

# PyRETIS — RETIS analysis

RETIS analysis report generated by PyRETIS version 3.0.0.dev0+098fc56 on 13.02.2023 09:18:59.

The main results are:

- The crossing probability:  $P_{\text{cross}} = 5.785553633 \times 10^{-7} \pm 3.093748387 \%$
- The initial flux (unit: 1/reduced):  $f_A = 0.441314103 \pm 0.153909975 \%$
- The rate constant (unit: 1/reduced):  $k_{AB} = 2.553246410 \times 10^{-7} \pm 3.097574432 \%$

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

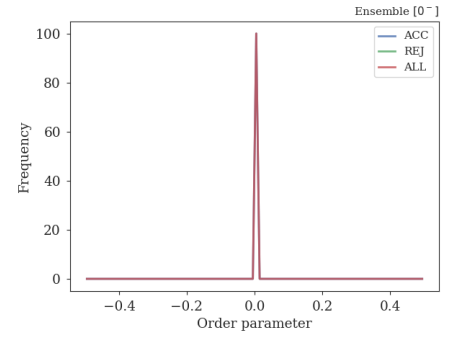
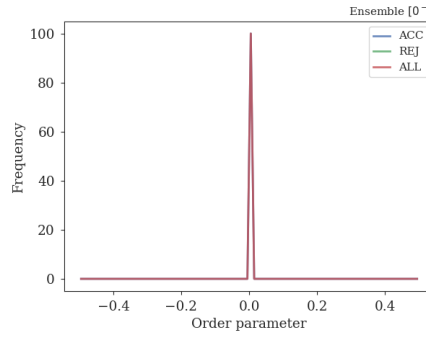
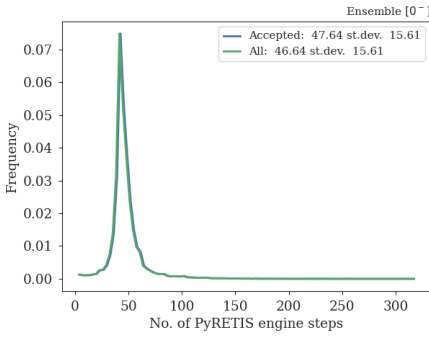
## 1 Results for $[0^-]$

Table 1: Interfaces

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

Table 2: Path lengths

Ensemble	Accepted	All	All/Accepted
$[0^-]$	47.635384	46.635384	0.979007



## 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
$[0^+]$	$-0.9900$	$-0.9900$	$1.0000$	$-0.8000$
$[1^+]$	$-0.9900$	$-0.8000$	$1.0000$	$-0.7000$
$[2^+]$	$-0.9900$	$-0.7000$	$1.0000$	$-0.6000$
$[3^+]$	$-0.9900$	$-0.6000$	$1.0000$	$-0.5000$
$[4^+]$	$-0.9900$	$-0.5000$	$1.0000$	$-0.4000$
$[5^+]$	$-0.9900$	$-0.4000$	$1.0000$	$-0.3000$
$[6^+]$	$-0.9900$	$-0.3000$	$1.0000$	$1.0000$

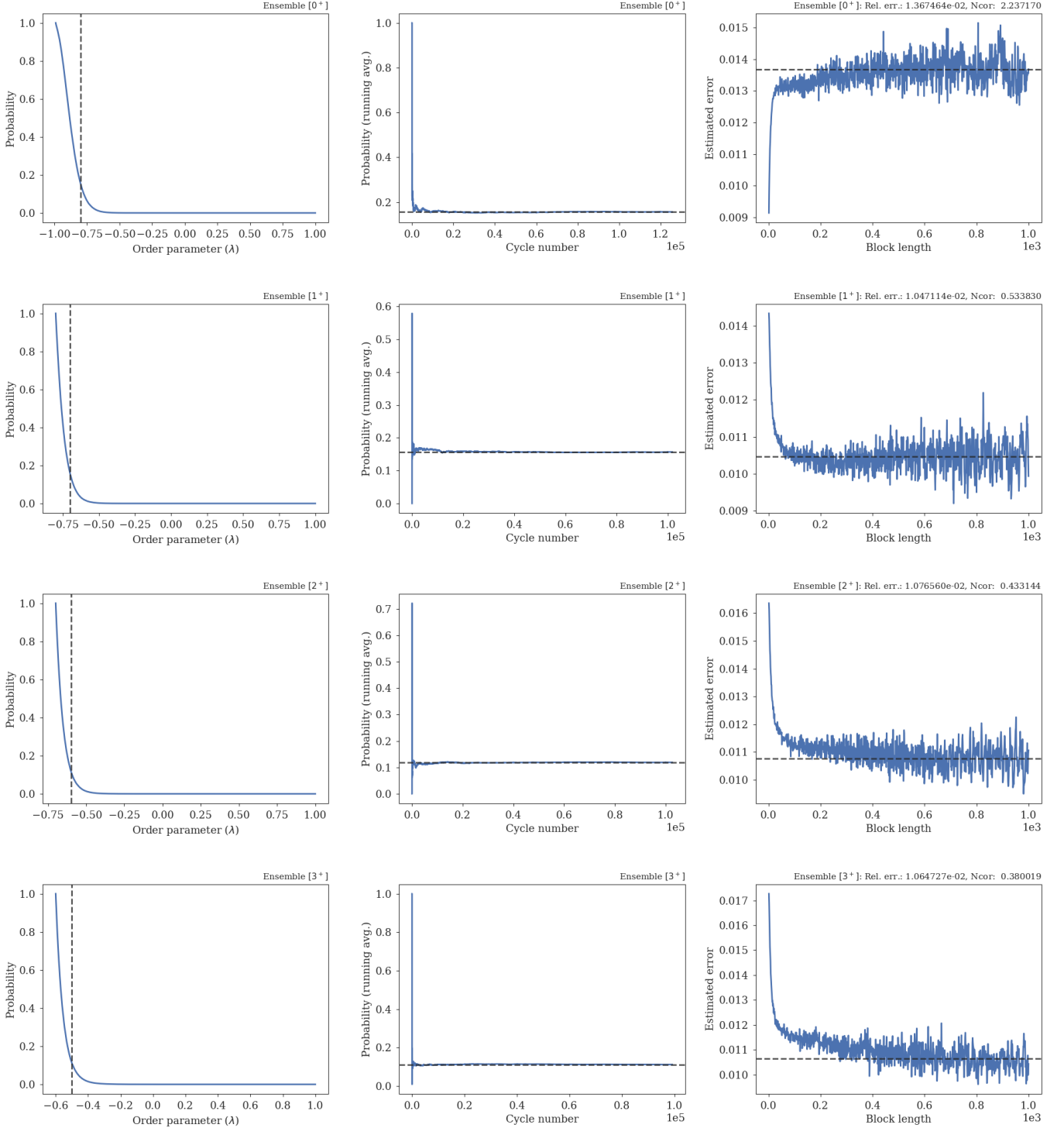
The calculated crossing probabilities are:

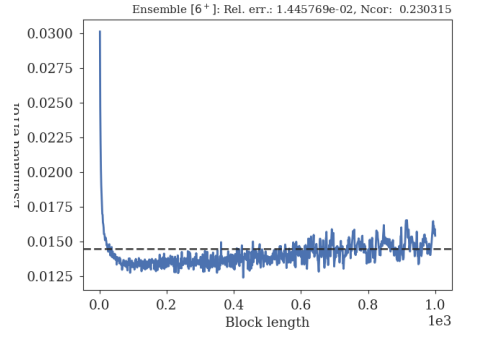
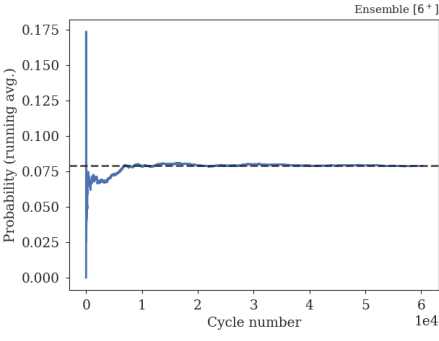
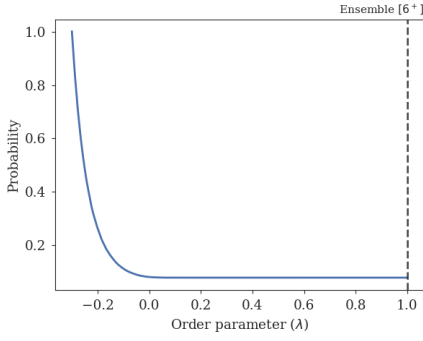
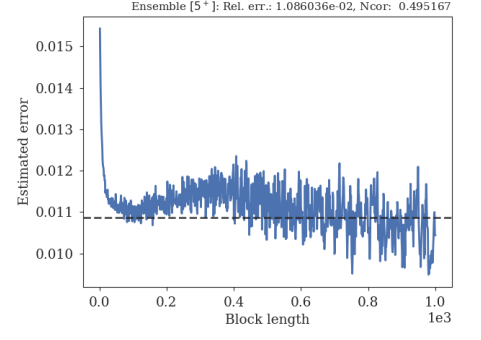
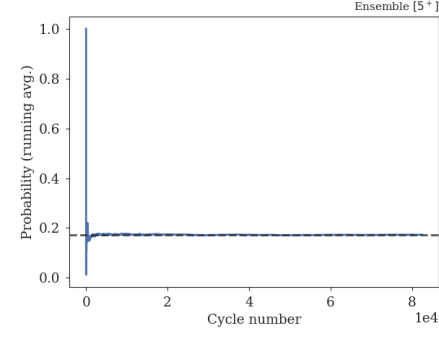
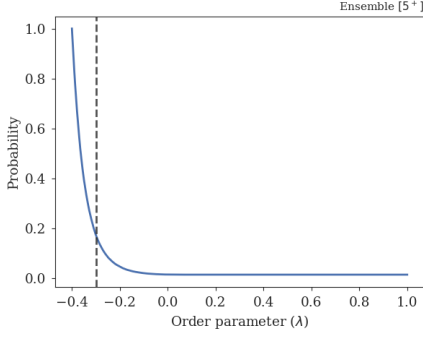
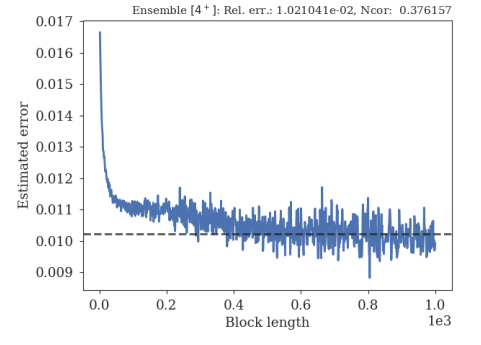
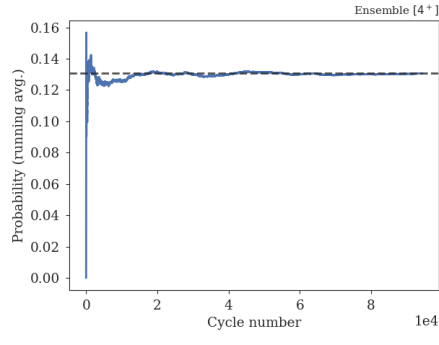
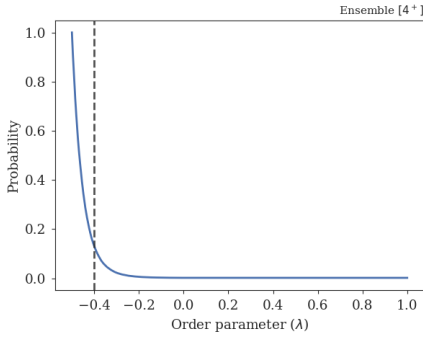
Table 4: Probabilities

Ensemble	$P_{\text{cross}}$	Error	Rel. error (%)
$[0^+]$	0.156005	0.002133	1.367464
$[1^+]$	0.156719	0.001641	1.047114
$[2^+]$	0.118881	0.001280	1.076560
$[3^+]$	0.111467	0.001187	1.064727
$[4^+]$	0.130639	0.001334	1.021041
$[5^+]$	0.173179	0.001881	1.086036
$[6^+]$	0.078932	0.001141	1.445769

The crossing probabilities are also displayed in the figures below

## 2.1 Crossing probabilities



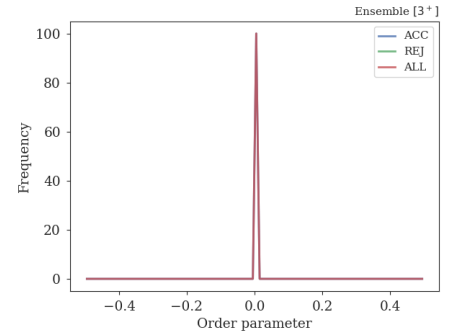
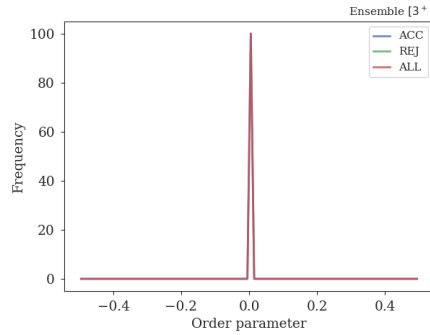
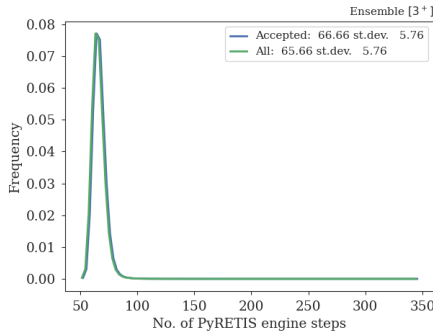
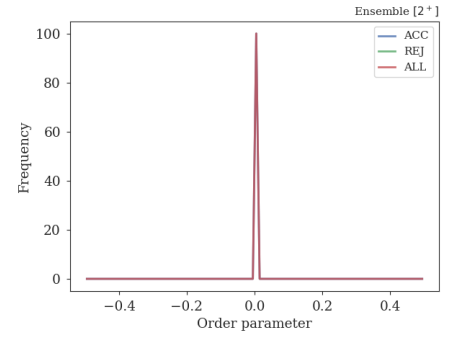
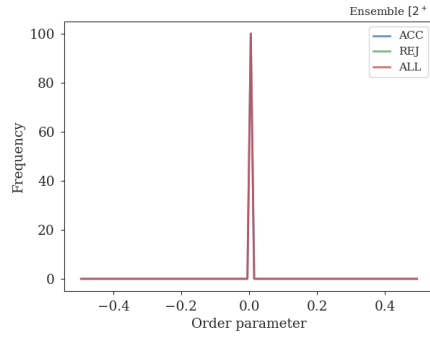
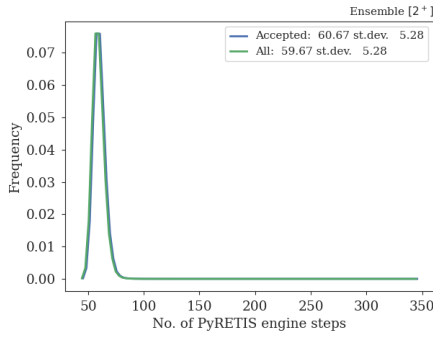
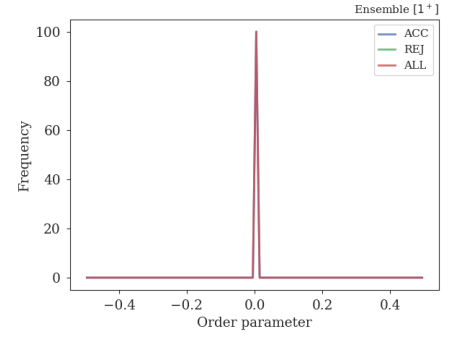
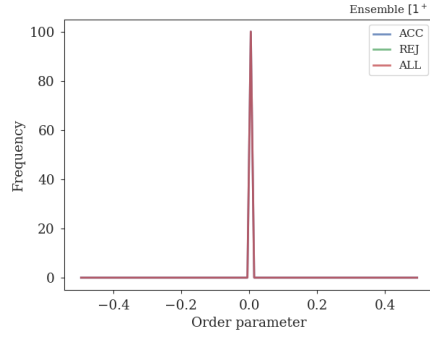
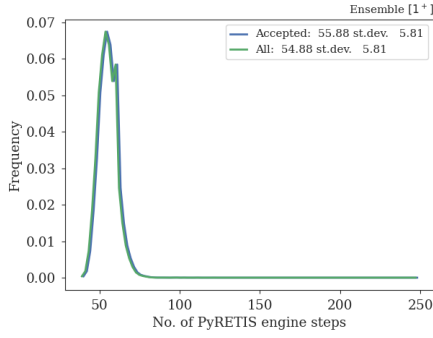
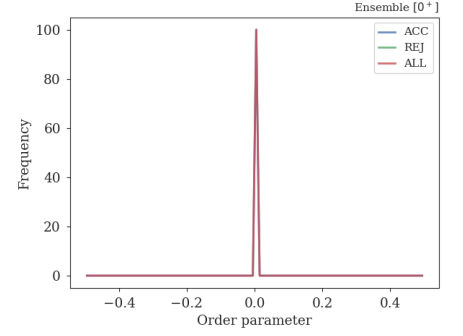
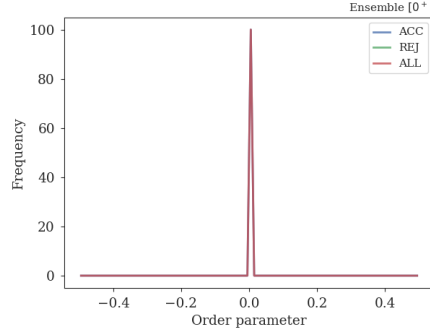
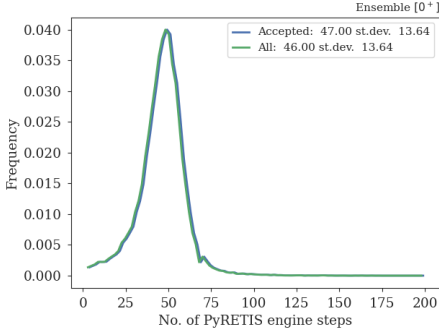


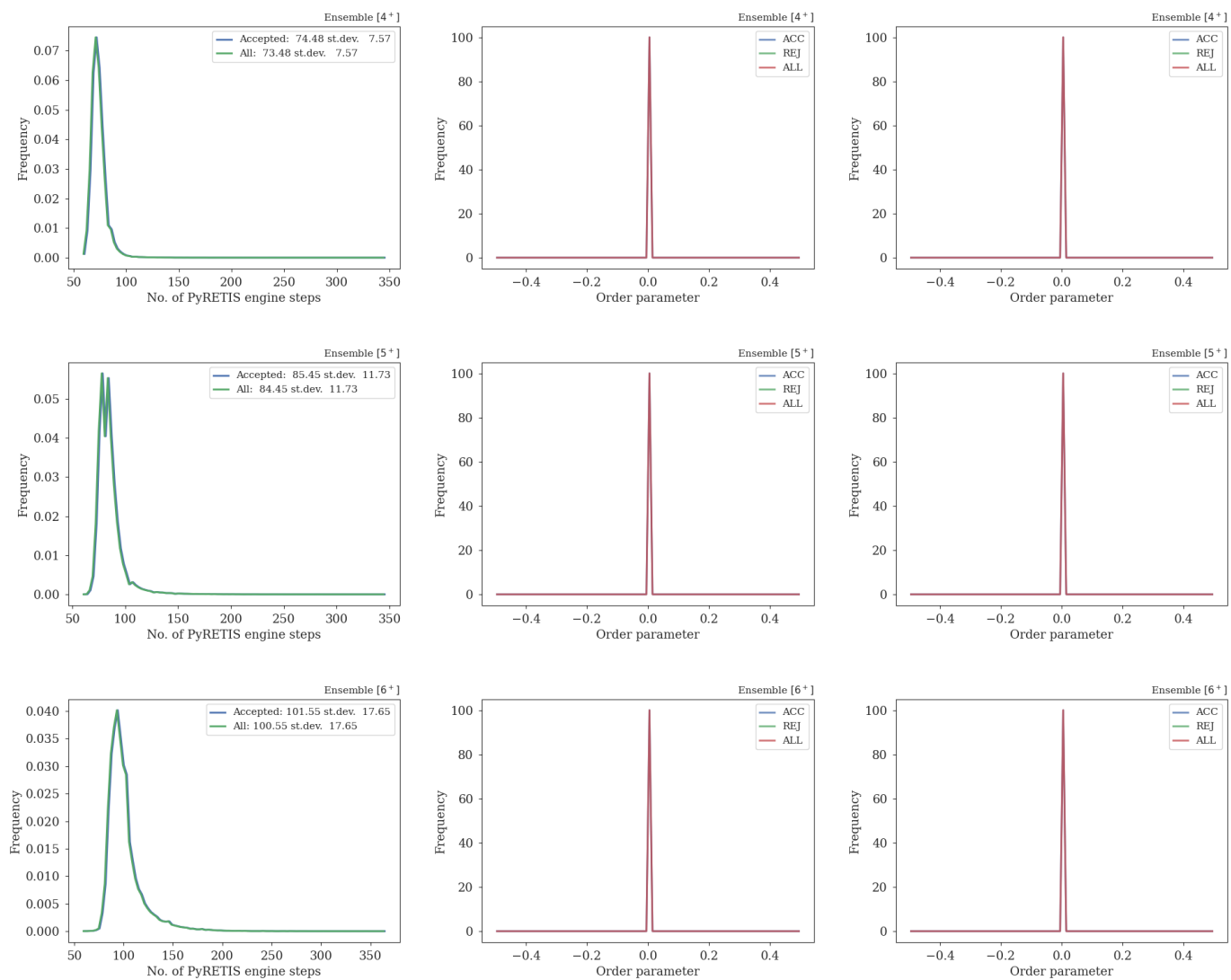
## 2.2 Distributions for path lengths and shooting moves

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 <sup>+</sup> ]	47.003006	46.003006	0.978725
[1 <sup>+</sup> ]	55.879187	54.879187	0.982104
[2 <sup>+</sup> ]	60.669014	59.669014	0.983517
[3 <sup>+</sup> ]	66.660125	65.660125	0.984999
[4 <sup>+</sup> ]	74.480284	73.480284	0.986574
[5 <sup>+</sup> ]	85.452567	84.452567	0.988298
[6 <sup>+</sup> ]	101.553359	100.553359	0.990153





## 2.3 Efficiency analysis

Table 6: Efficiency

Ensemble	TIS cycles	Tot sim.	Acceptance ratio	Correlation	Efficiency
[0 <sup>+</sup> ]	125658	$5.7806 \times 10^6$	1.000000	2.237170	$1.0810 \times 10^3$
[1 <sup>+</sup> ]	101788	$5.5860 \times 10^6$	1.000000	0.533830	612.480193
[2 <sup>+</sup> ]	102630	$6.1238 \times 10^6$	1.000000	0.433144	709.740196
[3 <sup>+</sup> ]	99154	$6.5105 \times 10^6$	1.000000	0.380019	738.054963
[4 <sup>+</sup> ]	94353	$6.9331 \times 10^6$	1.000000	0.376157	722.791416
[5 <sup>+</sup> ]	82456	$6.9636 \times 10^6$	1.000000	0.495167	821.341520
[6 <sup>+</sup> ]	60175	$6.0508 \times 10^6$	1.000000	0.230315	$1.2648 \times 10^3$

## 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.

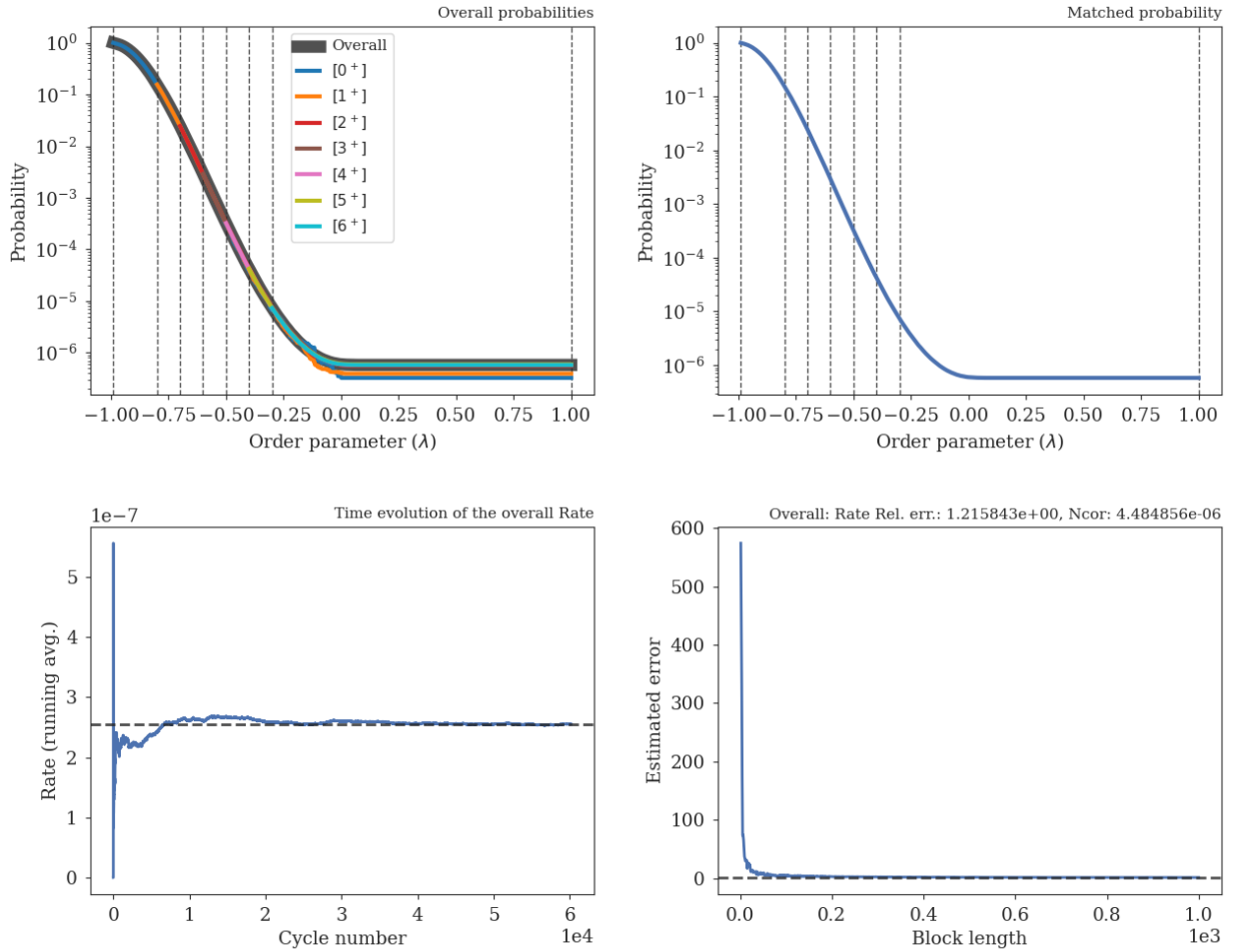


Table 7: Summary of main results

Property	Value	Relative error (%)
Crossing probability	$5.785553633 \times 10^{-7}$	3.093748387
Flux (1/reduced)	0.441314103	0.153909975
Rate constant (1/reduced)	$2.553246410 \times 10^{-7}$	3.097574432

Other statistics:

- sim.time:  $4.394848774 \times 10^7$
- $\tau_{\text{eff}} = 4.206432415 \times 10^4$

- $\tau_{\text{eff}}^{\text{opt}} = 4.102316613 \times 10^4$