Bootstrapping Quantum Mechanics

KEK Theory workshop
2025/12/16

Takeshi Morita (Shizuoka Univ.)

Refs.

2109.08033 (PLB 2022) , 2109.02701 (PRD 2022)

with Yu Aikawa (Shizuoka univ.), Kota Yoshimura (Notre Dame univ., USA)

2208.09370 (PTEP 2023) TM

2504.08586 (PTEP 2025) with Yu Aikawa (Shizuoka univ.)

Introduction:

What is the best numerical method for solving the eigenvalue problem in one-dimensional single-particle QM?

$$H = \frac{1}{2}p^2 + \frac{1}{2}x^2 + \frac{1}{4}x^4 \quad \rightarrow \quad E_n?$$

Numerically solving PDE by discretizing the space?

Variational method?

etc.

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One candidate is Bootstrap method. Han-Hartnoll-Kruthoff PRL 2020

- ✓ Error bar is ``exact”.
- ✓ Exact solutions can be obtained in solvable models.

Plan of This Talk

What is the best numerical method for solving the eigenvalue problem in one-dimensional single-particle QM?

$$H = \frac{1}{2}p^2 + \frac{1}{2}x^2 + \frac{1}{4}x^4 \quad \rightarrow \quad E_n ?$$

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- ✓ Error bar is ``exact".
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Sec.2 Review of the bootstrap method in QM

2. Review of the bootstrap method in QM

Han-Hartnoll-Kruthoff (PRL 2020)

Basic Idea: Two constraints on expectation values.

Uncertainty Relation

$$\langle \Delta x^2 \rangle \langle \Delta p^2 \rangle \geq \frac{\hbar^2}{4}$$

→ The expectation values of operators cannot take arbitrary values in QM.

Extension

$$\langle x^m \rangle, \langle p^n \rangle, \langle p^k x^l \rangle, \cdots$$

→ These quantities are also bounded.

Energy Eigenstate Relations

$$^{\forall}|\quad\rangle \to |E\rangle \quad \begin{cases} \langle HO \rangle = E\langle O \rangle \\ \langle OH \rangle = E\langle O \rangle \end{cases}$$

example) $\begin{cases} H = \frac{1}{2}p^2 + \frac{1}{2}x^2 + \frac{1}{4}x^4 \\ O = x^2 \end{cases}$

$$\rightarrow \langle HO \rangle = \langle p^2 x^2 \rangle / 2 + \langle x^4 \rangle / 2 + \langle x^6 \rangle / 4$$
$$= E\langle x^2 \rangle$$

2. Review of the bootstrap method in QM

Han-Hartnoll-Kruthoff (PRL 2020)

Basic Idea: Two con

Possible values of $E, \langle x \rangle, \langle x^2 \rangle, \langle p \rangle, \cdots$
are HIGHLY restricted.

Uncertainty Relation

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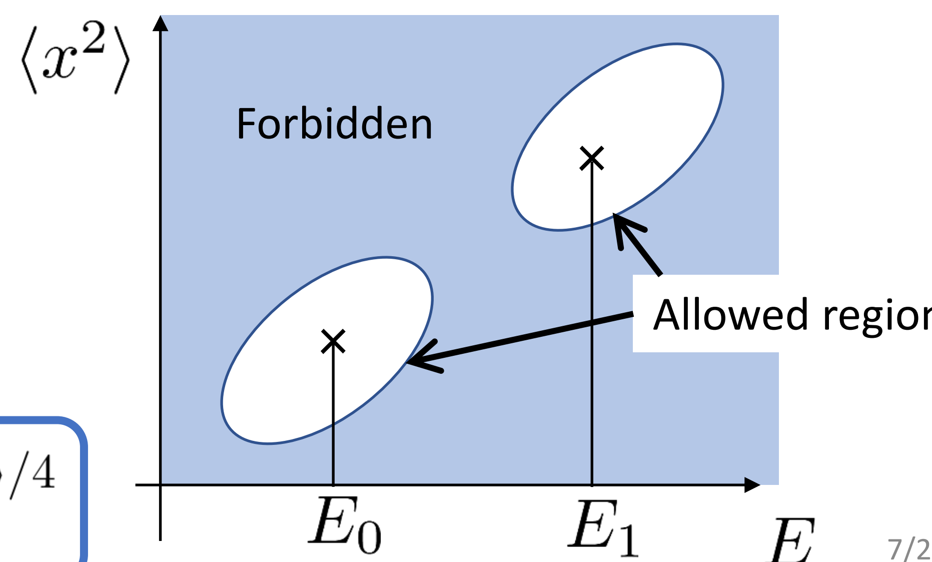

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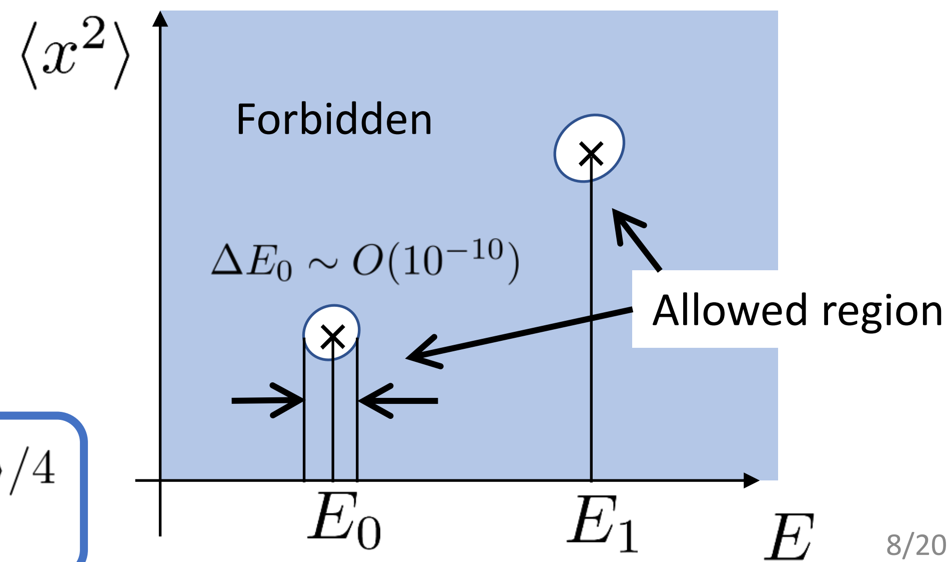

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Uncertainty Relation

$$\langle \Delta x^2 \rangle \langle \Delta p^2 \rangle \geq \frac{\hbar^2}{4}$$

Q1. How to obtain the bounds?

(Extension of the uncertainty relation)

…not take arbitrary values in QM.

Extension

$$\langle x^m \rangle, \langle p^n \rangle, \langle p^k x^l \rangle, \cdots$$

→ These quantities are also bounded.

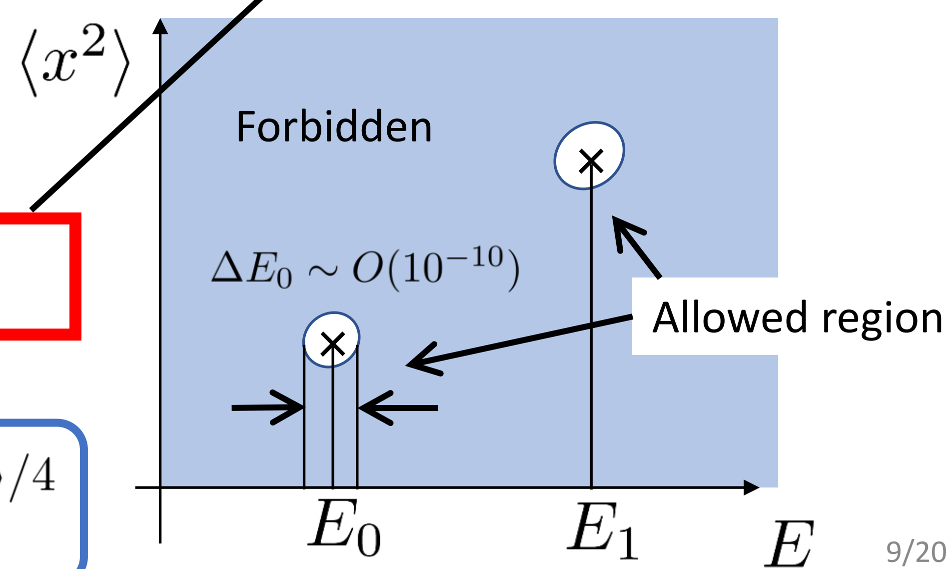
Energy Eigenstate Relations

$$^\forall | \ \ \rangle \to |E\rangle \quad \begin{cases} \langle HO \rangle = E \langle O \rangle \\ \langle OH \rangle = E \langle O \rangle \end{cases}$$

Q2. How to solve these constraints.

$O = x^2$

$$\to \langle HO \rangle = \langle p^2 x^2 \rangle /2 + \langle x^4 \rangle /2 + \langle x^6 \rangle /4$$
$$= E \langle x^2 \rangle$$



2.1 Extension of the Uncertainty Relation

Han-Hartnoll-Kruthoff (PRL 2020)
TM (PTEP 2023)

QM satisfies the following positivity: [Example: 1-dim single-particle QM]

O : Operators ex) $O = x^m p^n$

$\langle O^\dagger O \rangle = \left| O \rangle \right|^2 \geq 0$ is satisfied for $^\forall O,\ ^\forall | \ \rangle$, and we obtain the following relation:

$$\tilde{O} = \sum_{i=1}^{K} c_i O_i$$

- $\{O_i\}$: a set of K operators $(i = 1, \cdots, K)$
- $\{c_i\}$: constants
- K : an integer

ex) $\{O_i\} = \underbrace{\{x, p, xp, \cdots\}}_{K}$

$\Rightarrow 0 \leq \langle \tilde{O}^\dagger \tilde{O} \rangle = \vec{c}^{\,\dagger} M \vec{c}$ is satisfied for any $\{c_i\}$.

$$\vec{c}^{\,T} = (c_1, c_2, \cdots, c_K)$$

$$M := \begin{pmatrix} \ddots & \vdots & \\ \cdots & \langle O_i^\dagger O_j \rangle & \cdots \\ & \vdots & \end{pmatrix}$$

$K \times K$ hermite matrix

→All the eigenvalues of *M* are non-negative.

→ Called "positive-semidefinite matrix" and denoted by $M \succeq 0$.

$\langle O_i^\dagger O_j \rangle$ is highly constrained!

$M \succeq 0$ can be regarded as an extension of the uncertainty relation.

$$\langle \Delta x^2 \rangle \langle \Delta p^2 \rangle \geq \frac{\hbar^2}{4}$$

2.1 Extension of the Uncertainty Relation

Han-Hartnoll-Kruthoff (PRL 2020)
TM (PTEP 2023)

$$M := \begin{pmatrix} \ddots & \vdots & \\ \cdots & \langle O_i^\dagger O_j \rangle & \cdots \\ & \vdots & \end{pmatrix} \quad M \succeq 0$$

→ Extension of the uncertainty relation.

Why? $\tilde{O} = c_0 1 + c_1 x + c_2 p$

($\{O_i\} = \{1, x, p\}$)

Curtright-Zachos (2001)

$$M = \begin{pmatrix} 1 & \langle x \rangle & \langle p \rangle \\ \langle x \rangle & \langle x^2 \rangle & \langle xp \rangle \\ \langle p \rangle & \langle px \rangle & \langle p^2 \rangle \end{pmatrix} \xrightarrow{M \succeq 0}$$

The uncertainty relation

$$\langle \Delta x^2 \rangle \langle \Delta p^2 \rangle \geq \frac{\hbar^2}{4} \quad \text{for } ^\forall | \quad \rangle$$

→ Choosing $\tilde{O} = c_0 1 + c_1 x + c_2 p + c_3 x^2 + c_4 p^2 + \cdots$, $M \succeq 0$ provides constraints involving higher order expectation values $\langle x^m p^n \rangle$.

→ $M \succeq 0$ is an extension of the uncertainty relation.

Can we solve the condition $M \succeq 0$ and the following constraints?

$\langle HO \rangle = E \langle O \rangle$ $\qquad \langle HO \rangle = \langle p^2 x^2 \rangle /2 + \langle x^4 \rangle /2 + \langle x^6 \rangle /4 = E \langle x^2 \rangle$

2.1 Extension of the Uncertainty Relation

Han-Hartnoll-Kruthoff (PRL 2020)
TM (PTEP 2023)

Yes, such problems can be easily solved numerically as SemiDefinite Programming (SDP,半正定値計画問題).

$$M=\begin{pmatrix}1 & \langle x\rangle & \langle p\rangle & \cdots\\ \langle x\rangle & \langle x^2\rangle & \langle xp\rangle & \cdots\\ \langle p\rangle & \langle px\rangle & \langle p^2\rangle & \cdots\\ \vdots & \vdots & \vdots & \ddots\end{pmatrix}. \quad M\succeq 0$$

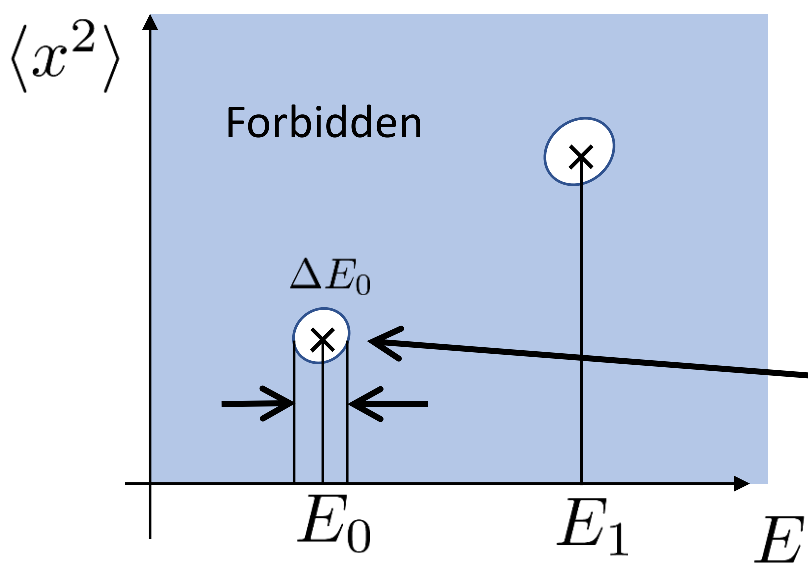
and

$$\begin{cases}\langle HO\rangle = E\langle O\rangle\\ \langle OH\rangle = E\langle O\rangle\end{cases}$$

$$\rightarrow \langle HO\rangle = \langle p^2x^2\rangle/2+\langle x^4\rangle/2+\langle x^6\rangle/4 = E\langle x^2\rangle$$

etc.

$$H=\frac{1}{2}p^2+\frac{1}{2}x^2+\frac{1}{4}x^4$$



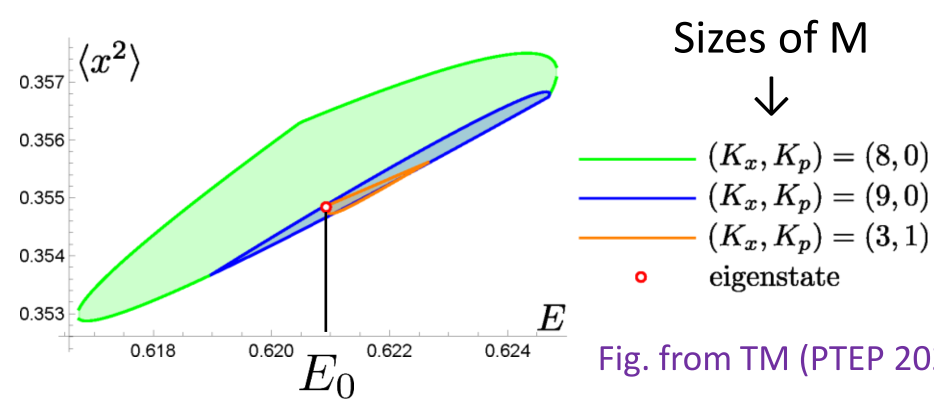


Fig. from TM (PTEP 2023)

2.1 Extension of the Uncertainty Relation

Han-Hartnoll-Kruthoff (PRL 2020)
TM (PTEP 2023)

Yes, such problems can

Programming (SDP,半正

- The size of M → A Cut off of bootstrap.
  A larger M provides better results.
  (But longer computation time.)
- Error bar is "Exact".
  E_n never takes the value in the forbidden region.

$$M = \begin{pmatrix} 1 & \langle x \rangle & \langle p \rangle & \cdots \\ \langle x \rangle & \langle x^2 \rangle & \langle xp \rangle & \cdots \\ \langle p \rangle & \langle px \rangle & \langle p^2 \rangle & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$$\rightarrow \langle HO \rangle = \langle p^2 x^2 \rangle /2 + \langle x^4 \rangle /2 + \langle x^6 \rangle /4$$
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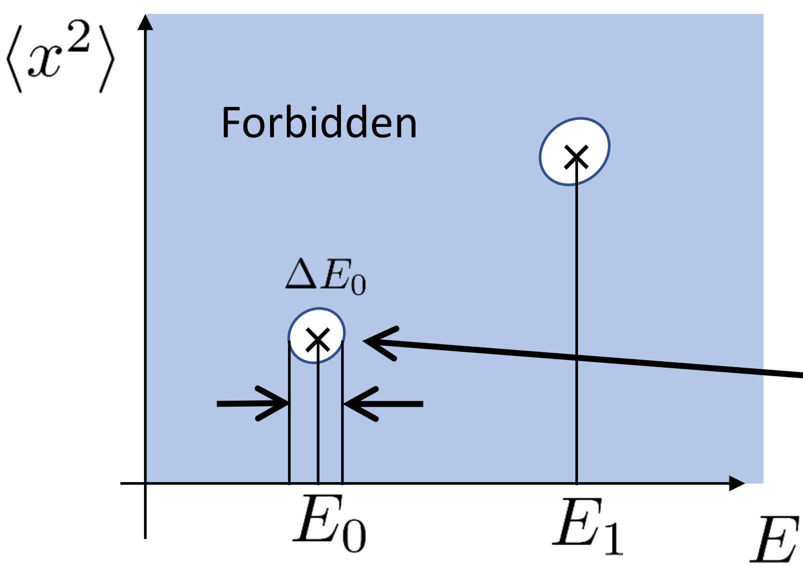
etc.



$$H = \frac{1}{2} p^2 + \frac{1}{2} x^2 + \frac{1}{4} x^4$$

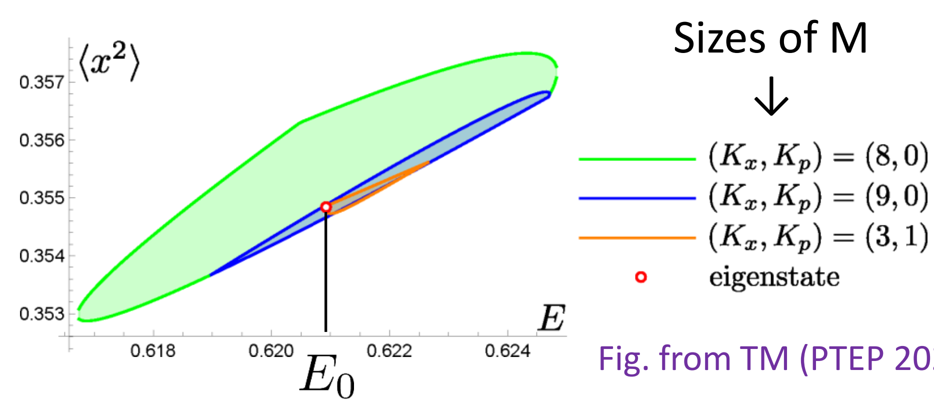


Fig. from TM (PTEP 2023)

Sec.3 Solvable models and the bootstrap method

3. Bootstrap → Exact results

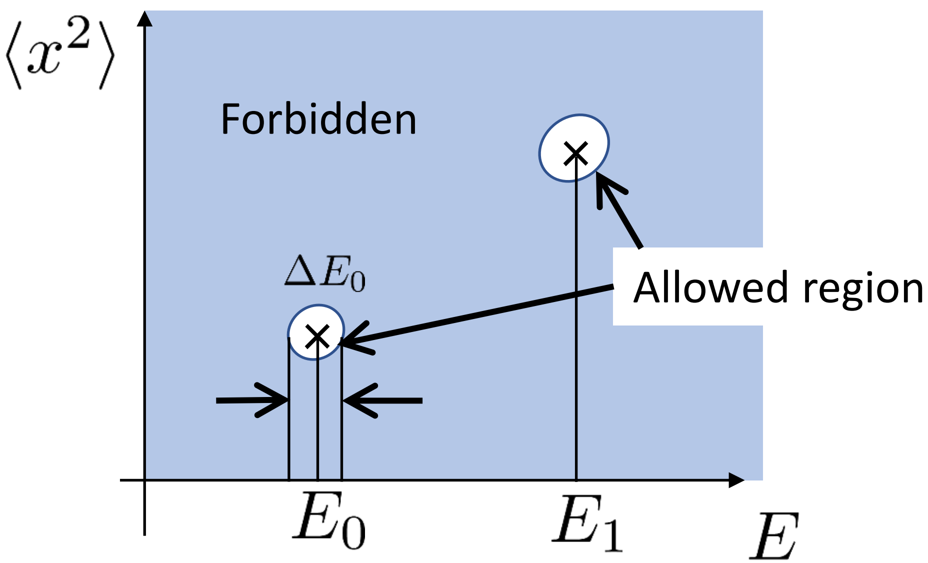
★What happens if we apply the bootstrap method to solvable systems?

$$M = \begin{pmatrix} 1 & \langle x \rangle & \langle p \rangle & \cdots \\ \langle x \rangle & \langle x^2 \rangle & \langle xp \rangle & \cdots \\ \langle p \rangle & \langle px \rangle & \langle p^2 \rangle & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \quad M \succeq 0$$

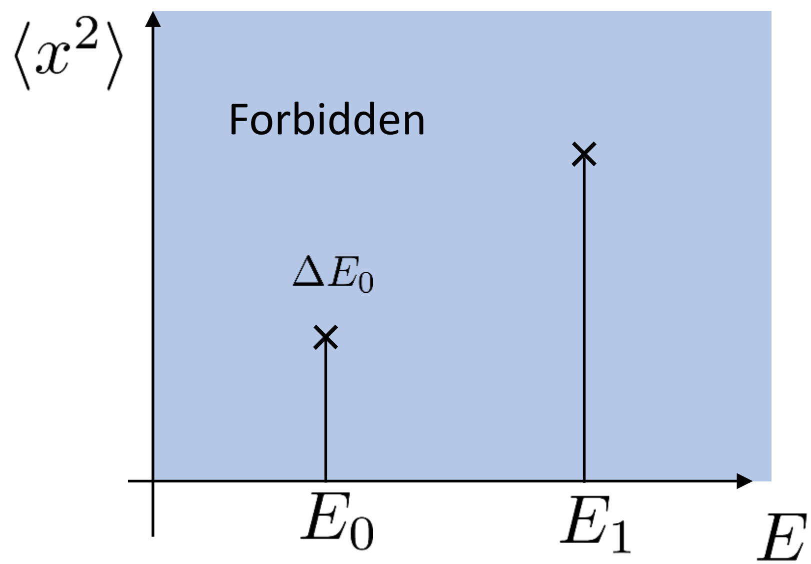
$$\begin{cases} \langle HO \rangle = E \langle O \rangle \\ \langle OH \rangle = E \langle O \rangle \end{cases} \qquad H = \frac{1}{2} p^2 + \frac{1}{2} x^2$$

Harmonic oscillator: Aikawa-TM-Yoshimura 2021
Pöschl–Teller potential: Sword-Vegh 2024

The allowed regions collapse to points!



Non-solvable system



Solvable systems
(at a finite size M)

3. Bootstrap → Exact results

★What happens if we apply the bootstrap method to solvable systems?

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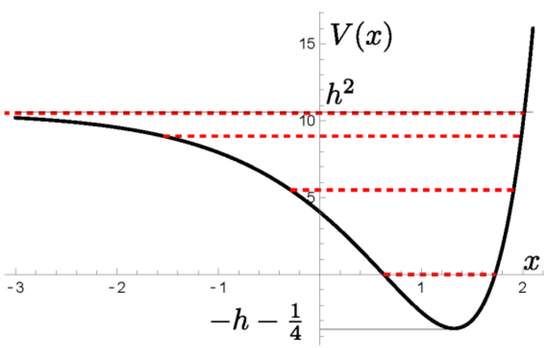
The allowed regions collapse to points!

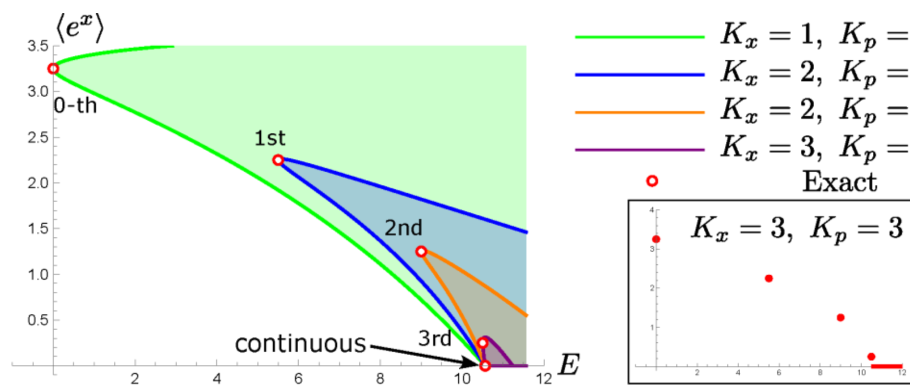
Ex) Morse potential

$$\mathcal{H} = p^2 + e^{2x} - (2h+1)e^x + h^2.$$



<u>Numerical bootstrap result</u>

$$\tilde{O} := \sum_{m=0}^{K_x} \sum_{n=0}^{K_p} c_{mn} e^{mx} p^n$$

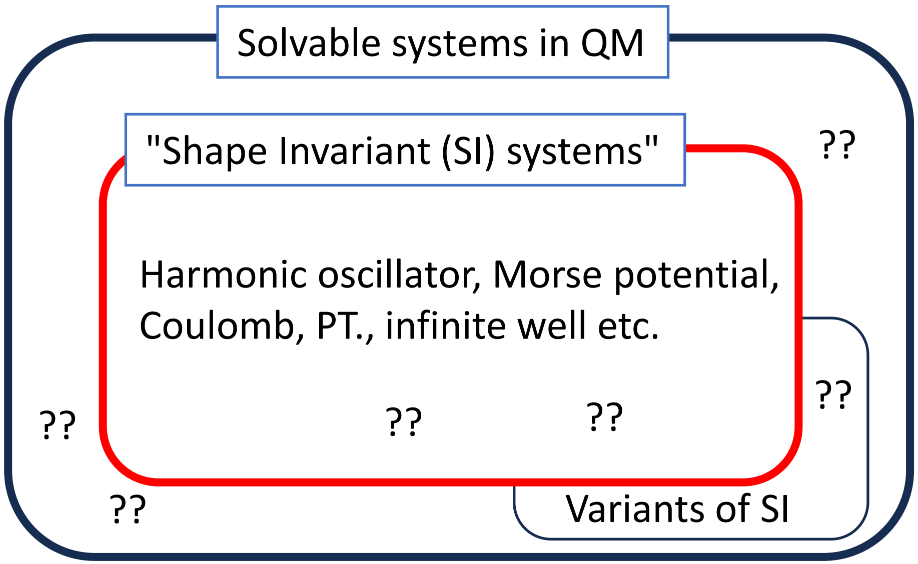


Aikawa-Morita (PTEP 2025)

3. Bootstrap → Exact results

Solvable models in QM

"Solvable"
= "Energy eigenvalues are obtained exactly."



Textbook by Sasaki-san

See also the PhD thesis of Nasuda-san
2403.20217

3. Bootstrap → Exact results

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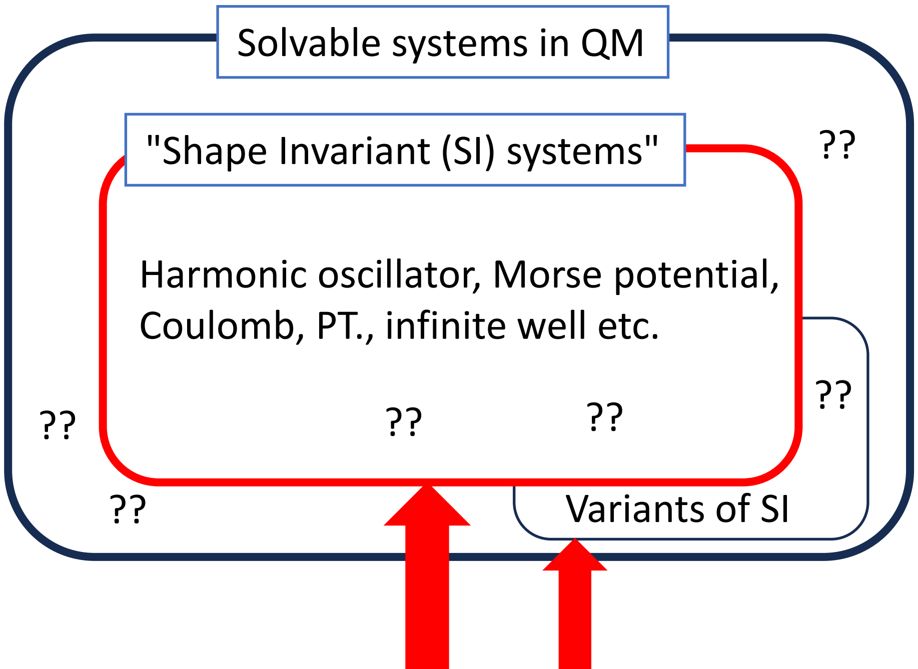

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Exact solutions are obtained by using the bootstrap method,
if the system satisfies the SI (or its variant).

→ Bootstrap method can be used as "<u>a detector</u>" of the solvable systems!

(I skip the proof today.)

Aikawa-Morita (PTEP 2025)

Summary

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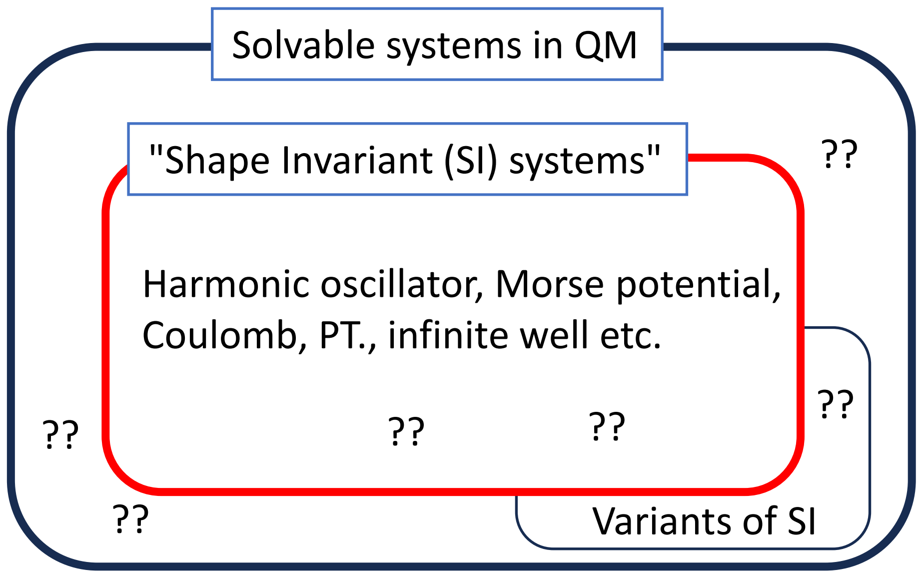
Bootstrap method

$$\langle \Delta x^2 \rangle \langle \Delta p^2 \rangle \geq \frac{\hbar^2}{4} \rightarrow M = \begin{pmatrix} 1 & \langle x \rangle & \langle p \rangle & \cdots \\ \langle x \rangle & \langle x^2 \rangle & \langle xp \rangle & \cdots \\ \langle p \rangle & \langle px \rangle & \langle p^2 \rangle & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \quad \begin{cases} \langle HO \rangle = E \langle O \rangle \\ \langle OH \rangle = E \langle O \rangle \end{cases}$$

$$M \succeq 0,$$

- Derivation of the spectrum through the extension of $\langle \Delta x^2 \rangle \langle \Delta p^2 \rangle \geq \frac{\hbar^2}{4}$.
- Error var is exact.
- Detector of the solvable systems.



Future Directions

- Other solvable systems?
- Many body systems.
- QFTs (Lattice gauge theories)
- gauge theories in the gauge/gravity correspondence

↑ Solvable?