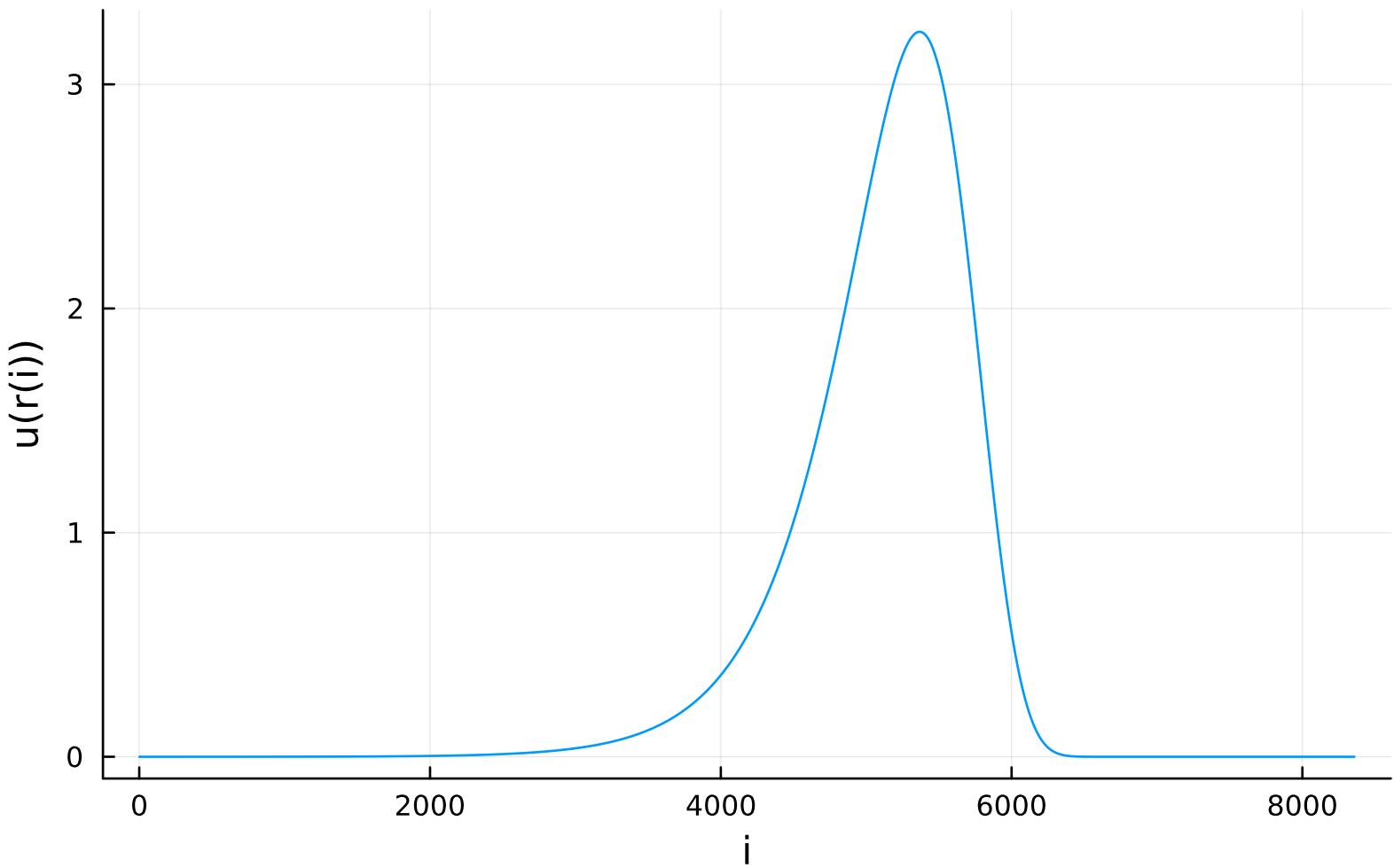
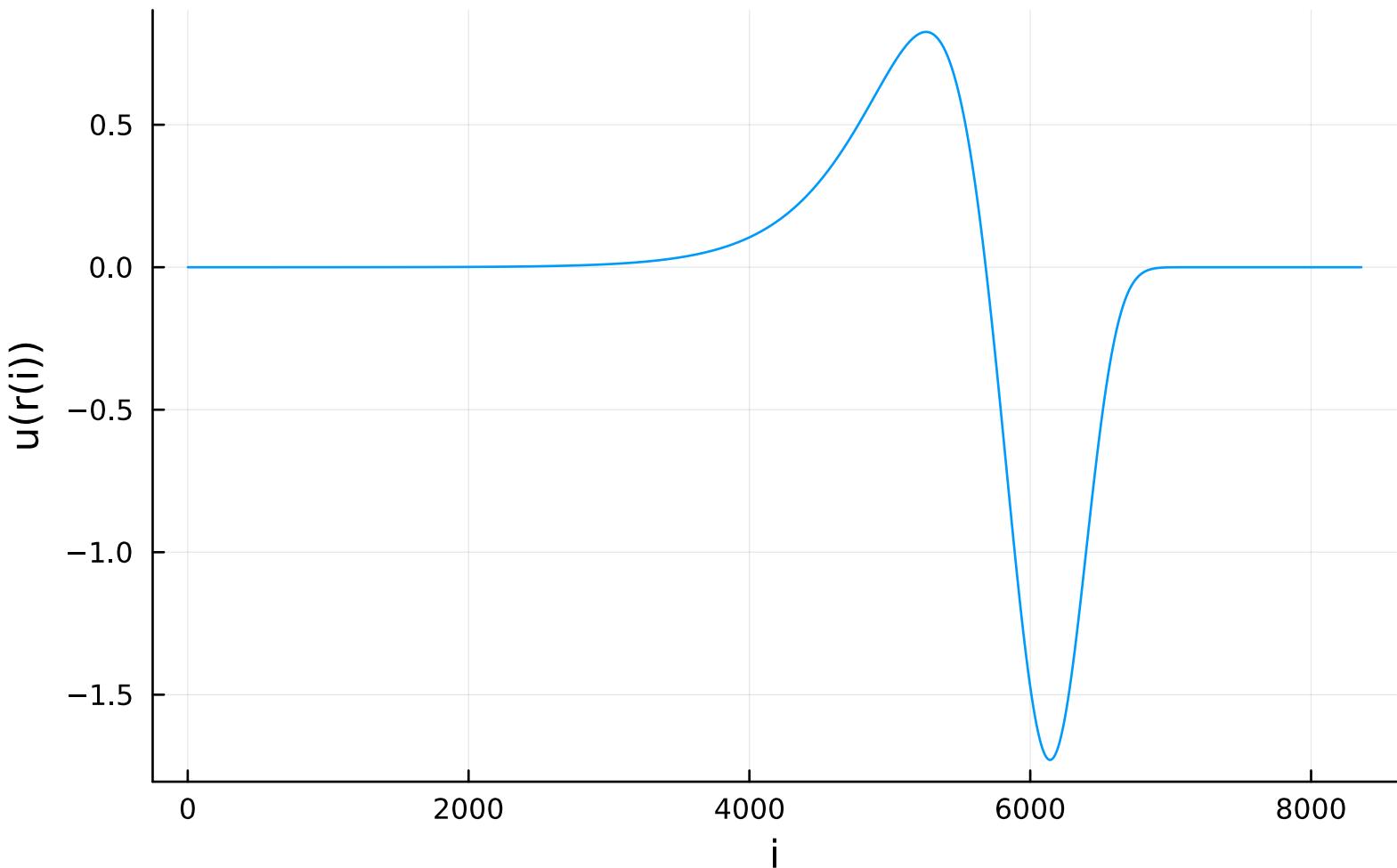


Calcium	E in Hartree			
Name	E NIST	E pred	ΔE	ΔE /E NIST
Ecoul	285.206130	285.201292	0.004838	0.000017
3p	-1.030572	-1.030736	0.000164	-0.000159
4s	-0.141411	-0.141710	0.000299	-0.002117
Etot	-675.742283	-675.742283	0.000000	-0.000000
2s	-15.046905	-15.047161	0.000256	-0.000017
3s	-1.706331	-1.706491	0.000160	-0.000093
Exc	-34.142538	-34.141772	0.000766	-0.000022
Ekin	674.657334	674.620490	0.036844	0.000055
2p	-12.285376	-12.285617	0.000241	-0.000020
1s	-143.935181	-143.936063	0.000882	-0.000006

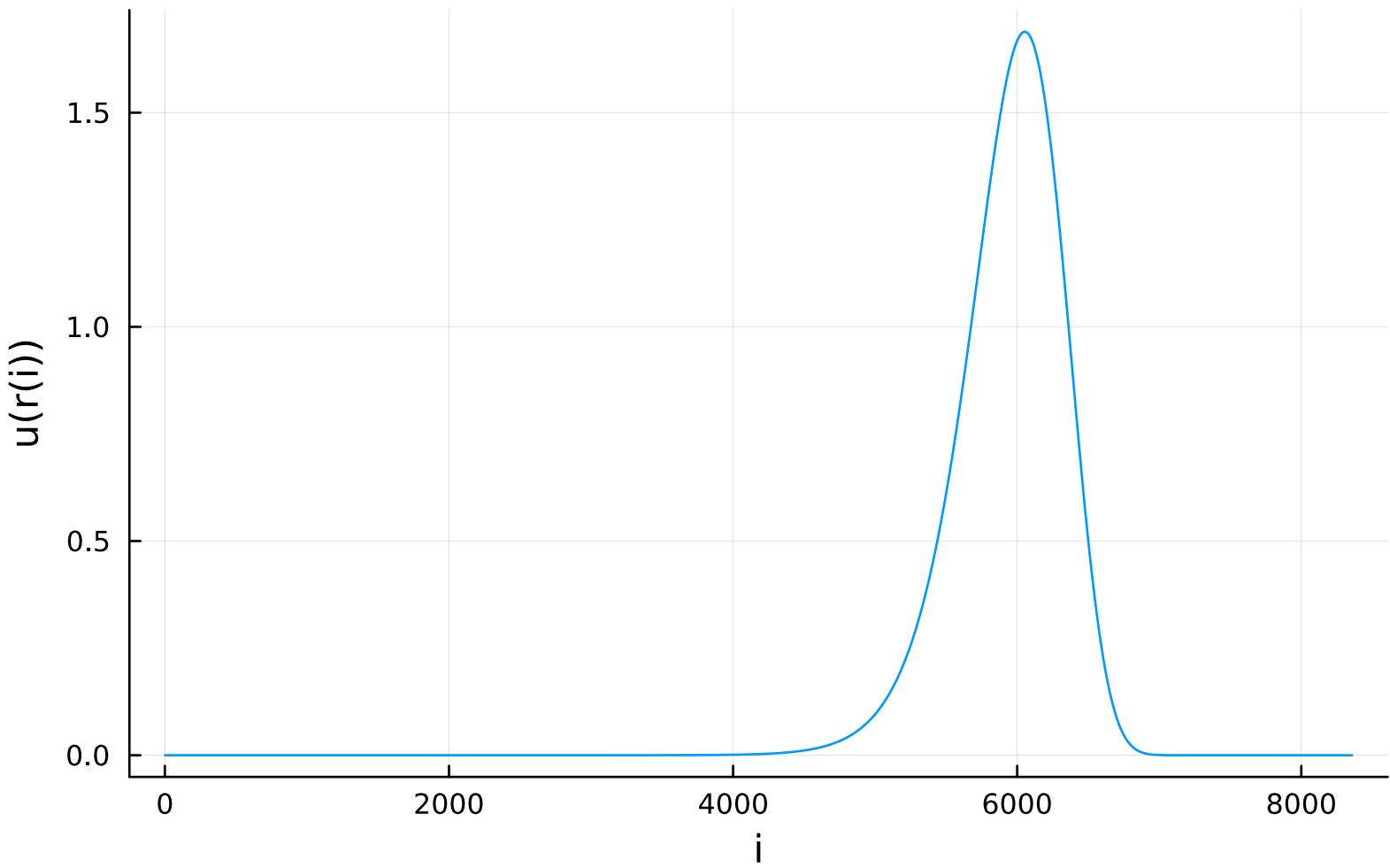
Orbital 1s eigen energy -143.9361



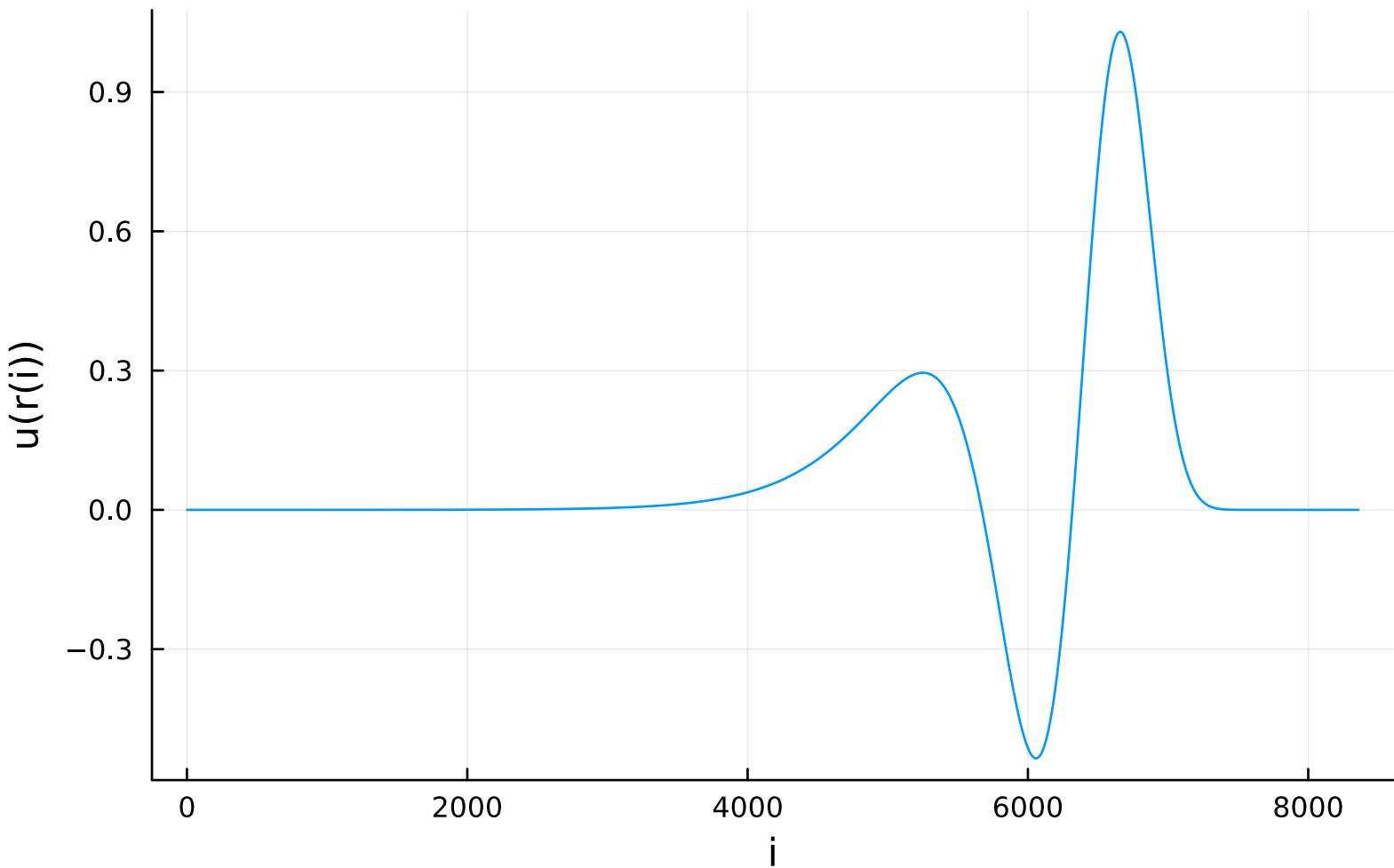
Orbital 2s eigen energy -15.0472



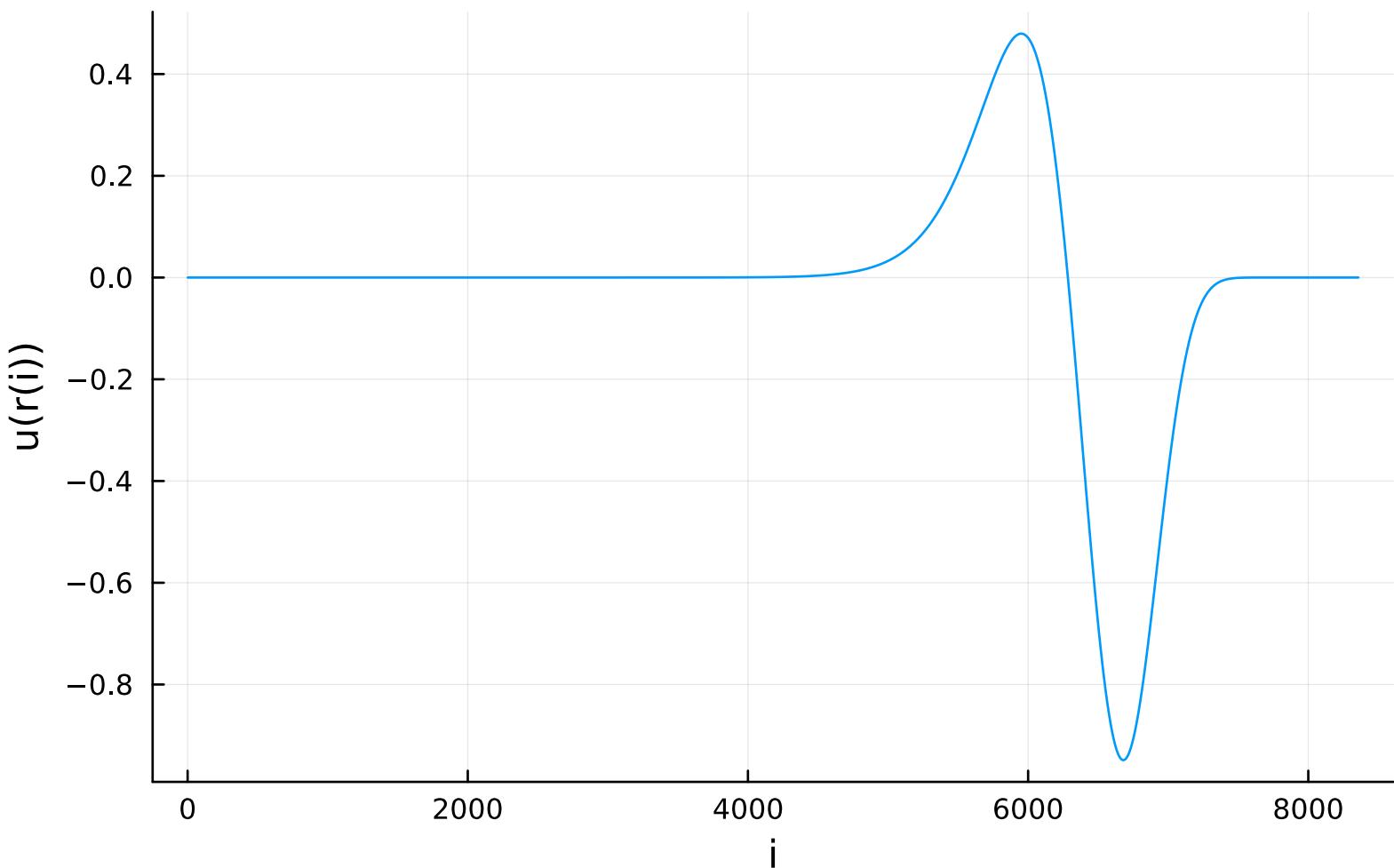
Orbital 2p eigen energy -12.2856



Orbital 3s eigen energy -1.7065



Orbital 3p eigen energy -1.0307



Orbital 4s eigen energy -0.1417

