In [1]:
```
import scipy.constants as cons
import numpy as np
h=cons.h
hb=cons.hbar
e=cons.e
c=cons.c
m_e=cons.m_e
a=cons.alpha
ry=cons.Rydberg*h*c
evtocm1=8065.45

def sl(l,j): #Skalarprodukt
    return 0.5*hb**2*(j*(j+1)-l*(l+1)-0.5*(0.5+1))

def E_ver(n,l,j): #Verschiebung wegen Spin-Bahn-Kopplung
    return a**4*m_e*c**2/(2*hb**2)*sl(l,j)/(n**3*l*(l+0.5)*(l+1))

def E_von_n(n): #Gesamtenergie
    return -ry/n**2

def E_mit_spin(n,l,j):
    if l==0:
        return E_von_n(n)
    return E_von_n(n)+_ver(n,l,j)
```

In [2]:
```
print(f"n=2,l=1,j=0.5    E={E_ver(2,1,0.5)/e*1e6}µeV")
print(f"n=2,l=1,j=1.5    E={E_ver(2,1,1.5)/e*1e6}µeV")
print(f"n=3,l=1,j=0.5    E={E_ver(3,1,0.5)/e*1e6}µeV")
print(f"n=3,l=1,j=1.5    E={E_ver(3,1,1.5)/e*1e6}µeV")
print(f"n=3,l=2,j=1.5    E={E_ver(3,2,1.5)/e*1e6}µeV")
print(f"n=3,l=2,j=2.5    E={E_ver(3,2,2.5)/e*1e6}µeV")
```

```
n=2,l=1,j=0.5    E=-30.188399499607854µeV
n=2,l=1,j=1.5    E=15.094199749803927µeV
n=3,l=1,j=0.5    E=-8.944710962846774µeV
n=3,l=1,j=1.5    E=4.472355481423387µeV
n=3,l=2,j=1.5    E=-2.683413288854032µeV
n=3,l=2,j=2.5    E=1.7889421925693545µeV
```

In [3]:
```
print(f"n=2,l=1,j=0.5    E={E_ver(2,1,0.5)/e*evtocm1}cm^-1")
print(f"n=2,l=1,j=1.5    E={E_ver(2,1,1.5)/e*evtocm1}cm^-1")
print(f"n=3,l=1,j=0.5    E={E_ver(3,1,0.5)/e*evtocm1}cm^-1")
print(f"n=3,l=1,j=1.5    E={E_ver(3,1,1.5)/e*evtocm1}cm^-1")
print(f"n=3,l=2,j=1.5    E={E_ver(3,2,1.5)/e*evtocm1}cm^-1")
print(f"n=3,l=2,j=2.5    E={E_ver(3,2,2.5)/e*evtocm1}cm^-1")
```

```
n=2,l=1,j=0.5    E=-0.24348302674411215cm^-1
n=2,l=1,j=1.5    E=0.12174151337205608cm^-1
n=3,l=1,j=0.5    E=-0.0721431190352925cm^-1
n=3,l=1,j=1.5    E=0.03607155951764625cm^-1
n=3,l=2,j=1.5    E=-0.02164293571058775cm^-1
n=3,l=2,j=2.5    E=0.0144286238070585cm^-1
```

In [4]:
```
E_von_n(1)/e
```

Out[4]:
```
-13.605693122994232
```

In [5]:
```
E_von_n(2)/e
```

Out[5]:
```
-3.401423280748558
```

In [6]:
```
E_von_n(3)/e
```

Out[6]:
```
-1.5117436803326925
```

In [7]:
```
a_=m_e*e**2/(4*np.pi*cons.epsilon_0*hb**2)
phi_quad_1=a_**3/np.pi
E_darwin_1=e**2*hb**2/(8*cons.epsilon_0*m_e**2*c**2)*phi_quad_1

E_rel=E_von_n(1)*(-a**2*(3/4-2))
(E_rel+E_darwin_1)/e
```

Out[7]:
```
-0.00018113039700813405
```

In [8]:
```
m,a,b,v0,grad=1.79e-25,0.05,0.08,500,1000

1.1e-3/(1/m*grad*(a/v0)*(1/2*a/v0+b/v0))
```

Out[8]:
```
9.376190476190475e-24
```

In [ ]:
```

```