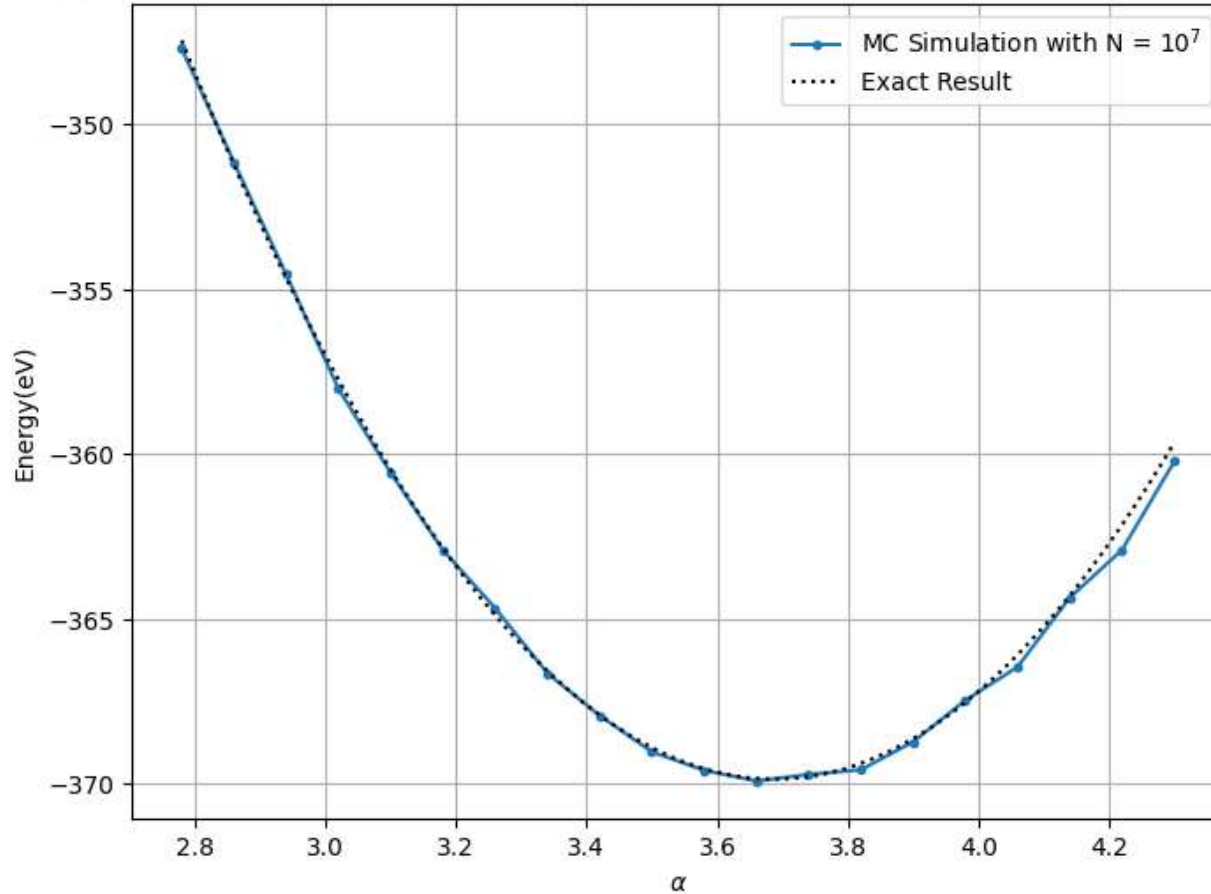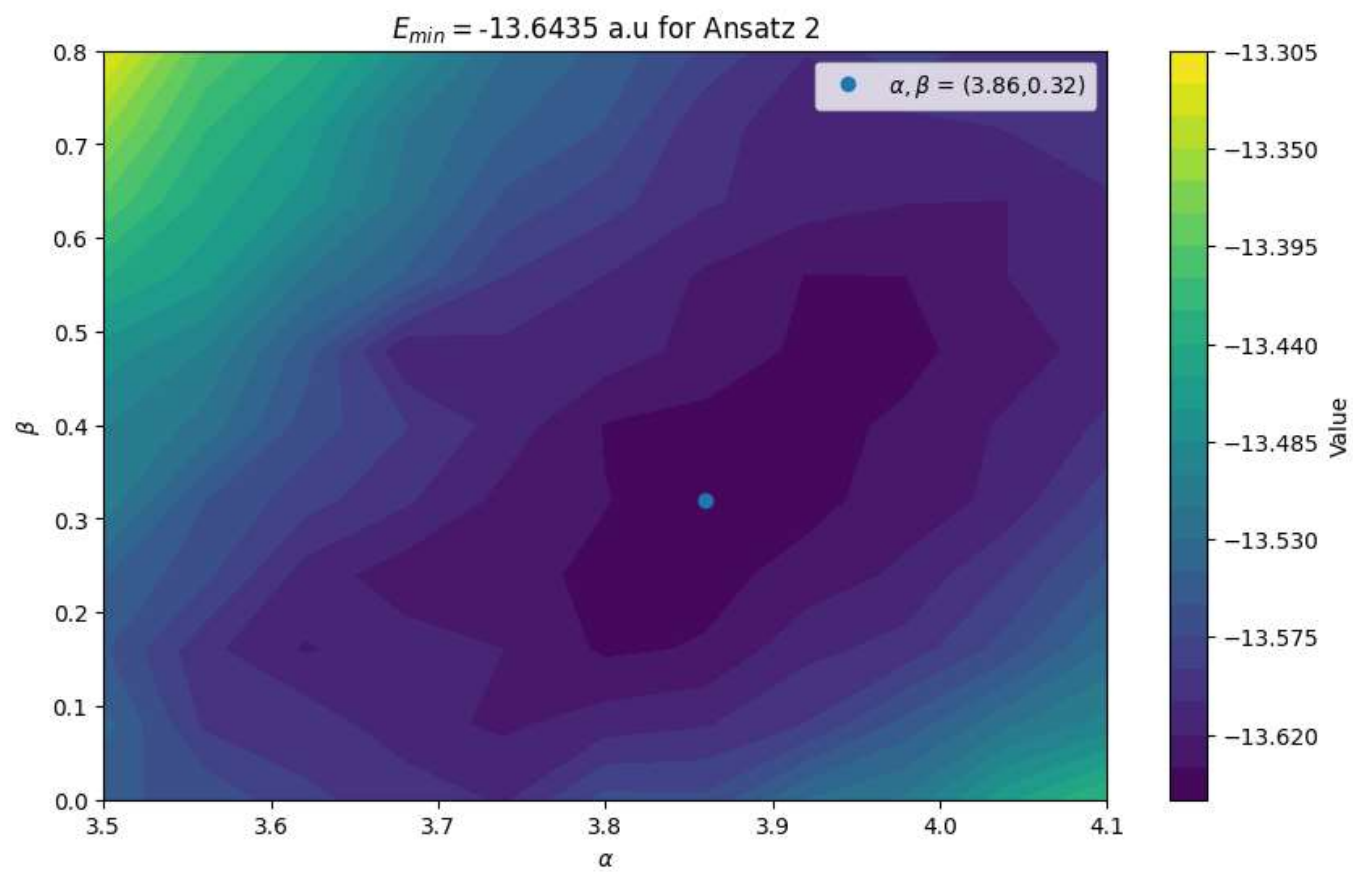# Beryllium VMC

Variational Monte Carlo Plot for Energy vs α (variational parameter) of Beryllium Ansatz 1

Beryllium Ansatz 1 VMC
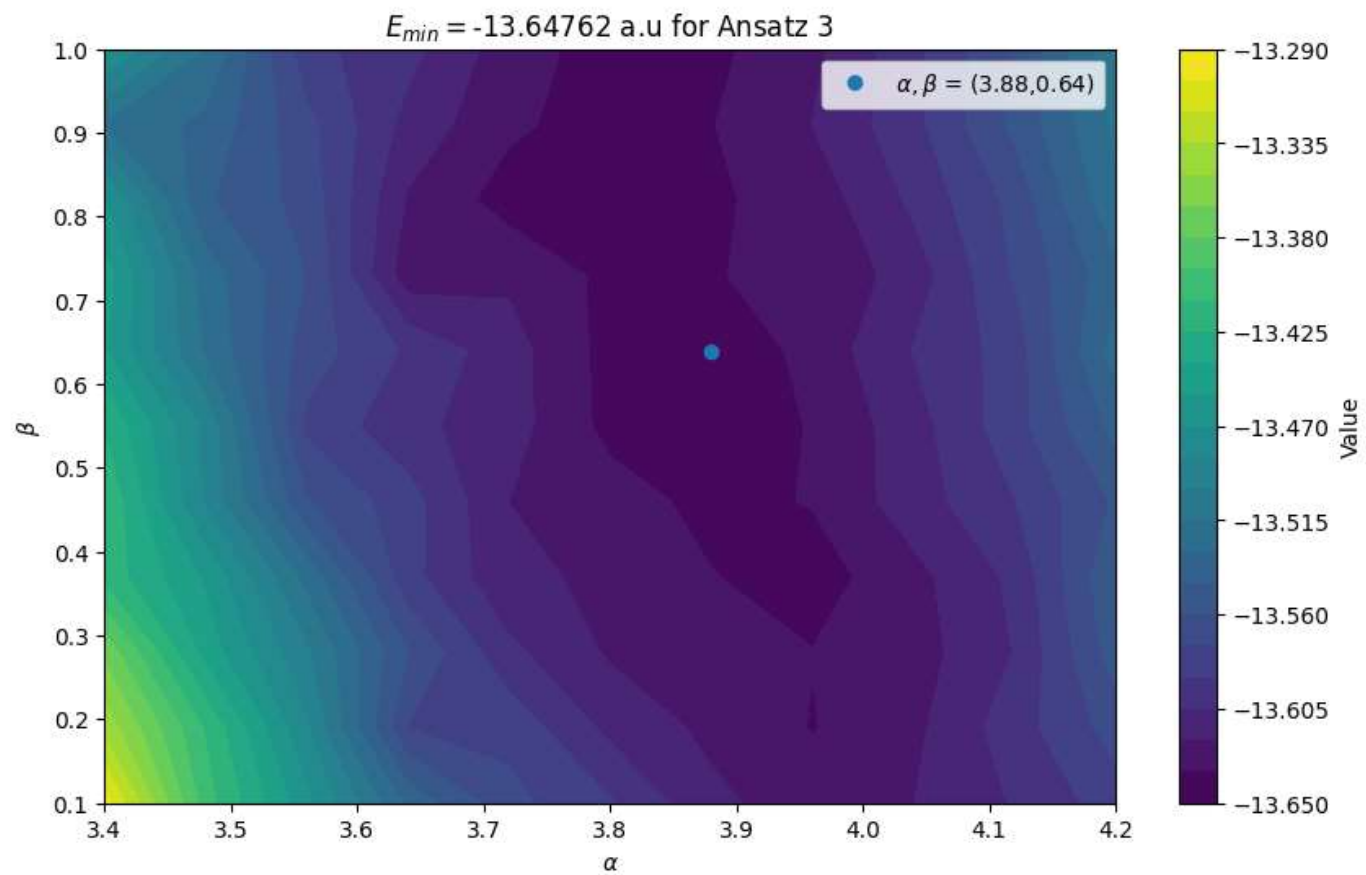
alpha	Energy(a.u)	Energy(eV)	Variance(a.u)
2.78	-12.78	-347.71	19.45
2.86	-12.91	-351.15	19.41
2.94	-13.03	-354.55	19.32
3.02	-13.16	-358.02	16.30
3.10	-13.26	-360.57	14.75
3.18	-13.34	-362.91	11.54
3.26	-13.41	-364.67	9.87
3.34	-13.48	-366.64	8.98
3.42	-13.53	-367.93	8.60
3.50	-13.57	-369.03	6.18
3.58	-13.59	-369.59	4.95
3.66	-13.60	-369.91	5.16
3.74	-13.59	-369.71	3.71
3.82	-13.59	-369.57	3.58
3.90	-13.56	-368.72	3.37
3.98	-13.51	-367.47	4.50
4.06	-13.47	-366.45	4.67
4.14	-13.40	-364.35	6.39
4.22	-13.34	-362.91	8.05
4.30	-13.24	-360.22	10.25

Average R12 for Ansatz 1 = 0.5968 bohr

E_{min} = -13.6435 a.u for Ansatz 2

α, β = (3.86, 0.32)

Beryllium Ansatz 2 VMC

α	β	Energy (a.u.)	Variance (a.u.)
3.80	0.24	-13.63825	1.042
3.80	0.32	-13.63451	0.876
3.80	0.40	-13.63627	1.109
3.86	0.24	-13.64018	0.803
3.86	0.32	-13.64353	0.596
3.86	0.40	-13.63992	0.696
3.92	0.24	-13.62952	0.720
3.92	0.32	-13.64021	0.442
3.92	0.40	-13.63896	0.438

Average R12 for Ansatz 2 = 0.6136bohr

$E_{min} = -13.64762$ a.u for Ansatz 3

● $\alpha, \beta = (3.88, 0.64)$

Beryllium Ansatz 3

alpha	beta	Energy (a.u.)	Variance (a.u.)
3.80	0.55	-13.63967	1.010
3.80	0.64	-13.64051	0.856
3.80	0.73	-13.63894	0.787
3.88	0.55	-13.64479	0.525
3.88	0.64	-13.64762	0.471
3.88	0.73	-13.63546	0.401
3.96	0.55	-13.63409	0.329
3.96	0.64	-13.63008	0.315
3.96	0.73	-13.63263	0.307

Average R12 for Ansatz 3 = 0.6037bohr