Quantum many-body bootstrap

2211.03819 with Colin Nancarrow

Also work in progress with

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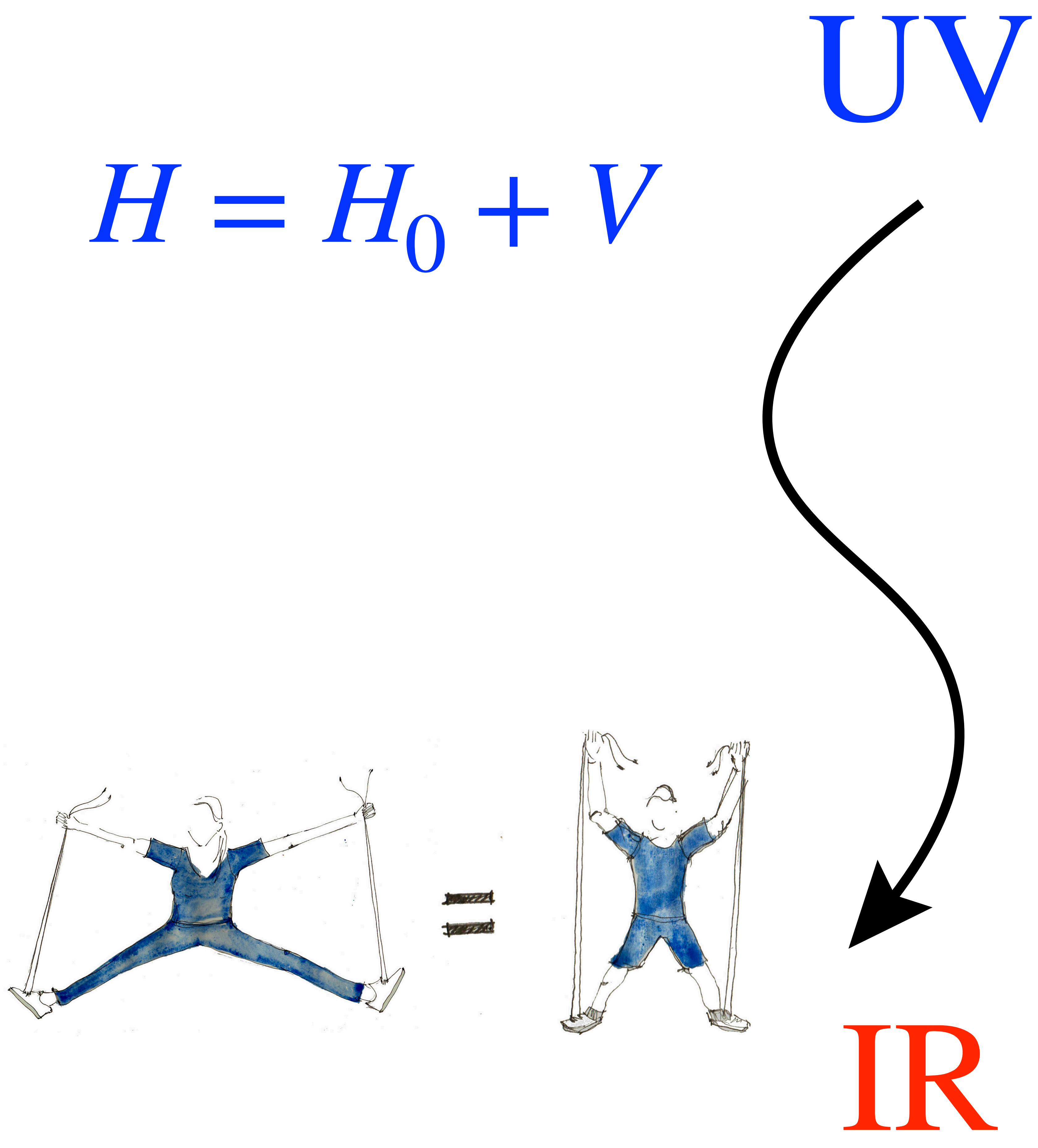
Yuan Xin 2024/01/08

Motivation

- Systems with large degrees of freedom can have interesting emergent behaviors, which are often strongly coupled and hard to compute.
- Bootstrap is a robust computational framework for making rigorous predictions in strongly coupled systems
- The setup for bootstrapping quantum many-body system is new, where a lot of progress was made recently.



Outline

- Introduction
- Bounding many-body ground state
- Bounding gap of many-body systems

Introduction

Introduction

Moment problem and Hankel matrix

- Moment Problem:
  - Organize observables as Hankel Matrix $M^K_{ij} = \langle x^{i+j} \rangle,\ 1 \le i, j \le K$
  - $$\langle x^n \rangle = \int x^n d\mu \quad \text{for a positive measure } \mu$$
    $$\Leftrightarrow$$
    $$M^K \text{ is positive semidefinite } M^K \succeq 0,\ \forall\ K$$
- $\langle x^n \rangle$ is further constrained by equations of motion, symmetry and locality.

Introduction

Warm up: Bootstrapping Anharmonic Oscillator [Han, Hartnoll, Kruthoff '20]

$$\begin{pmatrix} \langle 1 \rangle & \langle x \rangle & \cdots & \langle x^K \rangle \\ \langle x \rangle & \langle x^2 \rangle & \cdots & \langle x^{K+1} \rangle \\ \vdots & \vdots & \ddots & \\ \langle x^K \rangle & \langle x^{K+1} \rangle & & \langle x^{K+K} \rangle \end{pmatrix}$$

- $H = p^2 + \omega^2 x^2 + \lambda x^4$
- Bound from unitarity $M_{ij} \equiv \langle E | x^{i+j} | E \rangle \geqslant 0$
- Using defining equations of motions $\begin{cases} \langle [H, \mathcal{O}] \rangle = 0 \\ \langle H \mathcal{O} \rangle = E \langle \mathcal{O} \rangle \end{cases}$
- For diagonal matrix elements

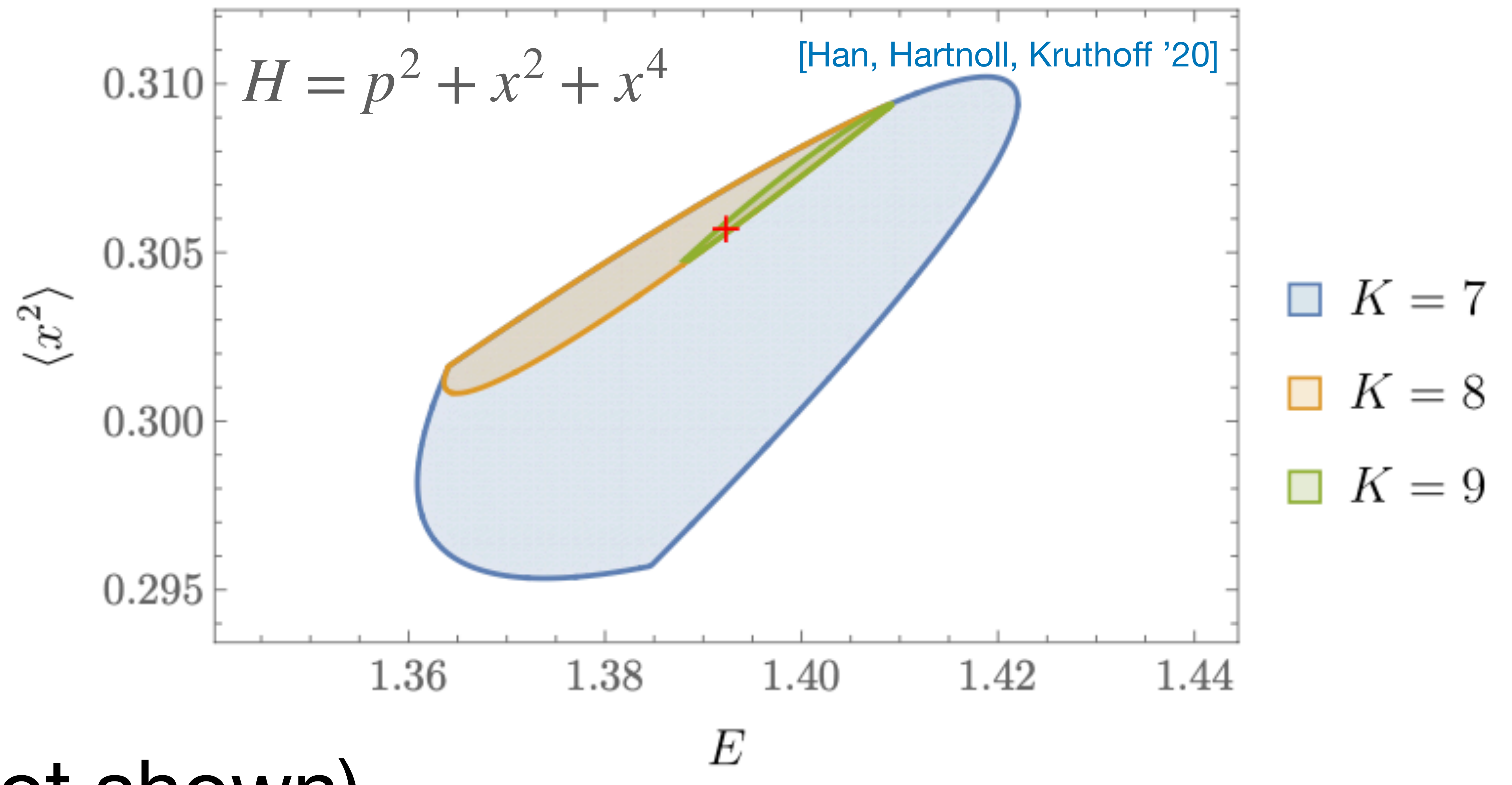
$$4tE\langle x^{t-1} \rangle - t(t-1)\langle x^{t+1} \rangle - 4\lambda(t+2)\langle x^{t+3} \rangle = 0$$

$\Rightarrow \ \langle x^{2n} \rangle = \# + \#' \langle x^2 \rangle$ $\qquad$ $\langle x^{2n+1} \rangle \propto \langle x \rangle = 0$ from parity

Introduction

Warm up: Bootstrapping Anharmonic Oscillator [Han, Hartnoll, Kruthoff '20]

- $M_{ij} \equiv \langle E | x^{i+j} | E \rangle \succcurlyeq 0$, $\langle x^{2n} \rangle = \# + \#' \langle x^2 \rangle$ $\quad 0 \leqslant i,j \leqslant K$
- Give E, $\langle x^2 \rangle$, ask if $M \succcurlyeq 0$
  - Yes: an eigenstate with E, $\langle x^2 \rangle$ is possible
  - No: an eigenstate with E, $\langle x^2 \rangle$ is impossible
- Bound also allows other eigenstates (not shown)



Introduction

Summarize & previous works

- For quantum mechanical systems, unitarity and equations of motion directly impose bounds on observables.

- See for example:
  [Anderson, Kruczenski ’16], [Lin ’20, ’23],
  [Han, Hartnoll, Kruthoff ’20], [Han ’20],
  [Kazakov, Zheng ’21 ’22], [Lawrence ’21, ’22],
  [Cho, Gabai, Lin, Rodriguez, Sandor, Yin ’22]
  [Li ’22] [Guo, Li ’22]
  [Kull, Schuch, Dive, Navascués’22]
  [Cho ’23], [Cho, Sun, ’23]
  [Fawzi, Fawzi, Scalet, ‘23],
  [Araújo, Klep, Vértesi, Garner, Navascues ’23]
  And more…

Bound $\langle \mathcal{O}_* \rangle$, E_0, etc.

Such that

$$\langle \mathcal{O}\bar{\mathcal{O}} \rangle \geqslant 0$$

$$\langle \delta\mathcal{O} + \mathcal{O}\delta S \rangle = 0$$

Or $\langle [H\mathcal{O}] \rangle = 0$

Bounding Many-body Ground State

Bounding Many-body Ground State

Generalize to Many-body Systems

- Vacuum energy diverges at infinite d.o.f. If we discard the corresponding equation, the energy does not explicitly show up in the bootstrap constraints.

$$\begin{cases} \langle [H, \mathcal{O}] \rangle = 0 \\ \cancel{\langle H \mathcal{O} \rangle = E \langle \mathcal{O} \rangle} \end{cases}$$

← satisfied by any static states and linear combination

- How do we specify that we are bounding ground state properties?
  - By definition, minimizing energy density leads to the ground state.
  - Or, add another constraint $\langle \mathcal{O}^\dagger [H, \mathcal{O}] \rangle \geq 0$ to isolate the ground state.

[Fawzi, Fawzi, Scalet, 2311.18706,
also Araújo, Klep, Vértesi, Garner, Navascues 2311.18707]

Bounding Many-body Ground State

Lower bounding ground state energy

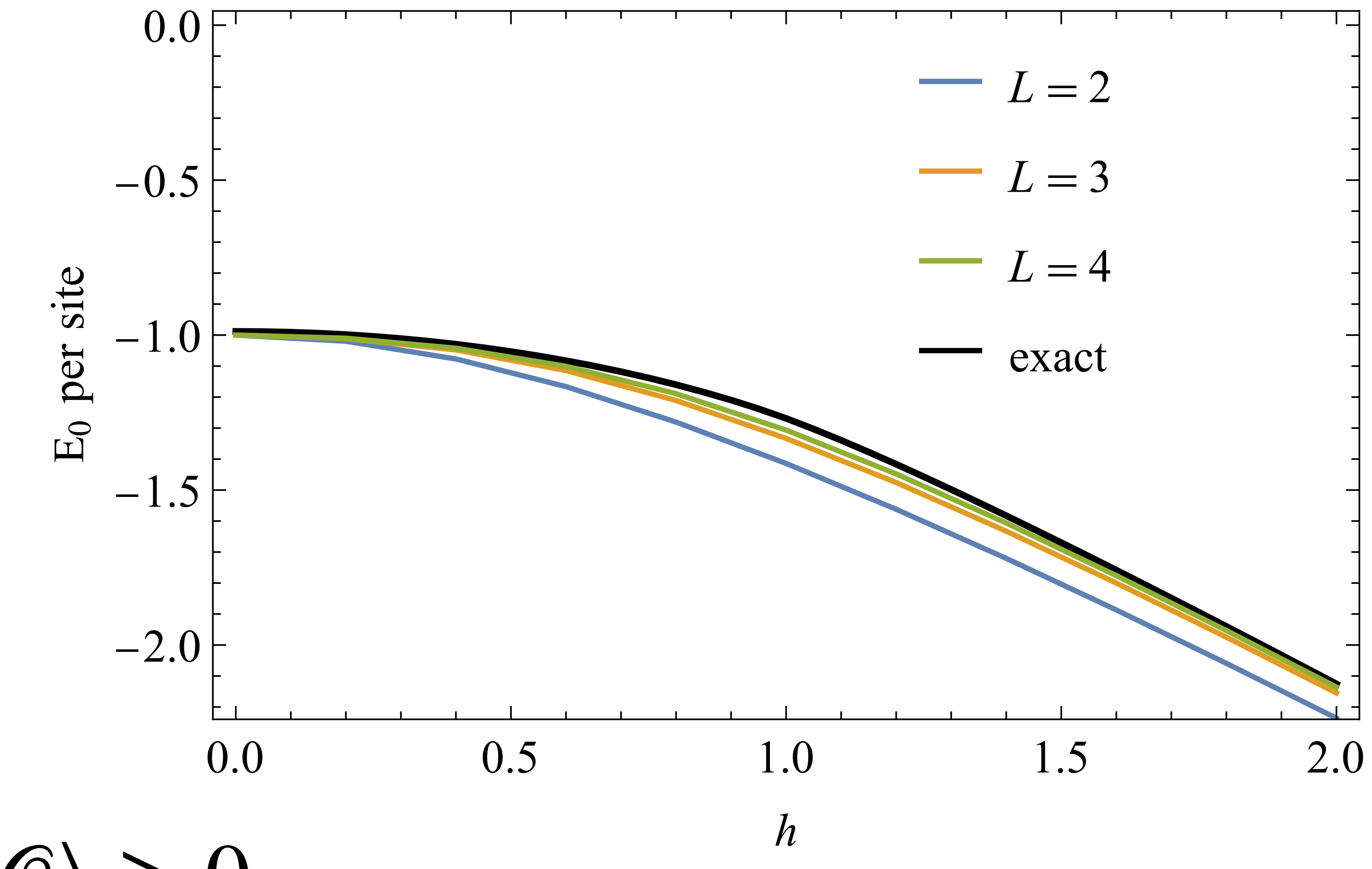
- Example: Transverse Field Ising Model (TFIM) on 1d infinite spin chain

$$H = \sum_i \sigma_i^z \sigma_{i+1}^z + h\sigma_i^x$$

- Infinitely many EOMs

$$0 = \langle [H, \sigma_1^{\mu_1}\sigma_2^{\mu_2}\cdots] \rangle = \langle \sum_{\{\nu\}} c^{\mu_1\mu_2\cdots}_{\nu_1\nu_2\cdots}\, \sigma_1^{\nu_1}\sigma_2^{\nu_2}\cdots \rangle$$

relate to infinitely many operators.
Restrict to operators within range L.



- Minimize $\langle H_{12} \rangle \equiv \langle \sigma_1^z \sigma_2^z + h\sigma_1^x \rangle$, constrained by $\langle \mathcal{O}^\dagger \mathcal{O} \rangle \geq 0$.

Bounding Many-body Ground State

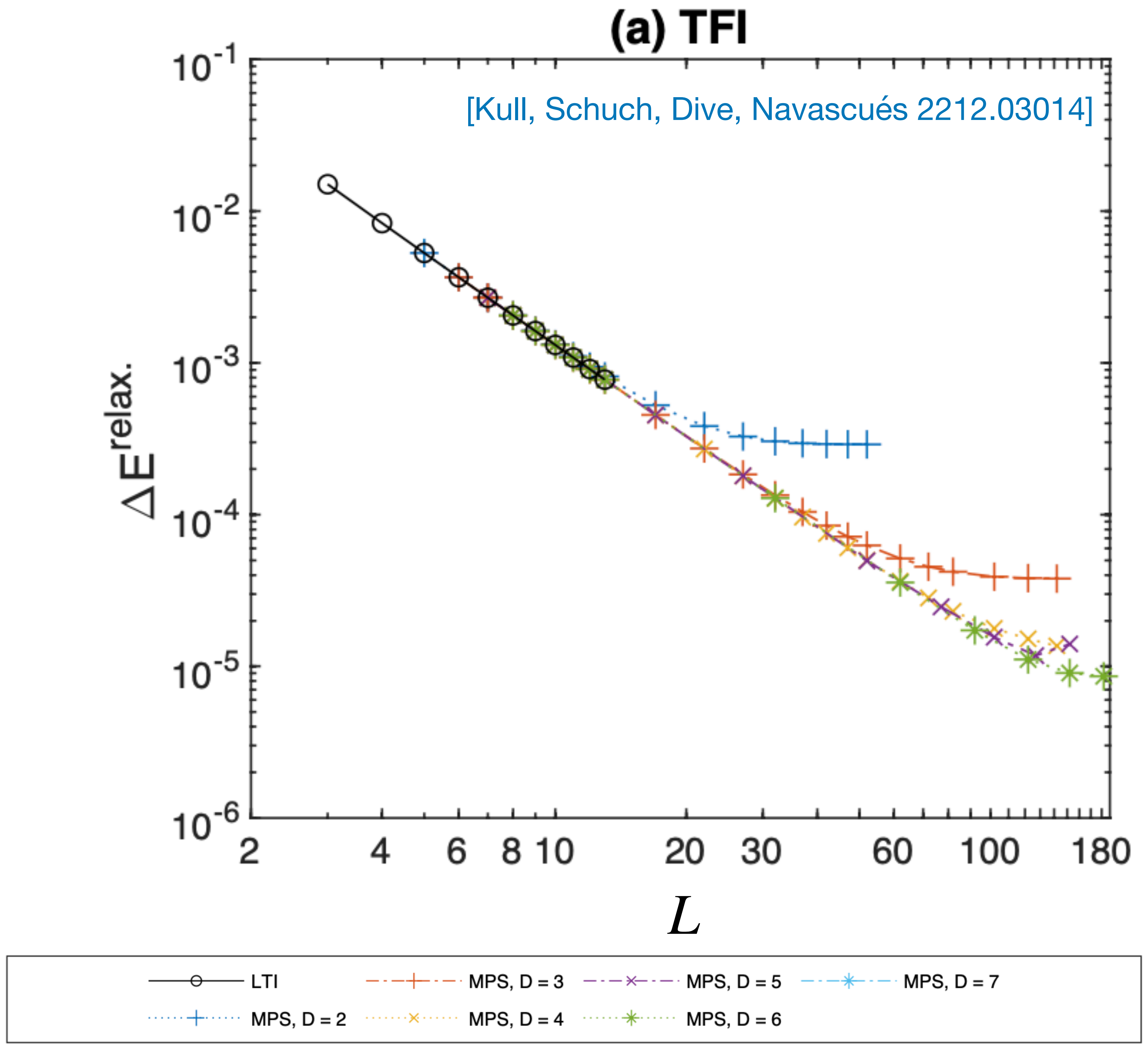
Optimizing the bound with Matrix Product State

- Bound converges as $\sim e^{-m_{gap}L}$,
  but dimension of $\langle \mathcal{O}_i^\dagger \mathcal{O}_j \rangle$ grows as 4^L .

- We do not need full 4^L variables
  to optimize bootstrap bound:
  Relaxing the constraint matrix
  $\langle \mathcal{O}_i^\dagger \mathcal{O}_j \rangle \succeq 0$ to $\langle B_{ij}^\dagger \mathcal{O}_j^\dagger \mathcal{O}_k B_{kl} \rangle \succeq 0$, where B
  is a $4^N \times O(D^2)$ matrix.

- B can be a Matrix Product State (MPS)

  [Kull, Schuch, Dive, Navascués 2212.03014]



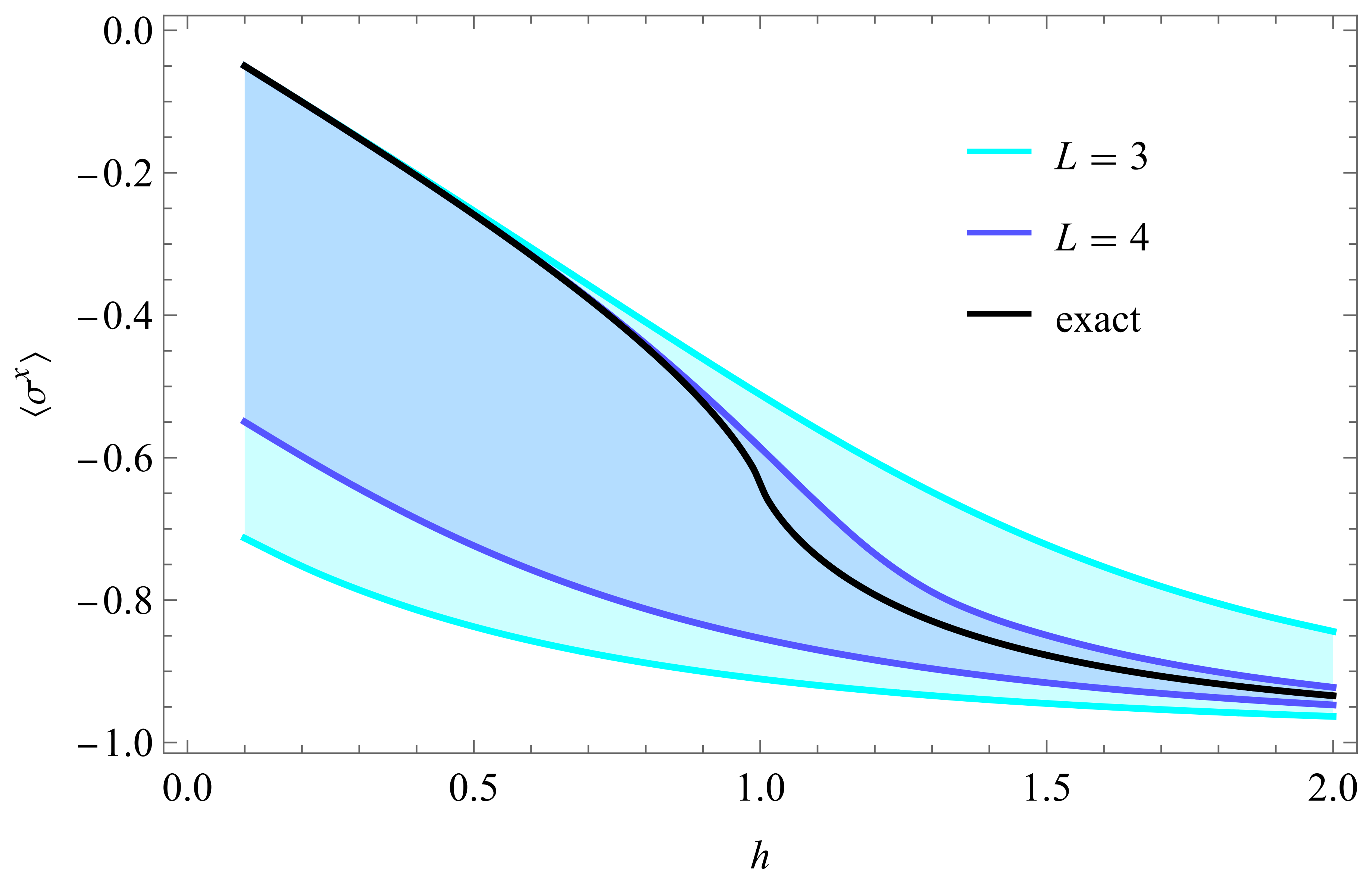
Bounding Many-body Ground State

Isolating the ground state

- If we want upper bound on ground state or other ground state expectation values, we will need to isolate the ground state.

- The additional condition is
  $\langle \mathcal{O}^\dagger [H, \mathcal{O}] \rangle \geq 0$

  [Fawzi, Fawzi, Scalet, 2311.18706,
  also Araújo, Klep, Vértesi, Garner, Navascues 2311.18707]



- Large L is still required to see convergence numerically. It is interesting to see if bound can be optimized using variational techniques.

Bounding Many-body Ground State

Our setup: optimize ground state bound using MPS

- Idea:

Moment matrix problem

$$\langle \mathcal{O}^\dagger \mathcal{O} \rangle \geq 0, \langle [H, \mathcal{O}] \rangle = 0$$

+

$$\langle \mathcal{O}^\dagger [H, \mathcal{O}] \rangle \geq 0$$

[Fawzi, Fawzi, Scalet, 2311.18706]

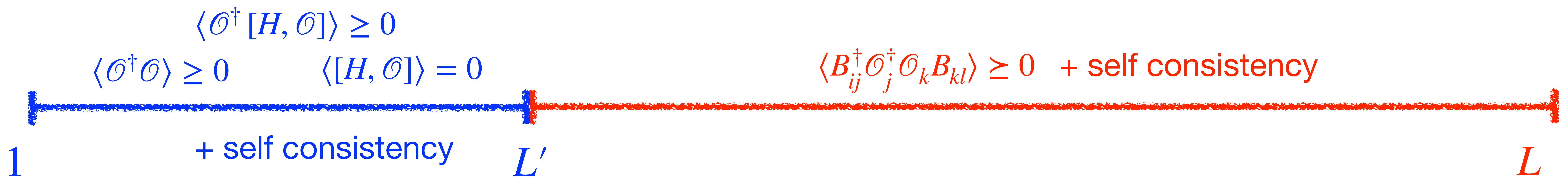
+

MPS relaxation $\langle B_{ij}^\dagger \mathcal{O}_j^\dagger \mathcal{O}_k B_{kl} \rangle \succeq 0$

[Kull, Schuch, Dive, Navascués 2212.03014]

Expensive, restrict to range L'

Cheap, go to range L that is very large



Bounding Many-body Ground State

Our setup: optimize ground state bound using MPS

- Full semidefinite problem

minimize: $\langle \mathcal{O}_b \rangle = \mathrm{Tr}(E^{ij}\mathcal{O}_b)\alpha_{ij}^{(L')}$

over: $\alpha_{ij}^{(r)},\ r = 1,2,\cdots,L',\cdots L$

with constraints:

$$\rho_r \succeq 0,\ \rho_r = \alpha_{ij}^{(r)}E^{ij},\ \text{for } r \leq L_1$$
$$\mathrm{Tr}_1\rho_r = \mathrm{Tr}_r\rho_r = \rho_{r-1},\ \mathrm{Tr}\rho_1 = 1$$
$$\omega_r \succeq 0,\ \omega_r = \alpha_{ij}^{(r)}E^{ij},\ \text{for } r \geq L' + 1$$
$$\mathrm{Tr}_1\omega_r = B \circ \omega_{r-1},\ \mathrm{Tr}_r\omega_r = \omega_{L'} \circ B$$
$$\mathrm{Tr}_1\omega_{L'+1} = B \circ \rho_{L'},\ \mathrm{Tr}_{L'+1}\omega_{L'+1} = \rho_{L'} \circ B$$

MPS ansatz, inspired by [Kull, Schuch, Dive, Navascués 2212.03014]

isolate ground state: $M \succeq 0,\ M_{ij} = \mathrm{Tr}(E^{rs}\mathcal{O}_i^\dagger[H,\mathcal{O}_j])\alpha_{rs}^{(L')}$

equations of motion: $\langle [H,\mathcal{O}_k] \rangle = \mathrm{Tr}(E^{rs}[H,\mathcal{O}_k])\alpha_{rs}^{(L')} = 0,\ \forall k\ .$

Moment matrix problem, with constraint that isolates the ground state, inspired by [Fawzi, Fawzi, Scalet, 2311.18706]

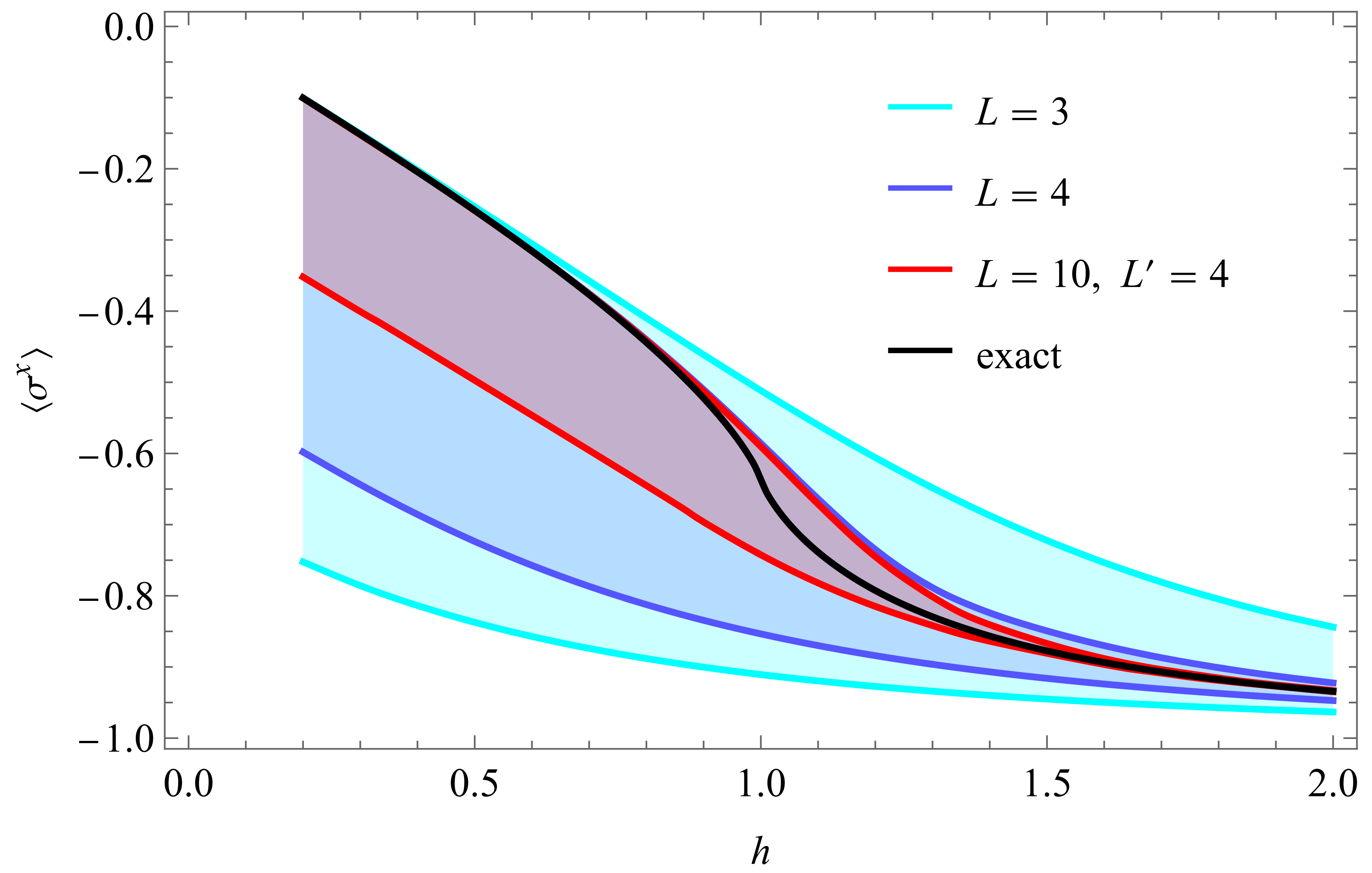
Bounding Many-body Ground State

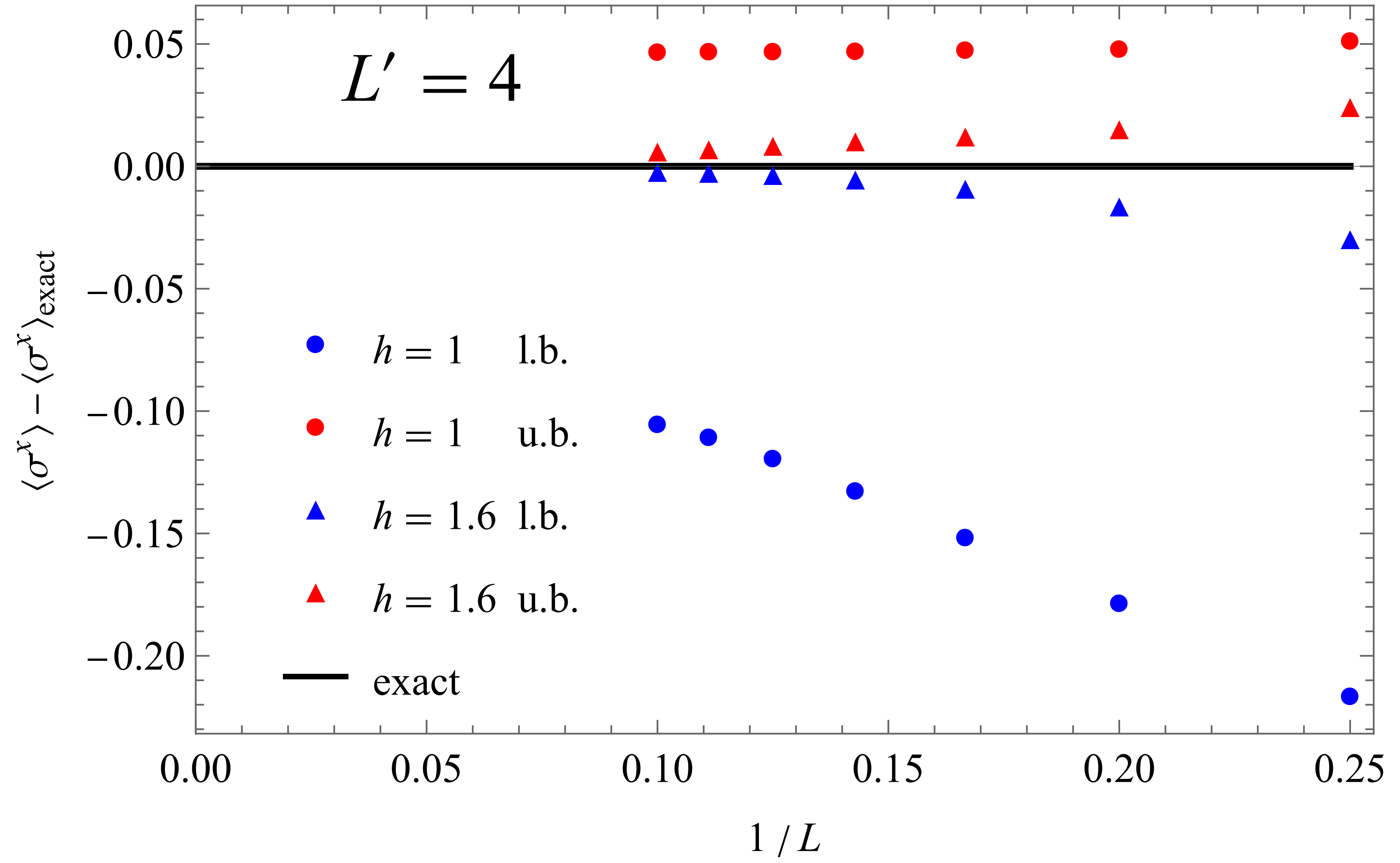
Numerical experiments

- Ongoing work. First result of $\langle \sigma^x \rangle$ upper and lower bound up to $L = 10$.
  (Note the system itself is infinite)

- Full positive matrix would be $4^{10} \times 4^{10} = 1048576 \times 1048576$. MPS relaxation drastically reduces it to 100~1000.

- Away from criticality result seems to be converging well, while at criticality $(h = 1)$ it seems to require more equations of motion beyond L'.





Bounding Gap of Many-body Systems

Bounding Gap of Many-body Systems

Bootstrapping spectral decomposition

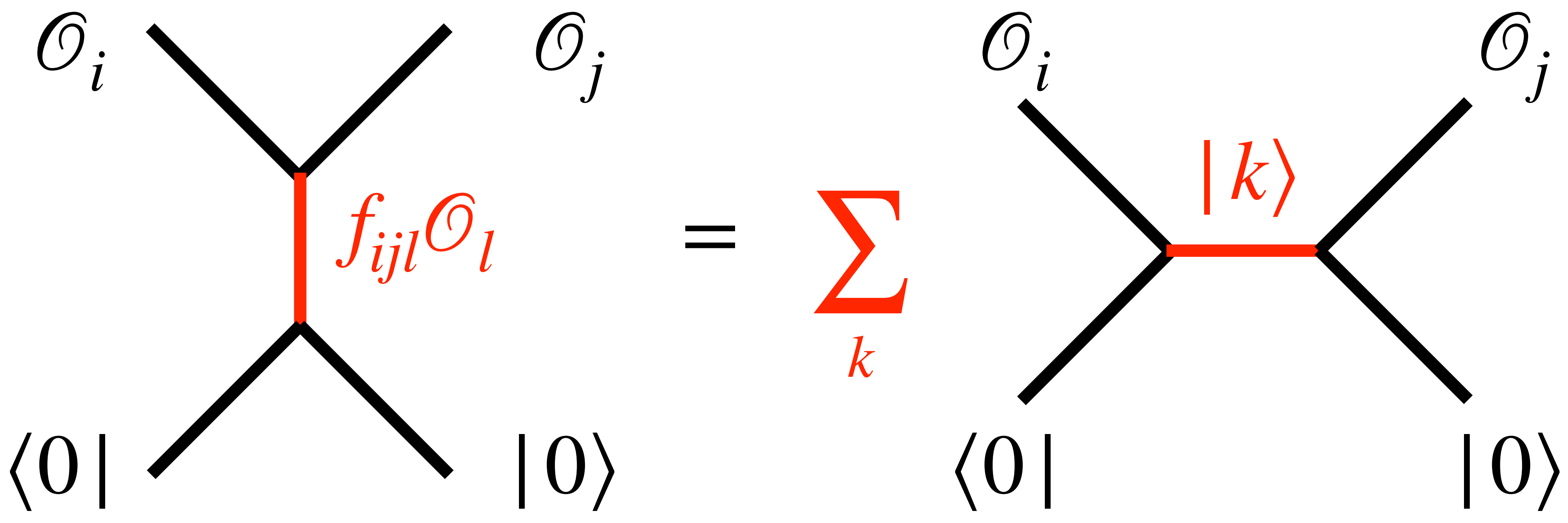
- Beyond the ground state observables, we are interested in gaps, correlators and excited state observables.
- For this purpose, we extend the moment matrix problem by inserting a complete basis of eigenstates:
- $$\langle 0|\mathcal{O}_i\mathcal{O}_j|0\rangle = \sum_k \langle 0|\mathcal{O}_i|k\rangle\langle k|\mathcal{O}_j|0\rangle$$
- The r.h.s. form a positive semidefinite matrix. If spectrum has a gap then sum over k starts from E_{gap} after E_0 itself. Positivity can be used to exclude such assumptions.
- $\langle \mathcal{O}^\dagger [H, \mathcal{O}]\rangle \geq 0$ can be taken as a relaxation from the above bootstrap equation.

Bounding Gap of Many-body Systems

Analogy to the conformal bootstrap

- The setup closely mirrors the conformal bootstrap. Many of the techniques in the conformal bootstrap can be directly applied here.

"Crossing equation":



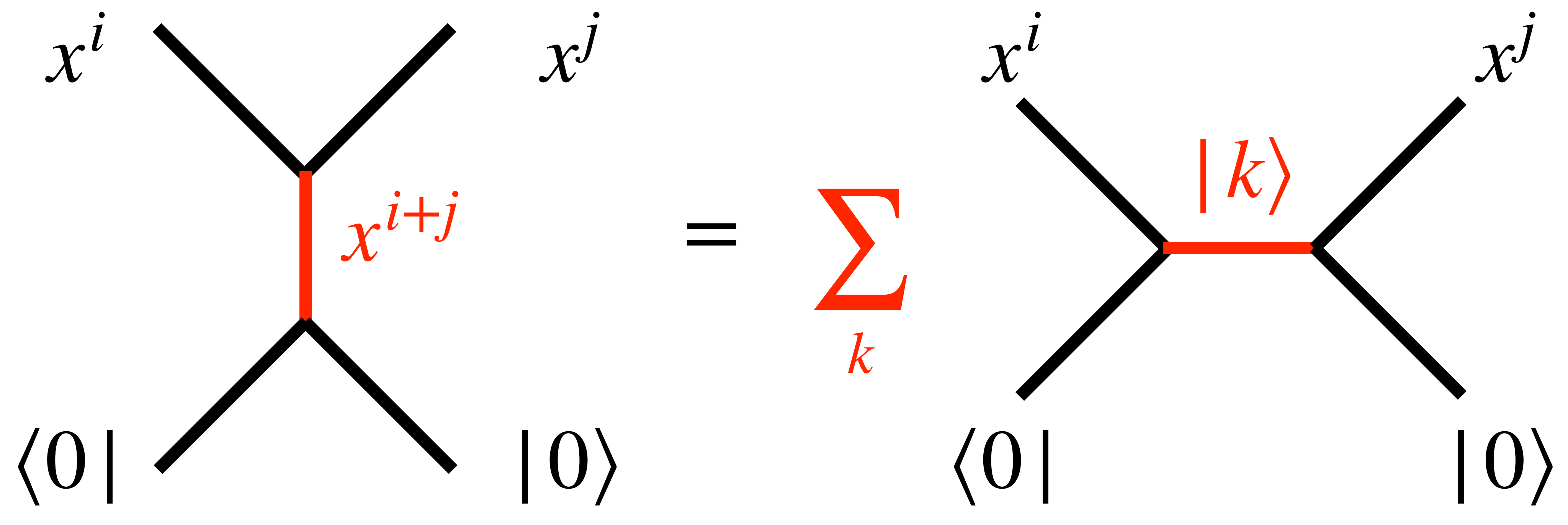
"OPE coefficients": $\langle k|\mathcal{O}_j|0\rangle$

$$\langle 0|\mathcal{O}_i\mathcal{O}_j|0\rangle = \sum_k \langle 0|\mathcal{O}_i|k\rangle\langle k|\mathcal{O}_j|0\rangle$$

Bounding Gap of Many-body Systems

Anharmonic operator revisited

- Revisit the moment problem of anharmonic oscillator using the new method:



$$\langle 0|x^{i+j}|0\rangle = \sum_k \langle 0|x^i|k\rangle\langle k|x^j|0\rangle$$

for $0 \leqslant i,j \leqslant K$

- Using equations of motion to reduce the unknowns

$$\begin{cases} \langle n|\left[H,\mathcal{O}\right]|m\rangle = (E_n - E_m)\langle n|\mathcal{O}|m\rangle \\ \langle n|H\,\mathcal{O}|m\rangle = E_n\langle n|\mathcal{O}|m\rangle \end{cases}$$

For diagonal matrix elements we had recursion relation

$$4tE\langle x^{t-1}\rangle - t(t-1)\langle x^{t+1}\rangle - 4\lambda(t+2)\langle x^{t+3}\rangle = 0$$

Bounding Gap of Many-body Systems

Anharmonic operator revisited

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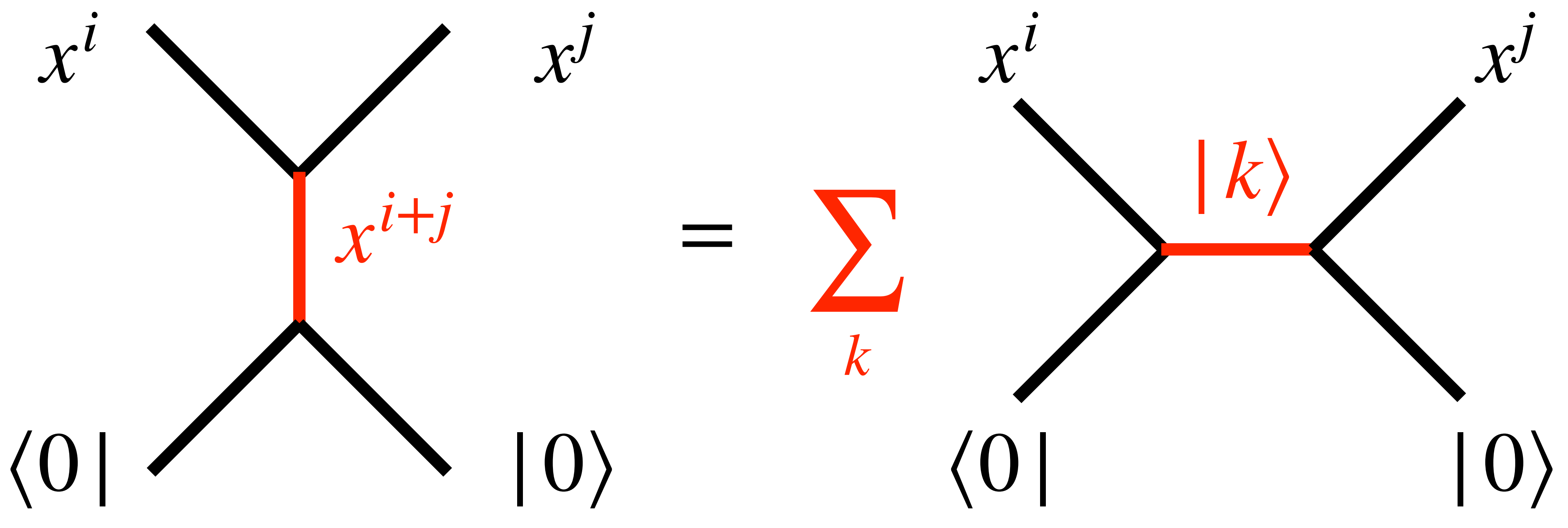


$$\langle 0|x^{i+j}|0\rangle = \sum_k \langle 0|x^i|k\rangle\langle k|x^j|0\rangle$$

for $0 \leqslant i,j \leqslant K$

- Using equations of motion to reduce the unknowns

For off-diagonal elements, we have similar relation

$$\langle n|x^i|m\rangle = g^i_I(E_n, E_m)\ \delta_{nm} + g^i_x(E_n, E_m)\ c_{nm,x} + g^i_{x^2}(E_n, E_m)\ c_{nm,x^2}$$

$$0 = \sum_k (c_{0k})^2\ \overrightarrow{F}^{E_0}_{E_k,P,\dots}$$

unknowns: $(c_{0k})^2$

$g^i_{\mathcal{O}}(E_n, E_m)$: $\overrightarrow{F}$

Bounding Gap of Many-body Systems

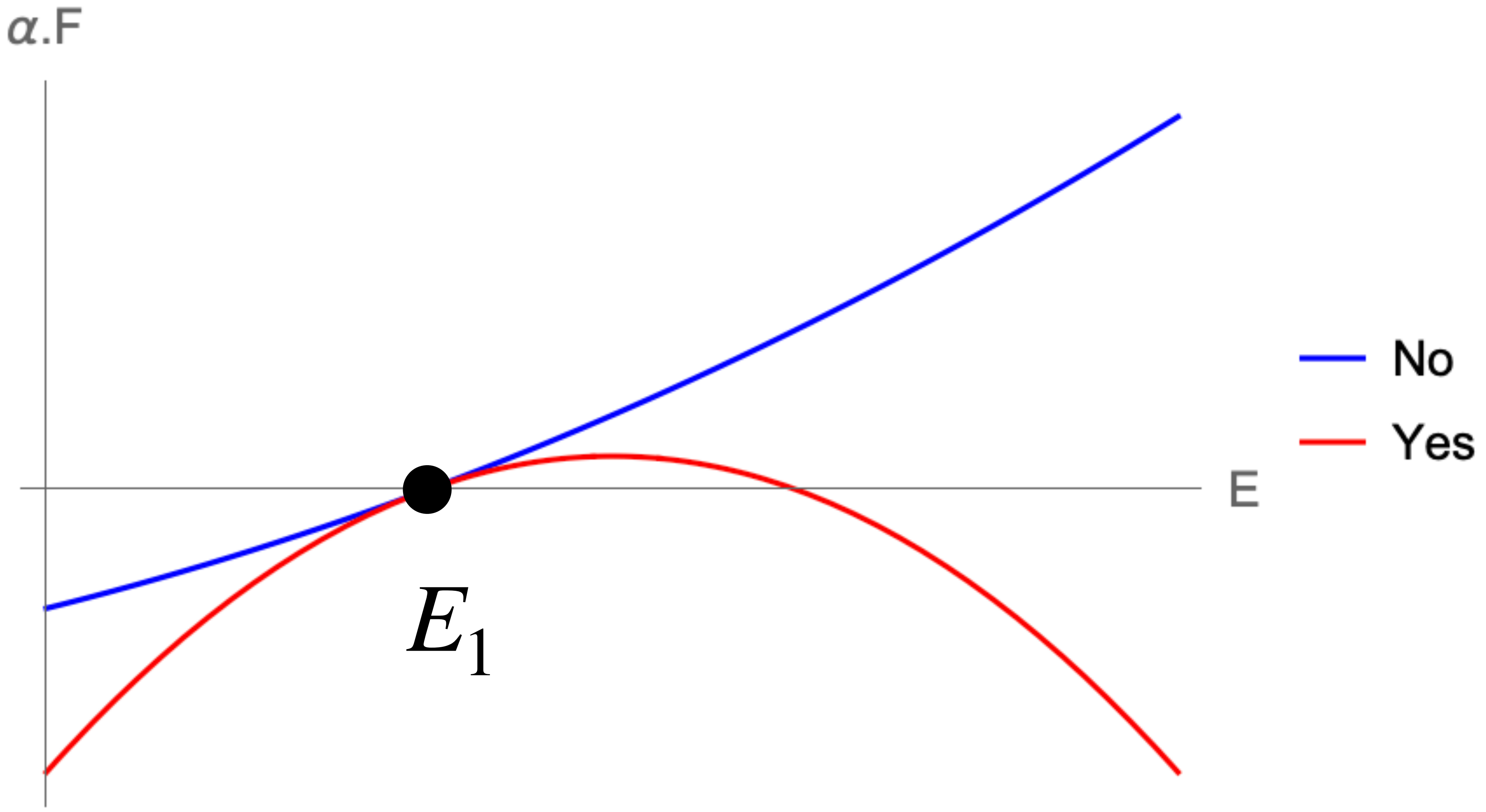
Anharmonic operator revisited

$$0 = \sum_k (c_{0k})^2 \; \vec{F}^{E_0}_{E_k, P, \cdots}$$

unknowns $\quad g^{i}_{\mathcal{O}}(E_n, E_m)$

$$0 = (1 \;\; c_{00,x^2})\left(\vec{\mathcal{S}}_0 - \vec{\mathcal{T}}_0\right)\begin{pmatrix} 1 \\ c_{00,x^2} \end{pmatrix} + \sum_{k_-} c^2_{0k_-,x}\vec{\mathcal{S}}_{k_-} + \sum_{k_+} c^2_{0k_+,x^2}\vec{\mathcal{S}}_{k_+} \,.$$

Schematically: find $\vec{\alpha}$ such that $\alpha \, . \, F \geq 0$



If there exists α_{ij} such that $\forall E_{k_\pm} \geqslant E_1$

$$\sum_{i,j \leqslant K} \alpha_{i,j} (1 \;\; c_{00,x^2})\left(\vec{\mathcal{S}}_0 - \vec{\mathcal{T}}_0\right)_{ij} \begin{pmatrix} 1 \\ c_{00,x^2} \end{pmatrix} = 1$$

$$\sum_{i,j \leqslant K} \alpha_{i,j} \left(\vec{\mathcal{S}}_{k_-}\right)_{ij} \geqslant 0$$

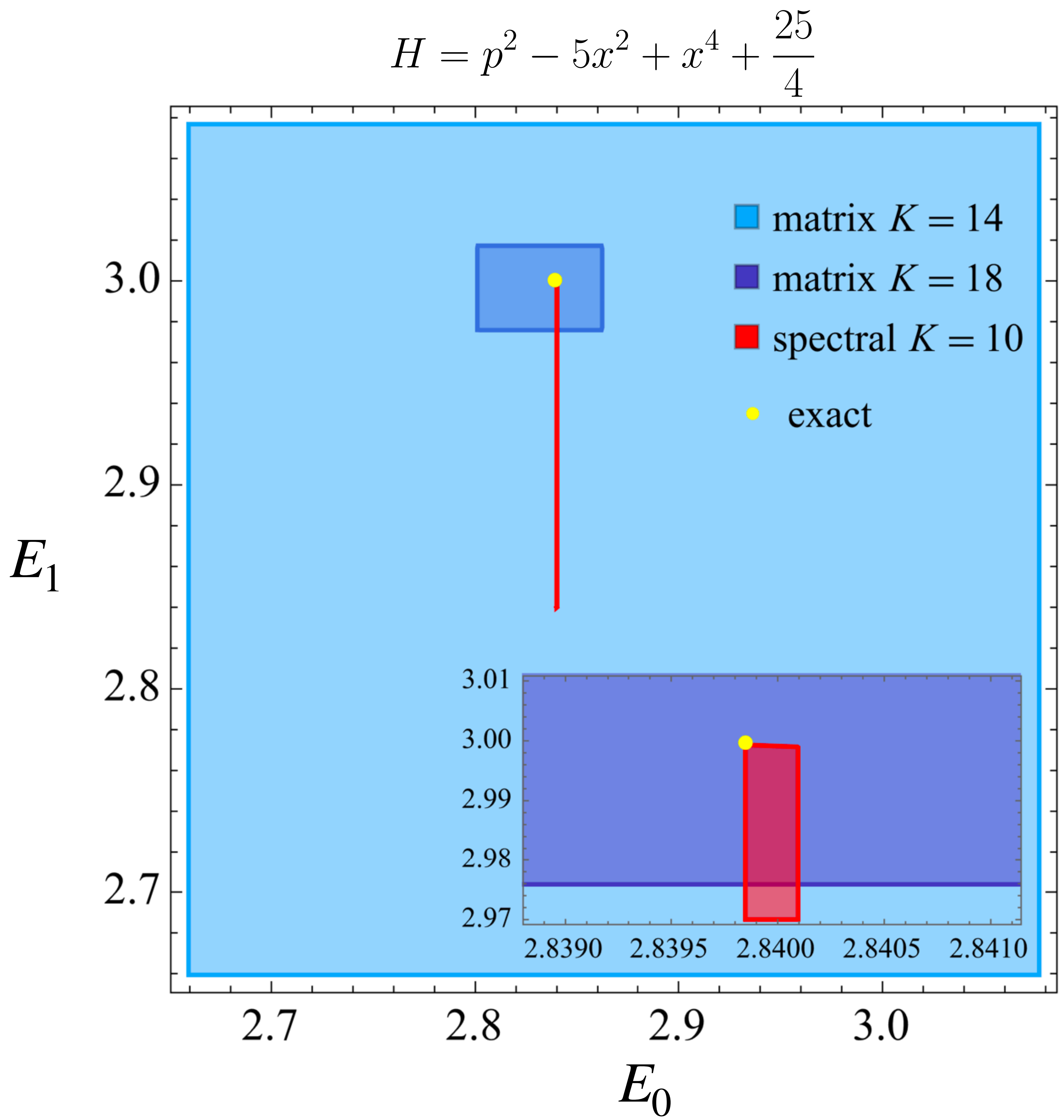
$$\sum_{i,j \leqslant K} \alpha_{i,j} \left(\vec{\mathcal{S}}_{k_+}\right)_{ij} \geqslant 0\,,$$

then all spectra with the prescribed (E_0, E_1) and c_{00,x^2} are ruled out.

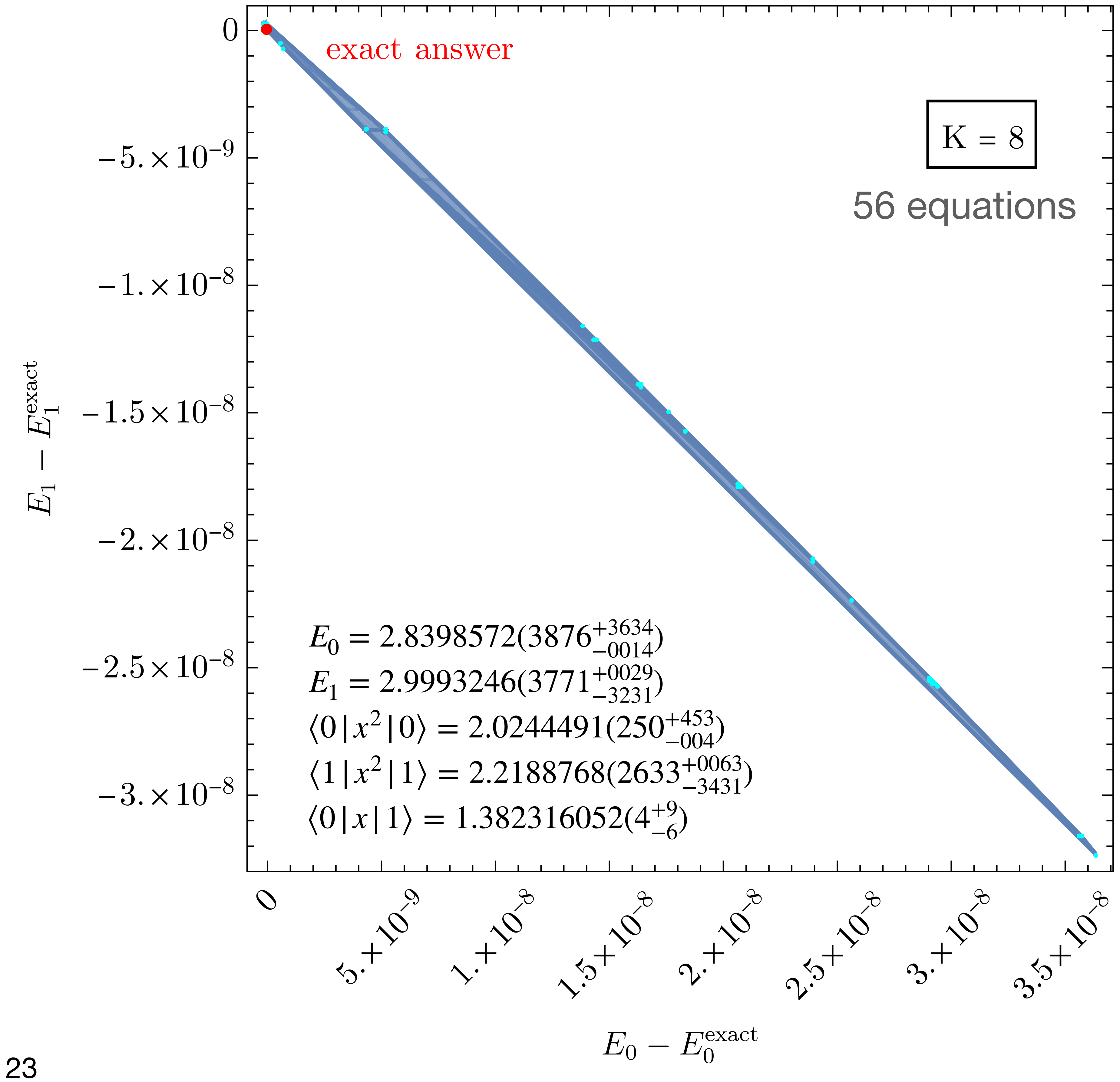
Bounding Gap of Many-body Systems

Anharmonic operator revisited

- Found upper bound on the gap E_1



- Much better results from mixed bootstrap study: $\langle 0 | x^{i+j} | 1 \rangle$

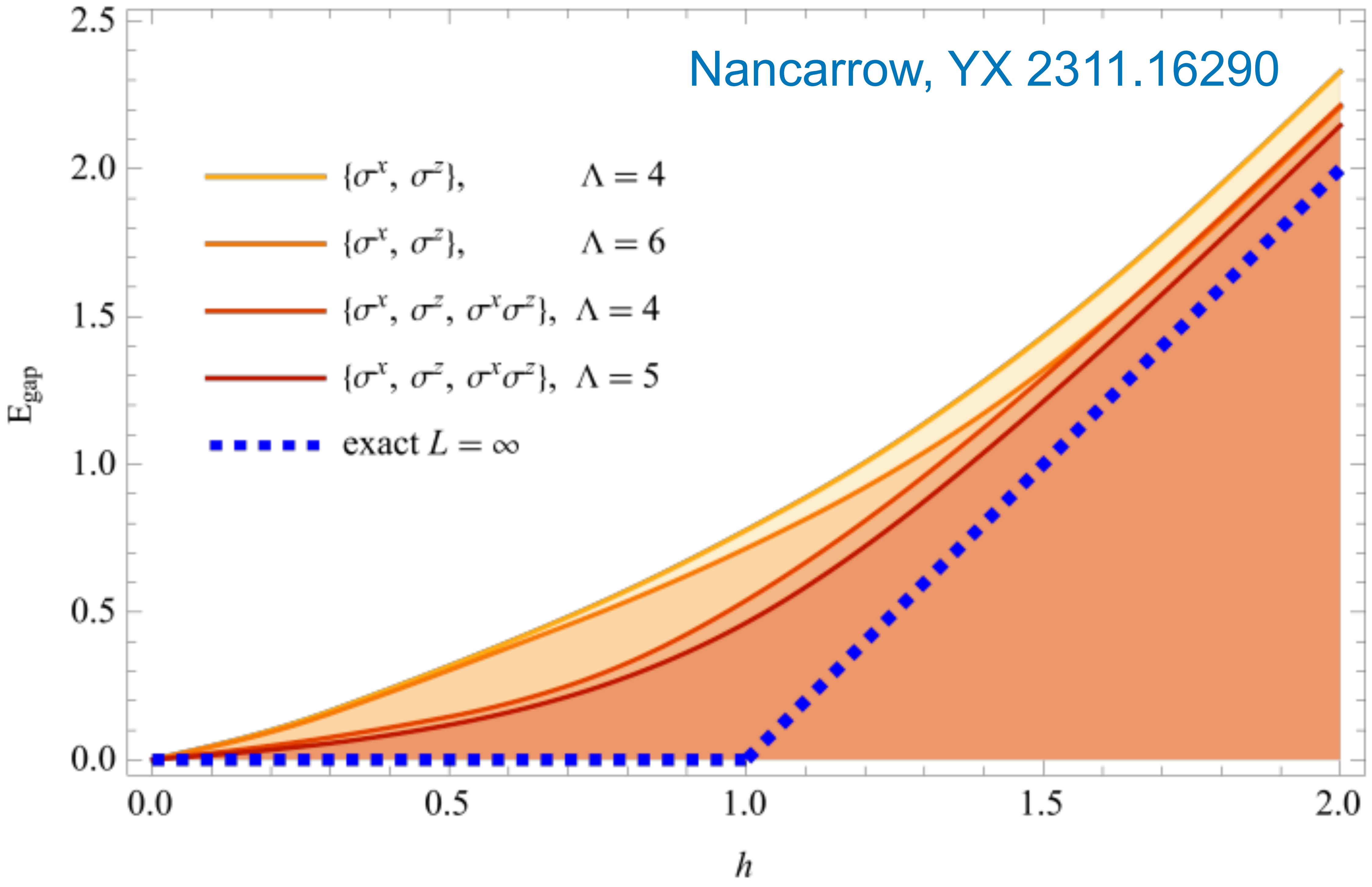


Bounding Gap of Many-body Systems

The gap of infinite chain

- For (1+1)D transverse field Ising Model, we obtain a rigorous upper bound on the gap

$$H = \sum_i \sigma_i^z \sigma_{i+1}^z + h\sigma_i^x$$



- Operator basis is:
  - "Primary operators" σ_1^x , σ_1^z and $\sigma_1^x\sigma_2^z$
  - All "descendants" by acting $[H, \cdot\,]$ on primary operators up to Λ times.
- $E_{gap} := E_1 - E_0$

Conclusion & Outlook

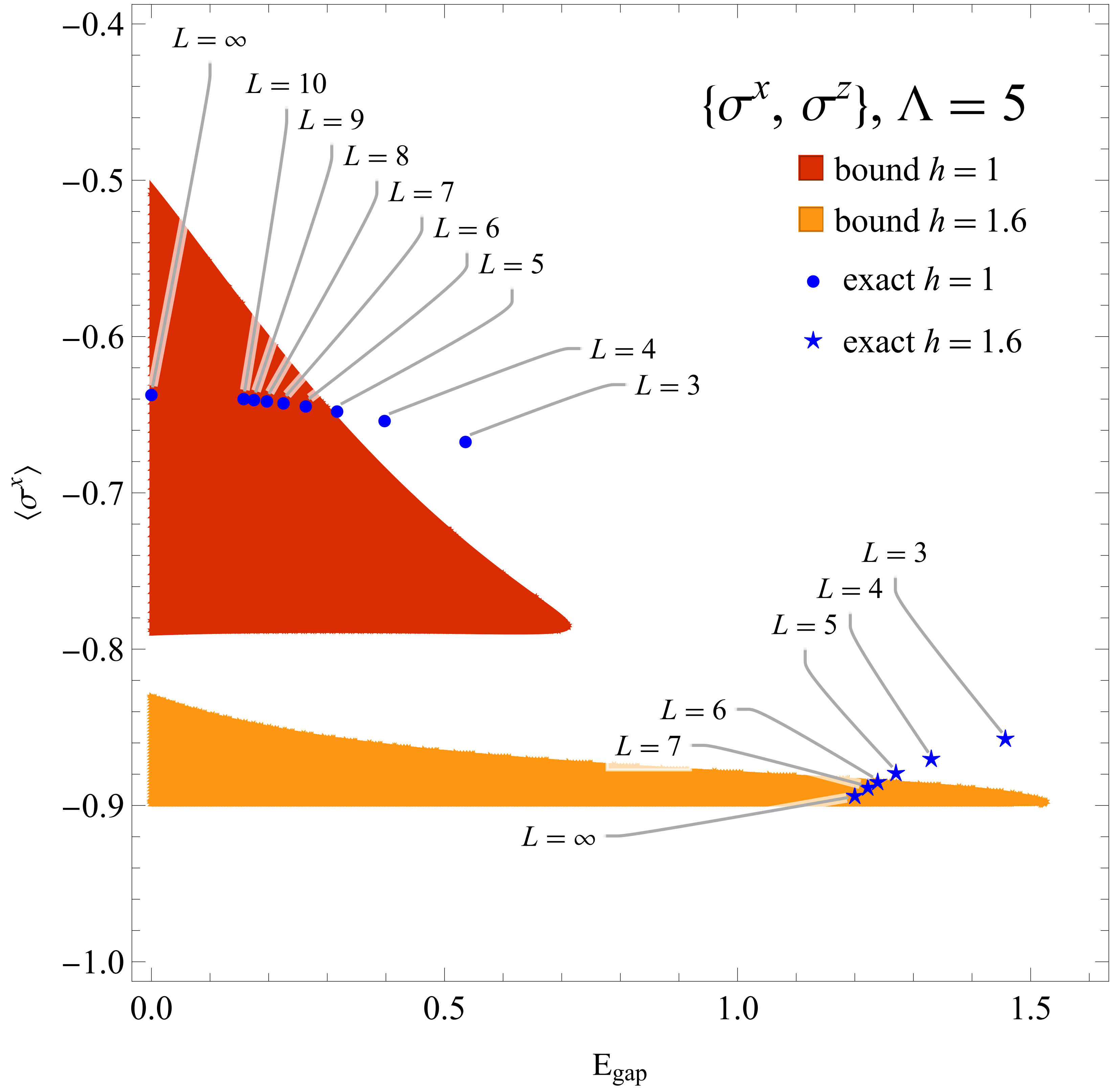
- Bootstrap is a useful tool to study Quantum Mechanics with infinite degrees of freedom.
- We have working setups to bound the ground state energy, ground state expectation value, gap and excited state expectation values.
- A relaxation based on variational methods can drastically reduce the cost.
- We are still working on a more general setup that combines bootstrap with variational methods, especially, one that preserves equations of motion.
- It would be interesting to generalize the new techniques to matrix quantum mechanics.

Thank You

Numerical Results of Infinite Spin Chain

Nancarrow, YX '22

- bounds on the correlators.



$$H = \sum_i \sigma_i^z \sigma_{i+1}^z + h\sigma_i^x$$

- Primary operators: σ_1^x , σ_1^z and $\sigma_1^x \sigma_2^z$
- Λ: Depth of $[H, \cdots]$
- $E_{\text{gap}} := E_1 - E_0$
- $h_{\text{crit}} = 1$
- Dots are finite volume exact diagonalization with lattice period L