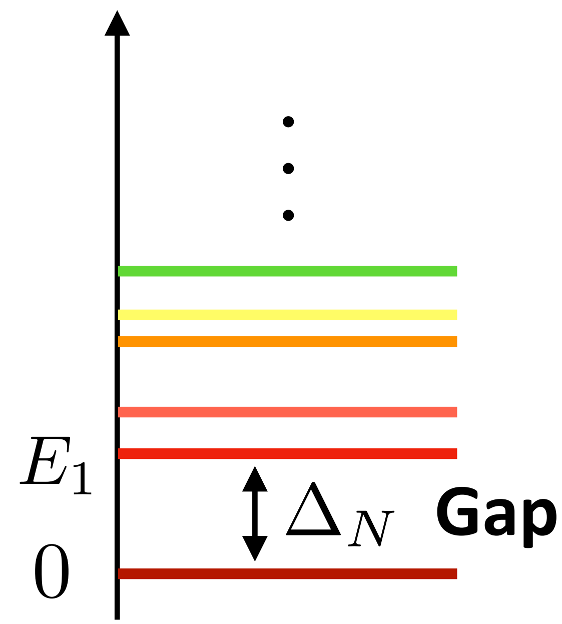
THE 1D SPECTRAL GAP PROBLEM

Translationally-invariant



$$H = \sum_{i=1}^{N} h_{i,i+1}$$

$$H = \sum_{k} E_k \, |\psi_k\rangle\langle\psi_k|$$

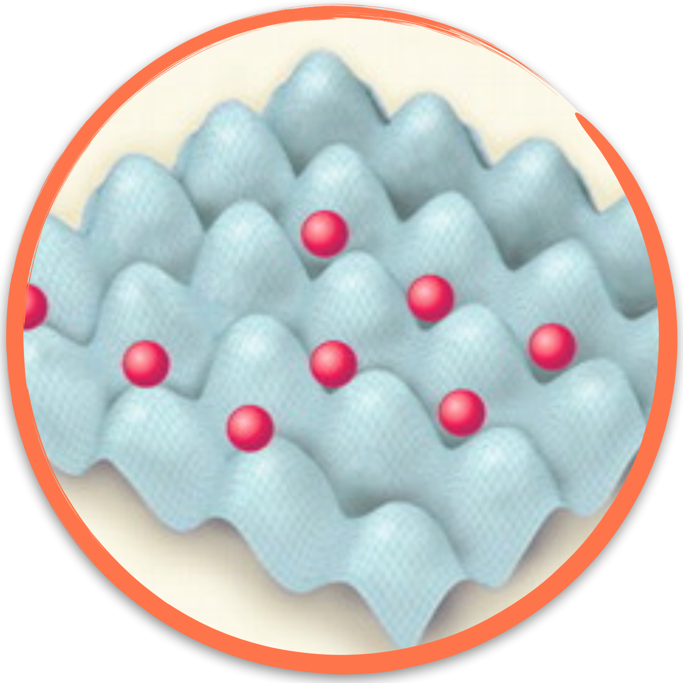


Frustration-Free $\quad E_0 = 0 \quad h_{i,i+1}\,|\psi_0\rangle = 0$

Thermodynamic limit $\quad \lim_{N\to\infty} \Delta_N = \Delta > 0$

Motivation

A BROAD RANGE OF APPLICATIONS



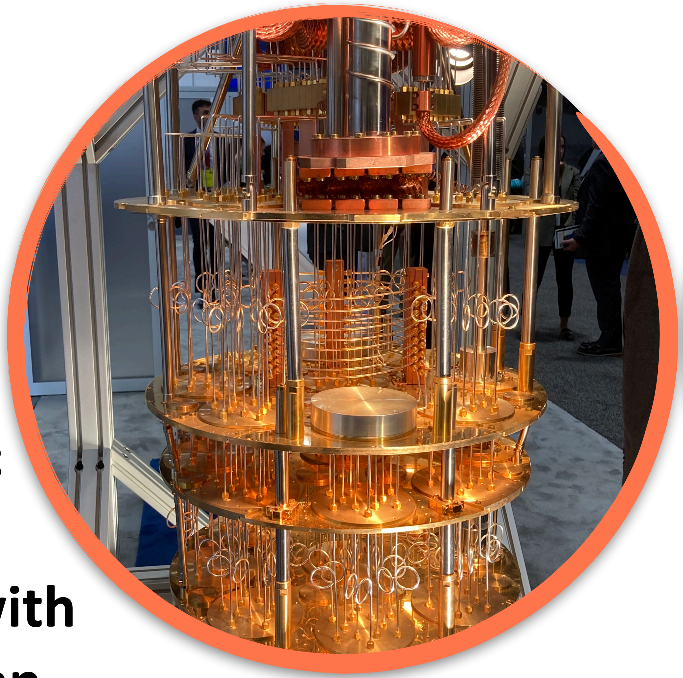
Many-body physics

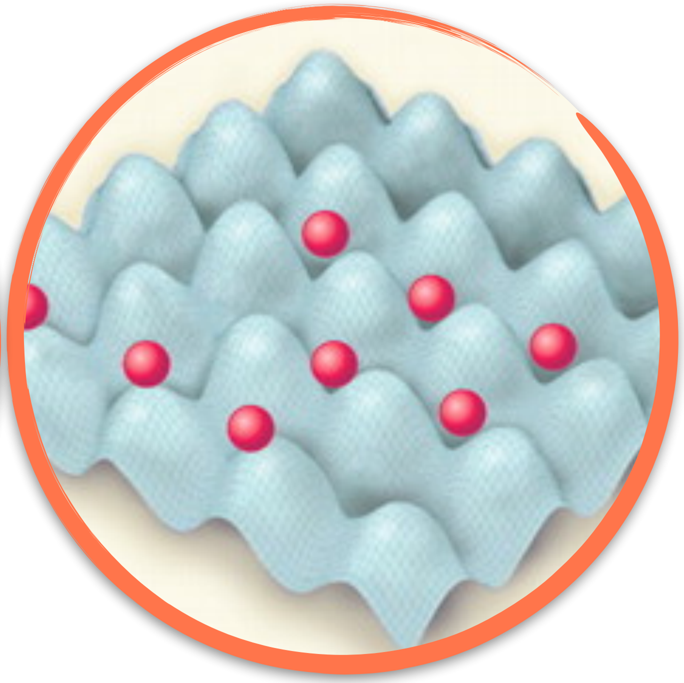
Physical consequences on the ground state:
- **decay of correlations,**
- **representability with tensor networks**

A BROAD RANGE OF APPLICATIONS

Quantum Information

Efficient adiabatic preparation of quantum states with parent hamiltonian (MPS, PEPS,…)





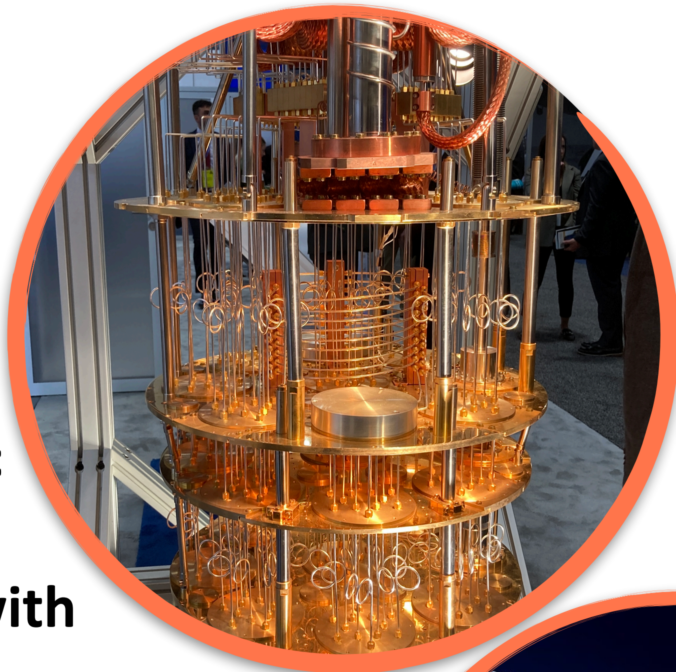
Many-body physics

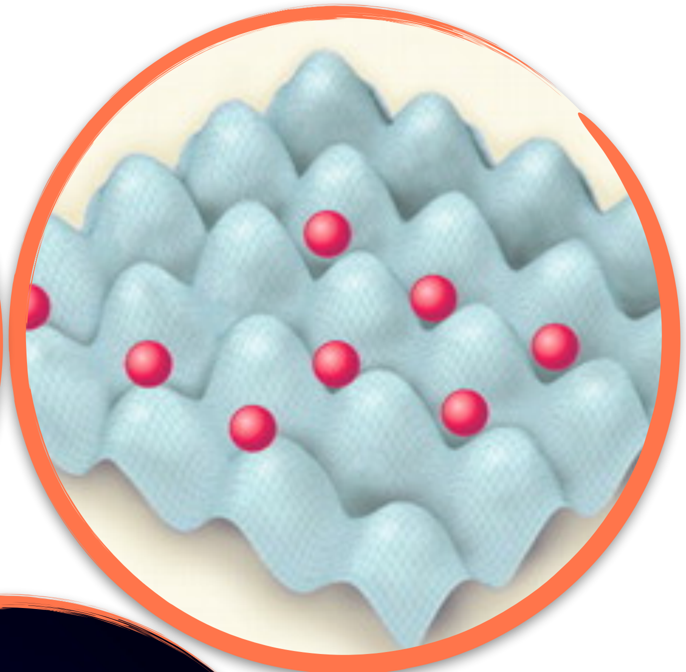
Physical consequences on the ground state:
- **decay of correlations,**
- **representability with tensor networks**

A BROAD RANGE OF APPLICATIONS

Quantum Information

Efficient adiabatic preparation of quantum states with parent hamiltonian (MPS, PEPS,…)





Many-body physics

Physical consequences on the ground state:
- **decay of correlations,**
- **representability with tensor networks**

Statistical physycs, Particle physics, Machine learning,…

Efficient Monte-Carlo sampling of classical distributions (rapid mixing)

A BROAD RANGE OF APPLICATIONS

Many-body physics

Physical consequences
on the ground state:
ay of correlations,
presentability with
nsor networks

C
In

Effic
prep
quar
pare
(MP

sycs,
ics,
ing,...

Carlo
sampling of classical
distributions (rapid mixing)

General setting

CONDITIONS FOR THE EXISTENCE OF THE GAP

H **has a spectral gap** Δ
If and only if

$$H^2 - \Delta H \succeq 0$$

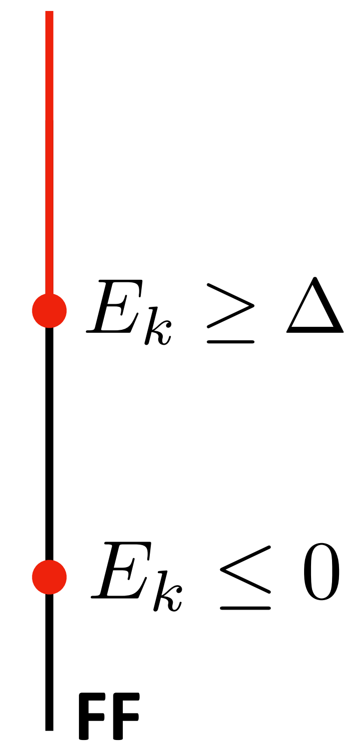
CONDITIONS FOR THE EXISTENCE OF THE GAP

H **has a spectral gap** Δ
If and only if

$$H^2 - \Delta H \succeq 0$$

intuition

$$E_k^2 - \Delta E_k = E_k(E_k - \Delta E_k) \geq 0$$



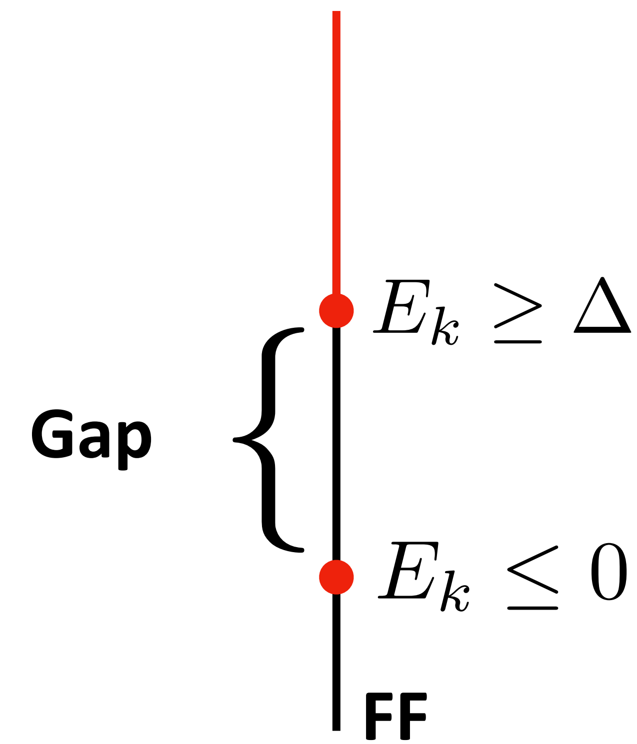
CONDITIONS FOR THE EXISTENCE OF THE GAP

H **has a spectral gap** Δ
If and only if

$$H^2 - \Delta H \succeq 0$$

intuition

$$E_k^2 - \Delta E_k = E_k(E_k - \Delta E_k) \geq 0$$



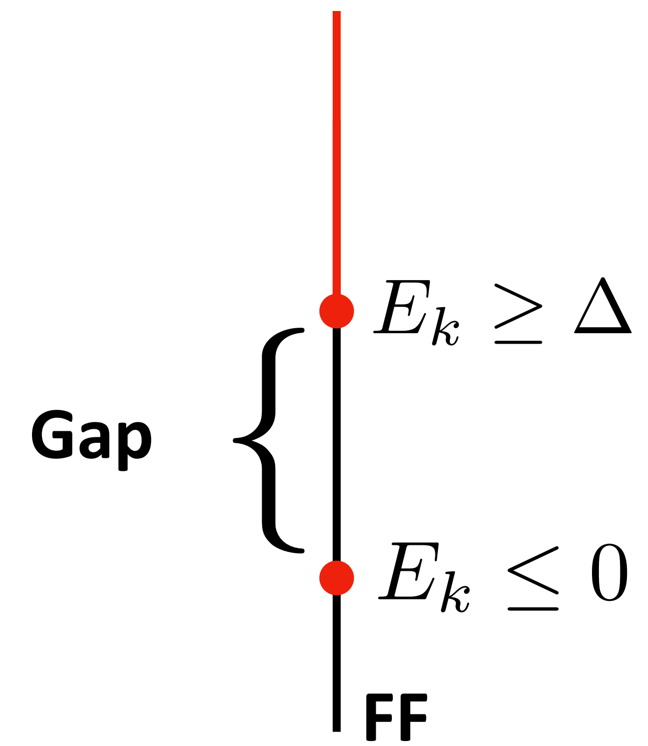
CONDITIONS FOR THE EXISTENCE OF THE GAP

H **has a spectral gap** Δ
If and only if

$$H^2 - \Delta H \succeq 0$$

intuition

$$E_k^2 - \Delta E_k = E_k(E_k - \Delta E_k) \geq 0$$



Widely used condition in previous methods

- **Finite-size criteria** (Knabe 1988, M. Lemm and D. Xiang 2022, …)
- **Eigenvalue problems** (Nachtergaele 1996, M. J. Kastoryano and A. Lucia 2018, …)

…

CONDITIONS FOR THE EXISTENCE OF THE GAP

H has a spectral gap Δ
If and only if

$$H^2 - \Delta H \succeq 0$$

Computing the eigenvalues
of an exponentially-large matrix

CONDITIONS FOR THE EXISTENCE OF THE GAP

H **has a spectral gap** Δ
If and only if

$$H^2 - \Delta H \succeq 0$$

Computing the eigenvalues of an exponentially-large matrix

The method

SIMPLIFICATIONS

H **has a spectral gap** Δ
If and only if

$$H^2 - \Delta H \succeq 0$$

Compu[illegible] the eigenvalues of an exp[illegible]tially-large matrix

1) Cut to a local operator

$$H^2 - \Delta H = \sum_{i=1}^{N} h_{i,i+1}^2 + \sum_{i \neq j} \{h_{i,i+1}, h_{j,j+1}\} - \Delta \sum_{i=1}^{N} h_{i,i+1}$$

SIMPLIFICATIONS

H **has a spectral gap** Δ
If and only if

$$H^2 - \Delta H \succeq 0$$

Compu… the eigenvalues
of an exp…tially-large matrix

1) Cut to a local operator

$$H^2 - \Delta H = \sum_{i=1}^{N} h_{i,i+1}^2 + \sum_{i \neq j} \{h_{i,i+1}, h_{j,j+1}\} - \Delta \sum_{i=1}^{N} h_{i,i+1}$$

$$= \sum_{i=1}^{N} (h_{i,i+1}^2 - \Delta h_{i,i+1}) + \sum_{i=1}^{N} \sum_{k} \{h_{i,i+1}, h_{i+k,i+k+1}\}$$

SIMPLIFICATIONS

H **has a spectral gap** Δ
If and only if

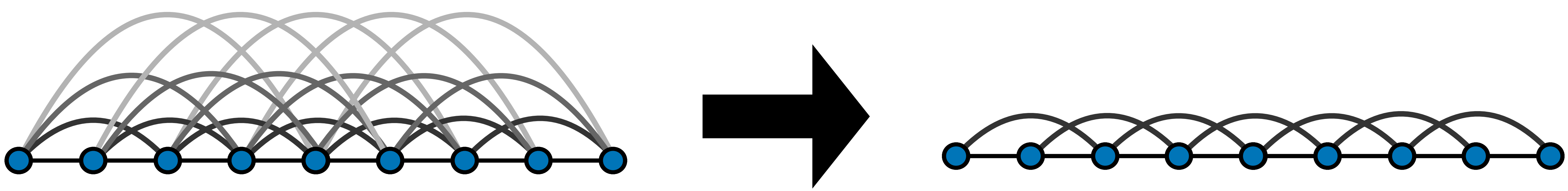
$$H^2 - \Delta H \succeq 0$$

Compu[illegible] the eigenvalues of an exp[illegible]tially-large matrix

1) Cut to a local operator

$$H^2 - \Delta H = \sum_{i=1}^{N} h_{i,i+1}^2 + \sum_{i \neq j} \{h_{i,i+1}, h_{j,j+1}\} - \Delta \sum_{i=1}^{N} h_{i,i+1}$$

$$= \sum_{i=1}^{N} (h_{i,i+1}^2 - \Delta h_{i,i+1}) + \sum_{i=1}^{N} \sum_{k} \{h_{i,i+1}, h_{i+k,i+k+1}\}$$



SIMPLIFICATIONS

H **has a spectral gap** Δ
If and only if

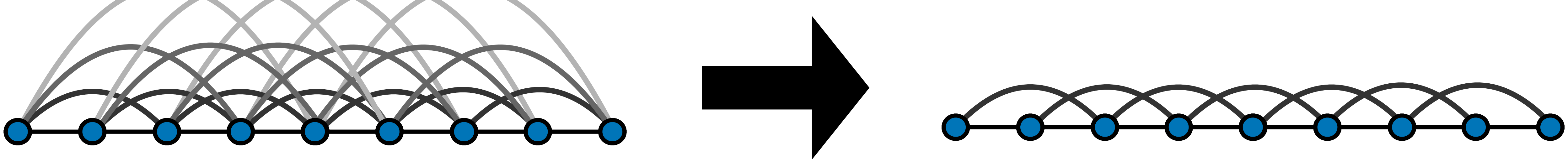
$$H^2 - \Delta H \succeq 0$$

Compu[illegible] the eigenvalues
of an exp[illegible]tially-large matrix

1) Cut to a local operator

$$H^2 - \Delta H = \sum_{i=1}^{N} h_{i,i+1}^2 + \sum_{i \neq j} \{h_{i,i+1}, h_{j,j+1}\} - \Delta \sum_{i=1}^{N} h_{i,i+1}$$

$$= \sum_{i=1}^{N} (h_{i,i+1}^2 - \Delta h_{i,i+1}) + \sum_{i=1}^{N} \sum_{k} \underbrace{\{h_{i,i+1}, h_{i+k,i+k+1}\}}_{\text{Distance k}}$$



SIMPLIFICATIONS

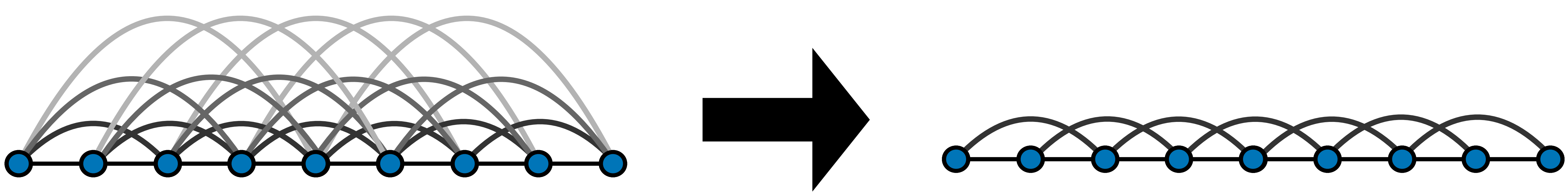
H **has a spectral gap** Δ
If and only if

$$H^2 - \Delta H \succeq 0$$

Computing the eigenvalues of an exponentially-large matrix

1) Cut to a local operator

$$Q_n(\Delta) = \sum_{i=1}^{N} (h_{i,i+1}^2 - \Delta h_{i,i+1}) + \sum_{i=1}^{N} \sum_{k \leq n} \{h_{i,i+1}, h_{i+k,i+k+1}\} \succeq 0$$



SIMPLIFICATIONS

H **has a spectral gap** Δ
If and only if

$$H^2 - \Delta H \succeq 0$$

Computing the eigenvalues of an exponentially-large matrix

1) Cut to a local operator

$$Q_n(\Delta) = \sum_{i=1}^{N} (h_{i,i+1}^2 - \Delta h_{i,i+1}) + \sum_{i=1}^{N} \sum_{k \leq n} \{h_{i,i+1}, h_{i+k,i+k+1}\} \succeq 0$$

$H^2 - \Delta H = Q_n(\Delta) +$ **Something positive semidefinite**

SIMPLIFICATIONS

H **has a spectral gap** Δ
If and only if

$$H^2 - \Delta H \succeq 0$$

~~**Compu[illegible] the eigenvalues of an exp[illegible]tially-large matrix**~~

1) Cut to a local operator

$$Q_n(\Delta) = \sum_{i=1}^{N} (h_{i,i+1}^2 - \Delta h_{i,i+1}) + \sum_{i=1}^{N} \sum_{k \leq n} \{h_{i,i+1}, h_{i+k,i+k+1}\} \succeq 0$$

$$H^2 - \Delta H = Q_n(\Delta) + \text{ Something positive semidefinite}$$

$$\{h_{i,i+1}, h_{i+k,i+k+1}\} \succeq 0$$

Because of frustration-freeness and commutation

SIMPLIFICATIONS

H **has a spectral gap** Δ
If and only if

$$H^2 - \Delta H \succeq 0$$

Computing the eigenvalues of an exponentially-large matrix

1) Cut to a local operator

$$Q_n(\Delta) = \sum_{i=1}^{N} (h_{i,i+1}^2 - \Delta h_{i,i+1}) + \sum_{i=1}^{N} \sum_{k \leq n} \{h_{i,i+1}, h_{i+k,i+k+1}\} \succeq 0$$

$$H^2 - \Delta H \succeq 0$$

SIMPLIFICATIONS

H **has a spectral gap** Δ
If and only if

$$H^2 - \Delta H \succeq 0$$

Compu the eigenvalues
of an exp tially-large matrix

1) Cut to a local operator

$$Q_n(\Delta) = \sum_{i=1}^{N} (h_{i,i+1}^2 - \Delta h_{i,i+1}) + \sum_{i=1}^{N} \sum_{k \leq n} \{h_{i,i+1}, h_{i+k,i+k+1}\} \succeq 0$$

2) Find a postive local generating operator

$$Q_n(\Delta) = \sum_i q_{n,i}$$

$$q_{n,i} \succeq 0$$

SIMPLIFICATIONS

H **has a spectral gap** Δ
If and only if

$$H^2 - \Delta H \succeq 0$$

Computing the eigenvalues of an exponentially-large matrix

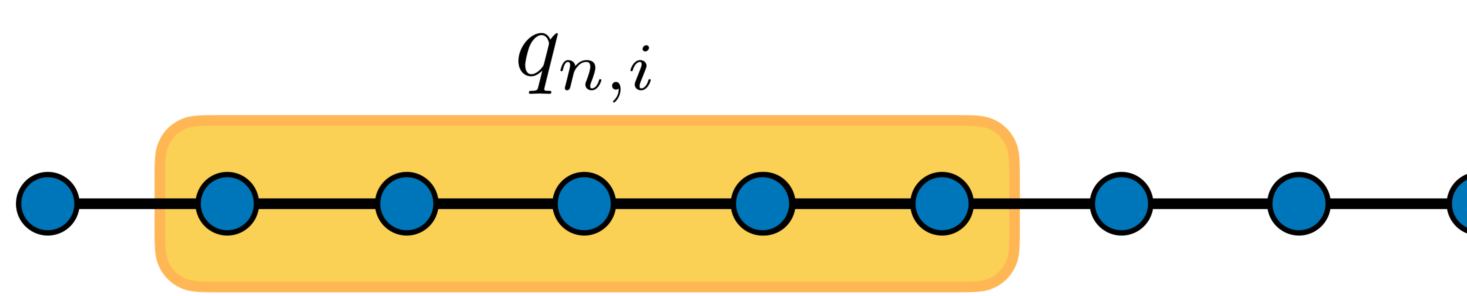
1) Cut to a local operator

$$Q_n(\Delta) = \sum_{i=1}^{N} (h_{i,i+1}^2 - \Delta h_{i,i+1}) + \sum_{i=1}^{N} \sum_{k \leq n} \{h_{i,i+1}, h_{i+k,i+k+1}\} \succeq 0$$

2) Find a postive local generating operator

$$Q_n(\Delta) = \sum_i q_{n,i}$$

$$q_{n,i} \succeq 0$$



SIMPLIFICATIONS

H **has a spectral gap** Δ
If and only if

$$H^2 - \Delta H \succeq 0$$

Compu[illegible] the eigenvalues of an exp[illegible]tially-large matrix

1) Cut to a local operator

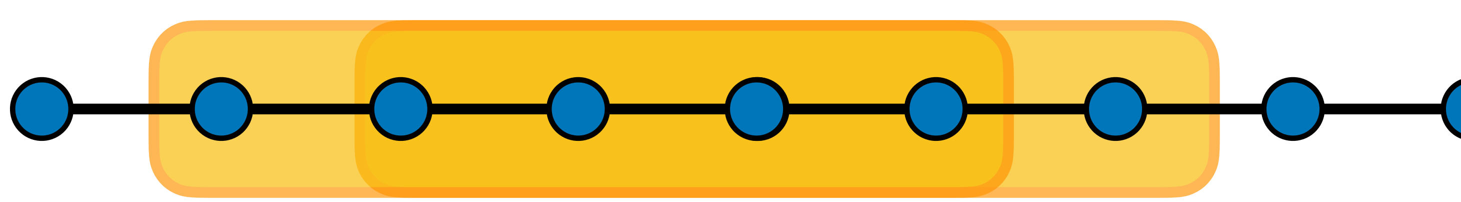
$$Q_n(\Delta) = \sum_{i=1}^{N} (h_{i,i+1}^2 - \Delta h_{i,i+1}) + \sum_{i=1}^{N} \sum_{k \leq n} \{h_{i,i+1}, h_{i+k,i+k+1}\} \succeq 0$$

2) Find a postive local generating operator

$$Q_n(\Delta) = \sum_i q_{n,i}$$

$$q_{n,i} \succeq 0$$

Translational invariant



SIMPLIFICATIONS

H has a spectral gap Δ
If and only if

$$H^2 - \Delta H \succeq 0$$

Computing the eigenvalues
of an exponentially-large matrix

1) Cut to a local operator

$$Q_n(\Delta) = \sum_{i=1}^{N} (h_{i,i+1}^2 - \Delta h_{i,i+1}) + \sum_{i=1}^{N} \sum_{k \leq n} \{h_{i,i+1}, h_{i+k,i+k+1}\} \succeq 0$$

2) Find a postive local generating operator

$$Q_n(\Delta) = \sum_i q_{n,i}$$

$$q_{n,i} \succeq 0$$

Once found, applies to any system size

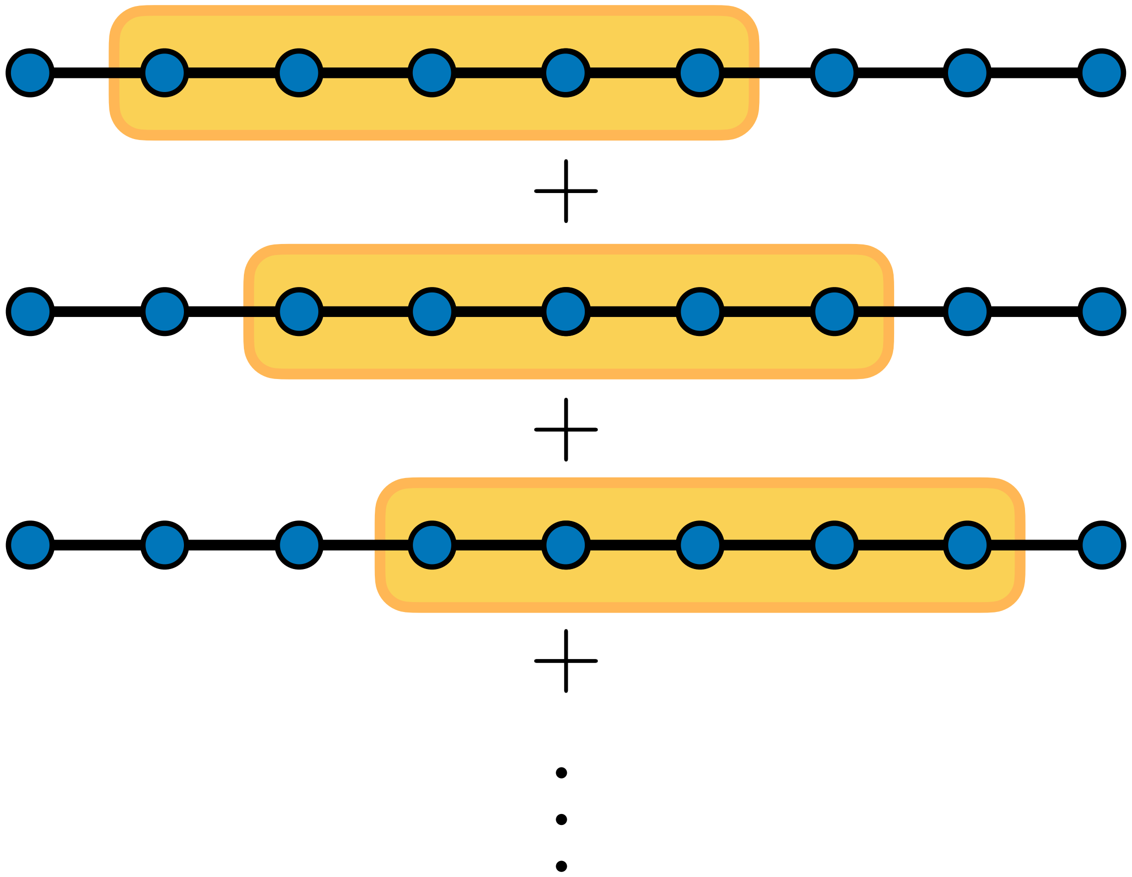
$$\lim_{N \to \infty} \Delta_N = \Delta > 0$$

THE LOCAL GENERATING TERM

$$Q_n(\Delta) = \sum_i q_{n,i}$$

Finding a suitable local generating term

$$q_{n,i} \succeq 0$$



$$= Q_n(\Delta)$$

THE LOCAL GENERATING TERM

$$Q_n(\Delta) = \sum_i q_{n,i}$$

Finding a suitable local generating term $q_{n,i} \succeq 0$

Easy to find a solution, but it is not $q_{n,i} \succeq 0$

A GENERAL SOLUTION

$$Q_n(\Delta) = \sum_i q_{n,i}$$

If and only if

$$q_{n,i} = g_{n,i} + \mathbb{1}_1 \otimes Y - Y \otimes \mathbb{1}_n$$

A GENERAL SOLUTION

$$Q_n(\Delta) = \sum_i q_{n,i}$$

If and only if

$$q_{n,i} = g_{n,i} + \mathbb{1}_1 \otimes Y - Y \otimes \mathbb{1}_n$$

Given

A GENERAL SOLUTION

$$Q_n(\Delta) = \sum_i q_{n,i}$$

If and only if

$$q_{n,i} = g_{n,i} + \mathbb{1}_1 \otimes Y - Y \otimes \mathbb{1}_n$$

Given

Supported on $n-1$ sites

A GENERAL SOLUTION

$$Q_n(\Delta) = \sum_i q_{n,i}$$

If and only if

$$q_{n,i} = g_{n,i} + \mathbb{1}_1 \otimes Y - Y \otimes \mathbb{1}_n$$

Given

Supported on $n-1$ sites

Look for Y such that

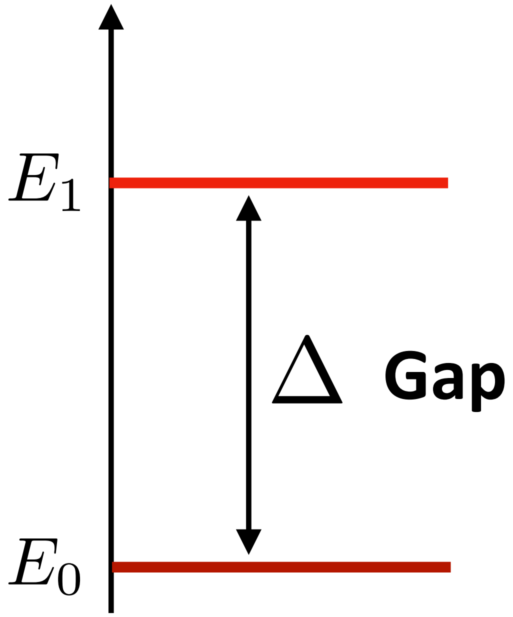
$$q_{n,i} \succeq 0$$

The numerical tool

A GENERAL SDP TO LOWER BOUND THE GAP

$$\Delta = \max_{\delta} \ \delta$$

$$s.t. \quad H^2 - \delta H \succeq 0$$

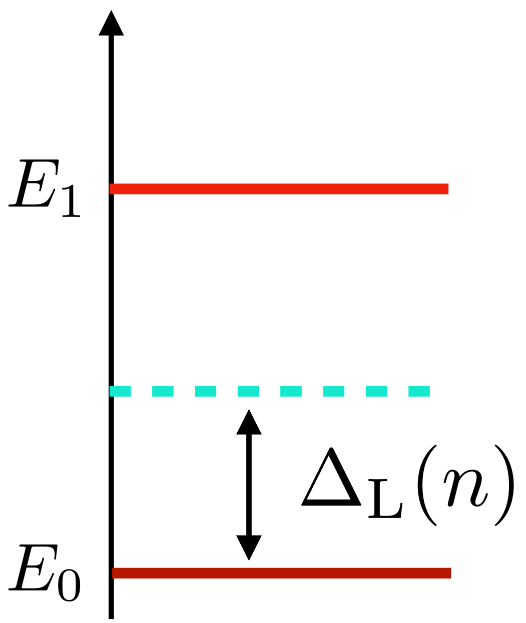


A GENERAL SDP TO LOWER BOUND THE GAP

$$\Delta = \max_{\delta} \ \delta$$

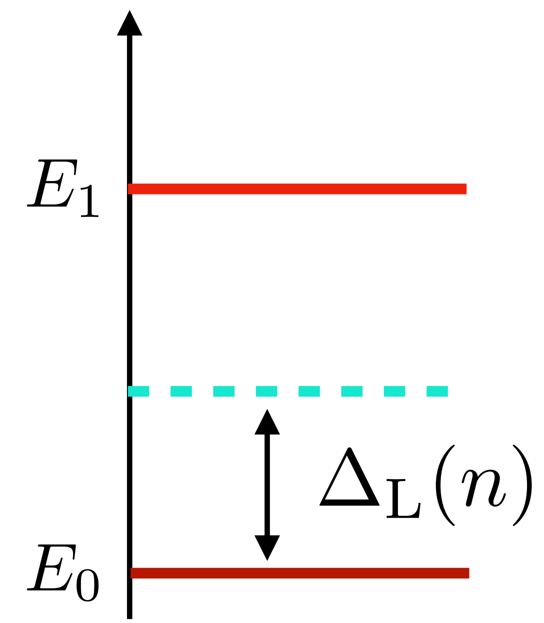
$$s.t. \quad H^2 - \delta H \succeq 0$$

Find a local and TI sum of squares



A GENERAL SDP TO LOWER BOUND THE GAP

$$\Delta = \max_{\delta} \ \delta$$
$$s.t. \quad H^2 - \delta H \succeq 0$$



Find a local and TI sum of squares

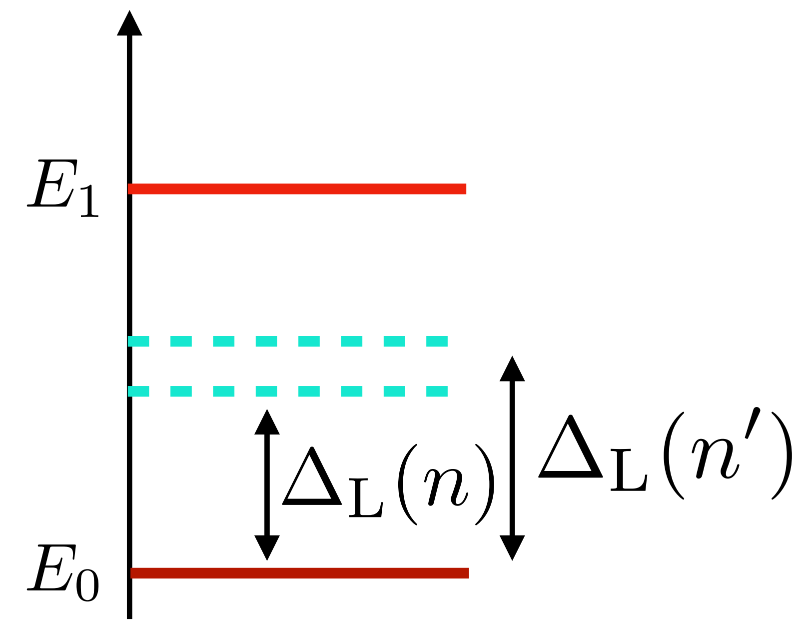
$$\Delta_{\mathrm{L}}(n) = \max_{\delta, Y} \ \delta$$
$$s.t. \quad q_{n,i} = g_{n,i}(\delta) + \mathbb{1}_1 \otimes Y - Y \otimes \mathbb{1}_n$$
$$q_{n,i} \succeq 0$$

Sufficient condition for

$$H^2 - \delta H \succeq 0$$

A GENERAL SDP TO LOWER BOUND THE GAP

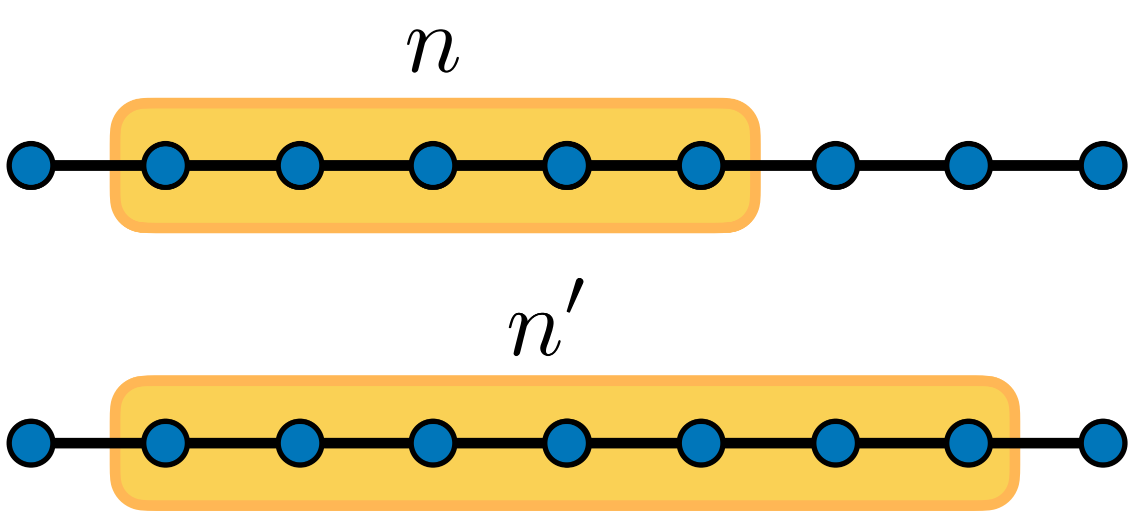
$$\Delta = \max_{\delta} \ \delta$$
$$s.t. \quad H^2 - \delta H \succeq 0$$



Find a local and TI sum of squares

$$\Delta_{\mathrm{L}}(n) = \max_{\delta, Y} \ \delta$$
$$s.t. \quad q_{n,i} = g_{n,i}(\delta) + \mathbb{1}_1 \otimes Y - Y \otimes \mathbb{1}_n$$
$$q_{n,i} \succeq 0$$

Systematic way of improving



A GENERAL SDP TO LOWER BOUND THE GAP

$$\Delta_{\mathrm{L}}(n) = \max_{\delta, Y} \ \delta$$

$$s.t. \quad q_{n,i} = g_{n,i}(\delta) + \mathbb{1}_1 \otimes Y - Y \otimes \mathbb{1}_n$$

$$q_{n,i} \succeq 0$$

Semidefinite programming = the global minimum can be found efficiently in the size of Y

Comparison to existing techniques

TWO MAIN TECHNIQUES

Global → **Local**

$$H^2 - \Delta H \succeq 0$$

$$q_{n,i} \succeq 0$$

TWO MAIN TECHNIQUES

Global

$$H^2 - \Delta H \succeq 0$$

→

Local

$$q_{n,i} \succeq 0$$

Previous methods have a similar spirit

- **Finite-size criteria** (Knabe 1988, M. Lemm and D. Xiang 2022, ...)

Requires estimating the gap for the size n system

TWO MAIN TECHNIQUES

Global **Local**

$$H^2 - \Delta H \succeq 0 \quad \Rightarrow \quad q_{n,i} \succeq 0$$

Previous methods have a similar spirit

- **Finite-size criteria** (Knabe 1988, M. Lemm and D. Xiang 2022, …)

  Requires estimating the gap for the size n system

- **Martingale-like methods** (Nachtergaele 1996, M. J. Kastoryano and A. Lucia 2018, …)

  Requires estimating the norm of size n projectors

TWO MAIN TECHNIQUES

Global

$$H^2 - \Delta H \succeq 0$$

Local

$$q_{n,i} \succeq 0$$

Previous methods have a similar spirit

- Finite-size criteria

- Martingale-like methods

Have been used to prove the gap in recent 2D results

M. Lemm, A. W. Sandvik, and L. Wang, ”Existence of a spectral gap in the Affleck-Kennedy-Lieb-Tasaki model on the hexagonal lattice." *PRL* 124.17 (2020)

N. Pomata and W. Tzu-Chieh, "Demonstrating the Affleck-Kennedy-Lieb-Tasaki spectral gap on 2D degree-3 lattices.”, *PRL* 124.17 (2020)

WE CAN RECOVER ALL OF THEM

Global → **Local**

$$H^2 - \Delta H \succeq 0 \quad \Rightarrow \quad q_{n,i} \succeq 0$$

Previous methods have a similar spirit

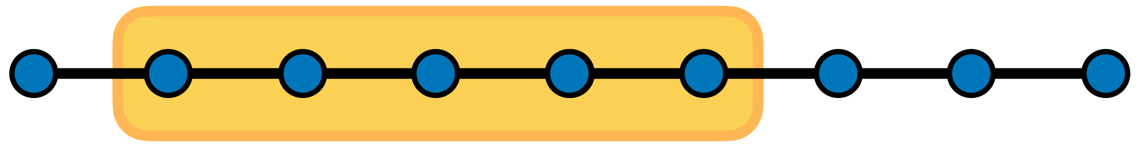
- **Finite-size criteria**

- **Martingale-like methods**

EXAMPLE: KNABE BOUND

Ansatz

$$q_{n,i}(\Delta_{\text{Knabe}}(n)) = \left(\frac{1-\epsilon_n}{n-2}\right) h_{n,i} + \sum_{x=1}^{n-2} \frac{1}{n-x-1} \sum_{j=0}^{n-x-2} \{h_{i+j}, h_{i+j+x}\} \succeq 0$$

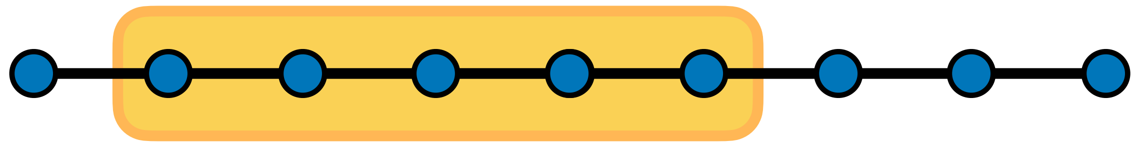


EXAMPLE: KNABE BOUND

Ansatz

$$q_{n,i}(\Delta_{\mathrm{Knabe}}(n)) = \left(\frac{1-\epsilon_n}{n-2}\right) h_{n,i} + \sum_{x=1}^{n-2} \frac{1}{n-x-1} \sum_{j=0}^{n-x-2} \{h_{i+j}, h_{i+j+x}\} \succeq 0$$

Finite size hamiltonian for n particles



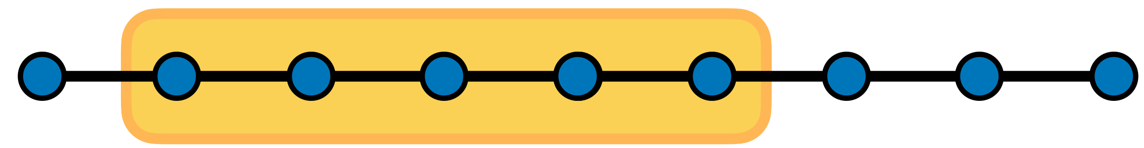
EXAMPLE: KNABE BOUND

Gap of the finite system

Ansatz

$$q_{n,i}(\Delta_{\mathrm{Knabe}}(n)) = \left(\frac{1-\epsilon_n}{n-2}\right) h_{n,i} + \sum_{x=1}^{n-2} \frac{1}{n-x-1} \sum_{j=0}^{n-x-2} \{h_{i+j}, h_{i+j+x}\} \succeq 0$$

Finite size hamiltonian for n particles



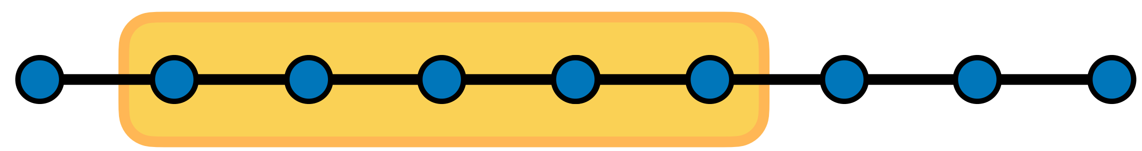
EXAMPLE: KNABE BOUND

Gap of the finite system

Ansatz

$$q_{n,i}(\Delta_{\text{Knabe}}(n)) = \left(\frac{1-\epsilon_n}{n-2}\right) h_{n,i} + \sum_{x=1}^{n-2} \frac{1}{n-x-1} \sum_{j=0}^{n-x-2} \{h_{i+j}, h_{i+j+x}\} \succeq 0$$

Finite size hamiltonian for
n **particles**



$$Q_n(\Delta_{\text{Knabe}}(n)) = \sum_i q_{n,i}(\Delta_{\text{Knabe}}(n)) \succeq 0$$

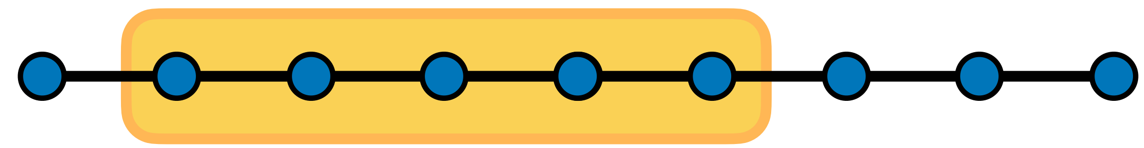
EXAMPLE: KNABE BOUND

Ansatz

Gap of the finite system

$$q_{n,i}(\Delta_{\text{Knabe}}(n)) = \left(\frac{1-\epsilon_n}{n-2}\right) h_{n,i} + \sum_{x=1}^{n-2} \frac{1}{n-x-1} \sum_{j=0}^{n-x-2} \{h_{i+j}, h_{i+j+x}\} \succeq 0$$

Finite size hamiltonian for n particles



$$Q_n(\Delta_{\text{Knabe}}(n)) = \sum_i q_{n,i}(\Delta_{\text{Knabe}}(n)) \succeq 0$$

Gap

$$\Delta_{\text{Knabe}}(n) = \frac{n-1}{n-2}\left(\epsilon_n - \frac{1}{n-1}\right)$$

Knabe 1988

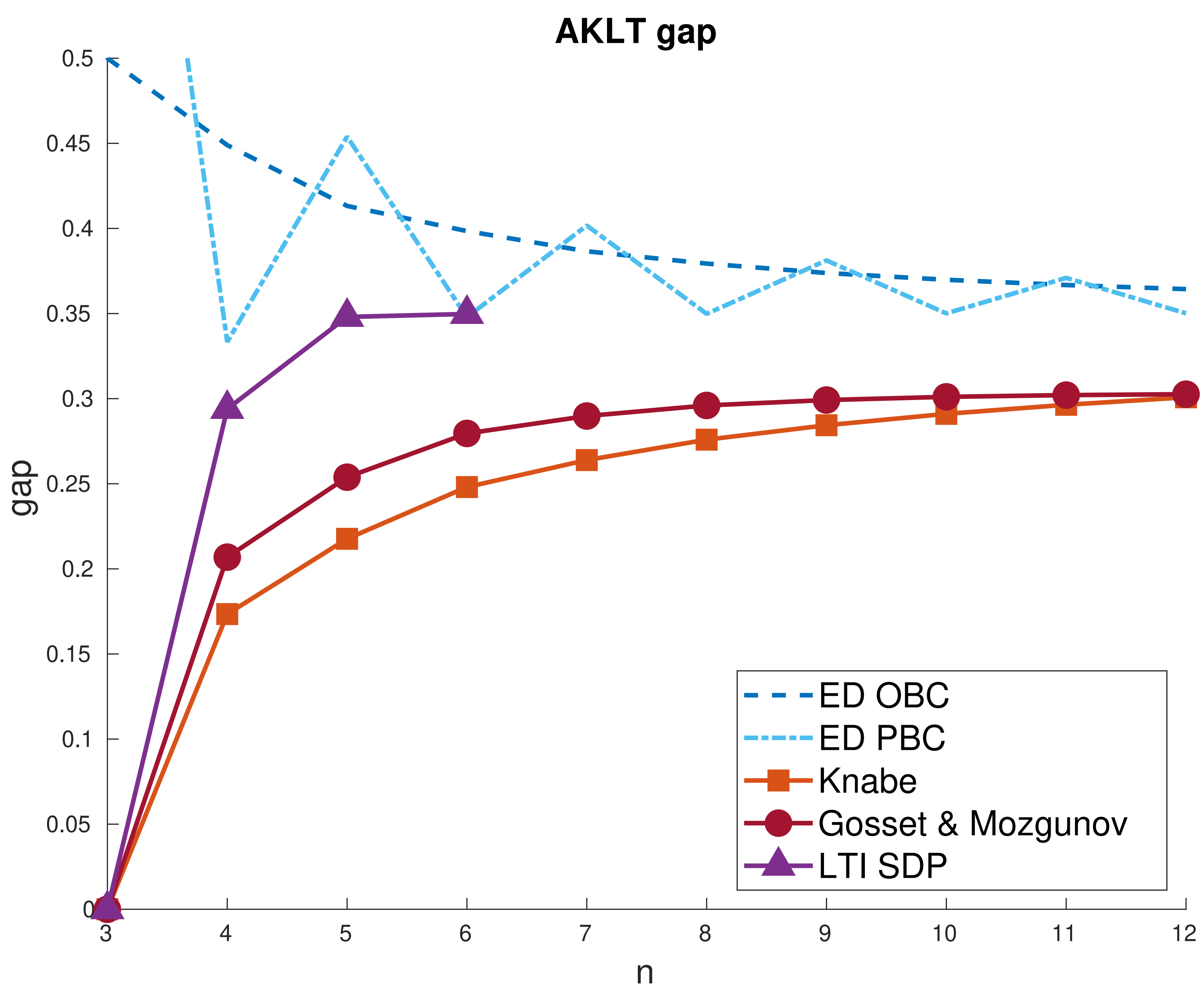
Numerical tests

THE AKLT MODEL

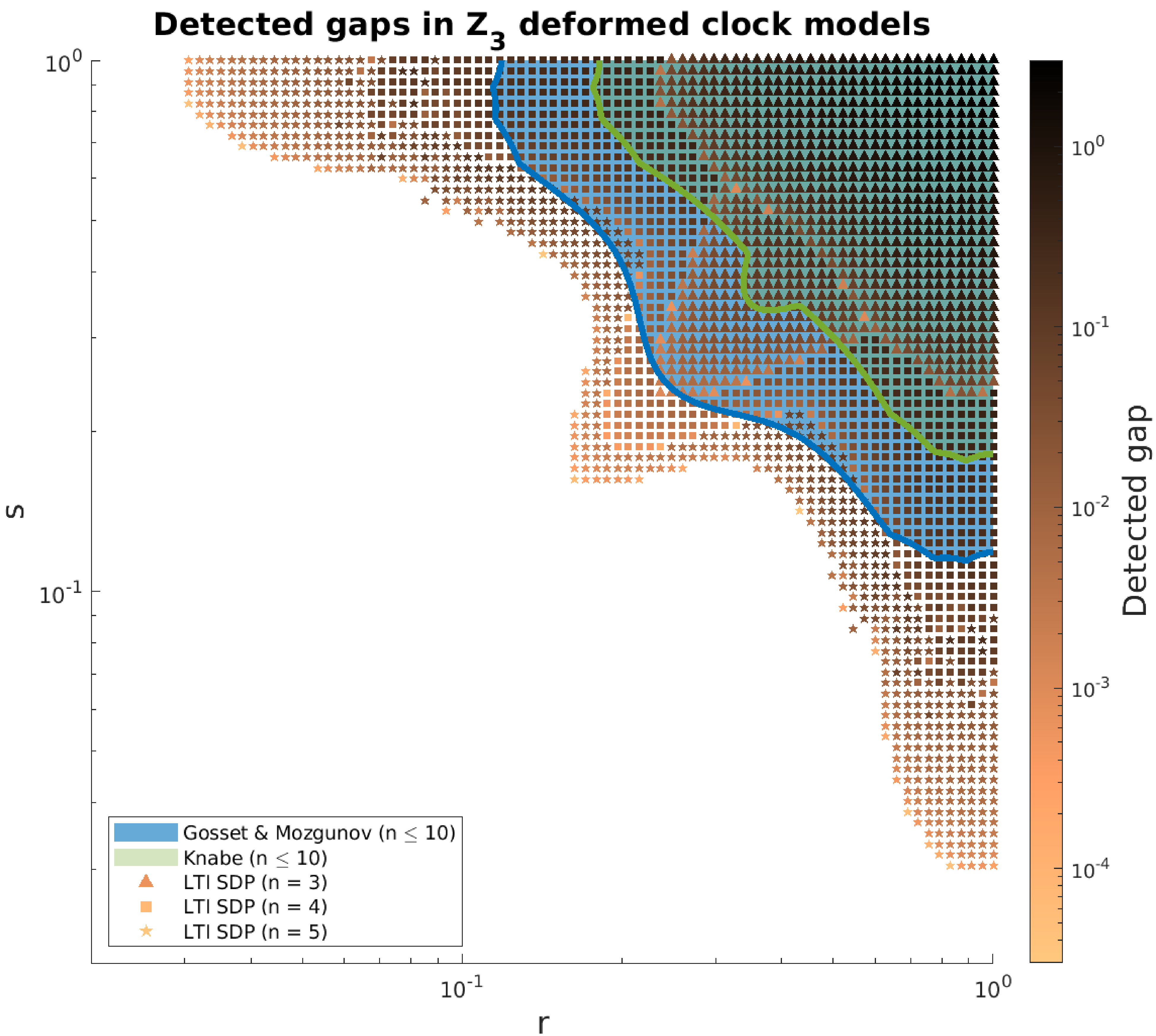
$$H = \frac{1}{2}\left[\sum_i \vec{S}_i \cdot \vec{S}_j + \frac{1}{3}\sum_i (\vec{S}_i \cdot \vec{S}_j)^2 + \frac{2}{3}\mathbb{1}\right]$$

THE AKLT MODEL

$$H = \frac{1}{2}\left[\sum_i \vec{S}_i \cdot \vec{S}_j + \frac{1}{3}\sum_i (\vec{S}_i \cdot \vec{S}_j)^2 + \frac{2}{3}\mathbb{1}\right]$$



COMPARISON WITH FINITE-SIZE CRITERIA



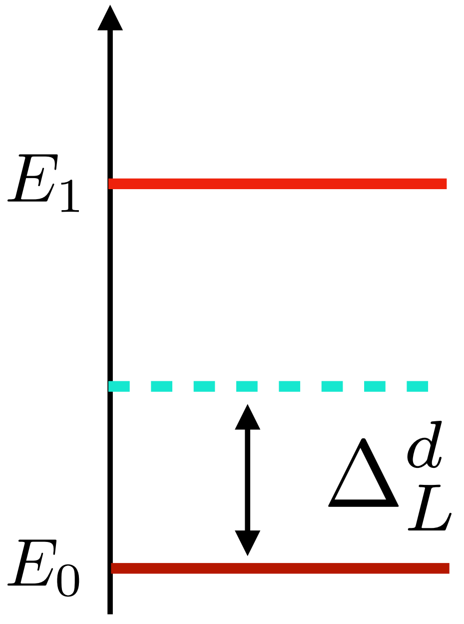
J. Wouters, H. Katsura, D. Schuricht, SciPost Phys. Core 4, 027 (2021)

Outlook

OUTLOOK

A numerical method to lower bound the gap for 1D systems

- **Efficient and with systematic improvement**
- **Recovers previous techniques as special cases**
- **Provides better results on benchmarks**



Future directions: 2D

THANKS

Kshiti Sneh Rai

Ilya Kull

Norbert Schuch

Patrick Emonts

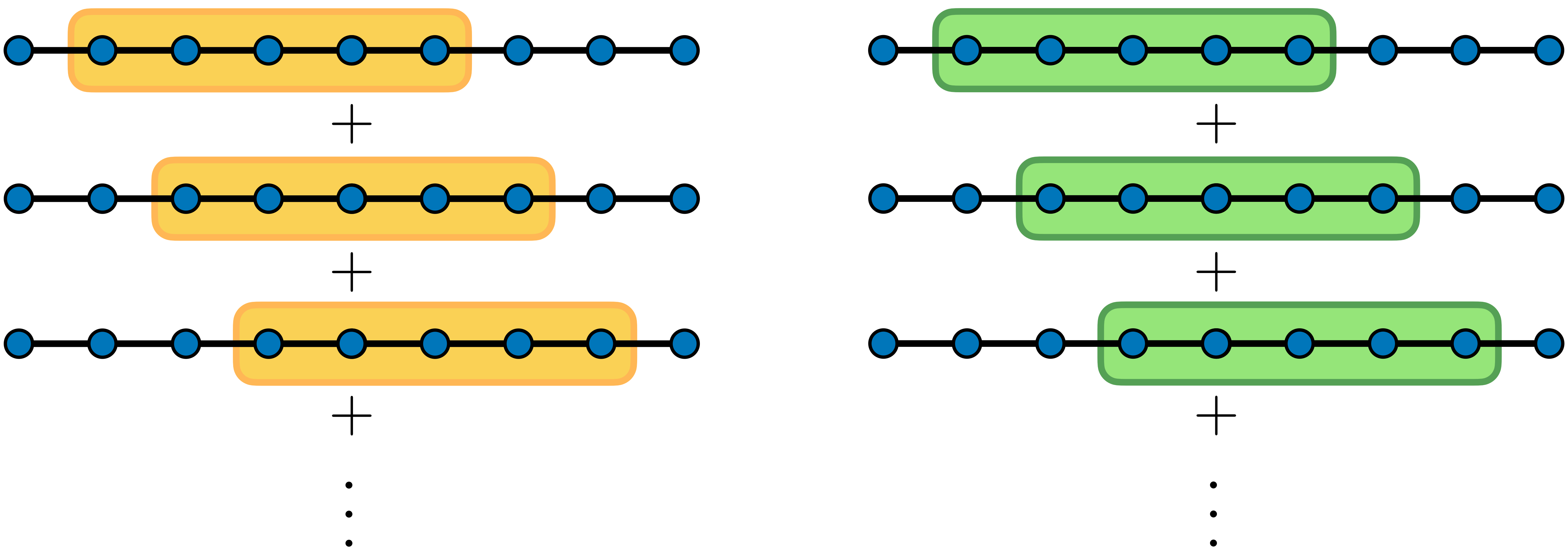
Jordi Tura

Thanks

Bonus

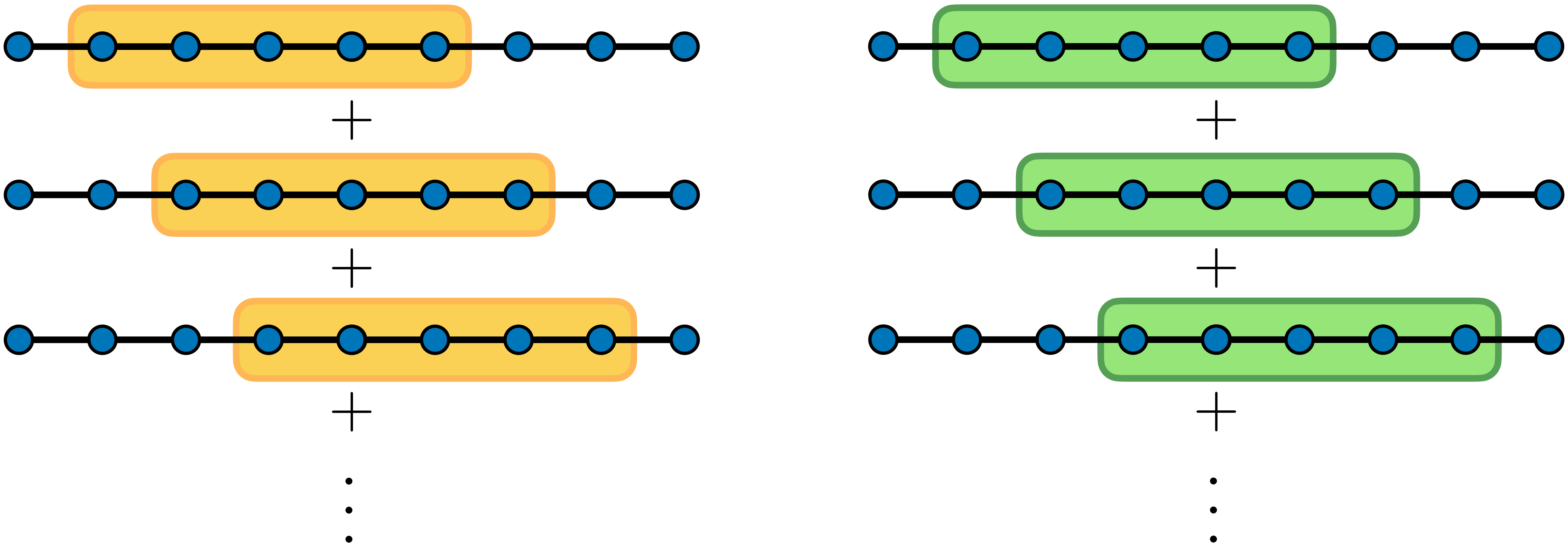
THE LOCAL GENERATING TERM

$$\sum_i g_{i,n} = \sum_i q_{i,n}$$



THE LOCAL GENERATING TERM

$$\sum_i g_{i,n} = \sum_i q_{i,n}$$



The solution is not unique

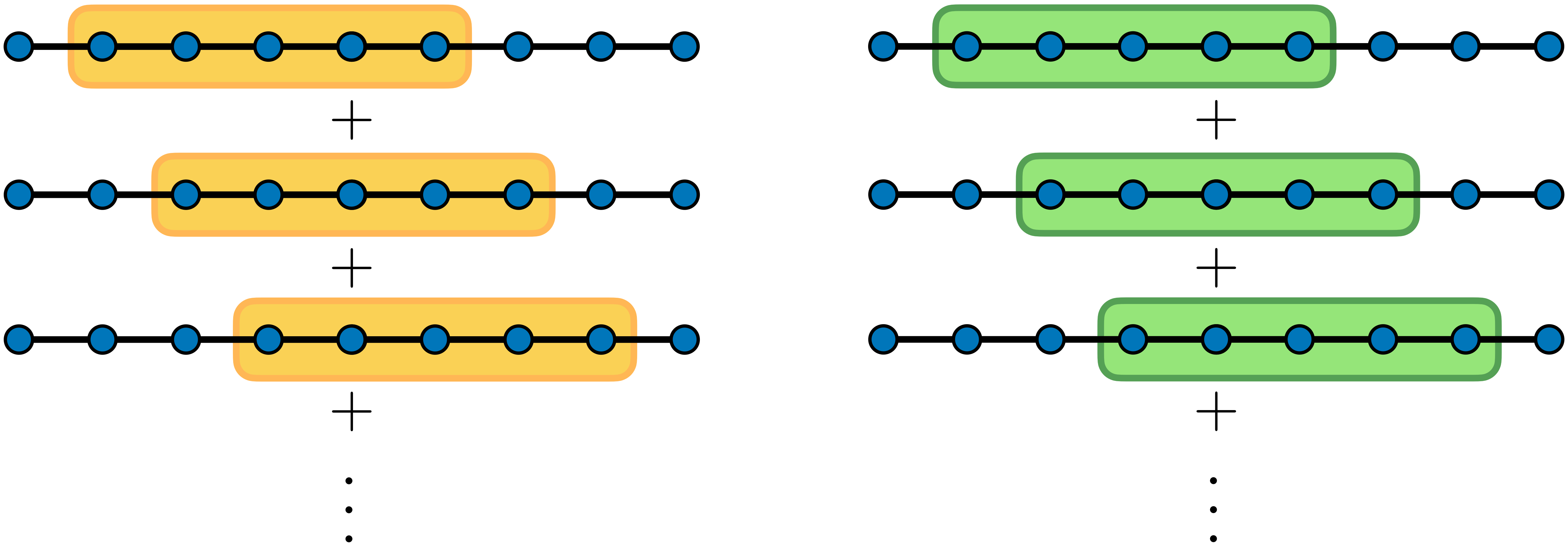
$$h_i = Z_i Z_{i+1} + X_i$$

$$h'_i = Z_i Z_{i+1} + \frac{1}{2} X_i + \frac{1}{2} X_{i+1}$$

$$H = \sum_i Z_i Z_{i+1} + \sum_i X_i$$

THE LOCAL GENERATING TERM

$$\sum_i g_{i,n} = \sum_i q_{i,n}$$



The solution is not unique

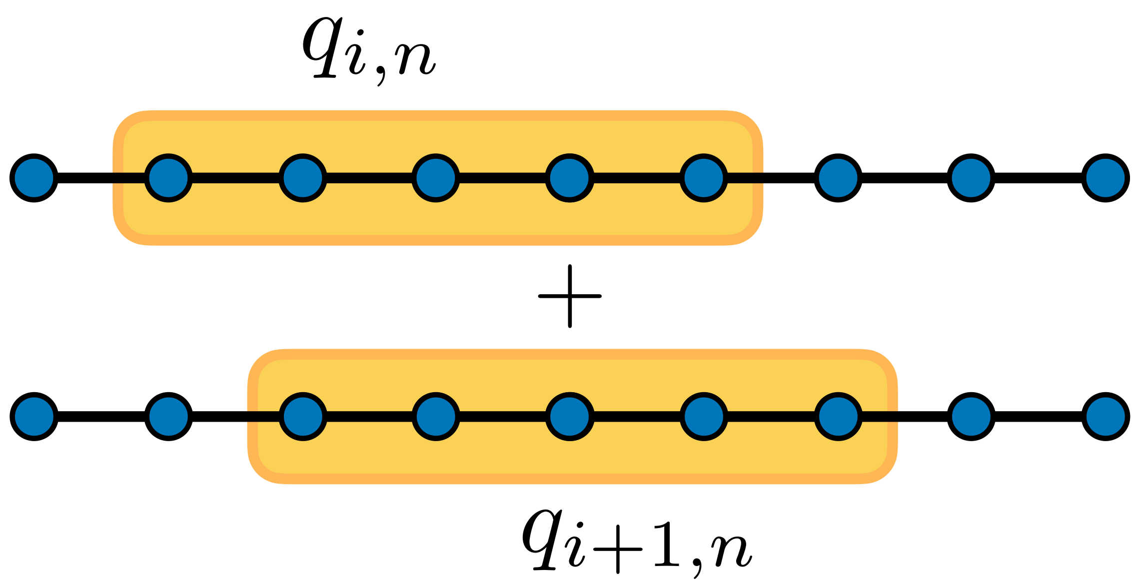
$$\left.\begin{aligned} h_i &= Z_i Z_{i+1} + X_i \\ h_i' &= Z_i Z_{i+1} + \frac{1}{2} X_i + \frac{1}{2} X_{i+1} \end{aligned}\right\} \quad H = \sum_i Z_i Z_{i+1} + \sum_i X_i$$

A GENERAL SOLUTION

$$\sum_i g_{i,n} = \sum_i q_{i,n}$$

If and only if

$$q_{n,i} = g_{n,i} + \mathbb{1}_1 \otimes Y - Y \otimes \mathbb{1}_n$$

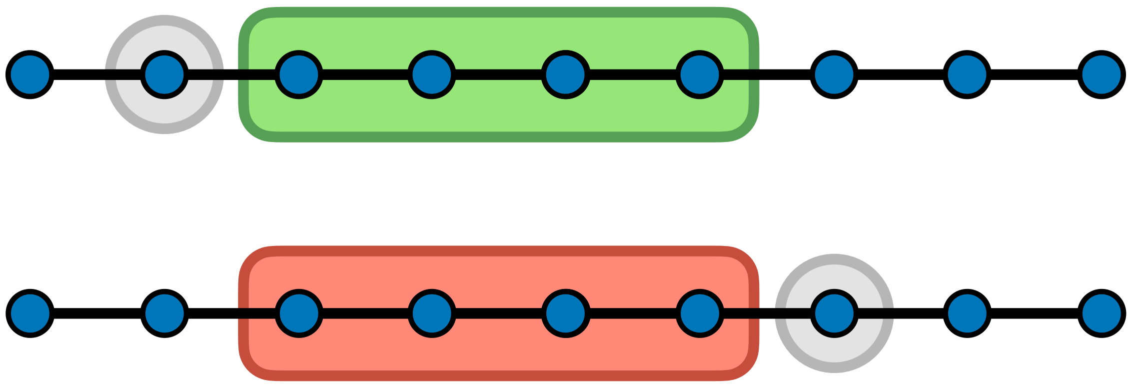


A GENERAL SOLUTION

$$\sum_i g_{i,n} = \sum_i q_{i,n}$$

If and only if

$$q_{n,i} = g_{n,i} + \mathbb{1}_1 \otimes Y - Y \otimes \mathbb{1}_n$$



$\mathbb{1}_1 \otimes Y$

$- Y \otimes \mathbb{1}_n$