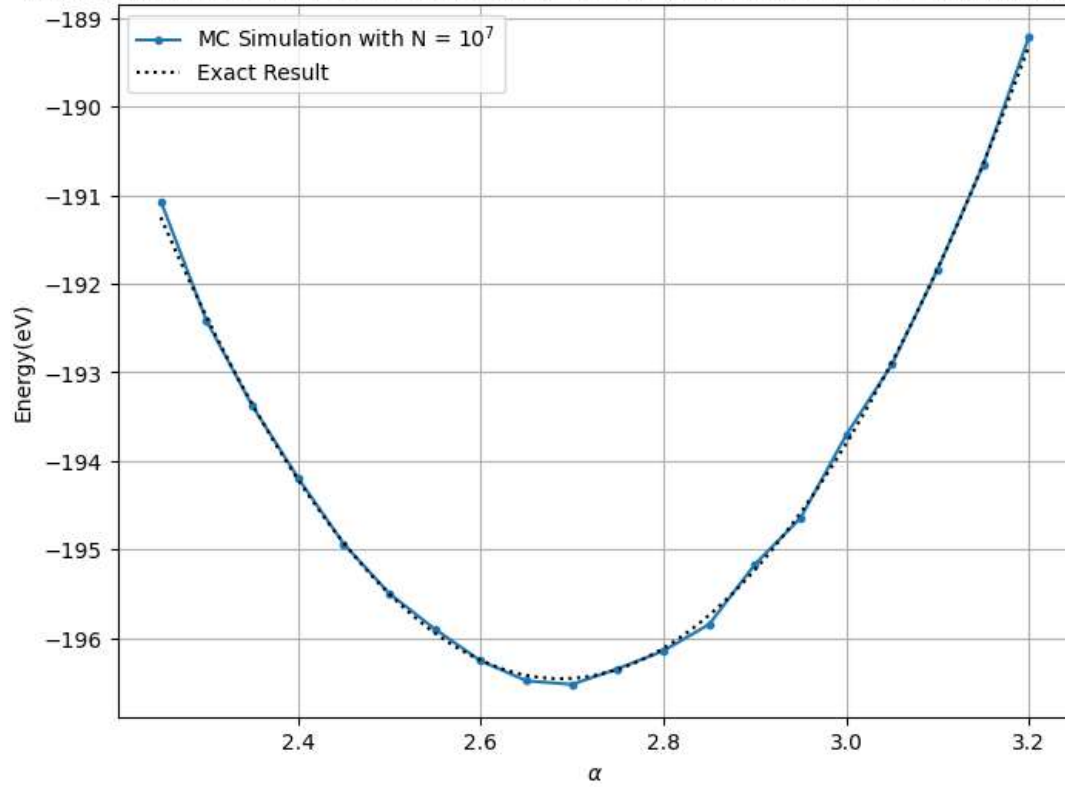


# Lithium VMC

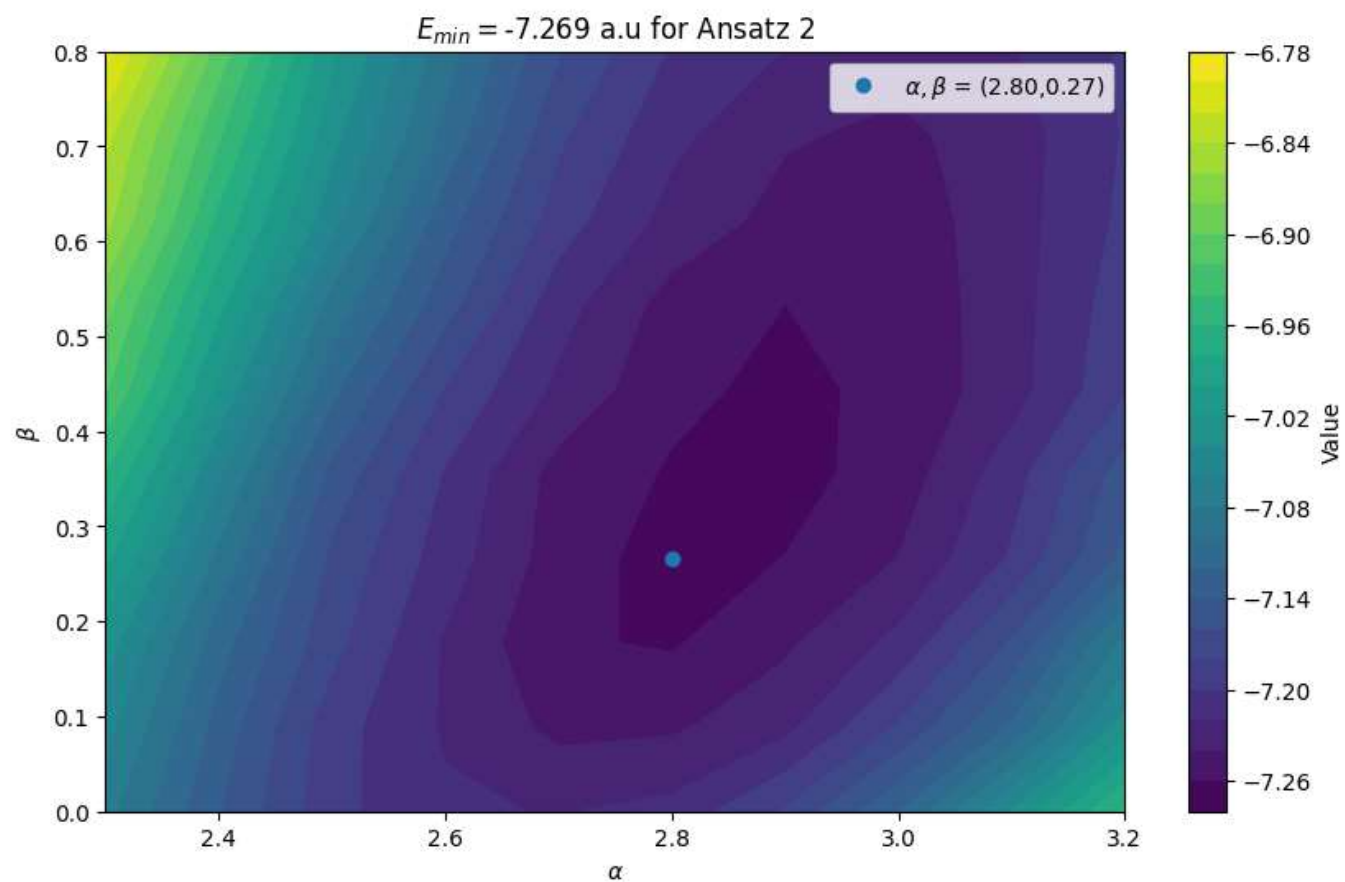
Variational Monte Carlo Plot for Energy vs  $\alpha$  (variational parameter) of Lithium(Ansatz 1)



Lithium VMC Ansatz 1

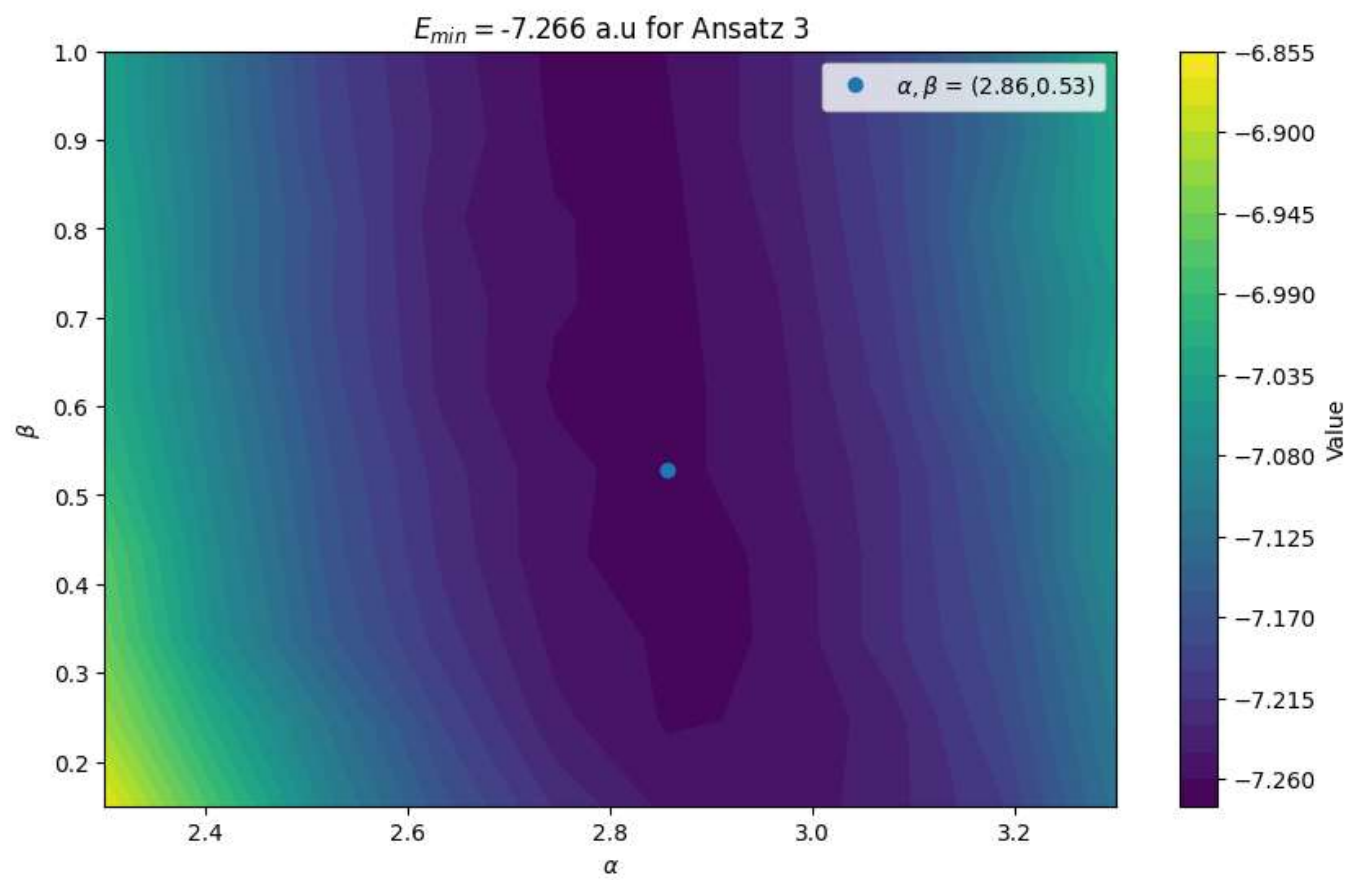
$\alpha$	Energy(a.u)	Energy(eV)	Variance(a.u)
2.25	-7.02	-191.07	5.04
2.30	-7.07	-192.42	5.42
2.35	-7.11	-193.37	4.39
2.40	-7.14	-194.19	3.98
2.45	-7.17	-194.93	3.56
2.50	-7.19	-195.49	3.25
2.55	-7.20	-195.90	2.92
2.60	-7.22	-196.25	2.50
2.65	-7.22	-196.48	2.36
2.70	-7.23	-196.52	2.26
2.75	-7.22	-196.34	2.04
2.80	-7.21	-196.14	1.96
2.85	-7.20	-195.84	1.86
2.90	-7.18	-195.17	1.99
2.95	-7.16	-194.64	2.15
3.00	-7.12	-193.70	2.45
3.05	-7.09	-192.91	2.77
3.10	-7.05	-191.84	3.18

Average R12 for Ansatz 1 = 0.8094 bohr



Ansatz 2			
$\alpha$	$\beta$	Energy (a.u.)	Variance (a.u.)
2.70	0.18	-7.25750	1.128
2.70	0.27	-7.25011	1.062
2.70	0.36	-7.24782	1.027
2.80	0.18	-7.26225	0.727
2.80	0.27	-7.26865	0.605
2.80	0.36	-7.26189	0.512
2.90	0.18	-7.24387	0.868
2.90	0.27	-7.25971	0.388
2.90	0.36	-7.26734	0.238

Average R12 for Ansatz 2 = 0.8511bohr



Ansatz 3

$\alpha$	$\beta$	Energy (a.u.)	Variance (a.u.)
2.74	0.43	-7.25764	0.785
2.74	0.53	-7.25631	0.675
2.74	0.62	-7.26215	0.680
2.86	0.43	-7.26598	0.356
2.86	0.53	-7.26610	0.286
2.86	0.62	-7.26599	0.280
2.97	0.43	-7.25772	0.178
2.97	0.53	-7.24947	0.172
2.97	0.62	-7.24931	0.173

Average R12 for Ansatz 3 = 0.8398bohr