Title: Quantum Many-body Bootstrap

Speakers: Yuan Xin

Series: Quantum Fields and Strings

Date: March 26, 2024 - 2:00 PM

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Abstract: Determining the long-range phase of matter of a strongly coupled system from its microscopic description has long been one of the central topics in physics. Simple microscopic systems often become strongly coupled at long range where we usually rely on clever approximations. Bootstrap is an alternative approach that uses positivity and equations of motion to make predictions in quantum many-body systems without making approximations. In this talk, I will show my recent work on using bootstrap to compute the ground state energy, local observables and gaps of a quantum many-body system in the thermodynamic limit with rigorous error bars.

Zoom link

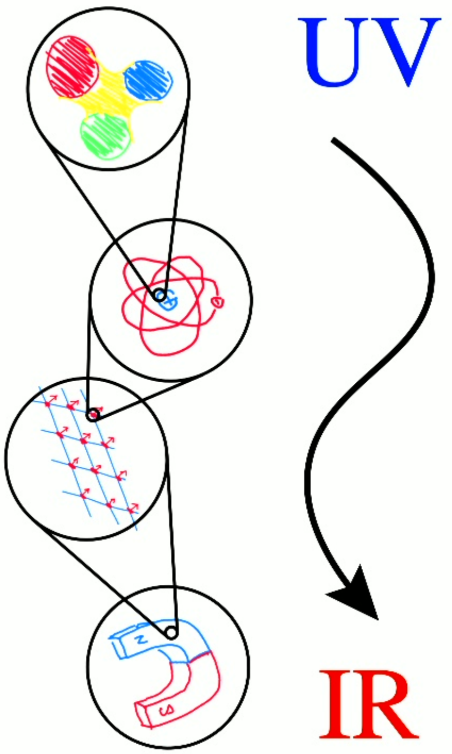
Quantum many-body bootstrap

2211.03819 with Colin Nancarrow
Also work in progress with
Minjae Cho, Colin Nancarrow, Peter Tadic, Zechuan Zheng

Yuan Xin 2024/03/26

Motivation

- Systems with large degrees of freedom can have interesting emergent behaviors, which are often strongly coupled and hard to compute.



Motivation

Simulation | vs. | Bootstrap

Known $H = H_0 + V$
$S = S + \delta S$
QFT, Lattice, …

Monte-Carlo,
Variational method …

?
Gapped? Not gapped?
Symmetry?
Spectrum?

Can have errors

?
Which UV theory?
Equation of motion?
Range of some parameters?

Rigorous self-consistency check

CFT data, S-matrix, …
Bound on parameters

Need a lot assumptions

Motivation

Simulation

Known

$H = H_0 + V$
$S = S + \delta S$
QFT, Lattice, …

Monte-Carlo,
Variational method …

?

Gapped? Not gapped?
Symmetry?
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Can have errors

Bootstrap

?

Which UV theory?
Equation of motion?
Range of some parameters?

Rigorous self-consistency check

CFT data, S-matrix, …
Bound on parameters

Need a lot assumptions

Desired method

Known

Self-consistency conditions,
No approximation made

Solution parameter space
Bound on parameters

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Outline

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

Introduction

Bounding many-body ground state

Bounding gap of many-body systems

Introduction

Moment problem and moment matrix

- Moment Problem:
  - Organize observables as Moment Matrix $M^K_{ij} = \langle x^{i+j} \rangle,\ 1 \le i,j \le K$
  - $$\boxed{\begin{gathered}\langle x^n \rangle = \int x^n d\mu \quad \text{for a positive measure } \mu \\ \Leftrightarrow \\ M^K \text{ is positive semidefinite } M^K \succeq 0,\ \forall\ K\end{gathered}}$$

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

- $\langle x^n \rangle$ is further constrained by equations of motion, symmetry and locality.

Introduction

Warm up: Bootstrapping Anharmonic Oscillator

[Han, Hartnoll, Kruthoff '20]

- $H = p^2 + \omega^2 x^2 + \lambda x^4$

- Ingredient 0: solution parameter space
  (Moment Matrix)
  assuming some energy eigenstate $|E\rangle$.

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

Truncated down to K

- Ingredient 1: Positivity $M_{ij} \equiv \langle E | x^{i+j} | E \rangle \succcurlyeq 0.$

- Ingredient 2: Equations of motion, $\langle [H, \mathcal{O}] \rangle = 0, \ \ \langle H \mathcal{O} \rangle = E \langle \mathcal{O} \rangle.$

- Can derive recursion relation:

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

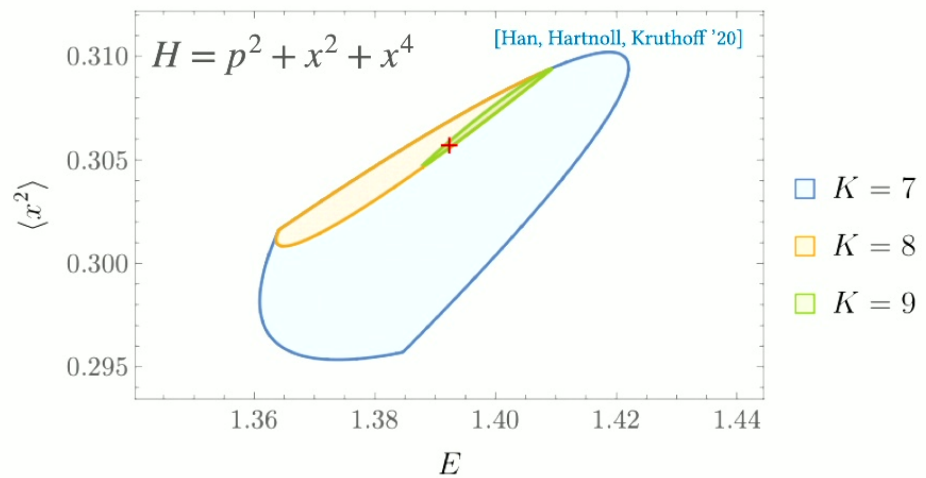
$$\Rightarrow \ \langle x^{2n} \rangle = \# + \#' \langle x^2 \rangle \ , \quad \langle x^{2n+1} \rangle \propto \langle x \rangle = 0 \text{ from parity}$$

Introduction

Warm up: Bootstrapping Anharmonic Oscillator

[Han, Hartnoll, Kruthoff '20]

- $M_{ij} \equiv \langle E | x^{i+j} | E \rangle \succcurlyeq 0$, $\langle x^{2n} \rangle = \# + \#' \langle x^2 \rangle$ $\qquad 0 \leqslant i,j \leqslant K$
- 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

Bounding Many-body Ground State

Bounding gap of many-body systems

Bounding Many-body Ground State

Generalize to Many-body Systems in thermodynamic limit

- Spin chain in thermodynamic limit: generalize Moment matrix to $M = \langle \mathcal{O}_i^\dagger \mathcal{O}_j \rangle$.

- Energy diverges. Simply discard the second type EOM.

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

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

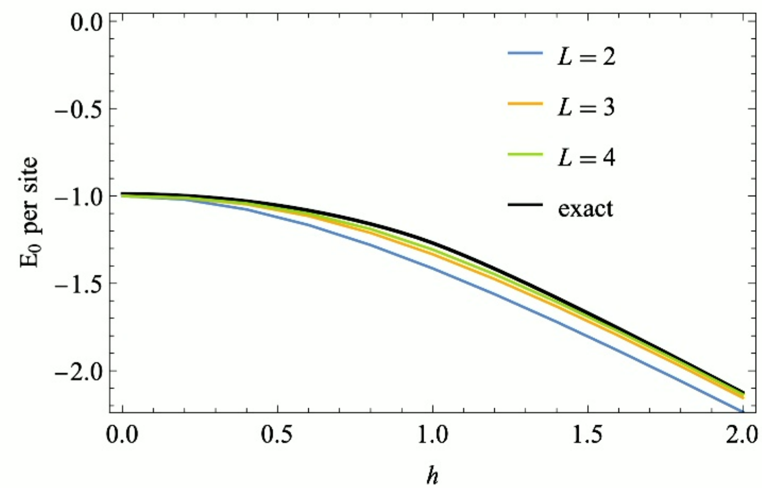
Lower bounding ground state energy

- TFIM example on 1d infinite spin chain $H = \sum_{i=-\infty}^{\infty} \sigma_i^z \sigma_{i+1}^z + h\sigma_i^x$.

- Bootstrap gives a lower bound on ground state energy which improves with L.

- Comment: rigorous bound, but to tighten the bound requires large L. Moment matrix grows as 4^L.

- Can we make it faster?



Bounding Many-body Ground State

Lower bounding ground state energy

- Example: Transverse Field Ising Model (TFIM) on 1d infinite spin chain
  $H = \sum_{i=-\infty}^{\infty} \sigma_i^z \sigma_{i+1}^z + h\sigma_i^x$
- Ingredient 0: Moment matrix on spin-1/2 chain:
  $M = \langle M_1 \otimes M_2 \otimes \cdots \otimes M_L \rangle$,
  truncate to L-local operators for finiteness.

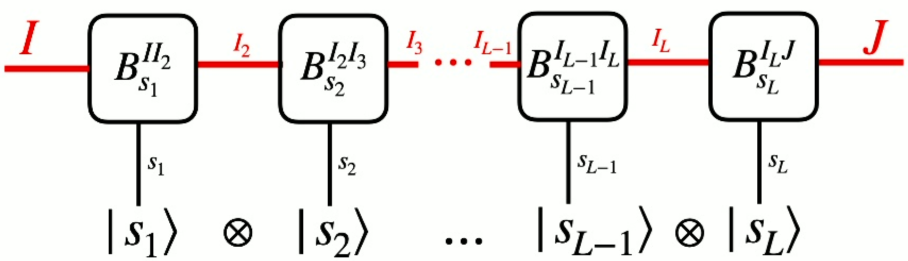
$$M_n = \begin{pmatrix} 1 & \sigma_n^1 & \sigma_n^2 & \sigma_n^3 \\ \sigma_n^1 & 1 & i\sigma_n^3 & -i\sigma_n^2 \\ \sigma_n^2 & -i\sigma_n^3 & 1 & i\sigma_n^1 \\ \sigma_n^3 & i\sigma_n^2 & -i\sigma_n^1 & 1 \end{pmatrix}$$

- Ingredient 1: Positivity: $M \succeq 0$.
- Ingredient 2: Minimize $\langle H_{12} \rangle \equiv \langle \sigma_1^z \sigma_2^z + h\sigma_1^x \rangle$ (assuming translation invariance)
- Turns out EOM $\langle [H, \sigma_1^{\mu_1} \sigma_2^{\mu_2} \cdots] \rangle = 0$ is not necessary for ground state minimization.

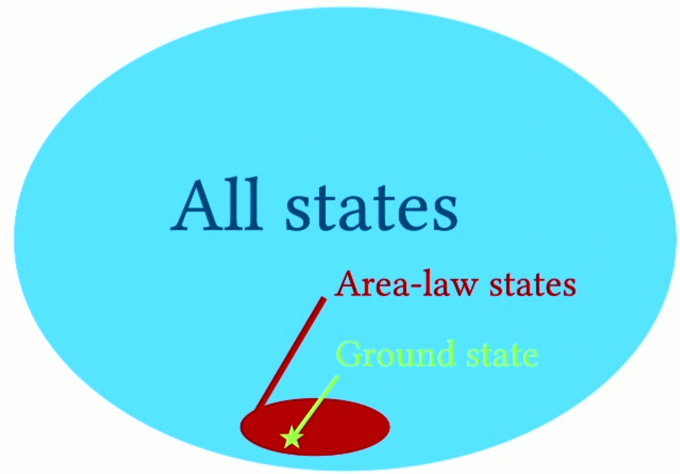
Bounding Many-body Ground State

Optimizing the bound with Matrix Product State (MPS)

- MPS is a variational ansatz
  $|\psi^{IJ}\rangle = B_{s_1}^{II_2} B_{s_2}^{I_2 I_3} \cdots B_{s_L}^{I_L J} \, | s_1 s_2 \cdots s_L \rangle$
  that efficiently approximates the many-body ground state.



$I_n, J = 1,2,\cdots D \quad D$: "bound dimension"



MPS is efficient because it captures the feature that ground state (in gapped phase) has area-law entanglement entropy.

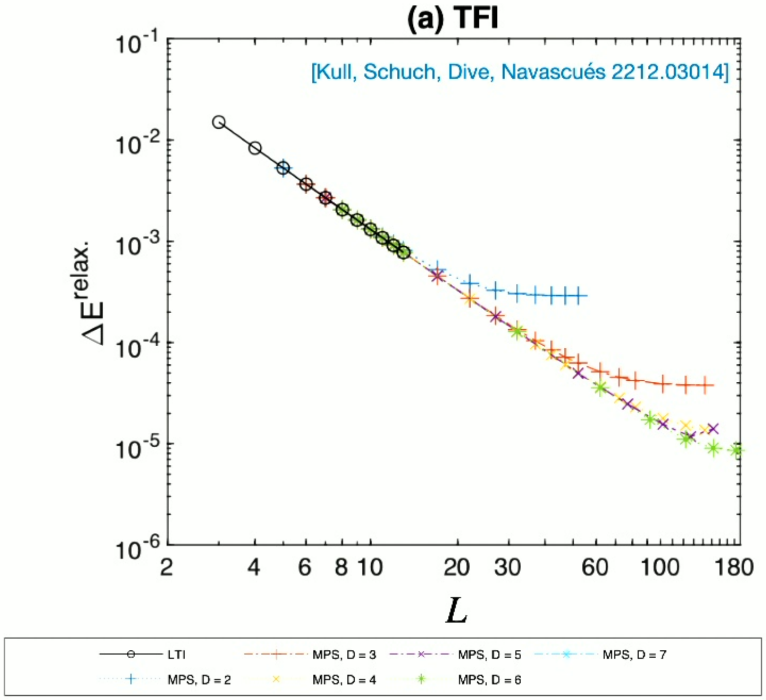
Bounding Many-body Ground State

Optimizing the bound with Matrix Product State (MPS)

- MPS is a variational ansatz $|\psi^{IJ}\rangle = B^{II_2}_{s_1} B^{I_2 I_3}_{s_2} \cdots B^{I_L J}_{s_L} | s_1 s_2 \cdots s_L \rangle$ that efficiently approximates the many-body ground state.
- Schematically, one relaxes positivity to $\langle | \psi^{IJ} \rangle \langle \psi^{IJ} | \rangle \geq 0$. Now problem scales as L^{power} and we can study much larger L.

[Kull, Schuch, Dive, Navascués 2212.03014]

$\dim 4^L \rightarrow \dim D^2$

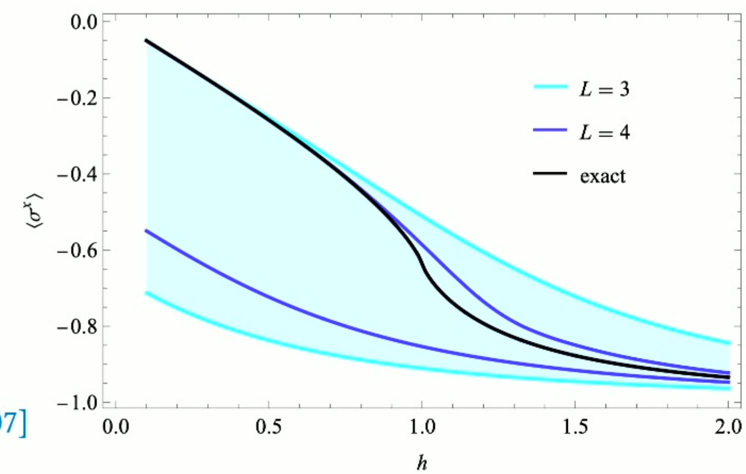


Bounding Many-body Ground State

Isolating the ground state

- It is much more interesting to obtain bounds on general observables.
- Requires two positivity conditions
  - $\langle \mathcal{O}^\dagger \mathcal{O} \rangle \geq 0$, i.e. $M \succeq 0$ (moment positivity).
  - $\langle \mathcal{O}^\dagger [H, \mathcal{O}] \rangle \geq 0$ (Perturbative positivity).

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

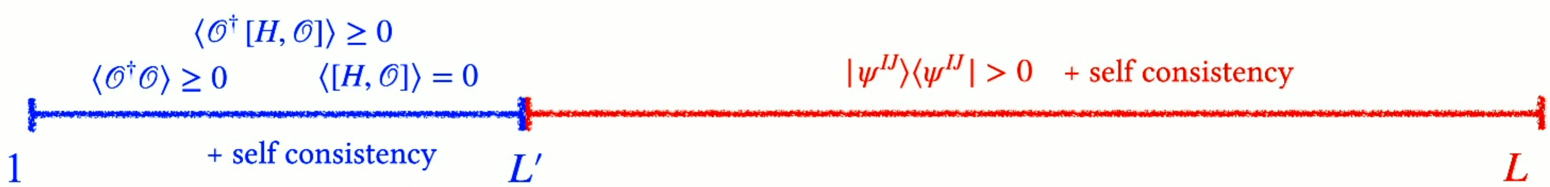


- EOMs are necessary: $\langle [H, \sigma_1^{\mu_1} \sigma_2^{\mu_2} \cdots] \rangle = 0$.
- Large L is still required to optimize bound. Combine with MPS?

Bounding Many-body Ground State

Our setup: optimize observable bound using MPS

- Unfortunately, naively the MPS relaxation doesn't play well with EOMs.
- For a generic element $A = |\psi^{IJ}\rangle\langle\psi^{KL}|$ in the relaxed moment matrix, action of Hamiltonian $[H, A] \notin \{\, |\psi^{IJ}\rangle\langle\psi^{KL}|\,\}$ brings it out of the MPS parameter space: Naively no EOMs to use in MPS relaxation.
- For now we can still proceed with a hybrid method using EOM and MPS in different parts of the problem.



Bounding Many-body Ground State

Our setup: optimize observable 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]

Expensive, restrict to range L'

$$+$$
MPS relaxation $|\psi^{IJ}\rangle\langle\psi^{IJ}| > 0$
[Kull, Schuch, Dive, Navascués 2212.03014]

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

$$
\begin{aligned}
\text{minimize :} \quad & \langle \mathcal{O}_b \rangle = \mathrm{Tr}(E^{ij}\mathcal{O}_b)\alpha_{ij}^{(L')} \\
\text{over :} \quad & \alpha_{ij}^{(r)},\ r = 1,2,\cdots,L',\cdots L \\
\text{with constraints :} \quad & \rho_r \geq 0,\ \rho_r = \alpha_{ij}^{(r)}E^{ij},\ \text{for } r \leq L_1 \\
& \mathrm{Tr}_1\rho_r = \mathrm{Tr}_r\rho_r = \rho_{r-1},\ \mathrm{Tr}\rho_1 = 1 \\
& \omega_r \geq 0,\ \omega_r = \alpha_{ij}^{(r)}E^{ij},\ \text{for } r \geq L'+1 \\
& \mathrm{Tr}_1\omega_r = B \circ \omega_{r-1},\ \mathrm{Tr}_r\omega_r = \omega_{L'} \circ B \\
& \mathrm{Tr}_1\omega_{L'+1} = B \circ \rho_{L'},\ \mathrm{Tr}_{L'+1}\omega_{L'+1} = \rho_{L'} \circ B \\
\text{isolate ground state :} \quad & M \geq 0,\ M_{ij} = \mathrm{Tr}(E^{rs}\mathcal{O}_i^\dagger[H,\mathcal{O}_j])\alpha_{rs}^{(L')} \\
\text{equations of motion :} \quad & \langle [H,\mathcal{O}_k] \rangle = \mathrm{Tr}(E^{rs}[H,\mathcal{O}_k])\alpha_{rs}^{(L')} = 0,\ \forall k\ .
\end{aligned}
$$

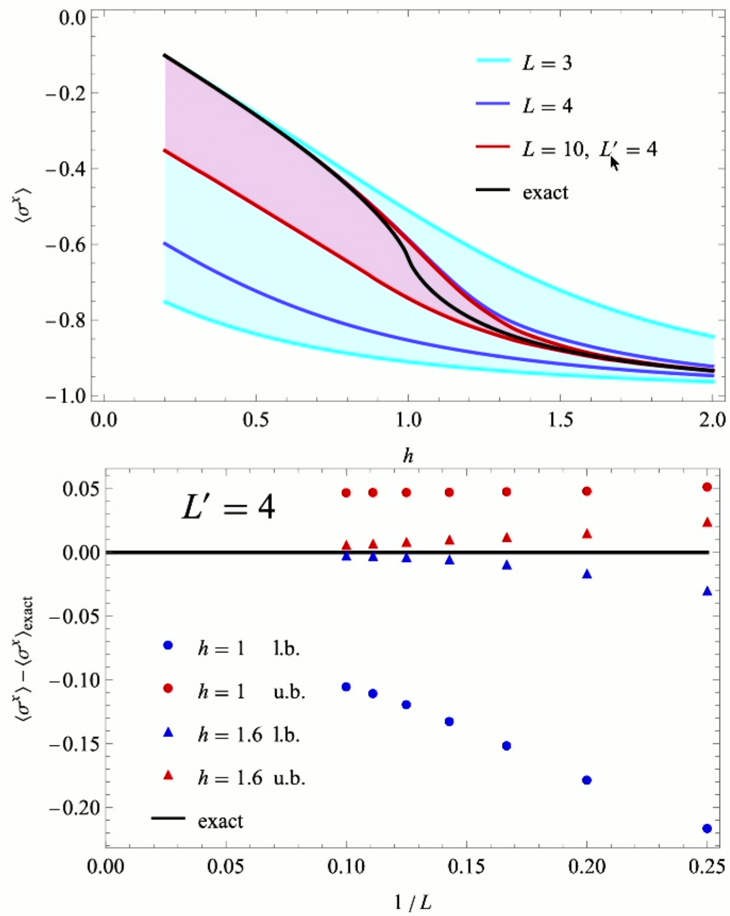
MPS ansatz, inspired by [Kull, Schuch, Dive, Navascués 2212.03014]

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)
- In full problem, we would have to do semidefinite programming for a matrix of $4^{10} \times 4^{10} = 1048576 \times 1048576$. MPS relaxation drastically reduces it to 100~1000.
- Away from criticality (e.g. $h = 1.6$) result seems to be converging well, while at criticality ($h = 1$) it seems to require more equations of motion beyond L'.



Introduction

Bounding many-body ground state

Bounding Gap of Many-body Systems

Bounding Gap of Many-body Systems

Bootstrapping spectral decomposition

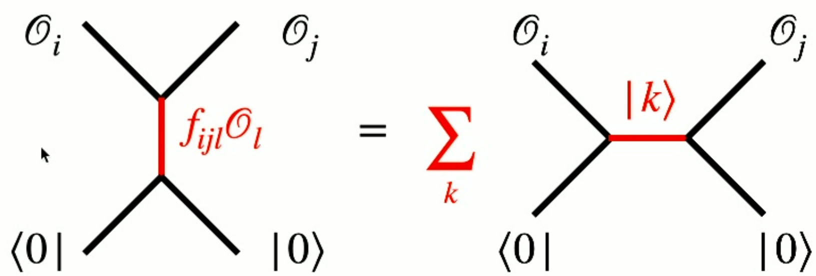
- Beyond the ground state observables, we are interested in gaps, correlators and excited state observables.
- For this purpose, we extend the moment matrix problem by inserting a complete basis of eigenstates:
- $$\langle 0 | \mathcal{O}_i \mathcal{O}_j | 0 \rangle = \sum_k \langle 0 | \mathcal{O}_i | k \rangle \langle k | \mathcal{O}_j | 0 \rangle$$
- 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":



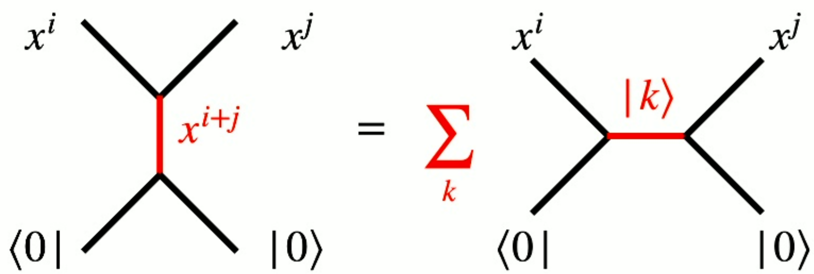
"OPE coefficients": $\langle k|\mathcal{O}_j|0\rangle$

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

Bounding Gap of Many-body Systems

Anharmonic oscillator 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

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

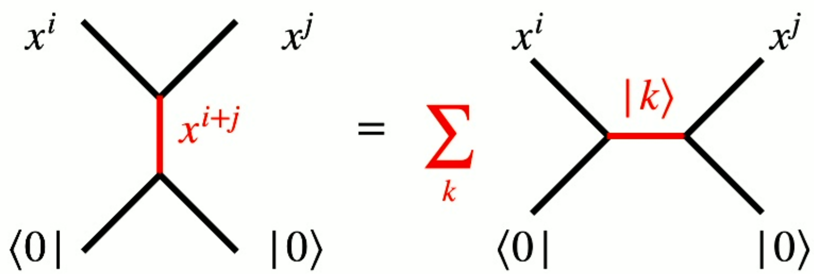
For diagonal matrix elements we had recursion relation

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

Bounding Gap of Many-body Systems

Anharmonic oscillator 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

For off-diagonal elements, we have similar relation, schematically:

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

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

unknowns $\qquad g^i_{\mathcal{O}}(E_n,E_m)$

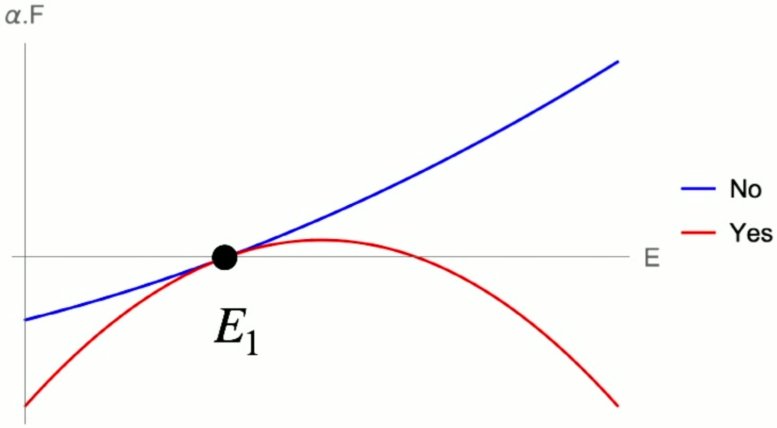
Bounding Gap of Many-body Systems

Anharmonic oscillator revisited

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

unknowns $\qquad g^i_{\mathcal{O}}(E_n, E_m)$

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



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

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

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

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

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

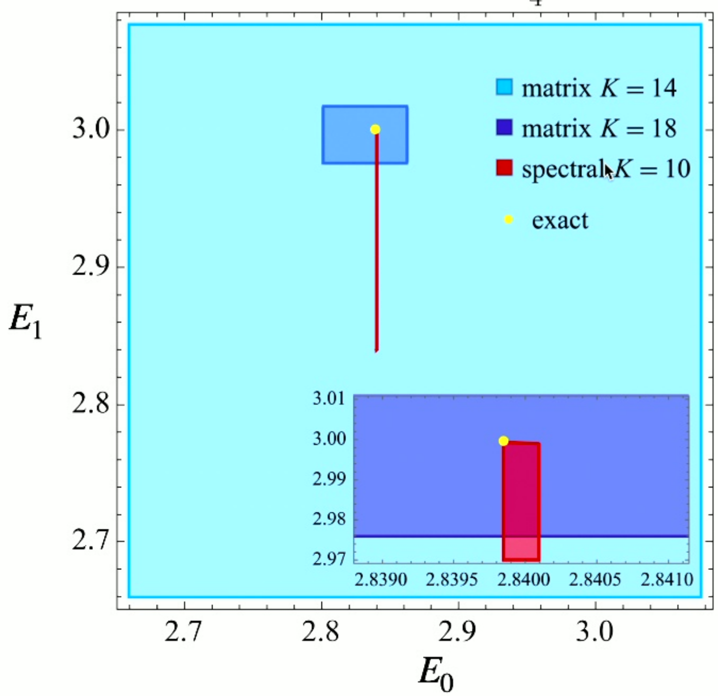
then all spectra with the prescribed (E_0, E_1) and c_{00,x^2} are ruled out.

Bounding Gap of Many-body Systems

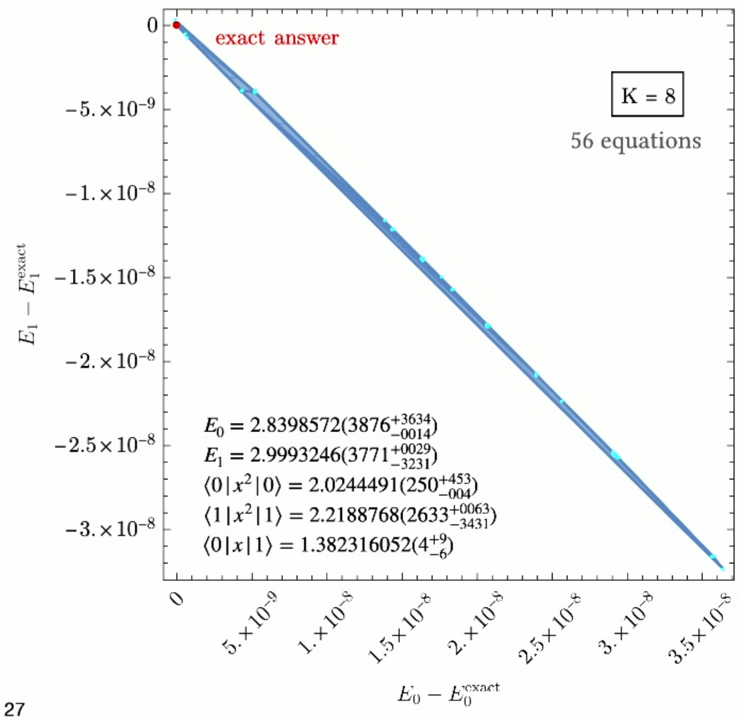
Anharmonic oscillator revisited

- Found upper bound on the gap E_1

$$H = p^2 - 5x^2 + x^4 + \frac{25}{4}$$



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

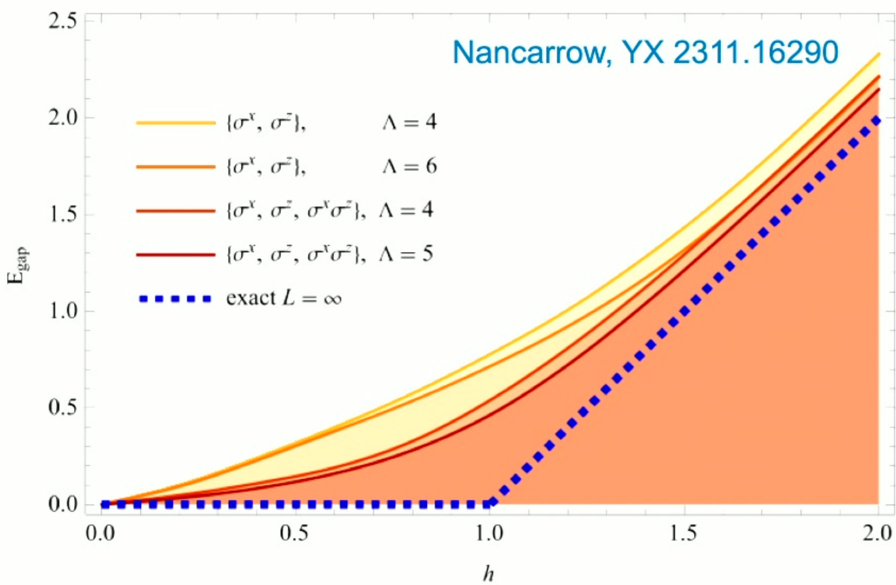


Bounding Gap of Many-body Systems

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.
- $E_{\text{gap}} := E_1 - E_0$

Conclusion & Outlook

- Bootstrap is a useful tool to study Quantum Mechanics with infinite degrees of freedom. It rigorously bounds the IR solution and knows about all its UV constraints.
- 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.

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QFT for Cosmology, Achim Kempf, **Lecture 21**

Perturbative quantization of inflaton field and the metric.

Recall:

- We decompose the inflaton field $\phi(x,\eta)$:

$$\phi(x,\eta) = \phi_0(\eta) + \varphi(x,\eta)$$

where:

- $\phi_0(\eta)$ is assumed large and is treated classically.
- $\varphi(x,\eta) =: \delta\phi(x,\eta)$ describes a field of small inhomogeneities and is to be quantized: $\hat{\varphi}(x,\eta)$

$$ds_s^2 = a^2(\eta)\Big[2\Phi(x,\eta)\,d\eta^2 - 2\sum_{i=1}\frac{\partial}{\partial x^i}B(x,\eta)\,dx^i d\eta - \sum_{i,j=1}^{3}\Big(2\Psi(x,\eta)\,\delta_{ij} - 2\frac{\partial}{\partial x^i}\frac{\partial}{\partial x^j}E(x,\eta)\Big)dx^i dx^j\Big]$$

$$ds_v^2 = a^2(\eta)\Big[2\sum_{i=1}^{3}V_i(x,\eta)\,dx^i d\eta - \sum^{3}\Big(\frac{\partial}{\partial x^j}W_i(x,\eta) + \frac{\partial}{\partial x^i}W_j(x,\eta)\Big)dx^i dx^j\Big]$$

- We decompose the metric $g_{\mu\nu}(x,\eta)$:

$$g_{\mu\nu}(x,\eta) = \underbrace{a_0^2(\eta)\,\eta_{\mu\nu}}_{\text{treated classically}} + \underbrace{\gamma_{\mu\nu}(x,\eta)}_{\text{assumed small, to be quantized}}$$

- Here, $\gamma_{\mu\nu}(x,\eta)$ can be decomposed into scalar, vector and tensor-type inhomogeneities, using functions $E, B, \Psi, \Phi, V_i, W_i, h_{ij}$.

namely: $ds^2 = g_{\mu\nu}(x,\eta)\,dx^\mu dx^\nu$

$$ds^2 = \overbrace{a^2(\eta)\Big(d\eta^2 - \sum_{i=1}^{3}(dx^i)^2\Big)}^{\text{zero-mode, i.e., homogeneous and isotropic part}} + \underbrace{ds_s^2}_{\text{scalar}} + \underbrace{ds_v^2}_{\text{vector}} + \underbrace{ds_t^2}_{\text{tensor}}$$

We insert the approximation

$$\phi(x,\eta) = \phi_0(\eta) + \varphi(x,\eta)$$

$$g_{\mu\nu} = a^2(\eta)\,\eta_{\mu\nu} + \gamma_{\mu\nu}(x,\eta)$$

with φ, γ assumed small, into the action:

$$S = \frac{-1}{16\pi G}\int R\sqrt{|g|}\,d^4x$$

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$$\phi(x,\eta) = \phi_0(\eta) + \varepsilon(x,\eta)$$

where:

- $\phi_0(\eta)$ is assumed large and is treated classically.
- $\varepsilon(x,\eta) =: \delta\phi(x,\eta)$ describes a field of small inhomogeneities and is to be quantized: $\hat{\varepsilon}(x,\eta)$

$$ds_S^2 = a^2(\eta)\Big[2\Phi(x,\eta)\,d\eta^2 - 2\sum_{i=1} \frac{\partial}{\partial x^i} B(x,\eta)\,dx^i d\eta$$
$$-\sum_{i,j=1}^{3}\Big(2\Psi(x,\eta)\,\delta_{ij} - 2\frac{\partial}{\partial x^i}\frac{\partial}{\partial x^j} E(x,\eta)\Big)\,dx^i dx^j\Big]$$

$$ds_V^2 = a^2(\eta)\Big[2\sum_{i=1}^{3} V_i(x,\eta)\,dx^i d\eta$$
$$-\sum_{i,j=1}^{3}\Big(\frac{\partial}{\partial x^j} W_i(x,\eta) + \frac{\partial}{\partial x^i} W_j(x,\eta)\Big)dx^i dx^j\Big]$$

$$ds_T^2 = a^2(\eta)\sum_{i,j=1}^{3} h_{ij}(x,\eta)\;dx^i dx^j$$

vector and tensor-type inhomogeneities, using functions

$$E, B, \Psi, \Phi, V_i, W_i, h_{ij}.$$

namely: $ds^2 = g_{\mu\nu}(x,\eta)\,dx^\mu dx^\nu$

$$ds^2 = \underbrace{a^2(\eta)\Big(d\eta^2 - \sum_{i=1}^{3}(dx^i)^2\Big)}_{\text{zero-mode, i.e., homogeneous and isotropic part}} + \underbrace{ds_S^2}_{\text{scalar}} + \underbrace{ds_V^2}_{\text{vector}} + \underbrace{ds_T^2}_{\text{tensor}}$$

We insert the approximation

$$\phi(x,\eta) = \phi_0(\eta) + \varepsilon(x,\eta)$$

$$g_{\mu\nu} = a^2(\eta)\,\eta_{\mu\nu} + \gamma_{\mu\nu}(x,\eta)$$

with ε, γ assumed small, into the action:

$$S = \frac{-1}{16\pi G}\int R\sqrt{|g|}\,d^4x$$

$$+\frac{1}{2}\int(\partial_\mu\phi)(\partial^\mu\phi) - V(\phi)\sqrt{|g|}\,d^4x$$

$$+ \text{neglected (other fields)}$$

One obtains many terms with $\Phi, \Psi, B, E, V, W, h$!

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(e.g., no preferred conformal time & space cds)

- But the choice of cds will affect the functions above, i.e. they are in part coordinate system dependent.

$\Rightarrow$ We may choose our spacelike hypersurfaces so that (and thus our notion of equal time) these functions $\Phi, \bar{\Psi}, E, B, v, w, h$ vanish or simplify.

It took on the order of 10 years to clarify this "gauge" question!

I) A spatial tensor field:

This is $h_{ij}(x,\eta)$ itself. It represents $T_{\mu\nu}$-independent, so-called Weyl curvature, namely gravitational waves. $h_{ij}(x,\eta)$ measures how much space is locally distorted against itself in different directions.

II) A spatially scalar field, r, made of φ and $g_{\mu\nu}$'s scalar part:

Due to the Einstein eqn,

$$\delta\phi(x,\eta) = \varphi(x,t)$$

combines with the scalar part of the metric inhomogeneities

$$\Psi(x,\eta),$$

to yield one dynamical entity, namely:

- **Result:**

  * For small inhomogeneities (1st order perturbation) nearly all inhomogeneities can be eliminated by suitable coordinate choice.

  * Except, there are two fields, which are coordinate system, i.e., "gauge" independent. Namely:

recall: $\phi_0(\tau)$ = classical homogeneous inflaton field.

$$r(x,\eta) := -\frac{a_0'}{a_0}\left(\phi_0(\eta)'\right)^{-1}\underset{\text{from inflaton}}{\varphi(x,\eta)} - \underset{\text{from "scalar" part of the metric}}{\Psi(x,\eta)}$$

Physically, what is $r(x,\eta)$?

* First term: $\Psi(x,\eta)$ is the (scalar) metric's fluctuation.

* Second term: In $\frac{a'}{a}\frac{1}{\phi_0'}\varphi$, the $\varphi(x,\eta)$ is the scalar field's fluctuation.

Consider now: 2 Useful choices for foliations of spacetime into spacelike hypersurfaces of equal time:

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II) A spatially scalar field, τ, made of φ and $g_{\mu\nu}$'s scalar part:

Due to the Einstein eqn,

$$\delta\phi(x,\eta) = \varphi(x,t)$$

combines with the scalar part of the metric inhomogeneities

$$\Psi(x,\eta),$$

to yield one dynamical entity, namely:

a.) Foliate so that on surfaces of equal time, η, one has: $\varphi \equiv 0$.

⇝ Equal time hypersurfaces chosen so that all points of equal value of ϕ have equal value of time.

Note: Only possible if ϕ decays over time (e.g. slow roll inflation, but not de Sitter).

⇝ We see that $\tau(x,\eta)$ expresses now purely metric fluctuations

⇝ Technically, these are fluctuations in the "intrinsic curvature". (Local bloating)

Physically, what is $\tau(x,\eta)$?

* First term: $\Psi(x,\eta)$ is the (scalar) metric's fluctuation.
* Second term: In $\frac{a'}{a}\frac{1}{\phi_0'}\varphi$, the $\varphi(x,\eta)$ is the scalar field's fluctuation.

Consider now: 2 Useful choices for foliations of spacetime into spacelike hypersurfaces of equal time:

b.) Foliate so that on surfaces of equal time, η, one has: $\Psi \equiv 0$

In this case, along each equal time surface there is no local bloating - but instead the inflaton field fluctuates.

Recall:

$$\tau(x,\eta) := -\frac{a_0'}{a_0}\left(\phi_0(\eta)'\right)^{-1}\varphi(x,\eta) - \Psi(x,\eta)$$

Question:

Why does the contribution of the inflaton in $\tau(x,\eta)$ take this particular form:

$$\frac{a'(\eta)}{a(\eta)}\frac{\varphi(x,\eta)}{\phi_0'(\eta)} \quad ?$$

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Note: Only possible if ϕ decays over time (e.g. slow roll inflation, but not de Sitter).

$\rightsquigarrow$ We see that $r(x,\eta)$ expresses now purely metric fluctuations

$\rightsquigarrow$ Technically, these are fluctuations in the "intrinsic curvature". (Local bloating)

Recall:

$$r(x,\eta) := -\frac{a_0'}{a_0}\left(\phi_0(\eta)'\right)^{-1}\varphi(x,\eta) - \Psi(x,\eta)$$

Question:

Why does the contribution of the inflaton in $r(x,\eta)$ take this particular form:

$$\frac{a'(\eta)}{a(\eta)}\,\frac{\varphi(x,\eta)}{\phi_0'(\eta)} \quad ?$$

Answer:

* The inflaton's inhomogeneities imply locally varying expansion rates.

$\Rightarrow$ some regions are ahead, others lag behind in their expansion.

* Changing the spacetime slicing from a) to b) has to turn pure intrinsic curvature, namely local bloating

$$\frac{\delta a(x,\eta)}{a(\eta)}$$

into pure inflaton fluctuations $\varphi(x,\eta)$.

* Indeed:

$\delta\eta(x)$ is the time "lag" between slicings a) and b)

$$\frac{\delta a}{a} = \frac{1}{a}\frac{\delta a}{\delta\phi}\delta\phi = \frac{1}{a}\frac{\delta a}{\delta\eta}\frac{\delta\eta}{\delta\phi}\delta\phi = \frac{a'}{a}\frac{1}{\phi'}\delta\phi$$

$$= \frac{a'}{a}\frac{1}{\phi'}\varphi \quad \checkmark$$

Ramifications:

* The intrinsic curvature inhomogeneities

very large when ϕ_0' is very small

$$r = -\Psi - \frac{a'}{a}\frac{1}{\phi_0'}\varphi$$

can become strongly enhanced, namely, as it happens, for close to de Sitter inflation:

i.e., for $a(t) \approx e^{Ht}$

i.e., for $H = \frac{\dot a}{a} \approx \text{const}$ (recall: $H \sim \sqrt{V(\phi)}$)

i.e., for $\phi \approx \text{const}$

i.e., for: $\phi' \approx 0$

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to turn pure intrinsic curvature, namely local stretching

$$\frac{\delta a(x,\eta)}{a(\eta)}$$

into pure inflaton fluctuations $\varphi(x,\eta)$.

* Indeed:

$\delta\eta(x)$ is the time "lag" between slicings a.) and b.)

$$\frac{\delta a}{a} = \frac{1}{a}\frac{\delta a}{\delta\phi}\delta\phi = \frac{1}{a}\frac{\delta a}{\delta\eta}\frac{\delta\eta}{\delta\phi}\delta\phi = \frac{a'}{a}\frac{1}{\phi'}\delta\phi$$

$$= \frac{a'}{a}\frac{1}{\phi'}\varphi \checkmark$$

... as it happens, for close to de Sitter inflation:

i.e., for $a(t) \approx e^{Ht}$

i.e., for $H = \frac{\dot a}{a} \approx \text{const}$ (recall: $H \sim \sqrt{V(\phi)}$)

i.e., for $\dot\phi \approx \text{const}$

i.e., for: $\phi' \approx 0$

□ Why? Recall that:

$$\frac{\delta a}{a} = \frac{1}{a}\frac{\delta a}{\delta\eta}\frac{\delta\eta}{\delta\phi}\delta\phi = \frac{a'}{a}\frac{1}{\phi'}\varphi$$

Thus: Assume $\phi' = \frac{\delta\phi}{\delta\eta} \ll 1$

$$\Rightarrow \frac{\delta\eta}{\delta\phi} \gg 1$$

□ Intuition:

$\frac{\delta\eta}{\delta\phi} \gg 1$ means that the local time-lag $\delta\eta$ between slicings a.) and b.) is large.

This could mean large $\varphi(x,\eta)$ against assumption.

Analogous to: A river in a plain meanders the more widely, the flatter the plain is.

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$$\Rightarrow \frac{\delta\eta}{\delta\phi} \gg 1$$

Intuition:

$\frac{\delta\eta}{\delta\phi} \gg 1$ means that the local time-lag $\delta\eta$ between slicings a.) and b.) is large. This could mean large $r(x,\eta)$ against assumption.

Could it be a problem?

Observations: We know the size of $|r|$ from the CMB. The curvature fluctuations r are of order 10^{-5}. Also, there is evidence that the Hubble radius increased during inflation. Namely, the fluctuations of modes that crossed it late are smaller. So inflation was significantly different from de Sitter.

Is there a preferred slicing of spacetime, say a) or b) in nature?

* Not during inflation, but at its end point!

So it is slicing type a.) * Why? At each point in space, inflation ends the moment the value of ϕ drops to its minimum. Thus, $r(x,\eta)$ is intrinsic curvature.

The expanded action

The action
$$S = \frac{-1}{16\pi G}\int R\sqrt{|g|}\,d^4x + \frac{1}{2}\int\left((\partial_\nu\phi)(\partial^\nu\phi) - V(\phi)\right)\sqrt{|g|}\,d^4x$$

must be expanded to second order in the inhomogeneities in order to obtain their equations of motion to first order:

$$S = S_S + S_T$$

The scalar part:

$$\boxed{S_S = \frac{1}{2}\int z^2(\eta)\left(\frac{\partial}{\partial x^\mu} r(x,\eta)\right)\left(\frac{\partial}{\partial x^\nu} r(x,\eta)\right)\eta^{\mu\nu}\,d^4x}$$

Here: $\boxed{z(\eta) := \frac{a_0^2(\eta)}{a_0'(\eta)}\phi_0'(\eta)} \approx \underbrace{\text{const}\cdot a_0(\eta)}$

because $a_0'(\eta) \approx \text{const}\, a(\eta)$ and $\phi_0' \approx \text{const}$ during inflation

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inflation. Namely, the fluctuations of modes that crossed it late are smaller. So inflation was significantly different from de Sitter.

Is there a preferred slicing of spacetime, say a) or b) in nature?

* Not during inflation, but at its end point!

So it is slicing type a) } * Why? At each point in space, inflation ends the moment the value of ϕ drops to its minimum. Then, $r(x,\eta)$ is intrinsic curvature.

Remark:

This action is similar to the scalar action which we considered so far:

$$S_{\phi} = \frac{1}{2}\int a^2(\eta)\left(\frac{\partial}{\partial x^\mu}\phi(x,\eta)\right)\left(\frac{\partial}{\partial x^\nu}\phi(x,\eta)\right)\eta^{\mu\nu}\,d^4x$$

The only difference is that $a(\eta)$ is now replaced by the more complicated (but still classical fixed background function) $z(\eta)$.

The tensor part: Each h_{ij} has exactly our well-known action:

$$\boxed{S_T' = \frac{1}{64\pi G}\sum_{i,j=1}^{3}\int a^2(\eta)\frac{\partial}{\partial x^\mu}\left(h'_{ij}(x,\eta)\right)\frac{\partial}{\partial x^\nu}\left(h'_{ij}(x,\eta)\right)\eta^{\mu\nu}\,d^4x \qquad !}$$

... be expanded to second order in the inhomogeneities in order to obtain their equations of motion to first order:

$$S' = S_S' + S_T'$$

The scalar part:

$$\boxed{S_S' = \frac{1}{2}\int z^2(\eta)\left(\frac{\partial}{\partial x^\mu}r(x,\eta)\right)\left(\frac{\partial}{\partial x^\nu}r(x,\eta)\right)\eta^{\mu\nu}\,d^4x}$$

Here: $\boxed{z(\eta) := \frac{a_0^2(\eta)}{a_0'(\eta)}\phi_0'(\eta)} \approx \underbrace{\text{const}\cdot a_0(\eta)}$

because $a_0'(\eta) \simeq \text{const}\,a(\eta)$ and $\phi_0' \simeq \text{const}$ during inflation

Quantization of r and h_{ij}:

The equations of motion come out to be:

Scalar:

$$r_k''(\eta) + \frac{2z'(\eta)}{z(\eta)}r_k'(\eta) + k^2 r_k(\eta) = 0$$

Tensor:

$$h_{ij_k}''(\eta) + \frac{2a'(\eta)}{a(\eta)}h_{ij_k}'(\eta) + k^2 h_{ij_k}(\eta) = 0$$

Exercise: verify

Strategy:

Define auxiliary fields, so that there will be no friction term in the equation of motion.

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The only difference is that $a(\eta)$ is now replaced by the more complicated (but still classical fixed background function) $z(\eta)$.

- The tensor part: Each h_{ij} has exactly our well-known action:

$$\boxed{S_T = \frac{1}{64\pi G}\sum_{i,j=1}^{3}\int a^2(\eta)\frac{\partial}{\partial x^\mu}\left(h^i{}_j(x,\eta)\right)\frac{\partial}{\partial x^\nu}\left(h^i{}_j(x,\eta)\right)\eta^{\mu\nu}d^4x \quad !}$$

Tensor:

$$h''_{ij_k}(\eta) + \frac{2a'(\tau)}{a(\tau)}h'_{ij_k}(\eta) + k^2 h_{ij_k}(\eta) = 0$$

- Exercise: verify

- Strategy:

Define auxiliary fields, so that there will be no friction term in the equation of motion.

- Recall: Previously in this course, this definition

$$\chi(x,\eta) := a(\eta)\,\phi(x,\eta)$$

achieved an eqn of motion without friction term:

$$\chi''_k(\eta) + \left(k^2 - \frac{a''}{a}\right)\chi_k(\eta) = 0$$

- Scalar components:

Since in their action a is replaced by z, we need:

$$u(x,\eta) := -z(\eta)\,r(x,\eta)$$

convenient factor

This yields the eqn. of motion without friction:

$$u''_k(\eta) + \left(k^2 - \frac{z''(\eta)}{z(\eta)}\right)u_k(\eta) = 0$$

- The tensor components:

Here, we can define as previously in the course:

$$p_{ij}(x,\eta) := \frac{1}{\sqrt{32\pi G}}\,a(\eta)\,h_{ij}(x,\eta)$$

convenient factor

to obtain the eqn of motion:

$$p''_{ij_k}(\eta) + \left(k^2 - \frac{a''(\eta)}{a(\eta)}\right)p_{ij_k}(\eta) = 0$$

Note: * The components of p_{ij} are not all independent, because h_{ij} obeys:

$$h_{ij} = h_{ji} \quad \text{and} \quad \sum_{i=1}^{3} h_{ii} = 0 \quad \text{and in particular:}$$

$$\sum_{i=1}^{3}\frac{\partial}{\partial x^i}h_{ij}(x,\eta) = 0 \quad \text{i.e.} \sum_{i=1}^{3} k_i\, h_{ij}(k,\eta) = 0$$

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Scalar components:

Since in their action a is replaced by z, we need:

$$u(x,\eta) := -z(\eta)\, r(x,\eta)$$

convenient factor

This yields the eqn. of motion without friction:

$$u_k''(\eta) + \left(k^2 - \frac{z''(\eta)}{z(\eta)}\right) u_k(\eta) = 0$$

to obtain the eqn of motion:

$$p_{ij_k}''(\eta) + \left(k^2 - \frac{a''(\eta)}{a(\eta)}\right) p_{ij_k}(\eta) = 0$$

Note: * The components of p_{ij} are not all independent, because h_{ij} obeys:

$$h_{ij} = h_{ji} \text{ and } \sum_{i=1}^{3} h_{ii} = 0 \text{ and in particular:}$$

$$\sum_{i=1}^{3} \frac{\partial}{\partial x_i} h_{ij}(x,\eta) = 0 \quad \text{i.e.} \sum_{i=1}^{3} k_i h_{ij}(k,\eta) = 0$$

* But $\vec{k}$ is the vector that points in the direction in which the mode $\vec{k}$ propagates.

$\Rightarrow$ The equation

$$\sum_{i=1}^{3} k_i h_{ij}(k,\eta) = 0$$

(For fixed j, the vectors h_{ij} and k_i are orthogonal) $\rightarrow$ means that h_{ij} has no component in the propagation direction:

$\Rightarrow$ h_{ij} describes transversal waves (like e.g. tectonic shear waves), not longitudinal waves.

$\rightsquigarrow$ h_{ij} possesses only 2 degrees of freedom:

$v_{k,\lambda}(\eta)$ with $\lambda = 1,2$ or $+\ \times$

* Polarization decomposition:

$$p_{ij}(k,\eta) := \sum_{\lambda=1,2} v_{k,\lambda}(\eta)\, \varepsilon_{ij}(k,\lambda)$$

Here, $\varepsilon_{ij}(k,\lambda)$ are for each k two arbitrary but fixed matrices, obeying $\sum_{i,j=1}^{3} \varepsilon_{ij}(k,1)\, \varepsilon_{ji}(k,2) = 0$ and:

$$\varepsilon_{ij} = \varepsilon_{ji}, \quad \sum_{i=1}^{3} \varepsilon_{ii} = 0, \quad \sum_{i=1}^{3} k_i \varepsilon_{ij} = 0$$

It is convenient to choose

$$\varepsilon_{ij}(-k,\lambda) = \varepsilon_{ij}^{*}(k,\lambda)$$

because then we have (as usual):

$$v_{k,\lambda}(\eta) = v_{-k,\lambda}^{*}(\eta)$$

$$\Rightarrow \quad v_{k,\lambda}''(\eta) + \left(k^2 - \frac{a''}{a}\right) v_{k,\lambda}(\eta) = 0$$

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(For fixed j, the vectors h_{ij} and k_i are orthogonal) $\rightarrow$ means that h_{ij} has no component in the propagation direction:

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but fixed matrices, obeying $\sum_{i,j=1}^{3} \varepsilon_{ij}(k,1)\,\varepsilon_{ji}(k,2) = 0$ and:

$$\varepsilon_{ij} = \varepsilon_{ji}, \quad \sum_{i=1}^{3} \varepsilon_{ii} = 0, \quad \sum_{i=1}^{3} k_i\,\varepsilon_{ij} = 0$$

It is convenient to choose

$$\varepsilon_{ij}(-k,\lambda) = \varepsilon^{*}_{ij}(k,\lambda)$$

because then we have (as usual):

$$v_{k,\lambda}(\eta) = v^{*}_{-k,\lambda}(\eta)$$

$$\Rightarrow \quad v''_{k,\lambda}(\eta) + \left(k^2 - \frac{a''}{a}\right) v_{k,\lambda}(\eta) = 0$$

The goal:
Quantize $\hat{u}_k(\eta)$, $\hat{p}_{ij}(\eta)$ and calculate $\delta\tau_k(\eta)$ and $\delta h_{ij}(\eta)$ from them at horizon crossing (after which they are constant).

Notice: We cannot simply re-use our de Sitter results b/c Mukhanov variable!

Expectations:
* Fluctuations of $\hat{\tau}$ yield local spacetime expansion (and thus eventually cooling) fluctuations
  $\rightarrow$ temperature spectrum in CMB
* Fluctuations of $\hat{h}$ yield grav. waves background. Should appear in polarization spectrum of CMB.

$\rightsquigarrow$ BICEP2 experiment almost found it!

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