I Encuentro Nacional de Dinámica Cuántica en la Materia

Implementación de Métodos de Aprendizaje Automatizado en problemas colisionales

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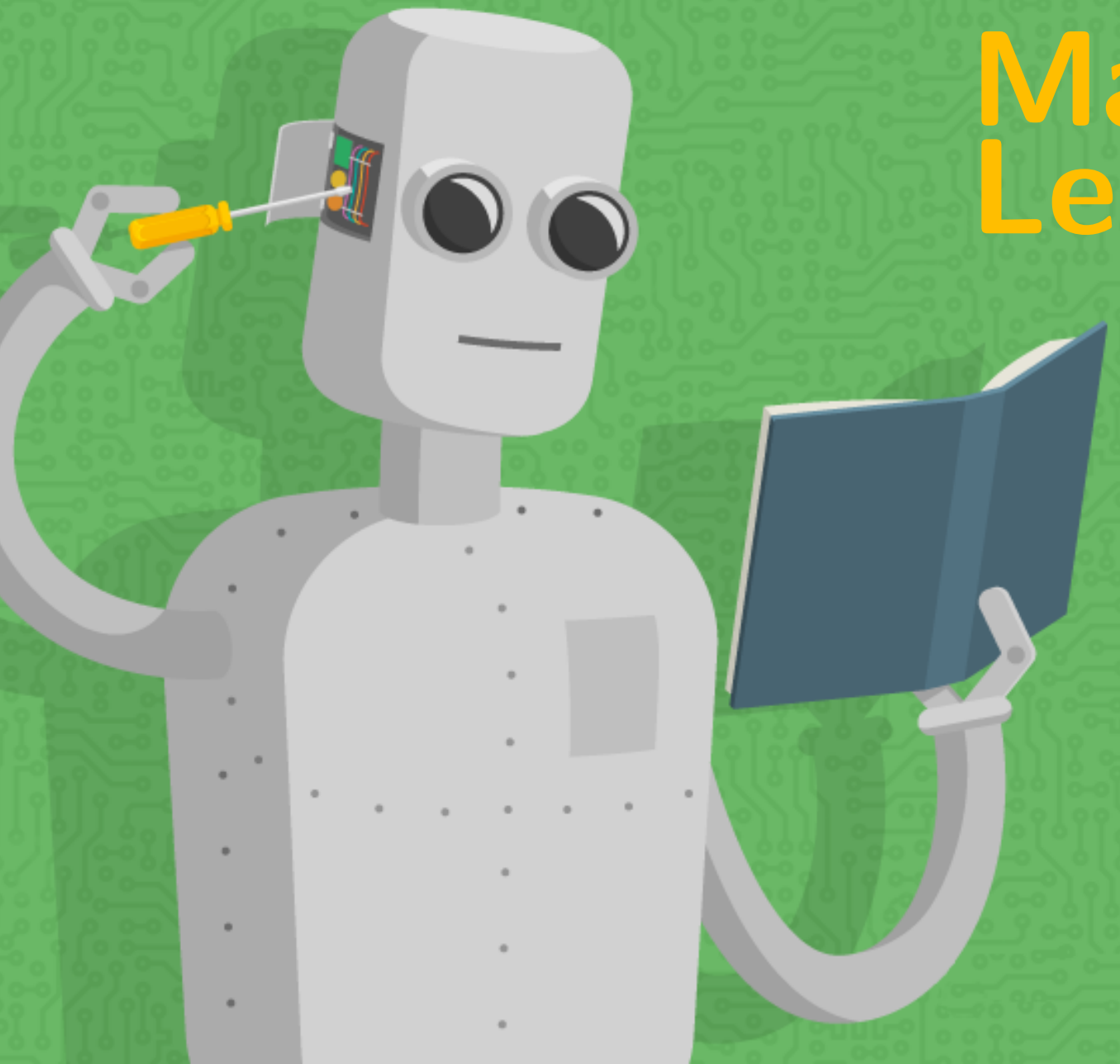
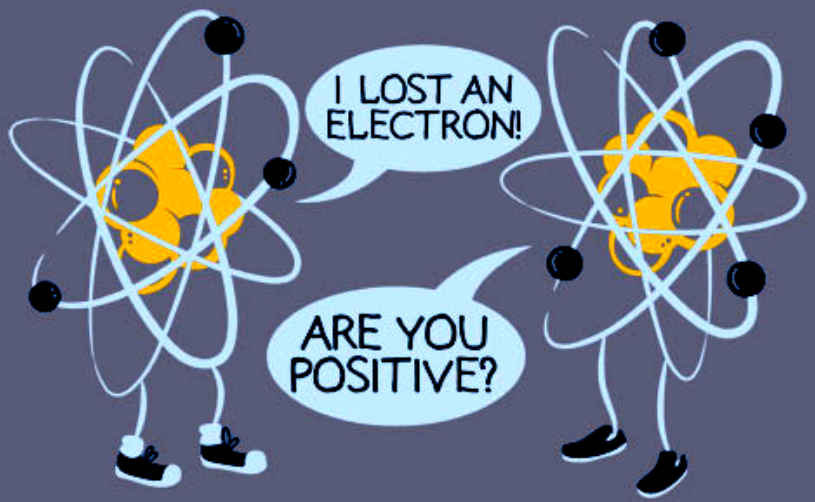
1 de Septiembre – Buenos Aires



Machine Learning


I LOST AN ELECTRON!
ARE YOU POSITIVE?

Método de Inversión Depurada (DIM)

$$T_{fi} = \left|\langle \psi_f | V | \psi_i \rangle\right|^2$$

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$$\left[-\frac{1}{2}\frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} - \frac{Z_{nl}(r)}{r} \right] P_{nl}(r) = E_{nl}\, P_{nl}(r)$$

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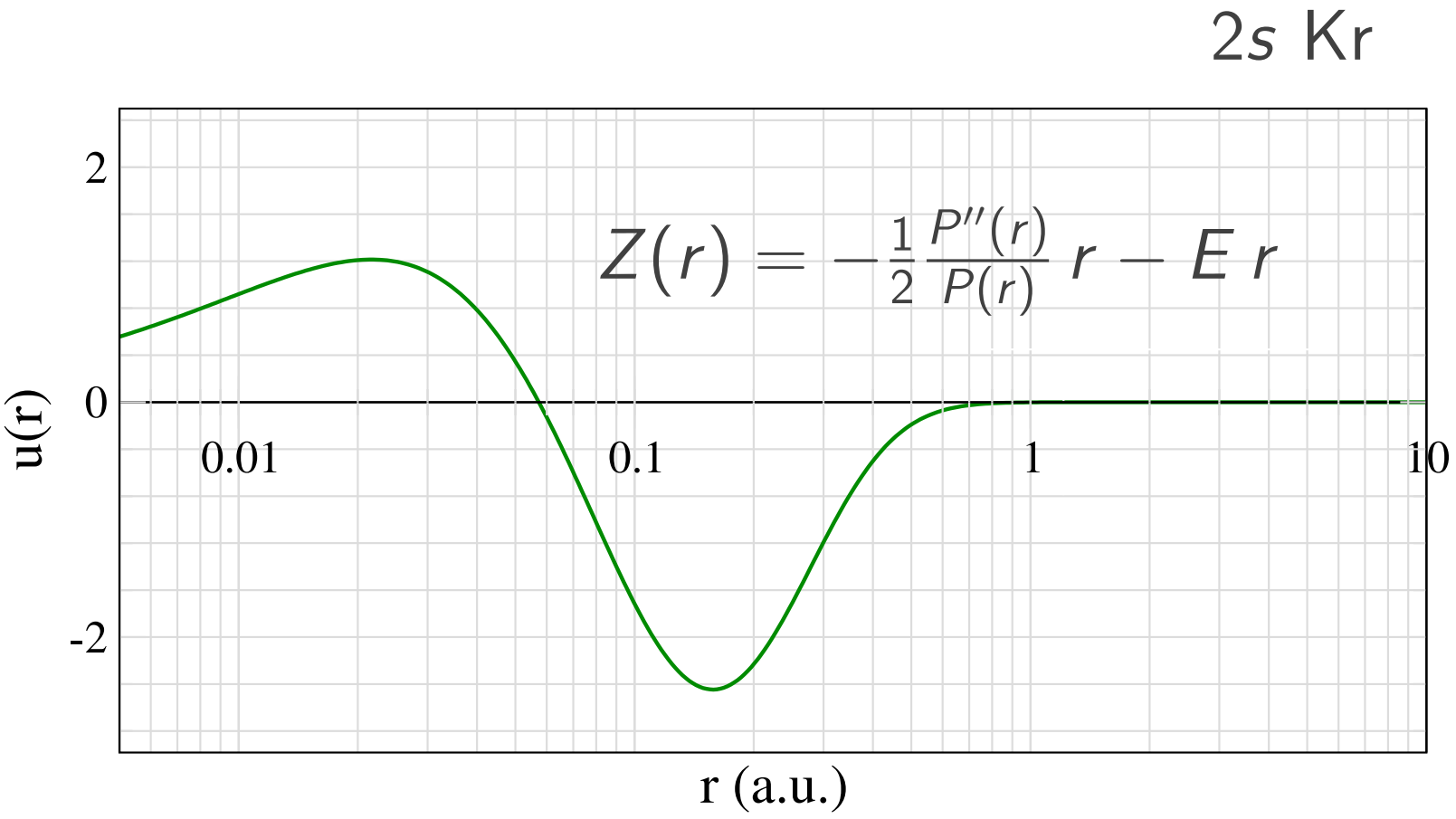
$$Z_{nl}(r) = -\frac{1}{2}\frac{P''_{nl}(r)}{P_{nl}(r)}\, r + \frac{l(l+1)}{2r} - E_{nl}\, r$$

Houston, we have a problem!



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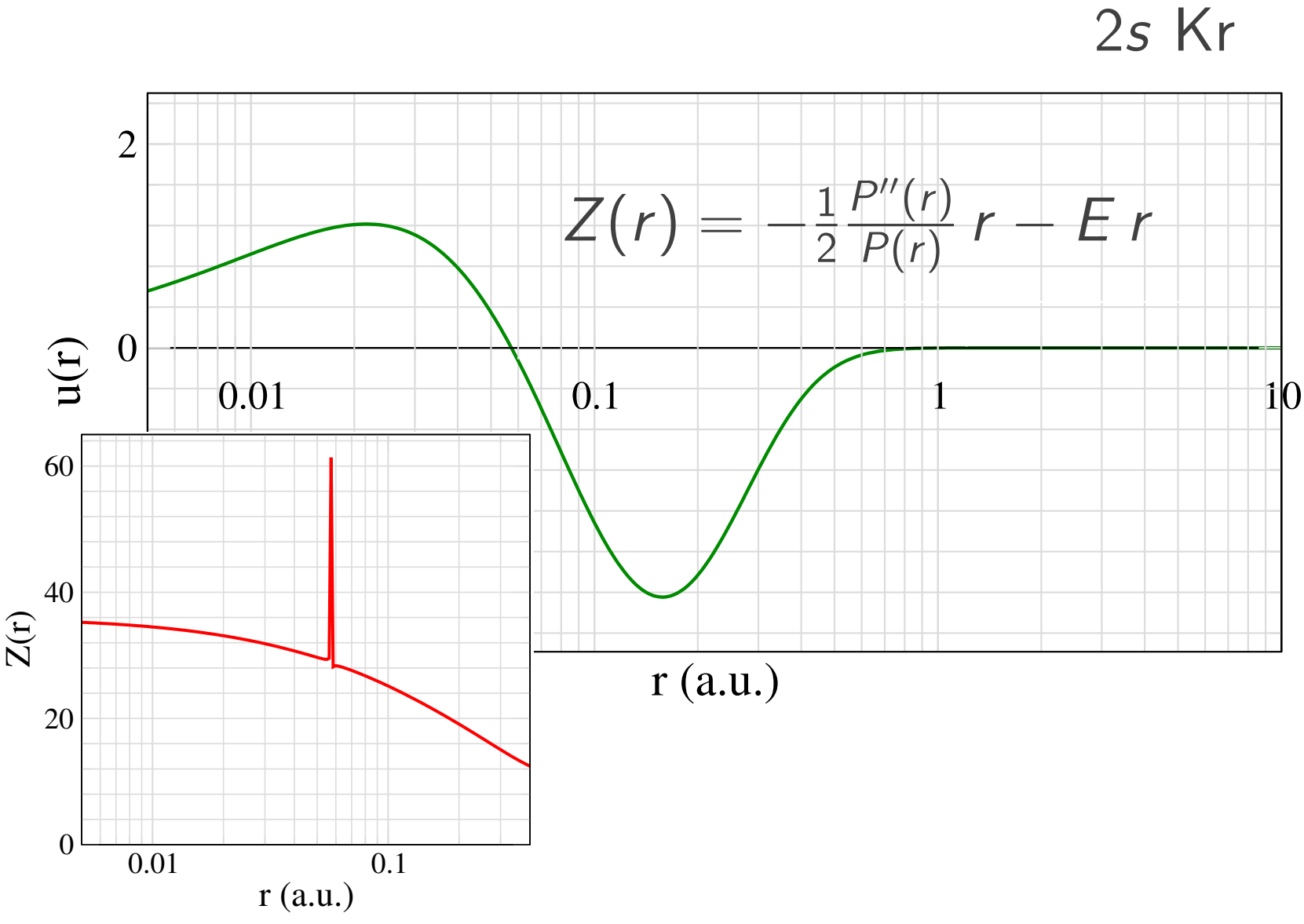

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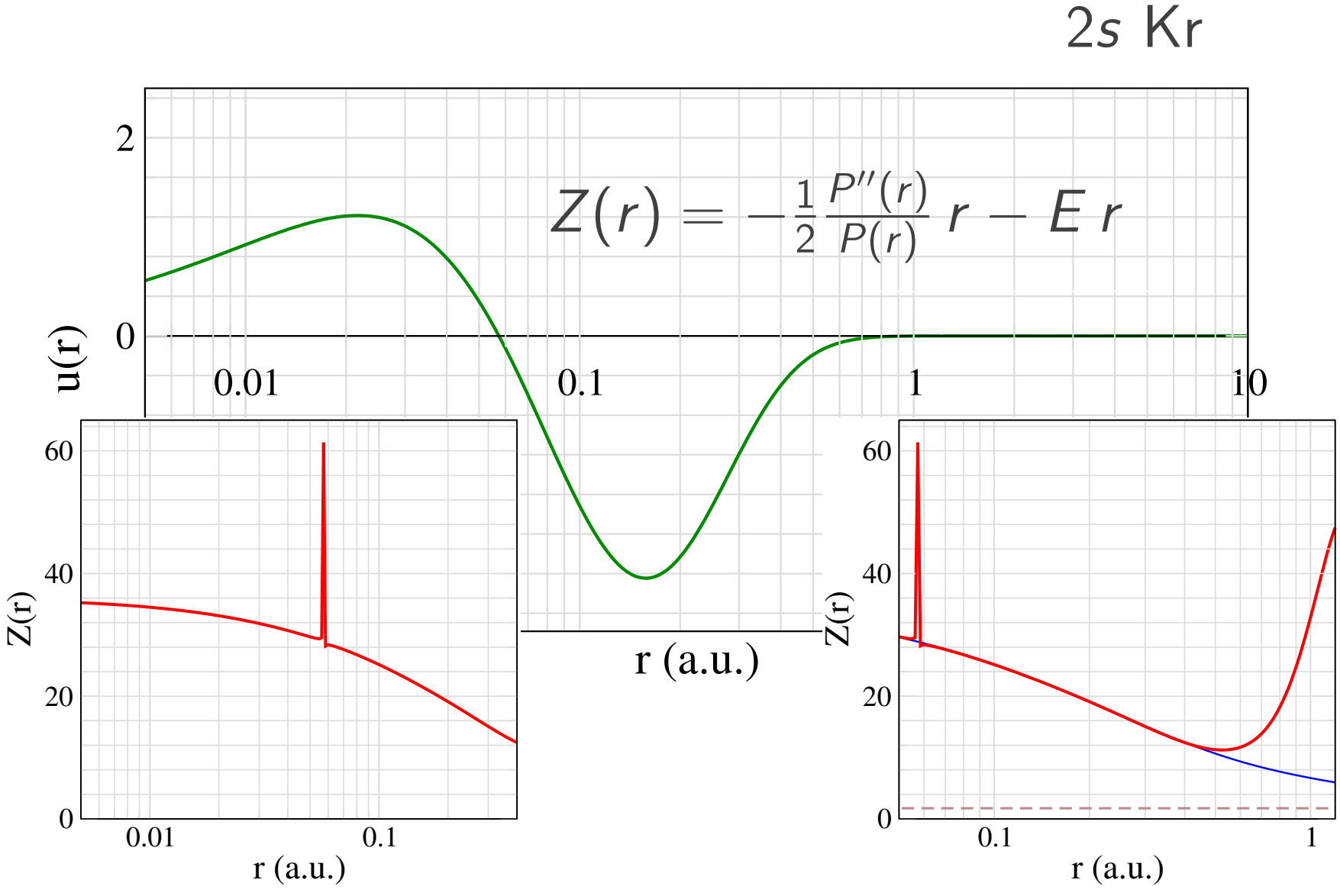
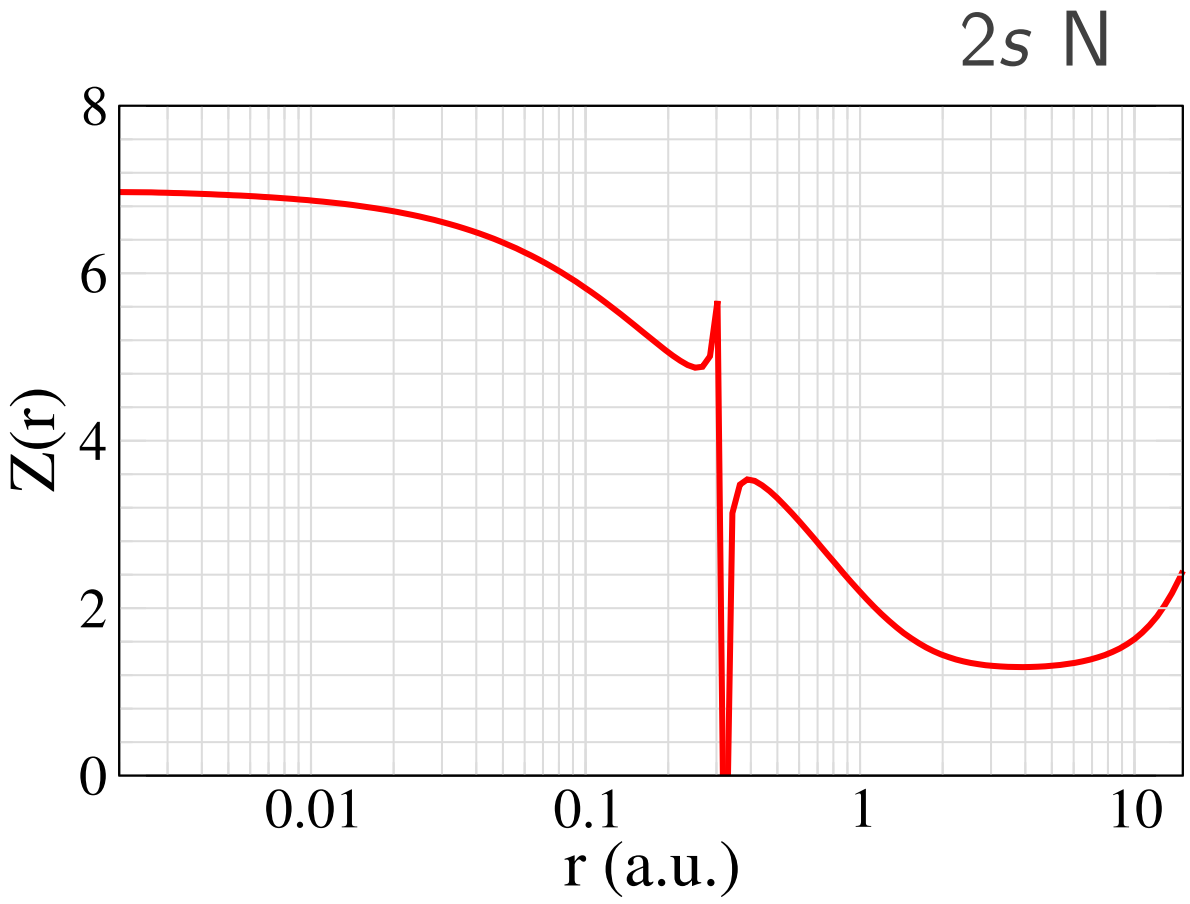
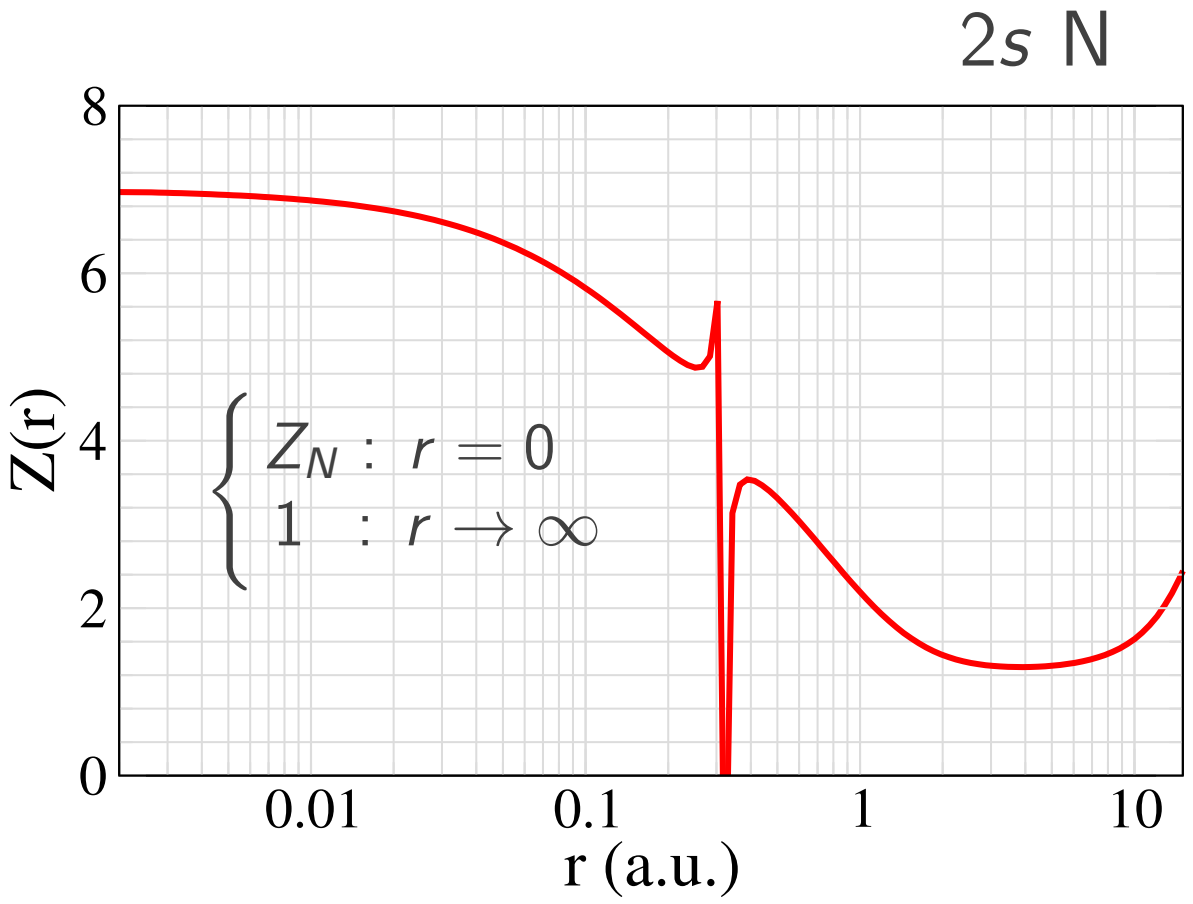


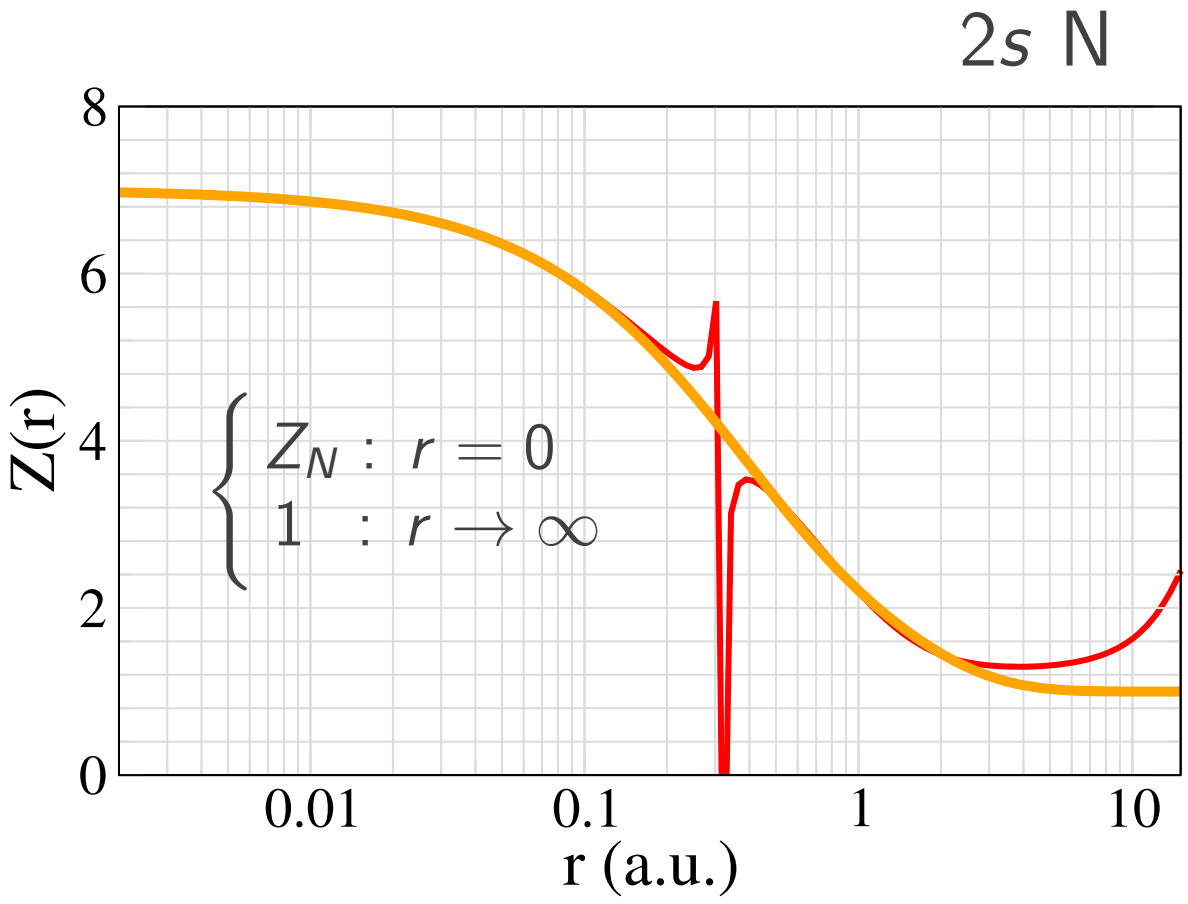
Depuración



Depuración

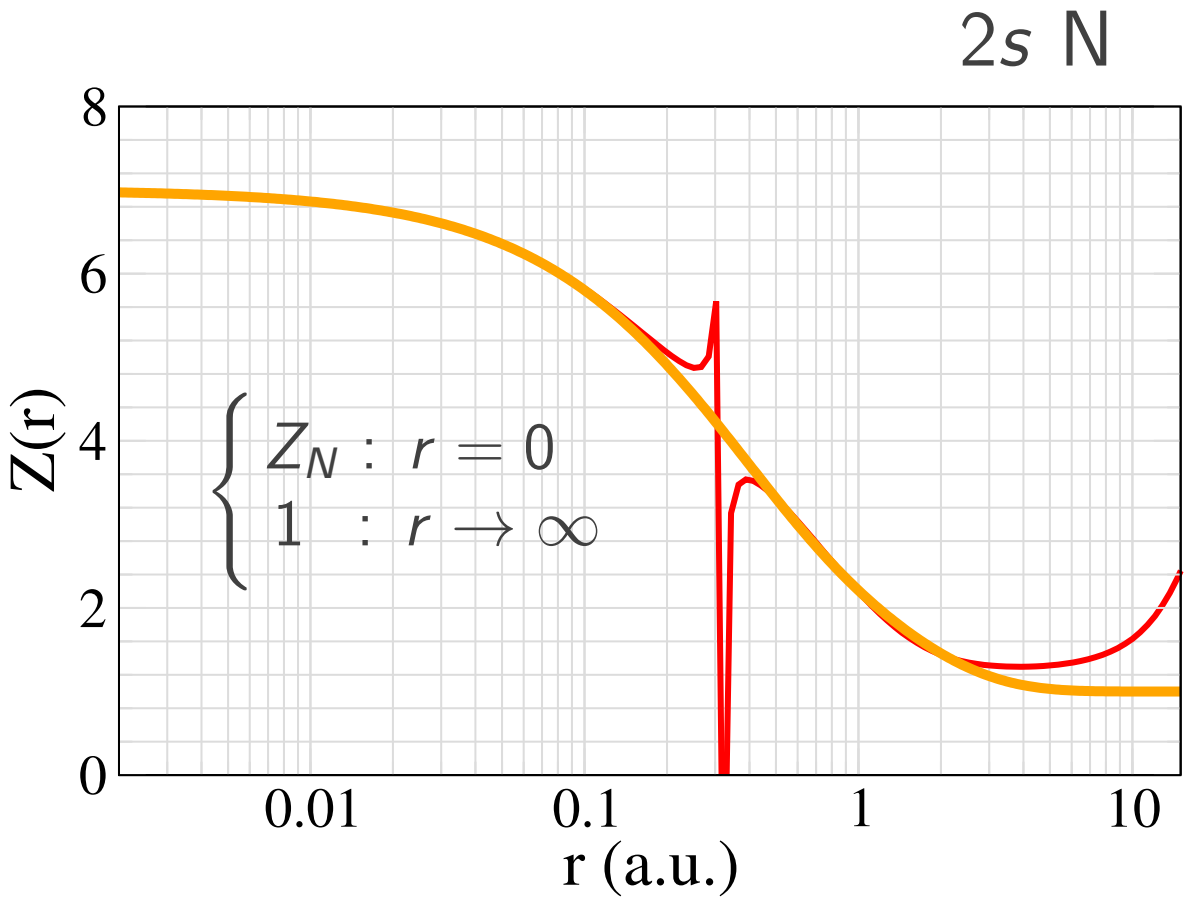

2s N
8
6
4
2
0
Z(r)
$\begin{cases} Z_N : r = 0 \\ 1 : r \to \infty \end{cases}$
0.01
0.1
1
10
r (a.u.)

Depuración



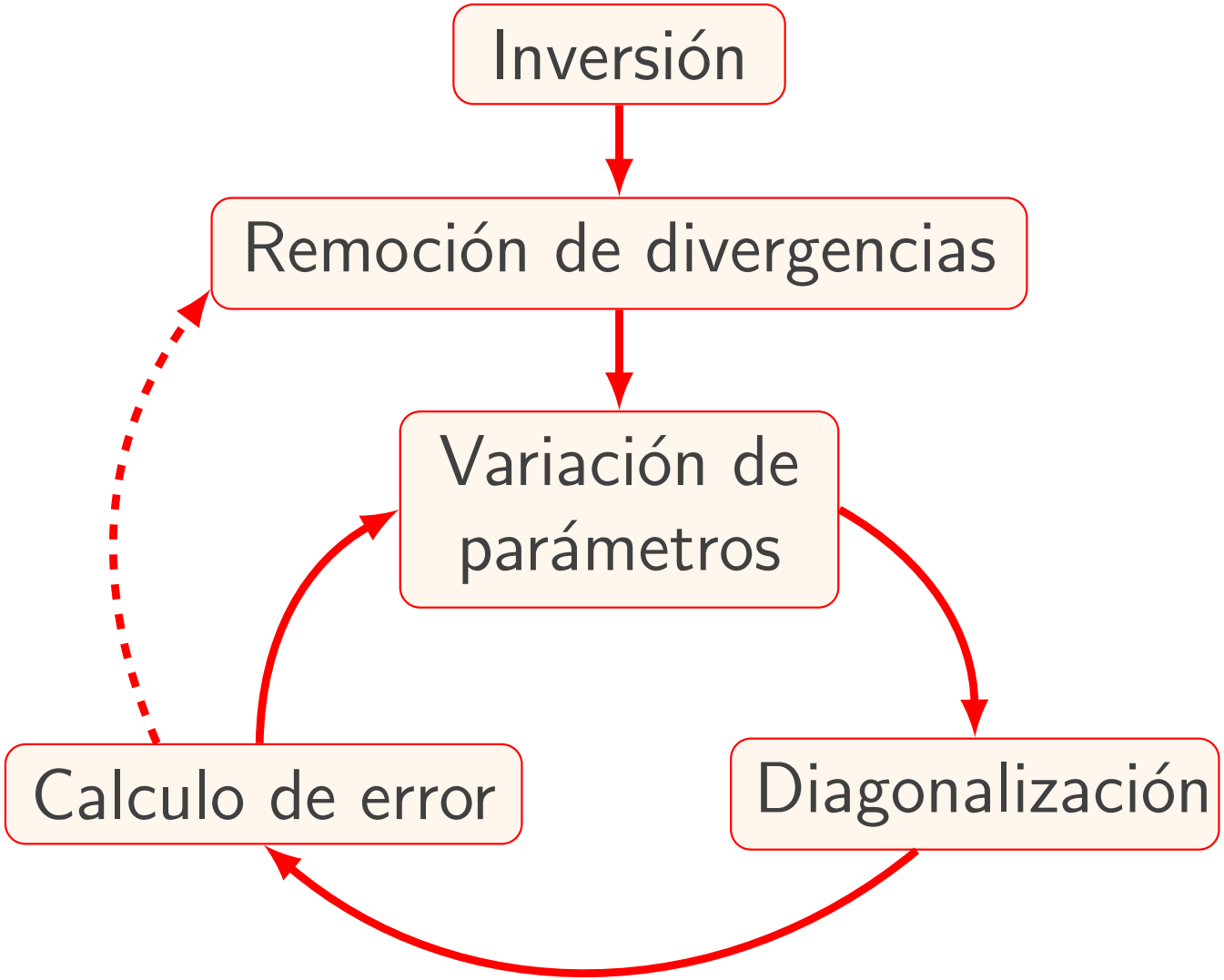
$$Z(r) = 1 + \sum_j \alpha_j e^{-\beta_j r}$$

Depuración

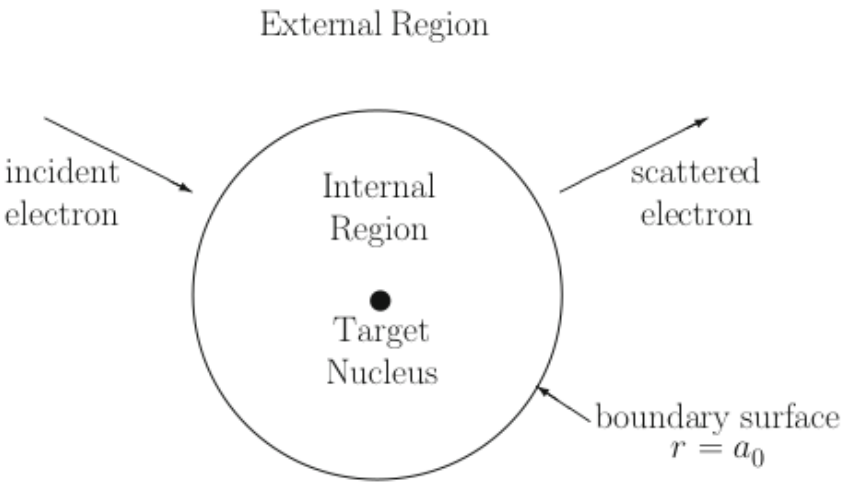


$$Z(r) = 1 + \sum_j \alpha_j e^{-\beta_j r}$$

Procedimiento



R–Matrix



Estructura del blanco

AUTOSTRUCTURE

↓

Región interna

RMATRXI

↓

Región externa

STGF

Descripción del blanco

$$\Phi_i(\mathbf{r}) = \sum_j c_{ji}\phi_j(\mathbf{r})$$

Configuration interaction

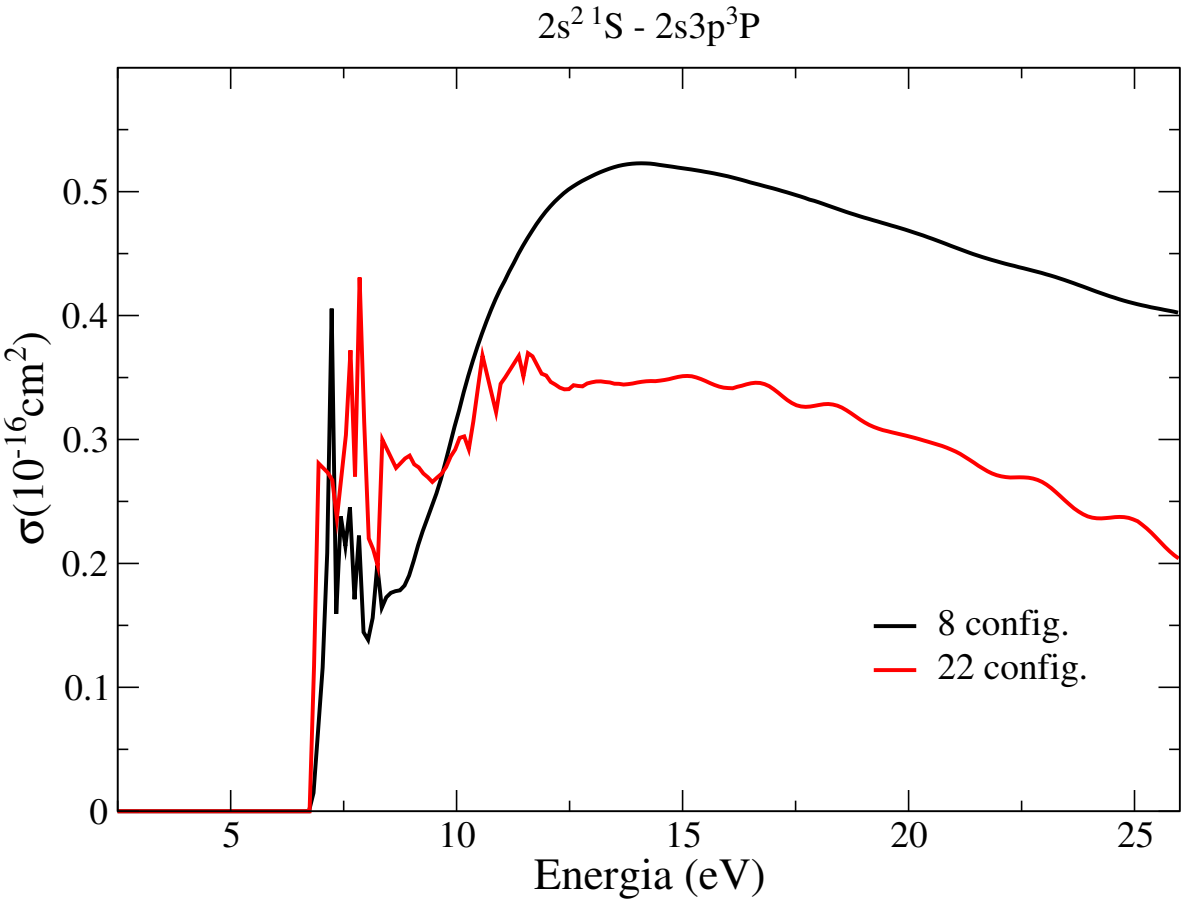
$$\left[\frac{1}{2}\frac{d^2}{dr^2} - \frac{l(l+1)}{2r^2} + V_{nl}^{\text{eff}}(\lambda_{nl}, r) + E_{nl}\right] P_{nl}(r) = 0$$

Thomas–Fermi–Dirac–Amaldi

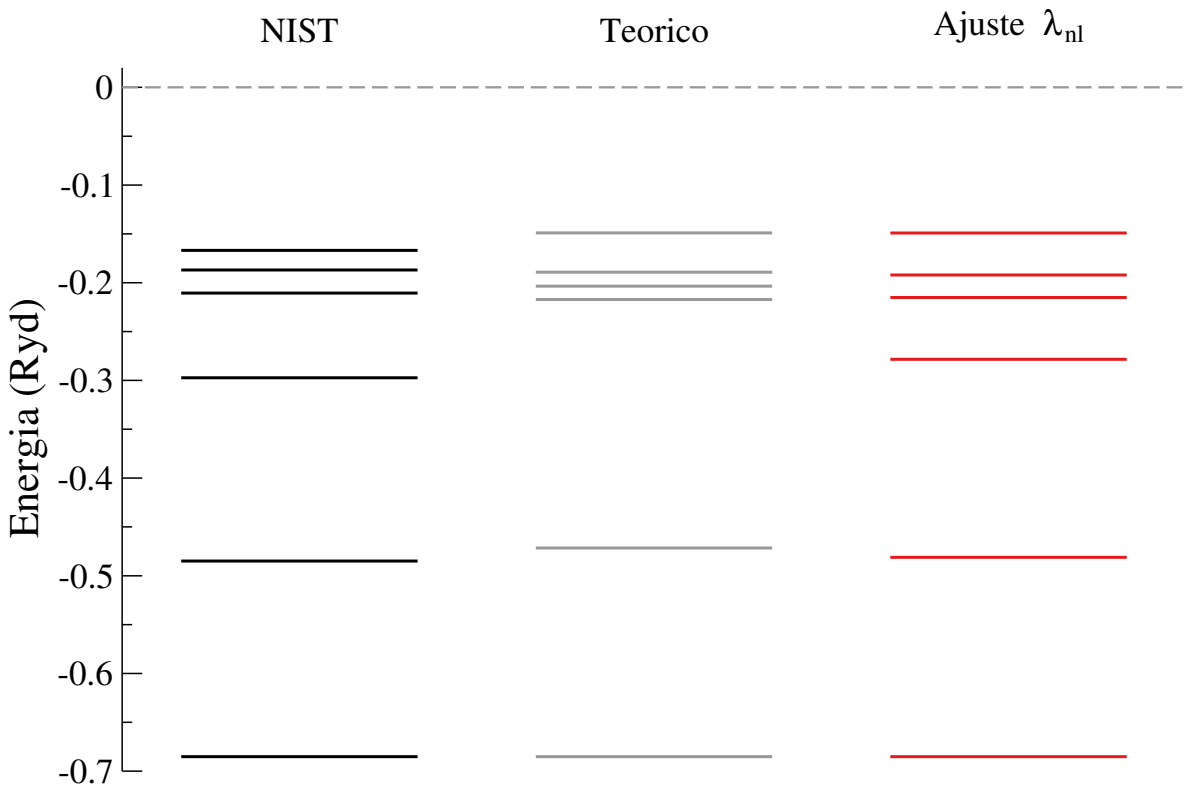
Slater-Type-Orbital de Burgess

Ejemplo: Berilio

$1s^2 2s^2$
$1s^2 2snl$
$1s^2 2p^2$
$1s^2 2pnl$



Ejemplo: Berilio



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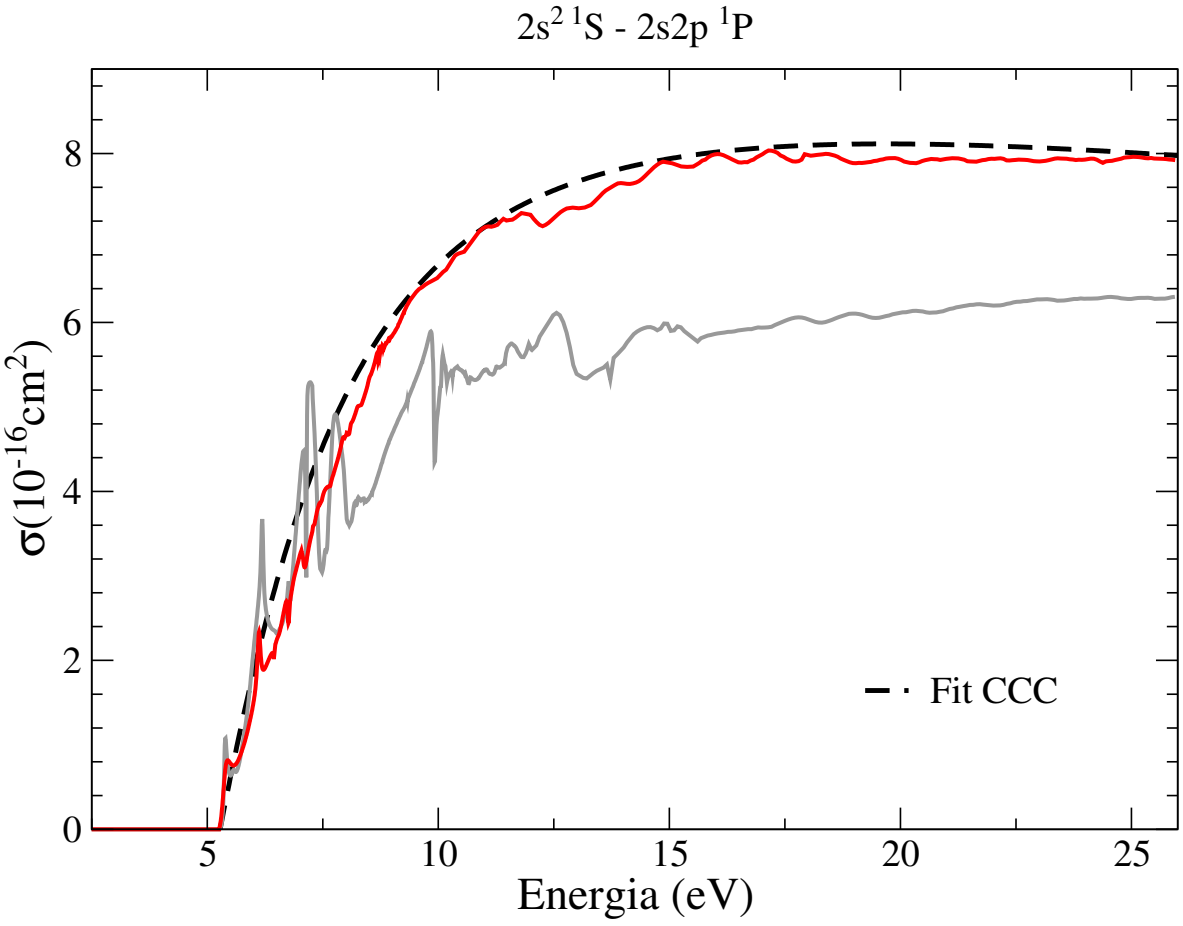
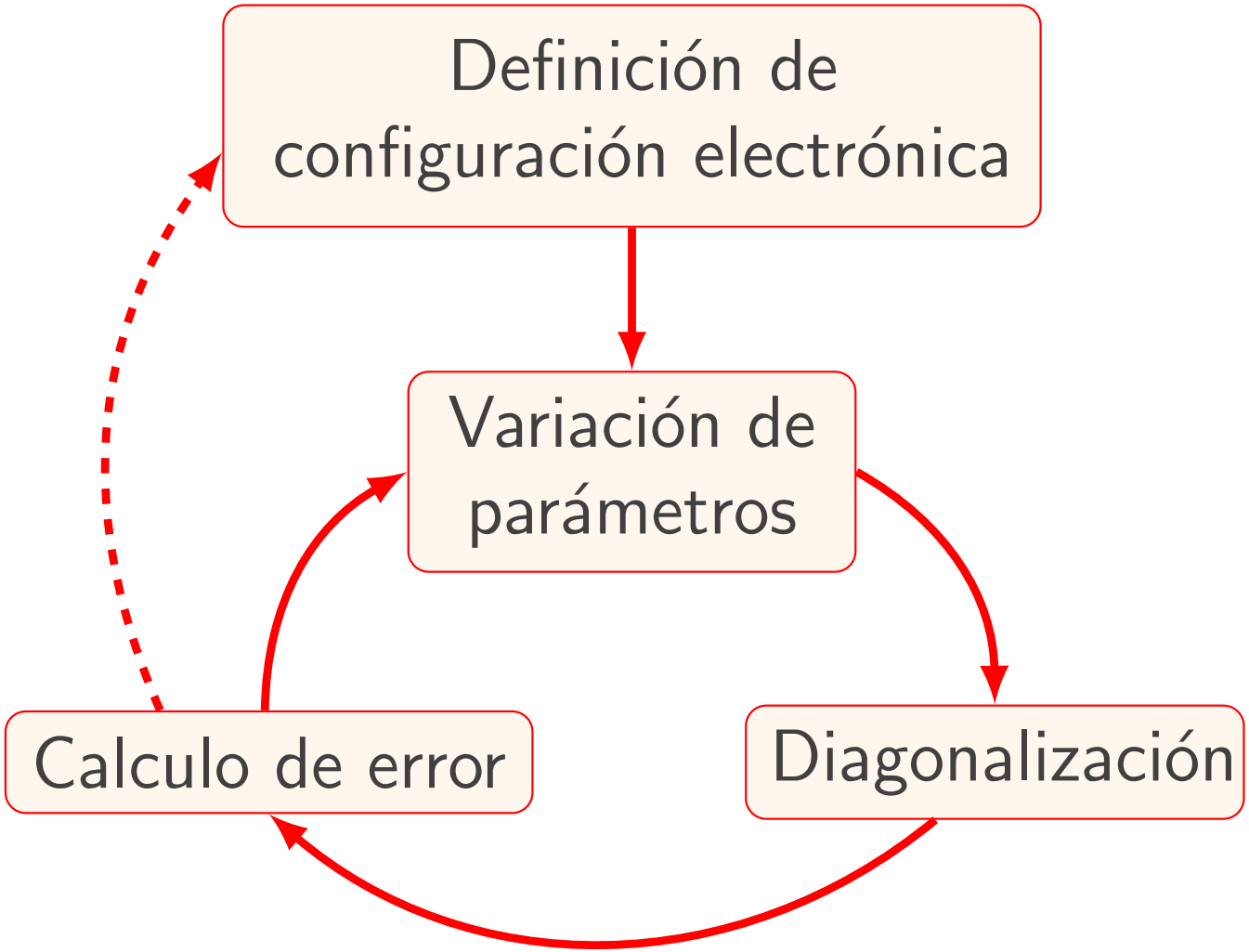


Procedimiento



Síntesis del problema

$$J = \sum_j \left| \frac{E_j^{\text{calc}}(\boldsymbol{\xi}) - E_j^{\text{teo}}}{E_j^{\text{teo}}} \right|$$

DIM: $\boldsymbol{\xi} = \{\boldsymbol{\alpha}, \boldsymbol{\beta}\}$

R–Matrix: $\boldsymbol{\xi} = \{\mathit{Configuraciones}, \boldsymbol{\lambda}\}$

Procesos Gaussianos

Resultados DIM

Resultados R–Matrix