

# Microscopic ensemble bootstrap in phase space

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## Abstract

The bootstrap method which has been studied under many quantum mechanical models turns out to be feasible in microcanonical ensembles as well. While the approach of Nakayama (2022 *Mod. Phys. Lett. A* 37 2250054) produces a sector when energy is negative, in this paper we report a method that has stronger constraints and results in a smaller region. We also study other models to demonstrate the effectiveness of our method.

Keywords: numerical bootstrap, microcanonical ensemble, Poisson bracket, bootstrap, oscillator

## 1. Introduction

Bootstrap, a novel yet promising method which has recently been studied in quantum mechanics, is a way to utilize the very general self-consistency condition and solve the system numerically. Developed in the 1960s and 70s [1], the method was later applied in large  $N$  systems [2–4], lattice theory [5–8], conformal field theory [9–13], as well as matrix models [14, 15]. This technique is also used to bootstrap the Dirac ensembles [16], some have integrated this method with artificial intelligence [17, 18]. And the bootstrap approaches used to find the eigen energies for bound states in recent papers are mostly inspired by Han [19]. Some papers have studied different systems using this method [20–25], and many have reported the accuracy and high precision of the method. In certain cases the bootstrap evolves into Dirac's ladder operator approach and can be solved analytically, suggesting some underlying mechanism of this method [26]. In this paper, we report an approach that can be seen as a classical correspondence to Han's.

Although widely studied in quantum mechanics, one can also apply the method to microcanonical ensembles as the fundamental relations of bootstrapping are still applicable and have their classical correspondence (3), (4), and (5) as  $\hbar \rightarrow 0$ .

Nakayama [27] first introduced this method into the classical scenario, despite reporting the feasibility of the approach, he mentioned a peninsula in  $E < 0$  which does not converge even for larger bootstrap matrices in the double-well potential. In this paper, we use a different approach that incorporates more information in phase space and thus exhibiting a much stronger constraint. We will see that the

result of the double-well bootstrap in phase space cancels the sector region in  $E < 0$  compared to the  $x$  only bootstrap. Also, it is worth mentioning that the similar approach is applied to the quantum anharmonic oscillator [28], which can be seen as the quantum version of our method.

We also investigate coulomb potential, a harmonic oscillator and a non-relativistic Toda model. The first two can be solved analytically (here by analytically, we mean that the averages of the observables can be written in a form of  $E$ ) via the bootstrap approach which, however, are trivial cases. As for the non-relativistic Toda model, our approach in phase space once again demonstrates a more powerful restriction, maybe so overly powerful that we can merely see a few points in the result if the sample is not large enough. Since Hu [29] has discussed many models and derived lots of bootstrap equations, most of our models are modified versions of his.

Although our approach may have a stronger constraint, it still cannot converge to the exact solution in some places, like the non-relativistic Toda model. Not to mention that our approach consumes much more computing power, as the size of our bootstrap matrix is  $O(n^4)$ . However, the benefit is that we can easily achieve high precision when the result converges.

## 2. Microcanonical ensemble bootstrap

### 2.1. Bootstrap equations and matrices

Starting with the Hamiltonian we have

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

for a microcanonical ensemble, the average of an observable  $\mathcal{O}(x, p)$  is

$$\langle \mathcal{O}(x, p) \rangle = \frac{\int dx dp \mathcal{O}(x, p) \delta(E - H)}{\int dx dp \delta(E - H)}, \quad (2)$$

and we can easily find that

$$\langle \{H, \mathcal{O}\} \rangle = 0, \quad (3)$$

$$\langle H\mathcal{O} \rangle = E \langle \mathcal{O} \rangle, \quad (4)$$

here  $\{H, \mathcal{O}\}$  is the poisson bracket. As for the positivity constraints, obviously for any observable  $\mathcal{O}$  we would have

$$\langle \mathcal{O}^* \mathcal{O} \rangle \geq 0, \quad (5)$$

and by writing the observable as a polynomial of certain observable  $o$ ,  $\mathcal{O} = \sum_{i=0}^k a_i o^i$ , one can construct a bootstrap matrix which can be defined as

$$\mathcal{M}_{ij} = \langle (o^*)^i o^j \rangle, \quad i, j = 0, 1, \dots, k-1, \quad (6)$$

we can then rewrite the constraints (5) with matrix and vectors

$$\alpha^\dagger \mathcal{M} \alpha \geq 0, \quad (7)$$

as (7) should hold true for any vector  $\alpha$ , the bootstrap matrix  $\mathcal{M}$  must embody the positive semi definiteness i.e.  $\mathcal{M} \succcurlyeq 0$ , which is essentially an eigenvalue problem

$$\forall (\mathcal{M})_{\text{eigenvalue}} \geq 0. \quad (8)$$

When the observable  $\mathcal{O}$  is a coupling of two observables, say,  $A$  and  $B$

$$\mathcal{O} = \sum_{i,j=0}^{k-1} a_i b_j A^i B^j, \quad (9)$$

$$\mathcal{O}^* \mathcal{O} = \sum_{i_1 j_1, i_2 j_2=0}^{k-1} a_{i_1}^* b_{j_1}^* (B^*)^{j_1} (A^*)^{i_1} A^{i_2} B^{j_2} a_{i_2} b_{j_2}, \quad (10)$$

we can define two auxiliary matrices  $\mathcal{M}_{ij}^0 = (B^*)^j (A^*)^i$  and  $\mathcal{M}_{ij}^1 = A^i B^j$ , the constraints can be written as

$$\mathcal{M}_{ij} = \langle (\mathcal{M}^0 \otimes \mathcal{M}^1)_{ij} \rangle, \quad i, j = 0, 1, 2, \dots, k^2 - 1, \quad (11)$$

$$\mathcal{M} \succcurlyeq 0. \quad (12)$$

## 2.2. Recursion formula

Taking  $\mathcal{O}$  as  $x^m p^n$  and substituting Hamiltonian (1) into (3) and (4), we immediately obtain

$$\begin{aligned} n \left\langle \frac{dV}{dx} x^m p^{n-1} \right\rangle &= 2Em \langle x^{m-1} p^{n-1} \rangle \\ &\quad - 2m \langle V x^{m-1} p^{n-1} \rangle, \\ E \langle x^m p^n \rangle &= \frac{1}{2m} \langle x^m p^{n+2} \rangle + \langle V x^m p^n \rangle, \end{aligned} \quad (13)$$

this would do the trick for the potential with polynomial of  $x$ . When the potential is in the form of exponentials, we need to

take  $\mathcal{O}$  as  $e^{mx} p^n$

$$\begin{aligned} n \left\langle \frac{dV}{dx} e^{mx} p^{n-1} \right\rangle &= 2Em \langle e^{mx} p^{n-1} \rangle - 2m \langle V e^{mx} p^{n-1} \rangle, \\ E \langle e^{mx} p^n \rangle &= \frac{1}{2M} \langle e^{mx} p^{n+2} \rangle + \langle V e^{mx} p^n \rangle. \end{aligned} \quad (14)$$

## 2.3. Methodology framework

With the recursion formula (13) or (14) and a few initial values we can construct a whole bootstrap matrix  $\mathcal{M}$ , and by testing the positive semi definiteness of the matrix the validity of the initial values can be determined. By doing so over all the possible initial values we will eventually find the allowed regions restricted by positivity constraint.

## 3. Numerical examples

### 3.1. Double-well potential

The Hamiltonian of a double-well potential can be written as

$$H = p^2 - x^2 + x^4, \quad (15)$$

taking  $M = \frac{1}{2}$  and with (13) we have

$$\begin{aligned} 2(2n + m) \langle x^{m+3} p^{n-1} \rangle &= 2(m + n) \\ &\quad \times \langle x^{m+1} p^{n-1} \rangle + 2mE \langle x^{m-1} p^{n-1} \rangle, \end{aligned} \quad (16)$$

$$\begin{aligned} \langle H x^m p^n \rangle &= E \langle x^m p^n \rangle = \langle x^m p^{n+2} \rangle \\ &\quad - \langle x^{m+2} p^n \rangle + \langle x^{m+4} p^n \rangle, \end{aligned} \quad (17)$$

plus  $\langle \{H, x^m\} \rangle = 0$ , we get

$$\langle x^{m-1} p \rangle = 0, \quad (18)$$

and for simplicity, here we assume that the average of  $x$  to the odd powers is 0,

$$\langle x^m \rangle = 0, \quad \text{for all odd } m \quad (19)$$

with (16), (17), (18) and (19), plus the initial parameters  $E$  and  $\langle x^2 \rangle$ , we can construct the bootstrap matrix  $\mathcal{M}$ . The result is shown in figure 1. We also reproduced the result in [27] to make a comparison, which is shown in figure 2.

In contrast with [27], our result shows no peninsula when  $E$  is negative, as we include the information of the momentum. Although this  $xp$  bootstrap performs poorly when  $k=3$ , the allowed region narrows down rapidly when  $k=4$  and it continues to shrink as  $k$  gets larger. Note that in our program the scale of the bootstrap matrix is  $k^4$ , which is much larger compared to the single observable bootstrap program with the scale of  $k^2$ . So in the case  $k=5$ , the size of our bootstrap matrix is 625, about seven times bigger than that of the  $x$  bootstrap. However, the allowed region still does not shrink even when we set  $k=25$  for the  $x$  only bootstrap program, so we conclude that this bootstrap in phase space does have a much stronger constraint than the single observable one.

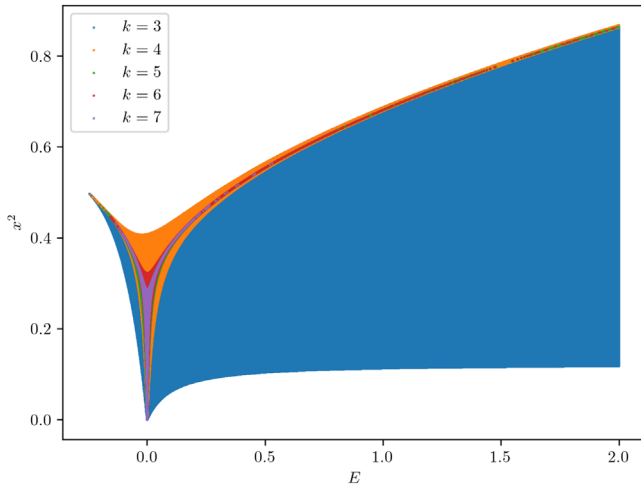


Figure 1. The allowed region in  $xp$  bootstrap.

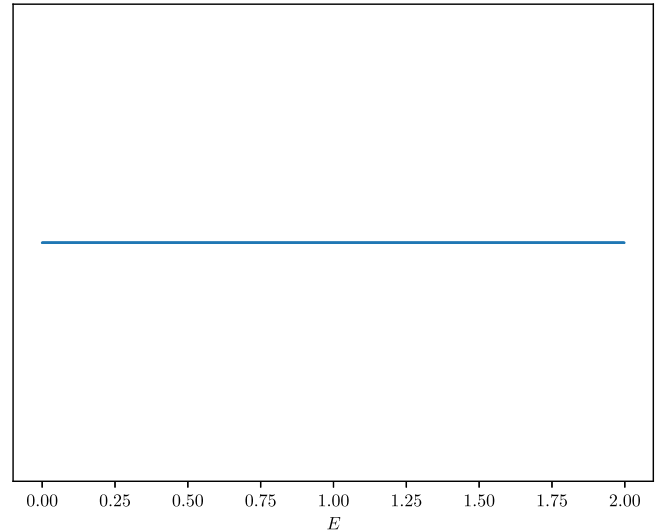


Figure 3. The allowed regions in  $xp$  bootstrap ( $k=4$ ) for harmonic oscillator.

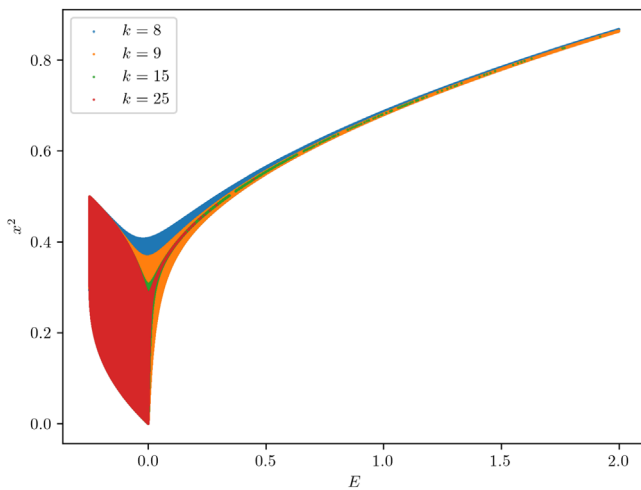


Figure 2. The allowed region in  $x$  bootstrap.

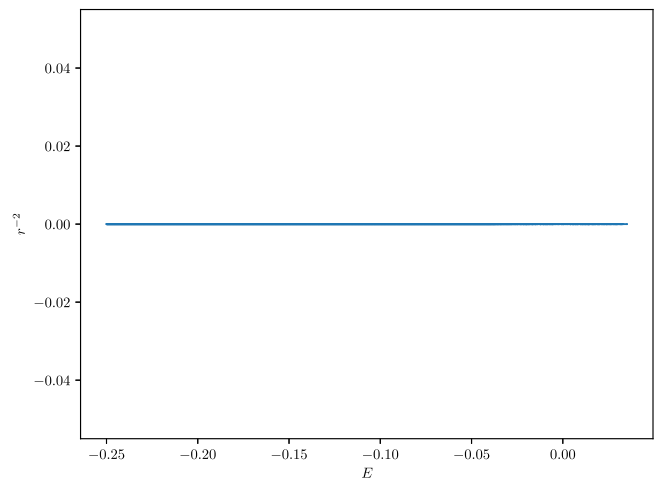


Figure 4. The allowed regions in  $x$  bootstrap ( $k=8$ ) for coulomb potential.

### 3.2. Harmonic oscillator and coulomb potential

Consider a harmonic oscillator, its Hamiltonian is

$$H = p^2 + x^2, \tag{20}$$

and again, we can obtain the recursion formula

$$\begin{aligned} 2n \langle x^{m+1} p^{n-1} \rangle &= 2Em \langle x^{m-1} p^{n-1} \rangle \\ &\quad - 2m \langle x^{m+1} p^{n-1} \rangle, \\ E \langle x^m p^n \rangle &= \langle x^m p^{n+2} \rangle + \langle x^{m+2} p^n \rangle, \end{aligned} \tag{21}$$

since  $\langle x^0 p^0 \rangle = 1$  and  $\langle x \rangle = 0$ , and (18) also holds true, we only need the initial energy  $E$  to bootstrap. The result of the bootstrap is shown in figure 3, as we sample  $E$  from negative to positive, we can see that the negative energies are rejected by the bootstrap program.

As for the coulomb potential, assume the Hamiltonian

$$H = p^2 - \frac{1}{r} + \frac{1}{r^2}, \tag{22}$$

here  $-\frac{1}{r} + \frac{1}{r^2}$  is the effective potential. The recursion

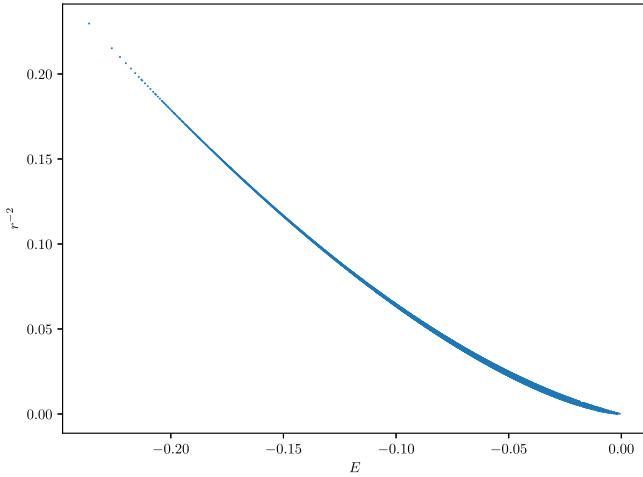
equations are

$$\begin{aligned} 2mE \langle r^{m-1} p^{n-1} \rangle &= 2(m-n) \langle r^{m-3} p^{n-1} \rangle \\ &\quad + (n-2m) \langle r^{m-2} p^{n-1} \rangle, \\ E \langle r^m p^n \rangle &= \langle r^m p^{n+2} \rangle - \langle r^{m-1} p^n \rangle + \langle r^{m-2} p^n \rangle. \end{aligned} \tag{23}$$

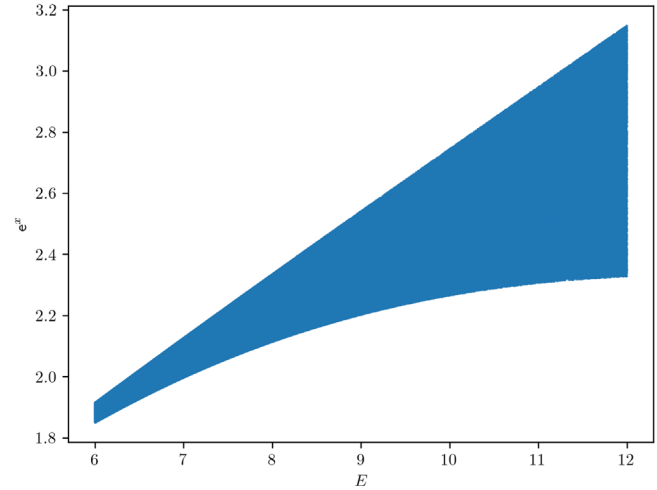
Substituting  $m=n=1$  into the first equation we can get

$$2E = -\langle r^{-1} \rangle, \tag{24}$$

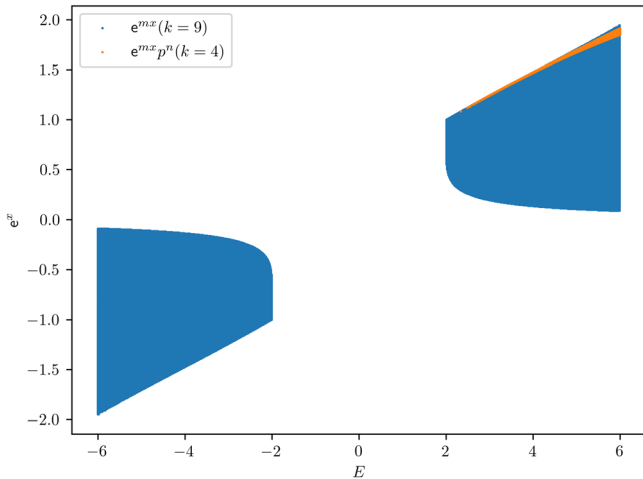
which is the Virial theorem. This time we only need  $E$  in the  $x$  bootstrap and the result is shown in figure 4. But for the  $xp$  bootstrap we also need the  $\langle r^{-2} \rangle$  because at some points the coefficients in (23) turn to 0, thus breaking the recursion. The initial value  $\langle r^{-2} \rangle$  gives the exact information we need to patch up these points, together with equation (18), the result of bootstrap is shown in figure 5. We can see that our  $xp$  bootstrap excludes the positive  $E$  which will cause the  $r$  to go negative, but the nuisance here is that we need to pay extra



**Figure 5.** The allowed regions in  $xp$  bootstrap ( $k=3$ ) for coulomb potential.



**Figure 7.** The allowed region diverges as  $E$  grows.



**Figure 6.** The allowed regions in  $xp$  bootstrap for non-relativistic Toda model.

attention to the numerical precision, for more details see the [appendix](#).

### 3.3. Non-relativistic Toda model

For a non-relativistic Toda model, the Hamiltonian could be written as

$$H = p^2 + e^x + e^{-x}, \tag{25}$$

the recursion equations are

$$\begin{aligned} (n + 2m)\langle e^{m+1}p^{n-1} \rangle &= 2E\langle e^m p^{n-1} \rangle \\ &+ (n - 2m)\langle e^{m-1}p^{n-1} \rangle, \\ E\langle e^{mx}p^n \rangle &= \langle e^{mx}p^{n+2} \rangle \\ &+ \langle e^{(m+1)x}p^n \rangle + \langle e^{(m-1)x}p^n \rangle, \end{aligned} \tag{26}$$

and studying  $\langle \{H, e^{mx}\} \rangle$  we have

$$\langle e^{(m-1)x}p \rangle = 0, \tag{27}$$

using the initial parameters  $E$  and  $\langle e^x \rangle$ , the bootstrap result is shown in figure 6.

The two observables bootstrap shows a much stronger constraint than the single one, in this non-relativistic Toda mode the  $e^{mx}$  bootstrap even fails to reject the negative  $E$ , and results in a much larger region. Our approach may have better precision, yet the allowed region still tends to diverge when  $E$  goes large in figure 7.

## 4. Conclusions

In this paper, we study two different bootstrap approaches in various models, our approach outperforms the single observable bootstrap program in most cases. We have seen that it cancels the sector region in a double-well potential, excludes some invalid  $E$ s in both the harmonic oscillator and non-relativistic Toda model. Although it performs better and achieves a much higher precision, it still fails to converge to the exact solution, and even tends to diverge. Like in the situations that  $E \rightarrow 0$  in the double-well potential,  $E \rightarrow \infty$  in the non-relativistic Toda model, we might still be missing some information to pin point the final answer.

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## Appendix. Numerical details

With the scale of the matrix growing at a fourth power rate, the floating-point precision becomes a bottleneck of our program as  $k$  grows. The typical double type in c++ no longer meets our need since the range of the eigenvalues can easily exceed  $10^{18}$ , thus leading to the loss of numerical precision in floating-point operations. In the coulomb potential above, this loss of precision will lead to some visible noise in the allowed region, resulting in a bulge where  $E$  is



**Figure A1.** The noise around  $E = 0$  in coulomb potential.

around 0 in figure A1. To eliminate this noise we set the precision in the code to 128 bits, as in figure 5.

The code is written in c++ with the Eigen library [30] for linear algebra and GNU MPFR [31] for multiple precision floating-point.

## References

- [1] Wikipedia contributors, Bootstrap model—Wikipedia, the free encyclopedia [https://en.wikipedia.org/w/index.php?title=Bootstrap\\_model&oldid=1195984682](https://en.wikipedia.org/w/index.php?title=Bootstrap_model&oldid=1195984682) (2024), [Online; accessed 28-January-2024]
- [2] Jevicki A, Karim O, Rodrigues J and Levine H 1983 Loop space Hamiltonians and numerical methods for large- $N$  gauge theories *Nucl. Phys.B* **213** 169
- [3] Jevicki A, Karim O, Rodrigues J and Levine H 1984 Loop-space Hamiltonians and numerical methods for large- $N$  gauge theories (II) *Nucl. Phys.B* **230** 299
- [4] Rodrigues J P 1985 Numerical solution of lattice Schwinger-Dyson equations in the large- $N$  limit *Nucl. Phys.B* **260** 350
- [5] Anderson P D and Kruczenski M 2017 Loop equations and bootstrap methods in the lattice *Nucl. Phys. B* **921** 702
- [6] Lawrence S 2021 Bootstrapping lattice vacua arXiv:2111.13007
- [7] Kazakov V and Zheng Z 2023 Bootstrap for lattice Yang–Mills theory *Phys. Rev.D* **107** L051501
- [8] Anderson P and Kruczenski M 2018 Loop equation in lattice gauge theories and bootstrap methods *EPJ Web Conf.* **175** 11011
- [9] Poland D, Rychkov S and Vichi A 2019 The conformal bootstrap: theory, numerical techniques, and applications *Rev. Mod. Phys.* **91** 015002
- [10] Guerrieri A, Penedones J a and Vieira P 2021 Where is string theory in the space of scattering amplitudes? *Phys. Rev. Lett.* **127** 081601
- [11] El-Showk S, Paulos M F, Poland D, Rychkov S, Simmons-Duffin D and Vichi A 2012 Solving the 3D Ising model with the conformal bootstrap *Phys. Rev. D* **86** 025022
- [12] El-Showk S, Paulos M F, Poland D, Rychkov S, Simmons-Duffin D and Vichi A 2014 Solving the 3d Ising model with the conformal bootstrap II. c-minimization and precise critical exponents *J. Stat. Phys.* **157** 869–914
- [13] Simmons-Duffin D 2017 The lightcone bootstrap and the spectrum of the 3d Ising cft *J. High Energy Phys.* **JHEP03(2017)086**
- [14] Lin H W 2020 Bootstraps to strings: solving random matrix models with positivity *J. High Energy Phys.* **JHEP06(2020)090**
- [15] Kazakov V and Zheng Z 2022 Analytic and numerical bootstrap for one-matrix model and “unsolvable” two-matrix model *J. High Energy Phys.* **JHEP06(2022)030**
- [16] Hessam H, Khalkhali M and Pagliaroli N 2022 Bootstrapping dirac ensembles *J. Phys. A: Math. Theor.* **55** 335204
- [17] Kántor G, Niarchos V and Papageorgakis C 2022 Conformal bootstrap with reinforcement learning *Phys. Rev.D* **105** 025018
- [18] Kántor G, Papageorgakis C and Niarchos V 2022 Solving conformal field theories with artificial intelligence *Phys. Rev. Lett.* **128** 041601
- [19] Han X, Hartnoll S A and Kruthoff J 2020 Bootstrapping matrix quantum mechanics *Phys. Rev. Lett.* **125** 041601
- [20] Bhattacharya J, Das D, Das S K, Jha A K and Kundu M 2021 Numerical bootstrap in quantum mechanics *Phys. Lett. B* **823** 136785
- [21] Berenstein D and Hulsey G 2022 Bootstrapping more QM systems *J. Phys. A* **55** 275304
- [22] Aikawa Y, Morita T and Yoshimura K 2022 Application of bootstrap to a  $\theta$  term *Phys. Rev.D* **105** 085017
- [23] Tchoumakov S and Florens S 2021 Bootstrapping bloch bands *J. Phys. A: Math. Theor.* **55** 015203
- [24] Bai D 2022 Bootstrapping the deuteron arXiv:2201.00551
- [25] Berenstein D and Hulsey G 2021 Bootstrapping simple qm systems arXiv:2108.08757
- [26] Aikawa Y, Morita T and Yoshimura K 2022 Bootstrap method in harmonic oscillator *Phys. Lett. B* **833** 137305
- [27] Nakayama Y 2022 Bootstrapping microcanonical ensemble in classical system *Mod. Phys. Lett.A* **37** 2250054
- [28] Du B-N, Huang M-X and Zeng P-X 2022 Bootstrapping Calabi-Yau quantum mechanics *Commun. Theor. Phys.* **74** 095801
- [29] Hu X 2022 Different bootstrap matrices in many QM systems arXiv:2206.00767
- [30] Guennebaud G *et al* 2010 Eigen v3 <http://eigen.tuxfamily.org>
- [31] Fousse L, Hanrot G, Lefèvre V, Pélissier P and Zimmermann P 2007 Mpfir: a multiple-precision binary floating-point library with correct rounding *ACM Transactions on Mathematical Software (TOMS)* **33** 13