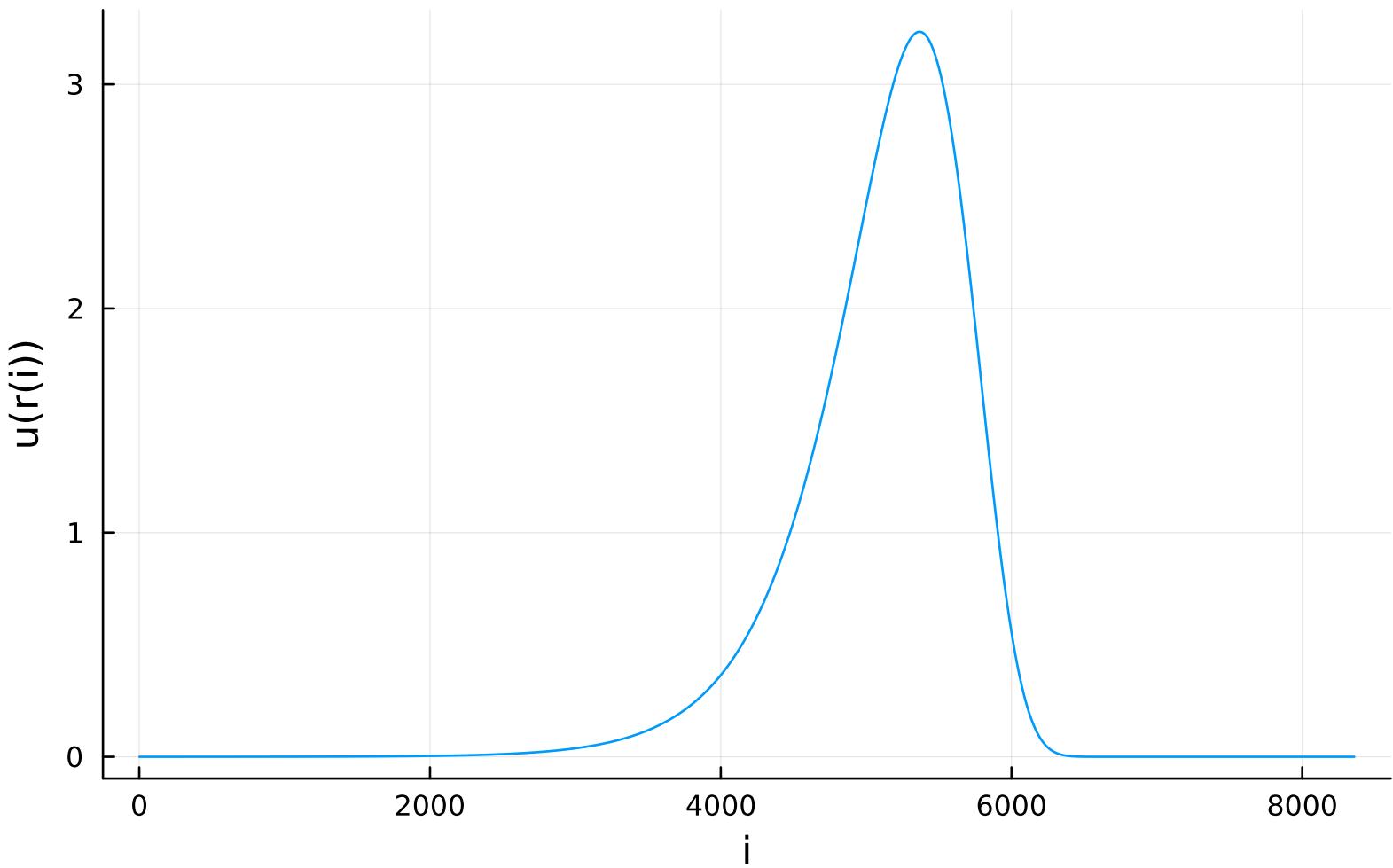
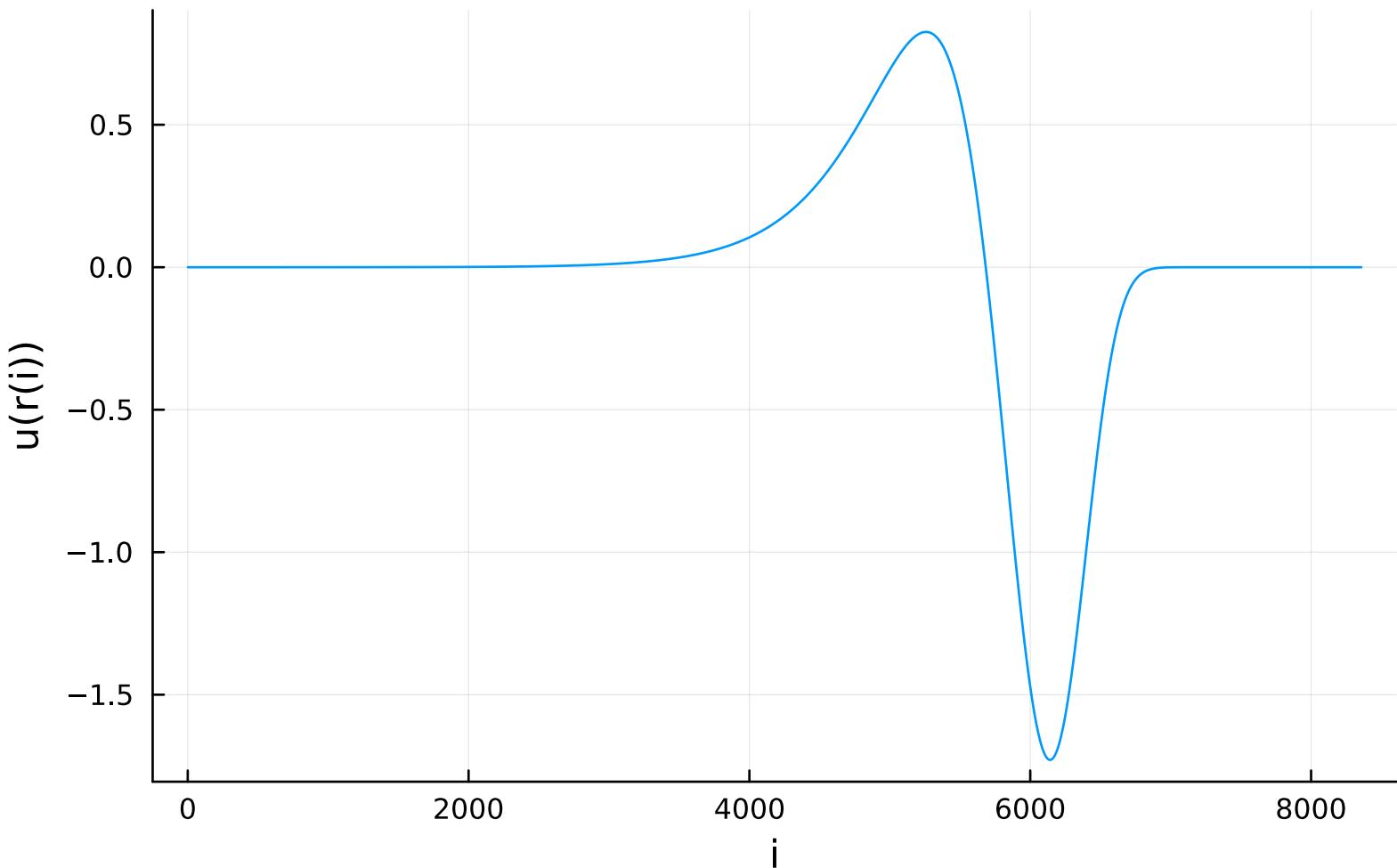


Calcium	E in Hartree			
Name	E NIST	E pred	ΔE	ΔE /E NIST
Ecoul	285.206130	285.206125	0.000005	0.000000
3p	-1.030572	-1.030572	0.000000	-0.000000
4s	-0.141411	-0.141410	0.000001	-0.000004
Etot	-675.742283	-675.742283	0.000000	-0.000000
2s	-15.046905	-15.046905	0.000000	-0.000000
3s	-1.706331	-1.706331	0.000000	-0.000000
Exc	-34.142538	-34.142538	0.000000	-0.000000
Ekin	674.657334	674.657333	0.000001	0.000000
2p	-12.285376	-12.285376	0.000000	-0.000000
1s	-143.935181	-143.935181	0.000000	-0.000000

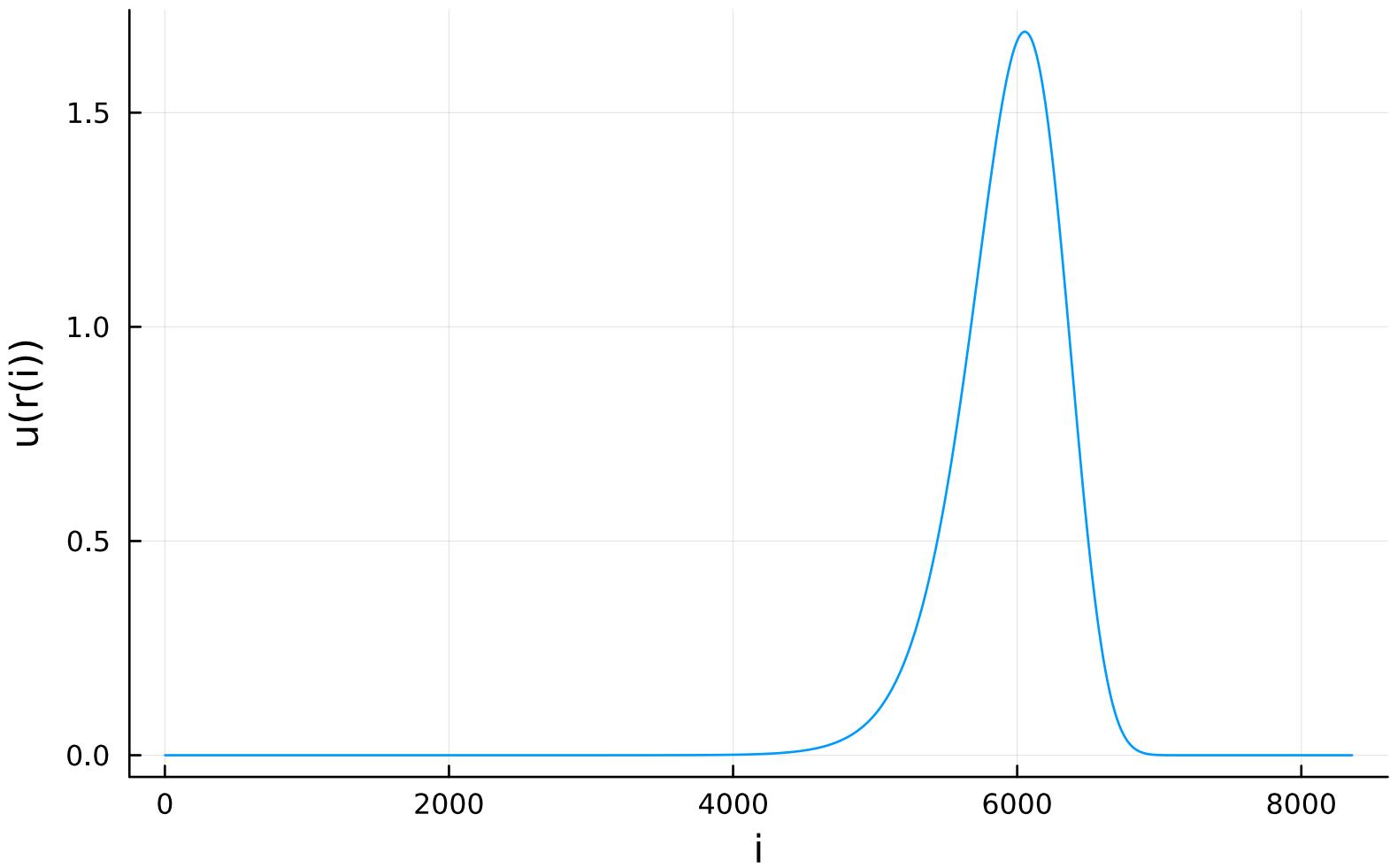
Orbital 1s eigen energy -143.9352



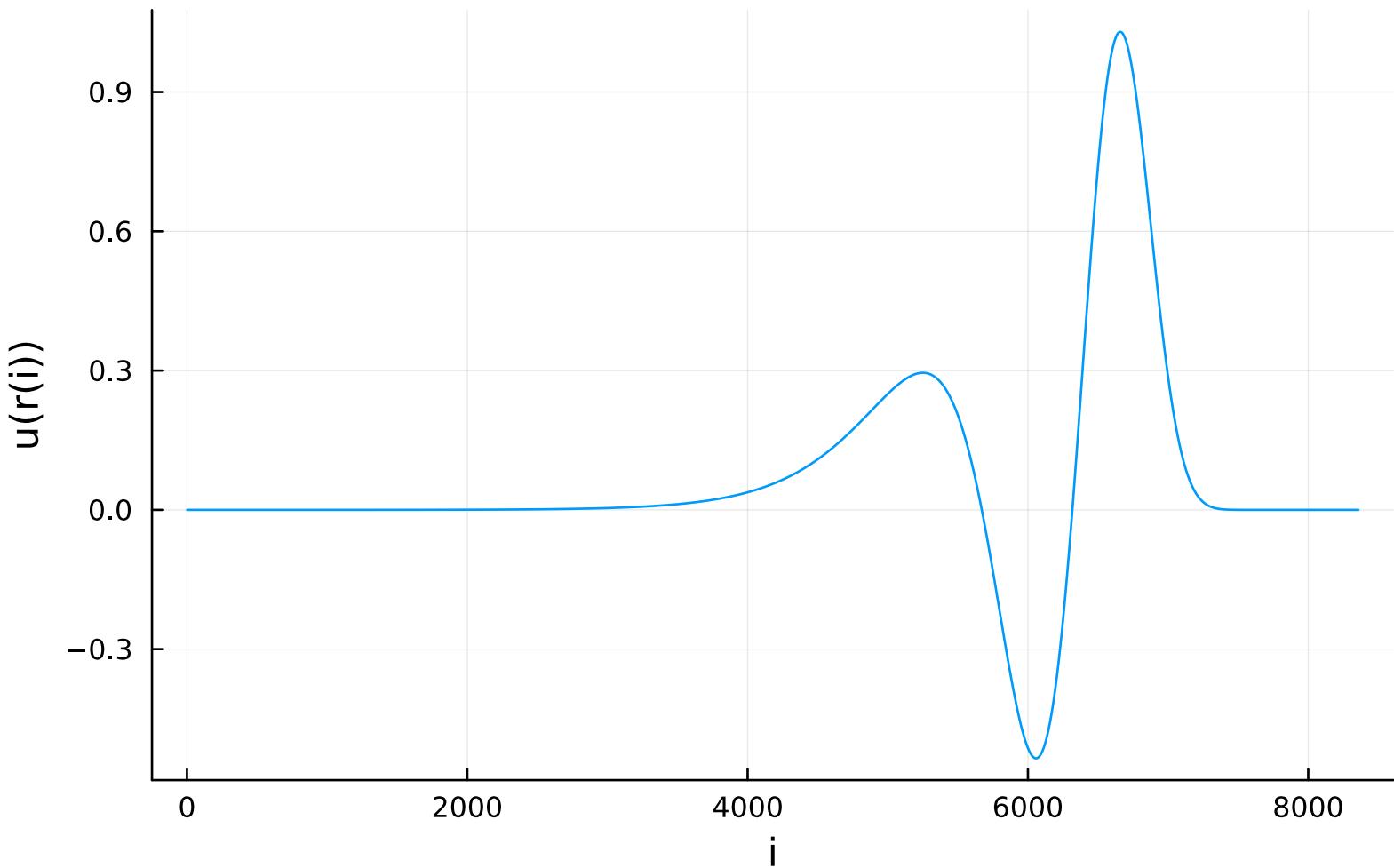
Orbital 2s eigen energy -15.0469



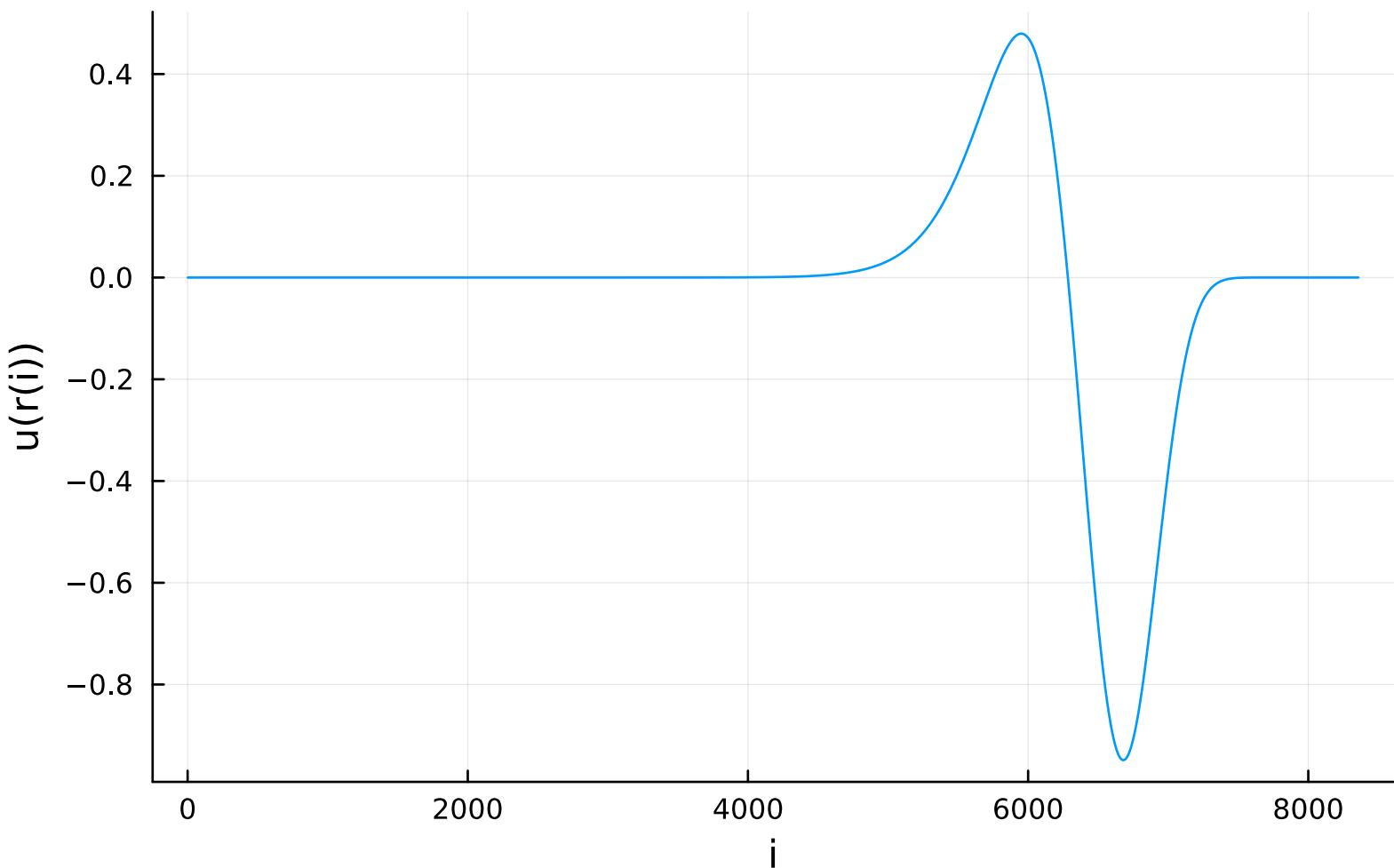
Orbital 2p eigen energy -12.2854



Orbital 3s eigen energy -1.7063



Orbital 3p eigen energy -1.0306



Orbital 4s eigen energy -0.1414

