I Encuentro Nacional de Dinámica Cuántica en la Materia

Implementación de Métodos de Aprendizaje Automatizado en problemas colisionales

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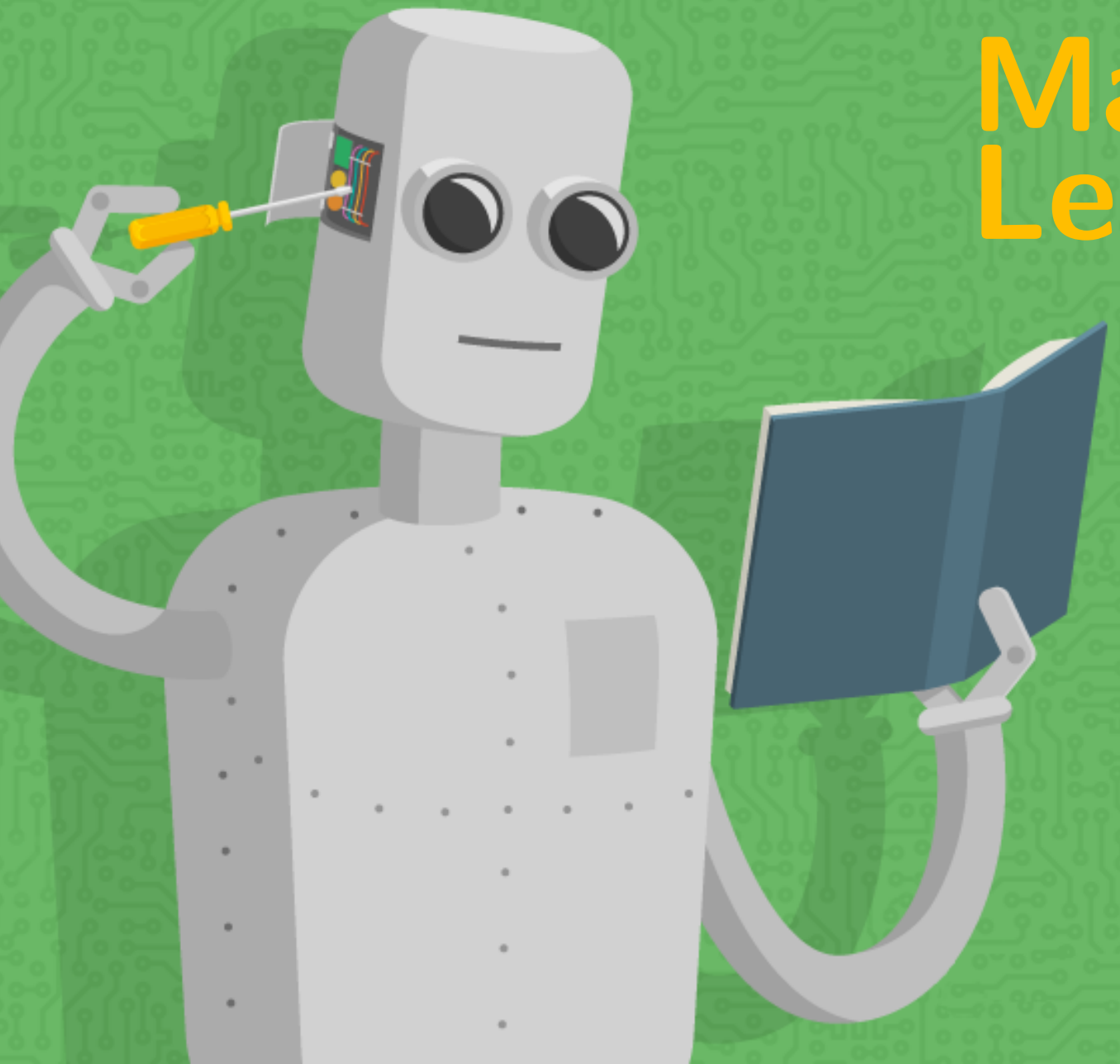
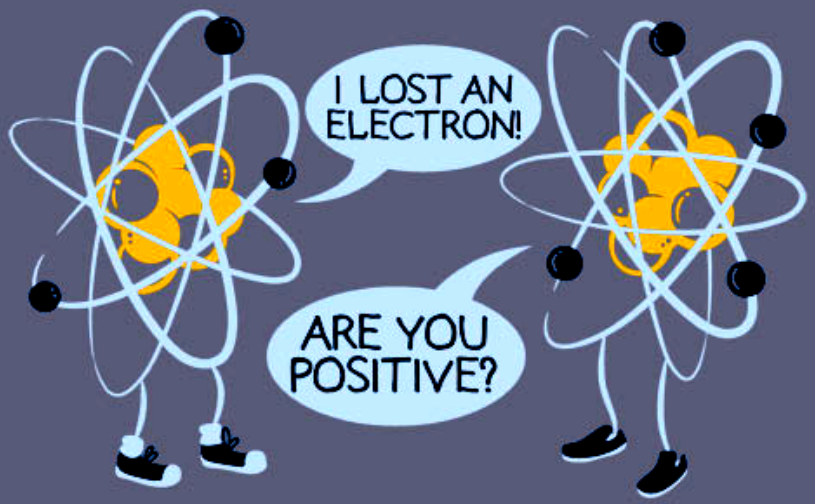


Machine Learning


I LOST AN ELECTRON!
ARE YOU POSITIVE?

Método de Inversión Depurada (DIM)

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

Método de Inversión Depurada (DIM)

¿Cómo conocemos V?

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$$\left[-\frac{1}{2}\frac{\partial^2}{\partial r^2} + \frac{l(l+1)}{2r^2} + \mathbf{V_{nl}(r)}\right] \varphi_{nl}(r) = E_{nl}\,\varphi_{nl}(r)$$

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$$\mathbf{V_{nl}(r)} = \frac{1}{2}\frac{\varphi''_{nl}(r)}{\varphi_{nl}(r)} - \frac{l(l+1)}{2r^2} + E_{nl}$$

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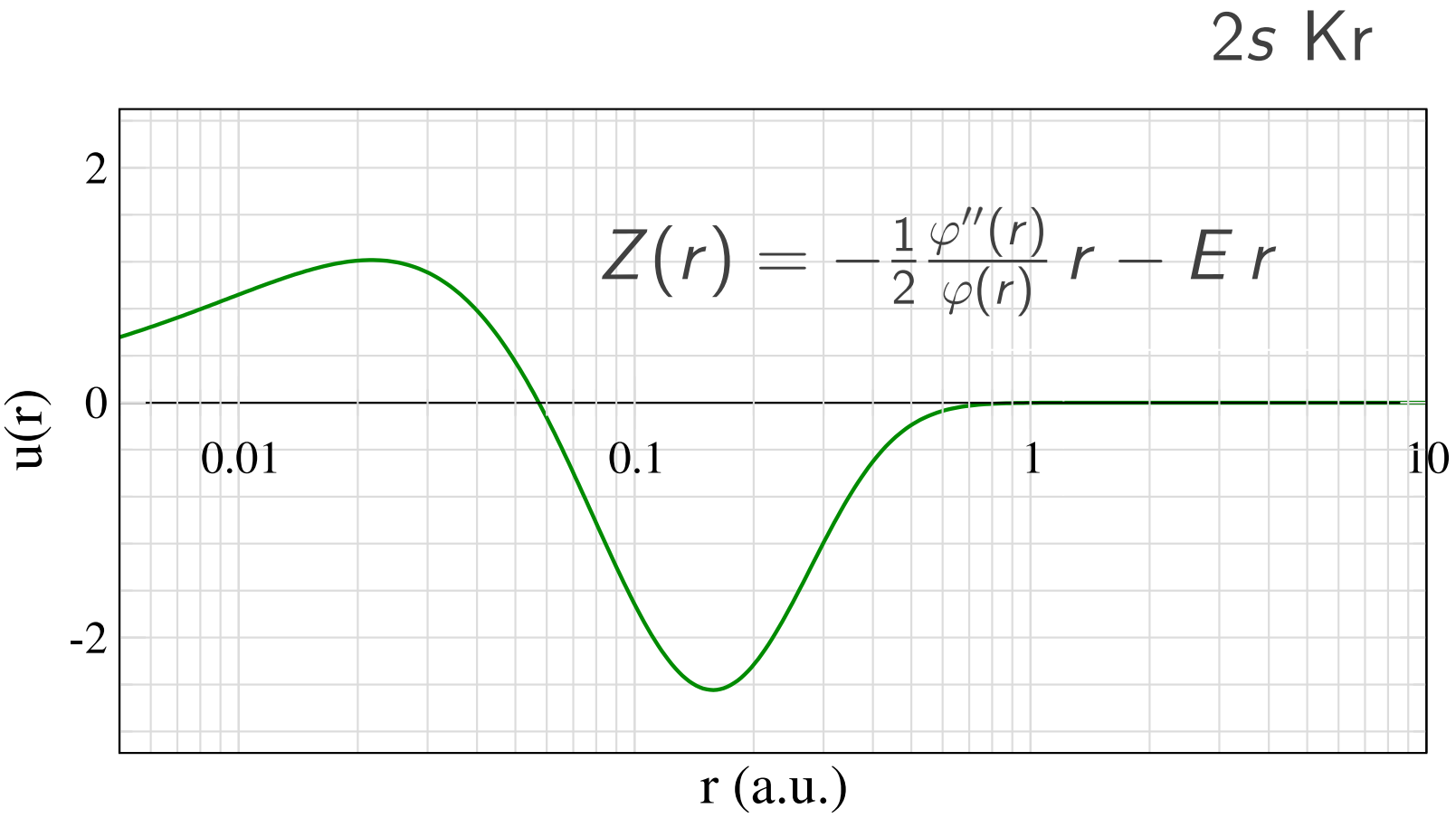
$$\mathbf{Z_{nl}(r)} = -\frac{1}{2}\frac{\varphi''_{nl}(r)}{\varphi_{nl}(r)}\,r + \frac{l(l+1)}{2r} - E_{nl}\,r$$

Houston, we have a problem!



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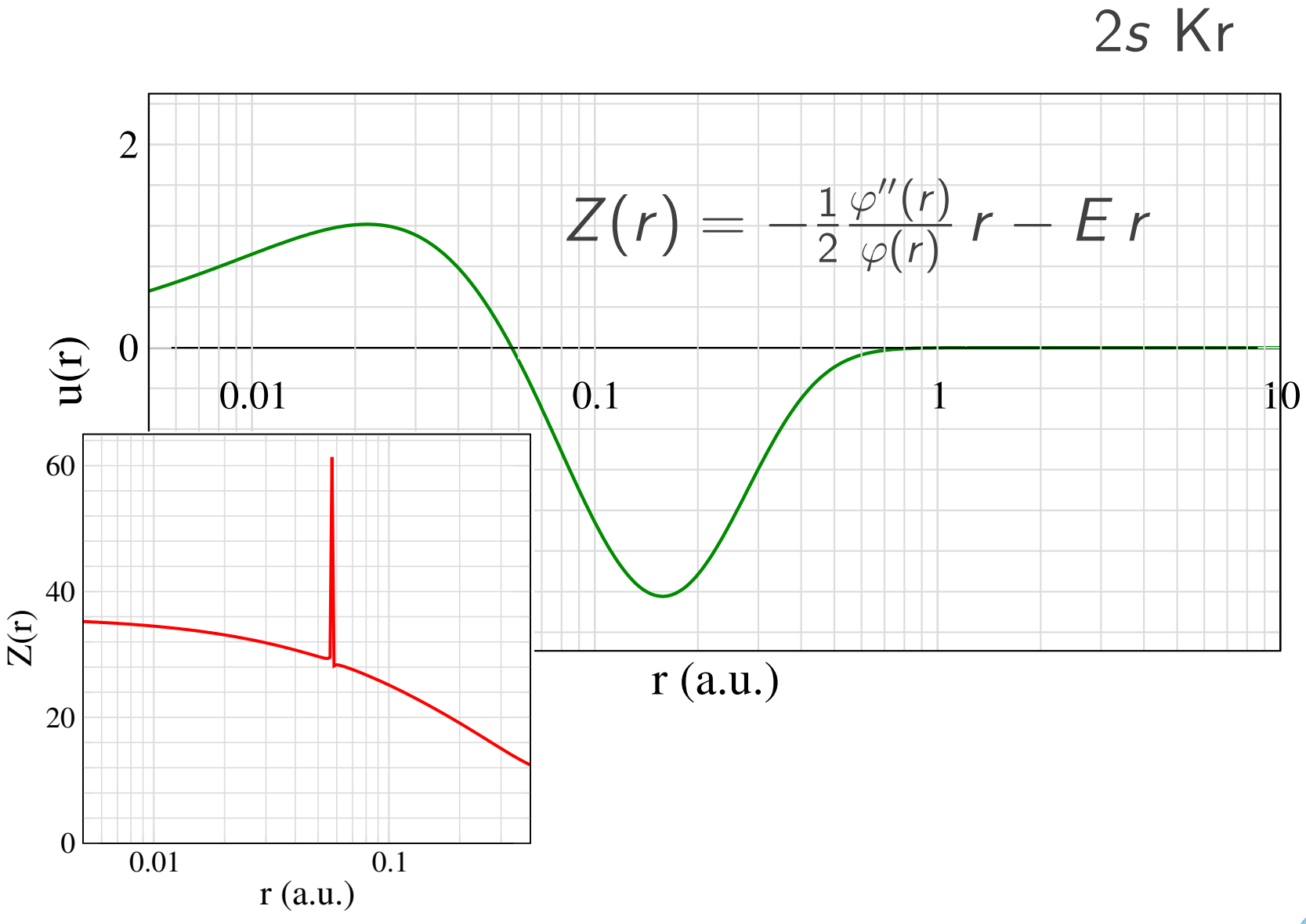

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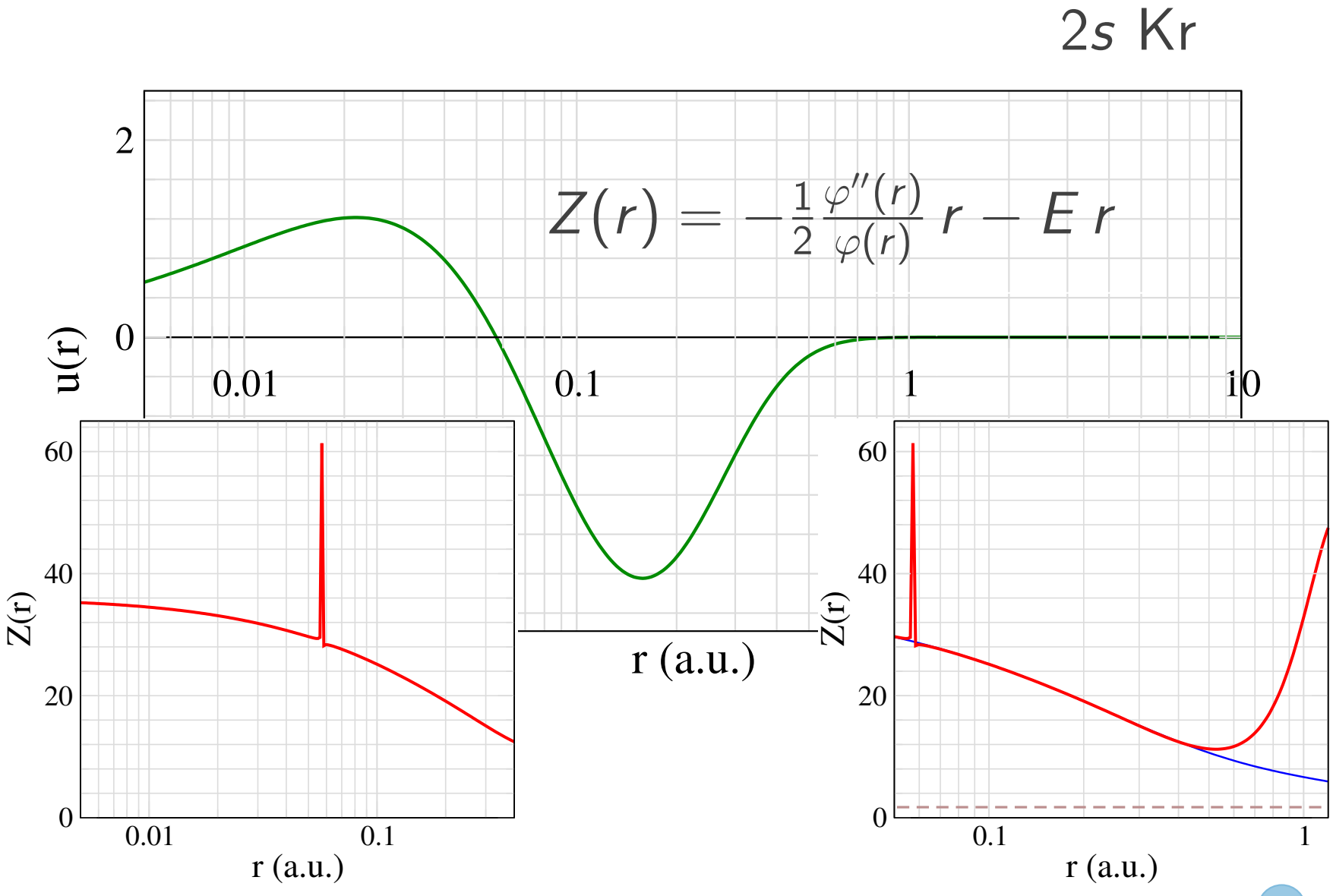
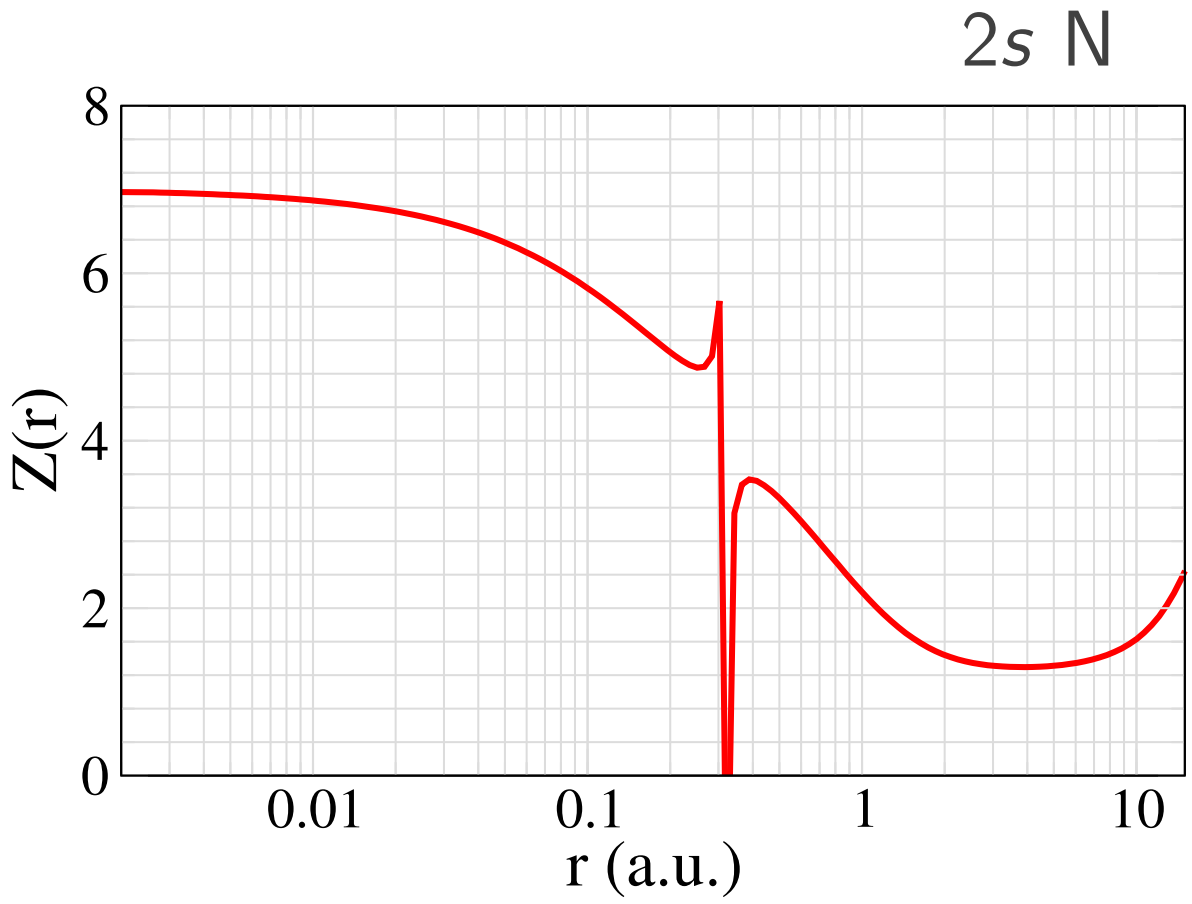
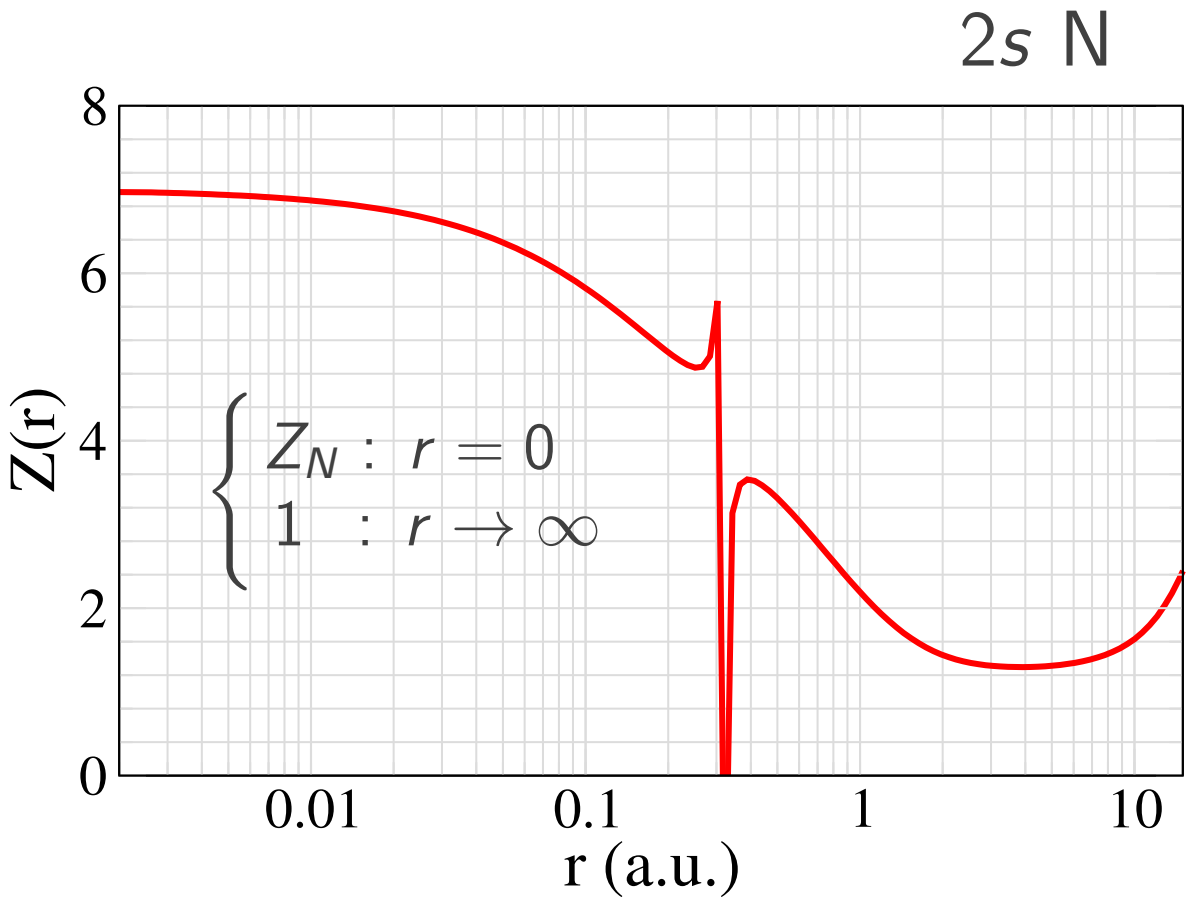


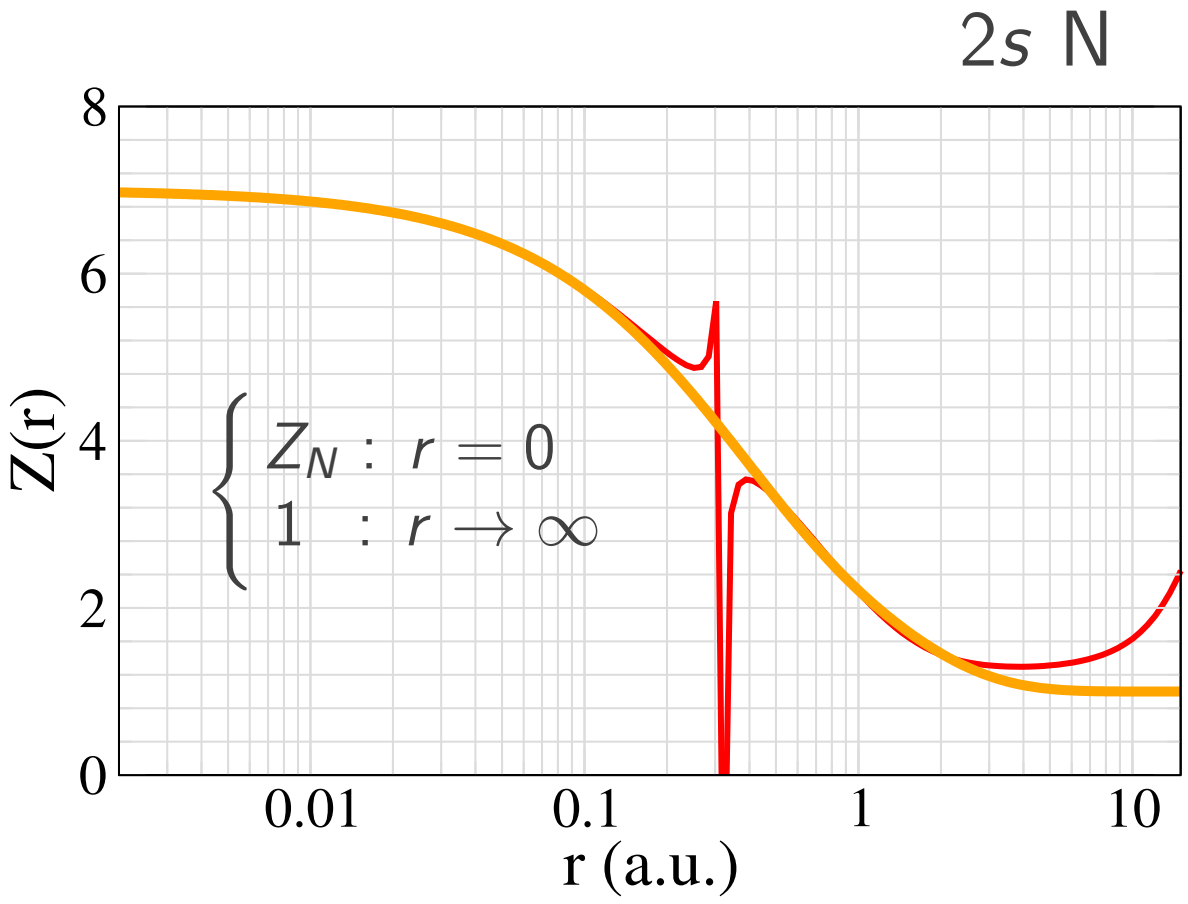
Depuración



Depuración

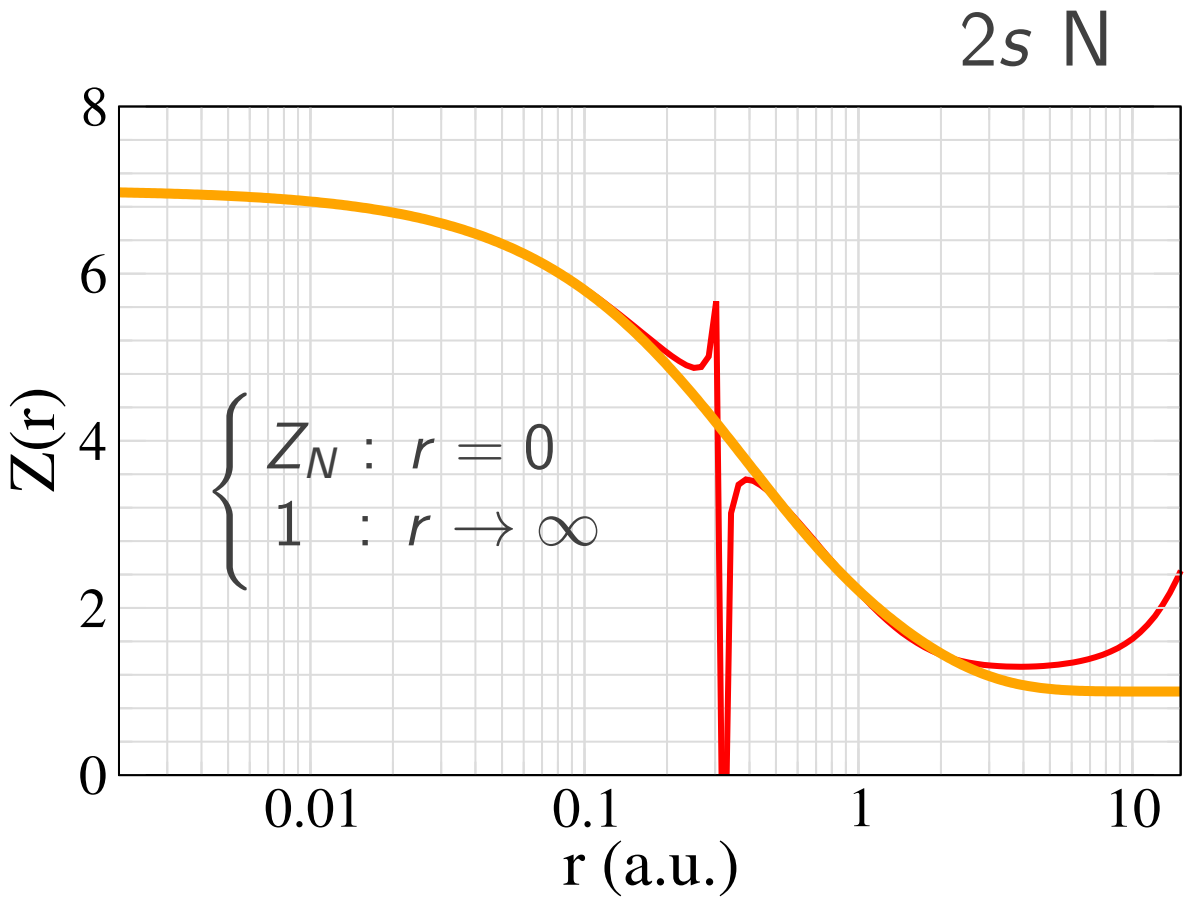

2s N
8
6
4
2
0
Z(r)
$\begin{cases} Z_N : r = 0 \\ 1 : r \to \infty \end{cases}$
0.01
0.1
1
10
r (a.u.)

Depuración



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

Depuración



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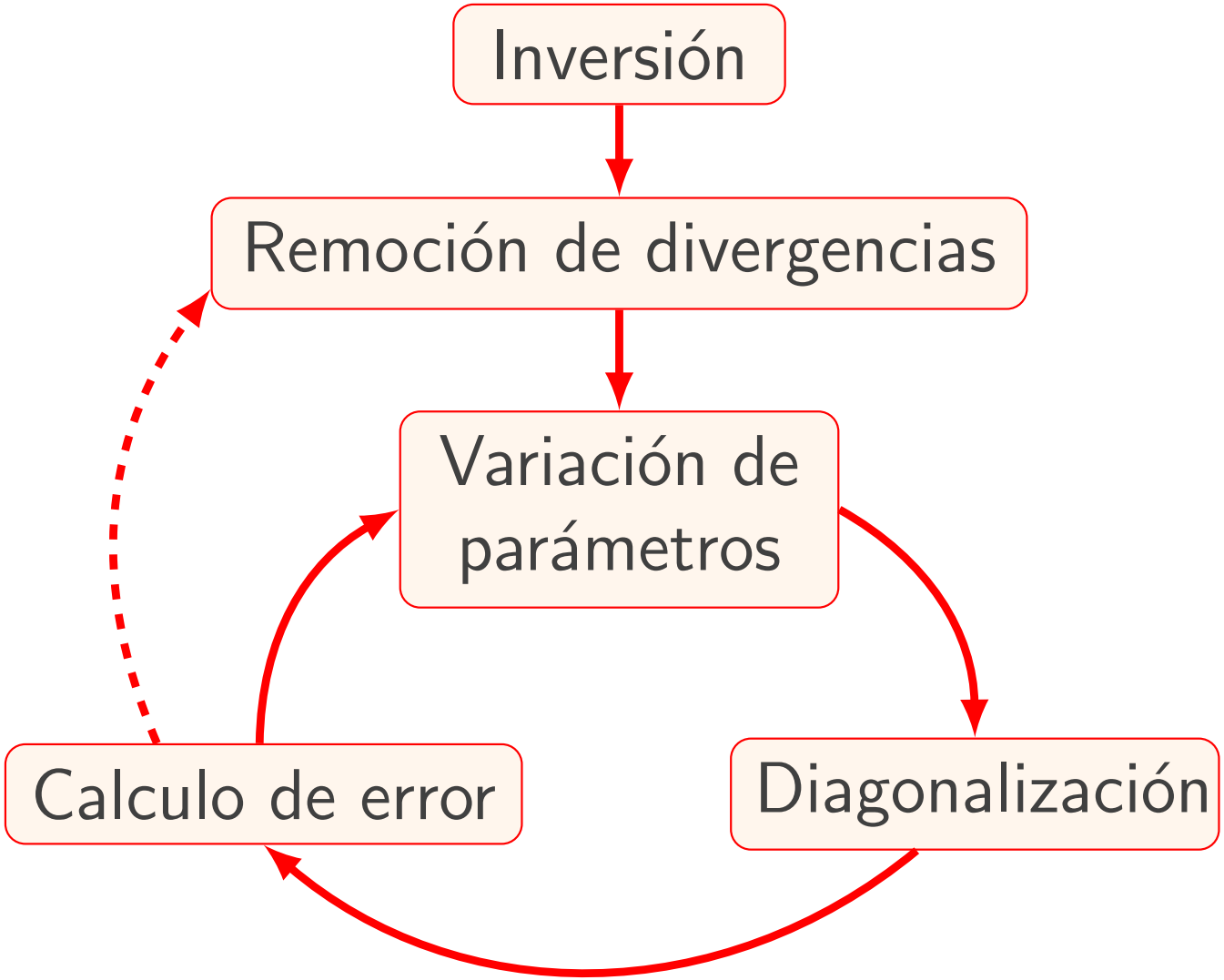
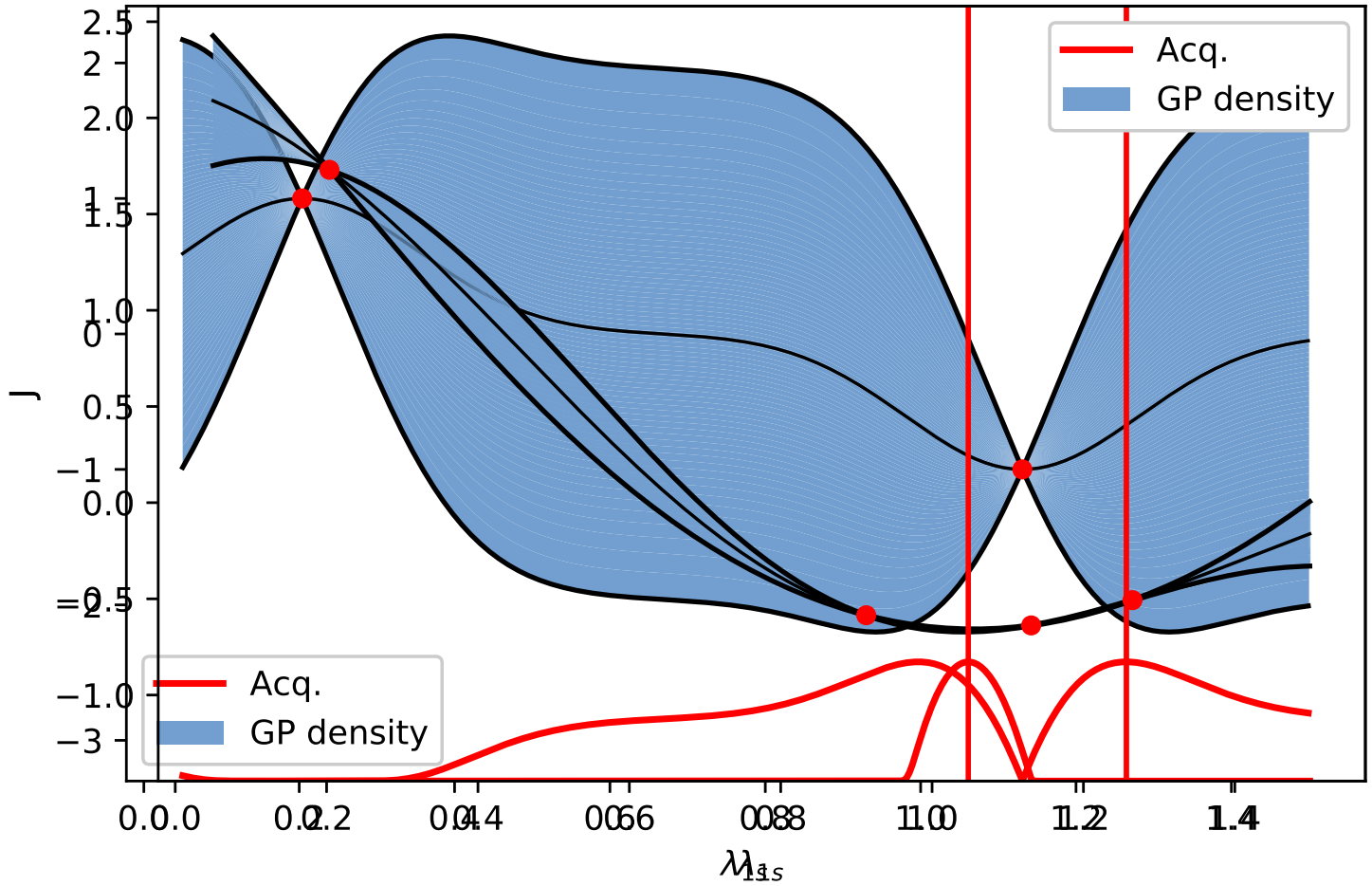
Procedimiento

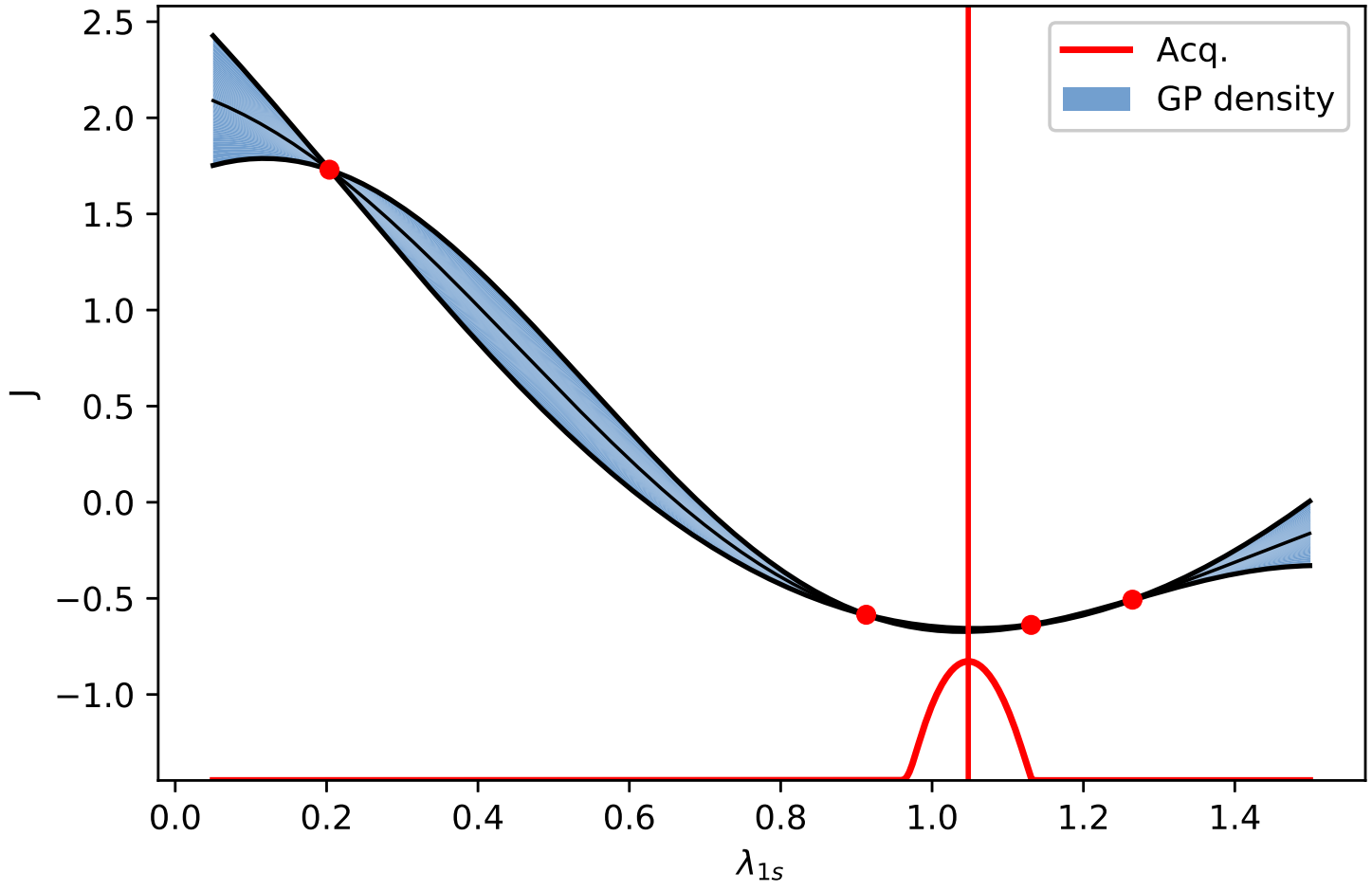


Optimización Bayesiana

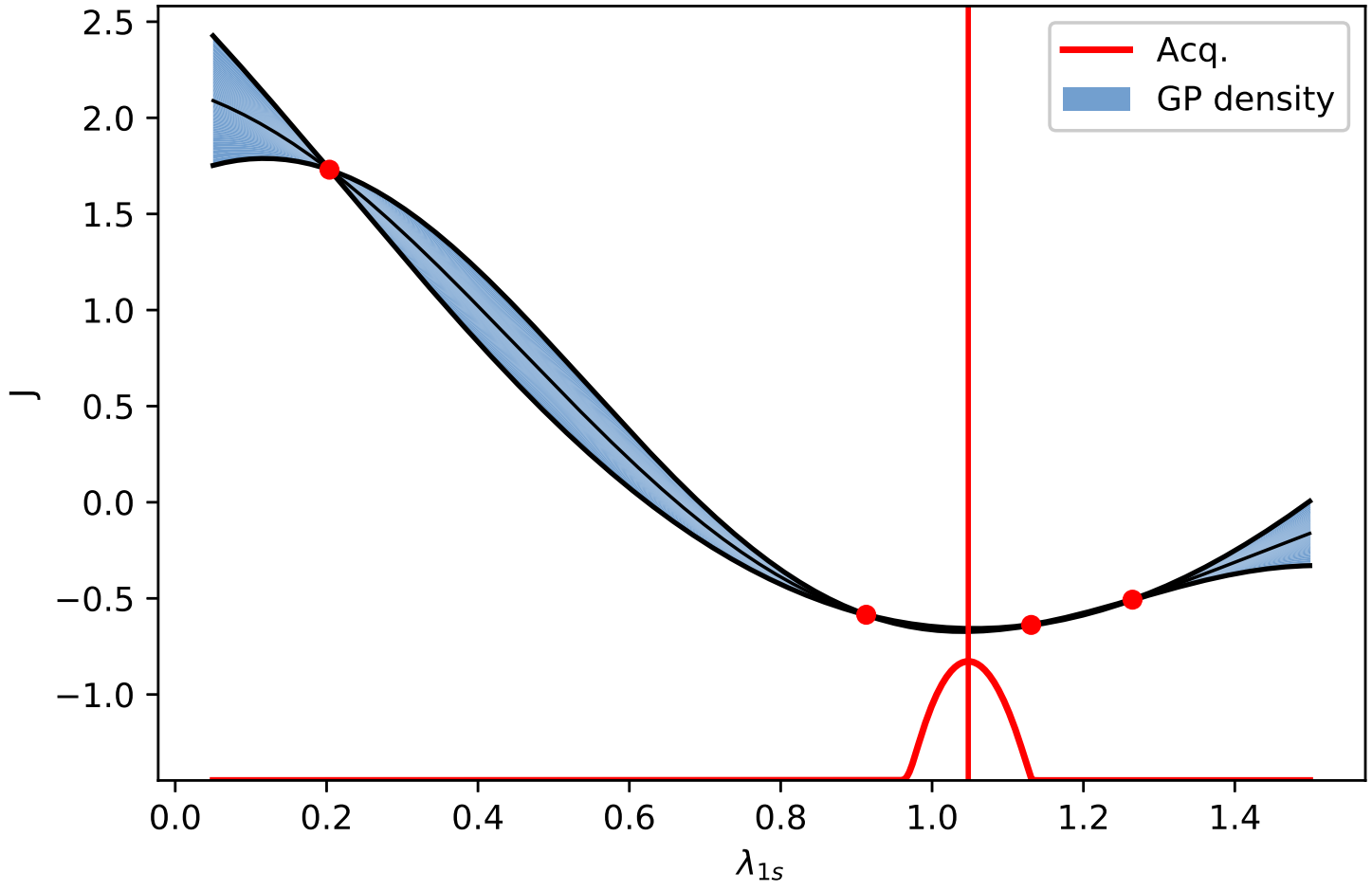
Gaussian Process



Gaussian Process



Gaussian Process



Gaussian Process