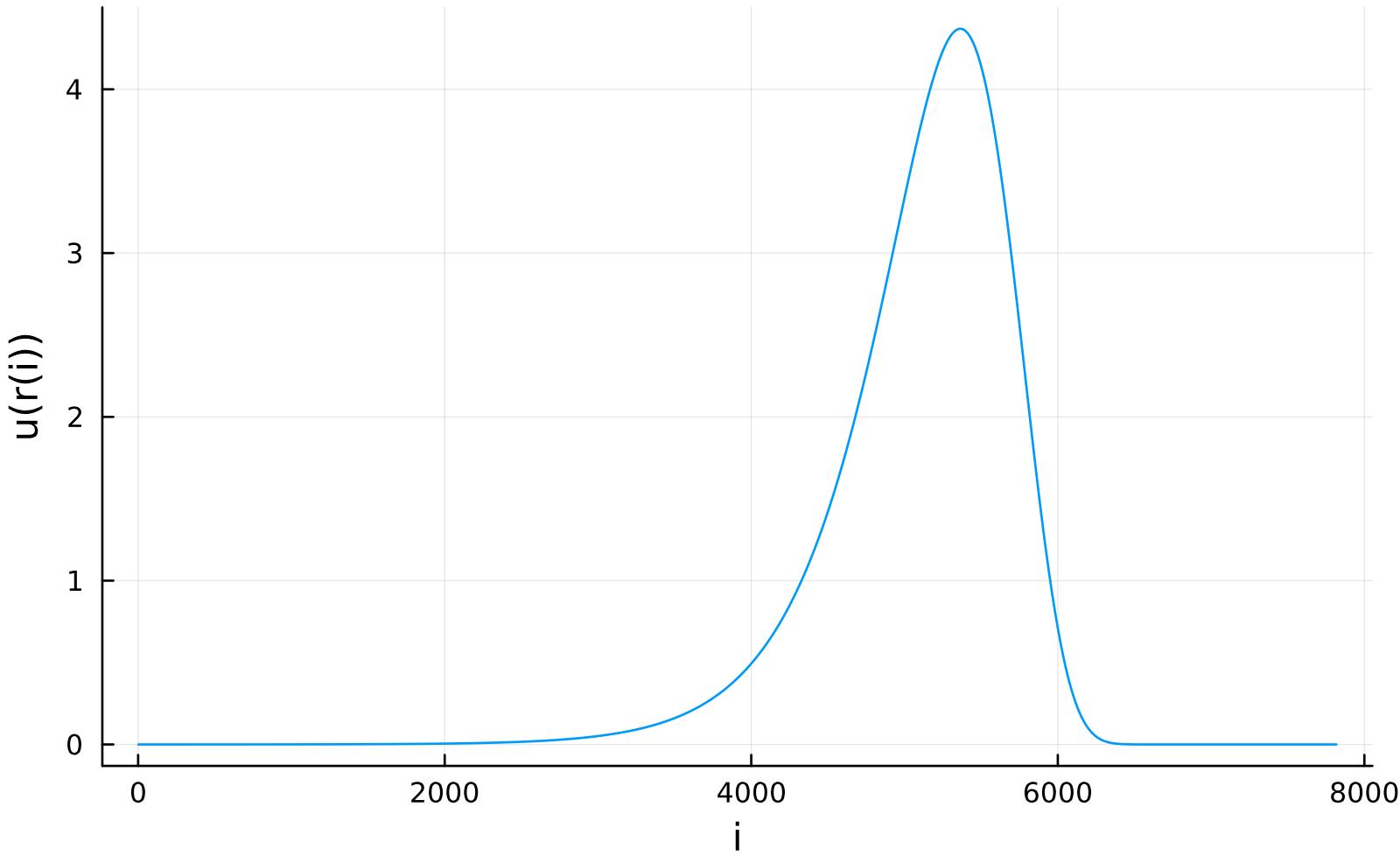
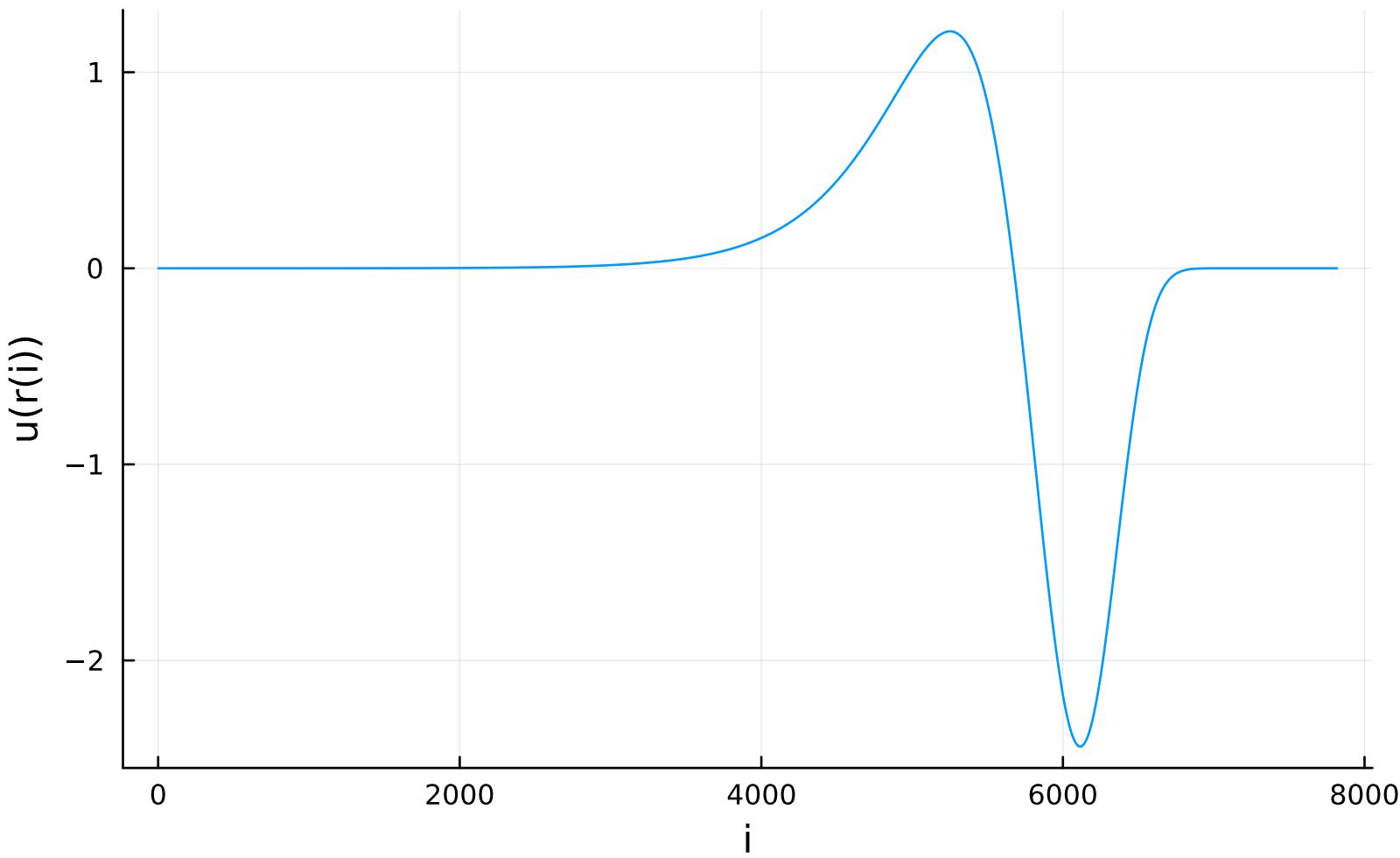


Krypton	E in Hartree			
Name	E NIST	E pred	ΔE	ΔE /E NIST
Ecoul	1171.723688	1172.457824	0.734136	0.000627
3p	-7.086634	-7.065211	0.021423	-0.003023
4p	-0.346340	-0.329568	0.016772	-0.048425
Exc	-91.819009	-91.846470	0.027461	-0.000299
2p	-60.017328	-59.995348	0.021980	-0.000366
4s	-0.820574	-0.803966	0.016608	-0.020240
Etot	-2750.147940	-2750.133222	0.014718	-0.000005
2s	-66.285953	-66.264043	0.021910	-0.000331
3s	-9.315192	-9.293759	0.021433	-0.002301
3d	-3.074109	-3.052749	0.021360	-0.006948
Ekin	2747.813142	2747.885161	0.072019	0.000026
1s	-509.982989	-509.961008	0.021981	-0.000043

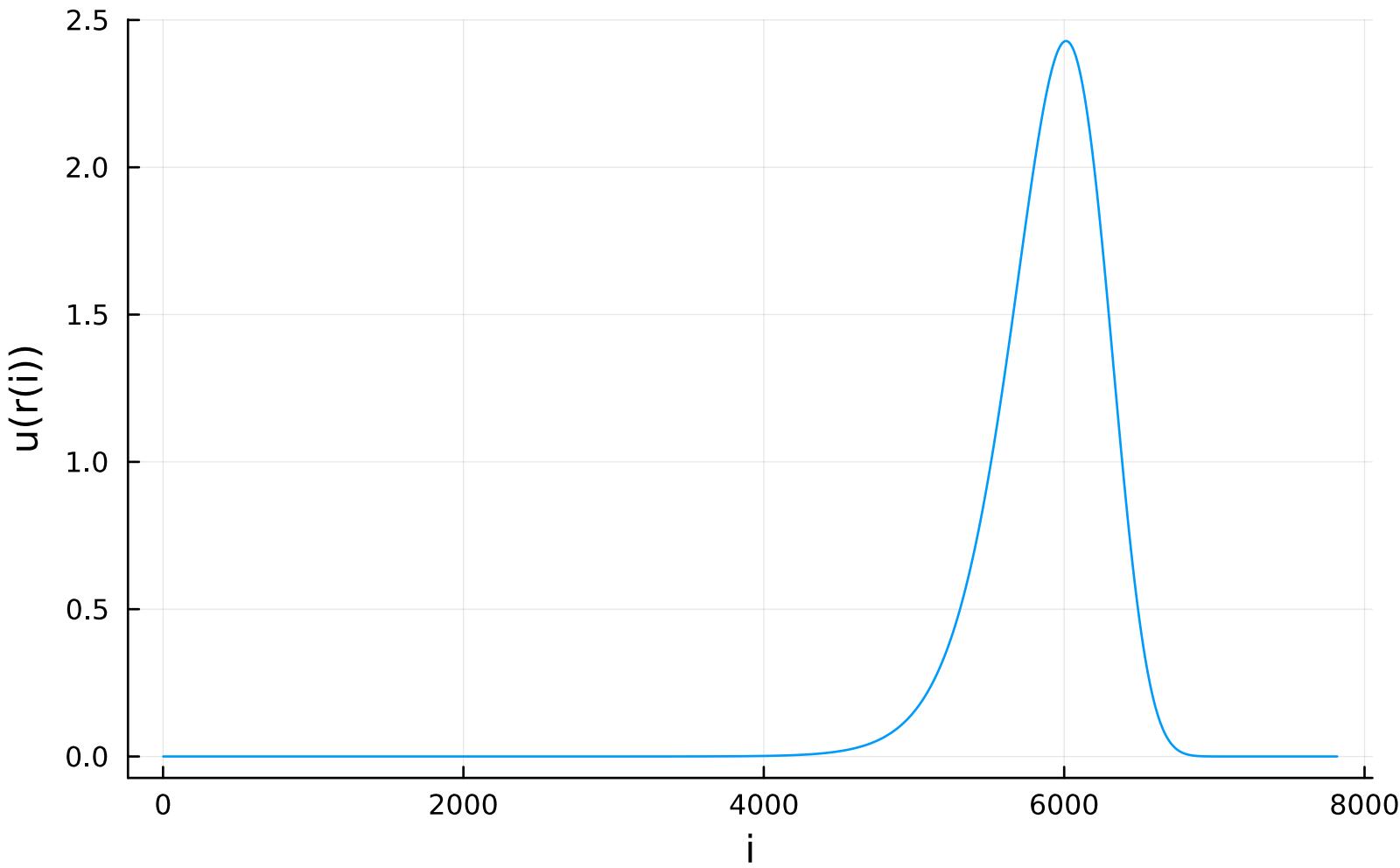
Orbital 1s eigen energy -509.9610



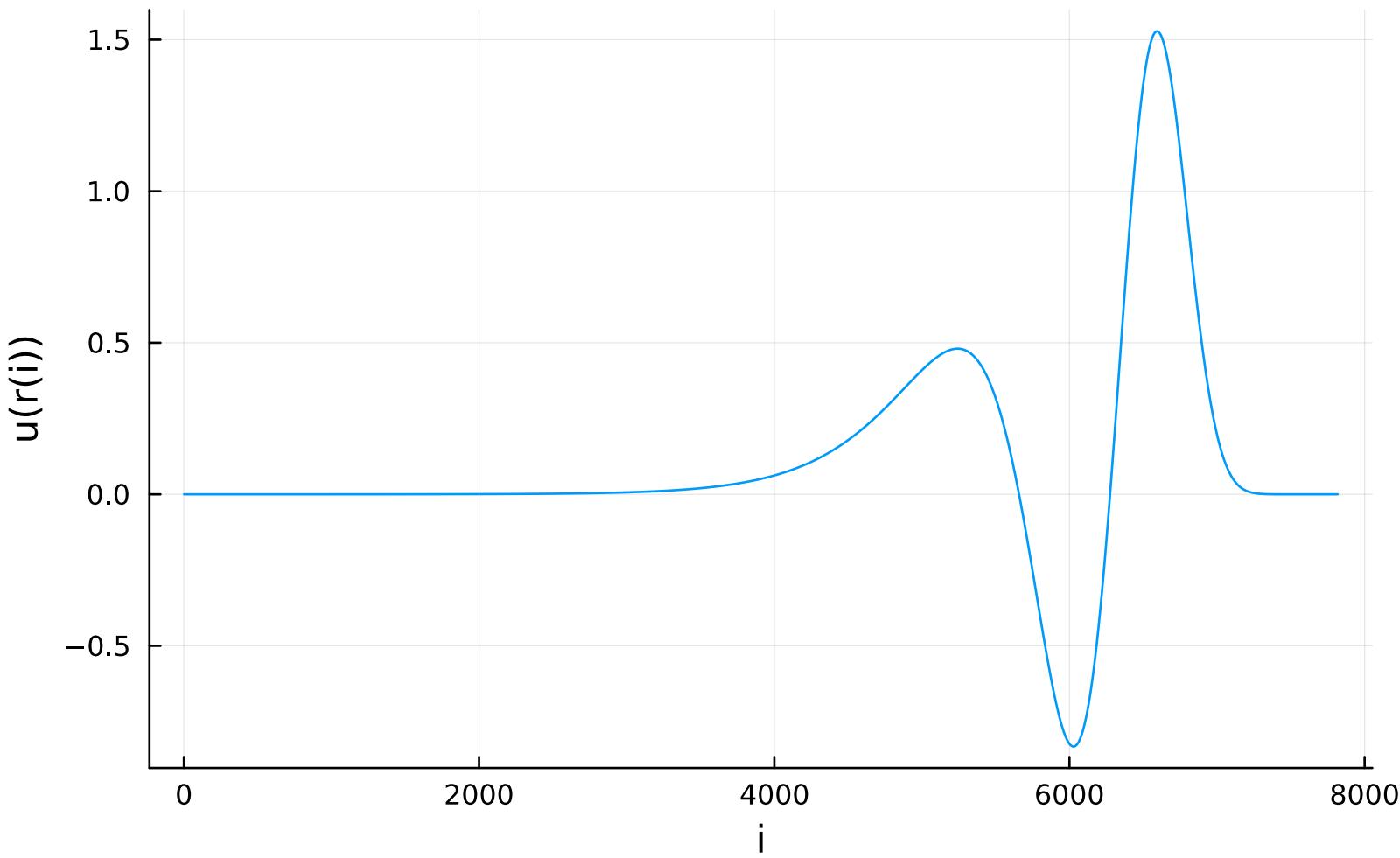
Orbital 2s eigen energy -66.2640



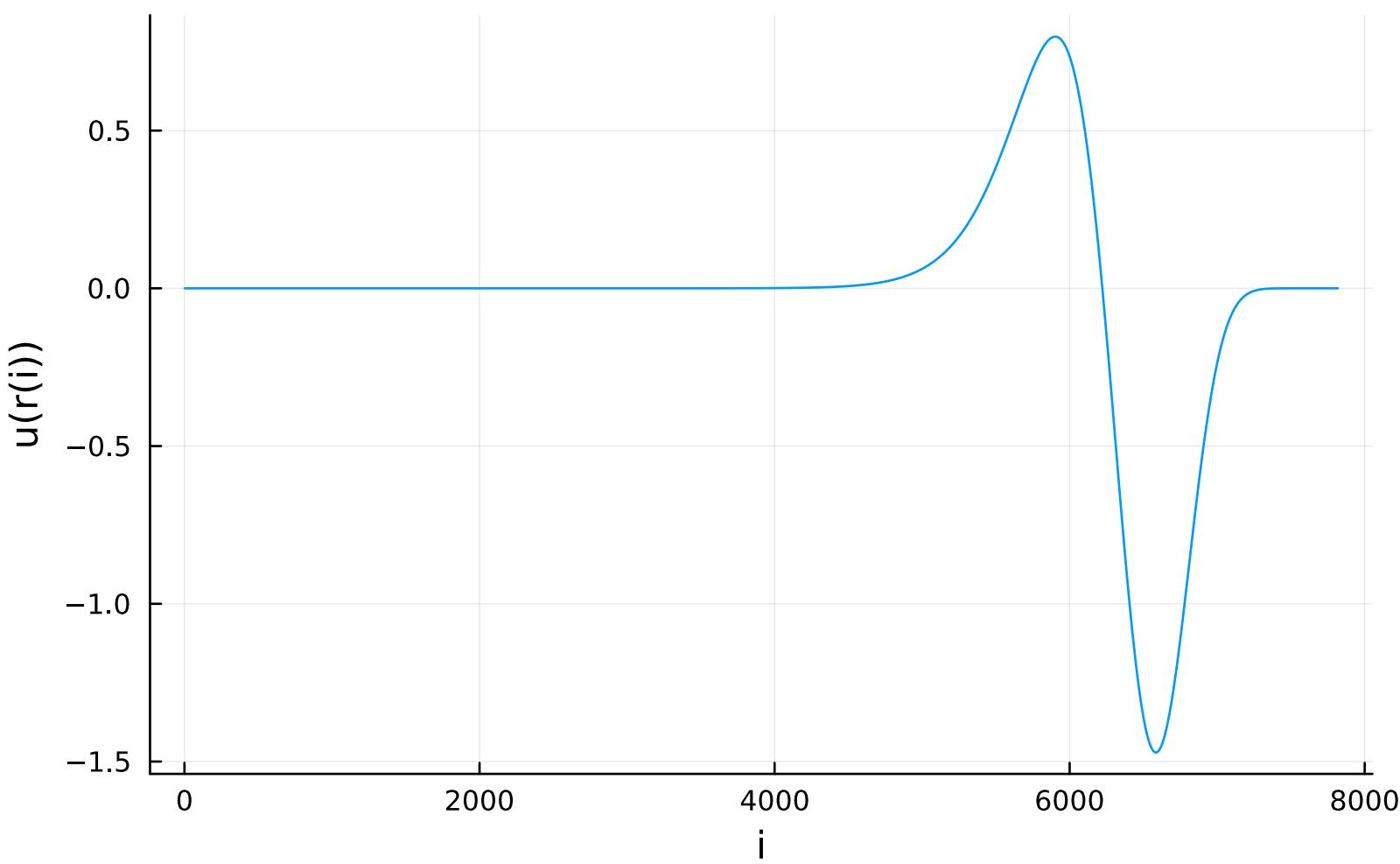
Orbital 2p eigen energy -59.9953



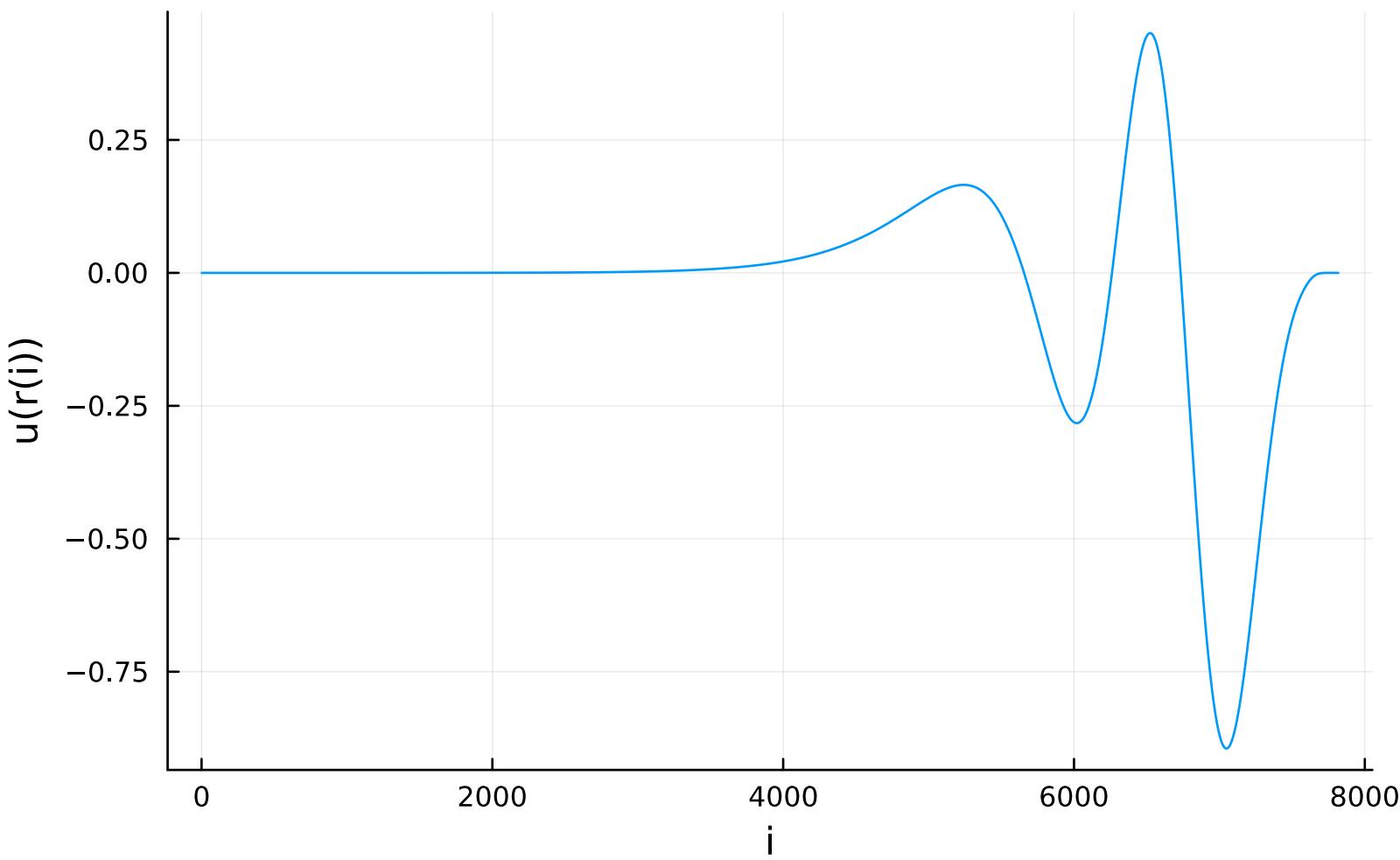
Orbital 3s eigen energy -9.2938



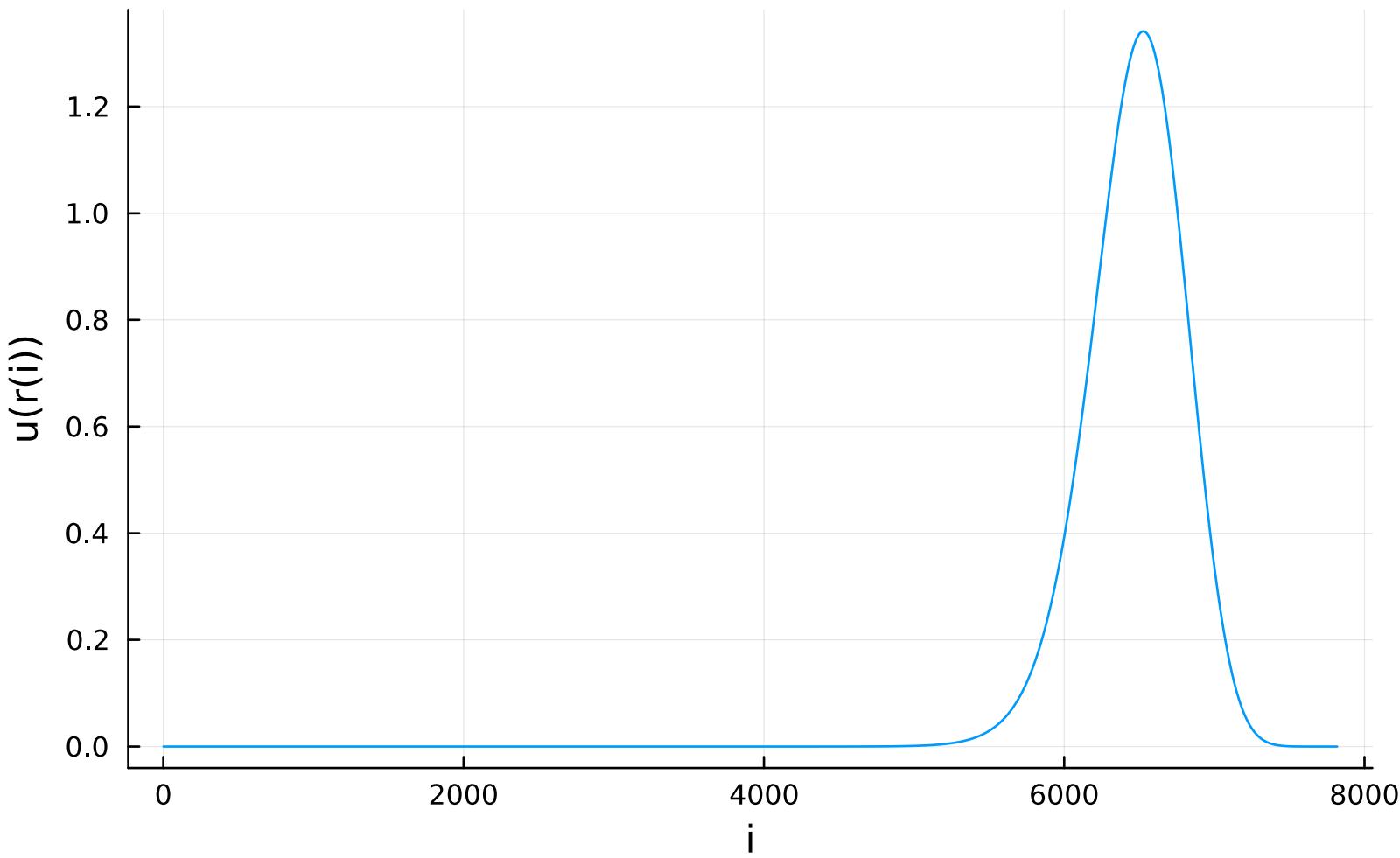
Orbital 3p eigen energy -7.0652



Orbital 4s eigen energy -0.8040



Orbital 3d eigen energy -3.0527



Orbital 4p eigen energy -0.3296

