Bootstrapping quantum mechanics

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August 2, 2024

Contents

Introduction

- the conformal bootstrap is a numerical method which leverages symmetries and consistency conditions
- used initially in Conformal Field Theory (CFT) – for example for estimating the 3d Ising model critical exponents
- we introduce and test the method on two simple quantum mechanical systems – the harmonic oscillator and the double-well – using our implementation in Python
- we estimate spectra of these systems and focus on the splitting of the ground state and the first excited state of the double-well
- obtained results are compared with the results gained analytically

Analytical methods

WKB approximation

- the approximation technique for a particular class of differential equations (in our case a time-independent Schrödinger equation)
- for a particle in a given potential, it will provide an ansatz for its wavefunction in classically allowed and forbidden regions

Path integral approach

- using the path integral formalism to express important quantities (such as the canonical partition function) and approximating these path integrals
- approximating the (Euclidean) action of the path integral around its saddle points to the second order (one-loop approximation) or to the higher orders (n-loop approximations)

Numerical bootstrap

- according to Oxford Learner's Dictionaries, bootstrap literally means an approach to creating something that uses the minimum amount of resources possible
- we will use just symmetry of the potentials and three basic identities true for any operator $\hat{O}$

$$\langle E|[\hat{H},\hat{O}]|E\rangle = \langle E|(\hat{H}\hat{O}-\hat{O}\hat{H})|E\rangle = E\langle E|\hat{O}|E\rangle - E\langle E|\hat{O}|E\rangle = 0 \quad (1)$$

$$\langle E|\hat{H}\hat{O}|E\rangle = E\langle E|\hat{O}|E\rangle \quad (2)$$

$$\langle E|\hat{O}^{\dagger}\hat{O}|E\rangle = (\hat{O}|E\rangle)^{\dagger}(\hat{O}|E\rangle) \geq 0 \quad (3)$$

- using the first two identities on operators $\hat{O} = \hat{x}^n$, $n \in \mathbb{N} \cup \{0\}$ and $\hat{O} = \hat{x}^m \hat{p}$, $m \in \mathbb{N}$, we can get rid of the momentum operators and have recursion relation for the coordinate moments

$$2mE\langle x^{m-1}\rangle + \frac{1}{4}m(m-1)(m-2)\langle x^{m-3}\rangle - \langle x^m V'(x)\rangle - 2m\langle x^{m-1}V(x)\rangle = 0 \tag{4}$$

- using the last identity on operator $\hat{O} = \sum_i c_i \hat{x}^i$, $c_i \in \mathbb{C}$ we get the consistency condition

$$0 \leq \langle O^\dagger O\rangle = \sum_{i,j} c_i^* \langle x^{i+j}\rangle c_j = \sum_{i,j} c_i^* M_{ij} c_j \tag{5}$$

- the matrix M, which elements are $M_{ij} = \langle x^{i+j}\rangle$, is called a Hankel matrix

Algorithmic structure

1. Select a subset of the search space $X \subset S$. For each point $p = (E, \langle x \rangle, \ldots) \in X$ generate the moment sequence $\{\langle x^m \rangle\}_0^{2K-2}$.

2. From $2K-2$ terms of this sequence for the point p construct the $K \times K$ Hankel matrix $M_{ij} = \langle x^{i+j} \rangle$, $0 \leq i, j \leq K-1$.

3. Check if the matrix M is positive definite. If it is not positive definite, then dismiss the point p. This way, we obtain the set of allowed points $X_K \subseteq X$ at depth K.

4. Repeat this procedure starting with the set of points X_K and depth $K+1$.

Applications

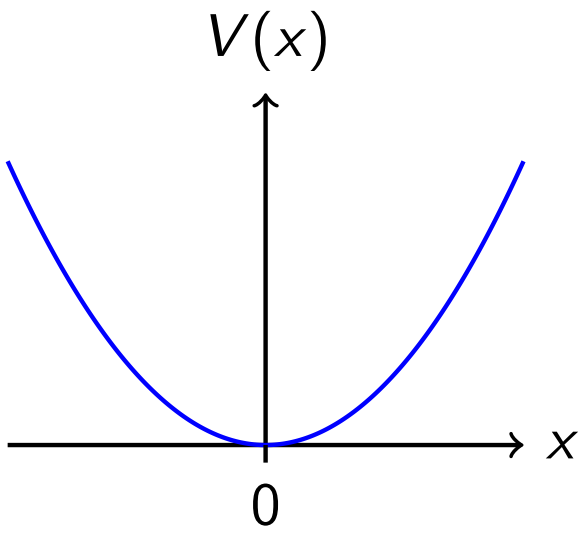

Figure 1: The harmonic oscillator potential $V(x) = \frac{1}{2}x^2$.

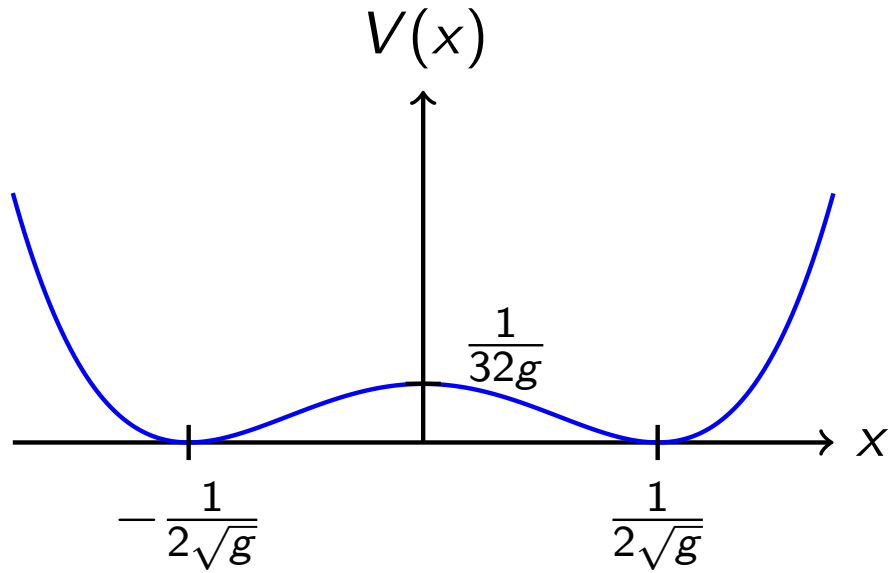

Figure 2: The double-well potential $V(x) = \frac{g}{2}\left(x^2 - \frac{1}{4g}\right)^2$, $g > 0$.

Harmonic oscillator

- using the recursion relation (4) for the harmonic oscillator potential $V(\hat{x}) = \frac{1}{2}\hat{x}^2$ we get for $s \in \{2, 3, 4, \ldots\}$

$$s\langle x^s \rangle = 2E(s-1)\langle x^{s-2} \rangle + \frac{1}{4}(s-1)(s-2)(s-3)\langle x^{s-4} \rangle \qquad (6)$$

- we have the recursion relation only for even moments, but the potential $V(x)$ is even, which means that all odd moments are equal to zero and from normalization, we know that $\langle x^0 \rangle = 1$
- the search space is one-dimensional $S = \{E\}$

n	E_n	Bootstrapped energy	Relative difference from the exact value
0	$1/2$	0.50 ± 0.01	$1.2 \cdot 10^{-50}$
1	$3/2$	$1.499999999999999996 \pm 9 \cdot 10^{-18}$	$2.8 \cdot 10^{-18}$
2	$5/2$	$2.500000000000001 \pm 3 \cdot 10^{-15}$	$4.6 \cdot 10^{-16}$
3	$7/2$	$3.4999999999998 \pm 4 \cdot 10^{-13}$	$5.4 \cdot 10^{-14}$
4	$9/2$	$4.50000000001 \pm 3 \cdot 10^{-11}$	$2.9 \cdot 10^{-12}$
5	$11/2$	$5.499999999 \pm 1 \cdot 10^{-9}$	$1.0 \cdot 10^{-10}$
6	$13/2$	$6.50000001 \pm 4 \cdot 10^{-8}$	$1.8 \cdot 10^{-9}$
7	$15/2$	$7.500000 \pm 1 \cdot 10^{-6}$	$5.5 \cdot 10^{-8}$
8	$17/2$	$8.50001 \pm 2 \cdot 10^{-5}$	$6.5 \cdot 10^{-7}$
9	$19/2$	$9.4999 \pm 2 \cdot 10^{-4}$	$6.9 \cdot 10^{-6}$

Table 1: Comparison of the bootstrapped energies – using the subsequent approach with $K = 50$ and $N = 10\ 000$ – with the exact spectrum of the harmonic oscilator $E_n = n + 1/2$ (in units of $\hbar\omega$).

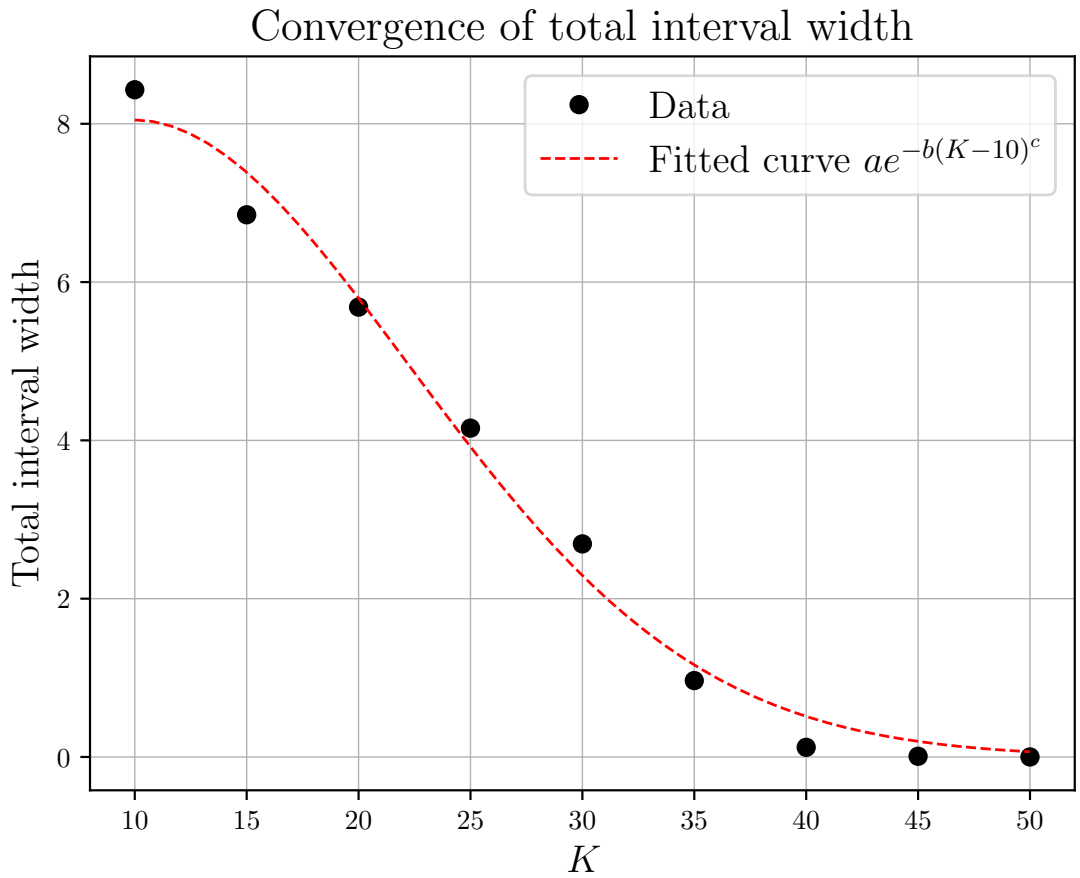

Figure 3: Convergence of the method for the harmonic oscillator. Fitted data are $a = 8.0 \pm 0.3$, $b = 0.004 \pm 0.002$, and $c = 1.9 \pm 0.2$.

Double-Well

- using the recursion relation (4) for the double-well potential $V(\hat{x}) = \frac{g}{2}\left(\hat{x}^2 - \frac{1}{4g}\right)^2$, $g > 0$ we get for $s \in \{4, 5, 6, \ldots\}$

$$\langle x^s \rangle = \frac{1}{2g}\frac{s-2}{s-1}\langle x^{s-2}\rangle + \frac{1}{g}\left(2E - \frac{1}{16g}\right)\frac{s-3}{s-1}\langle x^{s-4}\rangle + \\ + \frac{1}{4g}\frac{(s-3)(s-4)(s-5)}{s-1}\langle x^{s-6}\rangle \tag{7}$$

- we have the recursion relation only for even moments, but the potential $V(x)$ is even, which means that all odd moments are equal to zero and from normalization, we know that $\langle x^0 \rangle = 1$
- the search space is two-dimensional $S = \{E, \langle x^2 \rangle\}$

Bootstrapped energy at $g = 0.05$		
$0.3850 \pm 4 \cdot 10^{-4}$	~~$1.846 \pm 3 \cdot 10^{-3}$~~	$2.8316 \pm 4 \cdot 10^{-4}$
$0.4600 \pm 7 \cdot 10^{-4}$	~~$1.884 \pm 3 \cdot 10^{-3}$~~	$2.8556 \pm 5 \cdot 10^{-4}$
$0.4971 \pm 2 \cdot 10^{-4}$	$2.244 \pm 2 \cdot 10^{-3}$	$2.8798 \pm 6 \cdot 10^{-4}$
$1.0643 \pm 8 \cdot 10^{-4}$	$2.263 \pm 2 \cdot 10^{-3}$	$2.9040 \pm 6 \cdot 10^{-4}$
$1.598 \pm 3 \cdot 10^{-3}$	$2.283 \pm 2 \cdot 10^{-3}$	$2.9284 \pm 7 \cdot 10^{-4}$
~~$1.808 \pm 3 \cdot 10^{-3}$~~	$2.784123 \pm 9 \cdot 10^{-6}$	$2.9530 \pm 7 \cdot 10^{-4}$
~~$1.829 \pm 3 \cdot 10^{-3}$~~	$2.8078 \pm 2 \cdot 10^{-4}$	$2.9777 \pm 6 \cdot 10^{-4}$

Table 2: The bootstrapped energies for the double-well potential obtained by subsequently applying the bootstrap method with $K = 18$ and $N = 300$ (in units of $\hbar\omega$). Red ones are the impostors discarded by Figure 5 and Figure 6.

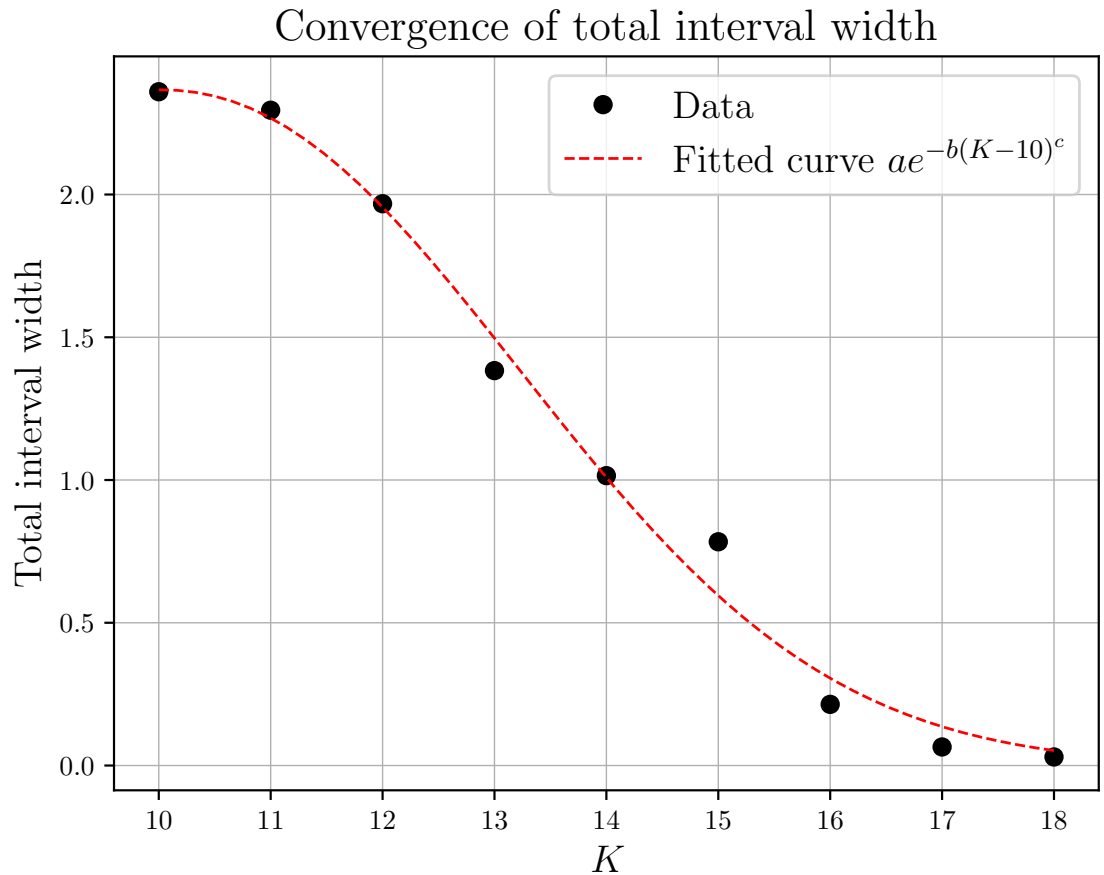

Figure 4: Convergence of the method for the double-well. Fitted data are $a = 2.37 \pm 0.08$, $b = 0.04 \pm 0.02$, and $c = 2.2 \pm 0.2$.

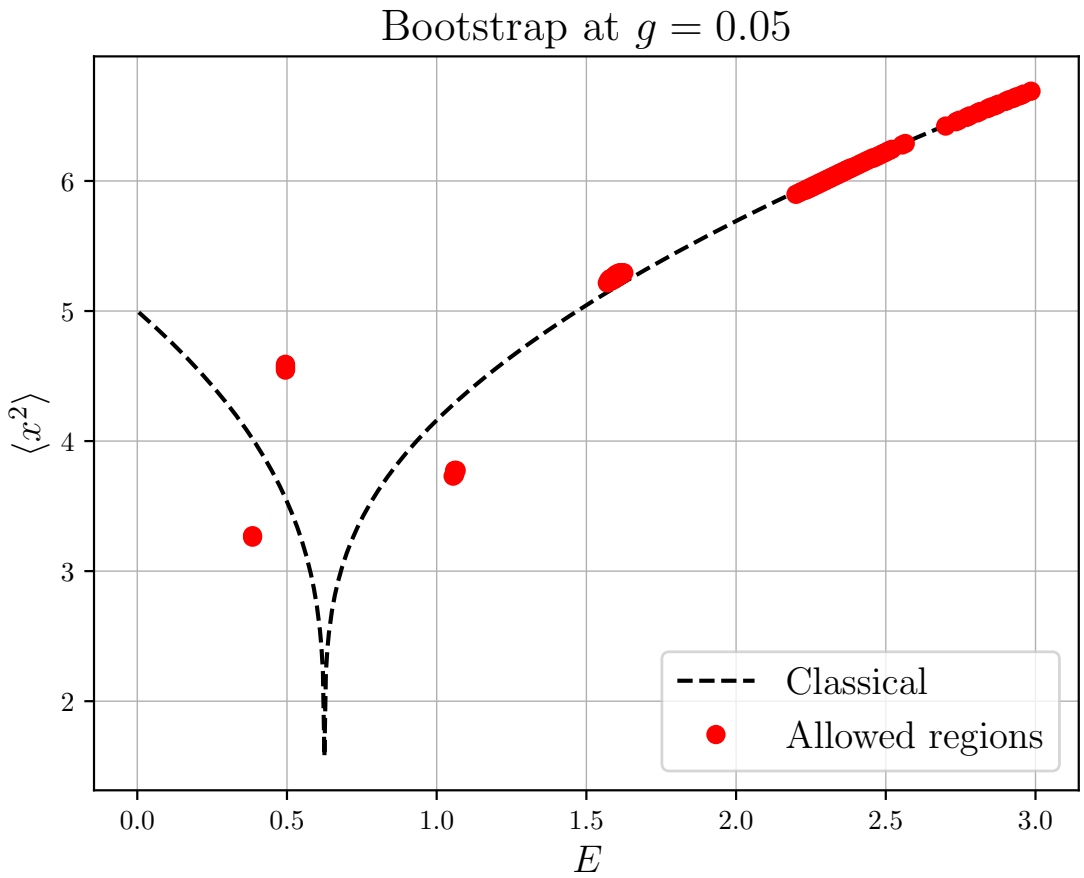

Figure 5: Reduced search space after one run of the bootstrap method for $K = 16$ and $N = 600$ together with the curve for the classical particle.

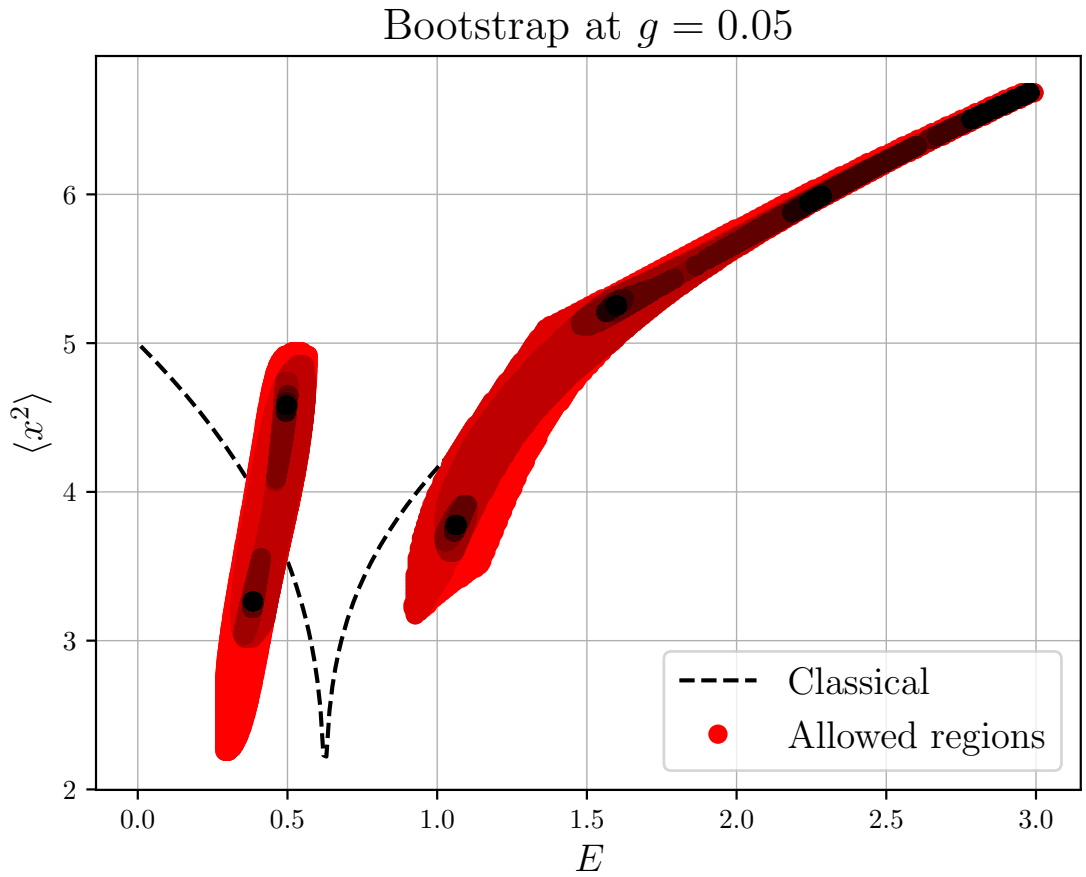

Figure 6: Reduced search space after subsequently running the bootstrap method for K from 10 (lightest) to 18 (darkest) and $N = 300$ together with the curve for the classical particle.

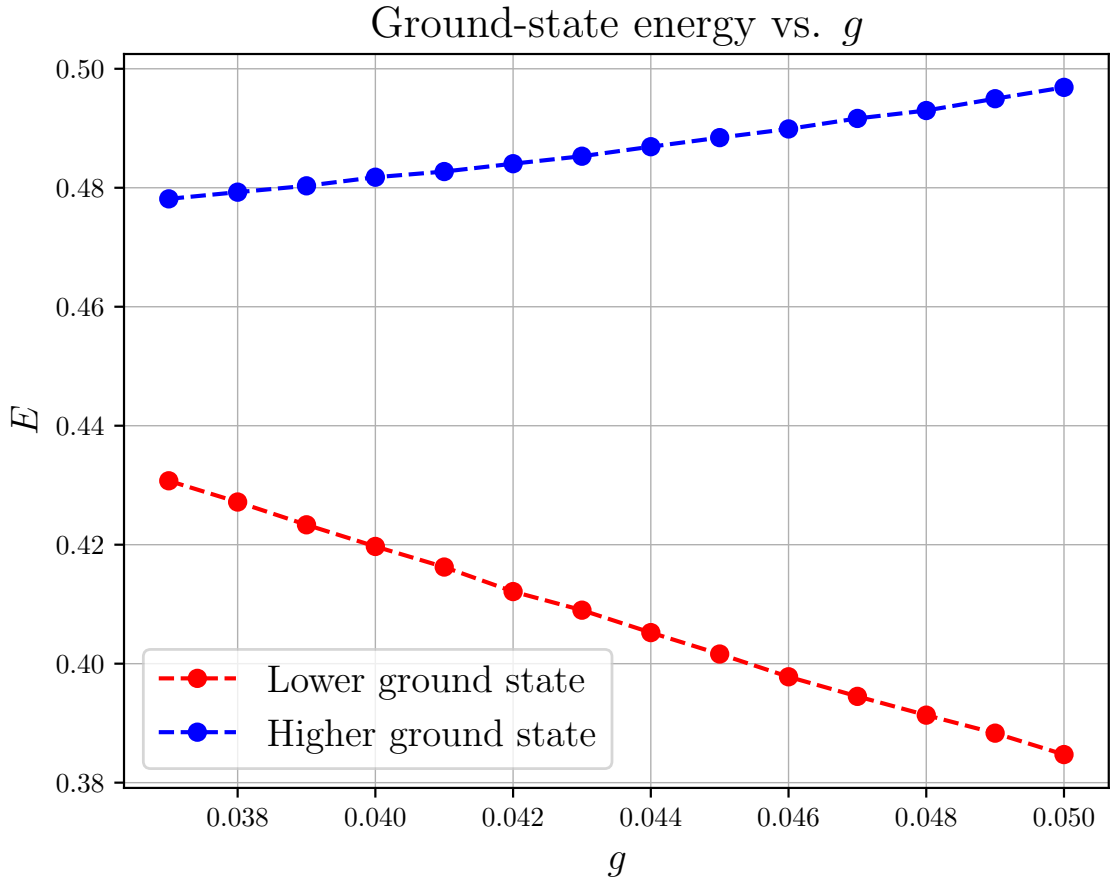

Figure 7: Dependence of energies of the ground and the first excited state on the coupling constant g. Both energies are closing on each other as $g \to 0$. We used one-run approach with $K = 18$ and $N = 900$.

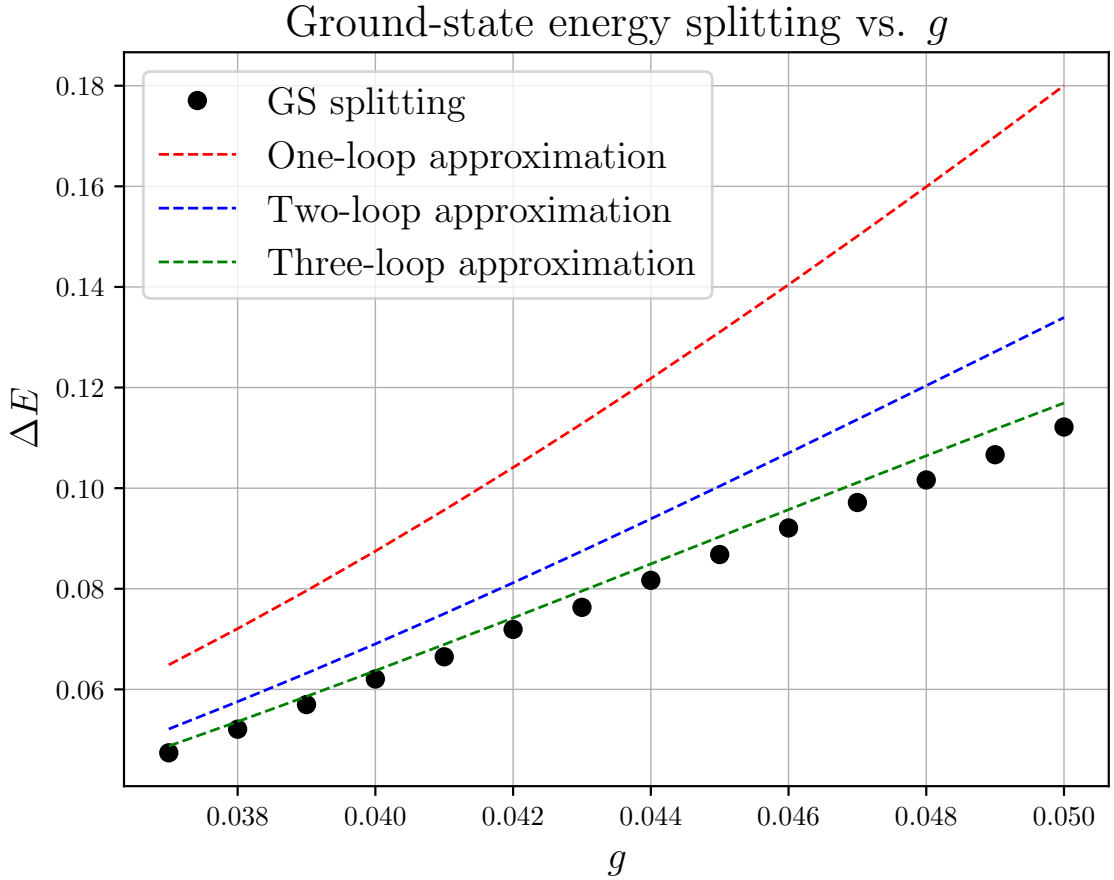

Figure 8: Dependence of energy difference of the ground and the first excited state on the coupling constant g in comparison with the one-loop (equivalent with the WKB), the two-loop, and the three-loop approximation method.We used one-run approach with $K = 18$ and $N = 900$.

Conclusion

- we found that the bootstrap method gave us better results than the standard approximation methods
- we explored two approaches to the bootstrap method – the one-run and the subsequent approach
- we found that the one-run approach is faster and more stable than the subsequent one and, therefore, more suitable for more complicated programs
- in systems with no prior knowledge, it is more convenient to use the subsequent approach because it is easier to spot that we missed some energies
- we recommend using the subsequent approach to get to know the new system and then using the one-run approach with calibrated parameters in more complicated programs