

# Plots for Exercise 1: Question 5: Lithium Ansatz 1

VMC Simulation for Ground State energy of Lithium Atom for Ansatz 1

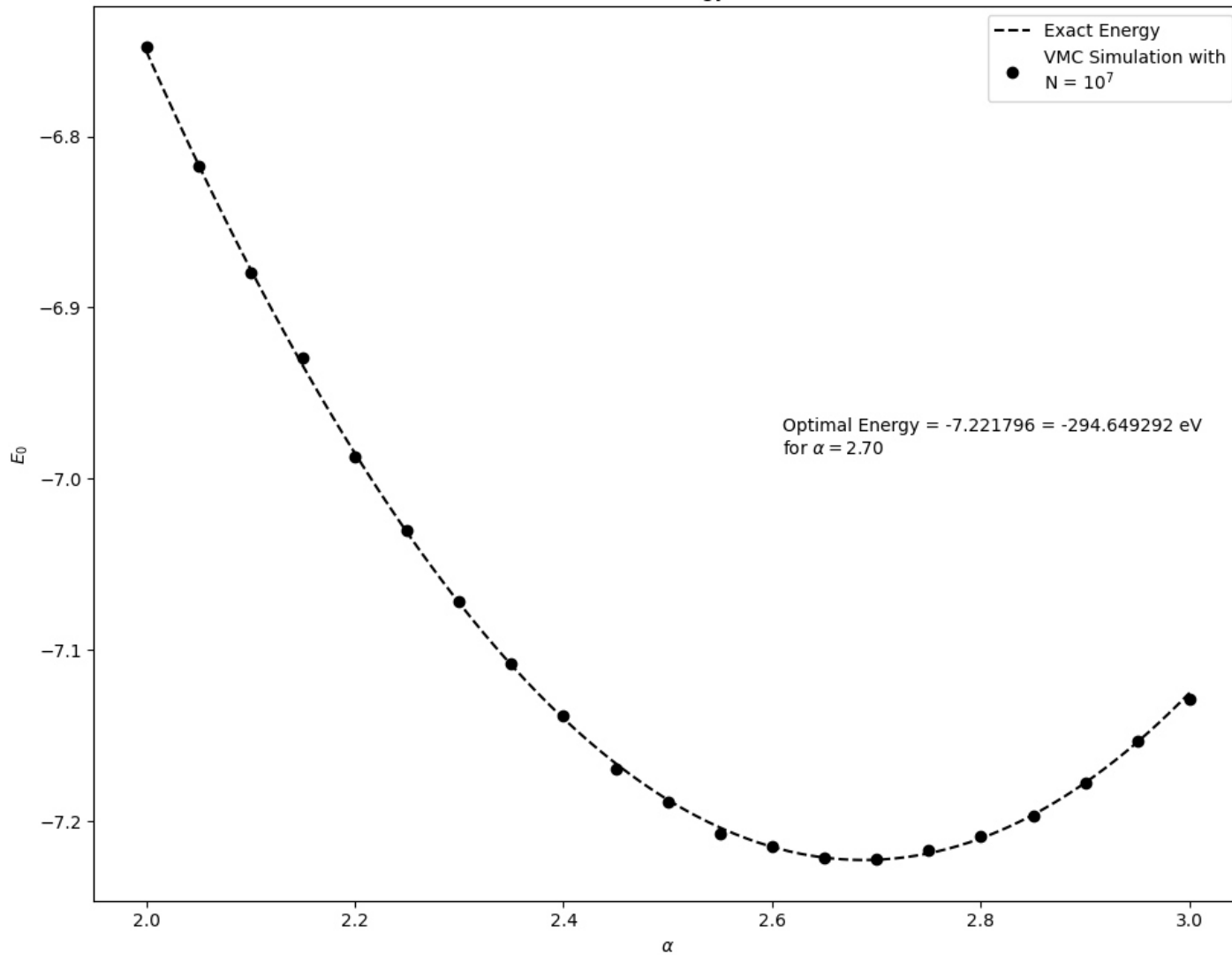


Table 4: Lithium: Ansatz 1

| alpha  | energy  | variance |
|--------|---------|----------|
| 2.0000 | -6.7479 | 6.8482   |
| 2.0500 | -6.8175 | 6.7456   |
| 2.1000 | -6.8793 | 6.1327   |
| 2.1500 | -6.9295 | 5.6893   |
| 2.2000 | -6.9874 | 5.4425   |
| 2.2500 | -7.0303 | 5.1732   |
| 2.3000 | -7.0719 | 4.7831   |
| 2.3500 | -7.1082 | 4.3054   |
| 2.4000 | -7.1387 | 4.4107   |
| 2.4500 | -7.1698 | 3.6296   |
| 2.5000 | -7.1891 | 3.3775   |
| 2.5500 | -7.2071 | 3.2824   |
| 2.6000 | -7.2147 | 2.5710   |
| 2.6500 | -7.2217 | 2.4588   |
| 2.7000 | -7.2218 | 2.1755   |
| 2.7500 | -7.2167 | 2.8505   |
| 2.8000 | -7.2088 | 2.1415   |
| 2.8500 | -7.1966 | 2.0171   |
| 2.9000 | -7.1775 | 2.4008   |
| 2.9500 | -7.1532 | 2.1370   |
| 3.0000 | -7.1290 | 2.2657   |

Optimal  $r_{12} = 0.811$

# Ansatz 2

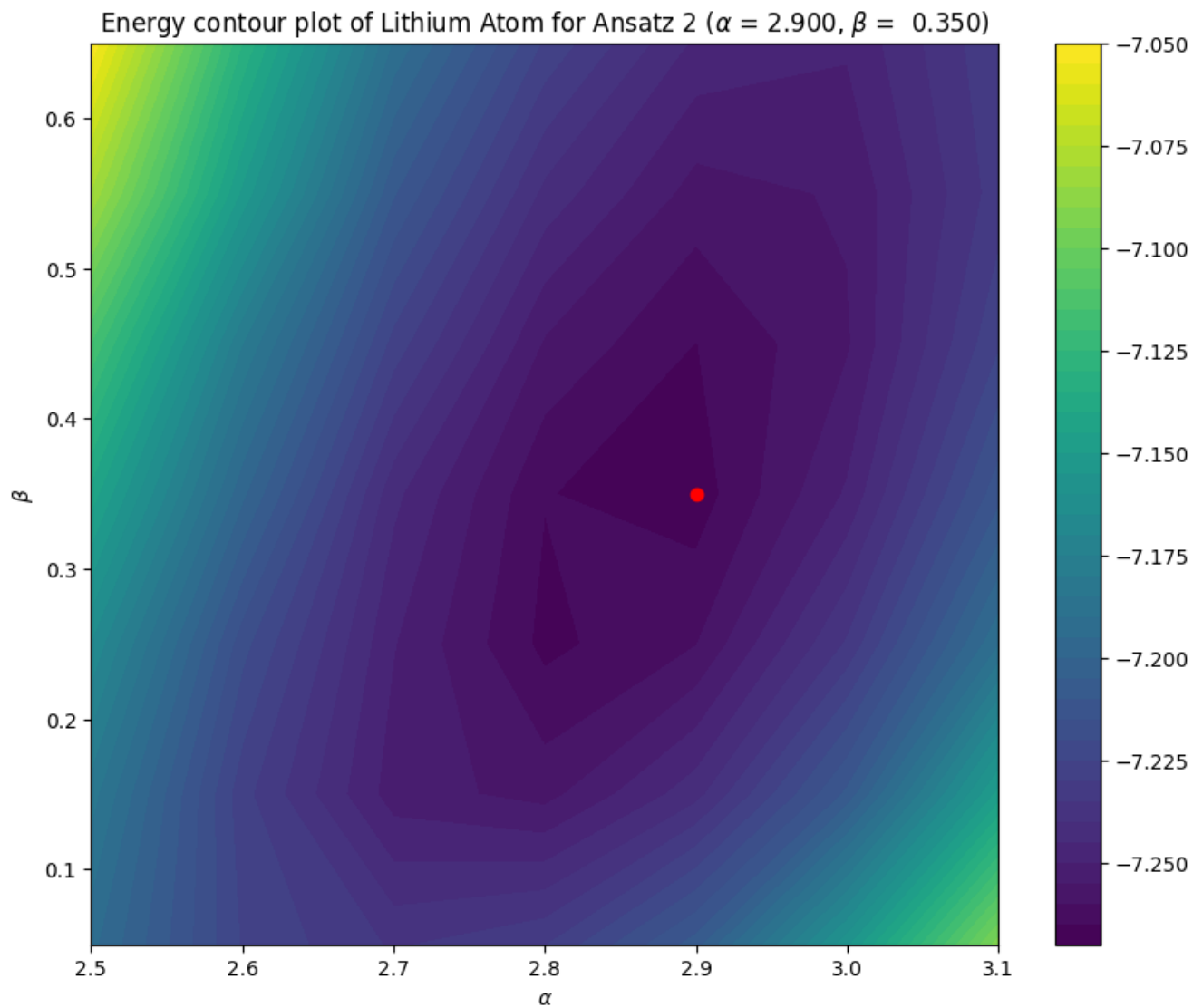


Table 5: Lithium: Ansatz 2

| alpha  | beta   | energy  | variance |
|--------|--------|---------|----------|
| 2.8000 | 0.2500 | -7.2665 | 0.5955   |
| 2.8000 | 0.3500 | -7.2648 | 0.5229   |
| 2.8000 | 0.4500 | -7.2558 | 0.5754   |
| 2.9000 | 0.2500 | -7.2603 | 0.3825   |
| 2.9000 | 0.3500 | -7.2679 | 0.2469   |
| 2.9000 | 0.4500 | -7.2651 | 0.2757   |
| 3.0000 | 0.2500 | -7.2343 | 0.4555   |
| 3.0000 | 0.3500 | -7.2494 | 0.2311   |
| 3.0000 | 0.4500 | -7.2557 | 0.2174   |

Optimal  $r_{12} = 0.838$

# Ansatz 3

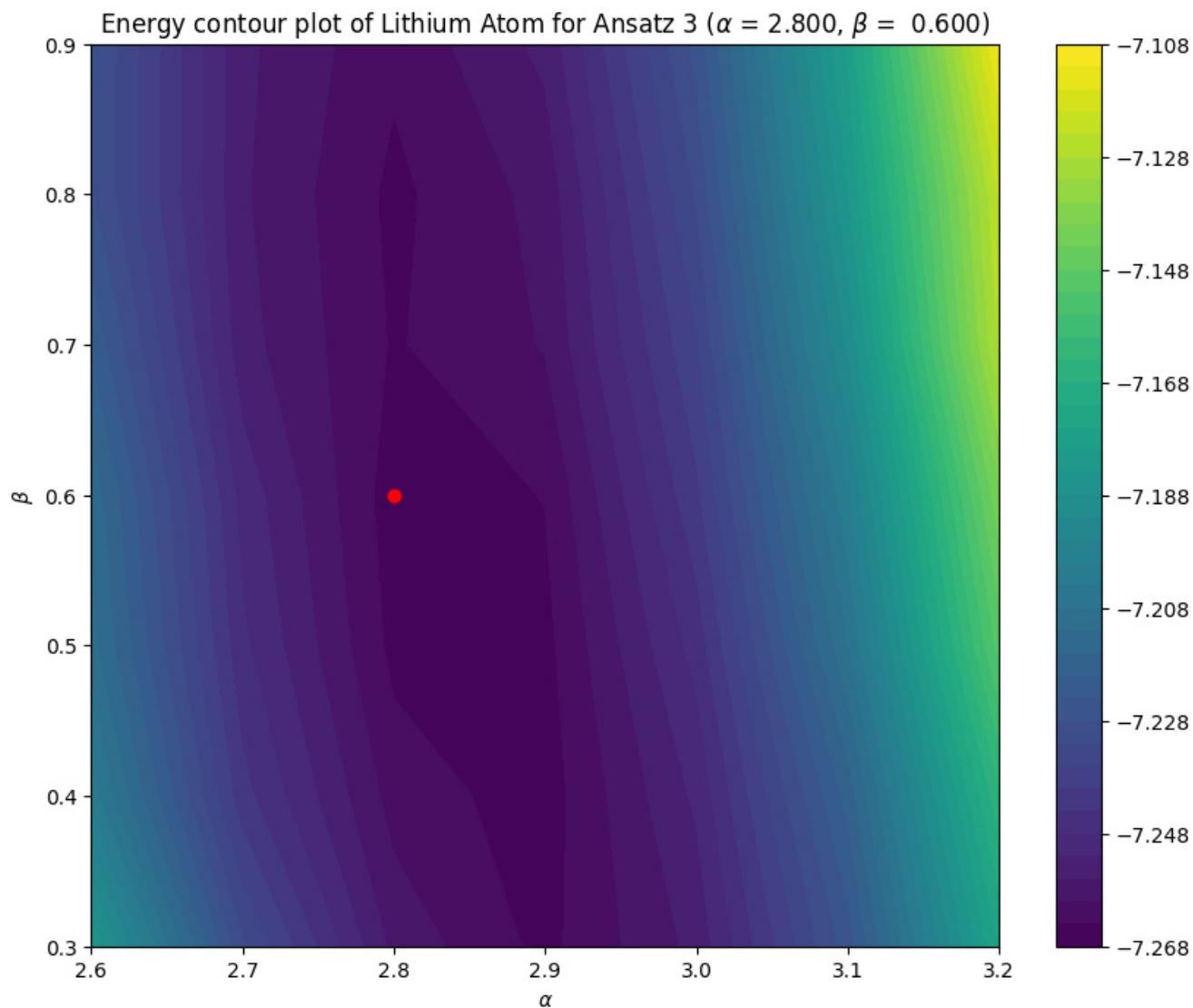


Table 6: Lithium: Ansatz 3

| alpha  | beta   | energy  | variance |
|--------|--------|---------|----------|
| 2.7000 | 0.5000 | -7.2471 | 1.0168   |
| 2.7000 | 0.6000 | -7.2496 | 0.9217   |
| 2.7000 | 0.7000 | -7.2546 | 0.9374   |
| 2.8000 | 0.5000 | -7.2652 | 0.4770   |
| 2.8000 | 0.6000 | -7.2662 | 0.4600   |
| 2.8000 | 0.7000 | -7.2644 | 0.4447   |
| 2.9000 | 0.5000 | -7.2653 | 0.2165   |
| 2.9000 | 0.6000 | -7.2639 | 0.2121   |
| 2.9000 | 0.7000 | -7.2597 | 0.1951   |

Optimal  $r_{12} = 0.851$