Numerical bootstrap

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Introduction

What's bootstrap

- A quantum theory = expectations of all Hermitian operators; Hamiltonian/Lagrangian $\Leftrightarrow$ "probability distribution"
- Constraint on the system $\Rightarrow$ relation between different $\langle O \rangle$'s ("**data**"); independent $\langle O \rangle$'s $\Leftrightarrow$ parameters in the model
- Inequality constraint (e.g. positivity of $\left\langle O^\dagger O \right\rangle$) $\Rightarrow$ allowed range of $\langle O \rangle$'s
- Solving a class of problems without mentioning explicitly the wave function/path integral: hence the name *bootstrap*

Example: conformal bootstrap

- The most famous example: **conformal bootstrap**
- Constraints: (spinless) two-point function

$$\langle \mathcal{O}(x)\mathcal{O}(y)\rangle = \frac{1}{|x-y|^{2\Delta_{\mathcal{O}}}}, \tag{1}$$

three-point function

$$\langle \mathcal{A}(x)\mathcal{B}(y)\mathcal{C}(z)\rangle = \frac{f_{\mathcal{A}\mathcal{B}\mathcal{C}}}{|x-y|^{\Delta_{\mathcal{A}}+\Delta_{\mathcal{B}}-\Delta_{\mathcal{C}}}|y-z|^{\Delta_{\mathcal{B}}+\Delta_{\mathcal{C}}-\Delta_{\mathcal{A}}}|z-x|^{\Delta_{\mathcal{C}}+\Delta_{\mathcal{A}}-\Delta_{\mathcal{B}}}} \tag{2}$$

Higher order correlation functions: OPEs.

- Independent parameters: $\{\Delta_{\mathcal{O}}, l_{\mathcal{O}}, f_{\mathcal{A}\mathcal{B}\mathcal{C}}\}$
- Inequality constraints (self-consistent conditions): determining the range of parameters

Bootstrap for generic systems

How to perform bootstrap for a generic system?

- Correlation functions cannot be determined by countably infinite parameters: no $\{\Delta_{\mathcal{O}}, l_{\mathcal{O}}, f_{\mathcal{ABC}}\}$.
  Solution Store $\{\langle O_1(x_1)O_2(x_2)\cdots O_n(x_n)\rangle\}$ separately. Using equational constraints to reduce the size of data. See next slide.

Bootstrap for generic systems

How to perform bootstrap for a generic system?

- How to get relations between correlation functions
  Solution Expanding each operator to a linear combination of normal ordered operators. (poor man's OPE)
  Density matrix is determined solely by H, then

$$\langle OH \rangle = \mathrm{tr}(\rho(H)OH) = \mathrm{tr}(H\rho(H)O) = \mathrm{tr}(\rho(H)HO) = \langle HO \rangle \quad (3)$$

  for all operators O. Similarly, suppose C is a symmetry of the system, we have

$$\langle OC \rangle = \langle CO \rangle . \quad (4)$$

  For energy eigenstates (i.e with definite E), we have

$$\langle OH \rangle = E \langle O \rangle , \quad E = \langle H \rangle . \quad (5)$$

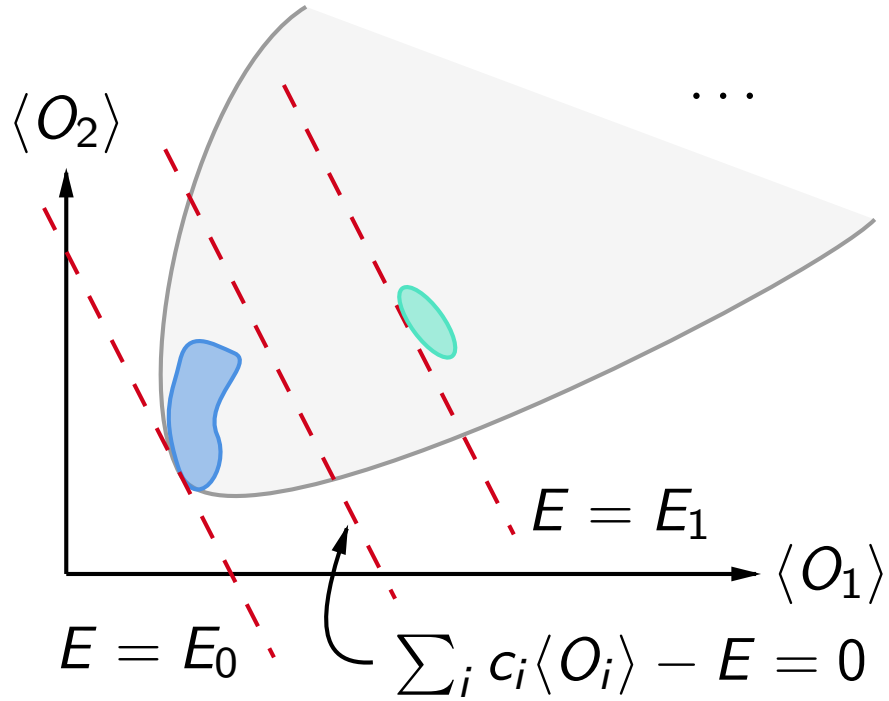
  Thus we break higher order correlation functions into lower order ones.

Bootstrap for generic systems

- The equality constraints used together with the positivity constraint

$$\langle O^\dagger O \rangle \geq 0 \tag{6}$$

  for every O defines an allowed region – the feasible domain for the following optimization.
- To get ground state information, minimize $\langle H \rangle$ globally.
- To get information about excited states, find local minima of $\langle H \rangle$.



Bootstrap for generic systems

The procedure of numerical bootstrap

Input data:

- N basis operators $\{O_i\}$, normal ordered with a length cutoff
- Data of equality constraints: Hamiltonian, symmetry, etc.
- Commutation rules, normal ordering rules, etc. so that $O_i O_j$ can be expanded in terms of $\{O_i\}$
- Hamiltonian $H = \sum_i c_i O_i$

Building the optimization problem:

1. Declare N variables $\{X_i\}$, $X_i = \langle O_i \rangle$ after optimization
2. Impose equality constraints on $\{X_i\}$ according to e.g. $\langle [H, O] \rangle = 0$
3. Imposing semidefinite constraint on $M_{ij} = \langle O_i^\dagger O_j \rangle$ (expanded into linear combination of $\{X_i\}$), so that after optimization $\langle O^\dagger O \rangle \geq 0$ for every O
4. Optimize $\sum_i c_i X_i$

Bootstrap for generic systems

Why we need numerical bootstrap

- Because it doesn't fail with strong non-perturbative effects.[1]
- Because if done correctly, it gives the *lower* bound of ground state energy
  - Density matrix = linear functional $\mathcal{F}$ from operators to numbers
  - Predicted $E_0 = \min_{\mathcal{F}\text{constrained}} \mathcal{F}[H]$
  - Real ground state also constrained $\Rightarrow$ real $E_0 >$ predicted E_0
  - Upper and lower bounds for all physical quantities:

$$\min_{E_{\text{lb}} \le \langle H \rangle_\rho \le E_{\text{ub}}} \langle O \rangle_\rho \le \langle O \rangle_{\rho_0} \le \max_{E_{\text{lb}} \le \langle H \rangle_\rho \le E_{\text{ub}}} \langle O \rangle_\rho \tag{7}$$

[1] arXiv 2108.11416

Bootstrap for generic systems

Some technical aspects of the problem

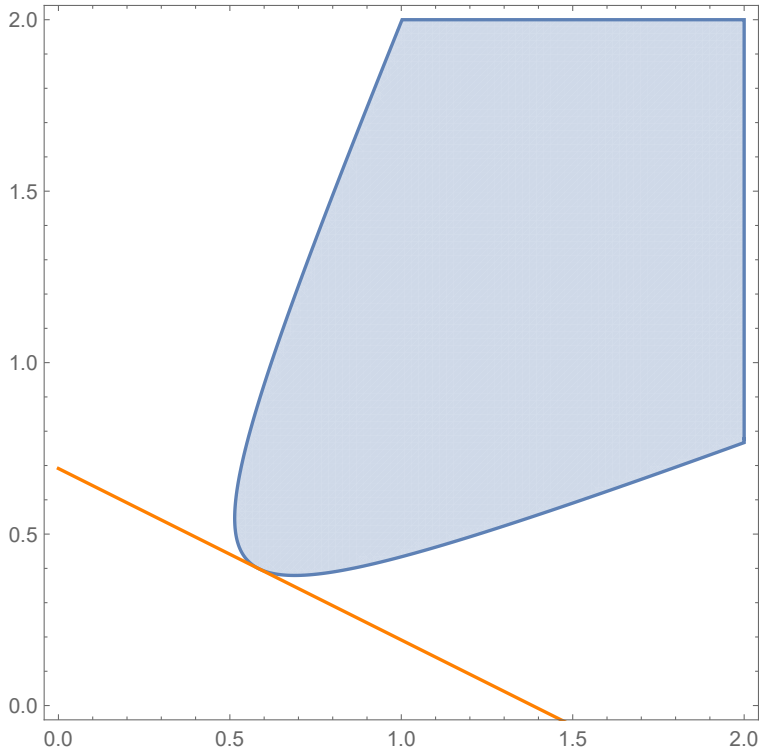
When building the optimization problem:

- A little symbolic calculation required
- Auto normal ordering of $O_i O_j$ given the operator algebra
- Auto commutator: $[A, B]$ = normal ordered AB - normal ordered BA

Bootstrap for generic systems

Optimization problem and algorithm: **semidefinite programming (SDP)**

- **Linear SDP**
  - $\langle [H, O] \rangle = 0$, thermal states allowed
  - Convex optimization[2], Linear objective $\Rightarrow$ minimum at the edge
  - Mature solvers like SCS or CSDP[3]
- **Nonlinear SDP**
  - $\langle HO \rangle = E \langle O \rangle$, there are optimization variables in E, eigenstates only
  - No solver mature enough[4]



[2] See Wikipedia

[3] https://github.com/cvxgrp/scs, https://github.com/coin-or/Csdp

[4] See the discussion before Sec. 1.1 in arXiv 2108.04830. Also, no nonlinear solver supporting SDP is listed in the solver list of JuMP.jl.

Examples

Anharmonic oscillator and Hubbard model

- Main topics of my thesis

Double-well potential[5]

- Non-perturbative: instanton effect
- Solved in a similar way of the anharmonic oscillator
- The dilute instanton approximation works when two wells are well separated.

Matrix model[6]

- Impossible to solve otherwise
- A specific case associated with M-theory[7]
- (Inherent) nonlinear constraints
  - Relaxed bootstrap in Sec. 4 in arXiv 2108.04830
  - trust-region sequential SDP in Xizhi Han's code

[5] See arXiv 2108.11416

[6] See arXiv 2108.04830 and arXiv 2004.10212

[7] arXiv hep-th 9610043

Example: x^4 anharmonic oscillator

The anharmonic oscillator[8]: famous failure of perturbation theory[9]

$$H = x^2 + p^2 + gx^4. \tag{8}$$

- Symmetry: $x \to -x \Rightarrow \langle x^n \rangle = 0$ with odd n
- Deriving equality constraints:
  - $\mathcal{O} = x^s$ and $\mathcal{O} = x^t p$ in $\langle [H, \mathcal{O}] \rangle = 0$
  - $\mathcal{O} = x^{t-1}$ in $\langle \mathcal{O} H \rangle = E \langle \mathcal{O} \rangle$
- So finally we have

$$\begin{aligned} &E = 2\left\langle x^2 \right\rangle + 3g\left\langle x^4 \right\rangle, \\ &4tE\left\langle x^{t-1} \right\rangle + t(t-1)(t-2)\left\langle x^{t-3} \right\rangle - 4(t+1)\left\langle x^{t+1} \right\rangle \\ &\quad - 4g(t+2)\left\langle x^{t+3} \right\rangle = 0 \end{aligned} \tag{9}$$

- Only independent variables: $\langle x^2 \rangle$ and E, so nonlinear SDP is possible
- SDP constraint: $M_{ij} = \left\langle x^{i+j} \right\rangle, M \geq 0$

[8] The example is provided in arXiv 2004.10212

[9] Carl M. Bender and Tai Tsun Wu, Anharmonic Oscillator. Phys. Rev. 184, 1231.

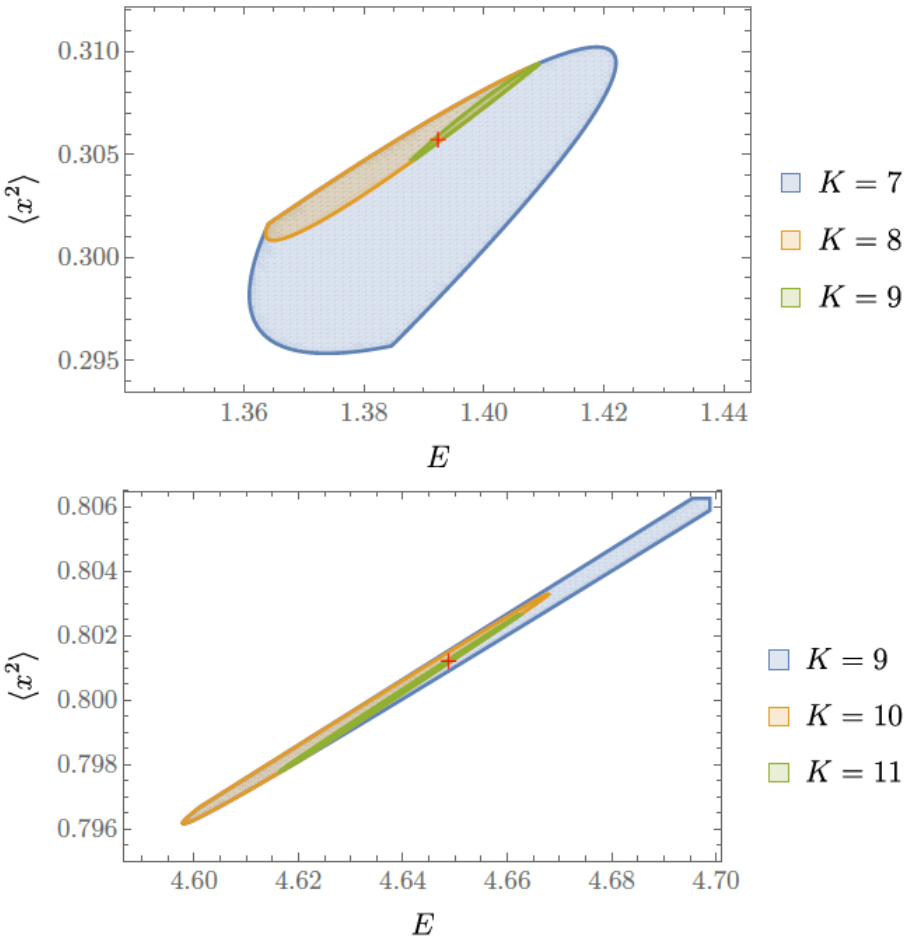
Example: x^4 anharmonic oscillator

- Reproduce Fig. 1 in arXiv 2004.10212 by brutal force searching
- Numerical bootstrap can be quite precise! (high resolution Mathematica plotting required to find the allowed region)

```
expectedX[0] := 1;
expectedX[2] := x2;
expectedX[4] := 1/(3 g) (E0 - 2 x2);
expectedX[u_?EvenQ] :=
1 / (4 g ((-3 + u) + 2)) *
(4 (-3 + u) E0 expectedX[(-3 + u) - 1]
+ (-3 + u) ((-3 + u) - 1) ((-3 + u) - 2)
    expectedX[(-3 + u) - 3]
- 4 ((-3 + u) + 1) expectedX[(-3 + u) + 1]);

matPositive[K_] :=
Table[expectedX[i+j], {i, 0, K}, {j, 0, K}];

RegionPlot[
AllTrue[Eigenvalues[matPositive[9] /. g -> 1]
    # >= 0 &],
{E0, 1.35, 1.44}, {x2, 0.294, 0.311},
PlotPoints -> 100]
```



Example: x^4 anharmonic oscillator

Benchmark

- Solving the Schrödinger equation with finite difference method with $\Delta x = 0.05$: $E_0 = 1.3919$
- Numerical bootstrap with $K = 11$: $E_0 = 1.3922$

Example: x^4 anharmonic oscillator

Linear SDP

- Solver: JuMP and COSMO[10]
- Operator algebra: McCoy formula

$$[x^n, p^m] = \sum_{k=1}^{\min(m,n)} \frac{-(-i\hbar)^k \, n! m!}{k! \, (n-k)! \, (m-k)!} x^{n-k} p^{m-k}. \tag{10}$$

- Operator basis and cutoff: $\{x^m p^n\}$, where $0 \leq m, n \leq 2L$
- Hence for $O_i = x^m p^n$ in $M_{ij} = \langle O_i^\dagger O_j \rangle$, $0 \leq m, n \leq L$
- COSMO only support real variables $\Rightarrow$ Declare two JuMP variables for $\mathrm{Re}\, O$ and $\mathrm{Im}\, O$ (odd $m+n \Rightarrow$ zero expectation, odd $n \Rightarrow$ imaginary, even $n \Rightarrow$ real),

$$M_{ij} \to \mathrm{Re}(M_{ij}) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \mathrm{Im}(M_{ij}) \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}. \tag{11}$$

[10] https://jump.dev/JuMP.jl/stable/, https://oxfordcontrol.github.io/COSMO.jl/stable/

Example: x^4 anharmonic oscillator

Result of linear SDP

- Successful when L is small
- But when L is 4. . . Severe convergent problem!
- Both stationary Schrödinger equation and nonlinear SDP estimate $E \approx 1.392$, $\langle x^2 \rangle \approx 0.306$. Not sure whether $L = 4$ converges.
- $L = 5$ takes 80000000 iterations and still doesn't converge.
- Only COSMO works for $L = 4$; SCS and CSDP report infeasibility
- False convergence when `eps_rel` is not small enough (1×10^{-5} not enough; 1×10^{-10} works for $L = 4$)

L	E	$\langle x^2 \rangle$	time consumption
2	1.381	0.313	0.752s, 958 iterations
3	1.387	0.305	2.501s, 1194 iterations
4	1.394	0.306	172375s, 79461867 iterations

Example: x^4 anharmonic oscillator

Possible reasons of the convergence problem

- Too much time is spent on tightening the constraints. Hints:
  - In the solver log of the $L = 4, 5$ cases, first energy goes down and residue goes up, then residue goes down and energy goes up, ...
  - False convergence
  - Solution: eliminate some variables in the optimization problem
- Float precision not enough, introducing fluctuation. Hints:
  - This is the case in conformal bootstrap.
  - Diagnosis: using less precise floats for $L = 2, 3$ and checking if the problem recurs.
  - Solution: same as conformal bootstrap
- The scheme

$$M_{ij} \to \mathrm{Re}(M_{ij}) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \mathrm{Im}(M_{ij}) \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \tag{12}$$

  is bad. Hints:
  - No convergence problem in Hubbard model. (strange but true ...)
  - Solution: rephrasing the anharmonic oscillator in terms of the creation and annihilation operators

Example: Hubbard model

Hubbard model[11]

$$H = -t \sum_{\langle \boldsymbol{i},\boldsymbol{j}\rangle,\sigma} c^{\dagger}_{\boldsymbol{i}\sigma} c_{\boldsymbol{j}\sigma} + U \sum_{\boldsymbol{i}} n_{\boldsymbol{i}\uparrow} n_{\boldsymbol{j}\downarrow} \tag{13}$$

is probably the most important strongly correlated electronic model.

- Half filling: small $U \Rightarrow$ Fermi liquid, large $U \Rightarrow$ Heisenberg model (Mott transition, spin-charge separation)
- Doping: t-J model, superconductivity
- Problems of various numerical approaches:
  - DQMC: sign problem when doped away from half-filling, can be tackled in some case[12] but no generic solution[13]
  - DMRG: works well in 1D but slow in 2D

[11] arXiv 2006.06002
[12] arXiv 2204.08777
[13] arXiv cond-mat 0408370

Example: Hubbard model

Linear SDP

- Solver: JuMP and COSMO
- Operator algebra: QuantumAlgebra.jl[14]
- Operator basis and cutoff: normal ordered $\{c^\dagger_{\boldsymbol{i}_1\sigma_1} c^\dagger_{\boldsymbol{i}_2\sigma_2} \cdots c_{\boldsymbol{i}_n\sigma_n}\}$, $n + \sum_{k=1}^{n} \|\boldsymbol{i}_k\|_1 \leq K$
- One JuMP variable for one operator $\Leftarrow$ the whole model is real
- Expectations of operators that do not keep particle number (e.g. $c^\dagger_{1\uparrow} c^\dagger_{2\uparrow} c^\dagger_{3\uparrow} c_{1\uparrow}$) and total spin (e.g. $c^\dagger_{1\uparrow} c_{1\downarrow}$) are zero
- Translational and inversion symmetry: $\langle c^\dagger_{1\uparrow} c_{1\uparrow} \rangle = \langle c^\dagger_{2\uparrow} c_{2\uparrow} \rangle$
- Electron filling: need to be explicitly imposed
  - half filling $\Rightarrow \langle n_1 \rangle = \langle n \rangle_2 = \cdots = 1$
  - doping $\Rightarrow \langle n_1 \rangle = \langle n \rangle_2 = \cdots = 0.75$, etc.
  - *Not* done by chemical potential (which is the case in DQMC but not in DMRG)

[14] https://github.com/jfeist/QuantumAlgebra.jl

Example: Hubbard model

DMRG benchmark

- Using ITensor's fixed quantum number DMRG to find reference values
- The DMRG solution is in the feasible domain (so the implementation is correct)

Example: Hubbard model

1D square lattice

$n_i = 1$		$U = 4$	$U = 6$	$U = 8$	$U = 10$
$K = 10$	E	-0.6202	-0.4580	-0.3574	-0.2913
	$n_{i\uparrow} n_{i\downarrow}$	0.1071	0.0639	0.0406	0.0275
$K = 12$	E	-0.6049	-0.4466	-0.3486	-0.2842
	$n_{i\uparrow} n_{i\downarrow}$	0.1027	0.0618	0.0394	0.0267
Exact	E	-0.5737	-0.4201	-0.3275	-0.2672
	$n_{i\uparrow} n_{i\downarrow}$	0.1002	0.0582	0.0366	0.0248

- Approximately correct, but not as good as Xizhi Han's results
- Converges rather quickly: 20 minutes for $K = 12$, 7×10^5 variables
- Larger $U \Rightarrow$ smaller absolute error, larger relative error

Example: Hubbard model

1D square lattice

- Accuracy with various U
  - Expected: large $U \Rightarrow$ localized electrons, so with our local operators large U means higher accuracy
  - Observed: Larger $U \Rightarrow$ smaller absolute error, larger relative error
  - What's the correct way to evaluate the accuracy of numerical bootstrap?
- Main performance bottleneck: *before* optimization, the step turning QuantumAlgebra.jl operators into JuMP variables

Example: Hubbard model

1D square lattice with doping

$n_i = 0.5$		$U = 4$	$U = 6$	$U = 8$	$U = 10$
$K = 12$	E	-0.7830	-0.7593	-0.7444	-0.7342
	$n_{i\uparrow} n_{i\downarrow}$	0.0168	0.0102	0.0068	0.0048
DMRG	E	-0.7534	-0.7243	-0.7059	-0.6939
	$n_{i\uparrow} n_{i\downarrow}$	0.0189	0.0114	0.0075	0.0052

- Comparison of accuracy between half filling and hole doping
  - Errors larger than half filling
  - Expected: hole doping $\Rightarrow$ iterant electrons, whose behavior can't be captured by local operators $\Rightarrow$ poorer accuracy ✓
- U increase $\Rightarrow$ relative and absolute errors increase??

Example: Hubbard model

2D square lattice

$n_i = 1$		$U = 2$	$U = 4$	$U = 6$	$U = 8$
$K = 8$	E	-1.3164	-1.0491	-0.8626	-0.7276
	$n_{i\uparrow} n_{i\downarrow}$	0.1602	0.1105	0.0784	0.0576
DMRG	E	-1.176(1)	-0.8605(5)	-0.6565(1)	-0.5241(1)
	$n_{i\uparrow} n_{i\downarrow}$	0.188(1)	0.126(1)	0.0809(3)	0.0539(1)

- Time consumption gets larger (no real large-scale results)
- Error analysis
  - The absolute error of E as U shows an increasing tendency (the relative error goes all the way higher)
  - The absolute error of the double occupation decreases, and the relative error shows a decreasing tendency
  - Expected: larger $U \Rightarrow$ smaller error
  - Possible reason: energy bound is not very tight

Future prospects

- Symmetry breaking: so the ground state ρ is not a function of H:

$$\lim_{\beta\to\infty}\frac{1}{Z}\mathrm{e}^{-\beta H}=\frac{1}{2}(|\uparrow\rangle\langle\uparrow|+|\downarrow\rangle\langle\downarrow|)\neq \underbrace{|\uparrow\rangle\langle\uparrow|}_{\text{true ground state}} \tag{14}$$

- Bootstrapping spin models: Heisenberg model, lattice frustration, next neighbor interaction induced frustration, spin liquids, etc.
- Bootstrapping a *class* of models (e.g. "all possible QM models")
  - Extending what is done in conformal bootstrap (e.g. "all possible CFTs made by σ and ϵ") to all kind of models
- Extracting thermal information from $\langle[O,H]\rangle=0$ bootstraps
  - What's the entropy?
  - What's the temperature in terms of operator expectations?
- What constraints are effective? (Important for scaling up and interpretation)
  - Can wave function ansatz (e.g. DMRG) provide some hints?
  - Constraints that are "almost" violated are the most important?
  - arXiv 2205.12325: bootstrap and perturbation theory