

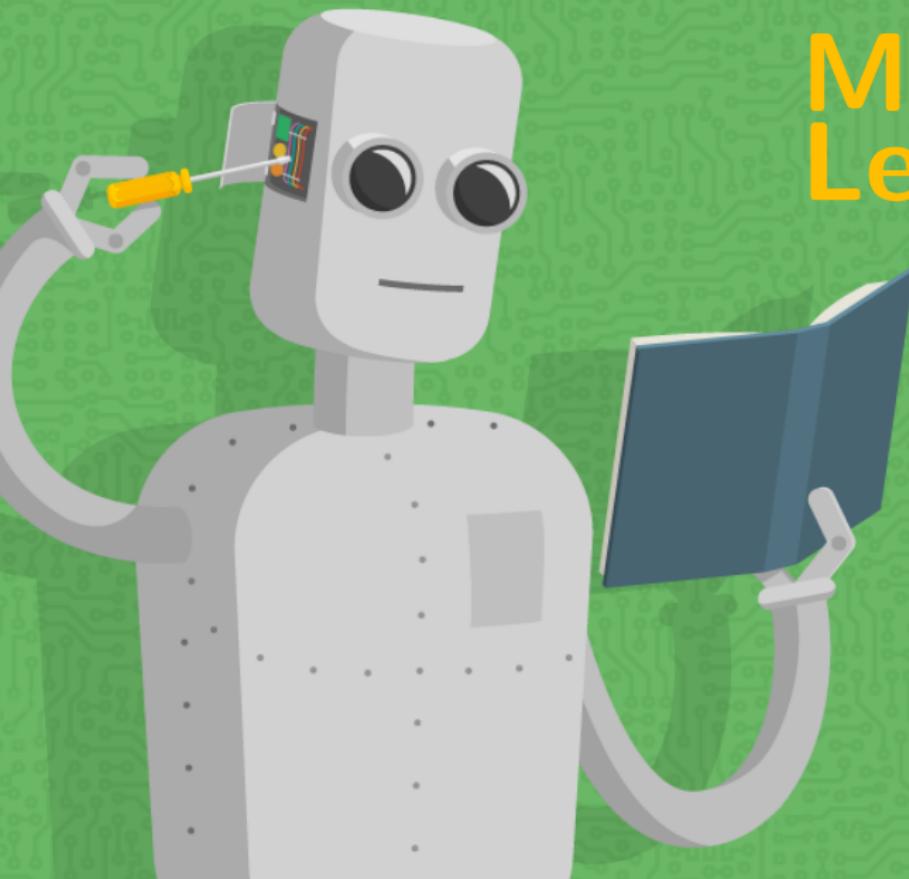
Implementación de Métodos de Aprendizaje Automatizado en problemas colisionales



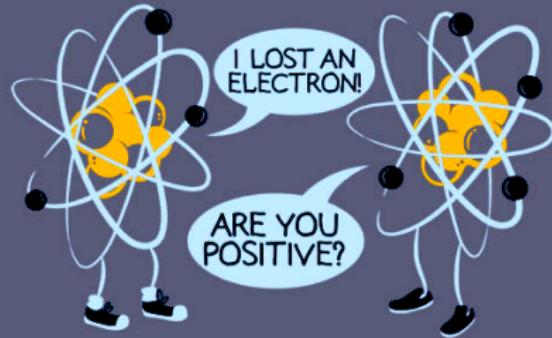
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1 de Septiembre – Buenos Aires



Machine Learning



Método de Inversión Depurada (DIM)

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

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¿Cómo
obtener V?

Método de Inversión Depurada (DIM)

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

Método de Inversión Depurada (DIM)

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

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

Método de Inversión Depurada (DIM)

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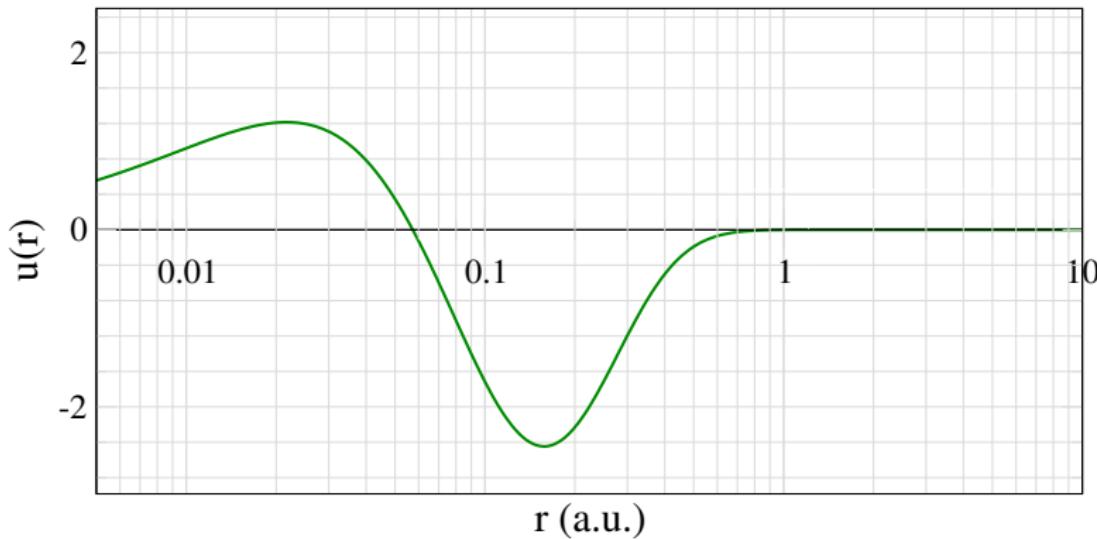
¿Cómo
obtener V?

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

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

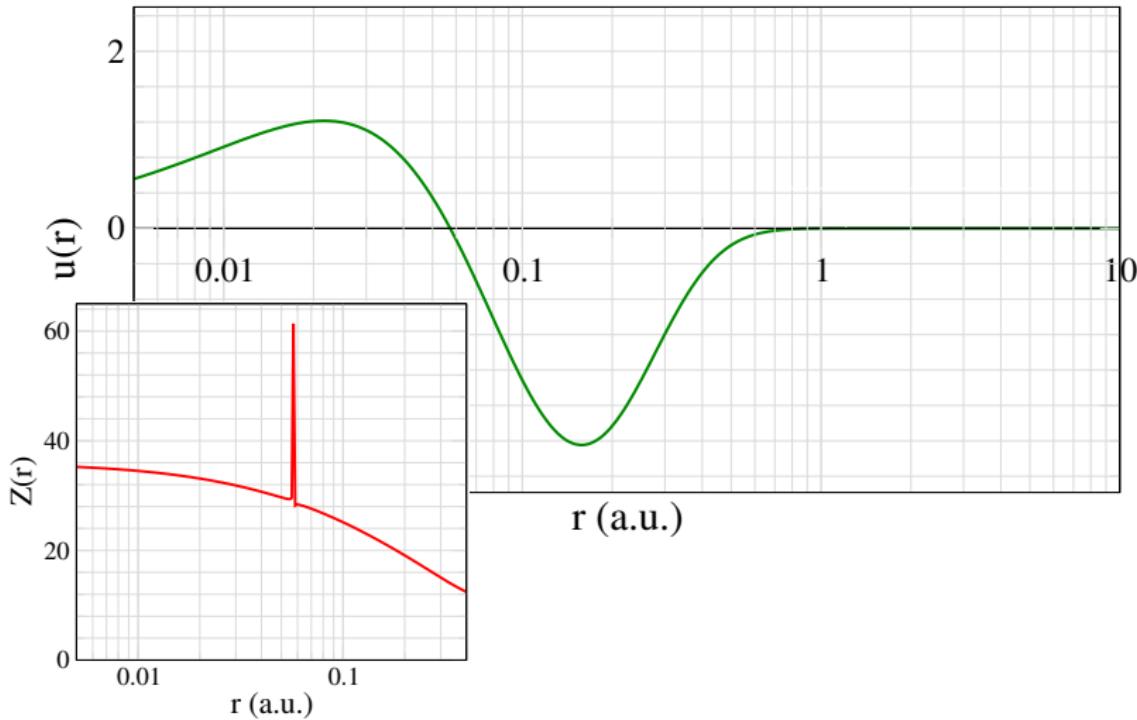
Houston, we have a problem!

$2s\ Kr$



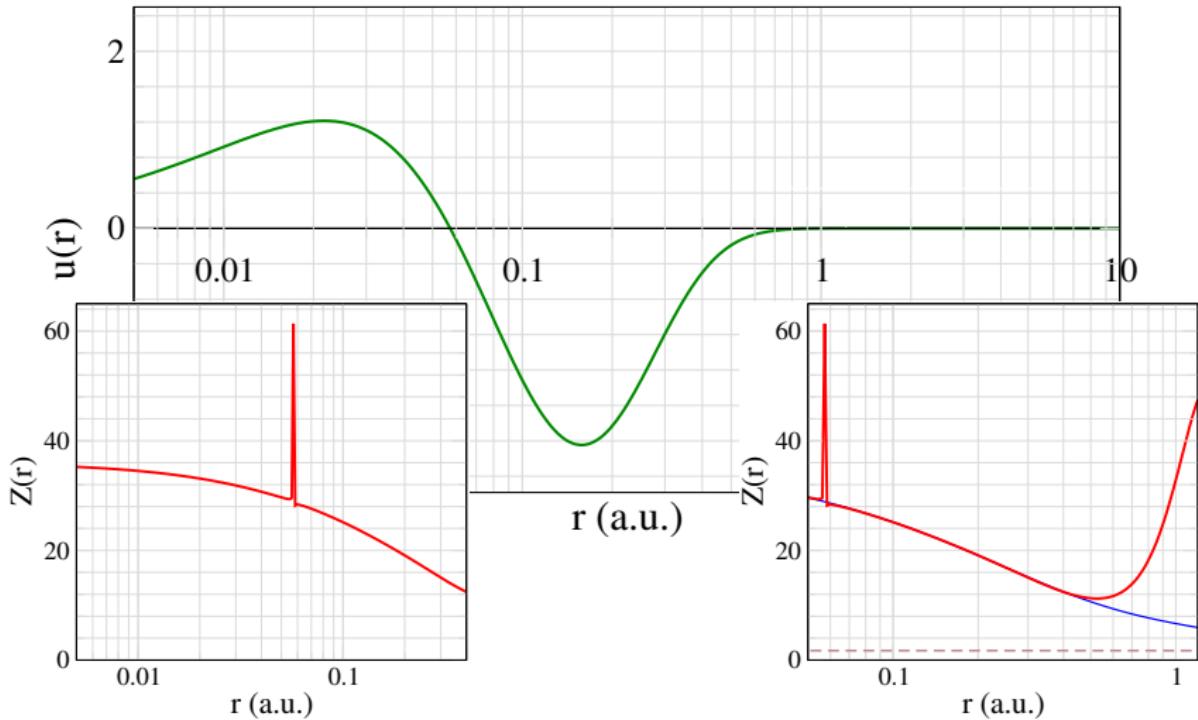
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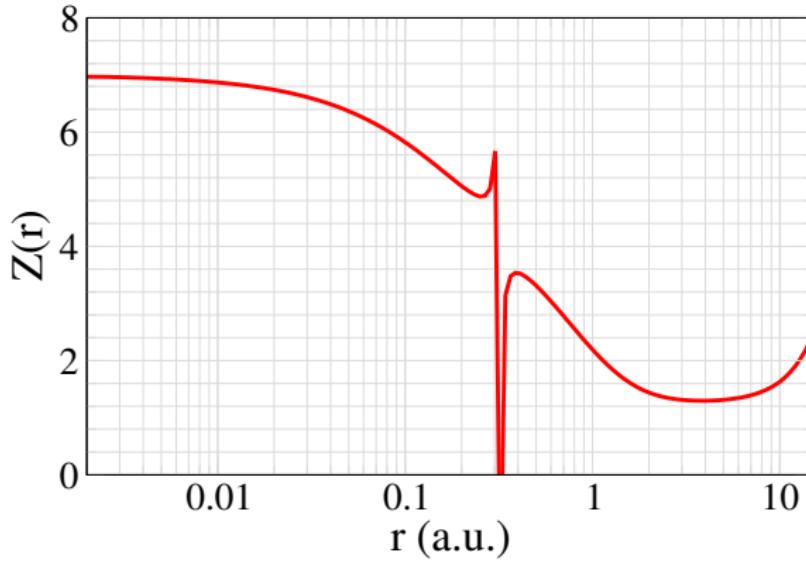
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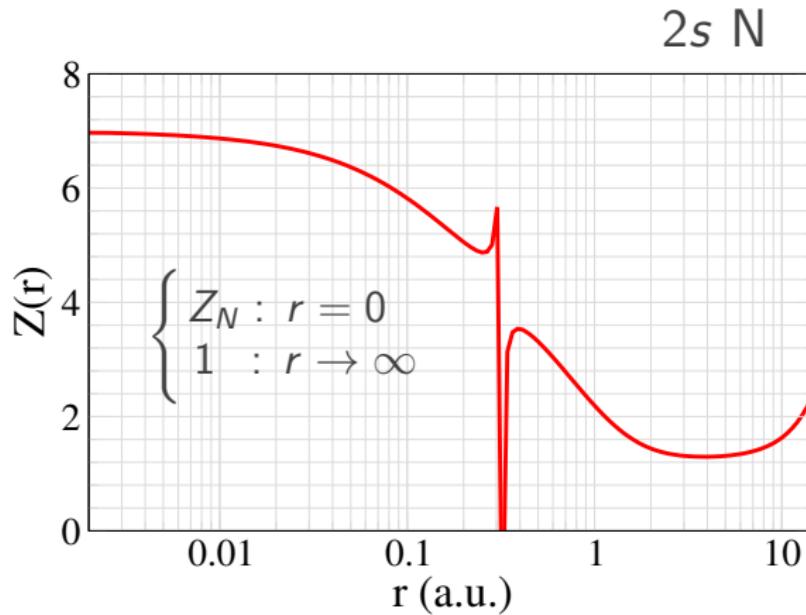


Depuración

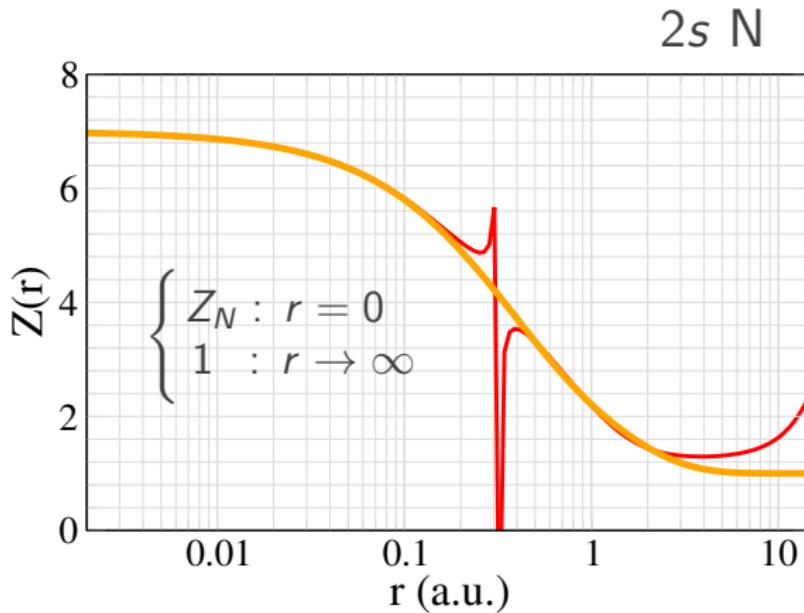
$2s\ N$



Depuración

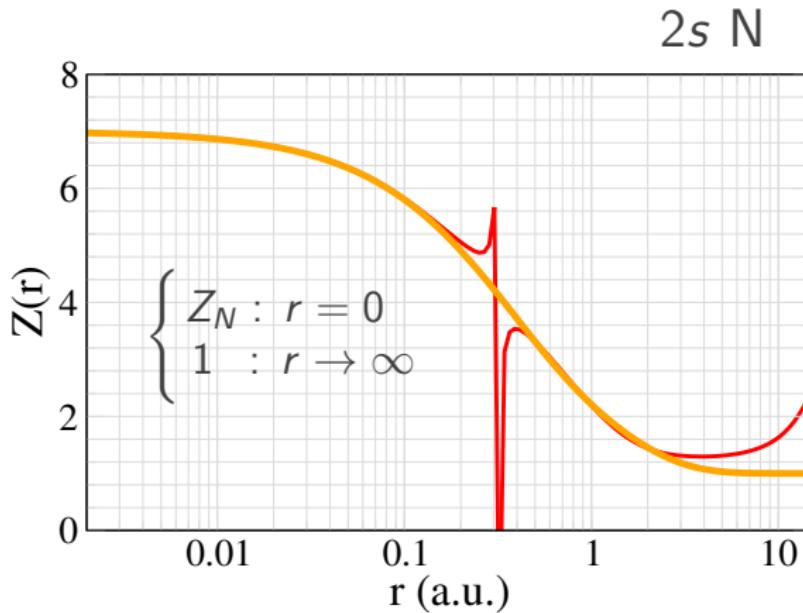


Depuración



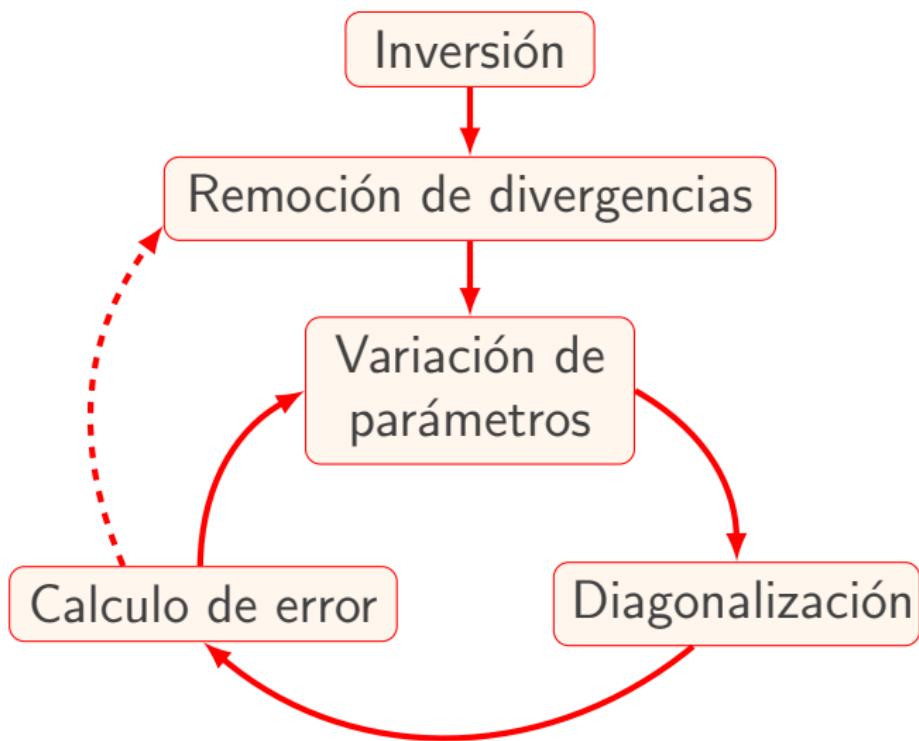
$$Z(r) = 1 + \sum_j \alpha_j e^{-\beta_j r}$$

Depuración

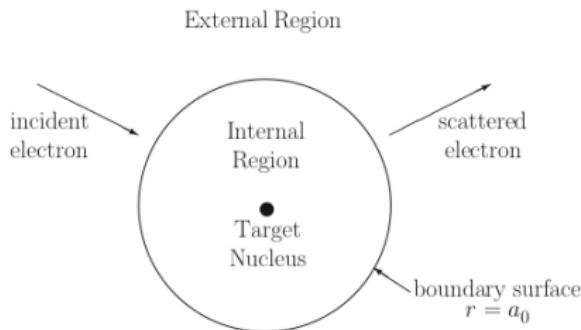


$$Z(r) = 1 + \sum_j \alpha_j e^{-\beta_j r}$$

Procedimiento



R-Matrix



Estructura del blanco

AUTOSTRUCTURE



Región interna

RMATRXI



Región externa

STGF

Descripción del blanco

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

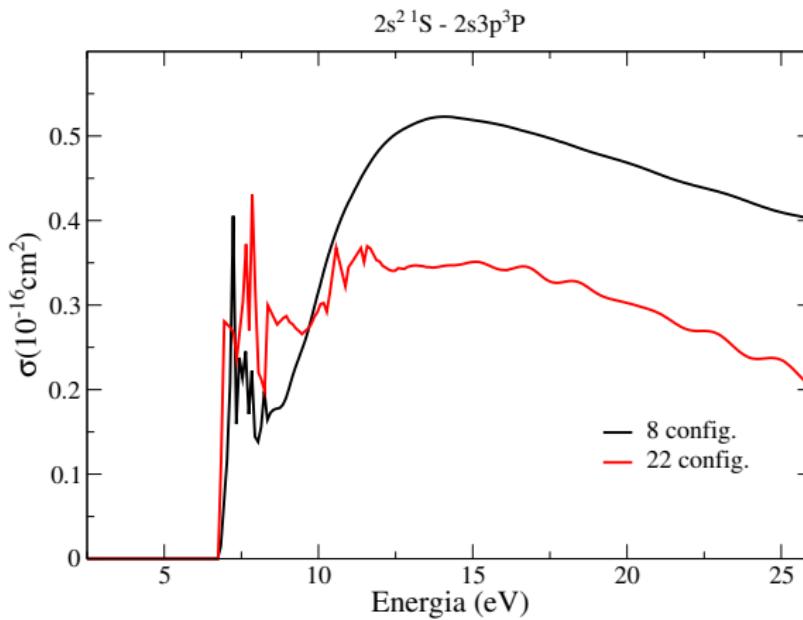
Configuration
interaction

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

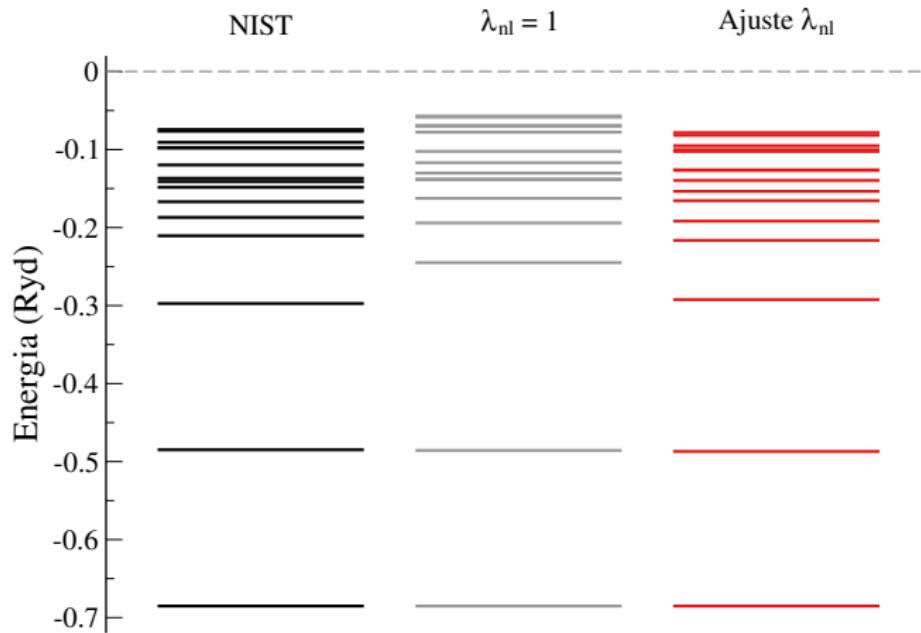
- Thomas–Fermi–Dirac–Amaldi
- Slater-Type-Orbital de Burgess

Ejemplo: Berilio

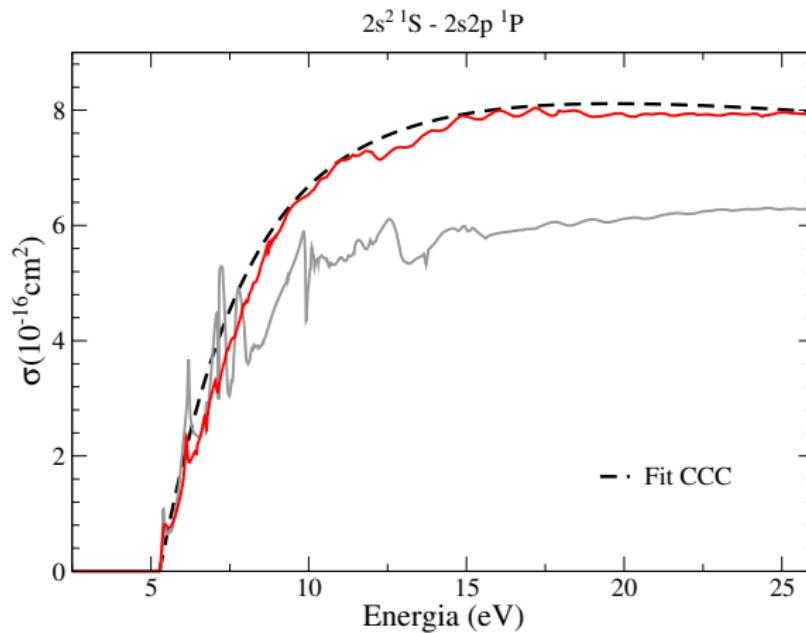
$1s^2 2s^2$
 $1s^2 2snl$
 $1s^2 2p^2$
 $1s^2 2pnl$



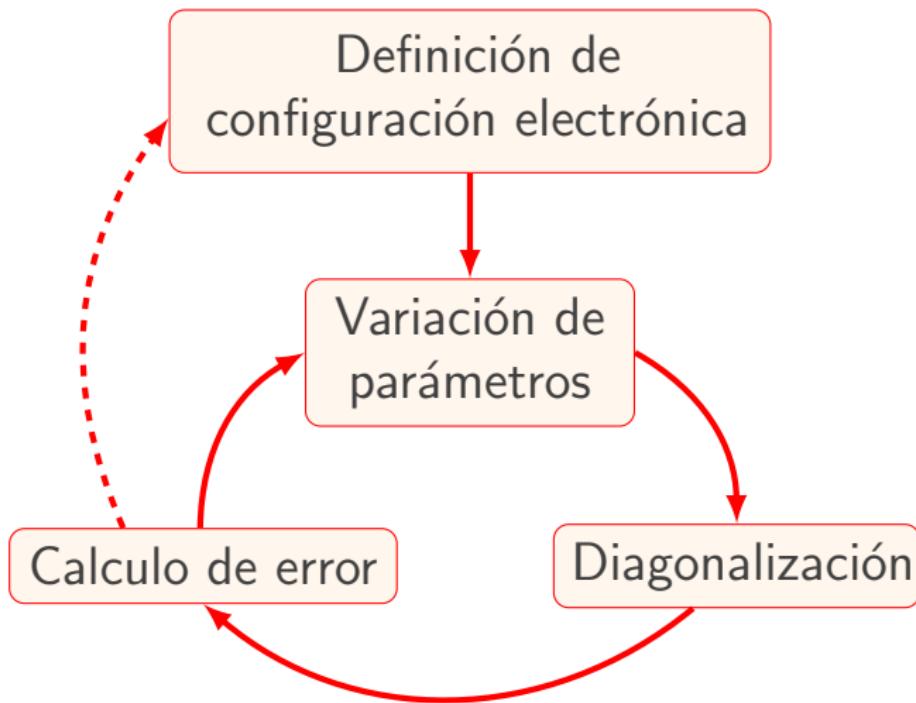
Ejemplo: Berilio



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Procedimiento

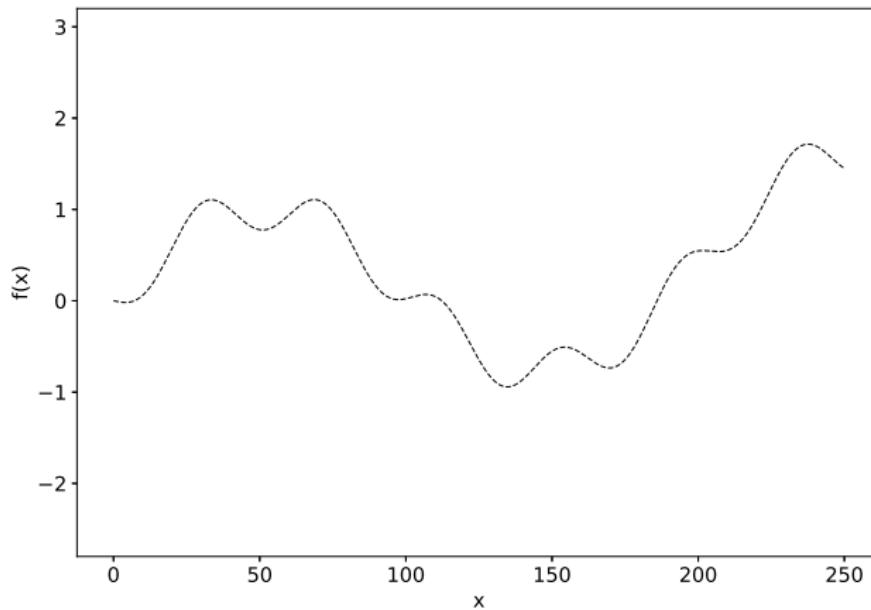


Síntesis del problema

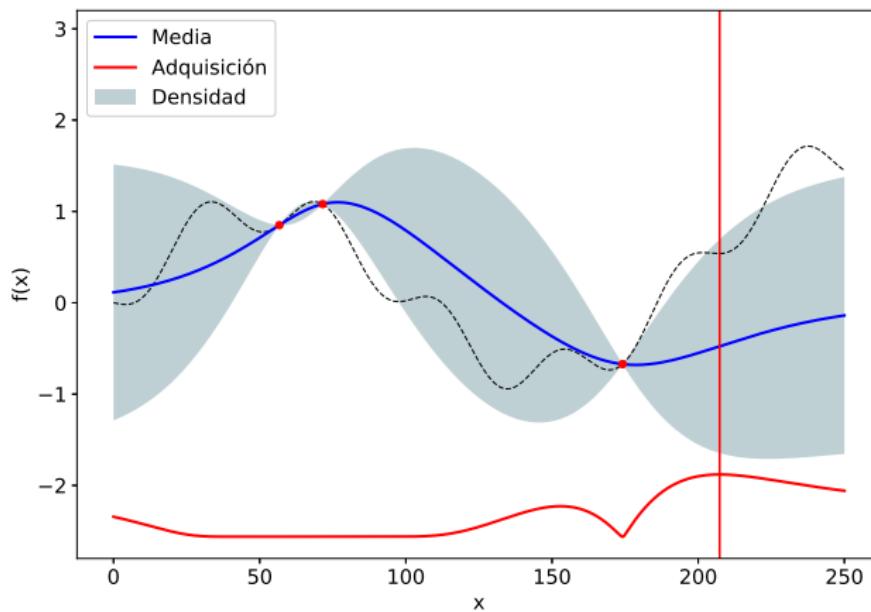
$$J = \sum_j \left| \frac{E_j^{\text{calc}}(\xi) - E_j^{\text{teo}}}{E_j^{\text{teo}}} \right|$$

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

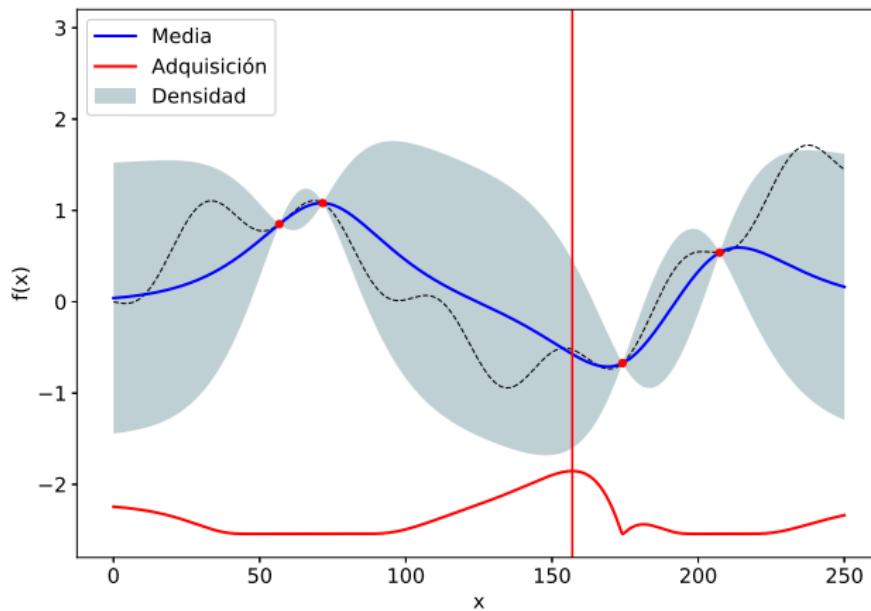
Procesos Gaussianos



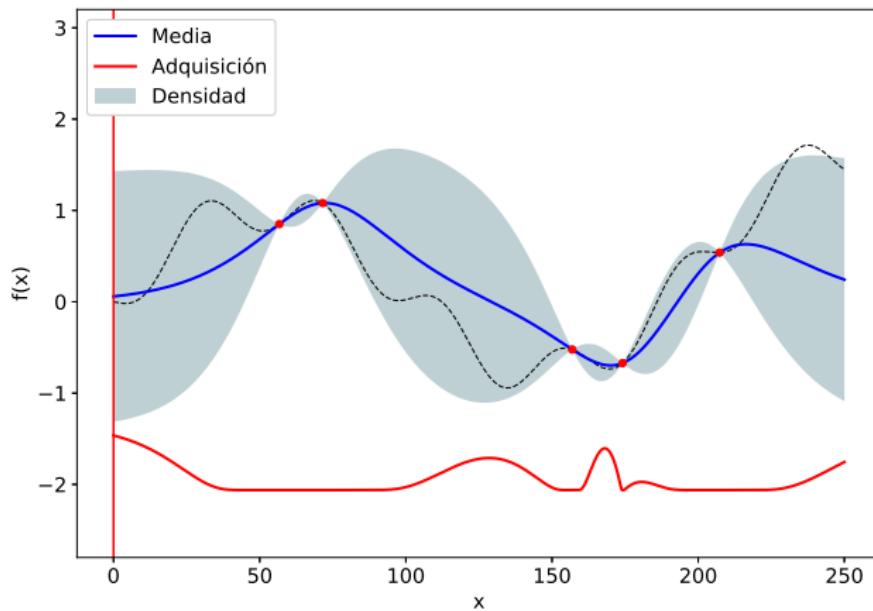
Procesos Gaussianos



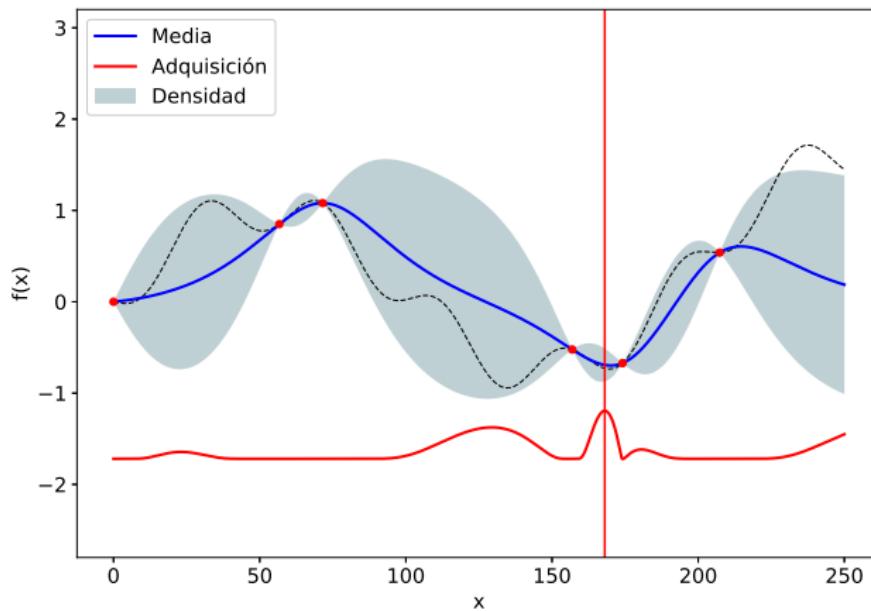
Procesos Gaussianos



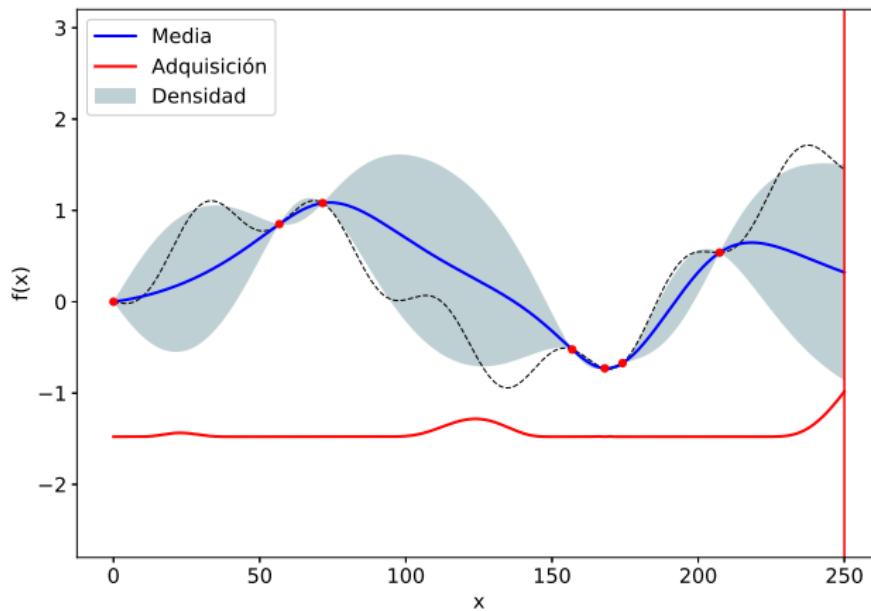
Procesos Gaussianos



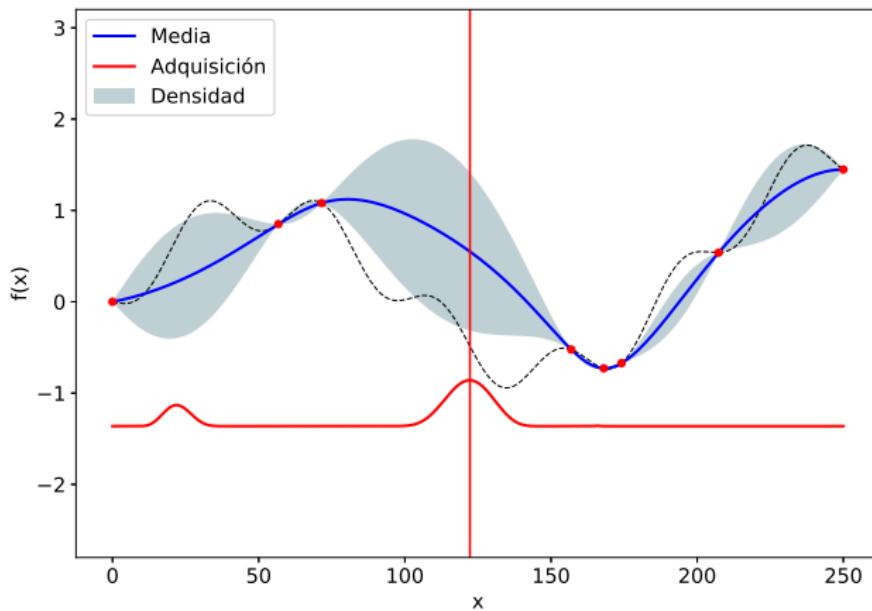
Procesos Gaussianos



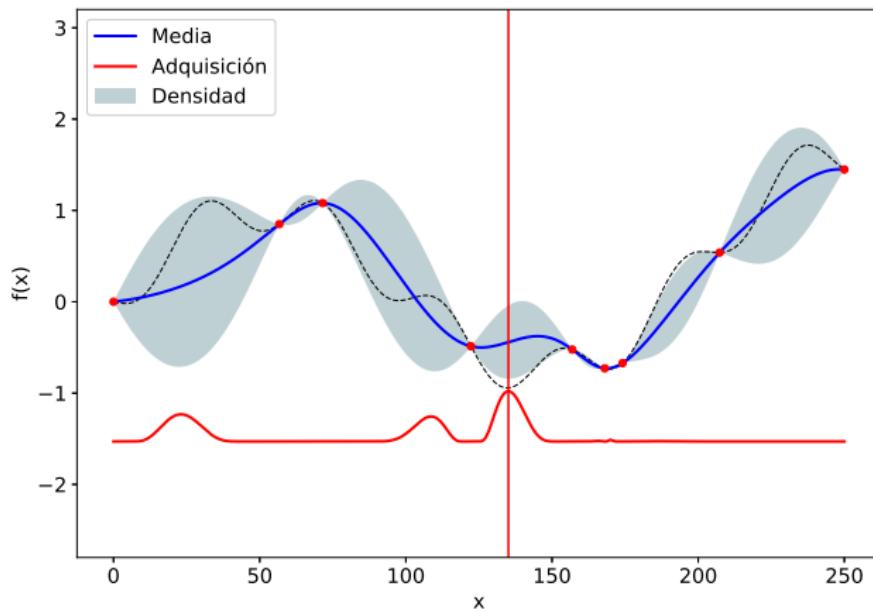
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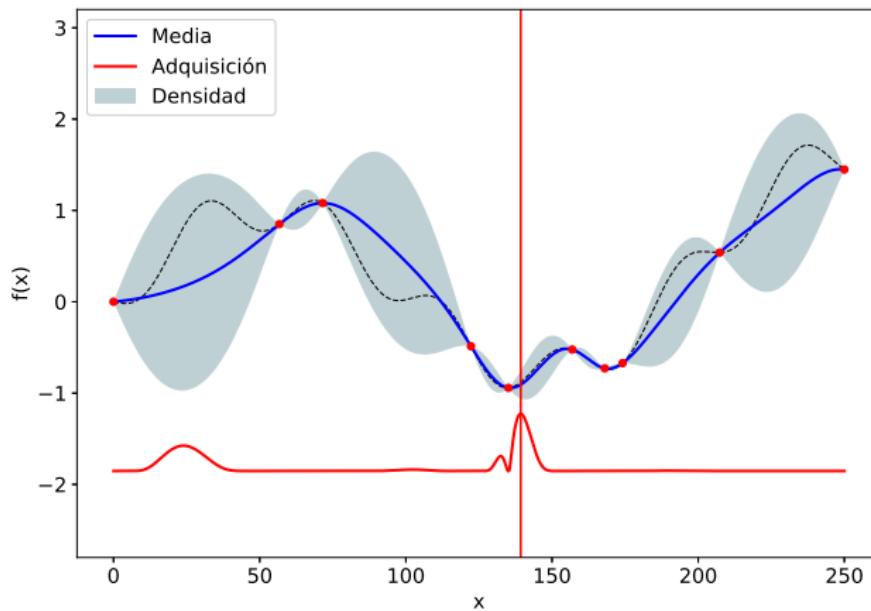
Procesos Gaussianos



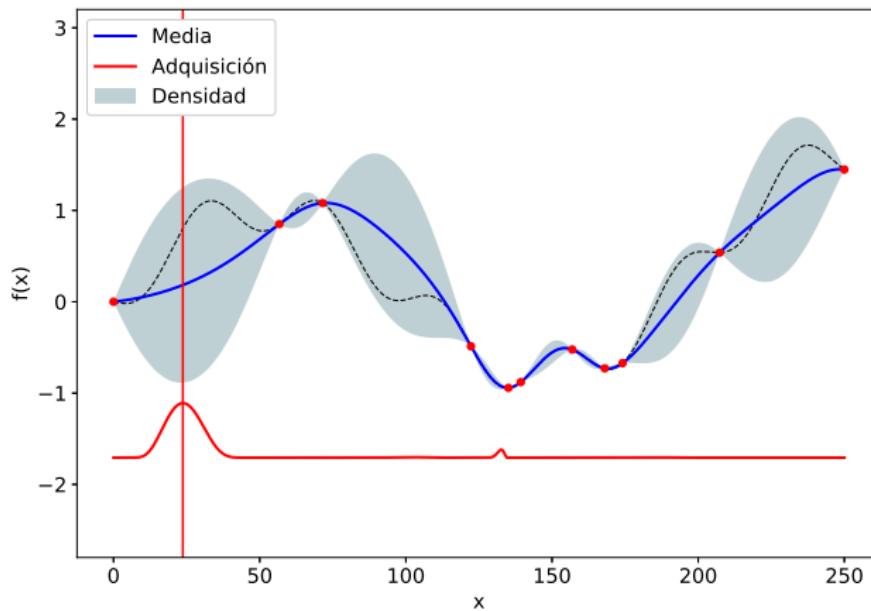
Procesos Gaussianos



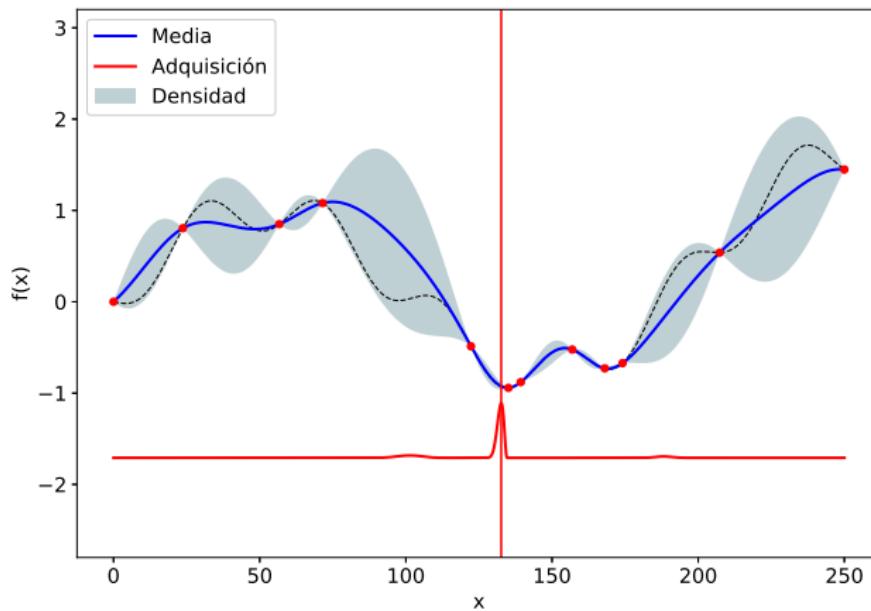
Procesos Gaussianos



Procesos Gaussianos

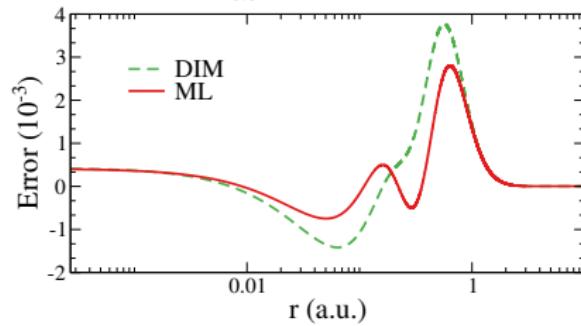
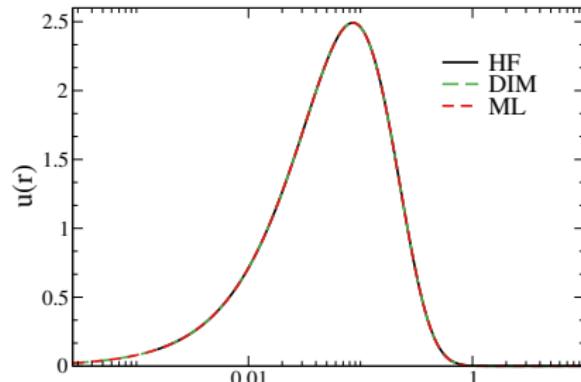
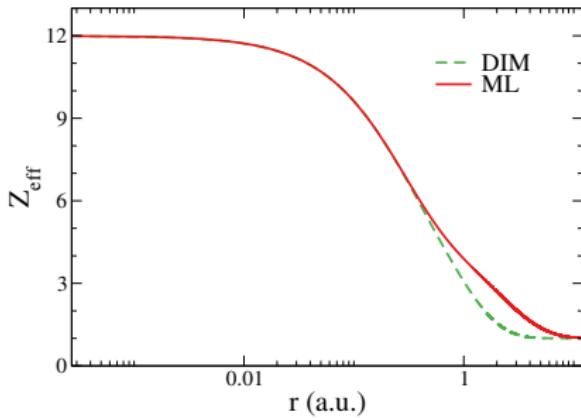


Procesos Gaussianos



DIM: Mg

1s



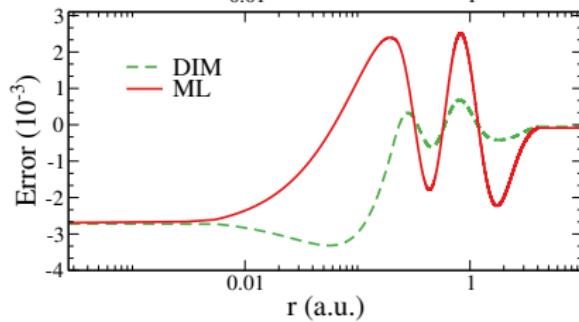
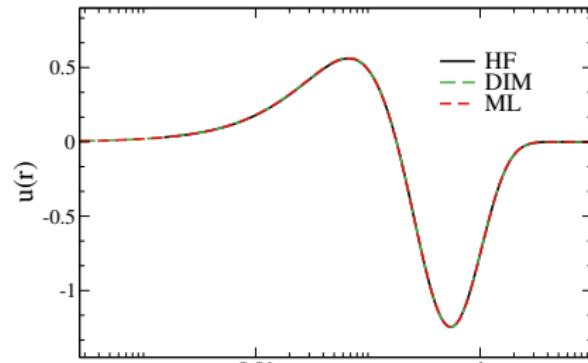
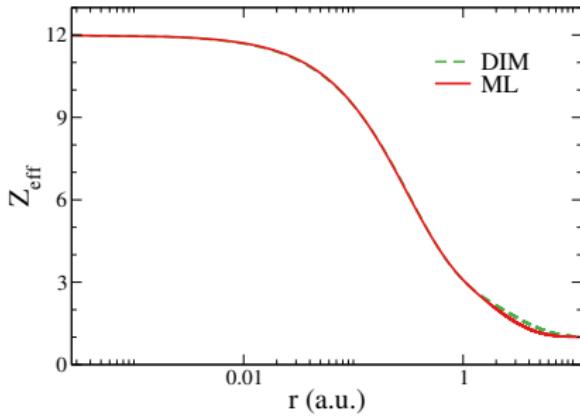
$$E \sim 10^{-6}$$

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



DIM: Mg

2s

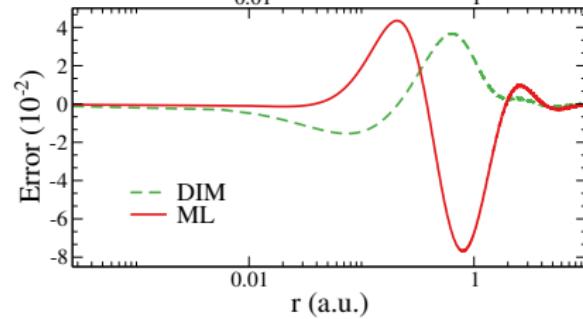
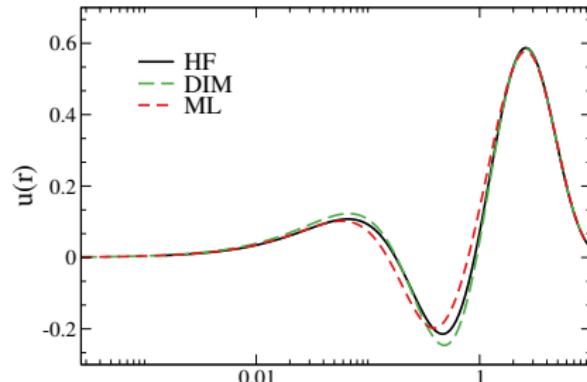
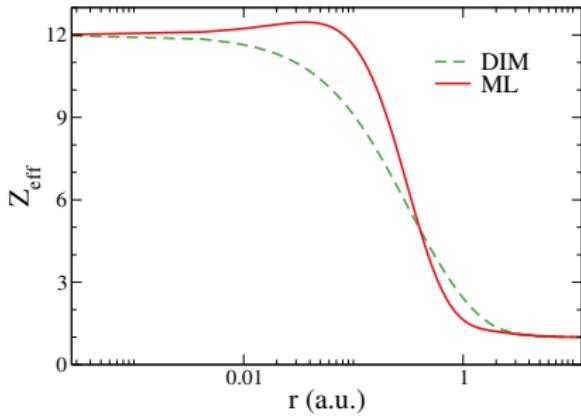


$$E \sim 10^{-7}$$

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

DIM: Mg

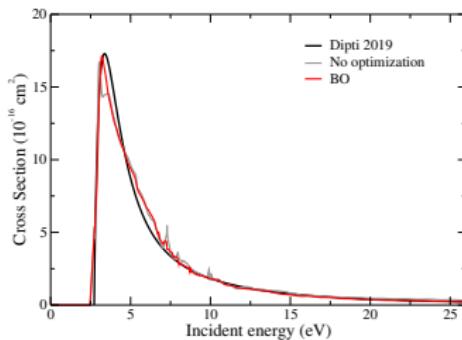
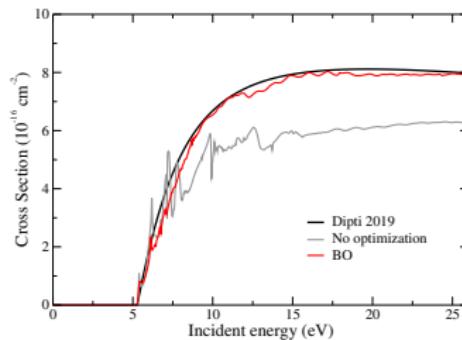
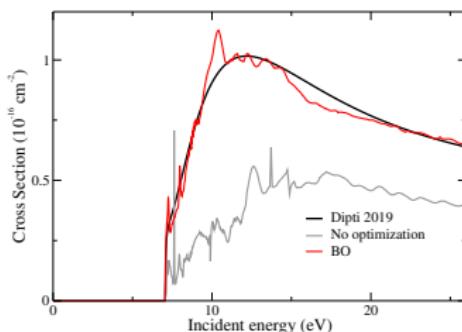
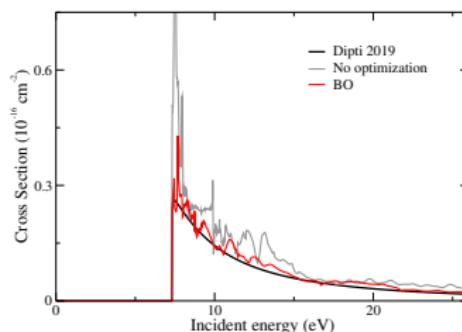
3s



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

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

R-Matrix: Berilio

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

Conclusiones