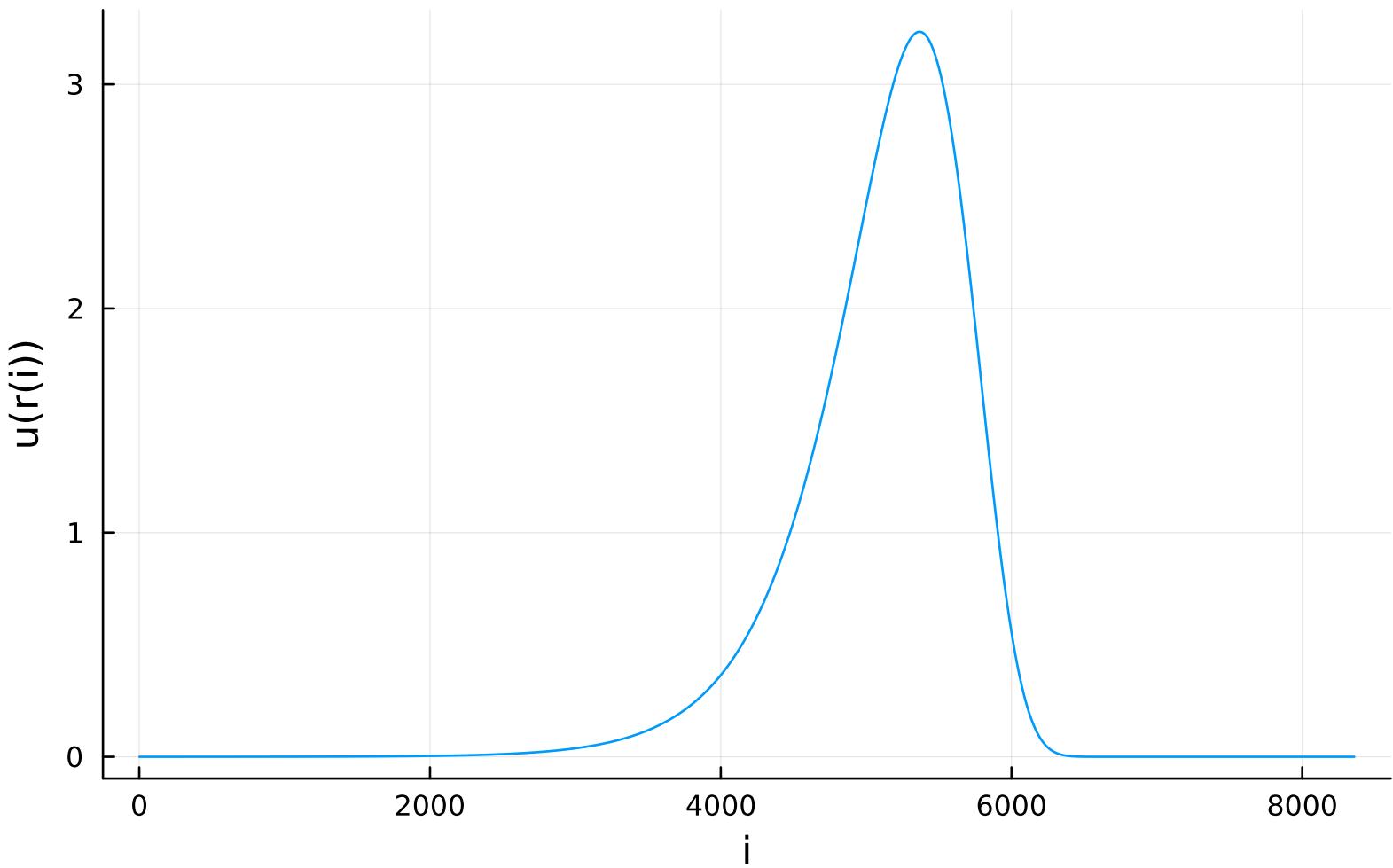
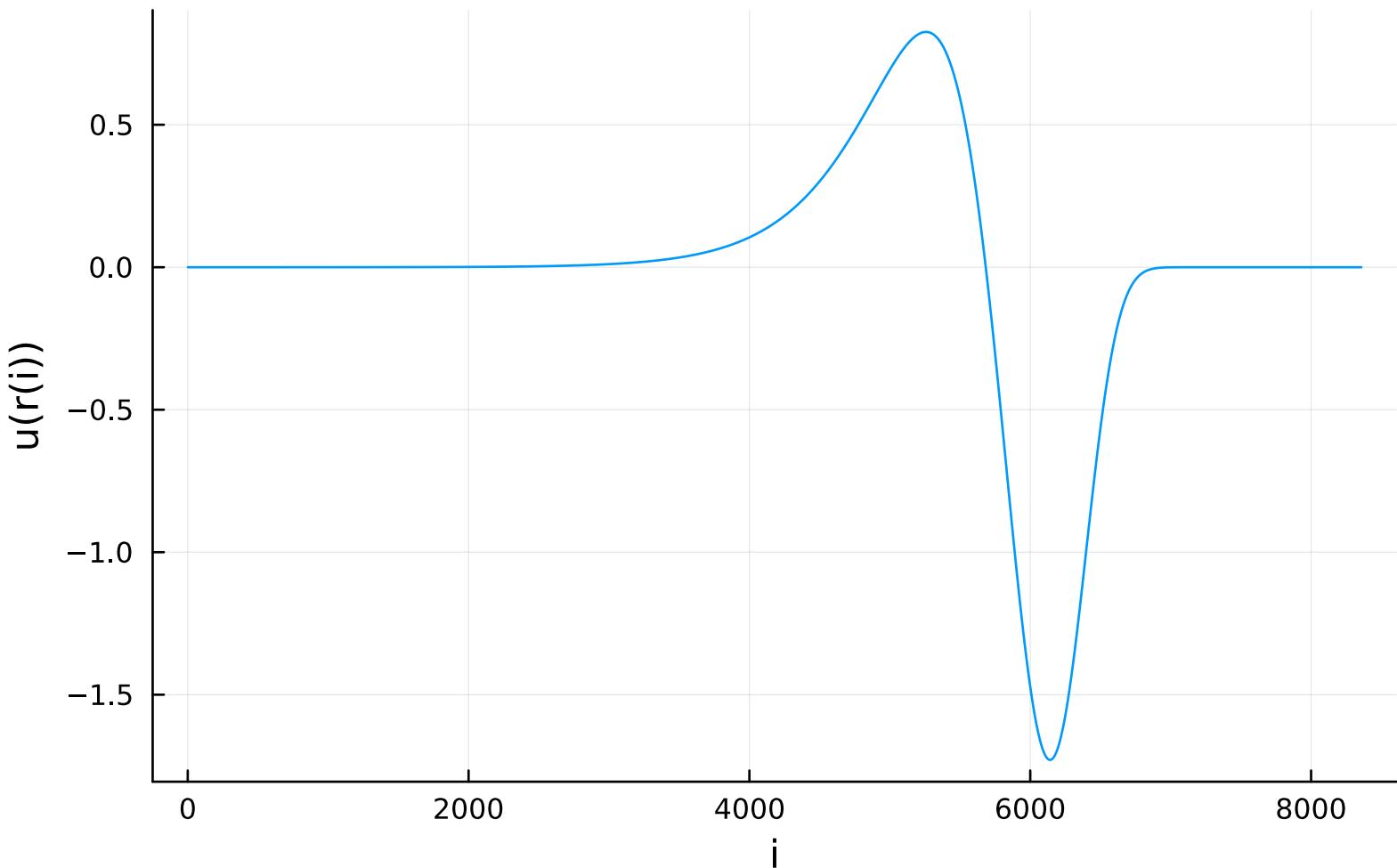


Calcium	E in Hartree			
Name	E NIST	E pred	ΔE	ΔE /E NIST
Ecoul	285.206130	285.205656	0.000474	0.000002
3p	-1.030572	-1.030520	0.000052	-0.000050
4s	-0.141411	-0.141388	0.000023	-0.000162
Etot	-675.742283	-675.742283	0.000000	-0.000000
2s	-15.046905	-15.046854	0.000051	-0.000003
3s	-1.706331	-1.706277	0.000054	-0.000032
Exc	-34.142538	-34.142514	0.000024	-0.000001
Ekin	674.657334	674.657176	0.000158	0.000000
2p	-12.285376	-12.285326	0.000050	-0.000004
1s	-143.935181	-143.935140	0.000041	-0.000000

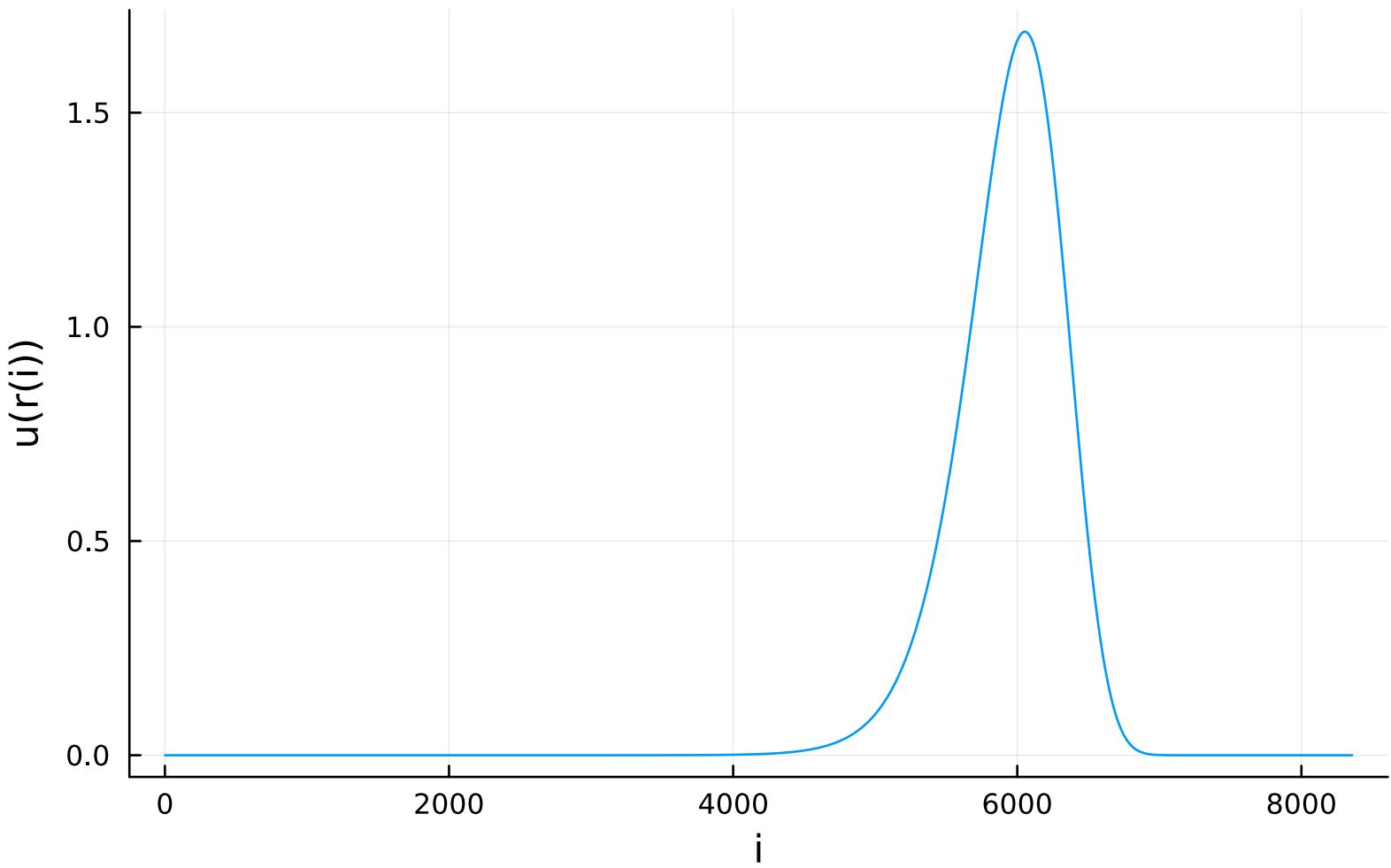
Orbital 1s eigen energy -143.9351



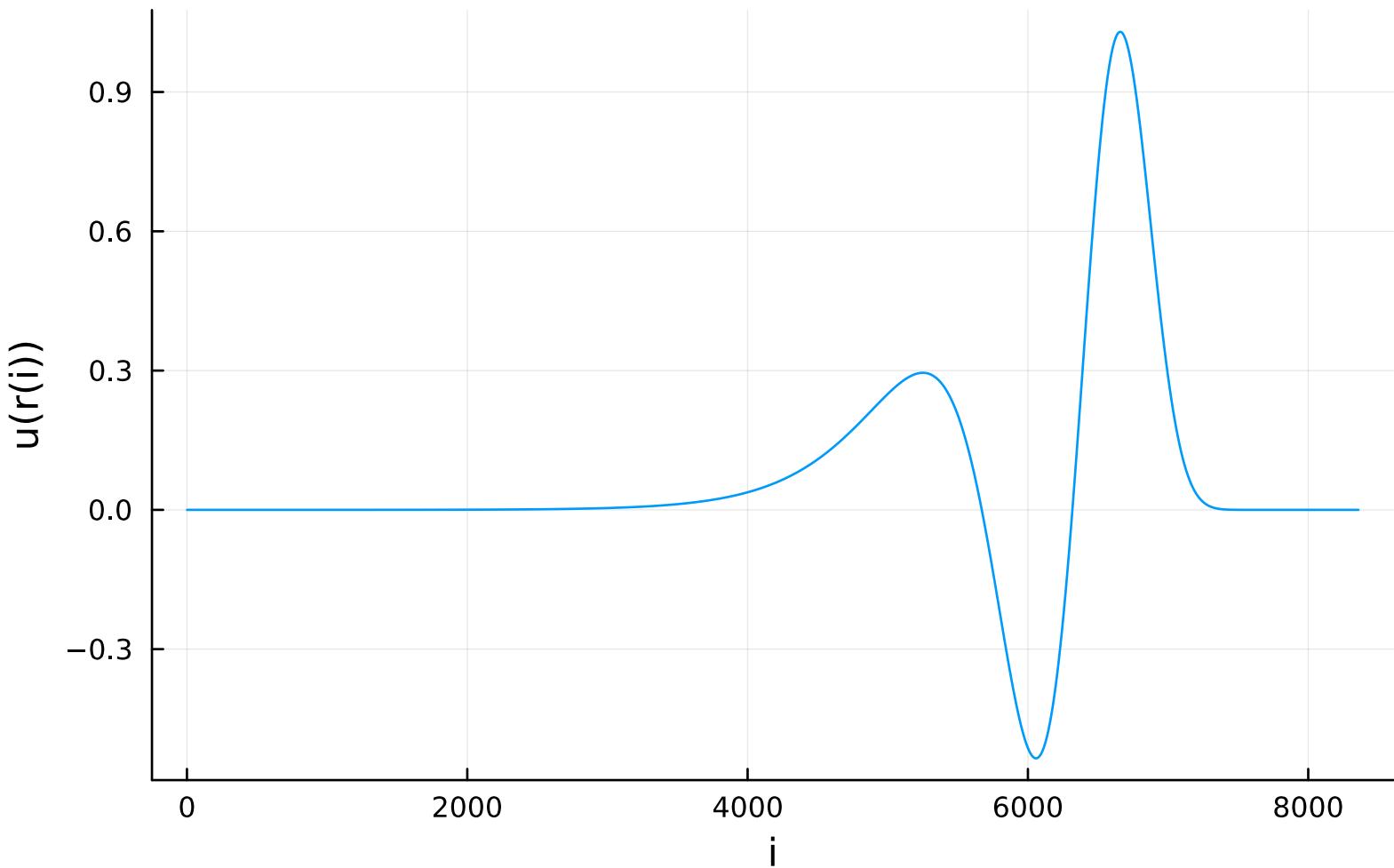
Orbital 2s eigen energy -15.0469



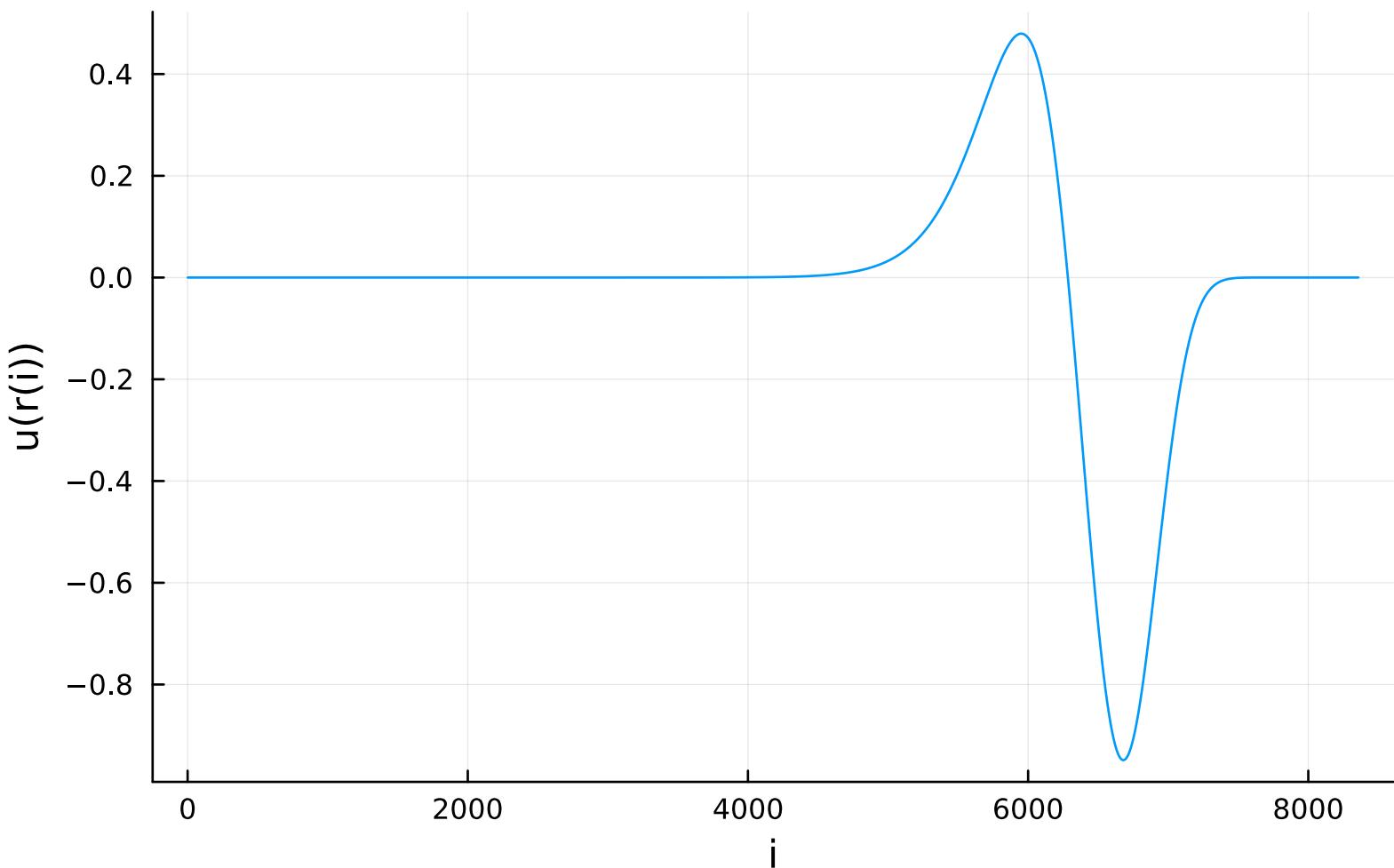
Orbital 2p eigen energy -12.2853



Orbital 3s eigen energy -1.7063



Orbital 3p eigen energy -1.0305



Orbital 4s eigen energy -0.1414

