

PyRETIS — RETIS analysis

RETIS analysis report generated by PyRETIS version 3.0.0.dev0+098fc56 on 13.02.2023 09:13:37.

The main results are:

- The crossing probability: $P_{\text{cross}} = 5.969870638 \times 10^{-7} \pm 3.013233817 \%$
- The initial flux (unit: 1/reduced): $f_A = 0.441235243 \pm 0.157589042 \%$
- The rate constant (unit: 1/reduced): $k_{AB} = 2.634117321 \times 10^{-7} \pm 3.017351876 \%$

Detailed results are given below for the different path ensembles and the overall results are summarized in the last section.

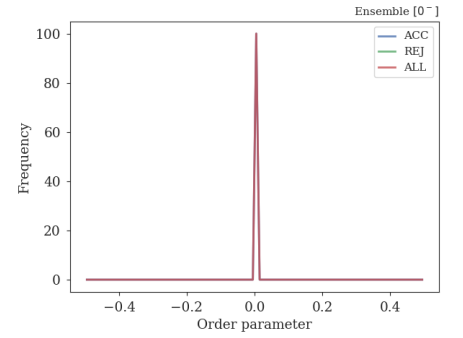
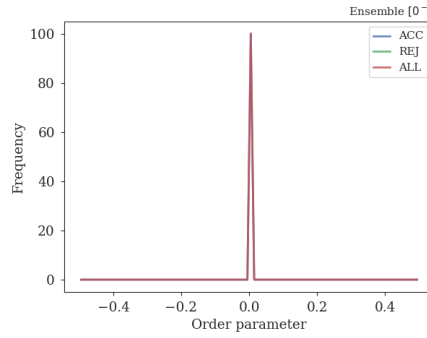
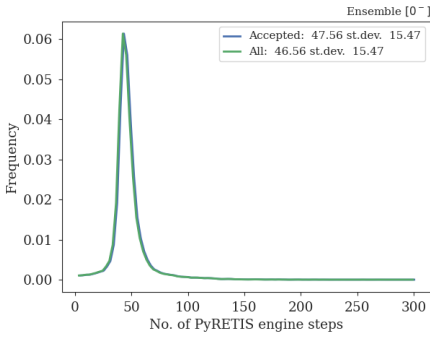
1 Results for $[0^-]$

Table 1: Interfaces

Ensemble	Left	Middle	Right
$[0^-]$	$-\text{inf}$	-0.9900	-0.9900

Table 2: Path lengths

Ensemble	Accepted	All	All/Accepted
$[0^-]$	47.556461	46.556461	0.978972



2 Results for path ensembles

The following interfaces were used in the simulation and in the analysis:

Table 3: Interfaces

Ensemble	Left	Middle	Right	Detect
$[0^+]$	-0.9900	-0.9900	1.0000	-0.8000
$[1^+]$	-0.9900	-0.8000	1.0000	-0.7000
$[2^+]$	-0.9900	-0.7000	1.0000	-0.6000
$[3^+]$	-0.9900	-0.6000	1.0000	-0.5000
$[4^+]$	-0.9900	-0.5000	1.0000	-0.4000
$[5^+]$	-0.9900	-0.4000	1.0000	-0.3000
$[6^+]$	-0.9900	-0.3000	1.0000	1.0000

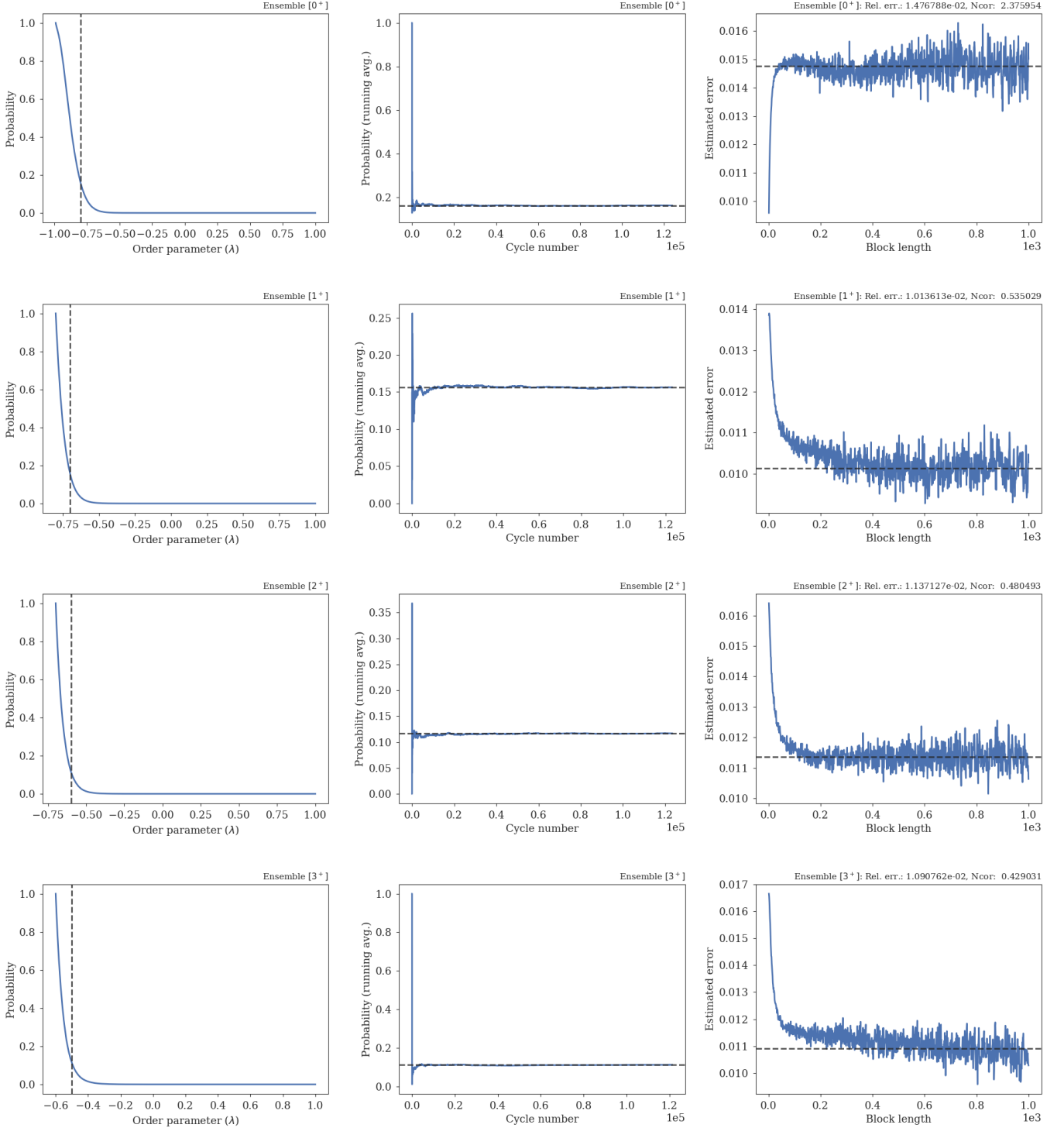
The calculated crossing probabilities are:

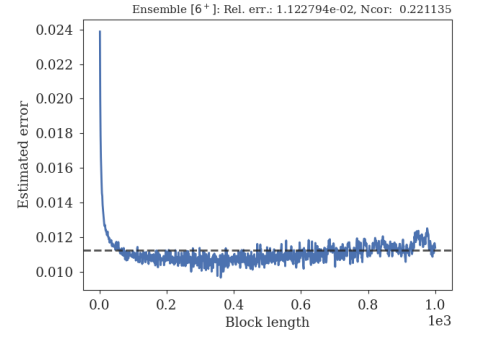
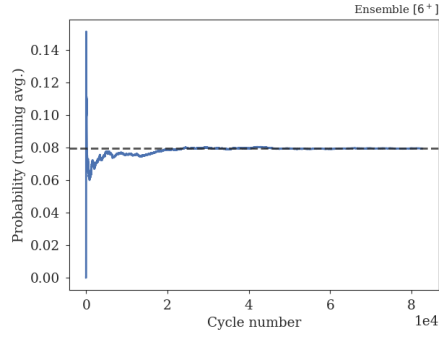
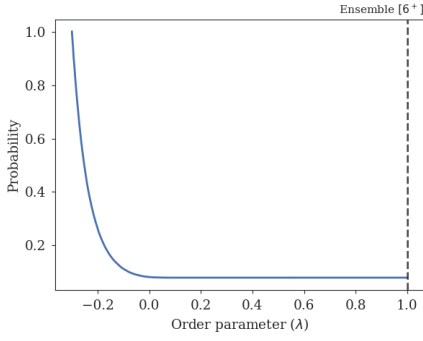
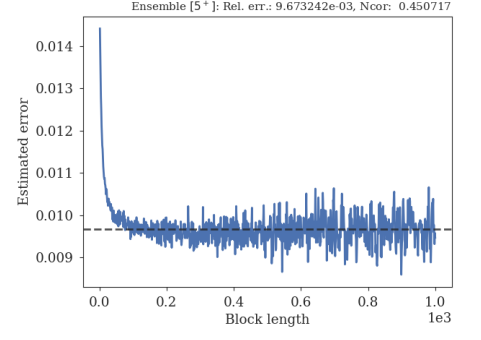
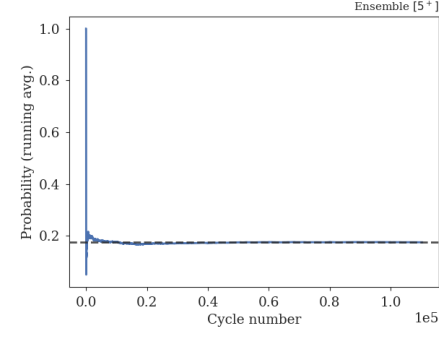
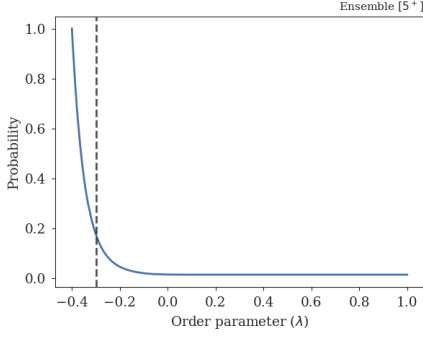
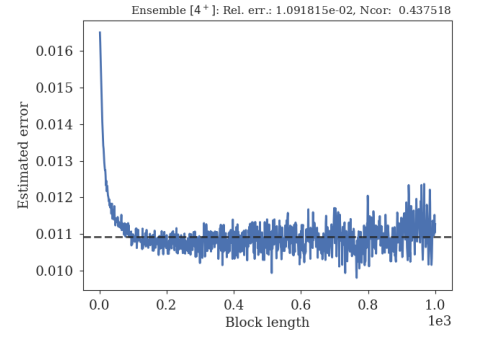
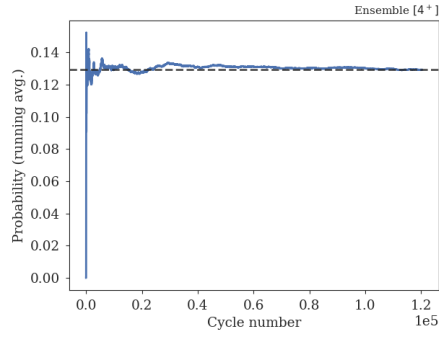
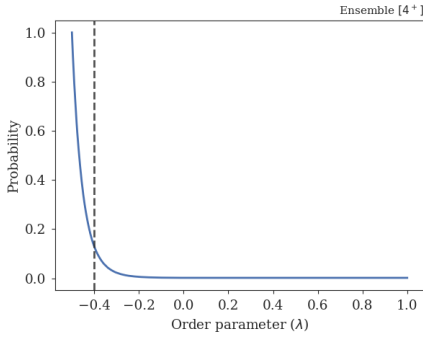
Table 4: Probabilities

Ensemble	P_{cross}	Error	Rel. error (%)
$[0^+]$	0.160847	0.002375	1.476788
$[1^+]$	0.156343	0.001585	1.013613
$[2^+]$	0.116772	0.001328	1.137127
$[3^+]$	0.112903	0.001231	1.090762
$[4^+]$	0.129205	0.001411	1.091815
$[5^+]$	0.175522	0.001698	0.967324
$[6^+]$	0.079400	0.000891	1.122794

The crossing probabilities are also displayed in the figures below

2.1 Crossing probabilities



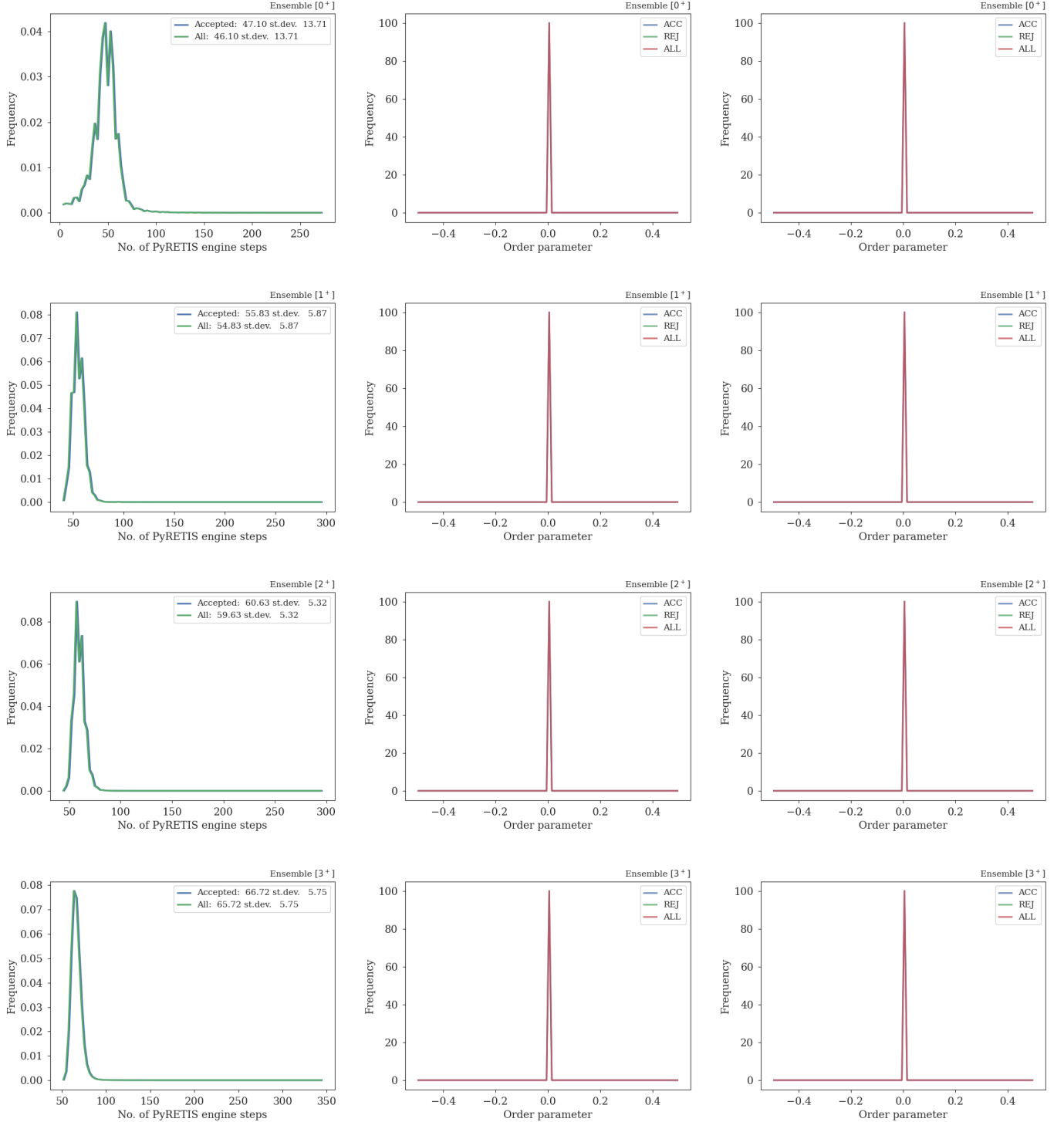


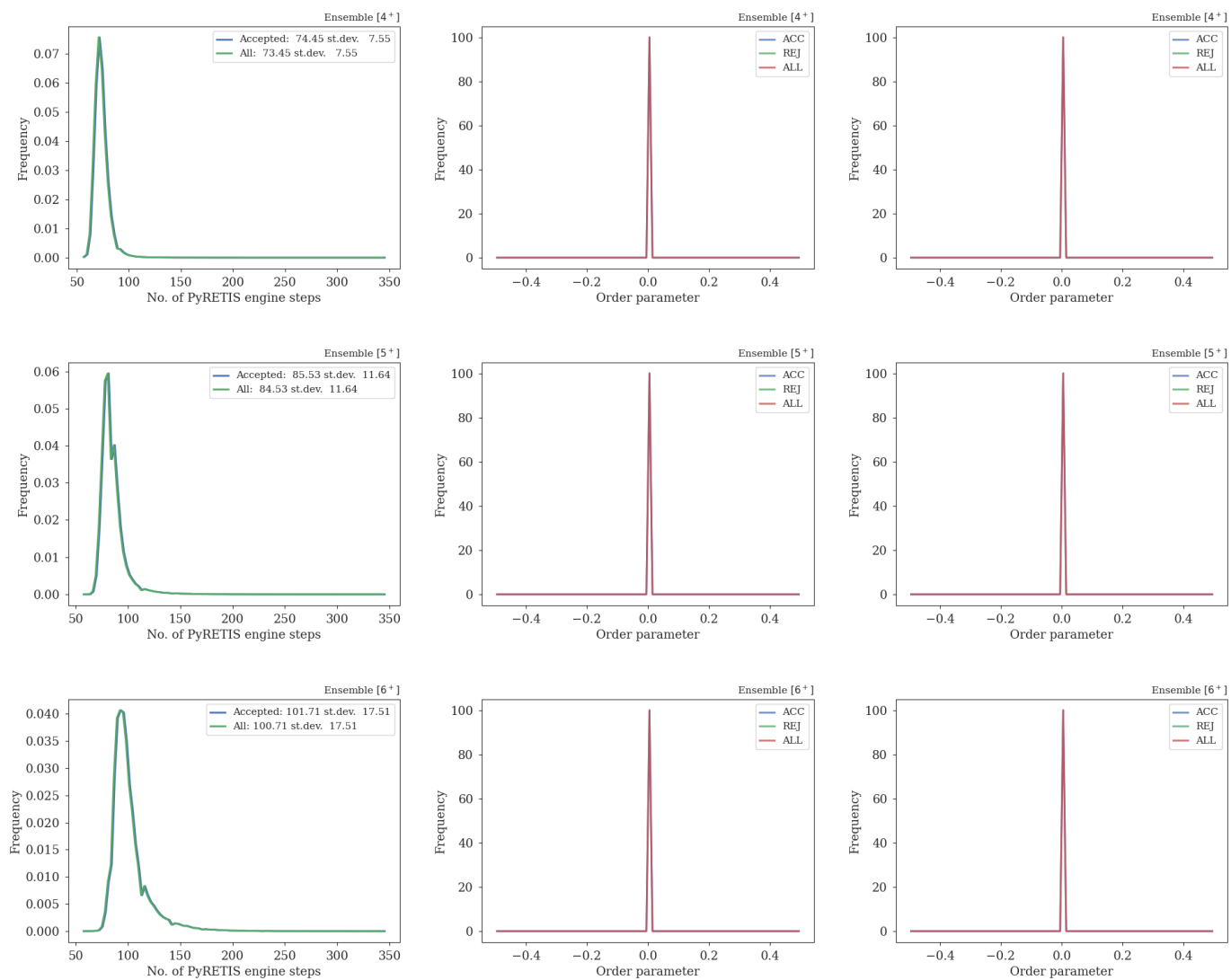
2.2 Distributions for path lengths and shooting moves

The average path lengths in the different ensembles are given in the table below and some distributions for the path lengths and shooting moves can also be found here:

Table 5: Path lengths

Ensemble	Accepted	All	All/Accepted
[0 ⁺]	47.098129	46.098129	0.978768
[1 ⁺]	55.831494	54.831494	0.982089
[2 ⁺]	60.633950	59.633950	0.983508
[3 ⁺]	66.720397	65.720397	0.985012
[4 ⁺]	74.450498	73.450498	0.986568
[5 ⁺]	85.534088	84.534088	0.988309
[6 ⁺]	101.705786	100.705786	0.990168





2.3 Efficiency analysis

Table 6: Efficiency

Ensemble	TIS cycles	Tot sim.	Acceptance ratio	Correlation	Efficiency
[0 ⁺]	123933	5.7131×10^6	1.000000	2.375954	1.2460×10^3
[1 ⁺]	123134	6.7516×10^6	1.000000	0.535029	693.669879
[2 ⁺]	123430	7.3606×10^6	1.000000	0.480493	951.770927
[3 ⁺]	121311	7.9726×10^6	1.000000	0.429031	948.549792
[4 ⁺]	120396	8.8431×10^6	1.000000	0.437518	1.0542×10^3
[5 ⁺]	110316	9.3255×10^6	1.000000	0.450717	872.598531
[6 ⁺]	82616	8.3199×10^6	1.000000	0.221135	1.0489×10^3

3 Combined results

The overall matched probability distributions are shown in the left figure while the matched probability distribution is shown in the right figure below. The overall crossing rate as a function of cycles and its relative error block analysis are reported in the two following plots, respectively.

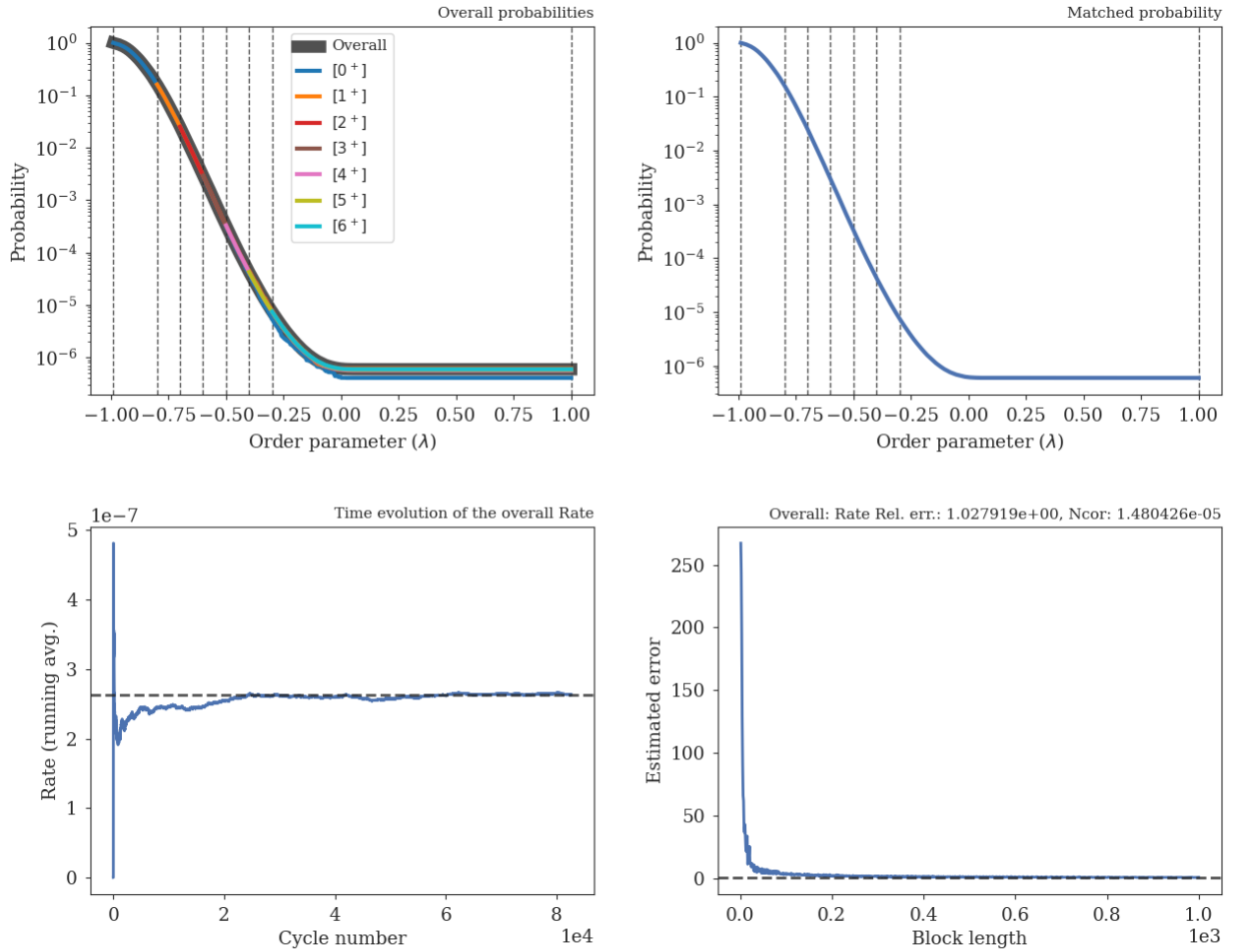


Table 7: Summary of main results

Property	Value	Relative error (%)
Crossing probability	$5.969870638 \times 10^{-7}$	3.013233817
Flux (1/reduced)	0.441235243	0.157589042
Rate constant (1/reduced)	$2.634117321 \times 10^{-7}$	3.017351876

Other statistics:

- sim.time: 5.428644383×10^7
- $\tau_{\text{eff}} = 4.928980031 \times 10^4$

- $\tau_{\text{eff}}^{\text{opt}} = 4.738410543 \times 10^4$