

# Implementación de Métodos de Aprendizaje Automatizado en problemas colisionales

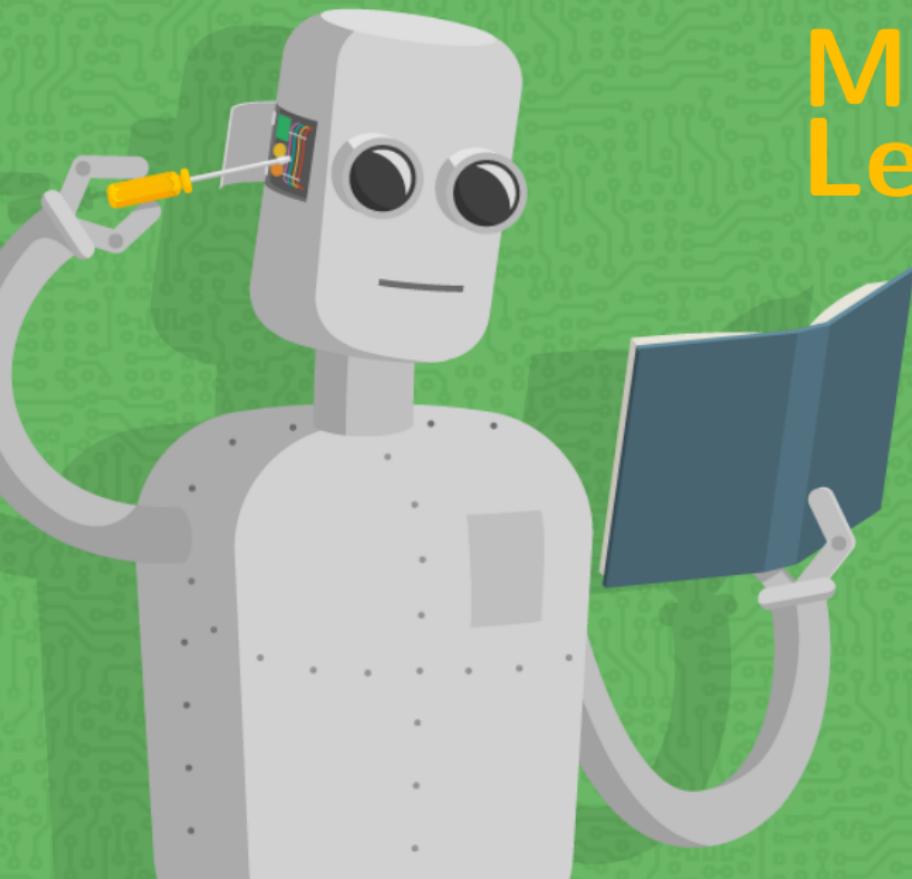
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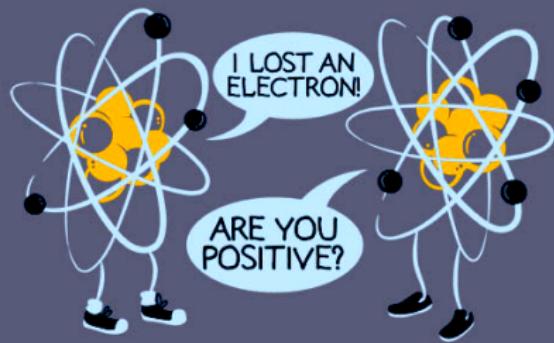
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# Machine Learning



# Método de Inversión Depurada (DIM)

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

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¿Cómo  
conocemos V?

# Método de Inversión Depurada (DIM)

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

¿Cómo  
conocemos  $V$ ?

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

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¿Cómo  
conocemos  $V$ ?

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

# Método de Inversión Depurada (DIM)

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

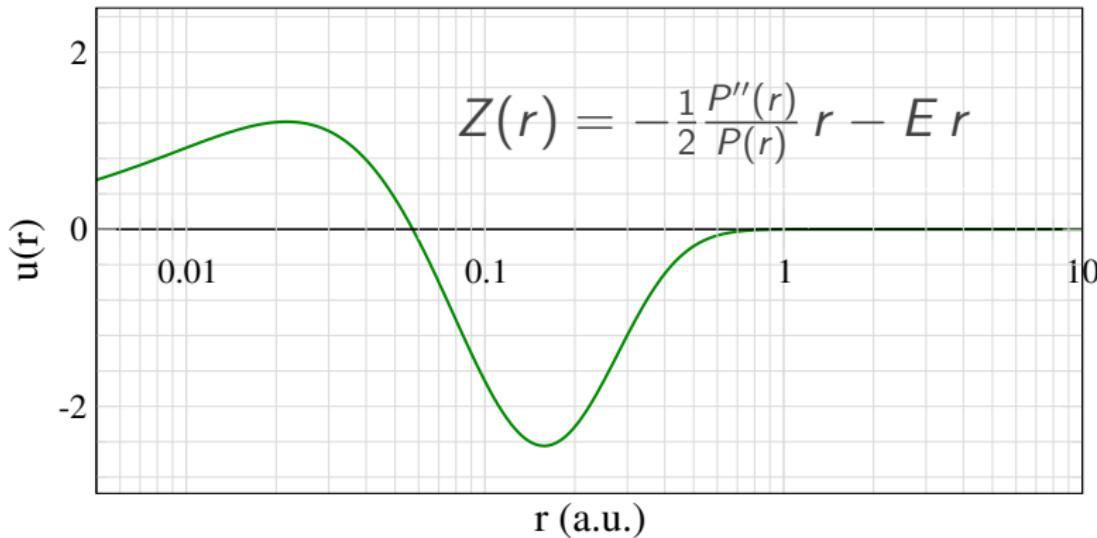
¿Cómo  
conocemos  $V$ ?

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

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

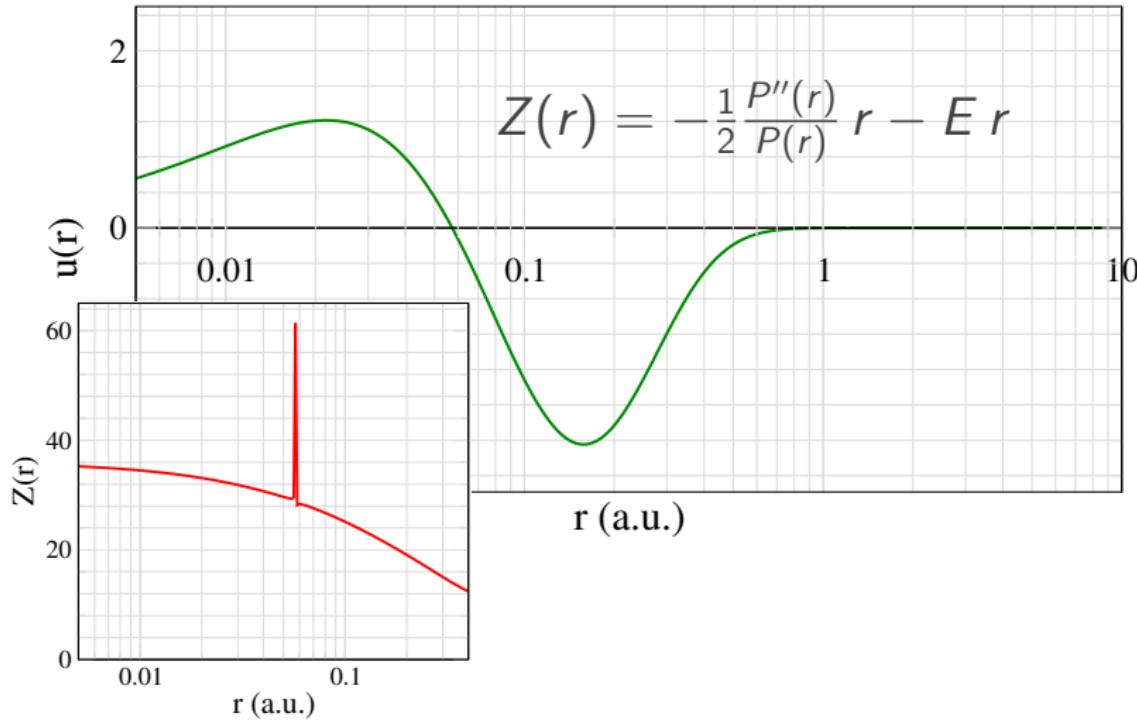
# Houston, we have a problem!

2s Kr



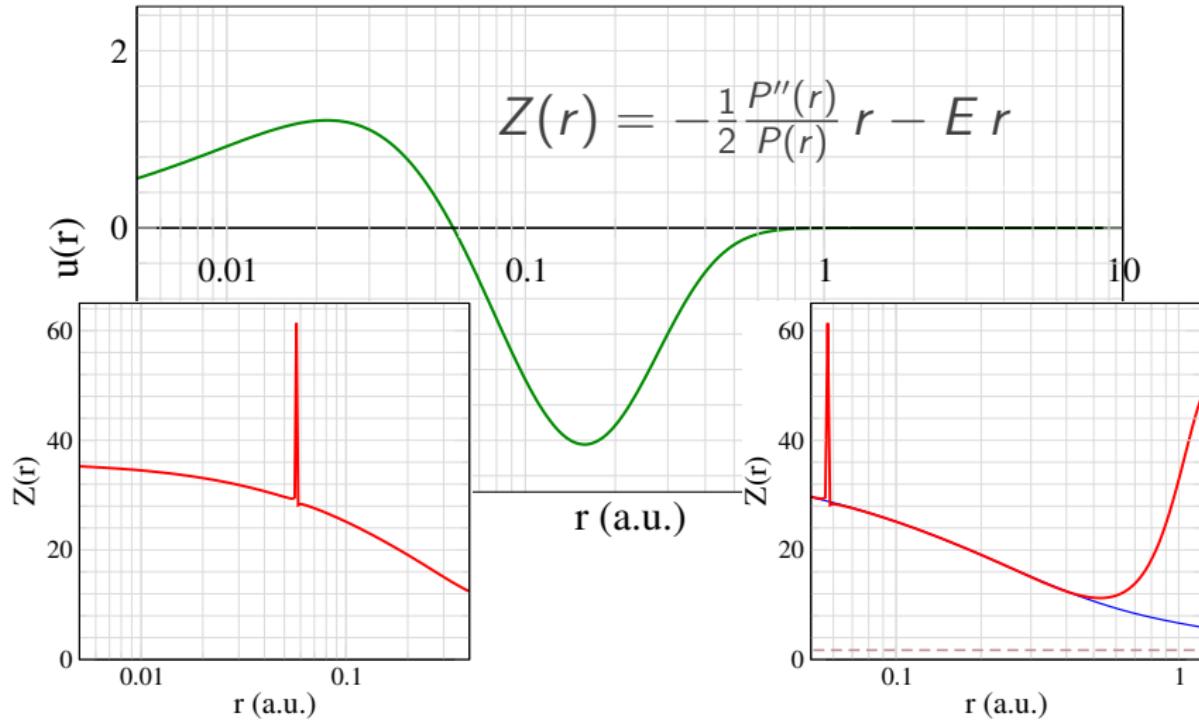
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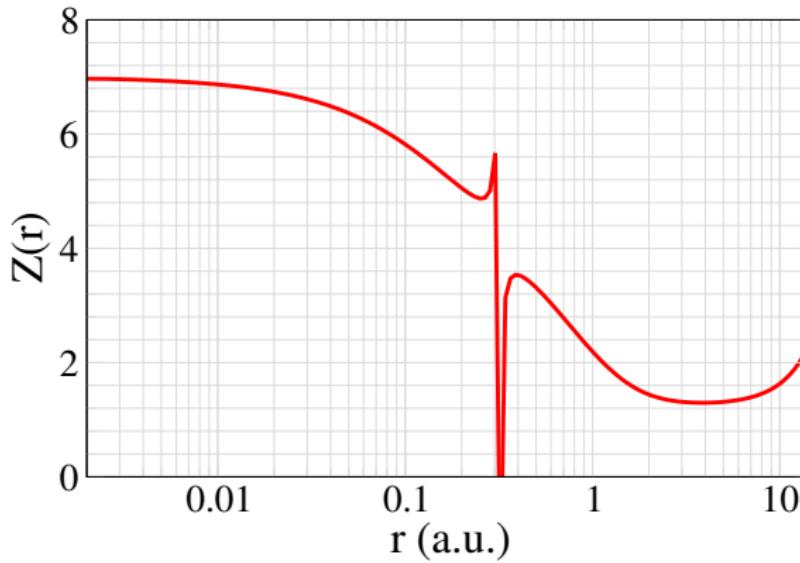
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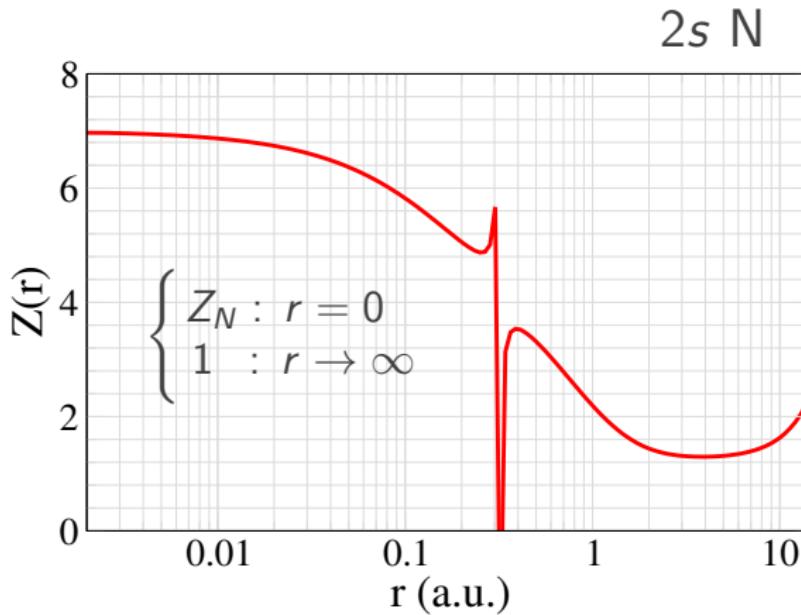


# Depuración

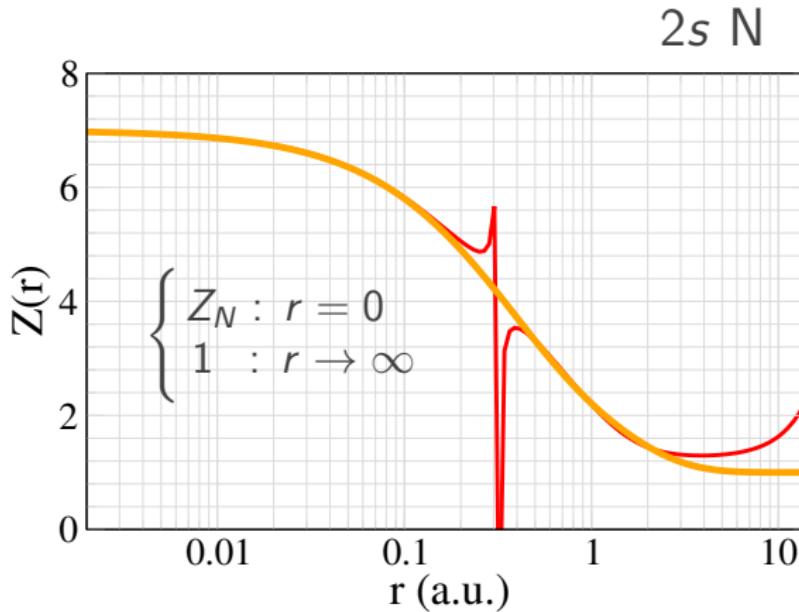
$2s\ N$



# Depuración



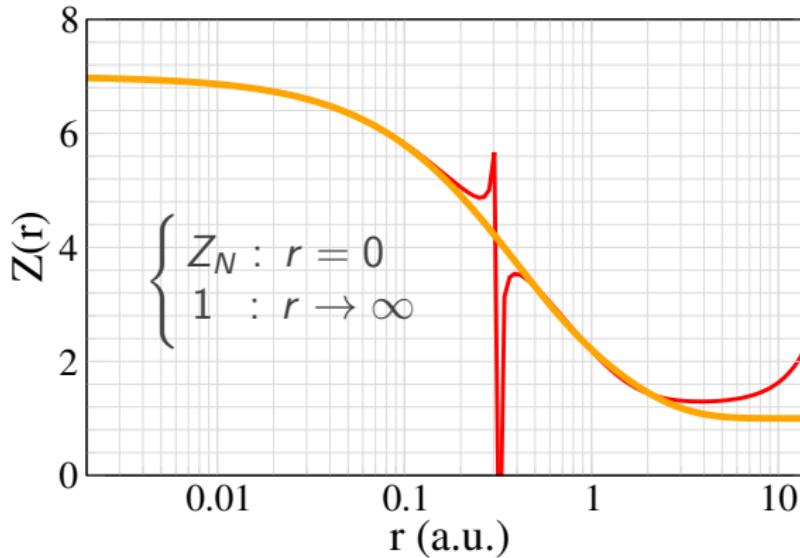
# Depuración



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

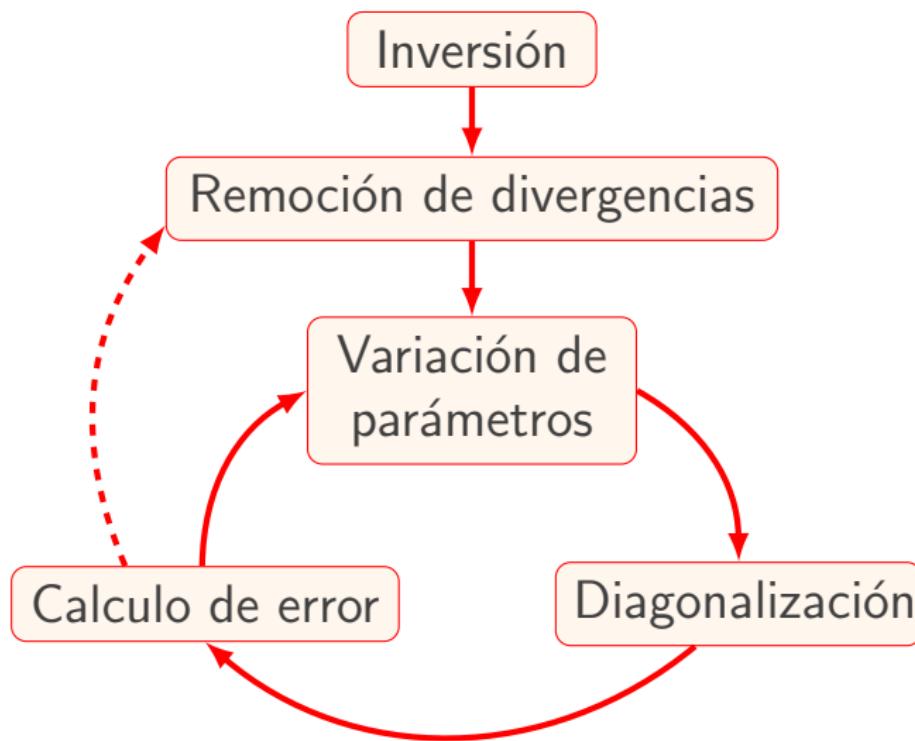
# Depuración

$2s\ N$

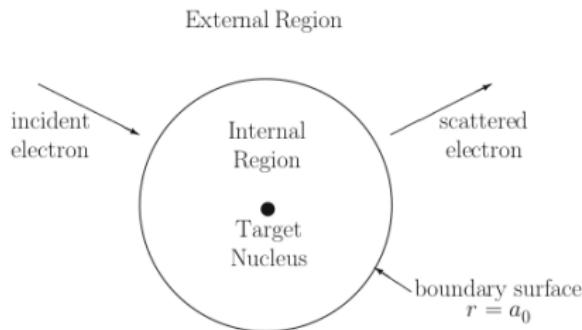


$$Z(r) = 1 + \sum_j \alpha_j e^{-\beta_j r}$$

# Procedimiento



# R-Matrix



Estructura del blanco

AUTOSTRUCTURE



Región interna

RMATRXI



Región externa

STGF

# Descripción del blanco

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

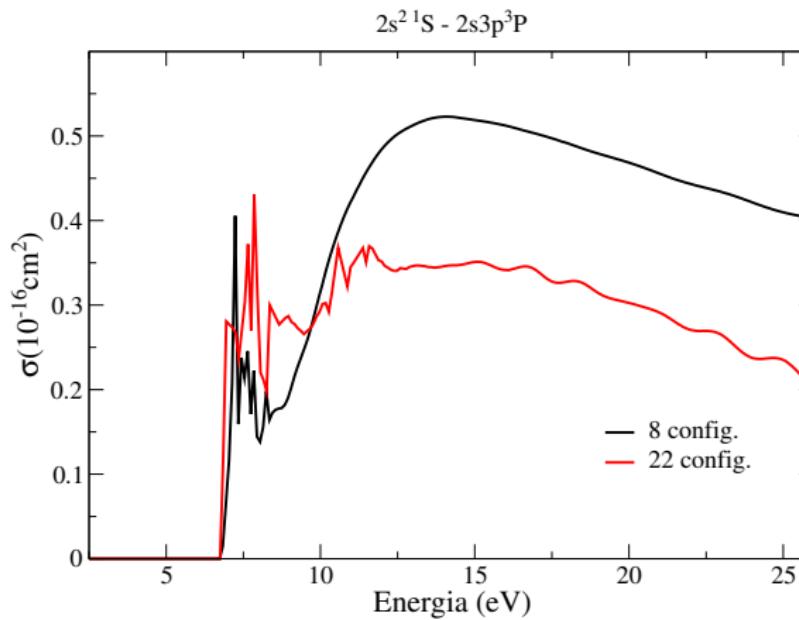
Configuration  
interaction

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

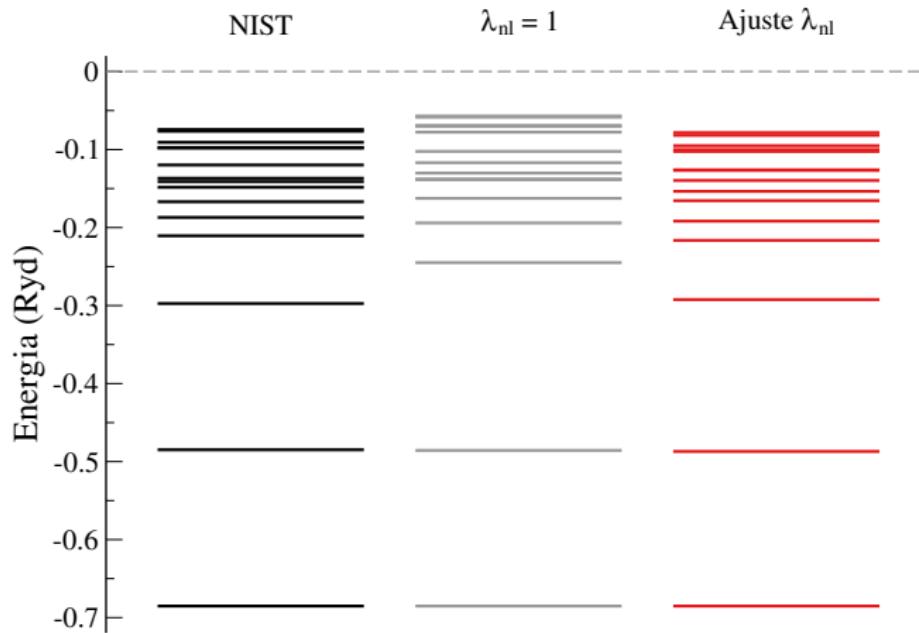
Thomas–Fermi–Dirac–Amaldi  
Slater-Type-Orbital de Burgess

# Ejemplo: Berilio

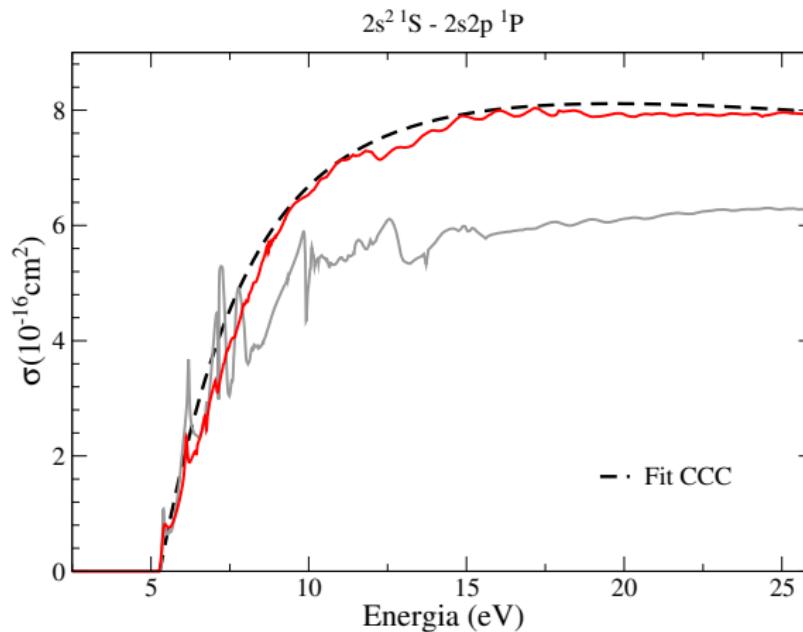
$1s^2 2s^2$   
 $1s^2 2snl$   
 $1s^2 2p^2$   
 $1s^2 2pnl$



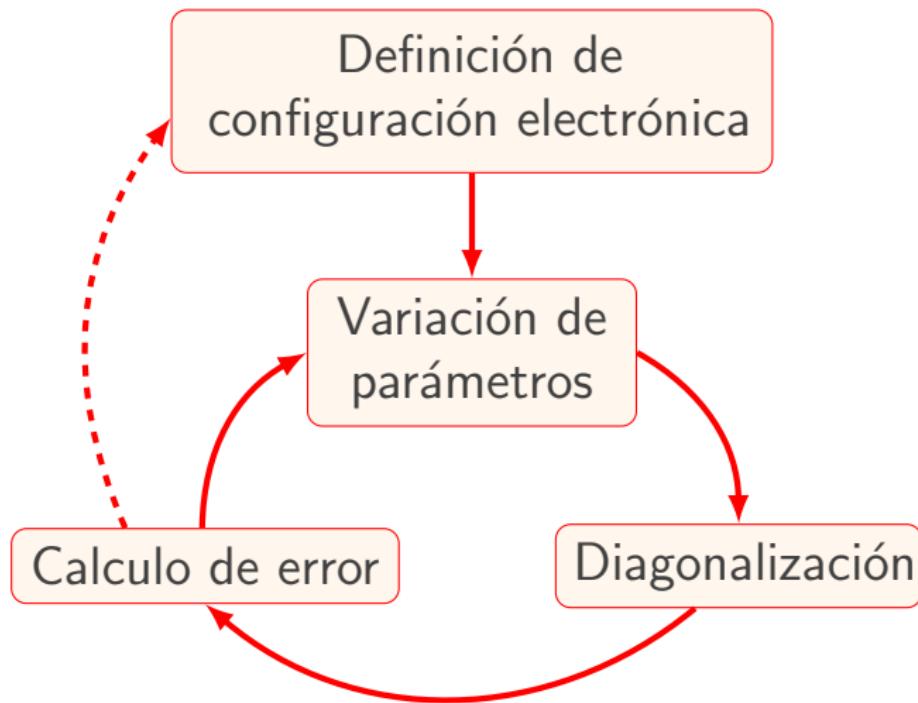
# Ejemplo: Berilio



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# Procedimiento



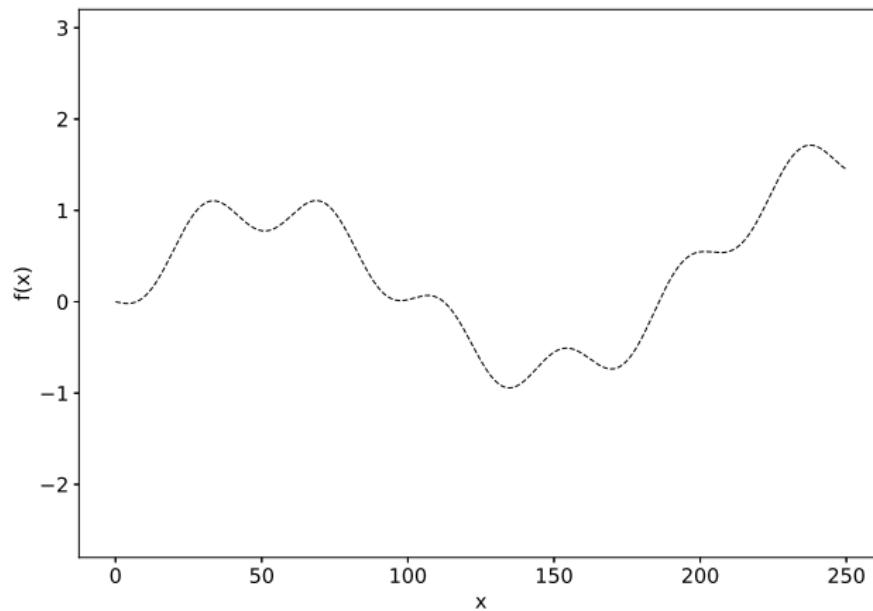
# Síntesis del problema

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

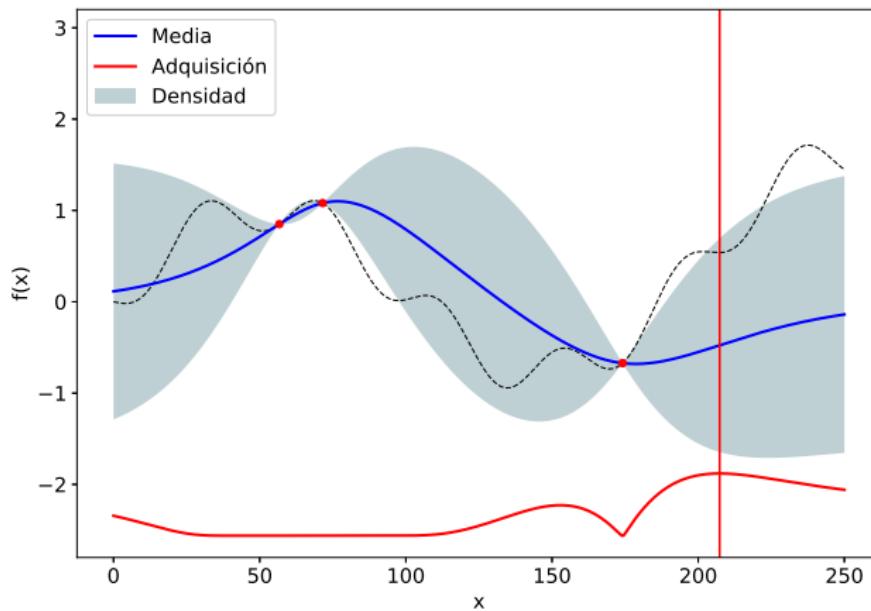
DIM:  $\xi = \{\alpha, \beta\}$

R-Matrix:  $\xi = \{Configuraciones, \lambda\}$

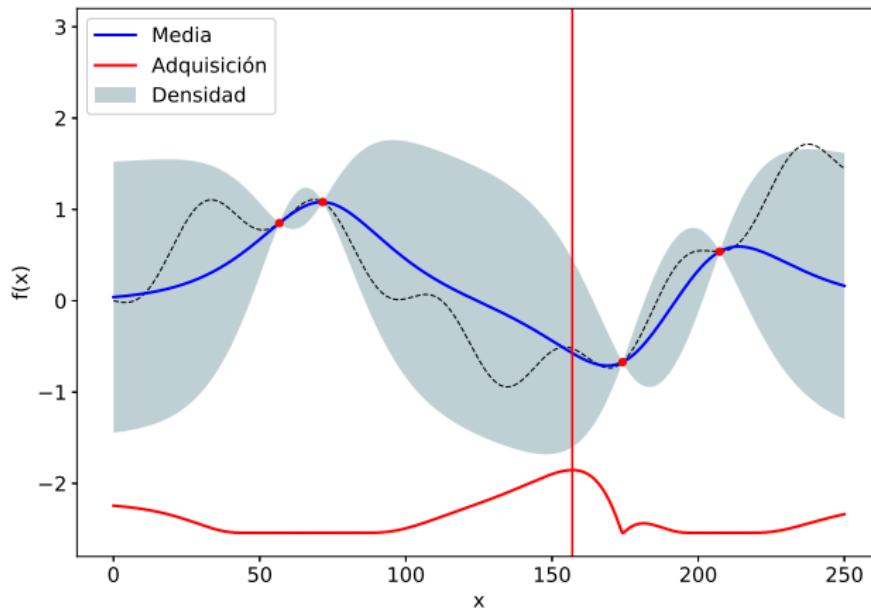
# Procesos Gaussianos



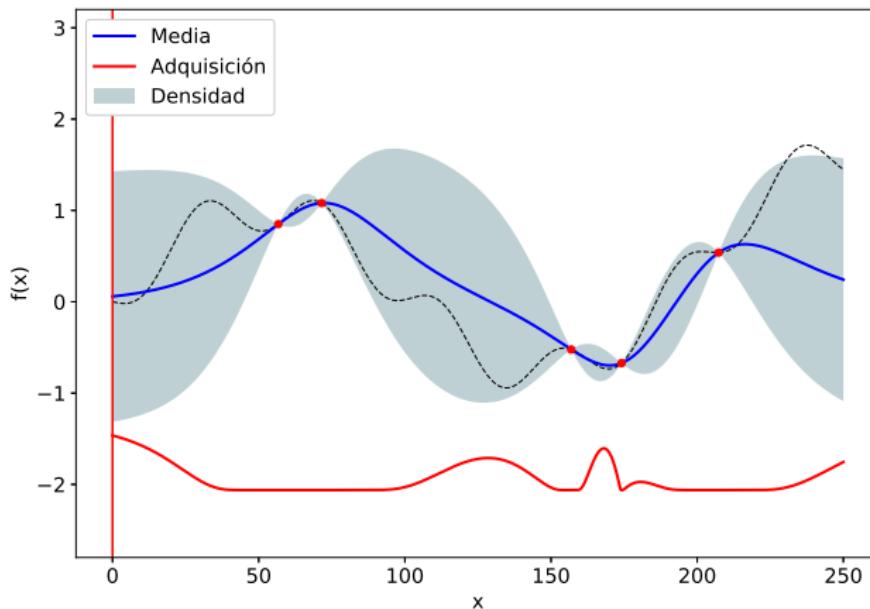
# Procesos Gaussianos



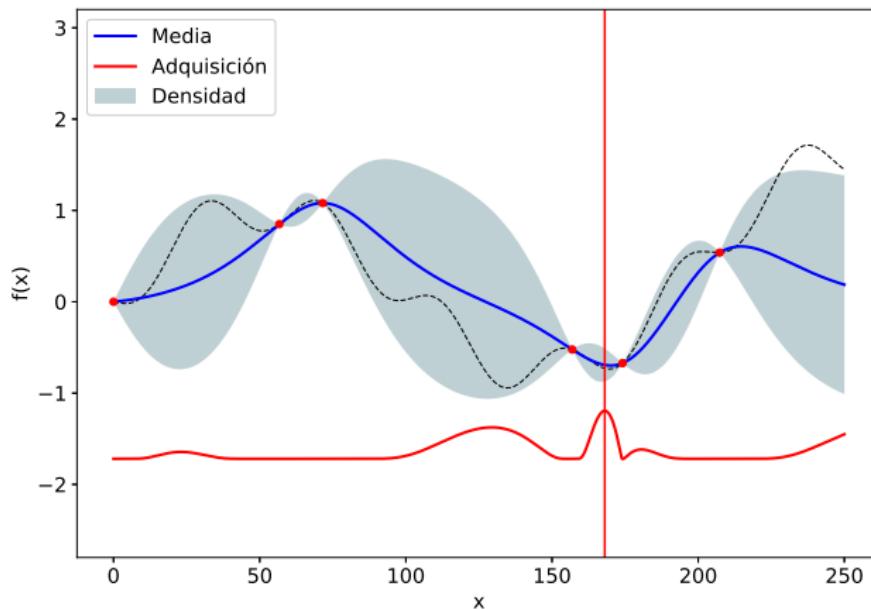
# Procesos Gaussianos



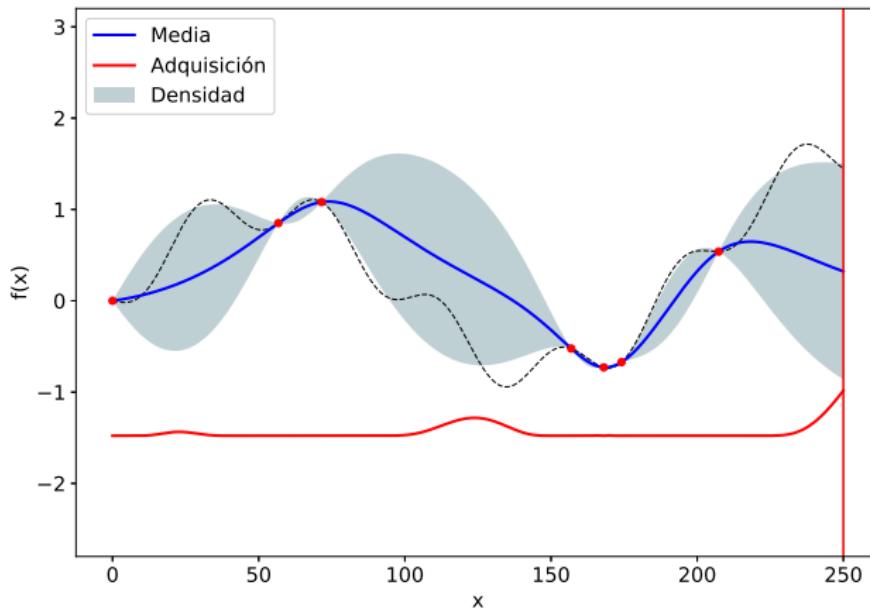
# Procesos Gaussianos



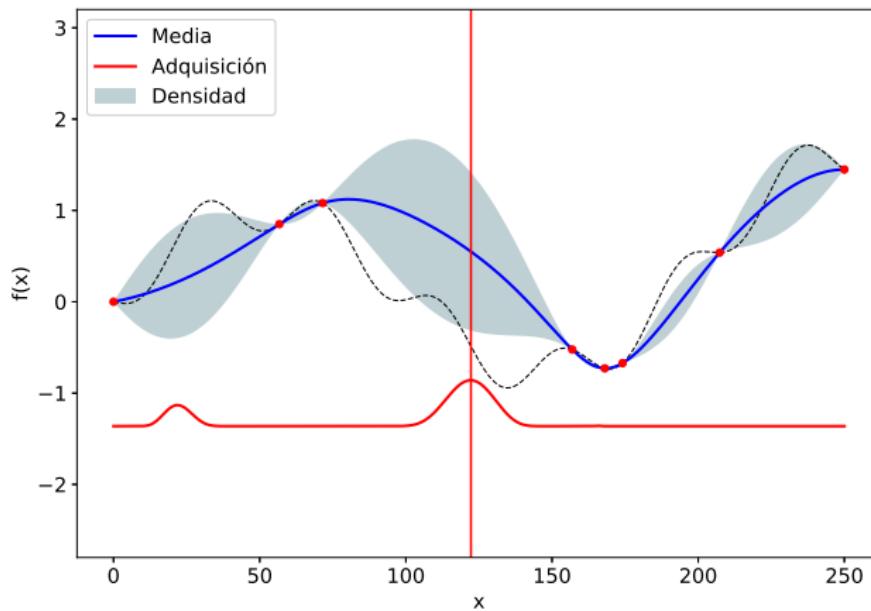
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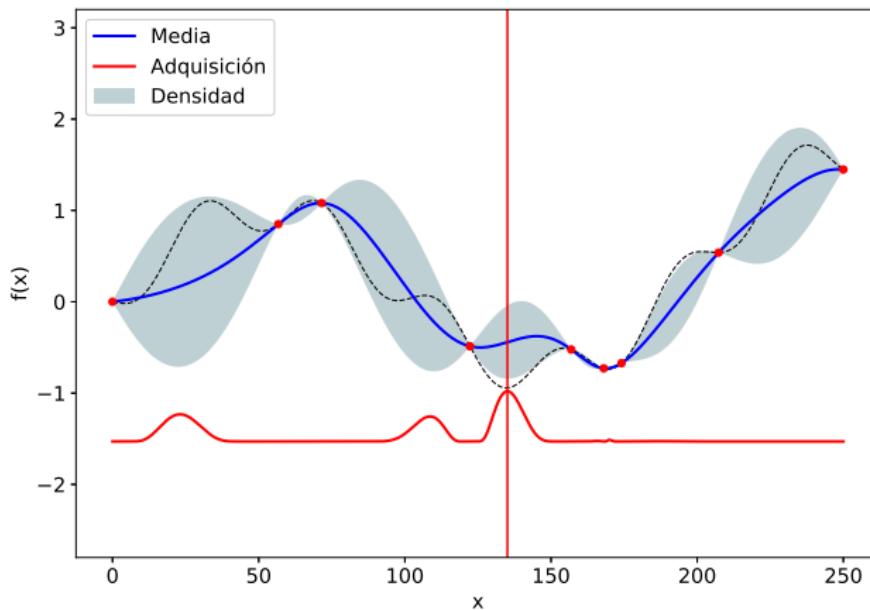
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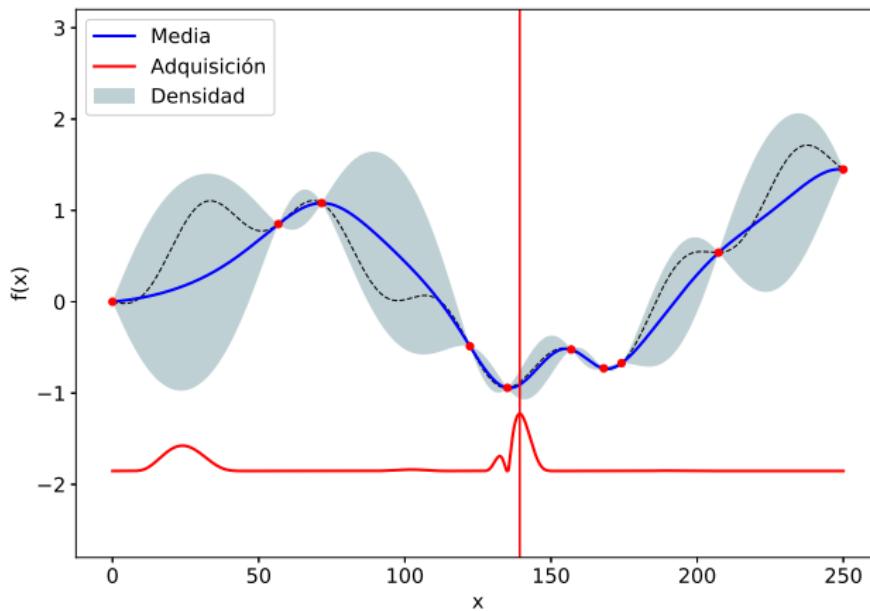
# Procesos Gaussianos



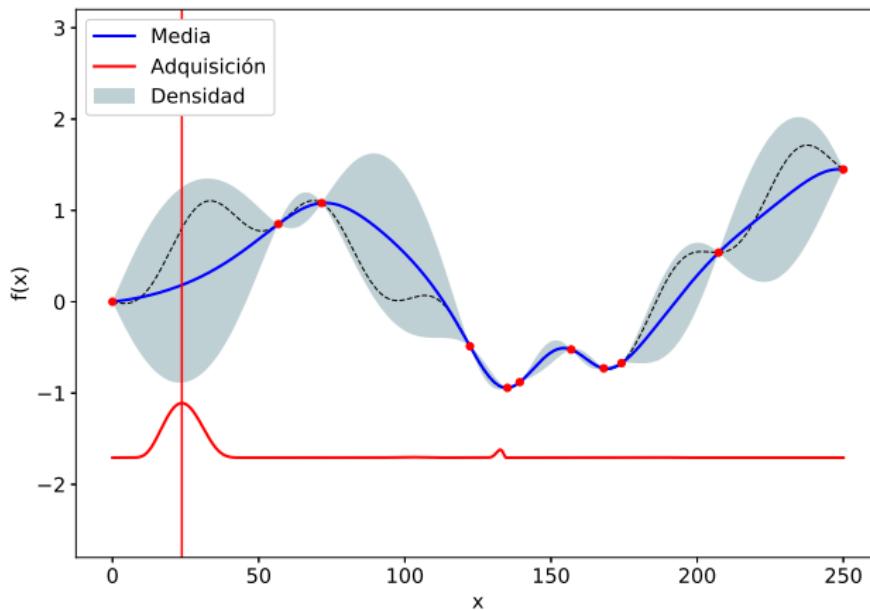
# Procesos Gaussianos



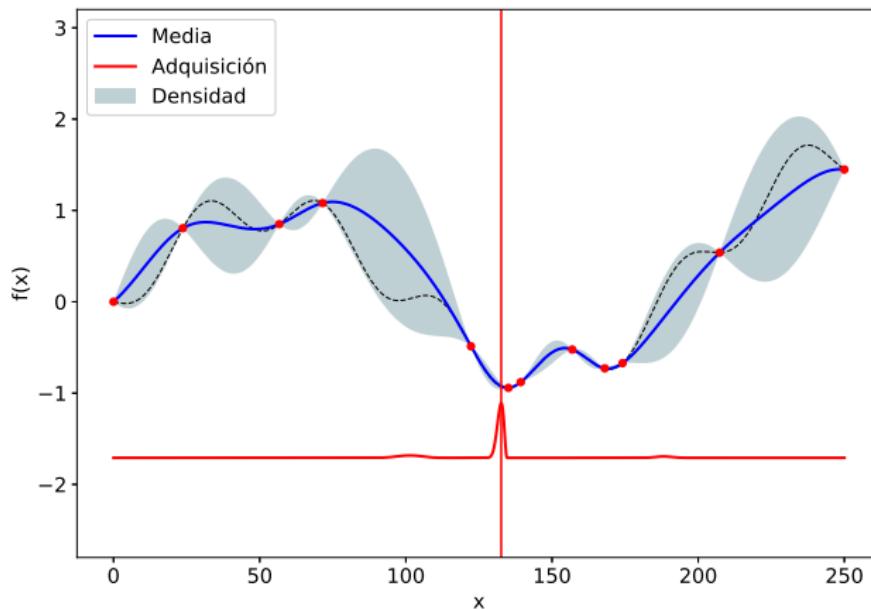
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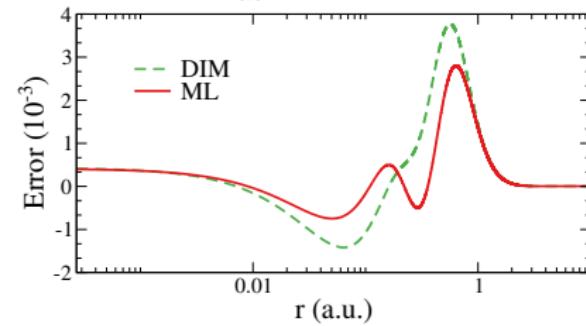
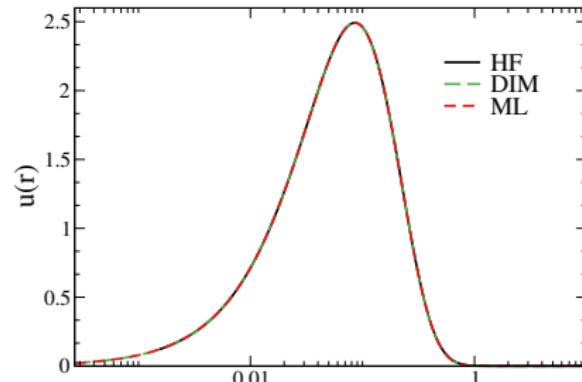
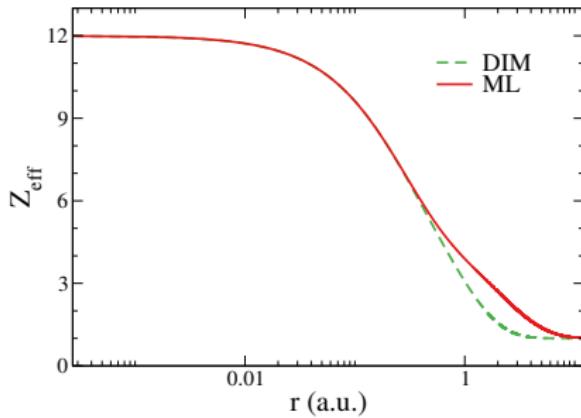


# Procesos Gaussianos



# DIM: Mg

1s

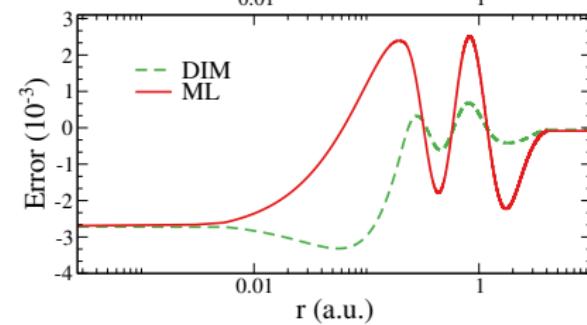
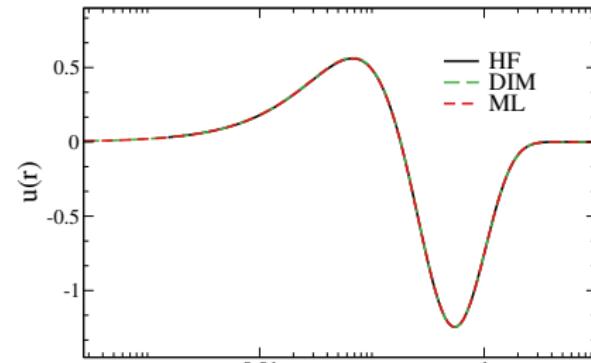
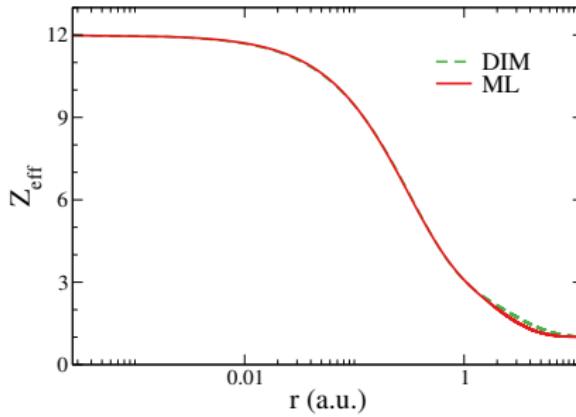


$$E \sim 10^{-6}$$

$$\langle r \rangle, \langle 1/r \rangle \sim 10^{-2}$$

# DIM: Mg

2s



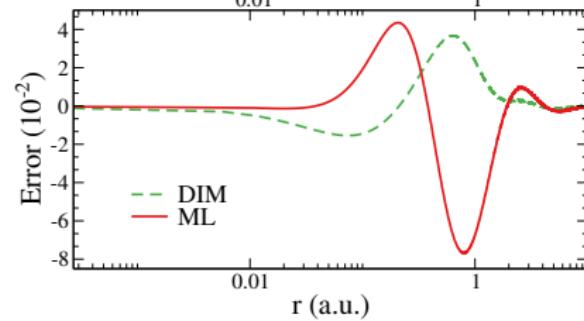
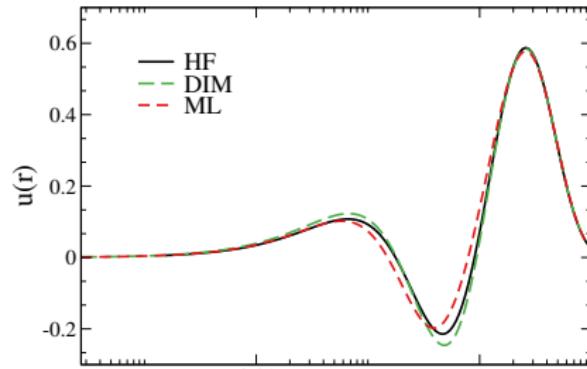
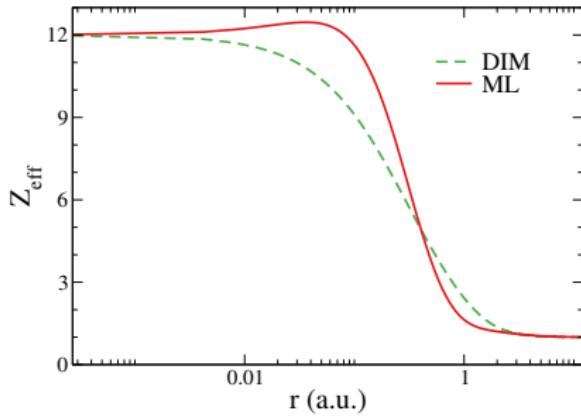
$$E \sim 10^{-7}$$

$$\langle r \rangle, \langle 1/r \rangle \sim 10^{-2}$$



# DIM: Mg

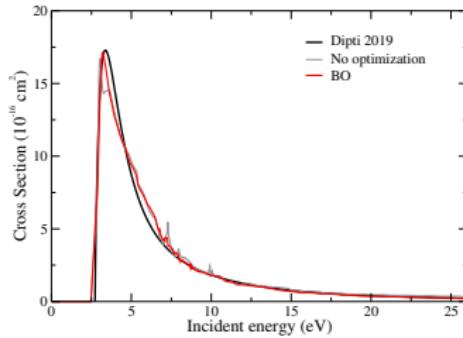
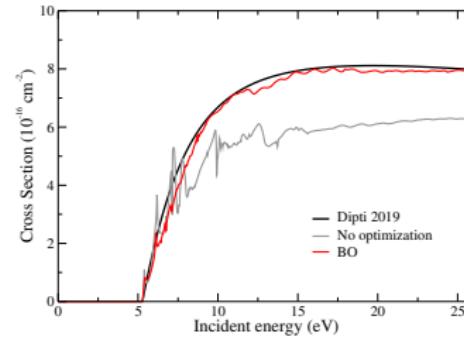
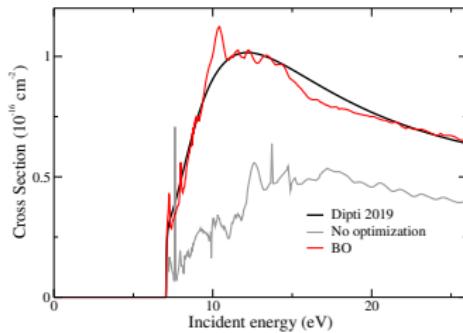
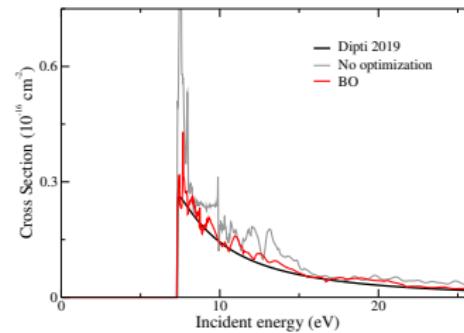
3s



$$E \sim 10^{-5}$$

$$\langle r \rangle, \langle 1/r \rangle \sim 10^{-1}$$

# R-Matrix: Berilio

 $2s\ ^2S - 2s2p\ ^3P$  $2s\ ^2S - 2s2p\ ^1P$  $2s\ ^2S - 2p\ ^2D$  $2s\ ^2S - 2s3p\ ^3P$ 

# Conclusiones