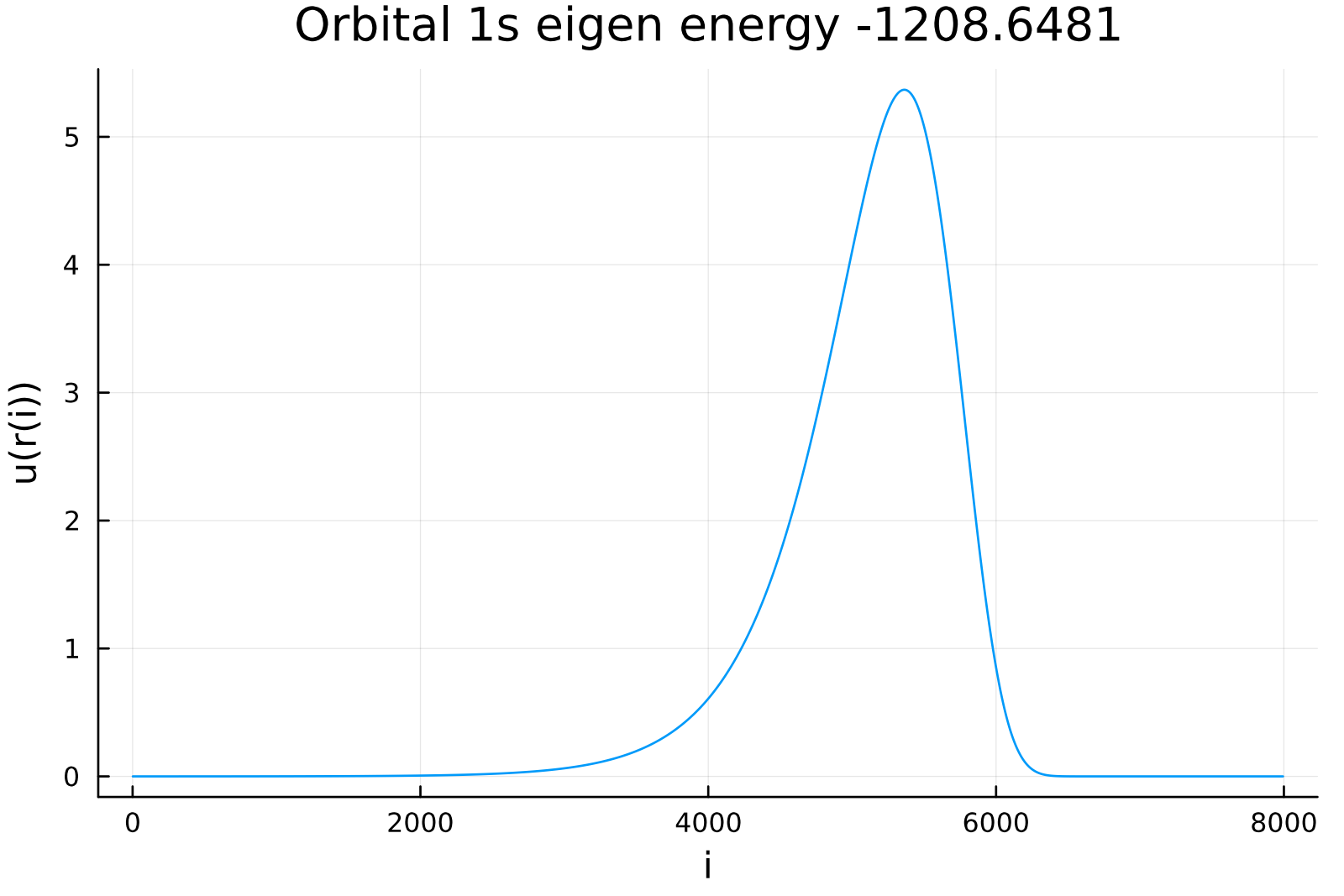
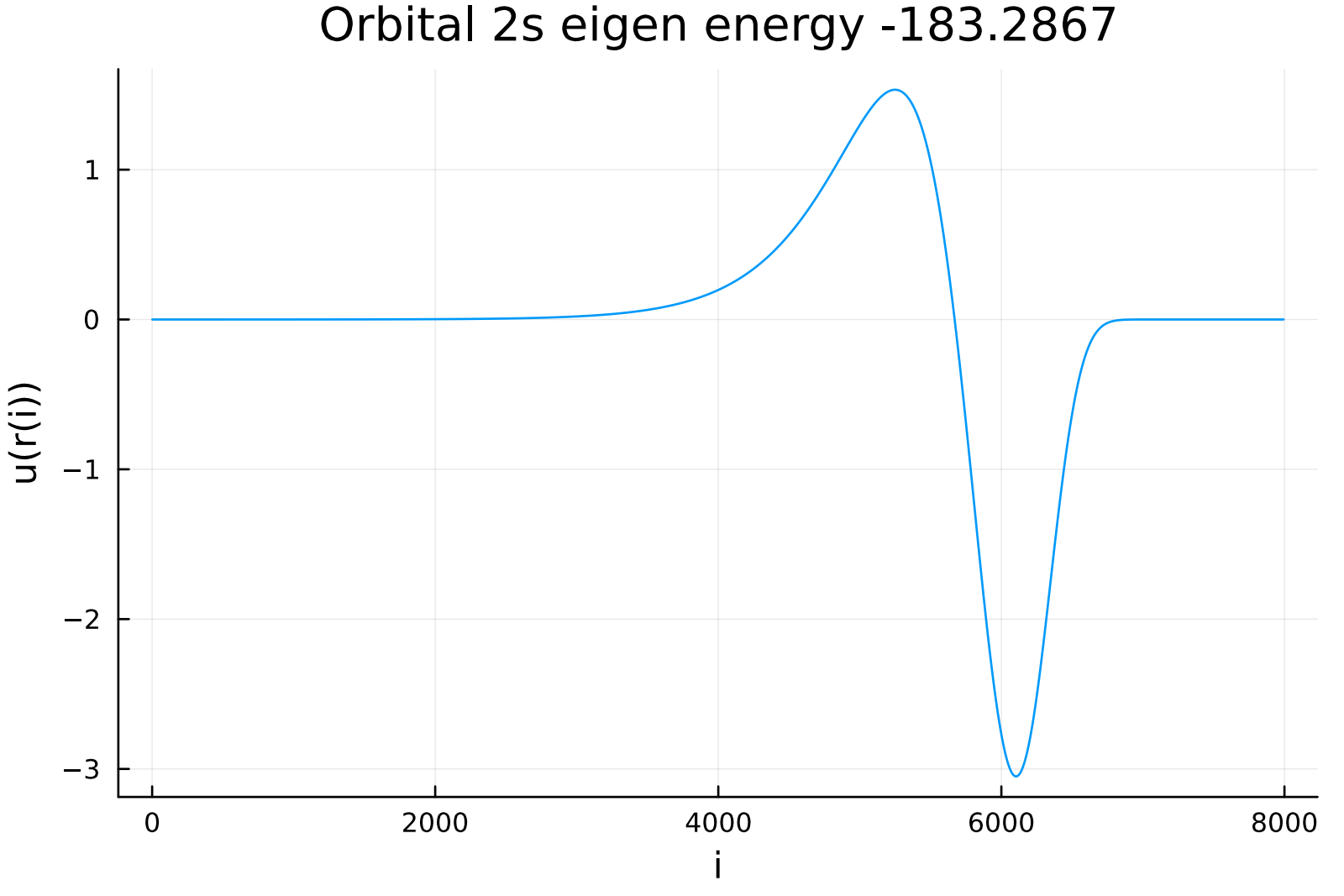
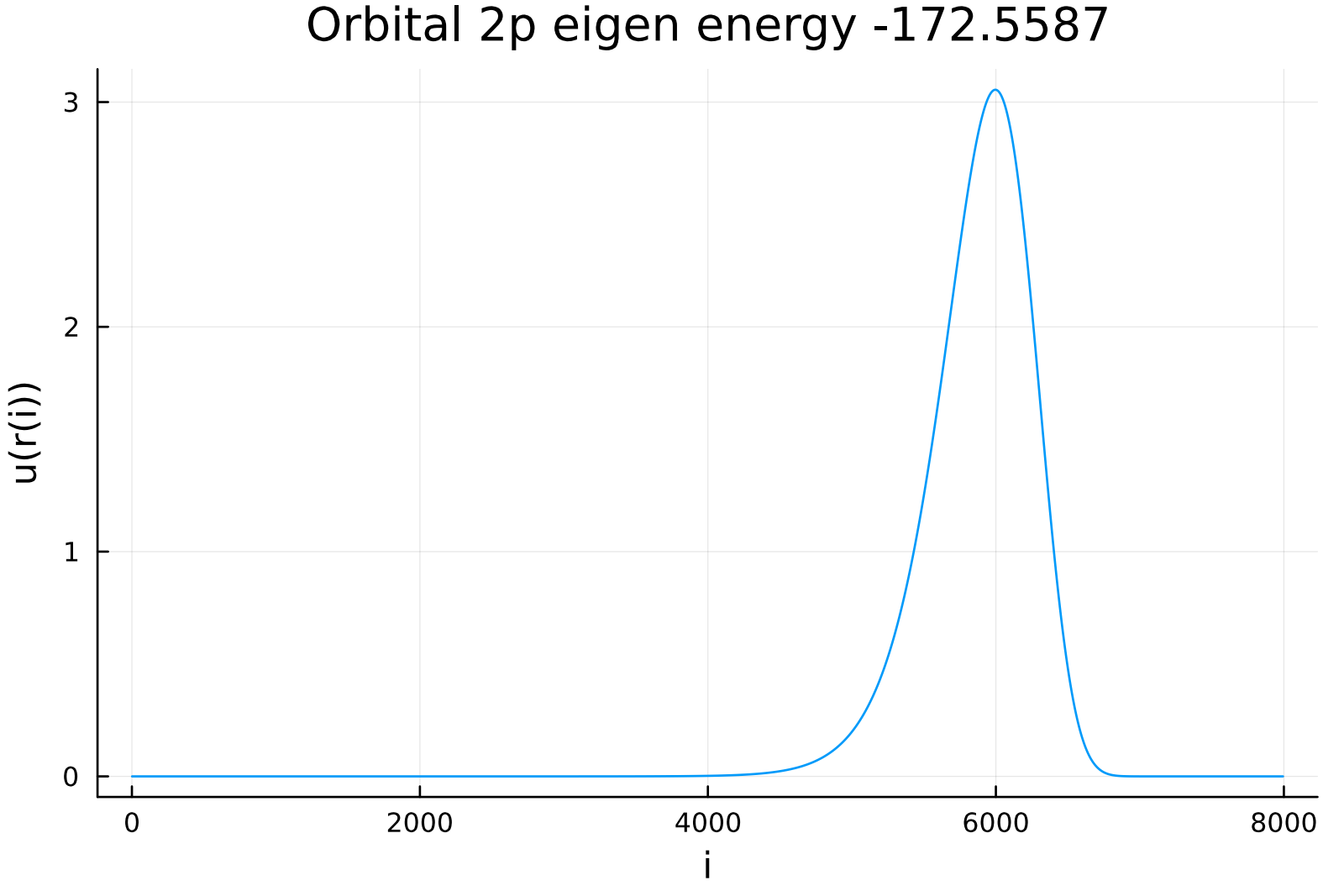
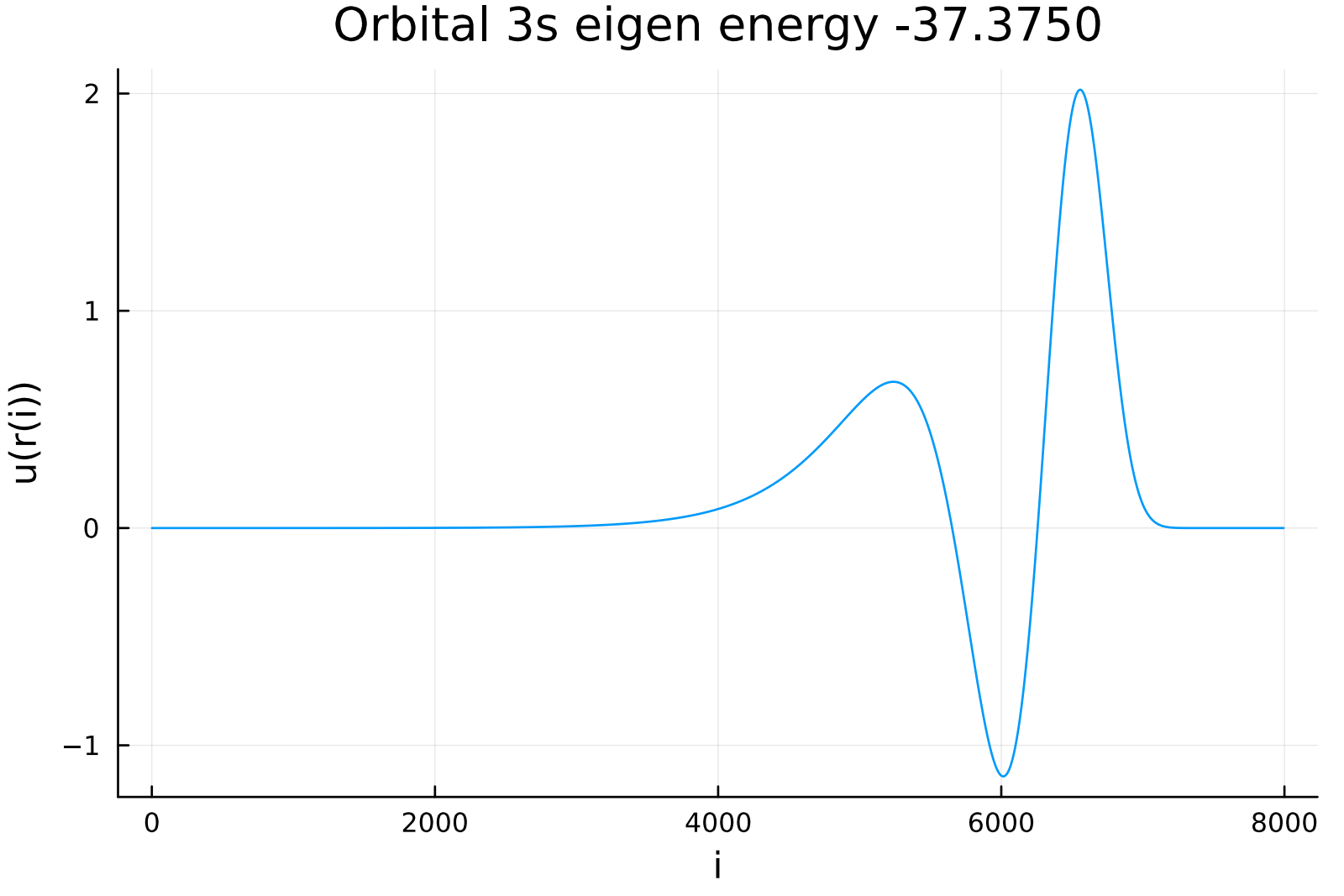
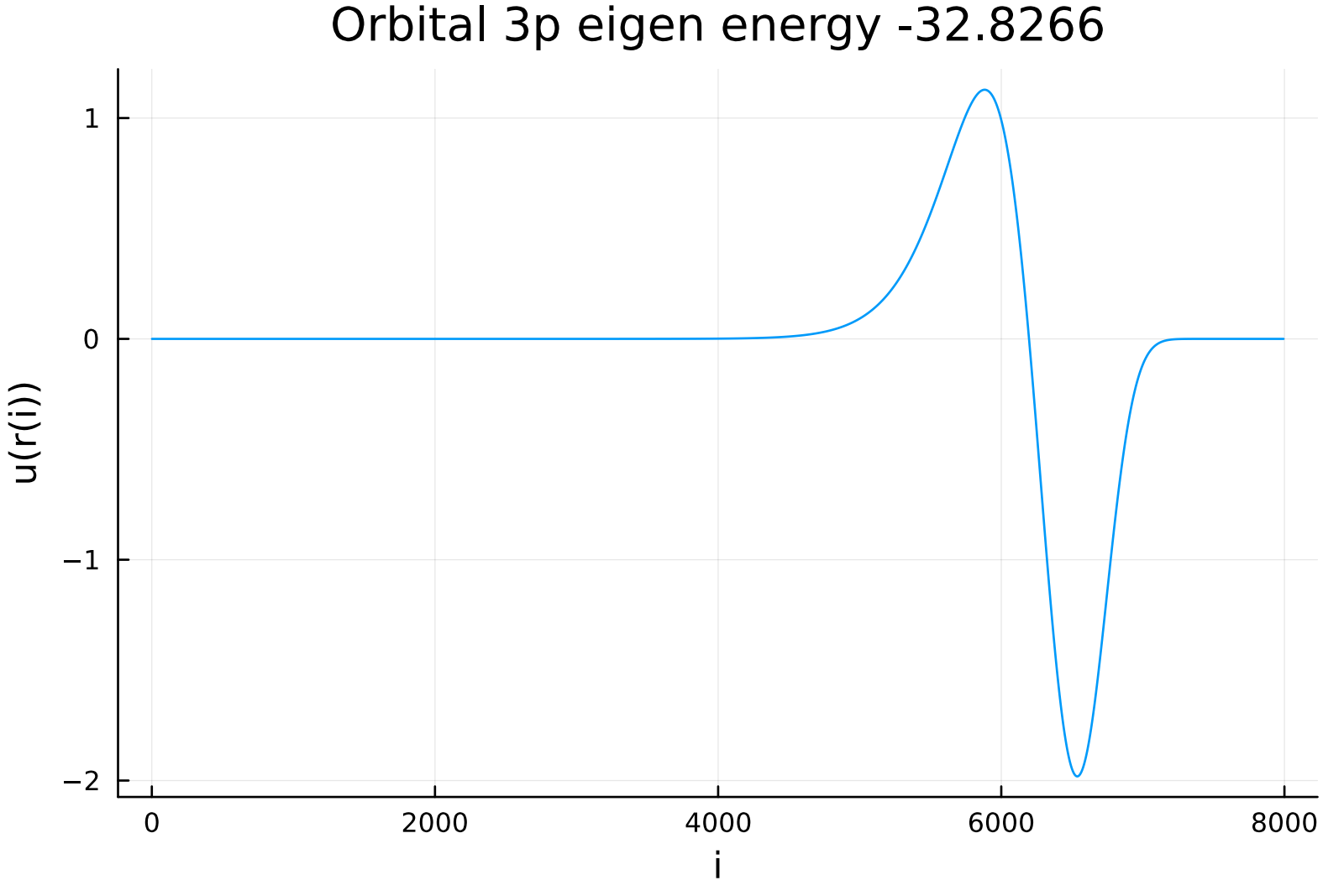
Xenon	E in Hartree			
Name	E NIST	E pred	|ΔE|	|ΔE|/E NIST
4d	-2.286666	-2.247945	0.038721	-0.016933
Ecoul	2880.919348	2882.990232	2.070884	0.000719
3p	-32.867042	-32.826601	0.040441	-0.001230
4p	-5.063802	-5.024636	0.039166	-0.007734
Exc	-175.713845	-175.770040	0.056195	-0.000320
5p	-0.309835	-0.278403	0.031432	-0.101448
2p	-172.599583	-172.558657	0.040926	-0.000237
5s	-0.672086	-0.641926	0.030160	-0.044875
4s	-6.678340	-6.639061	0.039279	-0.005882
Etot	-7228.856107	-7228.819657	0.036450	-0.000005
2s	-183.327495	-183.286651	0.040844	-0.000223
3s	-37.415454	-37.375042	0.040412	-0.001080
3d	-24.378230	-24.337731	0.040499	-0.001661
Ekin	7225.097817	7225.285697	0.187880	0.000026
1s	-1208.688993	-1208.648060	0.040933	-0.000034

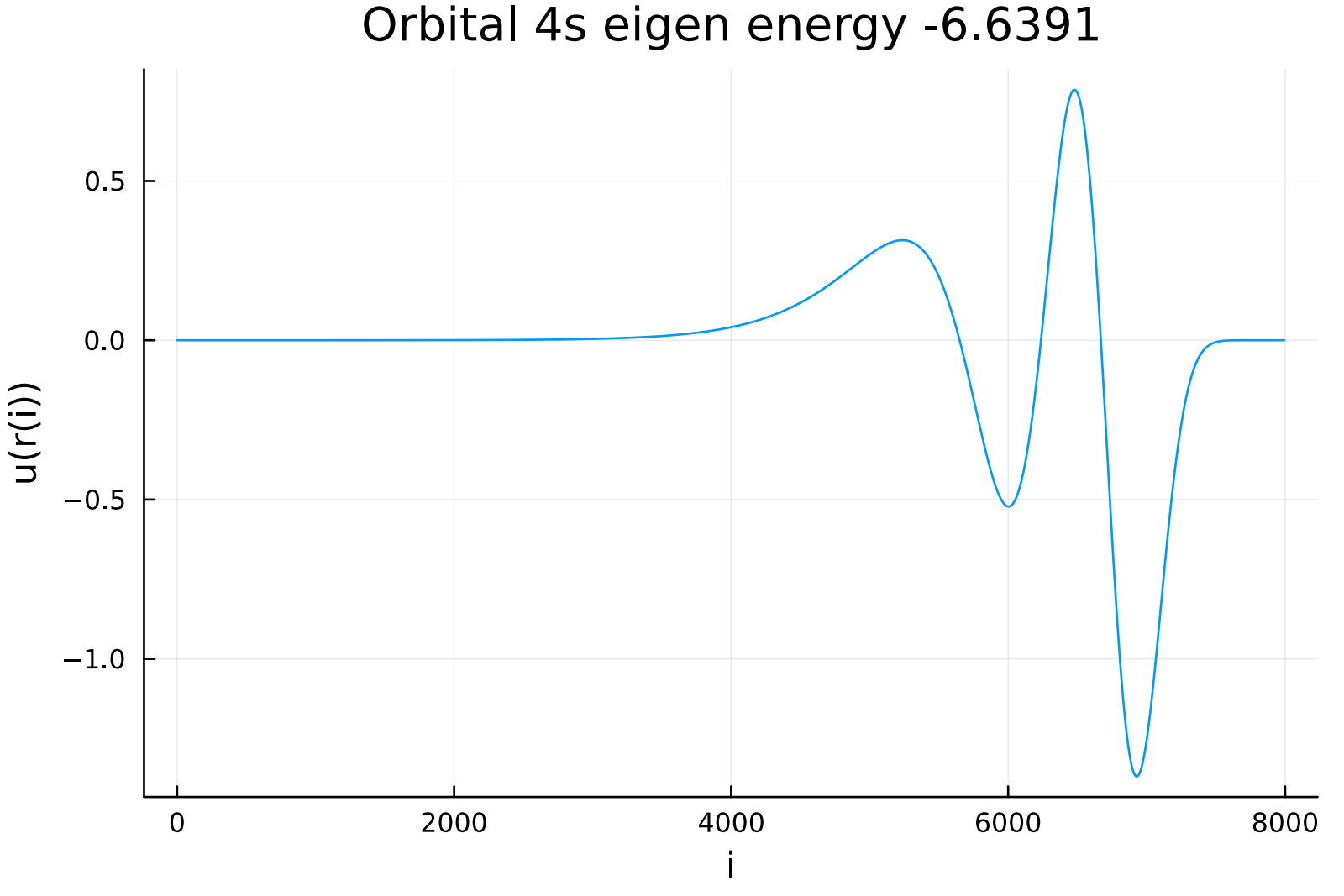

Orbital 1s eigen energy -1208.6481
u(r(i))
0
1
2
3
4
5
0
2000
4000
6000
8000
i

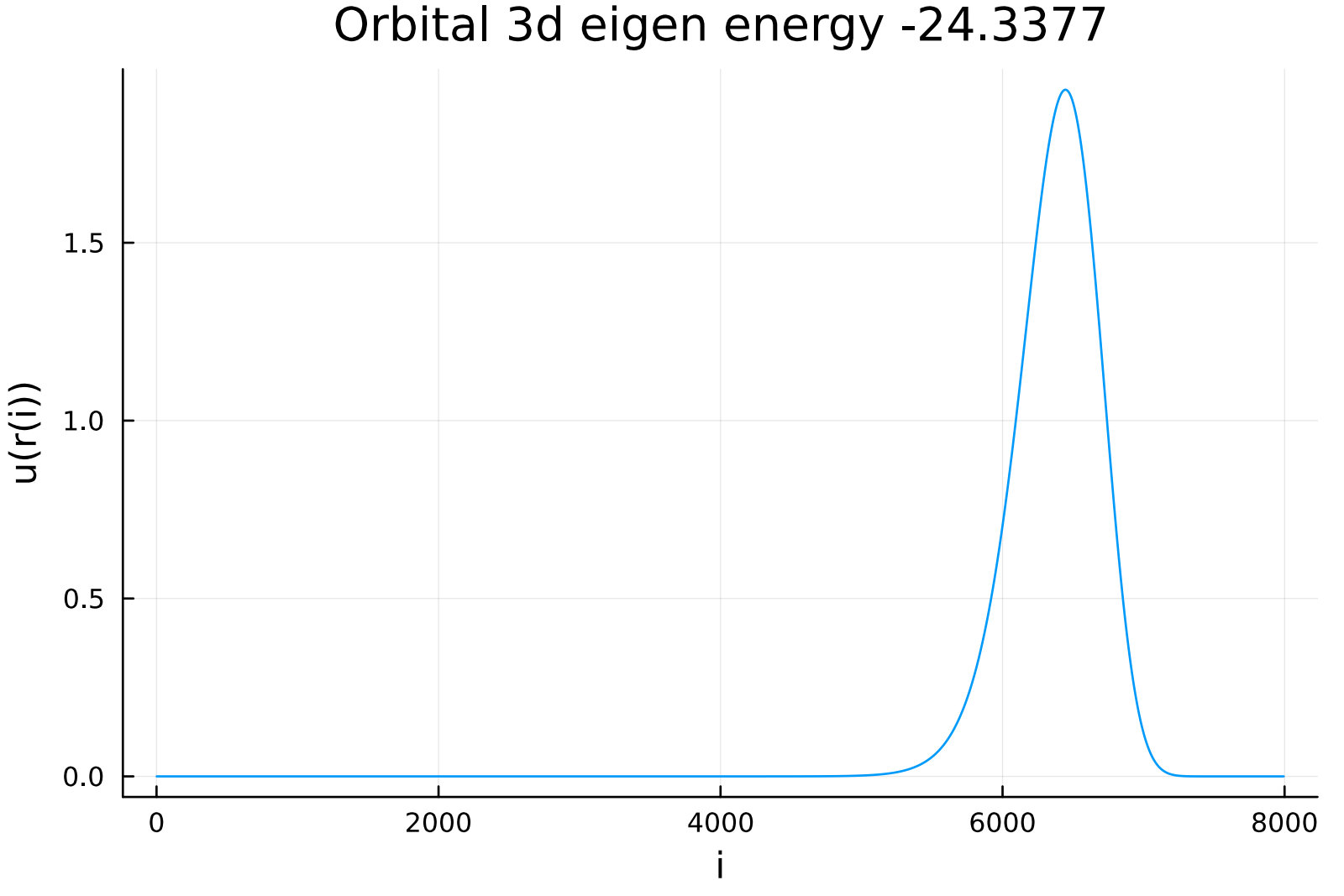

Orbital 2s eigen energy -183.2867
u(r(i))
1
0
−1
−2
−3
0
2000
4000
6000
8000
i

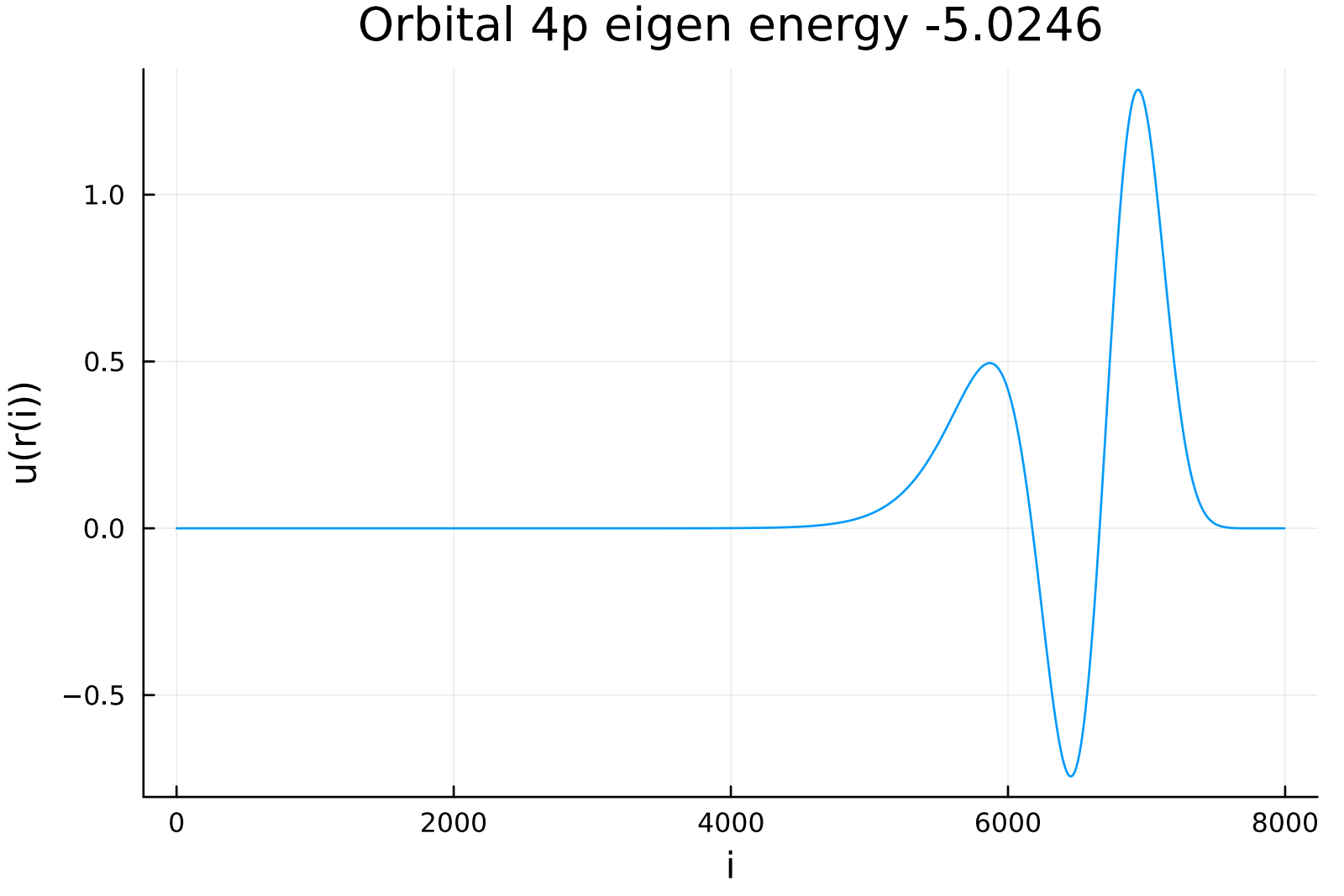

Orbital 2p eigen energy -172.5587
u(r(i))
i
0
1
2
3
0
2000
4000
6000
8000

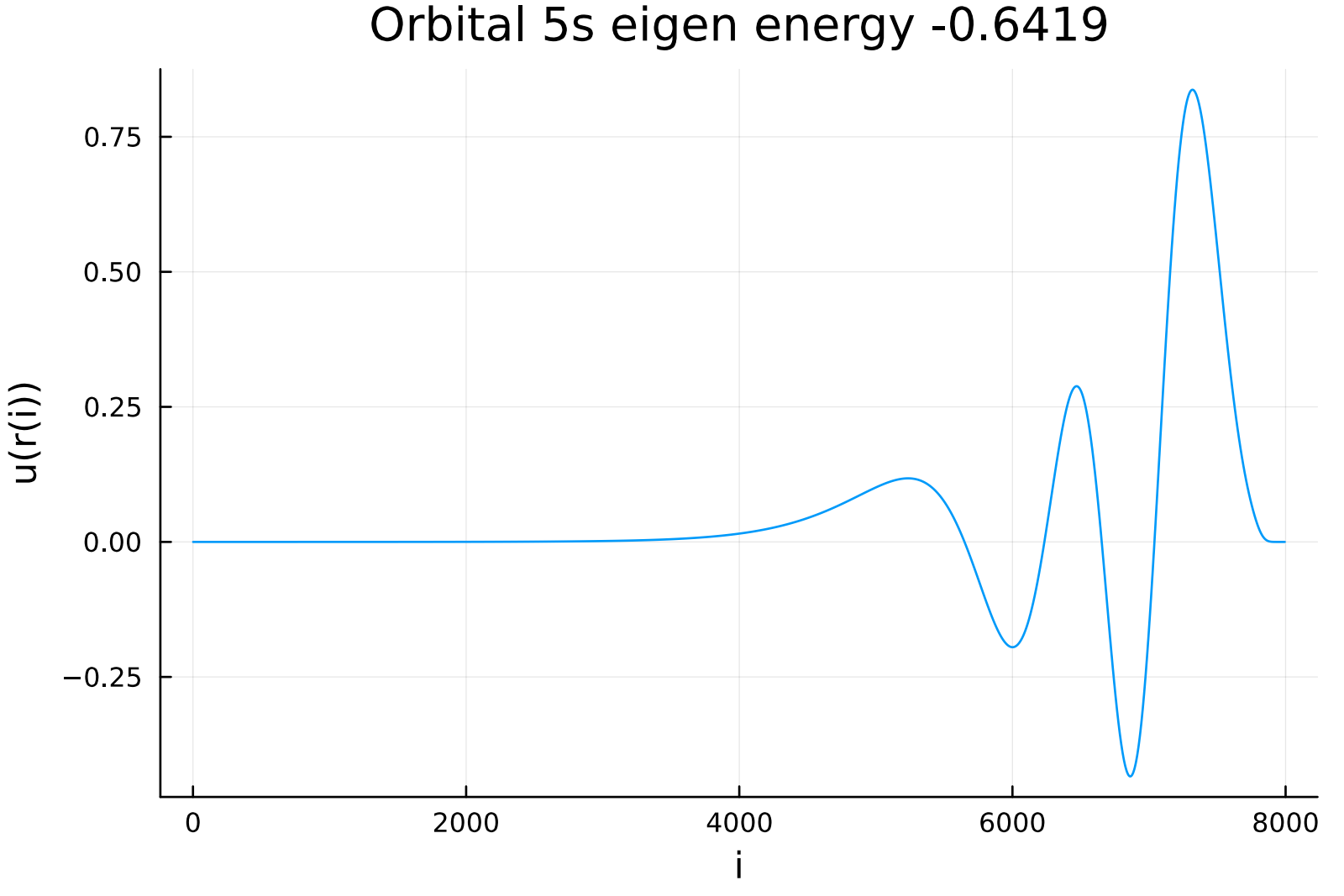

Orbital 3s eigen energy -37.3750
u(r(i))
i
2
1
0
−1
0
2000
4000
6000
8000

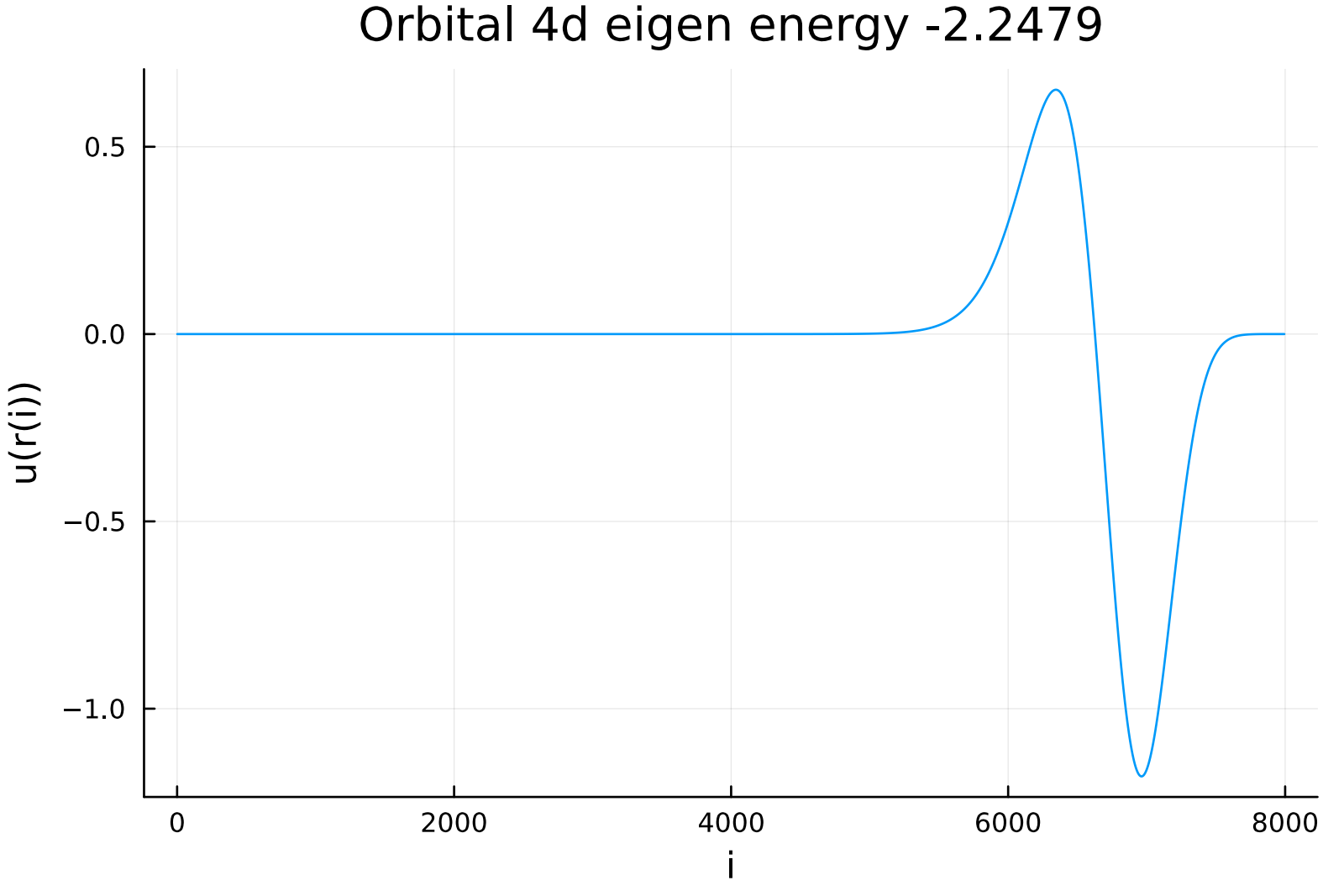

Orbital 3p eigen energy -32.8266
u(r(i))
1
0
−1
−2
0
2000
4000
6000
8000
i

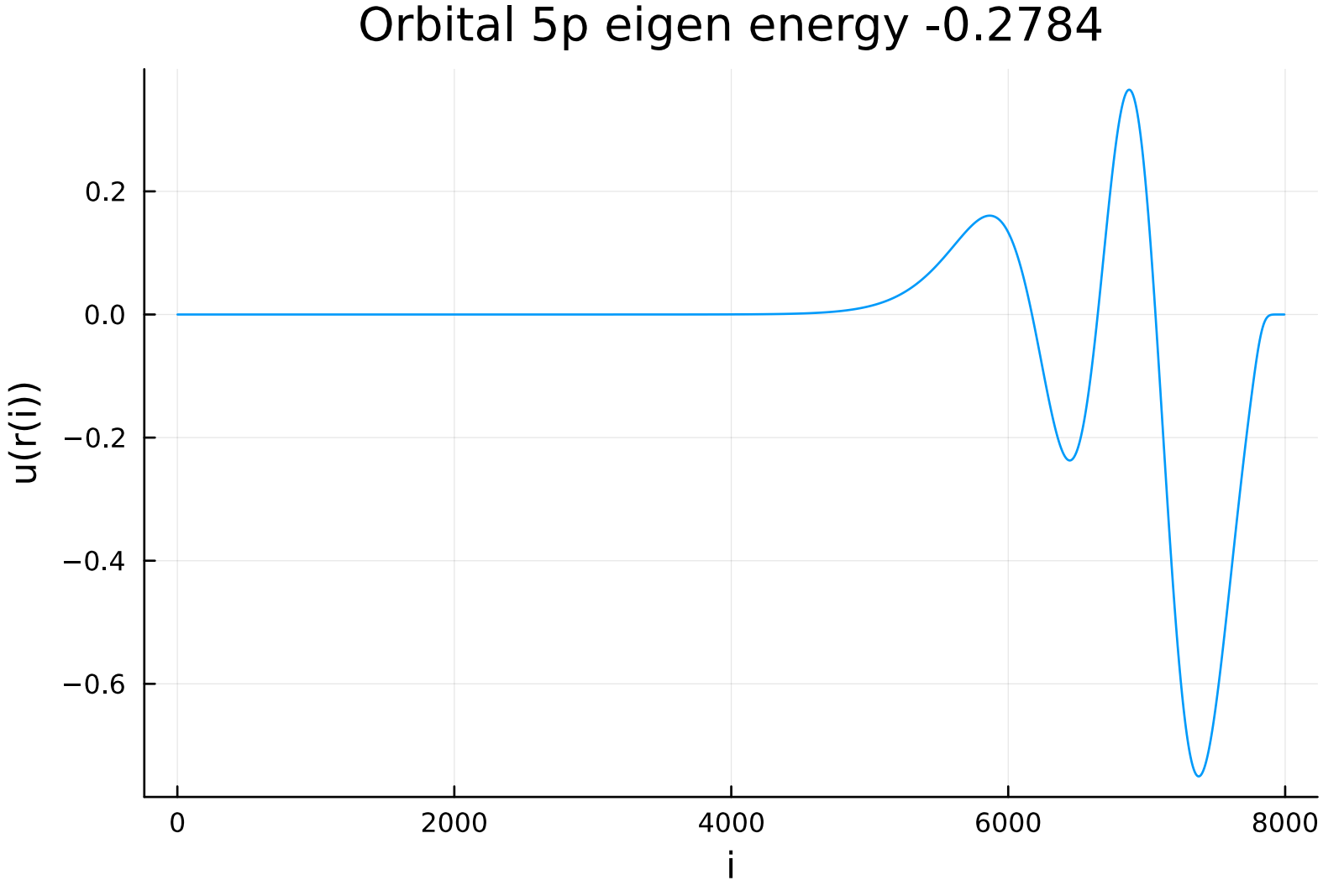

Orbital 4s eigen energy -6.6391
0.5
0.0
−0.5
−1.0
u(r(i))
0
2000
4000
6000
8000
i


Orbital 3d eigen energy -24.3377
u(r(i))
1.5
1.0
0.5
0.0
0
2000
4000
6000
8000
i


Orbital 4p eigen energy -5.0246
u(r(i))
1.0
0.5
0.0
−0.5
0
2000
4000
6000
8000
i


Orbital 5s eigen energy -0.6419
0.75
0.50
0.25
0.00
−0.25
u(r(i))
0
2000
4000
6000
8000
i


Orbital 4d eigen energy -2.2479
0.5
0.0
−0.5
−1.0
u(r(i))
0
2000
4000
6000
8000
i


Orbital 5p eigen energy -0.2784
0.2
0.0
−0.2
−0.4
−0.6
u(r(i))
0
2000
4000
6000
8000
i