

```
In[1]:= ClearAll["Global`*"]
borra todo
```

## Funciones radiales

```
In[2]:= R10[r_, Z_] := 2 (Z)^(3/2) Exp[-Z r];
           |exponencial

R21[r_, Z_] := 1/Sqrt[3] (Z/2)^(3/2) (Z r) Exp[-Z r/2];
           |exponencial

R20[r_, Z_] := 2 (Z/2)^(3/2) (1 - Z r/2) Exp[-Z r/2];
           |exponencial
```

## Integral de Coulomb

```
In[5]:= CoulombIntegral[r1_, r2_, Z_, n_, l_] :=
  Integrate[r2^2 * If[n == 2 && l == 0, R20[r2, Z], R21[r2, Z]] *
  |integra |si
  (Integrate[1/r2 r1^2 (R10[r1, Z])^2, {r1, 0, r2}]
  |integra
  + Integrate[1/r1 r1^2 (R10[r1, Z])^2, {r1, r2, Infinity}]),
  {r2, 0, Infinity};
```

## Integral de intercambio

```
In[6]:= ExchangeIntegral[r1_, r2_, Z_, n_, l_] :=
  
$$\frac{1}{2l+1} * \int_{\text{integra}} \left[ r2^2 R10[r2, Z] * \int_{\text{si}} \text{If}[n == 2 \&\& l == 0, R20[r2, Z], R21[r2, Z]] * \right.$$


$$\left. \left( \int_{\text{integra}} \left[ r1^2 R10[r1, Z] * \int_{\text{si}} \text{If}[n == 2 \&\& l == 0, R20[r1, Z], R21[r1, Z]] \frac{(r1)^1}{(r2)^{1+1}}, \right. \right.$$


$$\left. \{r1, 0, r2\} \right] + \int_{\text{integra}} \left[ \right.$$


$$\left. r1^2 R10[r1, Z] * \int_{\text{si}} \text{If}[n == 2 \&\& l == 0, R20[r1, Z], R21[r1, Z]] \frac{(r2)^1}{(r1)^{1+1}}, \{r1, r2, \infty\} \right] \right],$$


$$\{r2, 0, \infty\} \right]$$

```

## Integrales para n = 2 y l = 1

```
In[7]:= J20 = CoulombIntegral[r, ρ, 2, 2, 0]
Out[7]=  $-\frac{1296}{625}$ 

In[8]:= K20 = ExchangeIntegral[r, ρ, 2, 2, 0]
Out[8]=  $\frac{32}{729}$ 
```

## Integrales para n = 2 y l = 2

```
In[9]:= J21 = CoulombIntegral[r, ρ, 2, 2, 1]
Out[9]=  $\frac{2456}{625 \sqrt{3}}$ 

In[10]:= K21 = ExchangeIntegral[r, ρ, 2, 2, 1]
Out[10]=  $\frac{224}{6561}$ 
```

## Energía a primer orden de aproximación

### Estados $2^1 S$ y $2^3 S$

In[11]:= **FirstOrderCorrectionNL**[J\_, K\_] := J ± K;

In[12]:= **FirstOrderCorrection20** = **FirstOrderCorrectionNL**[J20, K20]

Out[12]=

$$-\frac{1296}{625} \pm \frac{32}{729}$$

### Estados $2^1 P$ y $2^3 P$

In[13]:= **FirstOrderCorrection21** = **FirstOrderCorrectionNL**[J21, K21]

Out[13]=

$$\frac{2456}{625 \sqrt{3}} \pm \frac{224}{6561}$$

## Energía imperturbada

In[14]:= **UnperturbedEnergyN**[Z\_, n\_] :=  $\frac{-Z^2}{2} \left(1 + \frac{1}{n^2}\right)$ ;

In[15]:= **UnperturbedEnergy2** = **UnperturbedEnergyN**[2, 2]

Out[15]=

$$-\frac{5}{2}$$

## Energía

### Energía para estados $2^1 S$ y $2^3 S$

In[16]:= **UnperturbedEnergy2** + **FirstOrderCorrection20**

Out[16]=

$$-\frac{5}{2} + \left(-\frac{1296}{625} \pm \frac{32}{729}\right)$$

## Energía para estados $2^1P$ y $2^3P$

In[17]:= **UnperturbedEnergy2 + FirstOrderCorrection21**

Out[17]=

$$-\frac{5}{2} + \left( \frac{2456}{625\sqrt{3}} \pm \frac{224}{6561} \right)$$