Bounds on expectation values in Quantum mechanics

KEK Theory Workshop 2022
(Dec. 9 2022)

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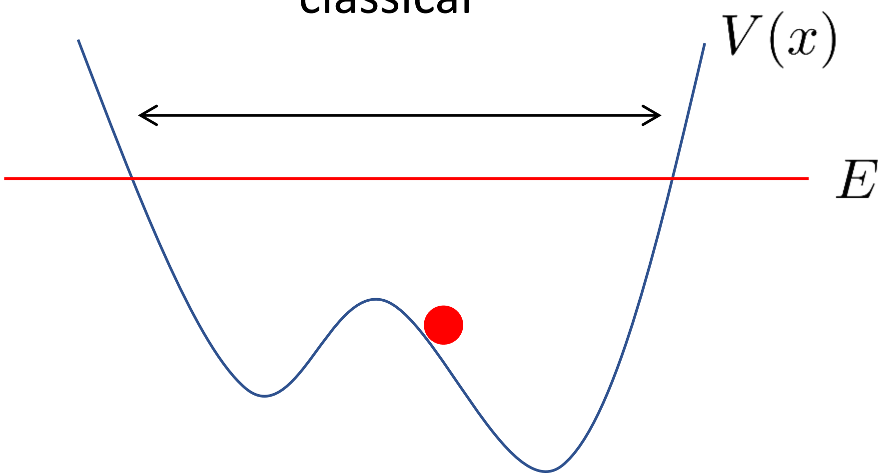
Ref.

2208.09370

TM

Introduction: 1dim non-relativistic system

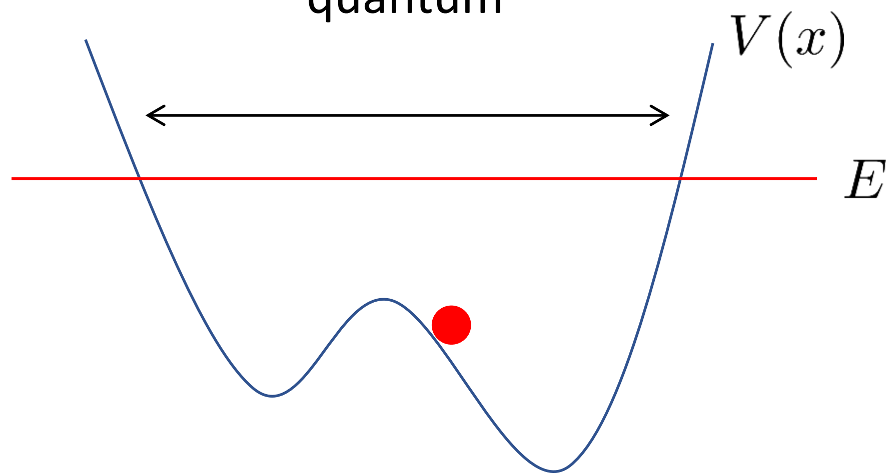
classical



Range of possible particle motion

→ Determined by Energy Conservation

quantum



Range of possible particle motion

→??

- (Correct but) Useless answer

$$-\infty \leq x \leq +\infty$$

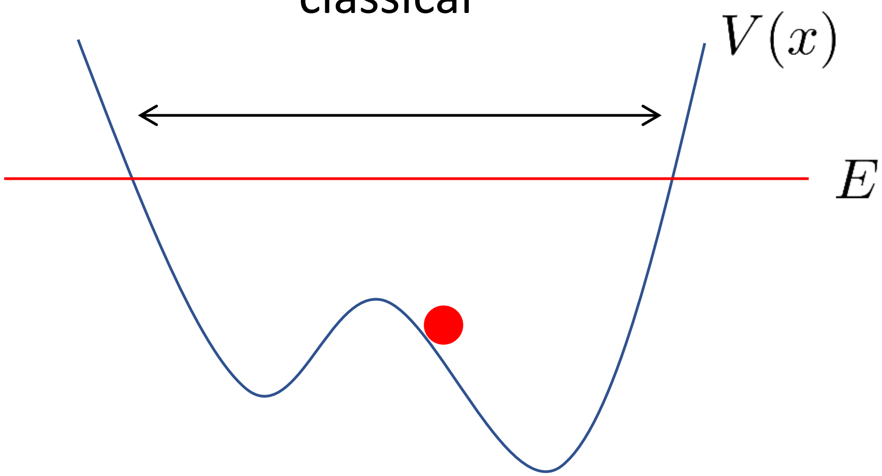
- Better answer

$$x_1 \leq \langle x \rangle \leq x_2, \qquad E = \langle H \rangle$$

Q. How to compute $x_1,\ x_2$?

Introduction: 1dim non-relativistic system

classical



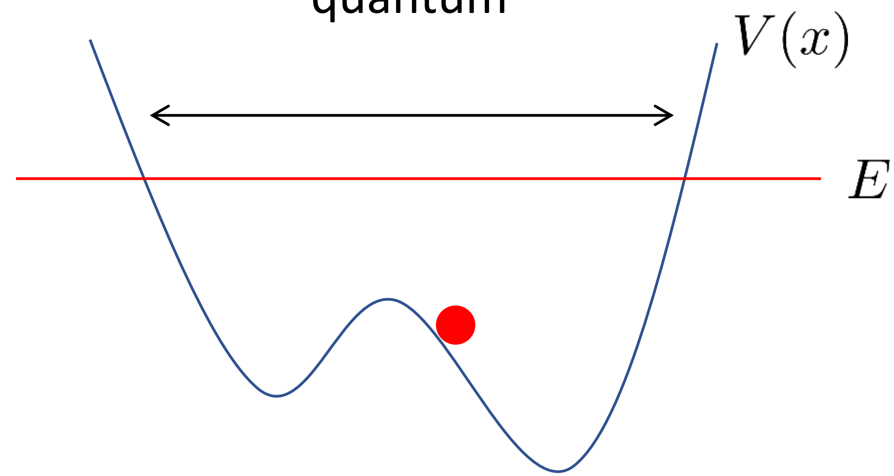
Range of possible particle motion

→ Determined by Energy Conservation

$x_1,\ x_2$ must depend on the particle state.
But universal bounds that are independent of states must exist.
→ We seek these universal bounds.

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

quantum



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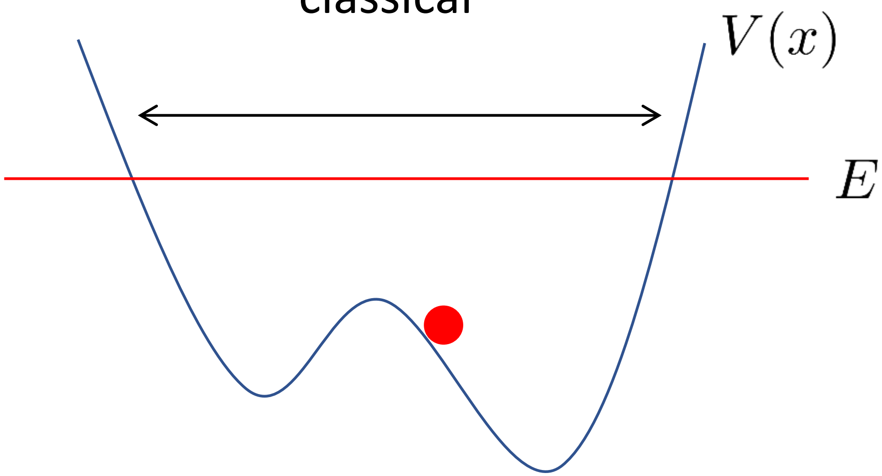

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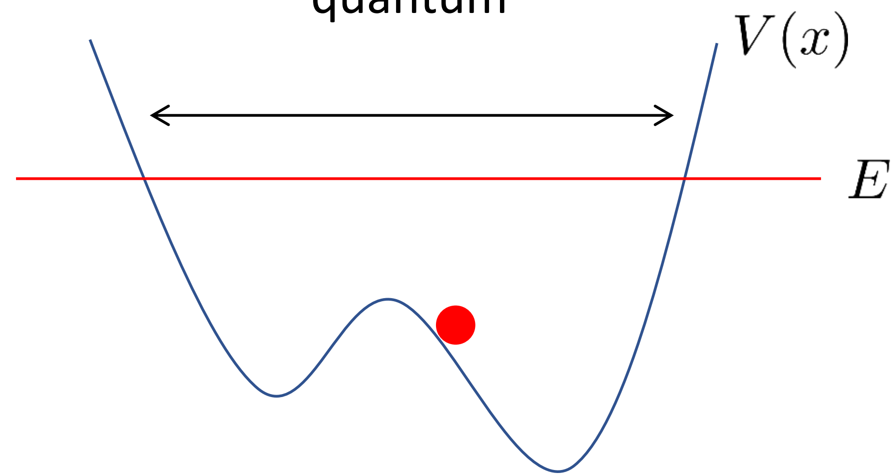

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A. Uncertainty Relation and its generalization (≒ Bootstrap method)

Han-Hartnoll-Kruthoff (2020)

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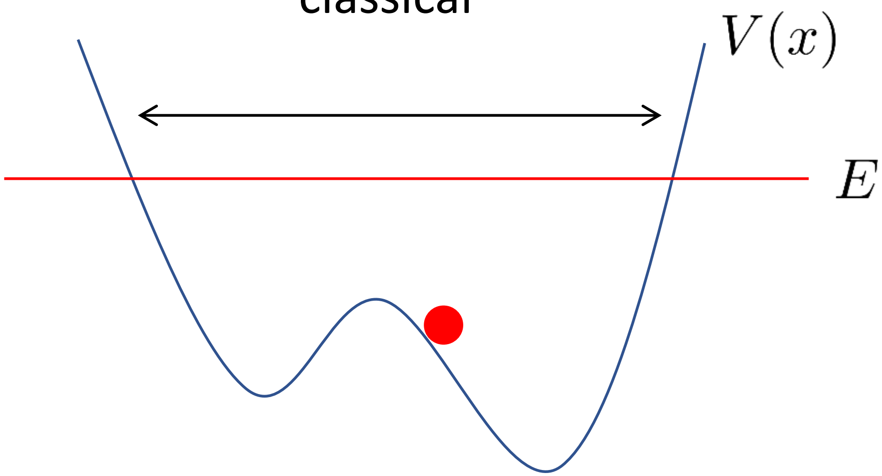

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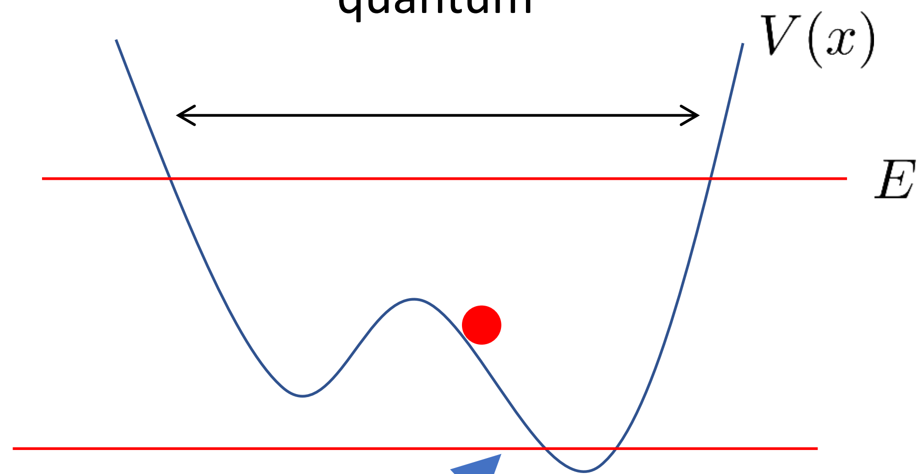

Range c … ossible particle motion

→ Determ …

Byproduct:
Uncertainty relations → Ground state

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A. Uncertainty Relation and its generalization (≒ Bootstrap method)

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1. Introduction

2. Harmonic Oscillator

   →Uncertainty Relation works.

3. General potential

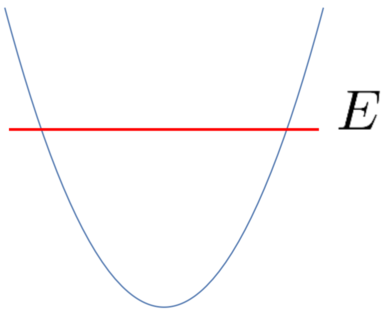
   →Numerical bootstrap method works.

   (Bootstrap = a generalized uncertainty relation)

   ◆ Comment on Ground State

4. Summary

2. Harmonic Oscillator



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

classical

$$-\sqrt{2E} \leq x \leq \sqrt{2E}$$

QM We use $E = \langle H \rangle$.

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

$$E = \frac{1}{2}\langle p^2 \rangle + \frac{1}{2}\langle x^2 \rangle = \frac{1}{2}\left(\langle \Delta p^2 \rangle + \langle p \rangle^2\right) + \frac{1}{2}\left(\langle \Delta x^2 \rangle + \langle x \rangle^2\right)$$

uncertainty relation ↓

$$\Longrightarrow \langle x \rangle^2 + \langle p \rangle^2 = 2E - \left(\langle \Delta x^2 \rangle + \langle \Delta p^2 \rangle\right) \leq 2E - 2\sqrt{\langle \Delta x^2 \rangle \langle \Delta p^2 \rangle} \leq 2E - \hbar.$$

↑ arithmetic mean

$$-\sqrt{2(E - \hbar/2)} \leq \langle x \rangle \leq \sqrt{2(E - \hbar/2)}$$

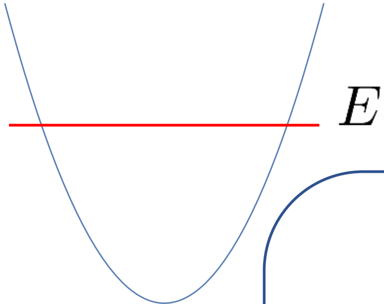
→ This result is equivalent to the classical result with $E \to E - \hbar/2$.

zero point energy

→ The classical result is corrected by the zero point energy.

✓ It is not difficult to show that this bound is saturated by coherent states.

2. Harmonic Oscillator



classical

$$-\sqrt{2E} \le x \le \sqrt{2E}$$

QM We us ...

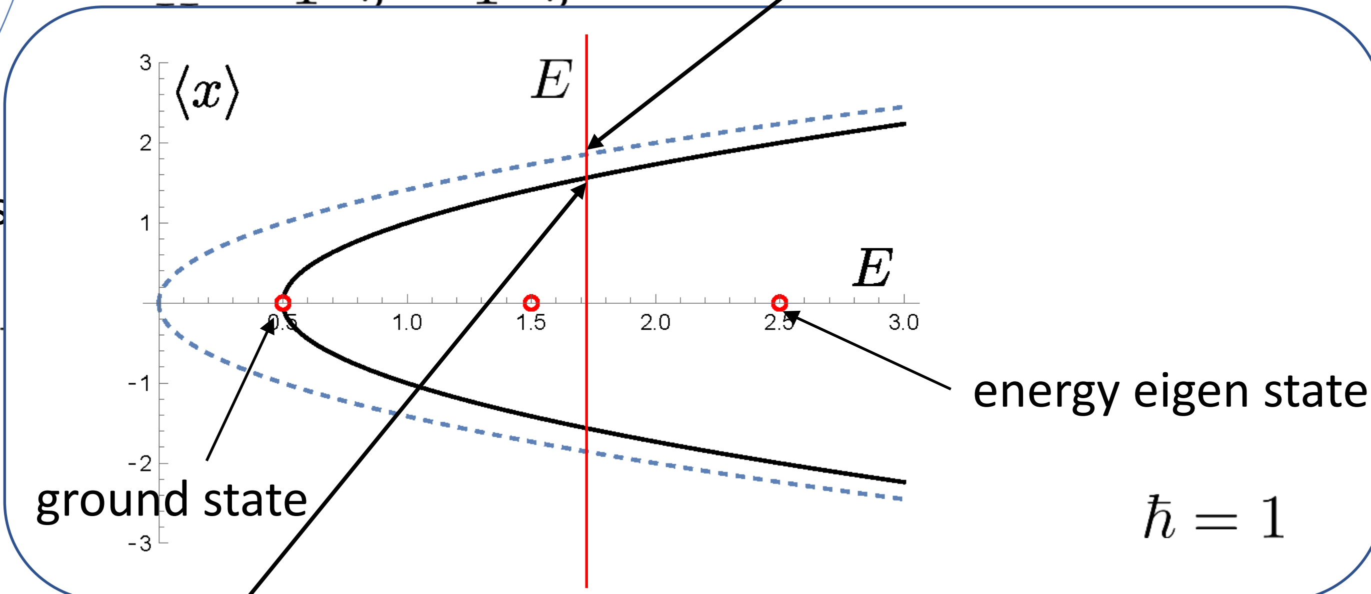
$$E = \frac{1}{2}\langle p^2\rangle \cdots$$

$$\Longrightarrow \langle x\rangle^2 \cdots$$

$\geq \frac{\hbar^2}{4}$

...elation

... $- \hbar.$



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   (Bootstrap = a generalized uncertainty relation)

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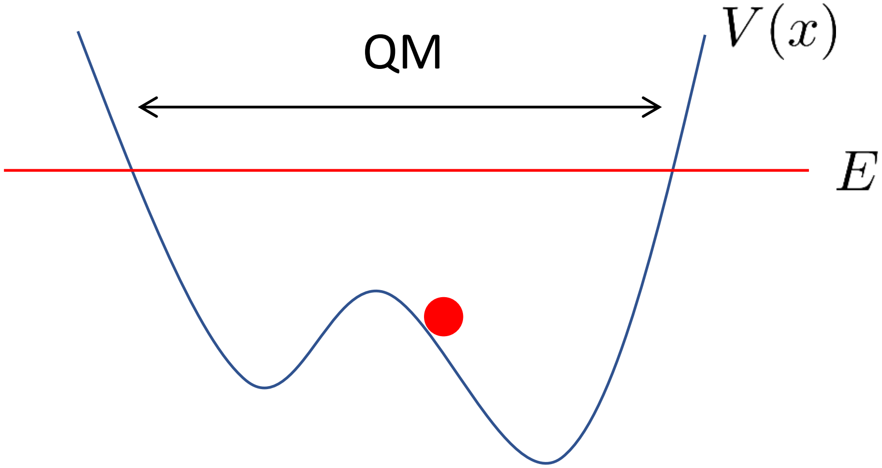
3. General Potential



$$H = \frac{1}{2}p^2 + V(x).$$

$$\text{ex)}\ V(x) = x^4$$

→ Uncertainty Relation is not enough. $\langle \Delta x^2 \rangle \langle \Delta p^2 \rangle \geq \frac{\hbar^2}{4} \overset{?}{\longleftrightarrow} \langle x^4 \rangle$

→ Even if we know all eigen states, it is hard to obtain the bound for $\langle x \rangle$.

→ We may need a generalization of the uncertainty relation involving

higher order moment observables $\{\langle x^m \rangle, \langle p^n \rangle, \langle p^k x^l \rangle\}$.

→ Bootstrap method Han-Hartnoll-Kruthoff (2020)

3. General Potential

Han-Hartnoll-Kruthoff (2020)

◆ Bootstrap method

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

If $\langle O^\dagger O \rangle \geq 0$ is satisfied for $^\forall O$, 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 $\sim$ cut off

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

$$\Leftrightarrow \langle \tilde{O}^\dagger \tilde{O} \rangle = \vec{c}^{\,\dagger} M \vec{c} \geq 0 \quad \text{for } ^\forall\{c_i\}$$

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

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

$K \times K$ matrix

Eigenvalues of M are all non-negative.

$$M \succeq 0$$

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

Han et al use it and obtain energy eigenstate.

3. General Potential

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◆ Bootstrap method and Uncertainty Relation

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

→ A Generalization of Uncertainty Relation

(Proof) $\tilde{O} = c_0 1 + c_1 x + c_2 p$

Curtright-Zachos (2001)

Uncertainty relation

$$M = \begin{pmatrix} 1 & \langle x \rangle & \langle p \rangle \\ \langle x \rangle & \langle x^2 \rangle & \langle xp \rangle \\ \langle p \rangle & \langle px \rangle & \langle p^2 \rangle \end{pmatrix} \xrightarrow{M \succeq 0} \langle \Delta x^2 \rangle \langle \Delta p^2 \rangle \geq \frac{\hbar^2}{4} \quad \text{for } {}^\forall | \quad \rangle$$

→ If we take $\tilde{O} = \underline{c_0 1 + c_1 x + c_2 p} + c_3 x^2 + c_4 p^2 + \cdots$, $M \succeq 0$ provides stronger constraints involving higher order moment $x^m p^n$.

→ $M \succeq 0$ is a generalized version of uncertainty relation.

3. General Potential

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Example: Anharmonic oscillator

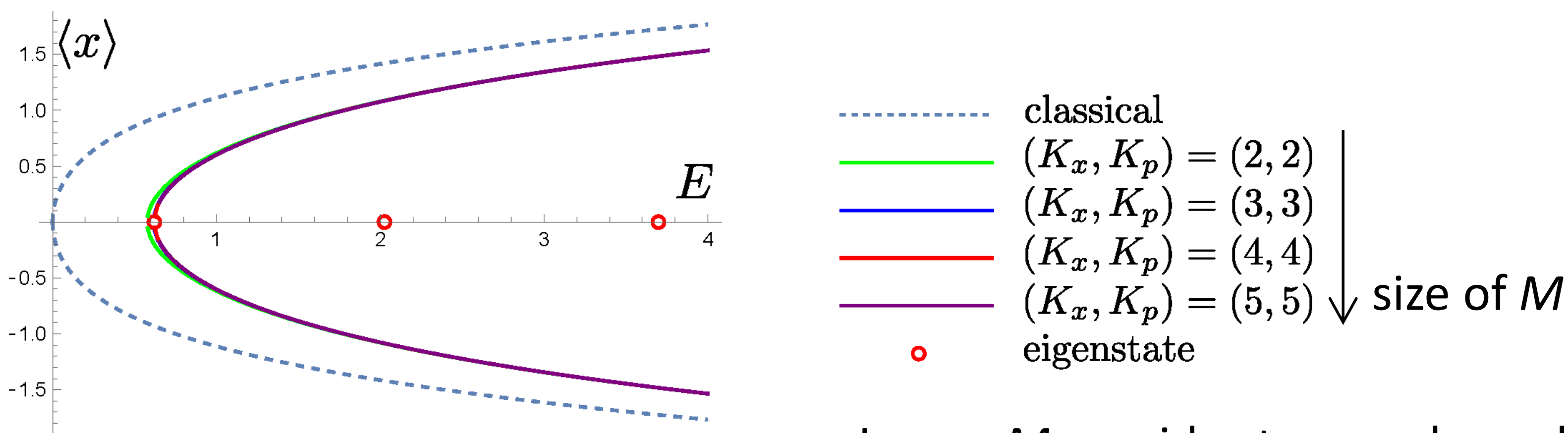
$$H = \frac{1}{2}p^2 + \frac{1}{2}x^2 + \frac{1}{4}x^4$$

$$M \succeq 0, \quad E = \langle H \rangle = \frac{1}{2}\langle p^2 \rangle + \frac{1}{2}\langle x^2 \rangle + \frac{1}{4}\langle x^4 \rangle$$

Find the maximum and minimum of $\langle x \rangle$.

→ "Linear Programming" (solvable)

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



Larger M provide stronger bounds.

3. General Potential

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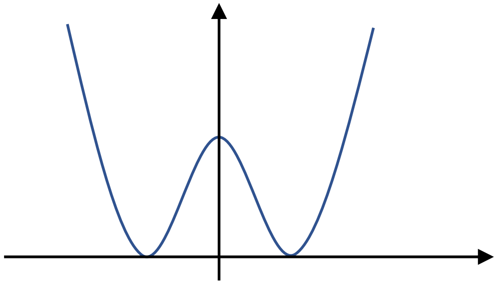
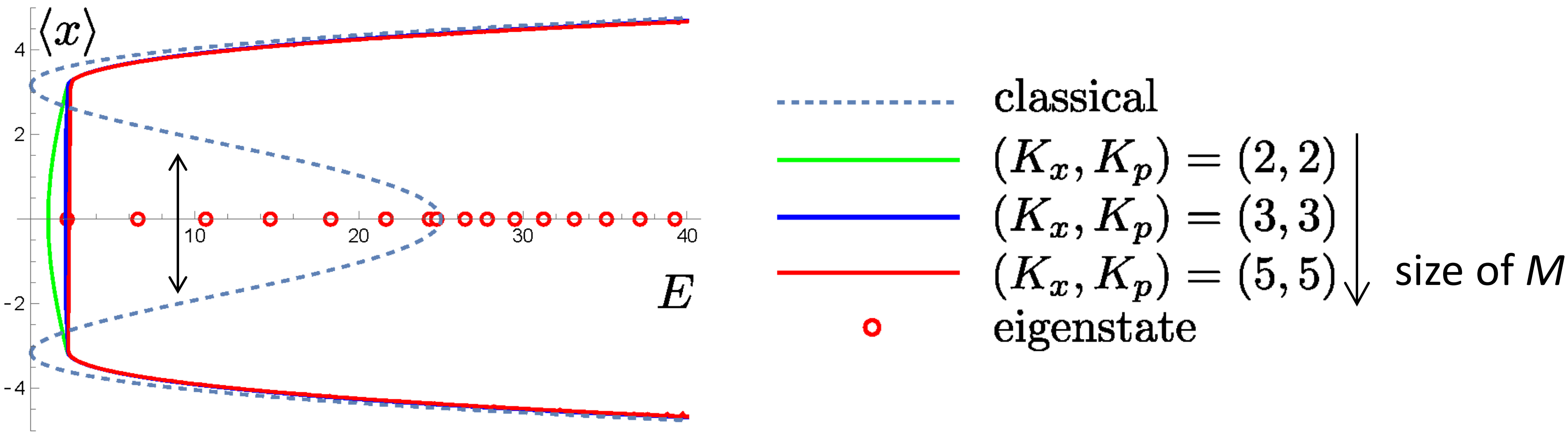
Example: Double well potential

$$H = \frac{1}{2}p^2 - 5x^2 + \frac{1}{4}x^4.$$





The conditions $E = \langle H \rangle$ and $M \succeq 0$ are strong enough to obtain the bounds on $\langle x \rangle$.

3. General Potential

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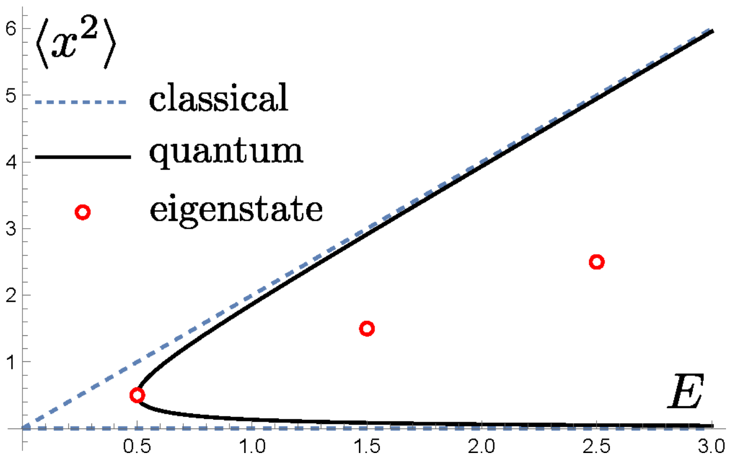
★ Other observables

Bounds on $\langle x \rangle$ → Bounds on $\langle x^m p^n \rangle$ Easy!

Example 1) $\langle x^2 \rangle$ in Harmonic Oscillator



$$E - \sqrt{E^2 - \hbar^2/4} \leq \langle x^2 \rangle \leq E + \sqrt{E^2 - \hbar^2/4}.$$

Example 2) $\langle p \rangle$

$$H = \frac{1}{2}p^2 + V(x). \quad \rightarrow \quad |\langle p \rangle| \leq p_* := \sqrt{2(E - E_0)}$$

E_0 :ground energy

$|0\rangle$: ground state

3. General Potential

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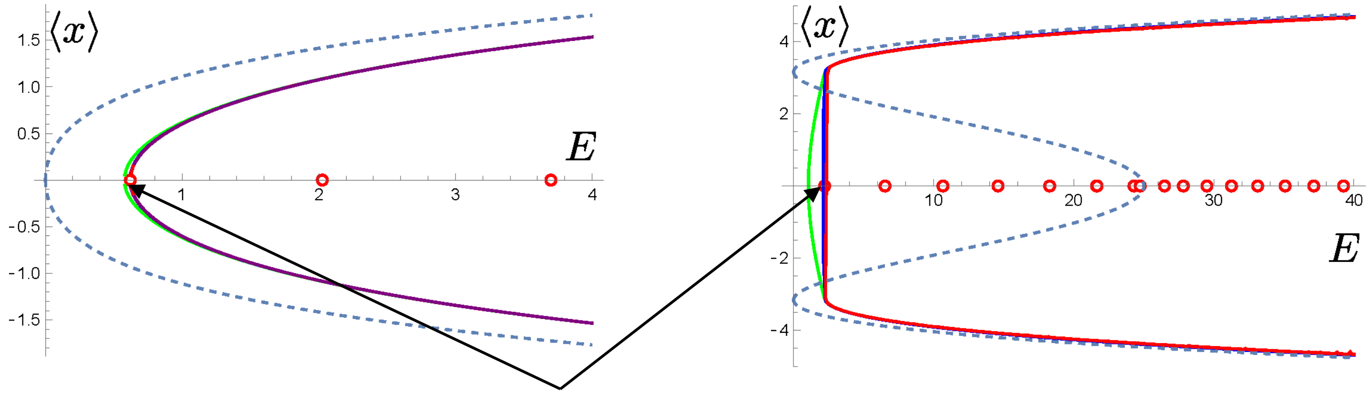
★ Uncertainty Relation → Ground state

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

$$H = \frac{1}{2}p^2 - 5x^2 + \frac{1}{4}x^4.$$



Lawrence (2021)

$M \succeq 0$ → Ground State

Summary

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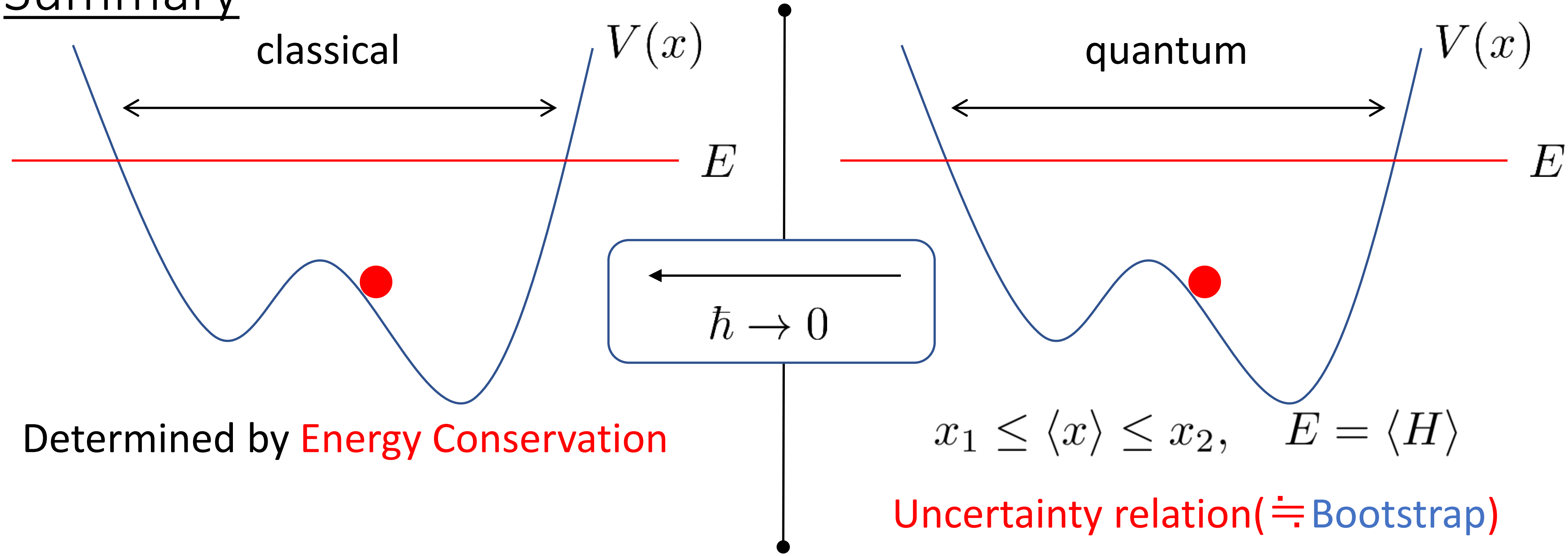

- ✓ Novel aspects of quantum mechanics:
  Uncertainty relations, Coherent states, Ground states.
- ✓ Uncertainty relation (bootstrap) → Ground states.

Issues

- ✓ Bosons and Fermions → Obtained bounds are weak.

Future directions

- ✓ Bounds for fixed charges, angular momentum and so on.
- ✓ Connection to other bounds in QM (chaos bound, viscosity bound, etc.)
- ✓ Application to other statistical models.