

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

## Funciones radiales

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

## Integral de intercambio

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


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


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


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

```

## Integrales para n = 2 y l = 1

```
In[*]:= J20 = CoulombIntegral[r, ρ, 2, 2, 0]
Out[*]=

$$\frac{34}{81}$$

In[*]:= K20 = ExchangeIntegral[r, ρ, 2, 2, 0]
Out[*]=

$$\frac{32}{729}$$

```

## Integrales para n = 2 y l = 2

```
In[*]:= J21 = CoulombIntegral[r, ρ, 2, 2, 1]
Out[*]=

$$\frac{118}{243}$$

In[*]:= K21 = ExchangeIntegral[r, ρ, 2, 2, 1]
Out[*]=

$$\frac{224}{6561}$$

```

## Energía a primer orden de aproximación

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

`In[*]:= FirstOrderCorrectionNL[J_, K_] := J ± K;`

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

`Out[*]=`

$$\frac{34}{81} \pm \frac{32}{729}$$

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

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

`Out[*]=`

$$\frac{118}{243} \pm \frac{224}{6561}$$

## Energía imperturbada

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

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

`Out[*]=`

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

## Energía

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

`In[*]:= UnperturbedEnergy2 + FirstOrderCorrection20`

`Out[*]=`

$$-\frac{5}{2} + \left(\frac{34}{81} \pm \frac{32}{729}\right)$$

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

`In[*]:= UnperturbedEnergy2 + FirstOrderCorrection21`

`Out[*]=`

$$-\frac{5}{2} + \left(\frac{118}{243} \pm \frac{224}{6561}\right)$$