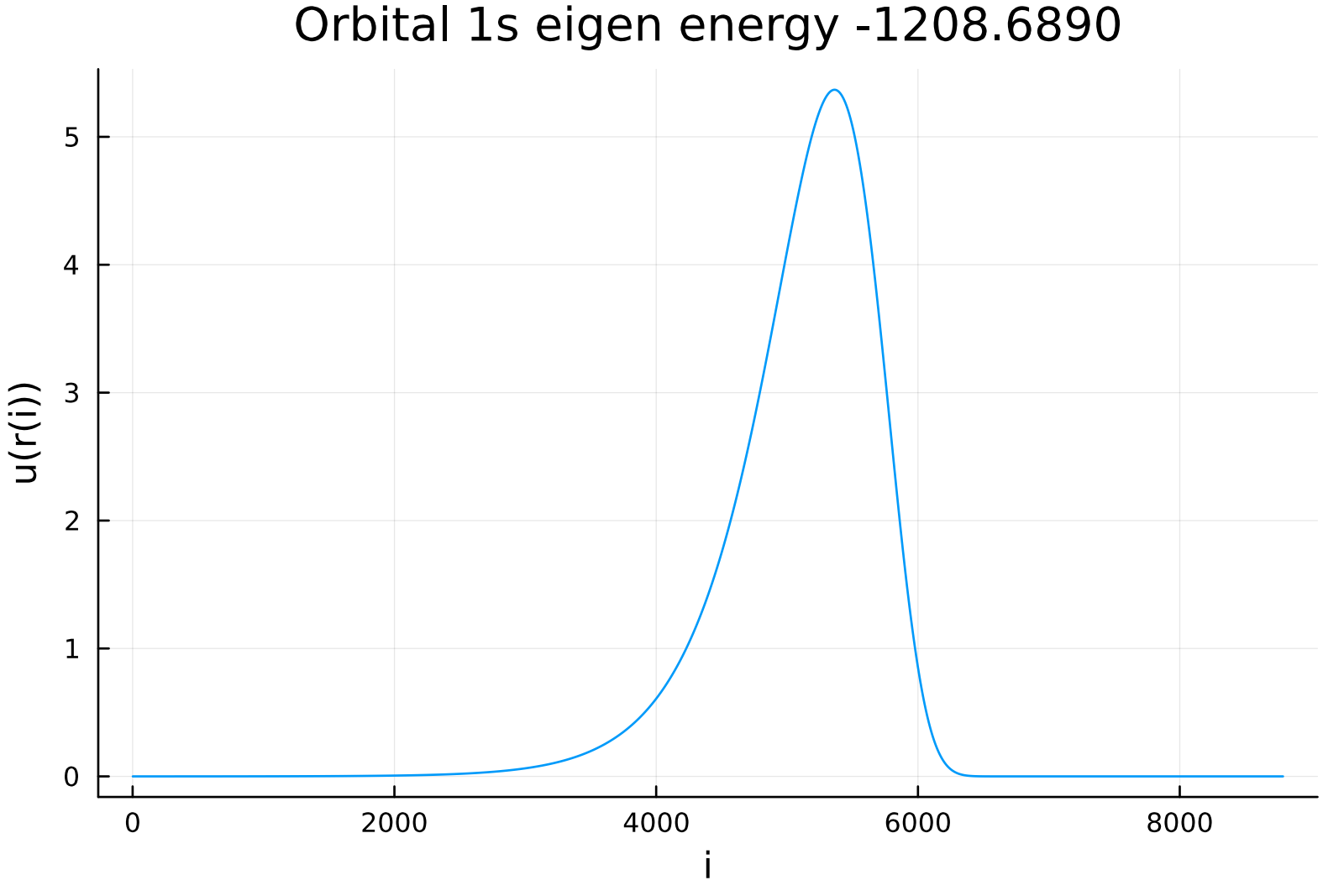
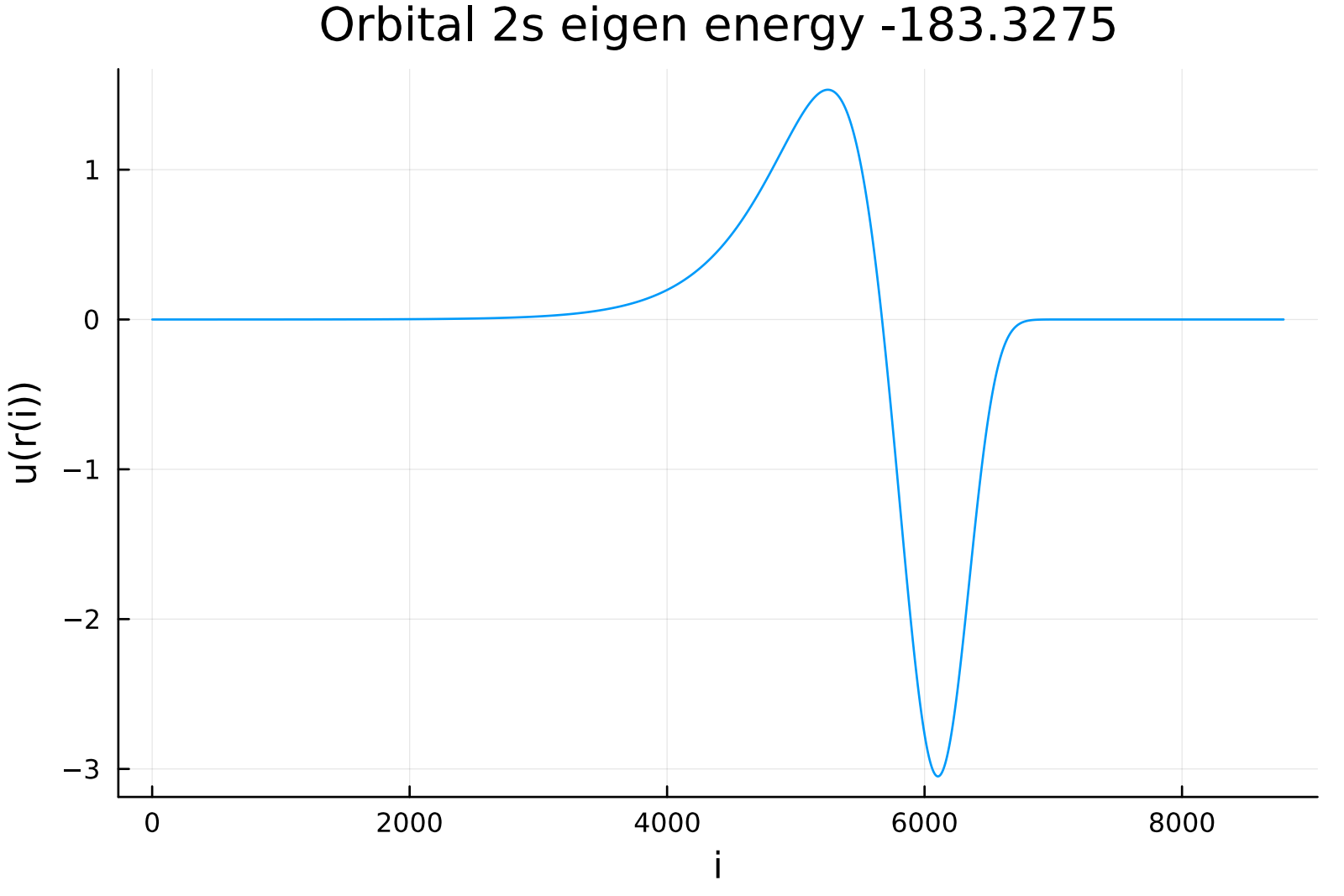
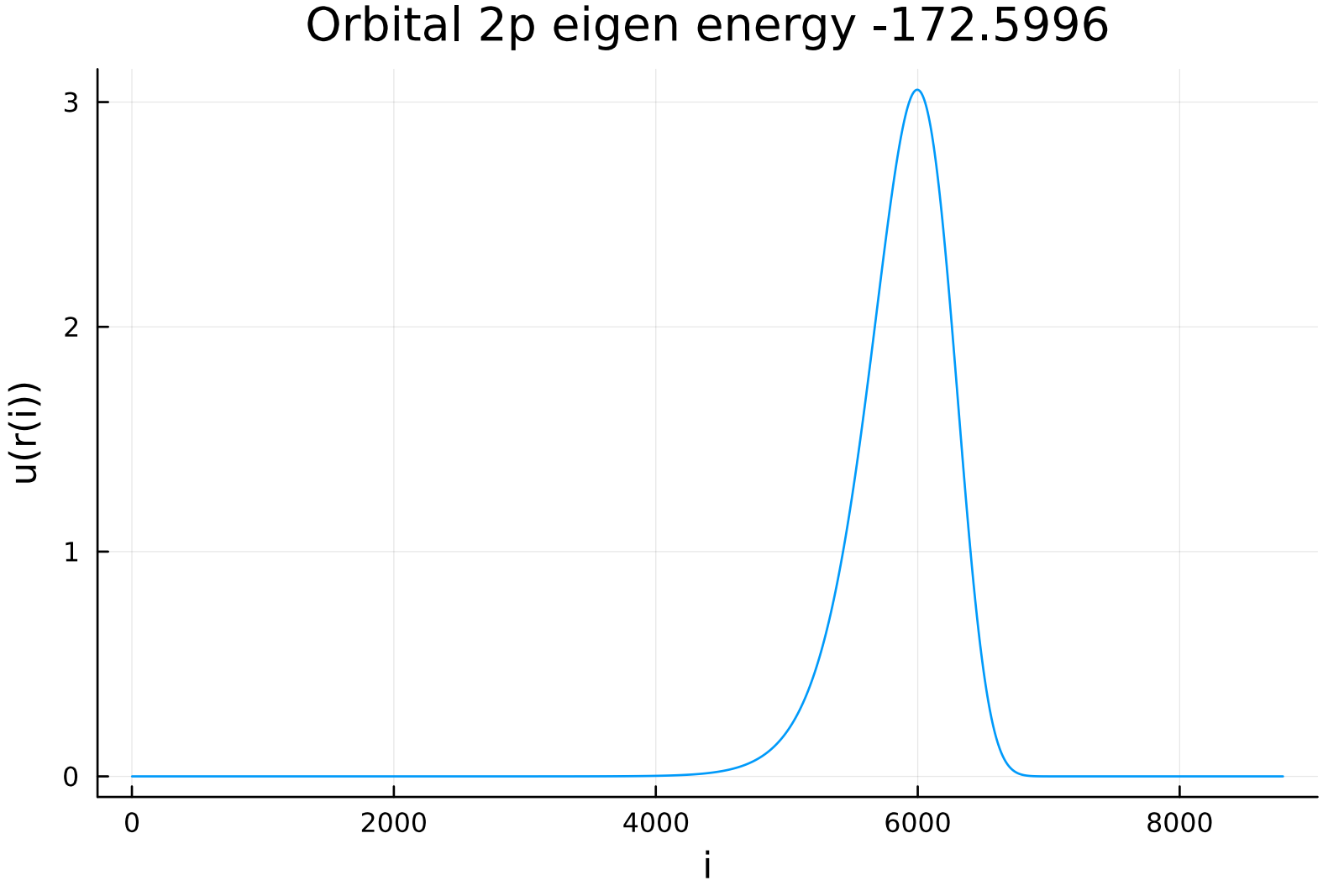
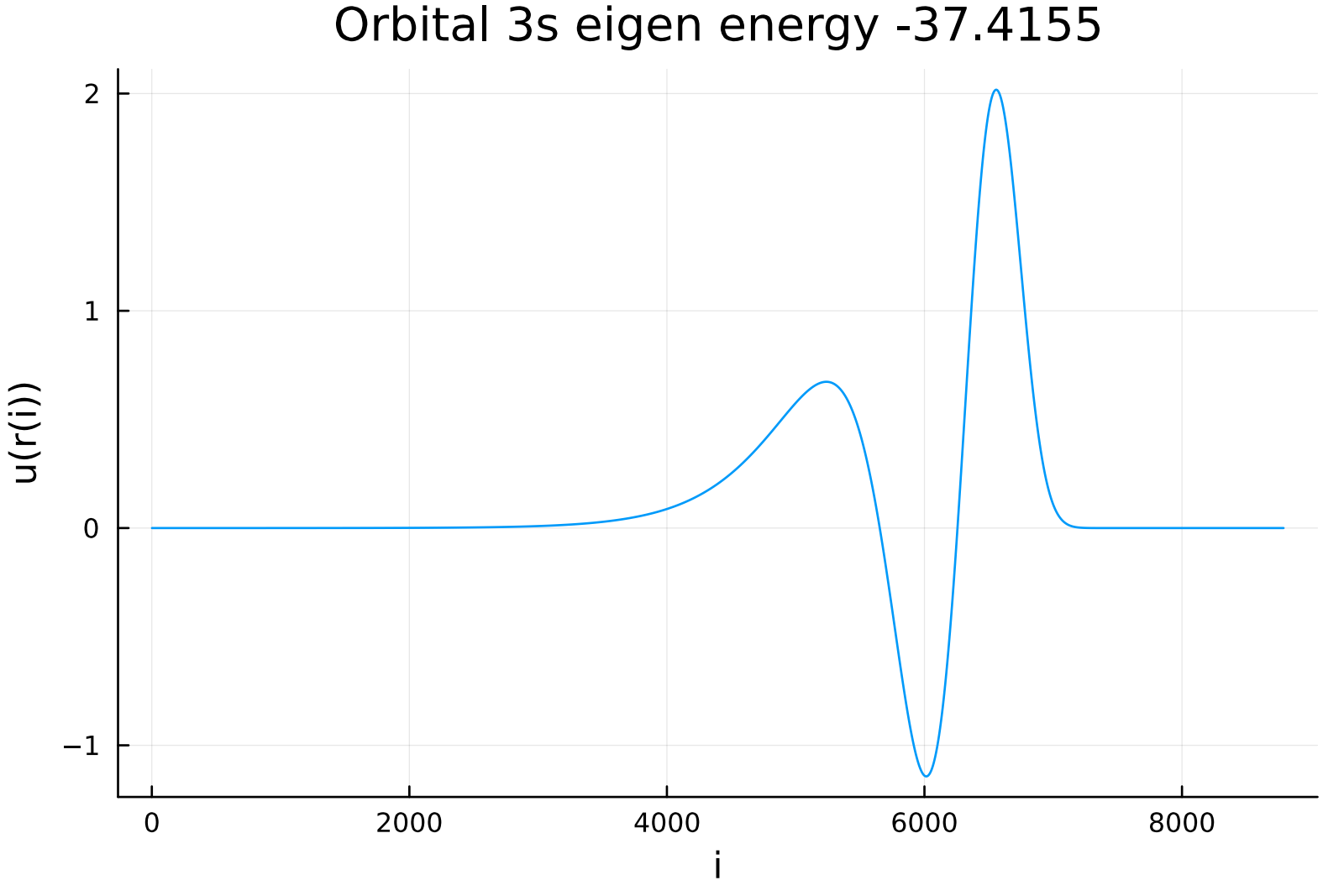
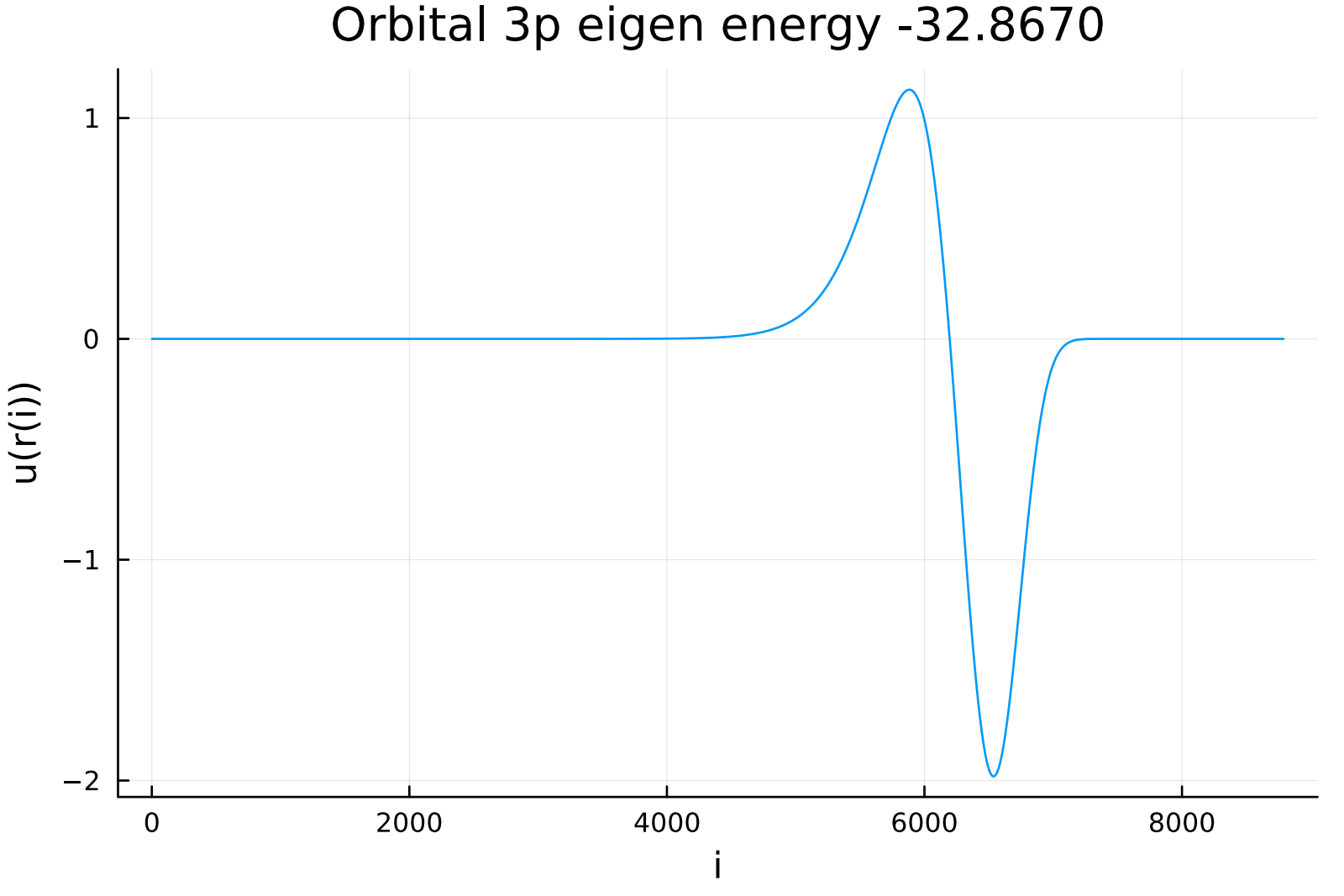
Xenon	E in Hartree			
Name	E NIST	E pred	|ΔE|	|ΔE|/E NIST
4d	-2.286666	-2.286666	0.000000	-0.000000
Ecoul	2880.919348	2880.919302	0.000046	0.000000
3p	-32.867042	-32.867042	0.000000	-0.000000
4p	-5.063802	-5.063801	0.000001	-0.000000
Exc	-175.713845	-175.713843	0.000002	-0.000000
5p	-0.309835	-0.309835	0.000000	-0.000000
2p	-172.599583	-172.599582	0.000001	-0.000000
5s	-0.672086	-0.672086	0.000000	-0.000000
4s	-6.678340	-6.678339	0.000001	-0.000000
Etot	-7228.856107	-7228.856106	0.000001	-0.000000
2s	-183.327495	-183.327495	0.000000	-0.000000
3s	-37.415454	-37.415453	0.000001	-0.000000
3d	-24.378230	-24.378230	0.000000	-0.000000
Ekin	7225.097817	7225.097725	0.000092	0.000000
1s	-1208.688993	-1208.688993	0.000000	-0.000000

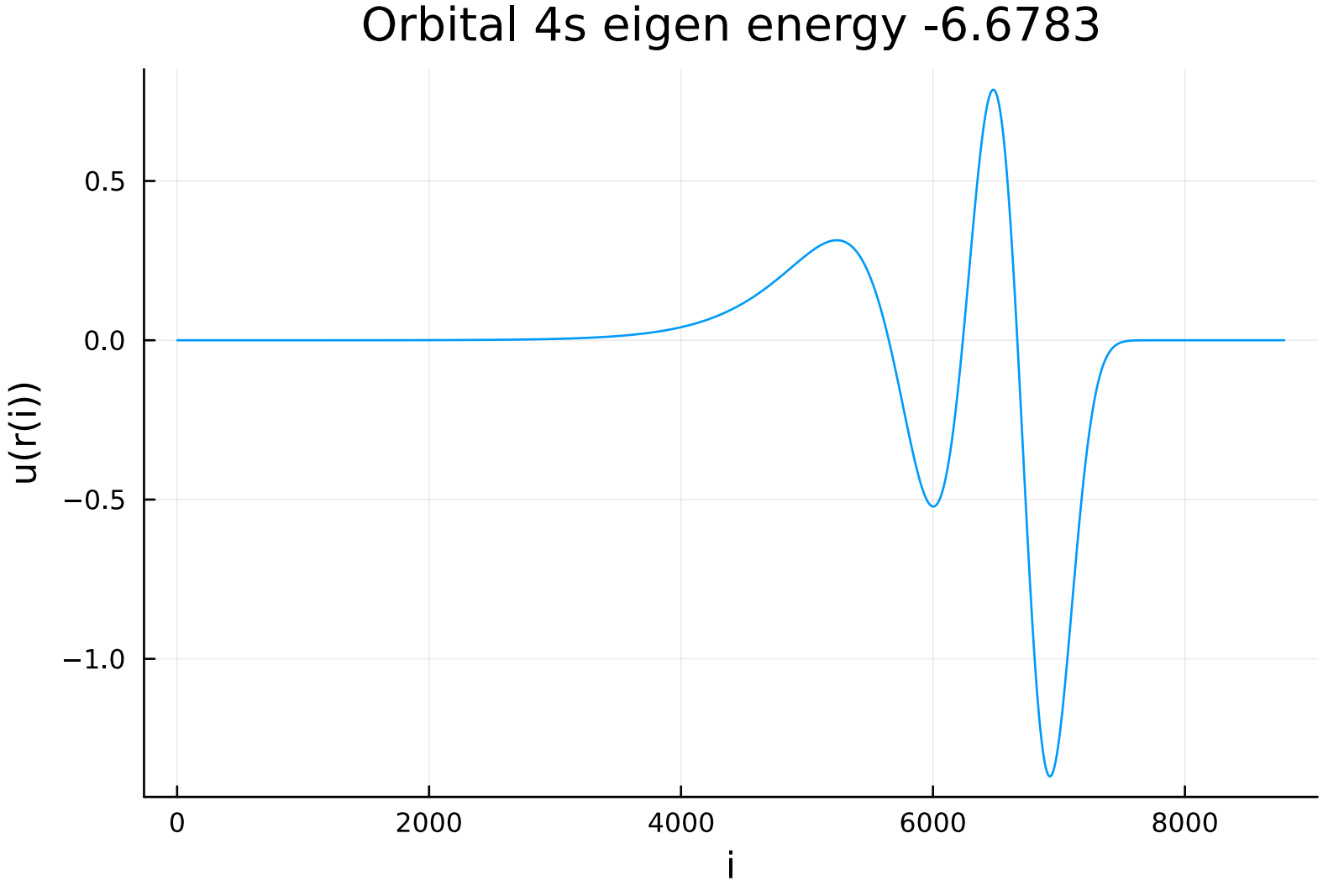

Orbital 1s eigen energy -1208.6890
u(r(i))
i
0
1
2
3
4
5
0
2000
4000
6000
8000

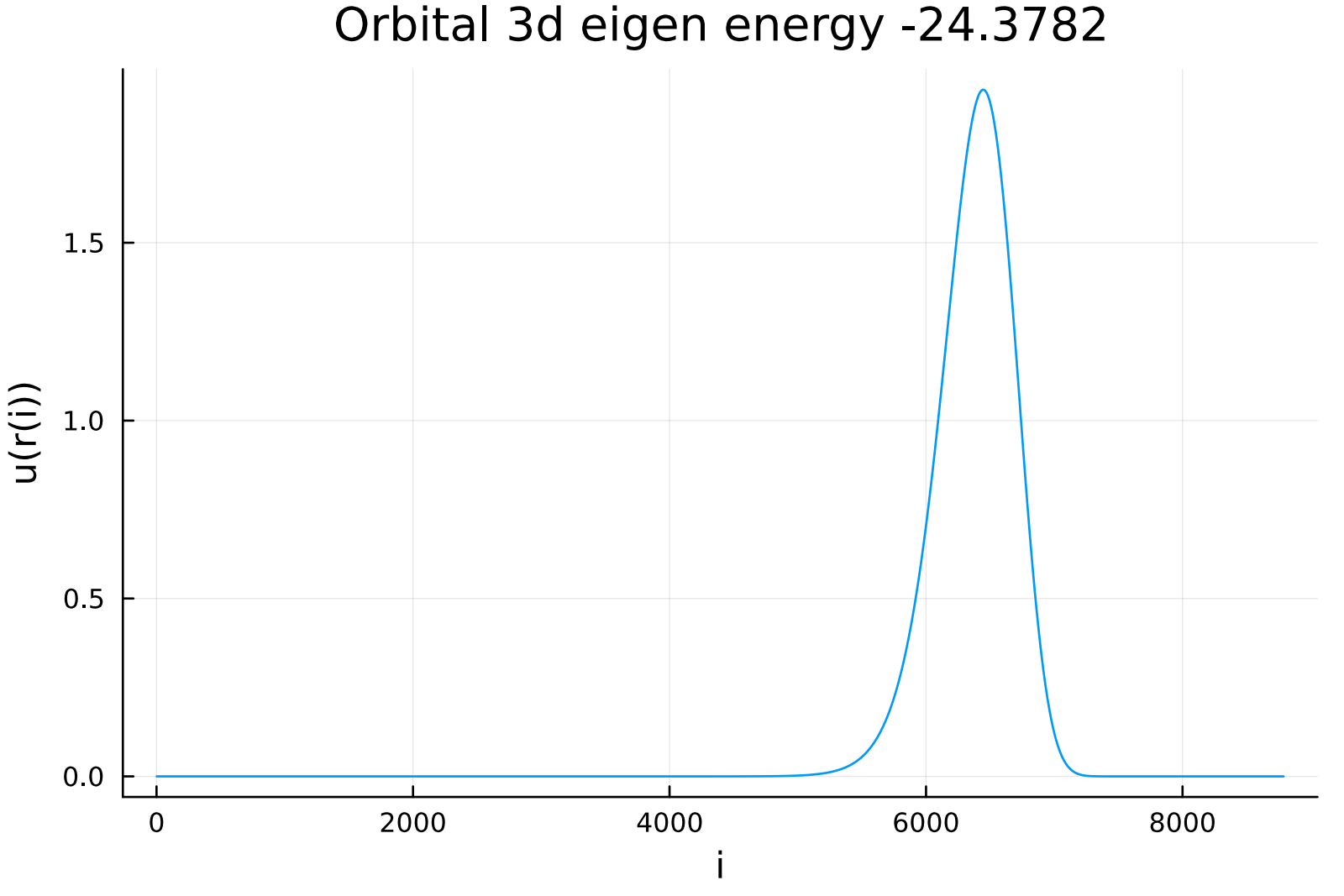

Orbital 2s eigen energy -183.3275
u(r(i))
1
0
−1
−2
−3
0
2000
4000
6000
8000
i

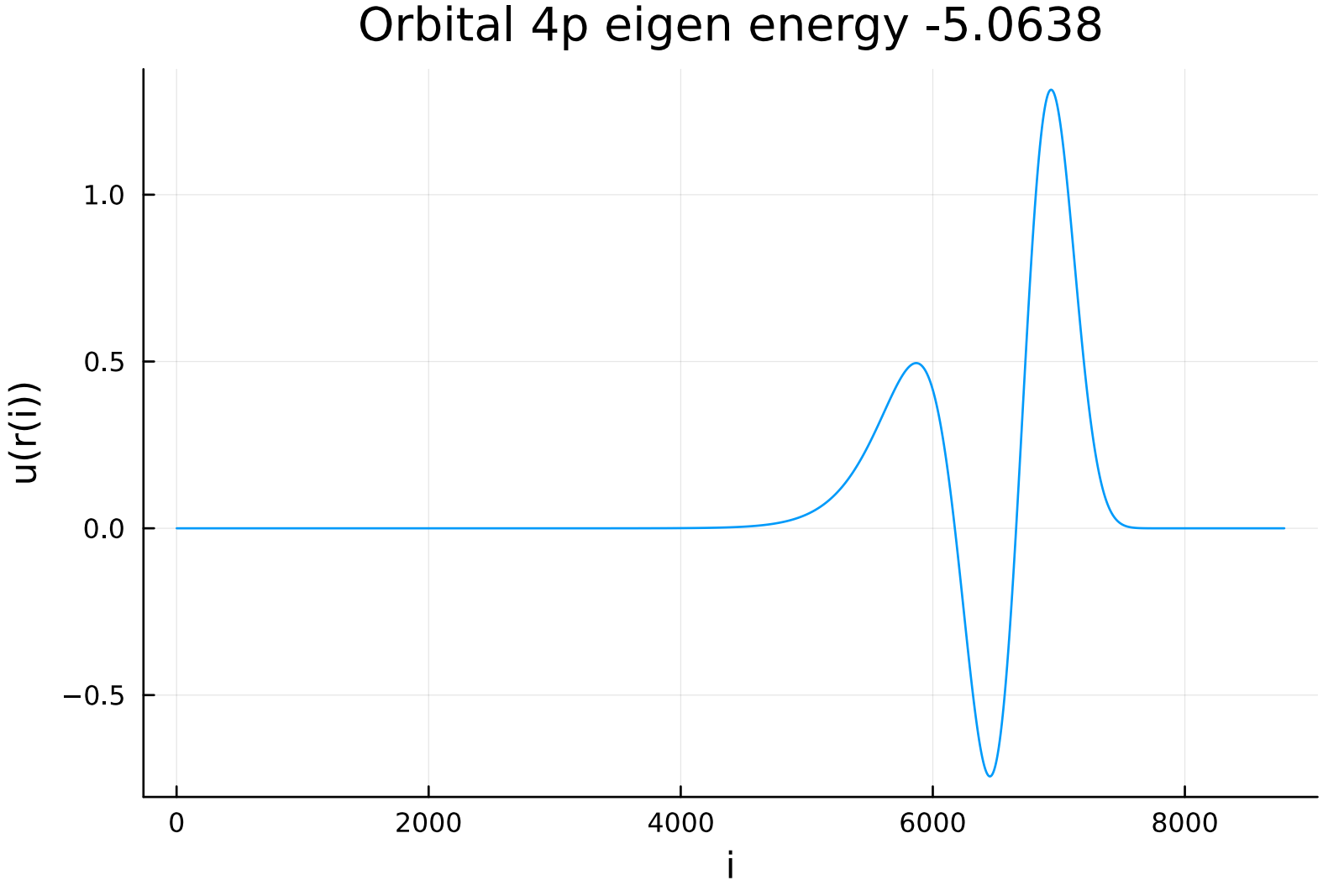

Orbital 2p eigen energy -172.5996
u(r(i))
i
0
1
2
3
0
2000
4000
6000
8000

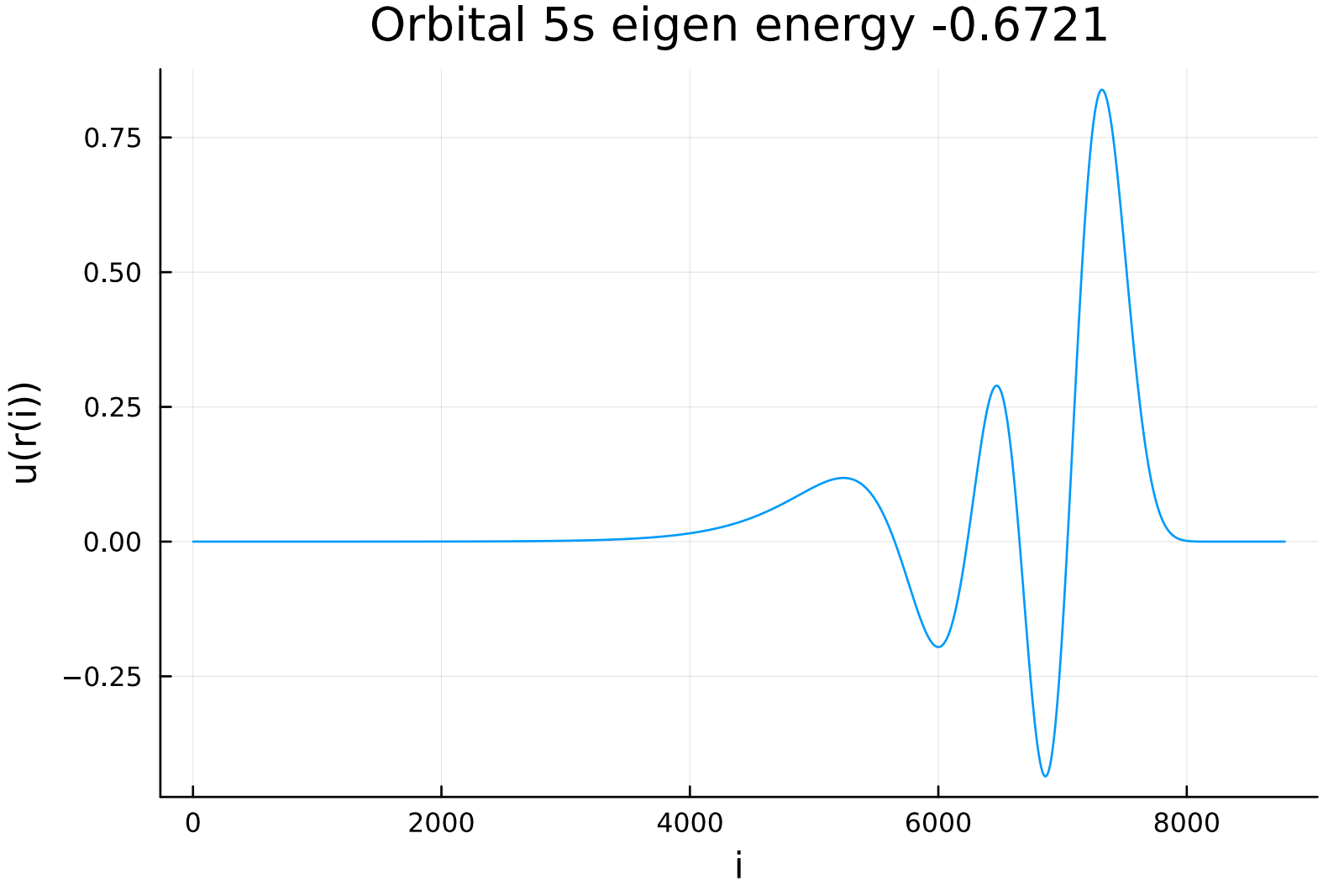

Orbital 3s eigen energy -37.4155
u(r(i))
2
1
0
−1
0
2000
4000
6000
8000
i

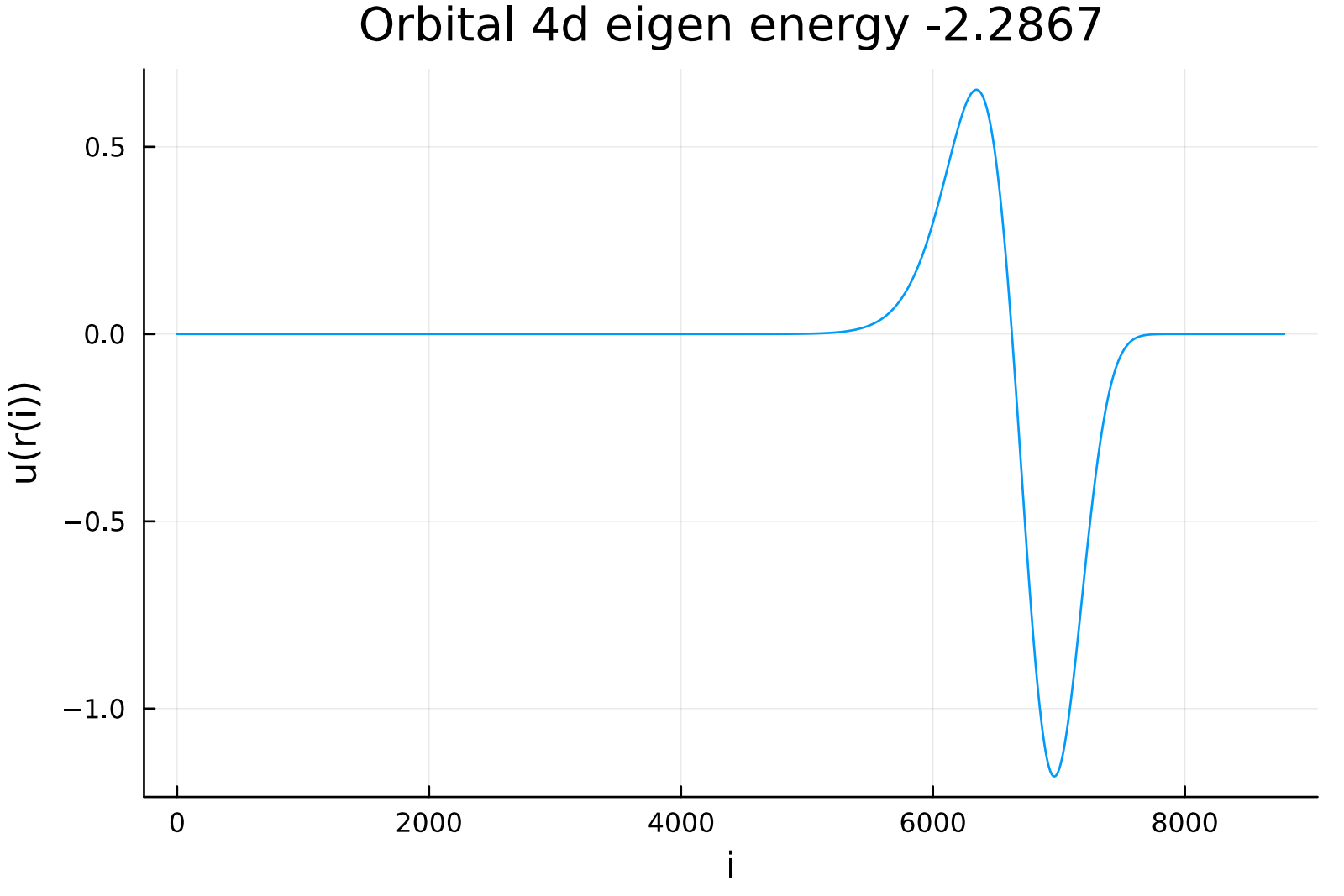

Orbital 3p eigen energy -32.8670
u(r(i))
1
0
−1
−2
0
2000
4000
6000
8000
i

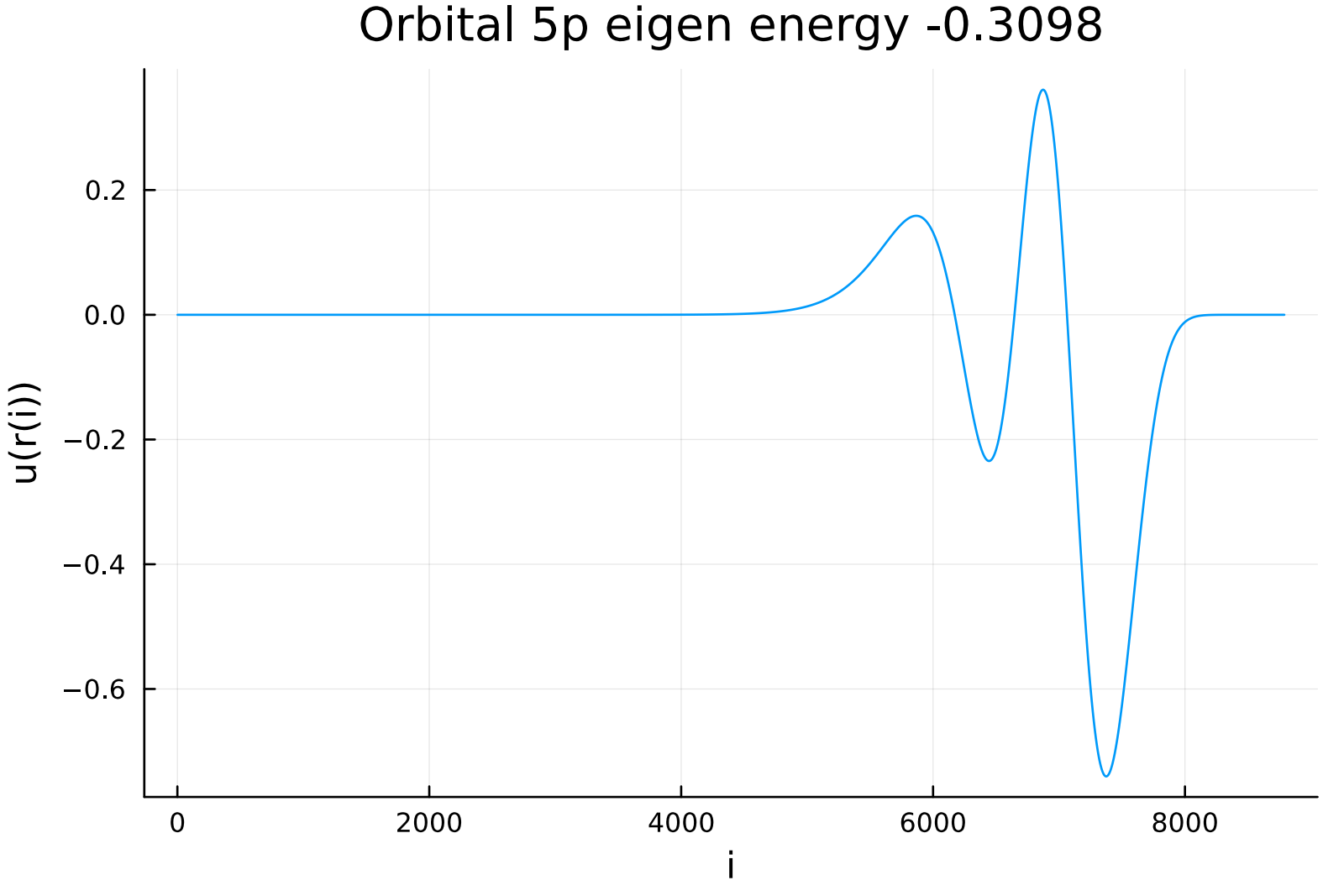

Orbital 4s eigen energy -6.6783
0.5
0.0
−0.5
−1.0
u(r(i))
0
2000
4000
6000
8000
i


Orbital 3d eigen energy -24.3782
u(r(i))
1.5
1.0
0.5
0.0
0
2000
4000
6000
8000
i


Orbital 4p eigen energy -5.0638
u(r(i))
1.0
0.5
0.0
−0.5
0
2000
4000
6000
8000
i


Orbital 5s eigen energy -0.6721
0.75
0.50
0.25
0.00
−0.25
u(r(i))
0
2000
4000
6000
8000
i


Orbital 4d eigen energy -2.2867
0.5
0.0
−0.5
−1.0
u(r(i))
0
2000
4000
6000
8000
i


Orbital 5p eigen energy -0.3098
0.2
0.0
−0.2
−0.4
−0.6
u(r(i))
0
2000
4000
6000
8000
i