I Encuentro Nacional de Dinámica Cuántica en la Materia

Implementación de Métodos de Aprendizaje Automatizado en problemas colisionales

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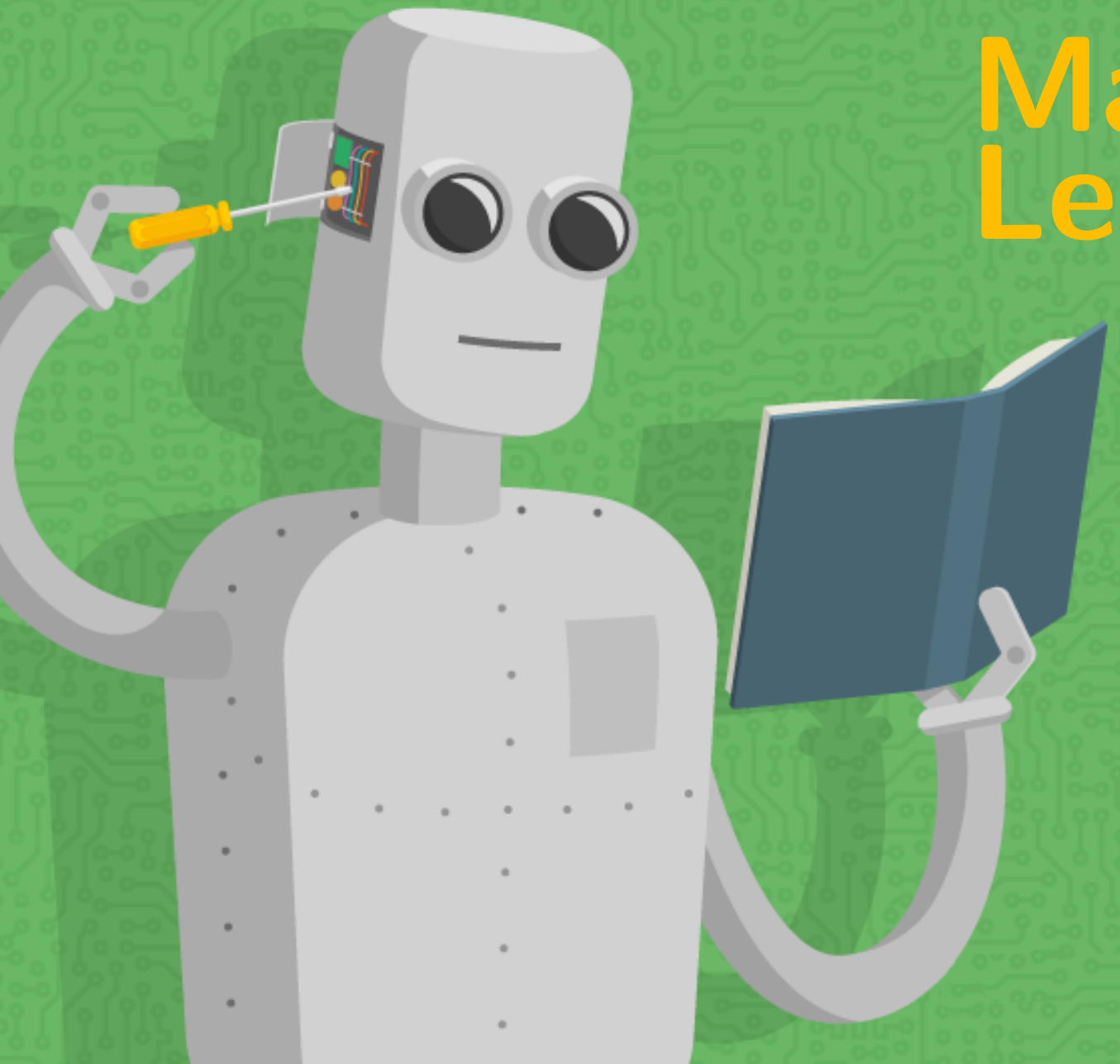
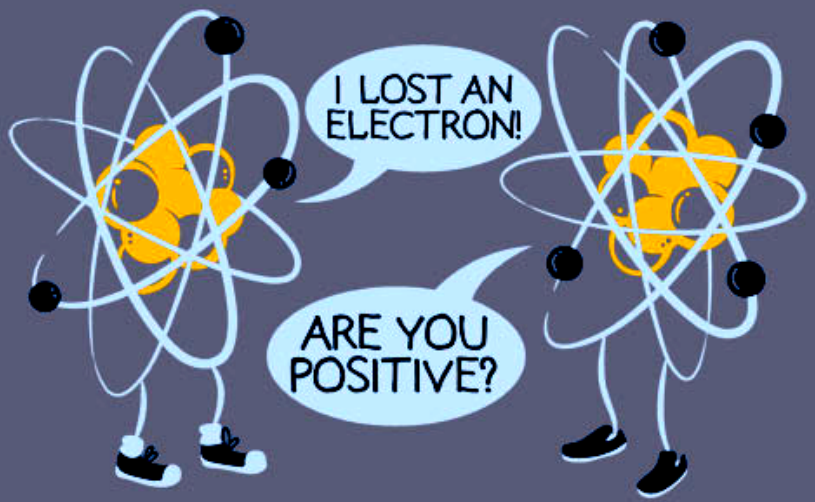


Machine Learning


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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¿Cómo conocemos V?

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

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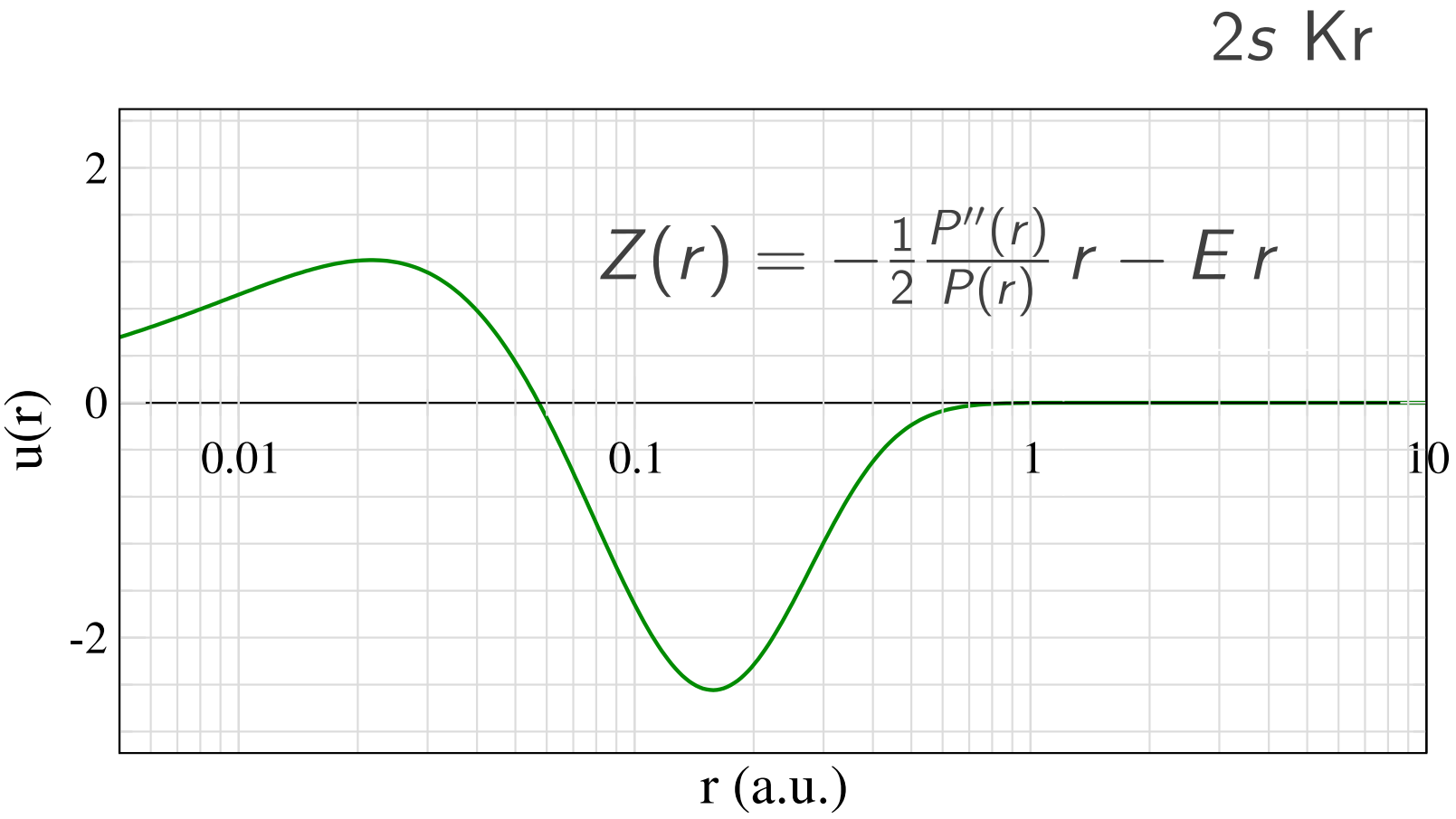
$$Z_{nl}(r) = -\frac{1}{2}\frac{P''_{nl}(r)}{P_{nl}(r)}\, r + \frac{l(l+1)}{2r} - \varepsilon_{nl}\, r$$

Houston, we have a problem!



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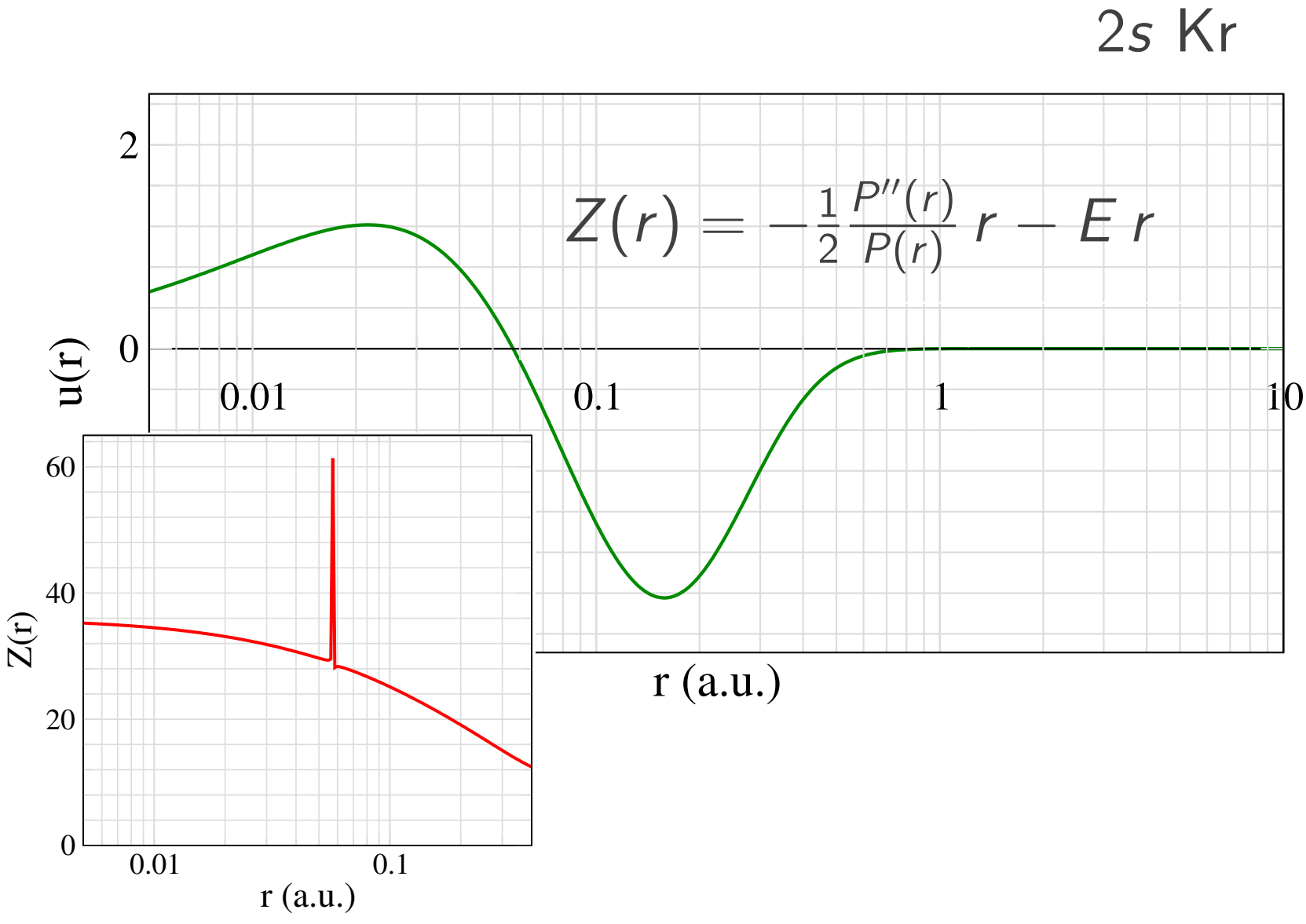

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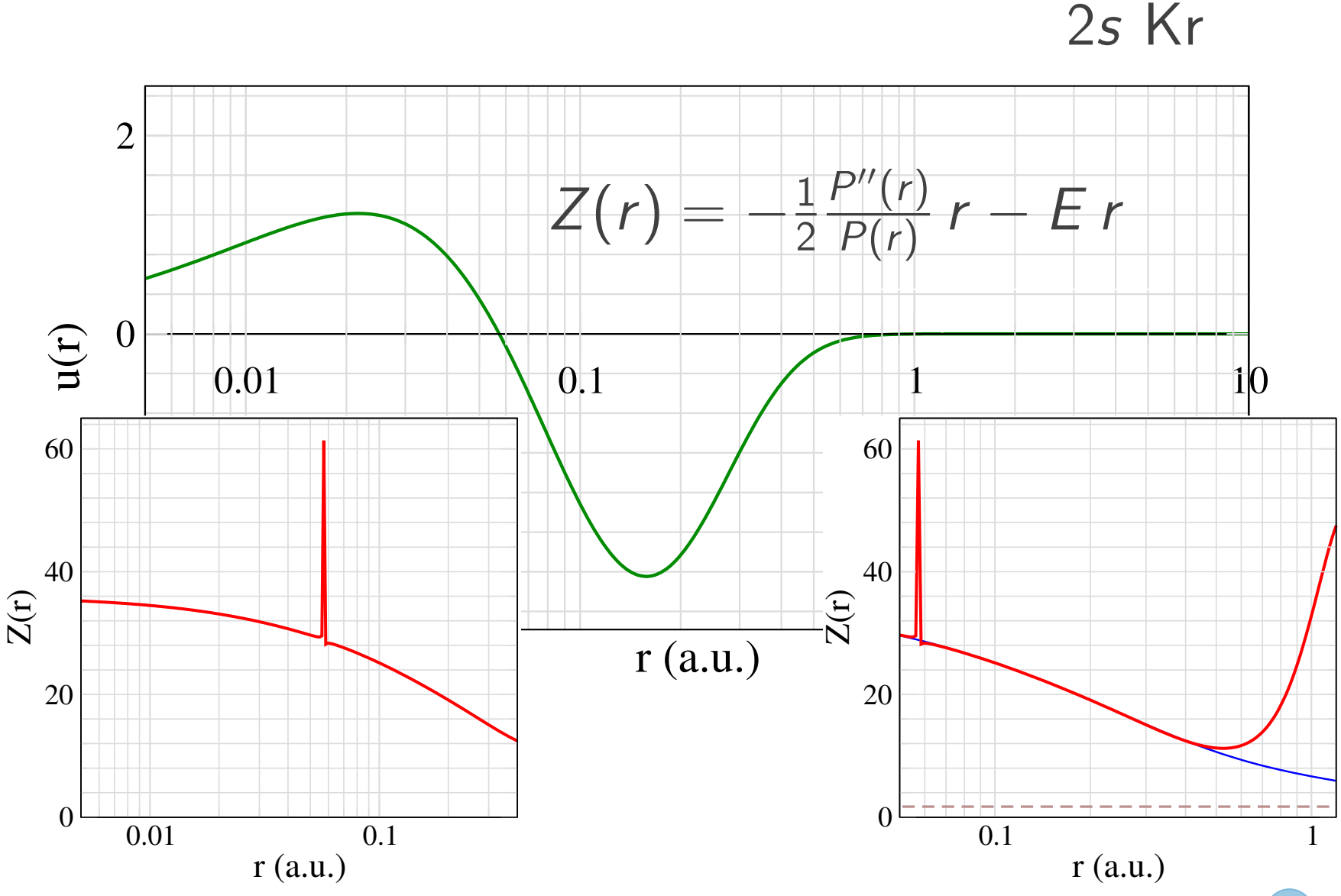
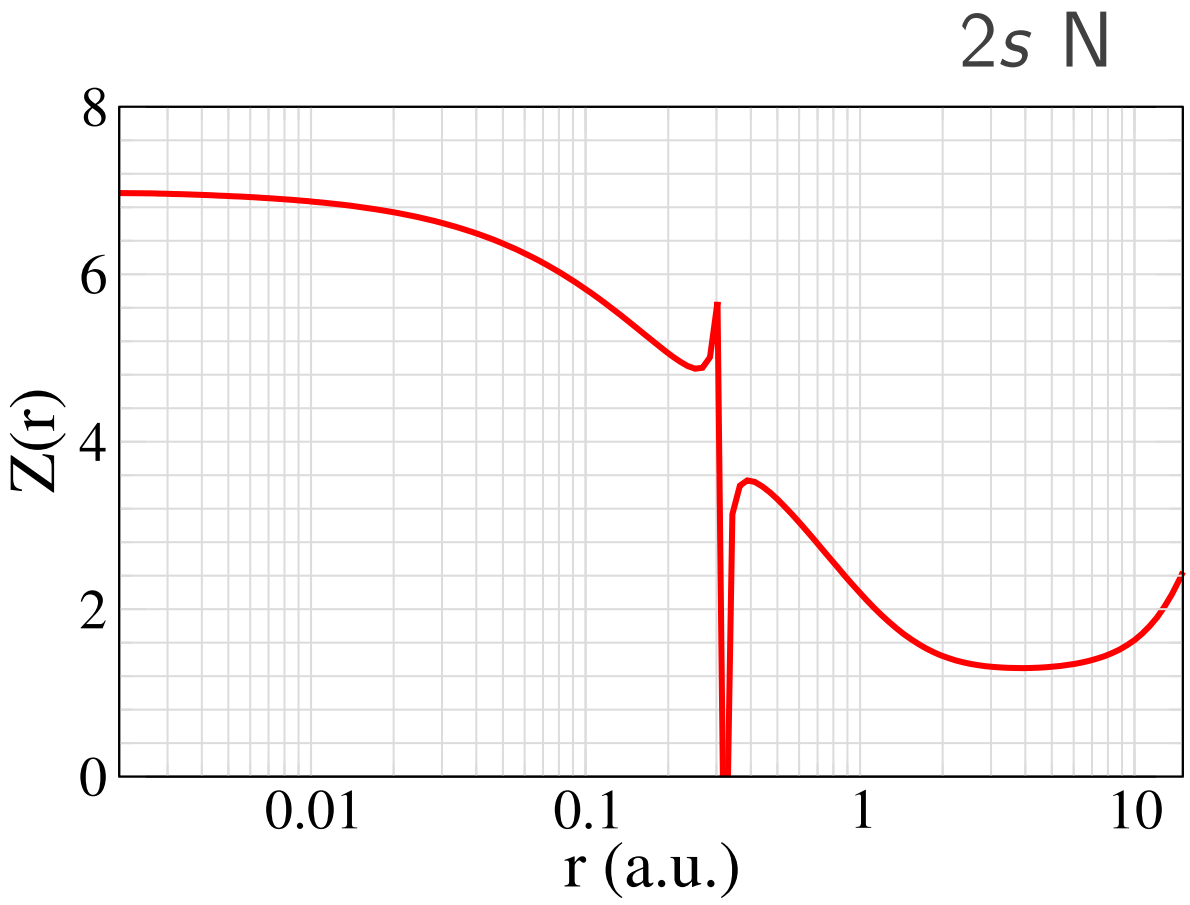
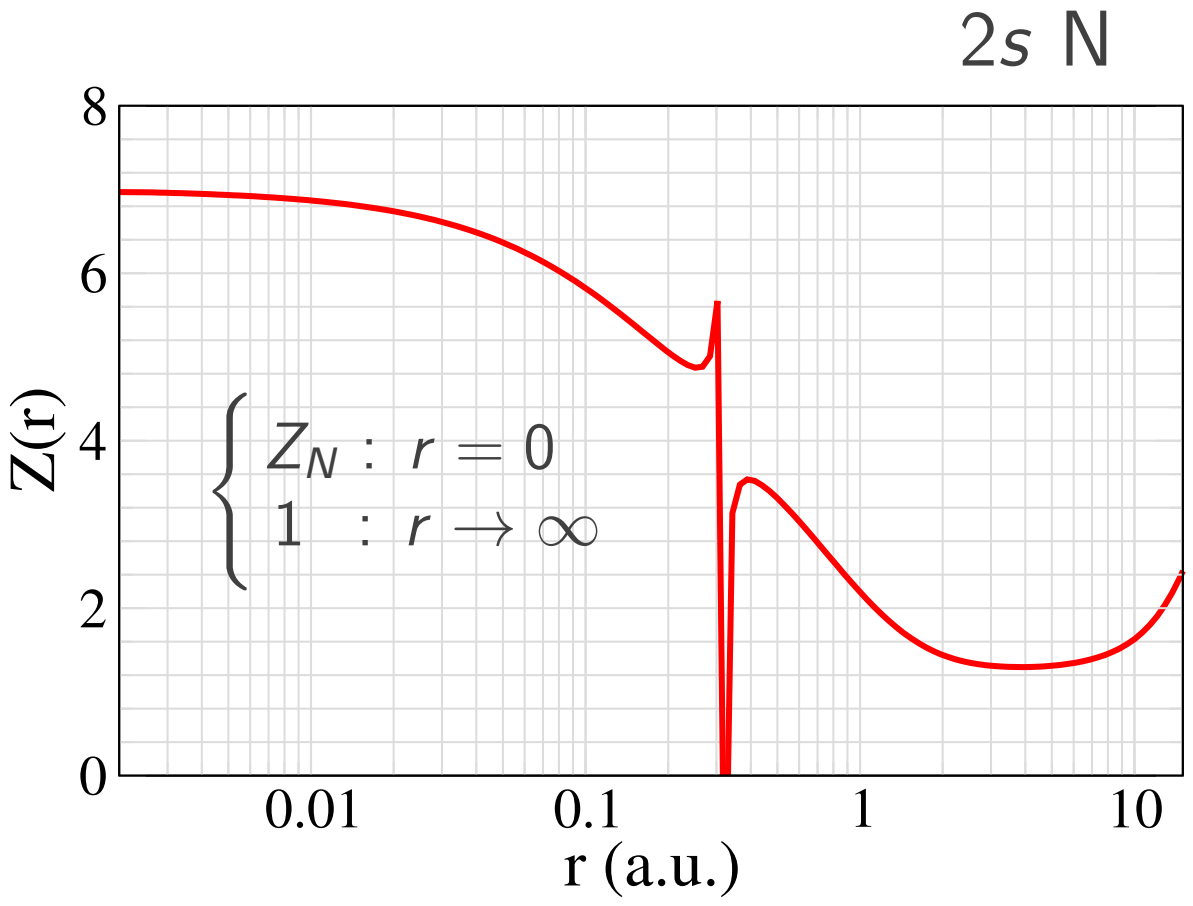


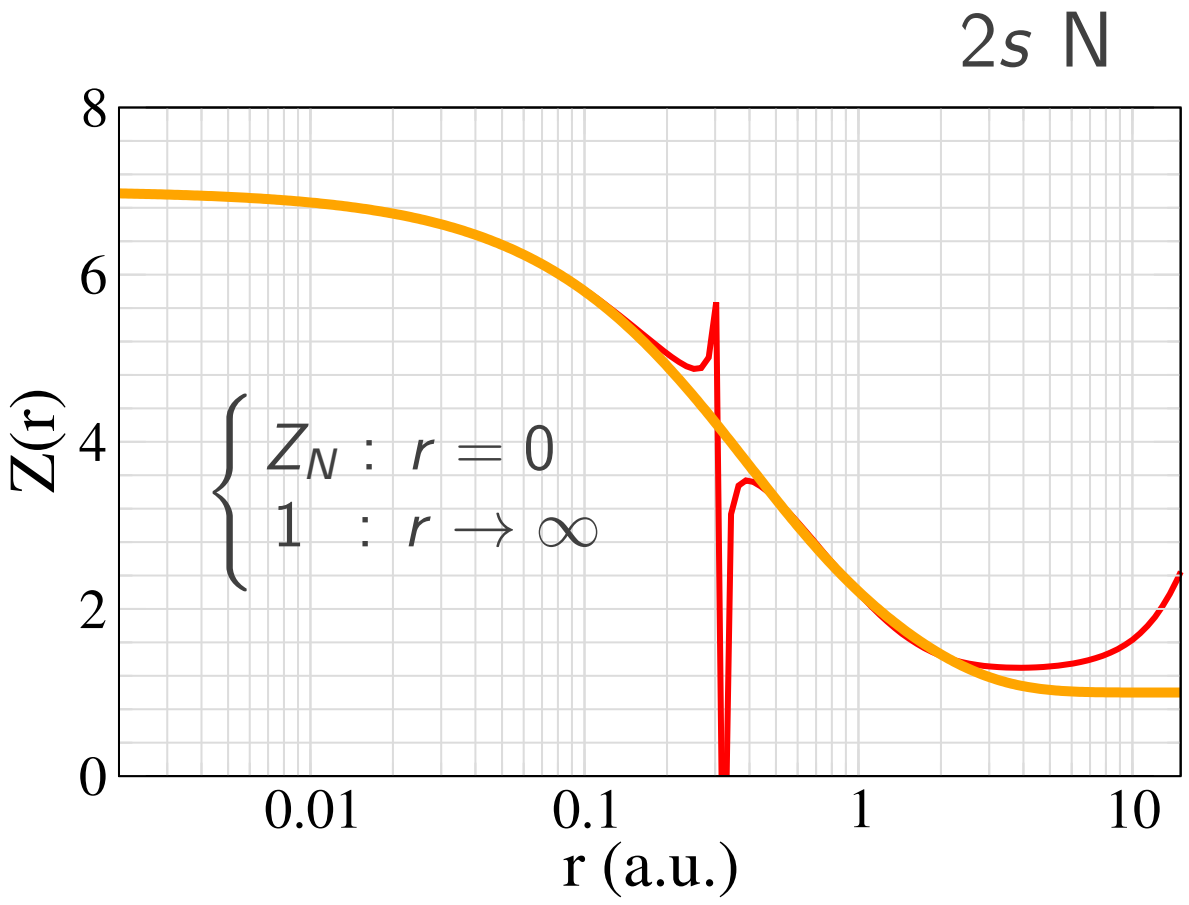
Depuración



Depuración

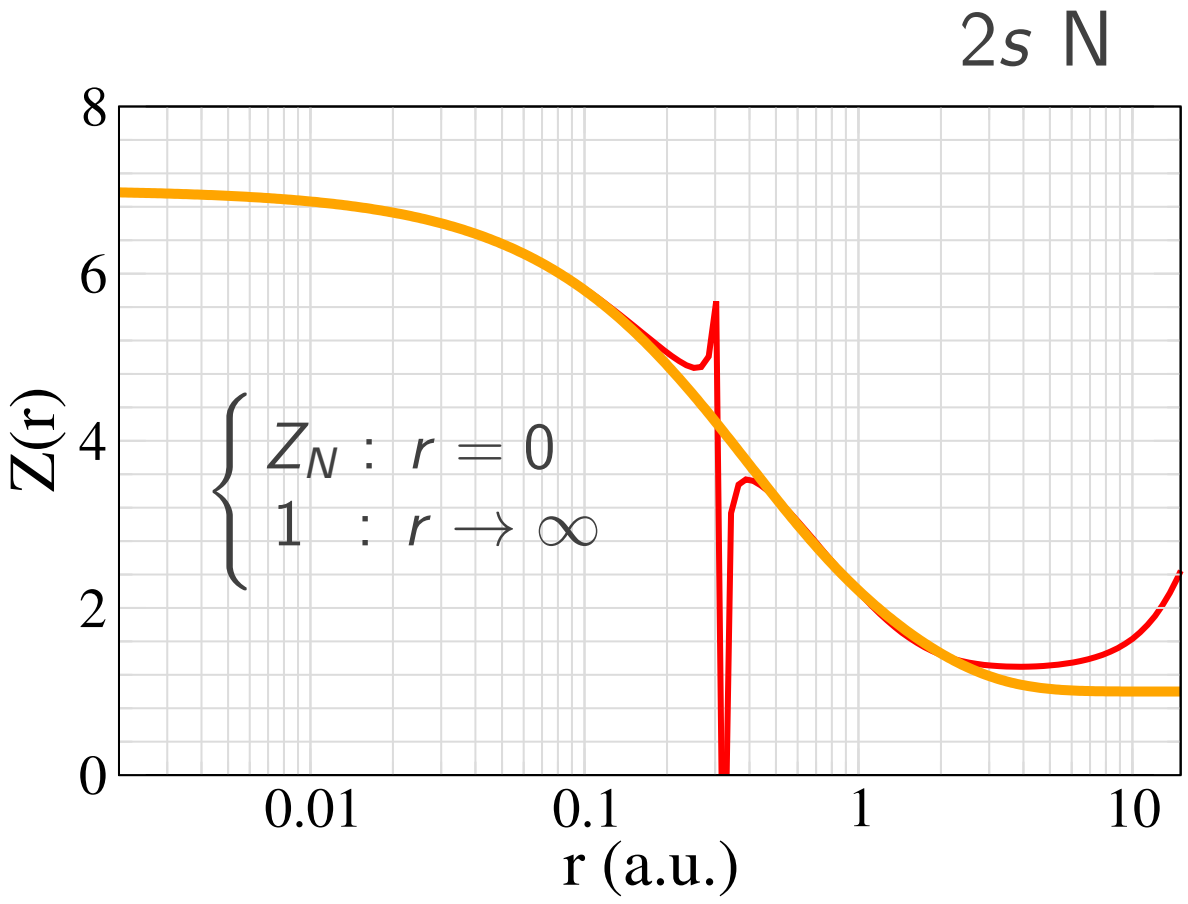

2s N
8
6
4
2
0
Z(r)
$\begin{cases} Z_N : r = 0 \\ 1 : r \to \infty \end{cases}$
0.01
0.1
1
10
r (a.u.)

Depuración



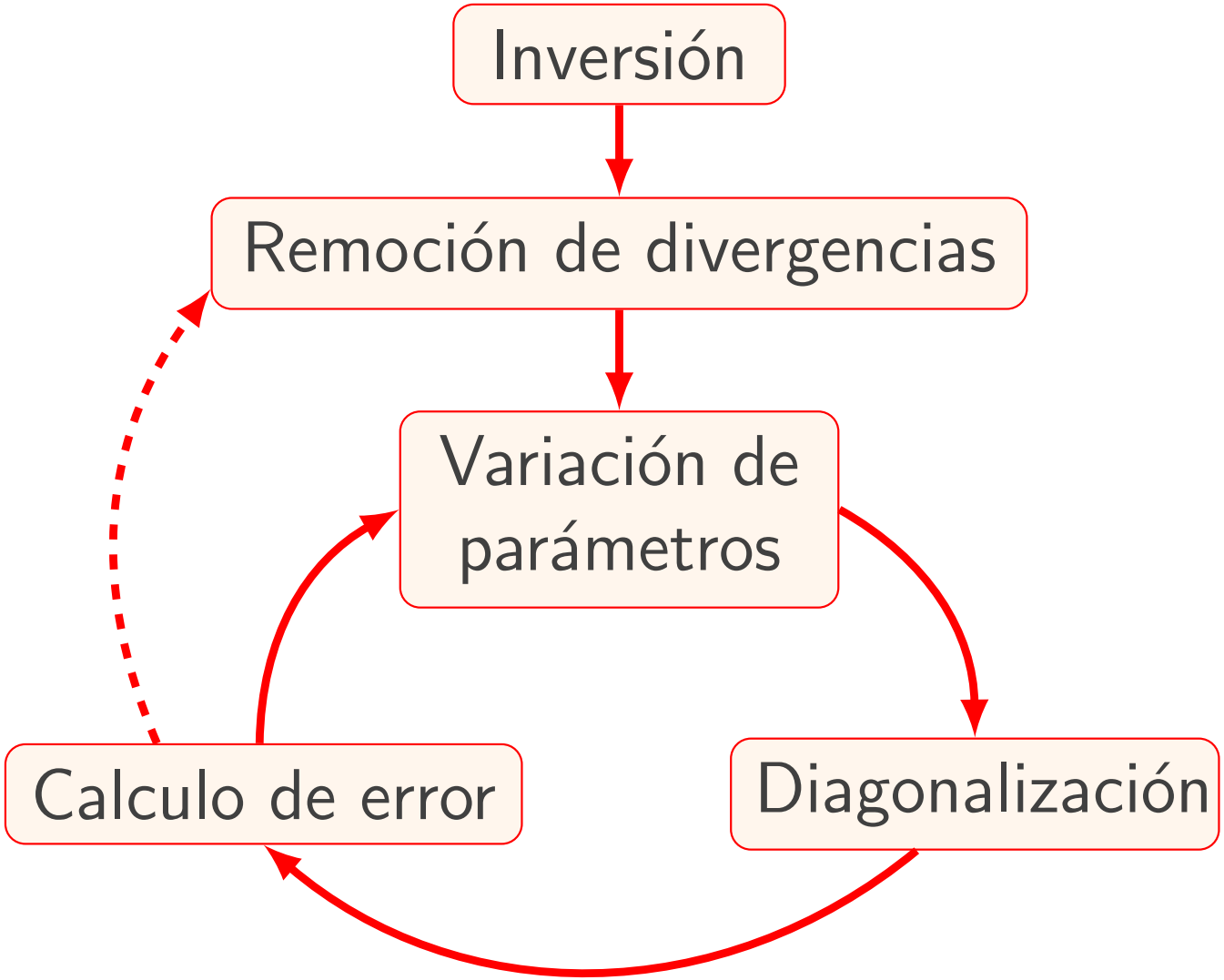
$$Z(r) = 1 + \sum_j \alpha_j e^{-\beta_j r}$$

Depuración



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

Procedimiento



Estructura atómica

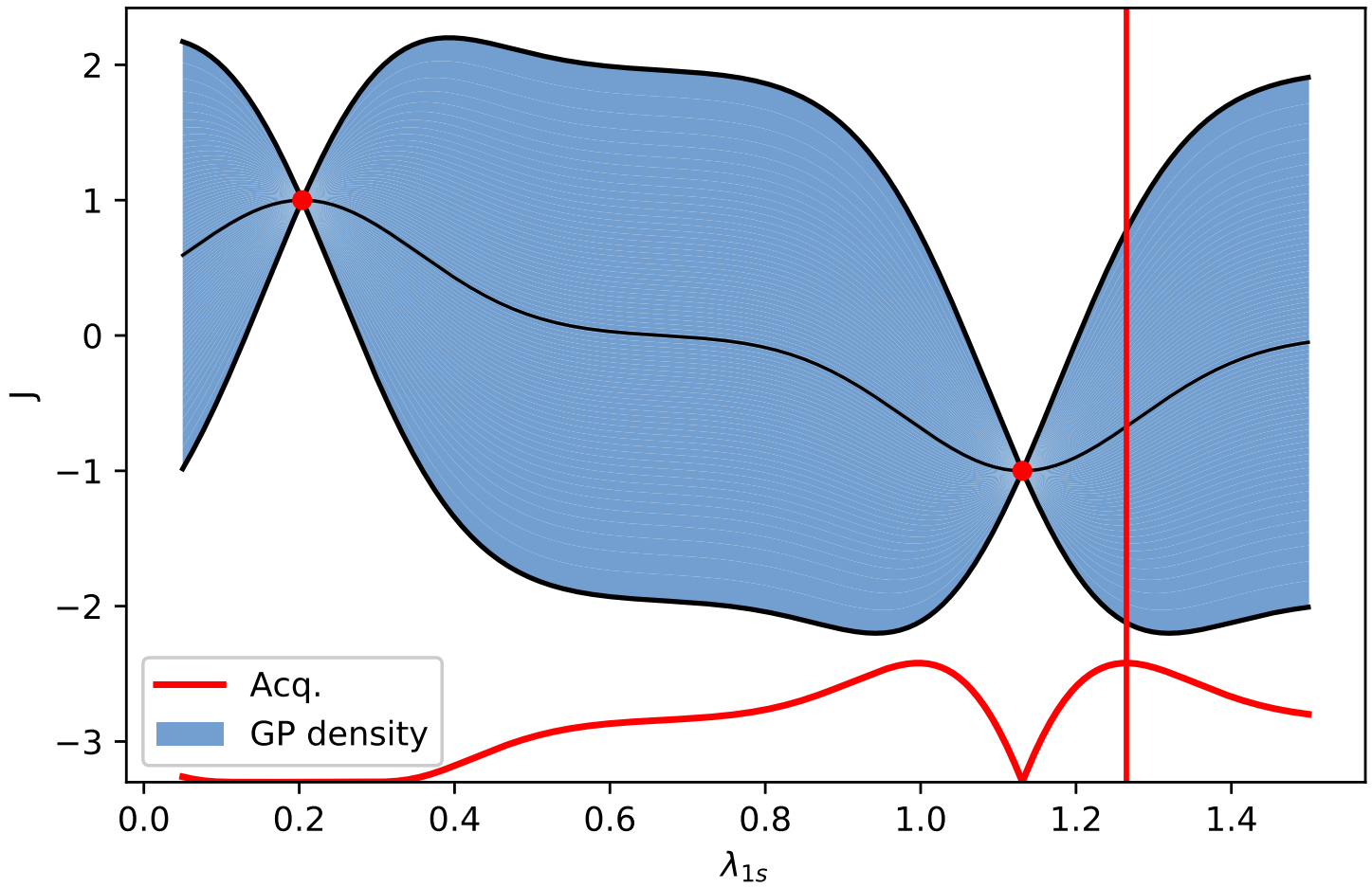
$$\left[\frac{1}{2}\frac{d^2}{dr^2} - \frac{l(l+1)}{2r^2} + V_{\text{eff}}(r) + \epsilon_{nl}\right] P_{nl}(r) = 0\,,$$

Model potential:

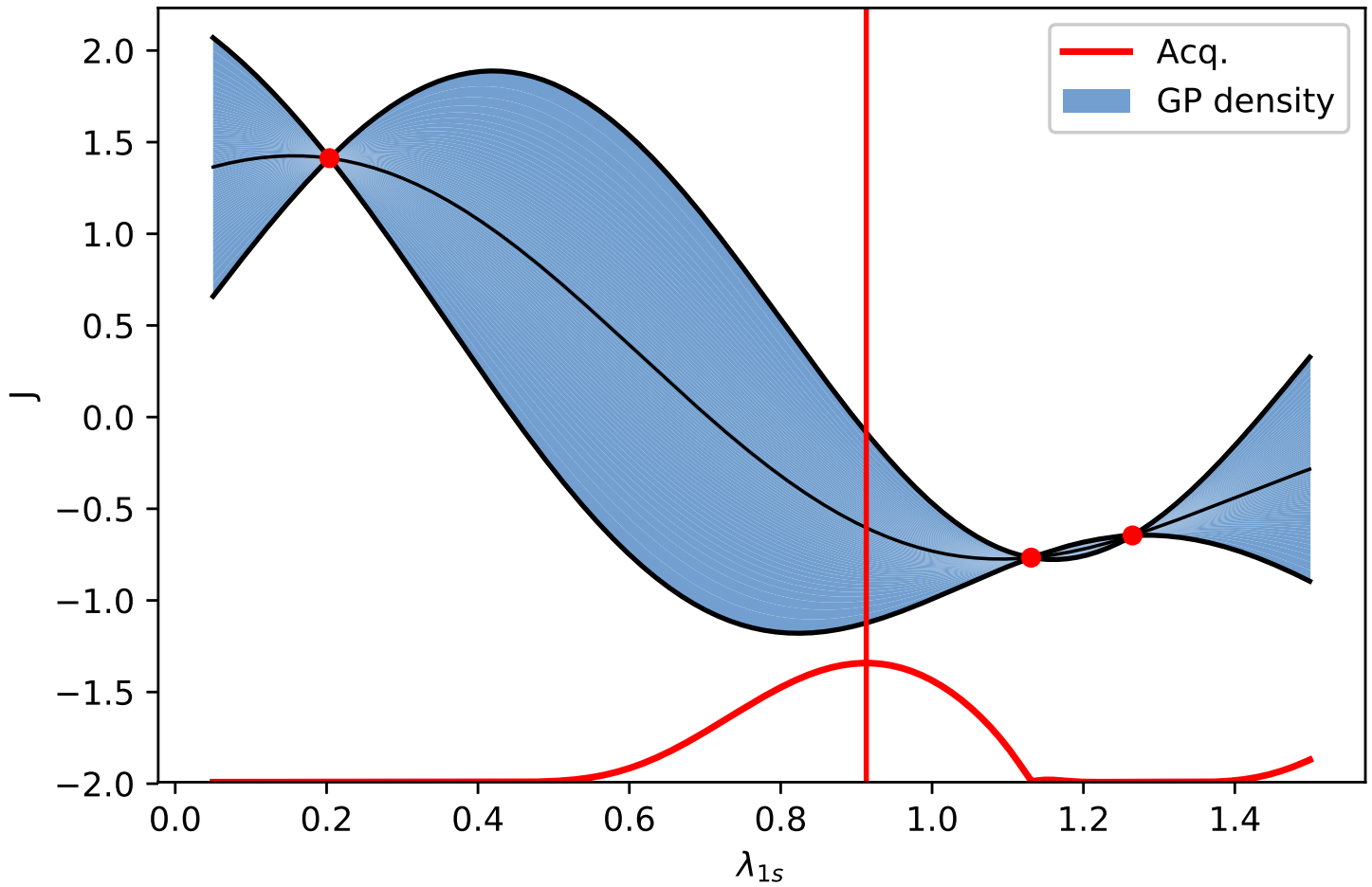
- Thomas–Fermi–Dirac–Amaldi [13].
- Slater-Type-Orbital potential of Burgess [23]
- Self-consistent configuration average potential of Cowan [7]

Optimización Bayesiana

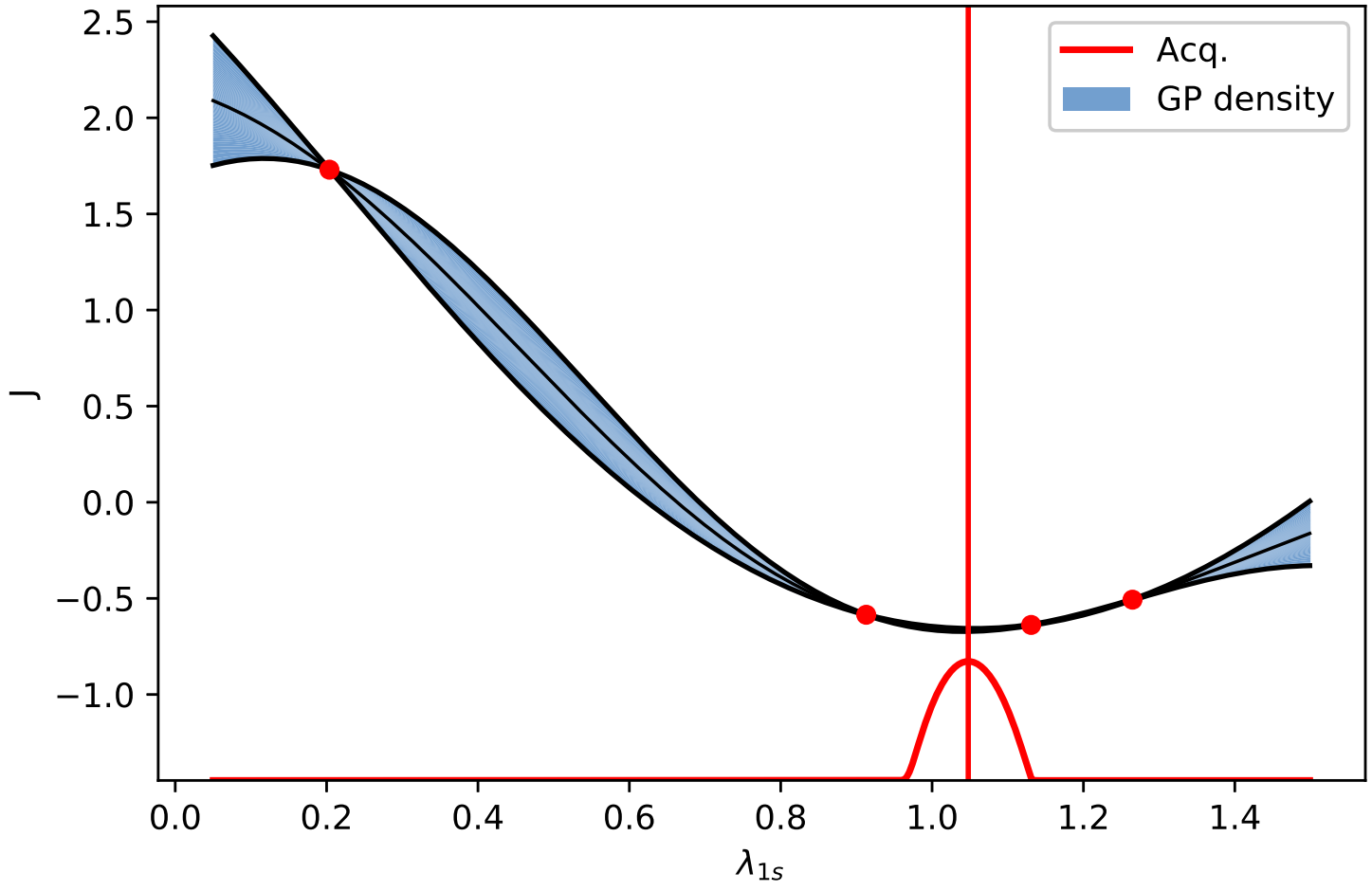
Gaussian Process



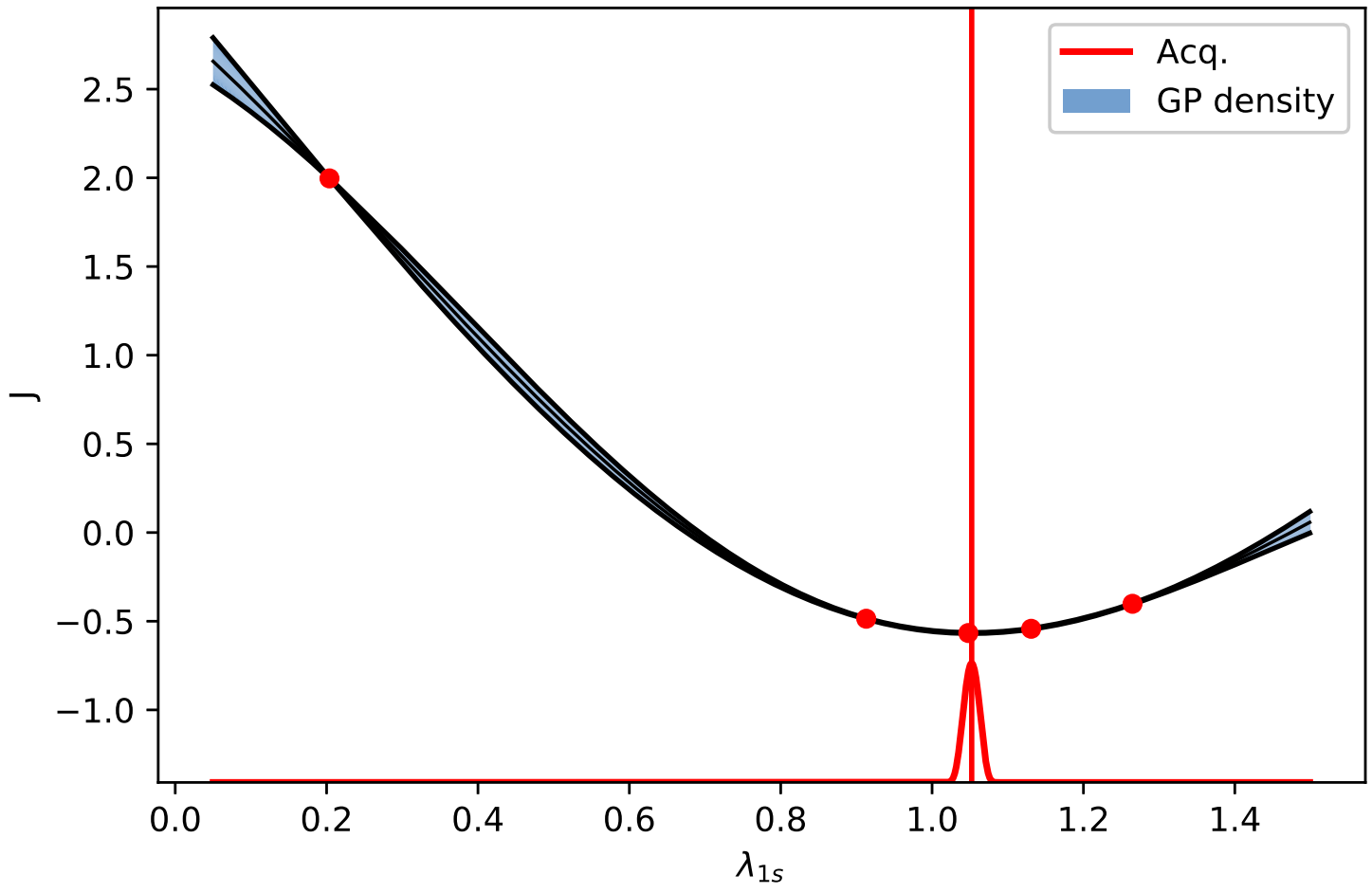
Gaussian Process



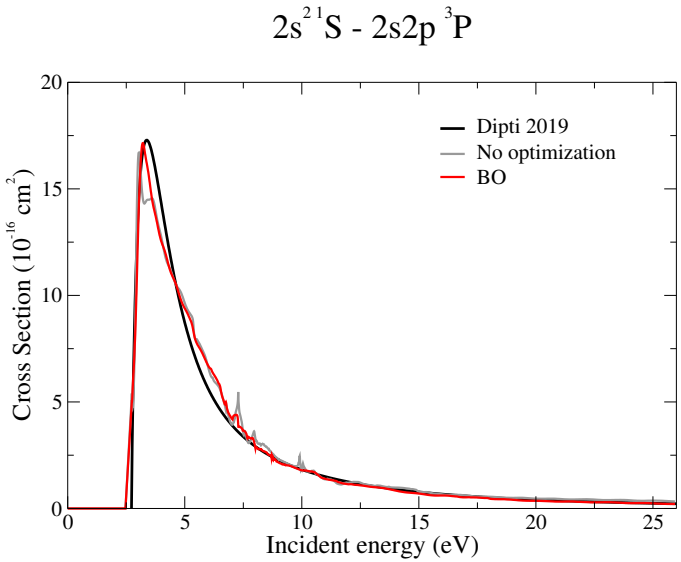
Gaussian Process

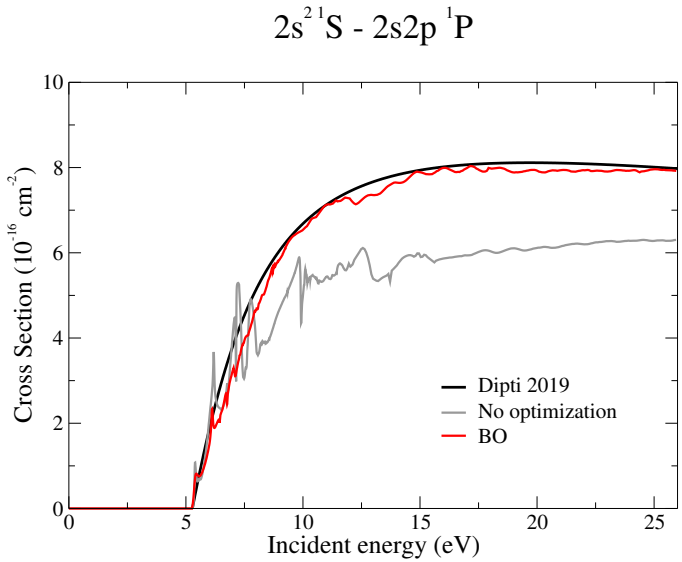


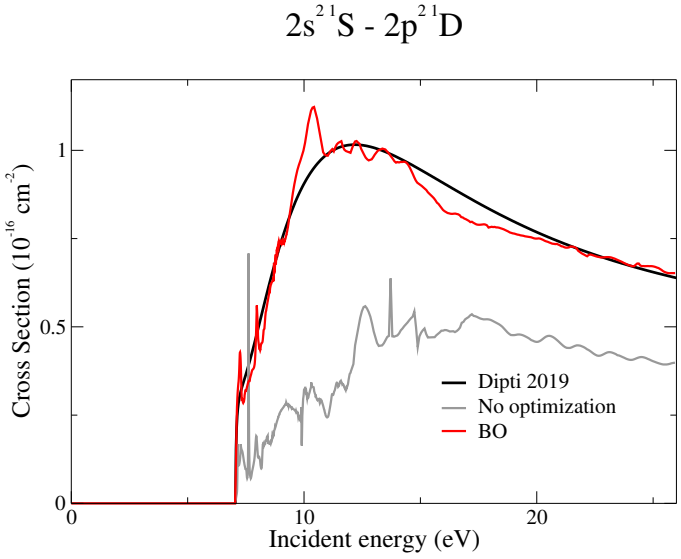
Gaussian Process

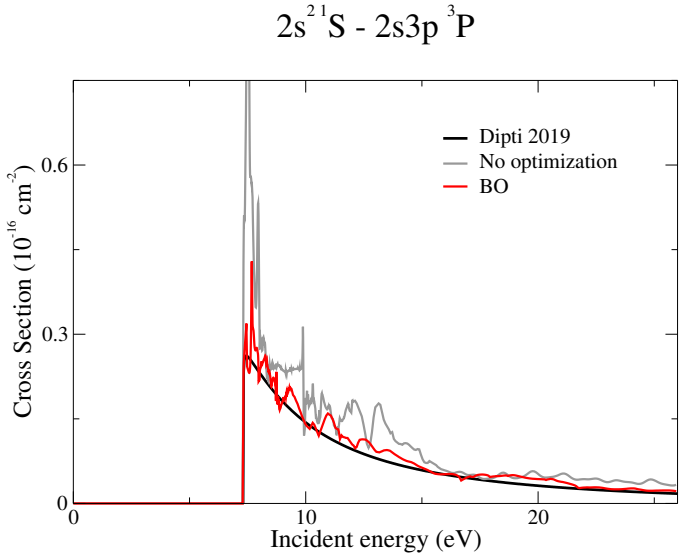


Resultados


2s² ¹S - 2s2p ³P
Dipti 2019
No optimization
BO
Cross Section (10⁻¹⁶ cm⁻²)
Incident energy (eV)


2s² ¹S - 2s2p ¹P
Dipti 2019
No optimization
BO
Cross Section (10⁻¹⁶ cm⁻²)
Incident energy (eV)


2s² ¹S - 2p² ¹D
Dipti 2019
No optimization
BO
Cross Section (10⁻¹⁶ cm⁻²)
Incident energy (eV)


2s² ¹S - 2s3p ³P
Dipti 2019
No optimization
BO
Cross Section (10⁻¹⁶ cm⁻²)
Incident energy (eV)