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 ensemble as well. In this paper we report a method as a improvement to [Y. Nakayama, Modern Physics Letters A **37**, 10.1142/s0217732322500547 (2022)].

I. INTRODUCTION

The bootstrap method aims at solving a system with its fundamental constraints, the so called positivity constraints. Although widely used in quantum mechanics, one can also apply the method into microcanonical ensembles which can be seen as classical correspondence to the quantum mechanical case when $\hbar \to 0$. Nakayama first introduced this method into the classical scenario [1], but he mentioned a peninsula in $E < 0$ which doesn't converge even for stronger constraints. In our work, we use both position x and momentum p in the phase space to bootstrap, we can see the peninsula shrinks vastly compared to the x only bootstrap program.

II. BOOTSTRAPPING METHOD

A. Bootstrap Equations and Matrices

Starting with the Hamiltonian we have

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

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

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

and we can easily find that

$$\langle \{H, \mathcal{O}\} \rangle = 0 \tag{3}$$

$$\langle H\mathcal{O} \rangle = E \langle \mathcal{O} \rangle \tag{4}$$

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

$$\langle \mathcal{O}^* \mathcal{O} \rangle \geq 0 \tag{5}$$

and by writing the observale 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

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

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

$$\boldsymbol{\alpha}^\dagger \boldsymbol{\mathcal{M}} \boldsymbol{\alpha} \geq 0 \tag{7}$$

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

$$\forall (\boldsymbol{\mathcal{M}})_{eigenvalue} \geq 0 \tag{8}$$

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

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

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

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

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

$$\boldsymbol{\mathcal{M}} \succeq 0 \tag{12}$$

B. Double Well Potential

The Hamiltonian of a double well potential can be written as

$$H = p^2 - x^2 + x^4 \tag{13}$$

here we consider the observable $\mathcal{O} = x^m p^n$, substitute it as well as the Hamiltonian into (3) and (4), we can obtain two recursion formulas

$$2(2n+m)\langle x^{m+3} p^{n-1} \rangle = 2(m+n)\langle x^{m+1} p^{n-1} \rangle + 2mE \langle x^{m-1} p^{n-1} \rangle \tag{14}$$

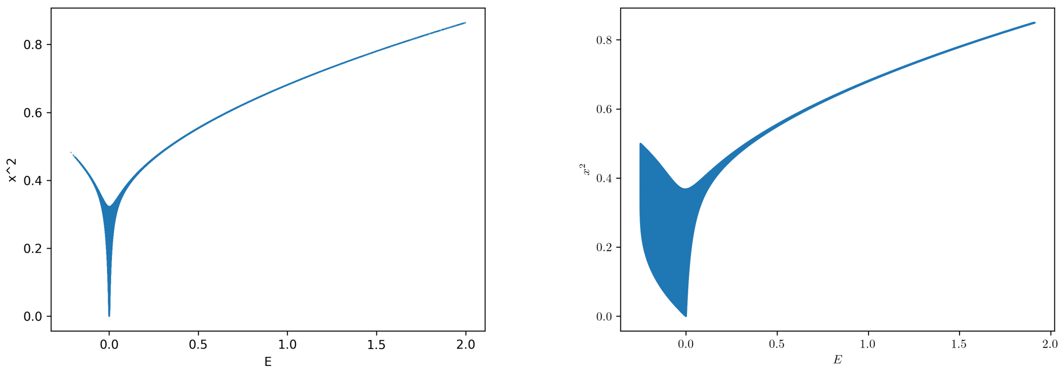

FIG. 1. xp bootstrap with $k = 5$(left), x only bootstrap with $k = 9$(right)

$$\langle H x^m p^n \rangle = E \langle x^m p^n \rangle = \langle x^m p^{n+2} \rangle - \langle x^{m+2} p^n \rangle + \langle x^{m+4} p^n \rangle$$

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

$$\langle x^{m-1} p \rangle = 0 \tag{15}$$

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

$$\langle x^m \rangle = 0, \quad \text{for all odd } m \tag{16}$$

with (14) (15) (15) (16) plus the initial paratemers E and $\langle x^2 \rangle$ we can construct the bootstrap matrix $\boldsymbol{\mathcal{M}}$.The result when $k = 5$ is shown in Fig. 1. We also reproduced the result in [1] to make a comparison.

In constrast with [1], our result shows no peninsula in where $E < 0$, as we include the information of the momentum. When E turns negative, the curve menifests a similar behavior as the positive part. 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 here the size of our bootstrap matrix is 625, about seven times to the x bootstrap. But the region still doesn't 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 constraints than the single observable one.

Like Nakayama has mentioned, $\langle x \rangle$ doesn't have to be zero in classical mechanics, but this method does produce a narrow region upon the assumption (16). So we then study the $\langle x \rangle$ and $\langle x^3 \rangle$ with fixed E and $\langle x^2 \rangle$ using the $\langle x^m p^n \rangle$ bootstrap program, which, still turns out to be a line in Fig. 2.

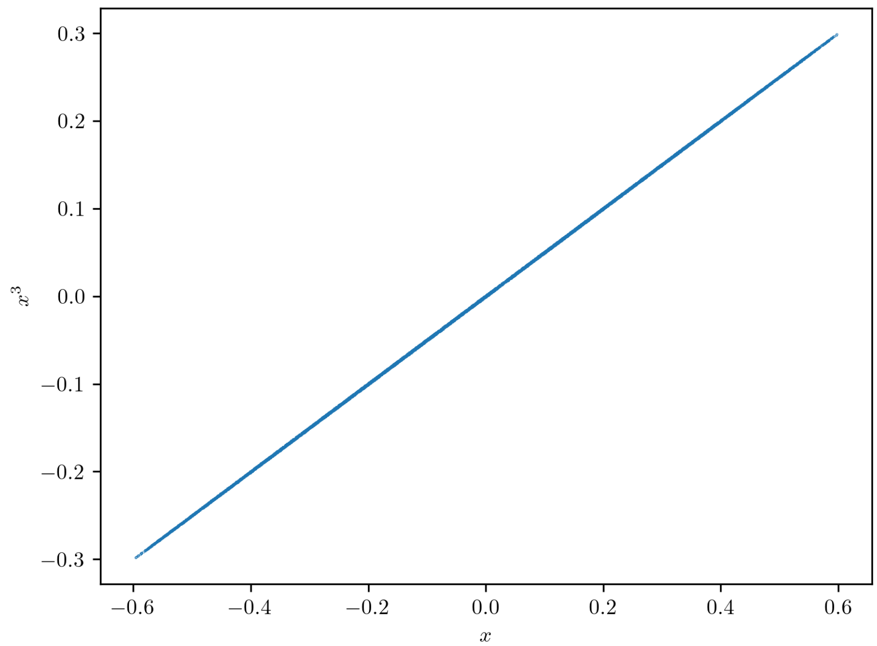

FIG. 2. $\langle x^m p^n \rangle$ bootstrap ($k = 5$) with fixed $E = -0.1$ and $\langle x \rangle = 0.4052$

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[1] Y. Nakayama, Bootstrapping microcanonical ensemble in classical system, Modern Physics Letters A **37**, 10.1142/s0217732322500547 (2022).