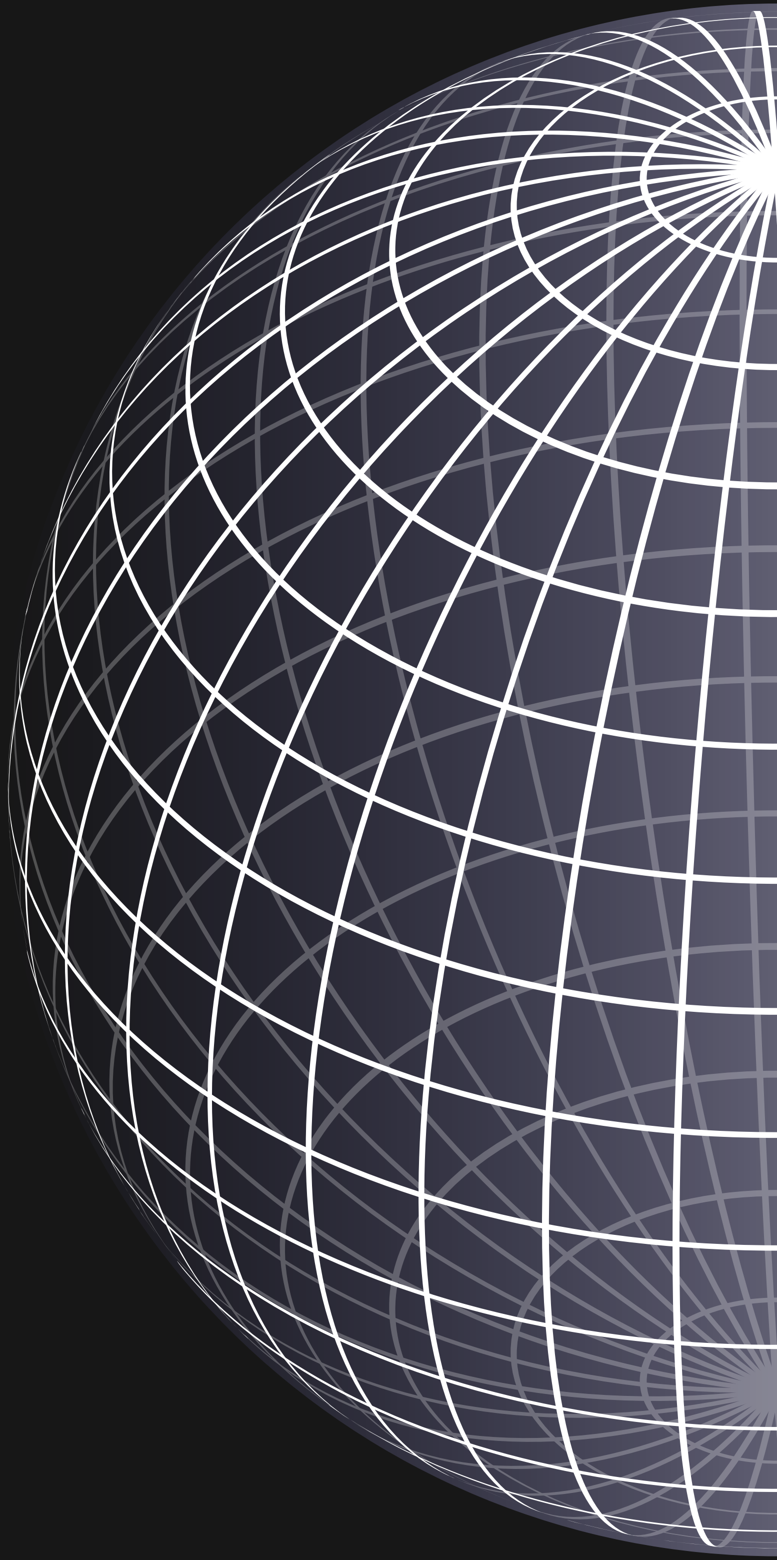
LINEAR FITS PT. 2



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TASKS

Prove that the mean value of σ_i & ΔE_i of each pair involved at avoided crossings decreases exponentially as a function of the energy.

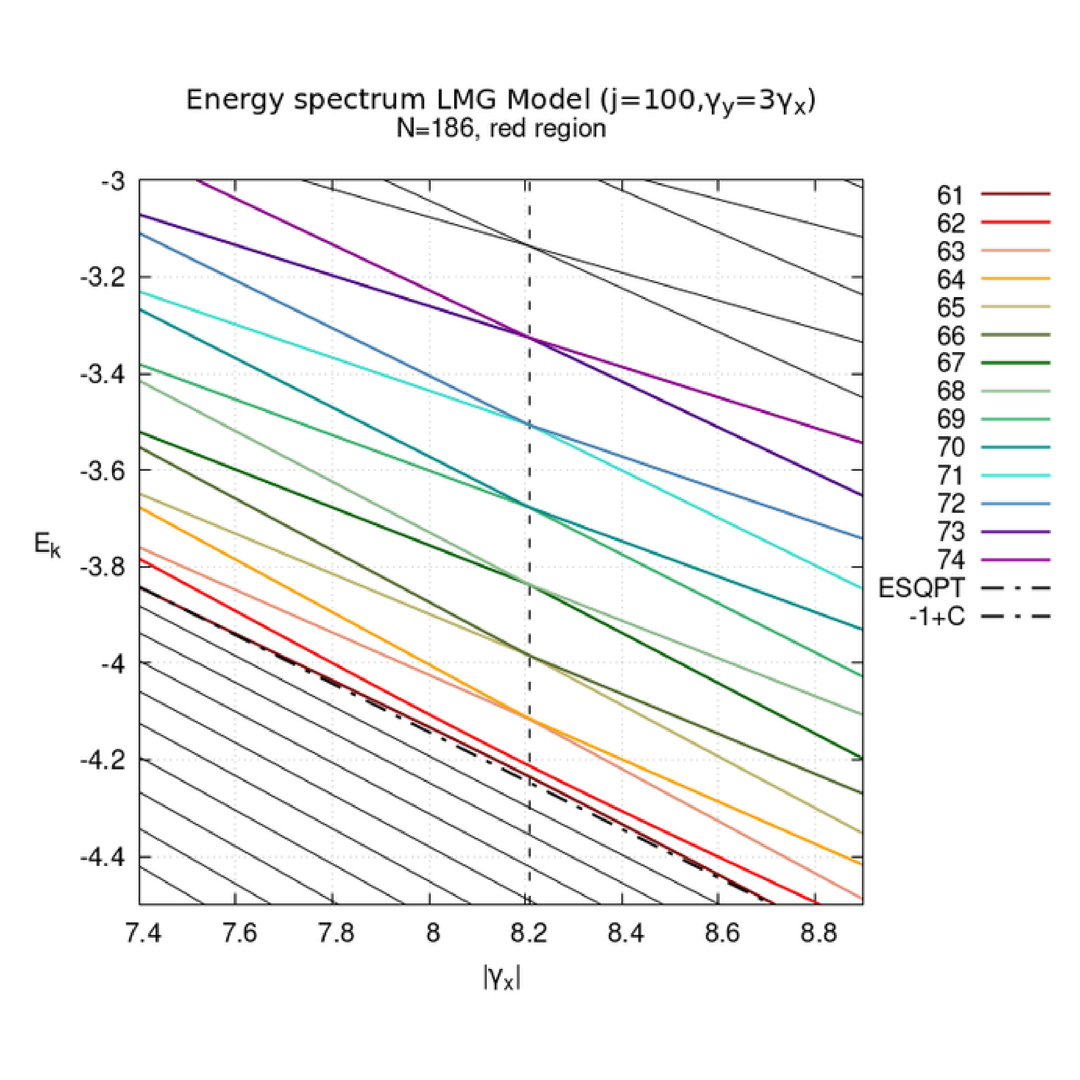
DESCRIPTION

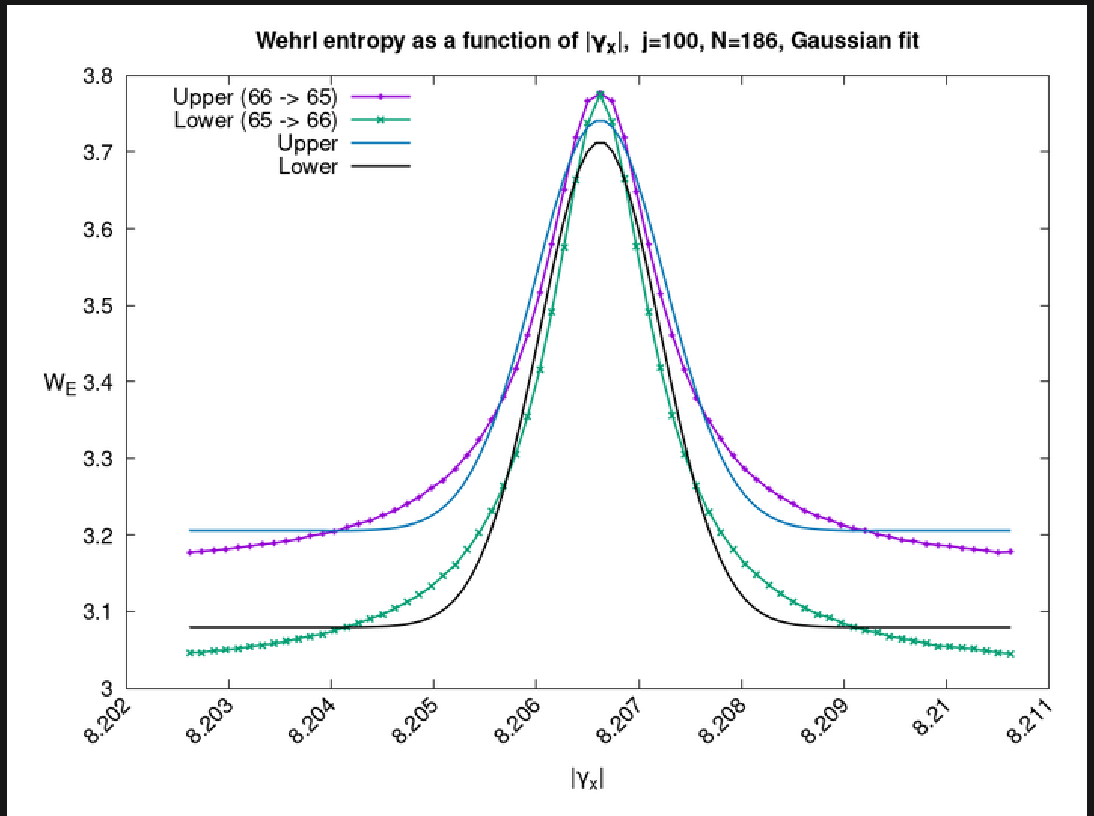
- E_i: Mean value of two energy levels at the value of γAC.
- $ESQPT_i$: Value of the ESQPT at γAC.
- σ_i : Width parameter of Gaussian Fits of the Wehrl Entropy.

EXPONENTIAL MODEL

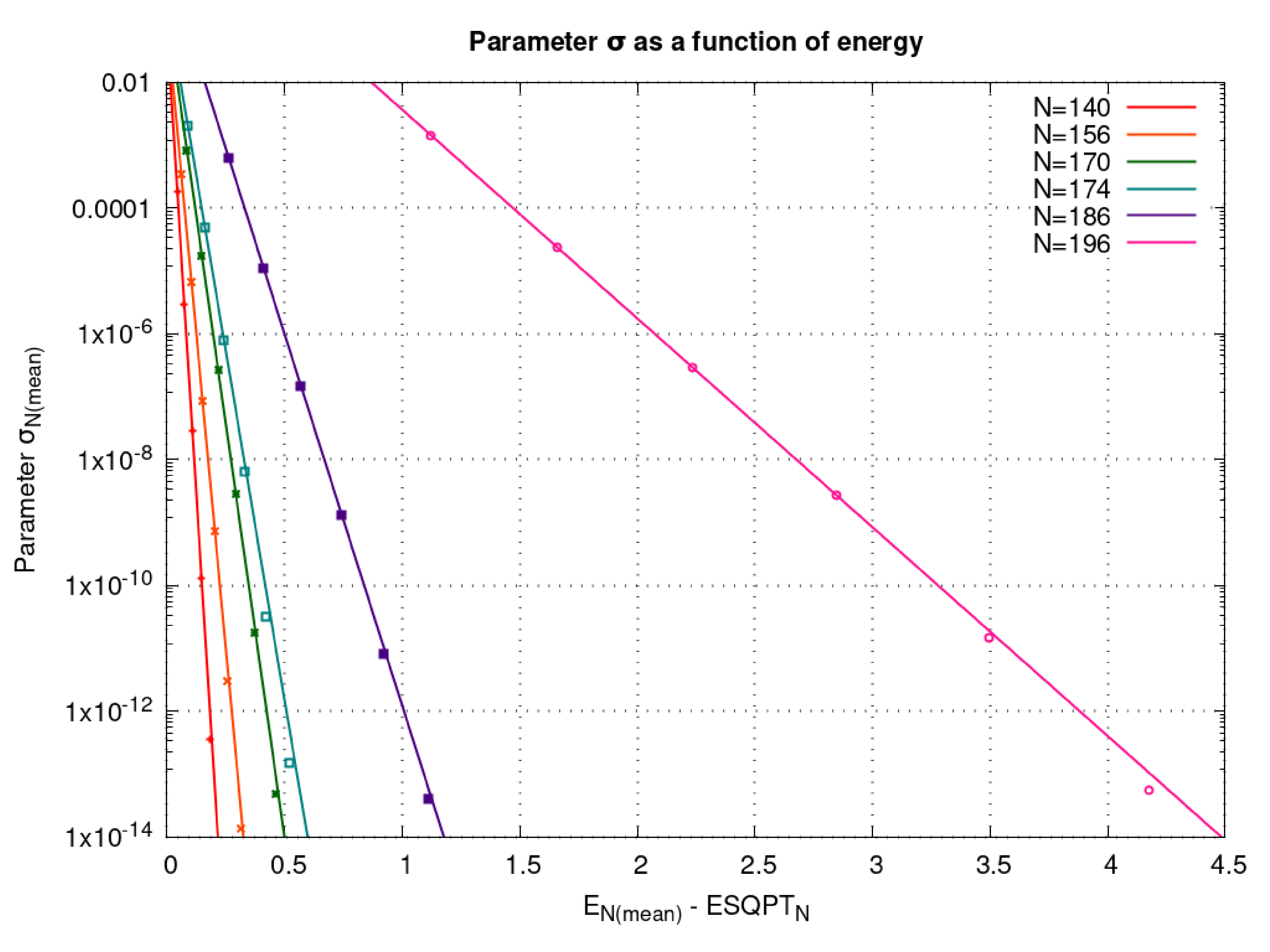
$$\sigma_N = A\, e^{-\alpha(E_N - ESQPT_N)}$$

$$\Delta E_N = B\, e^{-\beta(E_N - ESQPT_N)}$$





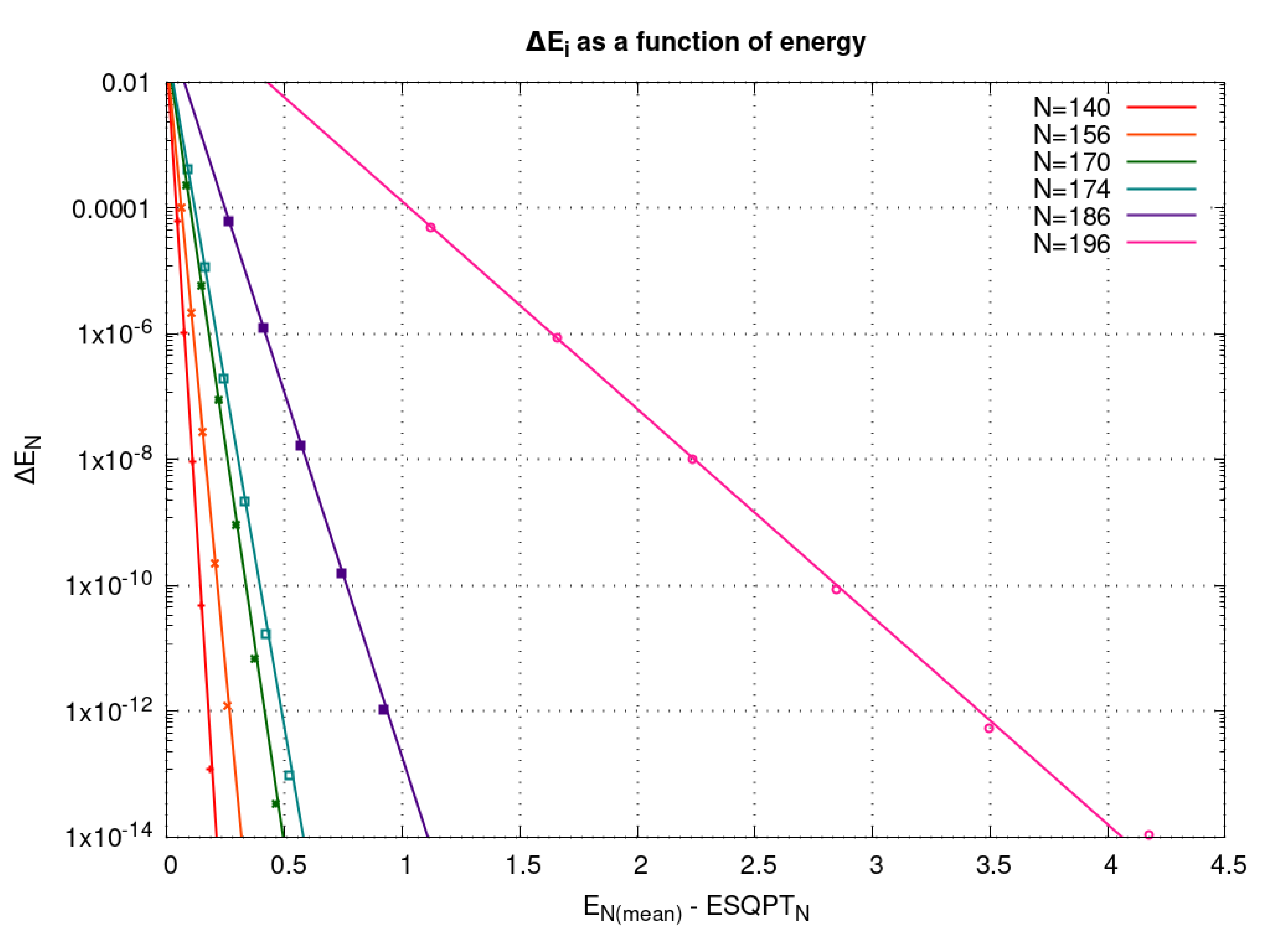
Parameter σ vs. E_i –ESQPT



$$\sigma_N = Ae^{-\alpha(E_N - ESQPT_N)}$$

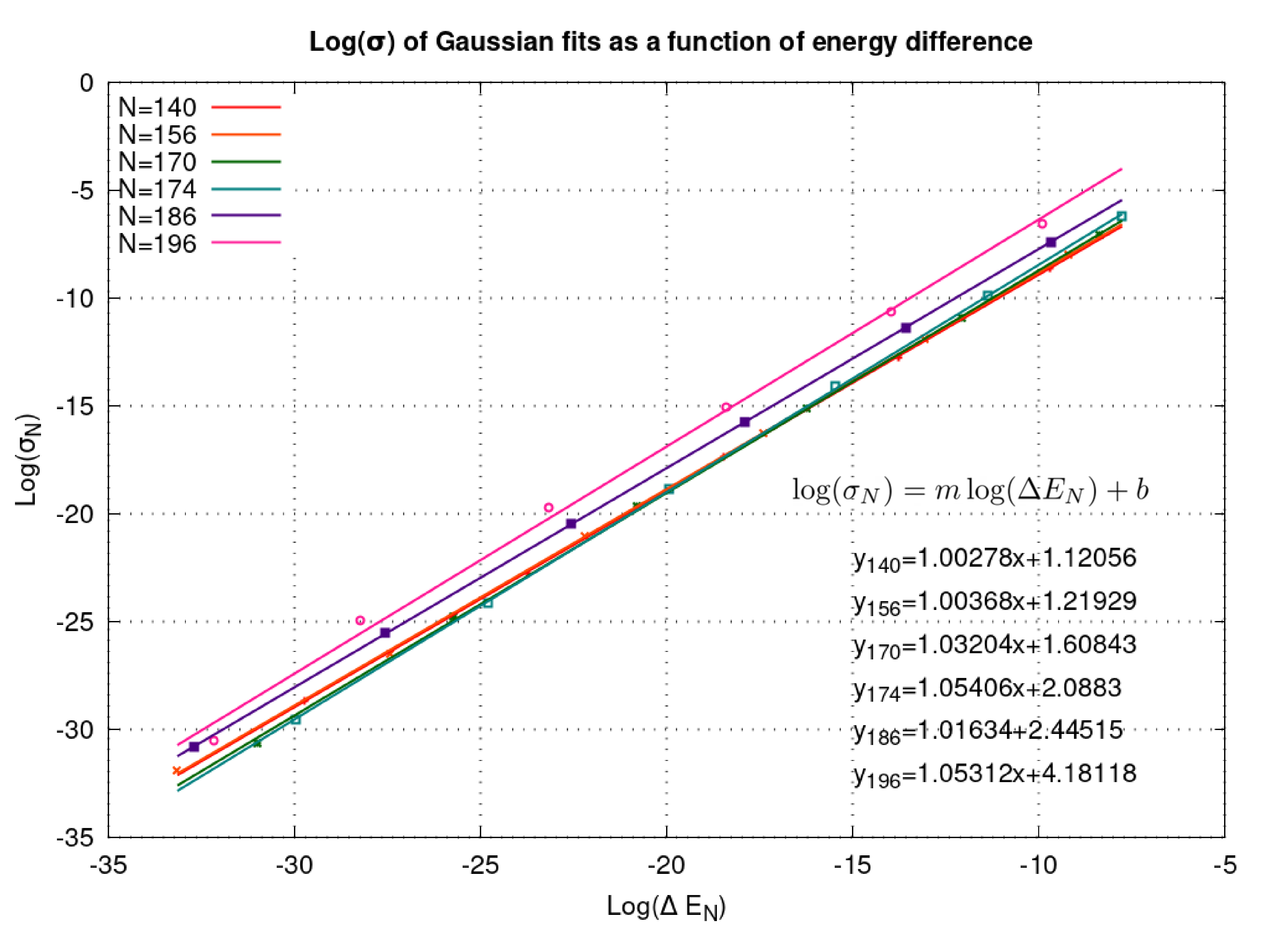
N	A	α
140	0.0661858	136.777
156	0.0887738	91.8037
170	0.135824	60.5679
174	0.186123	51.1451
186	0.777914	27.1767
196	7.62043	7.64105

ΔE_i vs. E_i –ESQPT



$$\Delta E_N = Be^{-\beta(E_N - ESQPT_N)}$$

N	B	β
140	0.0200315	134.813
156	0.0232367	89.9843
170	0.0311131	58.2432
174	0.0346337	49.8099
186	0.0699459	26.6627
196	0.25519	7.60061



From the following relations:

$$\sigma_N = A\, e^{-\alpha(E_N - ESQPT_N)}$$

$$\Delta E_N = B\, e^{-\beta(E_N - ESQPT_N)}$$

it's possible to show that:

$$\log(\sigma_N) = \underbrace{\frac{\alpha}{\beta}}_{m} \log(\Delta E_N) \underbrace{- \frac{\alpha}{\beta} \log(B) + \log(A)}_{+b}$$

Numerical comparison of the parameters

	N	m	alpha/beta	diff1	+b	cte	diff2
0	140	1.00278	1.014568	0.011788	1.12056	1.252129	0.131569
1	156	1.00368	1.020219	0.016539	1.21929	1.416423	0.197133
2	170	1.03204	1.039914	0.007874	1.60843	1.612236	0.003806
3	174	1.05406	1.026806	0.027254	2.08830	1.771727	0.316573
4	186	1.01634	1.019278	0.002938	2.44515	2.460174	0.015024
5	196	1.05312	1.005321	0.047799	4.18118	3.403846	0.777334