Hankel Matrices and Bootstrapping Quantum Mechanics

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2026 年 8 月 28 日

Background

Most quantum mechanical systems, even in one dimension, are not soluble by analytical methods. Finding a novel method to solve quantum mechanical systems is of great importance.

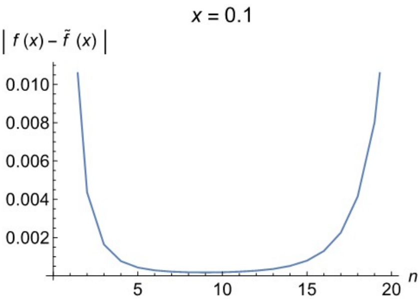
How to solve the spectrum problem of quantum mechanics?

- WKB approximation
- **Truncation method**
- (Thermodynamic) Bethe ansatz(TBA/BA)
- Topological string theory/Spectrum problem correspondence
- **Bootstrapping quantum mechanics**
- ......

Background

In theoretical physics, the precision of numerical calculations is not merely a technical concern; it also involves numerous physical considerations, such as nonperturbative effects.

$$f(x)=\int_0^\infty \frac{e^{-t}}{1+tx}dt \qquad \tilde{f}(x)=\sum_{n=0}^{\infty}(-1)^n n! x^n \tag{1}$$



Introduction

Bootstrapping quantum mechanics

Like the conformal bootstrp method, we do not solve the Schrödinger equation, but use some axioms(such as the positivity constraints) to derive the spectrum.

- 1. On an eigenstate of the Hamiltonian, it is true that certain expectation values vanish identically

$$\begin{aligned} \langle [H, \mathcal{O}] \rangle &= 0, \\ \langle H\mathcal{O} \rangle &= E\langle \mathcal{O} \rangle. \end{aligned} \tag{2}$$

- 2. Positivity constraints(for any operator $\mathcal{O}$).

$$\langle \mathcal{O}^\dagger \mathcal{O} \rangle \geq 0. \tag{3}$$

Introduction

Example: one dimensional quantum mechanics

$$H = \frac{p^2}{2} + V(x). \tag{4}$$

(1) First, we use the equation (2), which allows us to relate different moments of x, p. For example, take $\mathcal{O} = x^s$:

$$\langle [H, x^s] \rangle = 0 \Rightarrow s\langle x^{s-1} p \rangle = \frac{i}{2} s(s-1)\langle x^{s-2} \rangle. \tag{5}$$

(2) Second, take $\mathcal{O} = x^s p$

$$0 = s\langle x^{s-1} p^2 \rangle + \frac{1}{4} s(s-1)(s-2)\langle x^{s-3} \rangle - \langle x^s V'(x) \rangle. \tag{6}$$

Introduction

(3) Finally, we consider the second identity in (2), and taking $\mathcal{O} = x^{s-1}$

$$E\langle x^{s-1}\rangle = \frac{1}{2}\langle x^{s-1}p^2\rangle + \langle x^{s-1}V(x)\rangle. \tag{7}$$

Recursion relation

$$0 = 2sE\langle x^{s-1}\rangle + \frac{1}{4}s(s-1)(s-2)\langle x^{s-3}\rangle - \langle x^s V'(x)\rangle - 2s\langle x^{s-1}V(x)\rangle. \tag{8}$$

Virial theorem($s = 1$):

$$E = \langle V(x)\rangle + \frac{1}{2}\langle xV'(x)\rangle. \tag{9}$$

Choosing the minimal set $S = \{E, \langle x\rangle, \cdots\}$ as initial conditions

- $V(x) = \frac{1}{2}\omega^2 x^2; \quad S = E;$
- $V(x) = gx^3; \quad S = \{E, \langle x\rangle, \langle x^2\rangle\}$
- $V(x) = gx^4; \quad S = \{E, \langle x^2\rangle\}$

Introduction

Positivity constraint

For a given point $s \in S$, we can construct a moment sequence from the recursion relation. The positivity constrain can give us a physical way to accept or reject such a moment sequence $\{\langle x \rangle^n\}$.

Let $\mathcal{O} = \sum_{n=0}^{K} c_n x^n$, for any $c_n \in \mathbb{C}$, we have

$$\langle \mathcal{O}^\dagger \mathcal{O} \rangle = \sum_{n,m=0}^{K} c_n^* c_m \langle x^{n+m} \rangle \geq 0. \tag{10}$$

This is equivalent to the Hankel matrix $M_{ij} = \langle x^{i+j} \rangle$ being positive semidefinite.

The positivity of the Hankel matrix can be checked by the Sylvester's criterion, which states that a matrix is positive semidefinite if and only if all of its leading principal minors are nonnegative. This gives us a set of inequalities

$$\det(M_{ij})_{0\leq i,j\leq k} \geq 0, \quad k = 0, 1, \cdots, K, \tag{11}$$

which makes sure the allowed region can be shirnked as K increases. In the large K limit, the allowed region will converge to the physical spectrum.

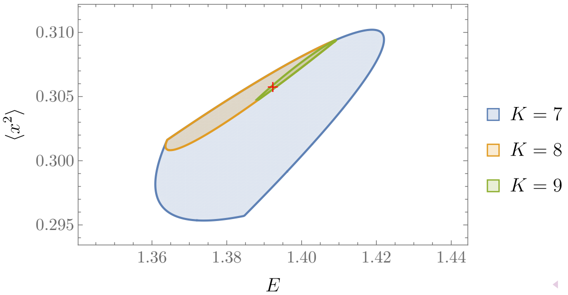
Introduction

Example: quantum anharmonic oscillator

$$H = p^2 + x^2 + gx^4, \qquad [x, p] = i \tag{12}$$

Recursion relation:

$$4g(s+2)\langle x^{s+3}\rangle = 4sE\langle x^{s-1}\rangle + s(s-1)(s-2)\langle x^{s-3}\rangle - 4(s+1)\langle x^{s+1}\rangle. \tag{13}$$



Introduction

This method can not directly yield the energy spectrum; instead, it determines the interval where the spectrum resides by scanning the allowed parameter regions. As a result, it consumes substantial computational resources and suffers from limited precision.

One approach to improve precision introduces two-dimensional operators of the form $\mathcal{O} = \sum_{i,j=0}^{K} c_{ij} x^i p^j$, which expands the dimension of the matrix from the original $K+1$ to $(K+1)^2$.

Another methods, like null bootstrap method, also need to scan the allowed parameter regions, which is also computationally expensive.

Hankel matrix and Quantization condition

The bootstrapping matrix is positive semidefinite, and the spectrum can be determined by semidefinite programming(SDP).

Another way to determine the spectrum is to find the boundary of the allowed region in the parameter space. The boundary is determined by the quantization condition, which is equivalent to the Hankel matrix being singular.

For the example of the quantum anharmonic oscillator, the Hankel matrix is $M_{ij} = \langle x^{i+j} \rangle, \quad 0 \leq i, j \leq K.$, and $M_{ij} = 0$, for $i + j$ odd. The determinant can be factorized as

$$\mathrm{Det}(M_{ij})_{0\leq i,j\leq K} = \mathrm{Det}(M_{2i,2j})_{0\leq i,j\leq K/2} \mathrm{Det}(M_{2i+1,2j+1})_{0\leq i,j\leq K/2}. \tag{14}$$

Hankel matrix and Quantization condition

Quantization condition

$$\mathrm{Det}(M_{2i,2j})_{0\leq i,j\leq K/2} = \mathrm{Det}(M_{2i+1,2j+1})_{0\leq i,j\leq K/2} = 0. \tag{15}$$

Question:

What are the quantization conditions for Hamiltonian systems that require three or more initial conditions?

For the general cases, the bootstrap matrices can be factorized by

$$\mathrm{Det}(M_{ij}) = \prod_{i=1}^{N+1} \lambda_i. \tag{16}$$

Hankel matrix and Quantization condition

A nature conjecture is that the first s smallest eigenvalues all converge to zero, where s is the number of initial conditions. In the large N limit, the determinant of bootstrapping matrix must be vanish, so it is surffient to determine the spectrum.

For a positive measure μ, we can define the moments as

$$s_n = \int x^n d\mu(x), \quad n = 0, 1, 2, \cdots \tag{17}$$

The smallest eigenvalue of the Hankel matrix can be defined as $H_n = (s_{i+j})_{i,j=0}^{n-1}$ is $\lambda_1(H_n)$. And the following theorem holds:

定理

(Berg, Chen, and Ismail, 2002) *If μ is determinate, then $\lim_{n\to\infty} \lambda_1(H_n) = 0$. And if there exists a strictly positive constant such that all λ_N are greater than this constant, then the measure μ is indeterminate.*

Hankel matrix and Quantization condition

Index of Determinacy

For a determinate measure μ, the index of determinacy is defined as

$$\mathrm{ind}_z(\mu) = \sup\{k \in \mathbb{N} |\ |t - z|^{2k}\mu \text{ is determinate}\}. \tag{18}$$

定理

(Berg and Duran, 1997) *If a measure is continuous, its determinacy index is infinite. A finite determinacy index exists only when the measure is discrete.*

Quantization condition

$$\lim_{N\to\infty} \lambda_1(H_N) = 0, \quad \lim_{N\to\infty} \lambda_2(H_N) = 0, \cdots, \quad \lim_{N\to\infty} \lambda_s(H_N) = 0. \tag{19}$$

Hankel matrix and Quantization condition

Although these smallest eigenvalues all tend to zero, their rates of convergence to zero differ. A superior approach is to construct distinct Hankel matrices, compute the determinants of these Hankel matrices, and impose the condition that all these determinants converge to zero. This method is more efficient and exhibits a faster convergence rate than directly solving for the eigenvalues.

$$\mathrm{Det}(M_{ij})_{0\leq i,j\leq K} = \mathrm{Det}(M_{ij})_{1\leq i,j\leq K+1} = \cdots = \mathrm{Det}(M_{ij})_{s-1\leq i,j\leq K+s-1} = 0 \tag{20}$$

Recursion relation for the anharmonic oscillator

For the quartic oscillator the Hamiltonian is

$$H = p^2 + x^2 + gx^4, \qquad [x, p] = i. \tag{21}$$

The stationarity relation $\langle [H, x^s] \rangle = 0$ gives the bootstrap recursion

$$4g(s+2)\langle x^{s+3}\rangle = 4sE\langle x^{s-1}\rangle + s(s-1)(s-2)\langle x^{s-3}\rangle - 4(s+1)\langle x^{s+1}\rangle. \tag{22}$$

Writing $\nu_k = \langle x^{2k}\rangle$, the moments form the affine family

$$\nu_k = a_k(E) + b_k(E)\nu_1. \tag{23}$$

Hankel matrix for the anharmonic oscillator

The Hankel matrix is

$$H_n(E, \nu_1) = \left(\nu_{i+j}\right)_{0 \leq i,j \leq n-1} = A_n(E) + \nu_1 B_n(E). \tag{24}$$

For fixed E, the boundary of the positivity region is determined by

$$\det\left(A_n(E) + \nu_1 B_n(E)\right) = 0. \tag{25}$$

This is the generalized eigenvalue problem

$$A_n(E)v = -\nu_1 B_n(E)v. \tag{26}$$

Hankel matrix for the anharmonic oscillator

For the x^4 model the free parameters are E and ν_1. At finite dimension, the physical value of ν_1 is obtained by looking for a repeated generalized eigenvalue of the pencil $A_n(E) + \nu_1 B_n(E)$. Equivalently, one scans E and minimizes

$$\Delta_n(E) = \min_{i \neq j} \left| \lambda_i(E) - \lambda_j(E) \right|. \tag{27}$$

The double-root condition

$$\det H_n(E, \nu_1) = 0, \qquad \det H_{n+1}(E, \nu_1) = 0 \tag{28}$$

is therefore the finite-dimensional quantization condition. Its $n \to \infty$ limit is the physical spectrum.

Numerical spectrum for $g = 1$

Using the generalized-eigenvalue method at finite Hankel dimension, the first six levels are reproduced to high accuracy.

Level	E_{double}	Absolute error
0	1.392351645161	3.63×10^{-9}
1	4.648812958900	2.55×10^{-7}
2	8.655051281534	1.32×10^{-6}
3	13.156728822338	7.51×10^{-5}
4	18.057581043076	2.36×10^{-5}
5	23.297388664818	5.28×10^{-5}

At finite truncation some nonphysical double roots are also present. These do not converge as $n \to \infty$ and are therefore excluded by the infinite-dimensional condition.

Some limitations of bootstrapping quantum mechanics

The bootstrap method is powerful but is not universal. Three typical obstructions are as follows.

- Ambiguity: for $H = p^2 + (x - L)^2 + \cosh x$, the bootstrap data do not distinguish different real values of L.
- Higher-dimensional potentials: for $H = p^2 + x^2 + y^2 + g(x^2 + y^2)^2$, the moments $\langle x^n y^m \rangle$ satisfy the recursion, but positivity can still fail.
- Divergent moments: for $H = e^x + e^{-x} + e^p + e^{-p}$, the moment $\langle x^n \rangle$ diverges once $n \geq 2\pi/\hbar$.

Question:

When is the Bootstrapping quantum mechanics equivalent to the spectral problems?

Spectrum problem for a general polynomial potential

Let

$$V(x) = v_{2m}x^{2m} + \sum_{k=0}^{2m-1} v_k x^k, \qquad v_{2m} > 0,\ m \geq 1, \tag{29}$$

and set $H = -\frac{d^2}{dx^2} + V(x)$. Its spectrum is discrete and simple:

$$E_0 < E_1 < E_2 < \cdots, \qquad E_n \to +\infty. \tag{30}$$

For fixed E, write $u_E = V - E$. The symmetric-square operator is

$$\mathcal{L}_E = \frac{d^3}{dx^3} - 4u_E\frac{d}{dx} - 2V'. \tag{31}$$

Hankel positivity is exact at infinite dimension

Call E admissible if there is a positive probability measure μ_E with all moments finite,

$$s_n = \int_{\mathbb{R}} x^n \, d\mu_E(x) < \infty, \tag{32}$$

such that

$$H_N(\mu_E) = \left(s_{i+j}\right)_{0 \le i,j \le N} \succeq 0, \qquad N = 0, 1, 2, \ldots, \tag{33}$$

and

$$\mathcal{L}_E \mu_E = 0 \qquad \text{in} \quad \mathcal{D}'(\mathbb{R}). \tag{34}$$

Then

$$\boxed{E \in \mathrm{Spec}(H) \iff E \text{ is admissible}}. \tag{35}$$

If E is an eigenvalue, the admissible measure is unique and equals

$$\mu_E(dx) = \psi_E(x)^2 \, dx. \tag{36}$$

Proof, part 1: the symmetric square

The Schrödinger equation is

$$\psi'' = u_E \psi. \tag{37}$$

For $\rho = \psi_i \psi_j$, a direct calculation gives

$$\rho''' - 4u_E \rho' - 2u_E' \rho = 0. \tag{38}$$

If ψ_1, ψ_2 are two independent solutions, then the general solution of this third-order equation is

$$\rho = A\psi_1^2 + B\psi_1\psi_2 + C\psi_2^2. \tag{39}$$

Proof, part 2: integrability selects ψ_E^2

Assume that E is not an eigenvalue. Let f_+ decay at $+\infty$ and f_- decay at $-\infty$. Then

$$\rho = Af_+^2 + Bf_+f_- + Cf_-^2. \tag{40}$$

At $+\infty$, f_-^2 dominates, so $C = 0$; at $-\infty$, f_+^2 dominates, so $A = 0$. Hence $\rho = Bf_+f_-$. Liouville–Green asymptotics give

$$\left|f_+(x)f_-(x)\right| \sim \frac{1}{2\sqrt{V(x) - E}} \sim |x|^{-m}. \tag{41}$$

The requirement that all moments be finite forces $B = 0$, a contradiction. Thus E must be an eigenvalue.

Proof, part 2: the eigenvalue case

If E is an eigenvalue, choose the normalized eigenfunction ψ_E and an independent solution y_2. The general solution is

$$\rho = A\psi_E^2 + B\psi_E y_2 + Cy_2^2. \tag{42}$$

At both infinities y_2^2 dominates, so $C = 0$. Since

$$\left|\psi_E y_2\right| \sim |x|^{-m}, \tag{43}$$

the condition that all moments be finite forces $B = 0$. Normalization gives $A = 1$, hence

$$\mu_E = \psi_E^2\, dx. \tag{44}$$

Summary

- We putforward a new bootstrap method to determine the spectrum of quantum mechanical systems.
- For a general polynomial potential, the spectrum problem is equivalent to the existence of a positive measure satisfying a third-order symmetric-square equation.
- The spurious roots of finite truncation are inevitable.

$$\boxed{E \in \mathrm{Spec}(H) \iff E \text{ is admissible}}. \tag{45}$$

Thanks!