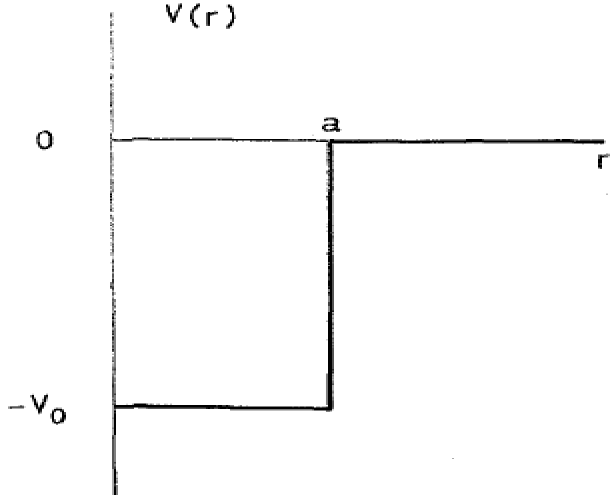
Pozo de potencial esférico finito



$$V(r) = \begin{cases} 0 \ \ si \ \ r > a \\ -V_0 \ si \ \ r < a \end{cases}$$

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\Psi + V(r)\Psi = E\Psi \qquad (3)$$

$$\Psi(r,\theta,\phi) = \mathrm{R(r)Y}(\theta,\phi)$$

$$\frac{d^2R}{d\rho^2} + \frac{2}{\rho}\frac{dR}{d\rho} + \left[1 - \frac{\ell(\ell+1)}{\rho^2}\right]R = 0$$

$\rho = \alpha r \quad para \ \ r < a \quad y \ \rho = i\beta r \quad para \ r > a$

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l = 0

$\Psi(r,\theta,\phi) = R(r)Y(\theta,\phi)$ $\qquad \chi(r) = R(r)/r$

$- \frac{h^2}{8m\pi^2}\frac{d^2\chi}{dr^2} - V_0\,\chi = E\,\chi \qquad r < a$

$- \frac{h^2}{8m\pi^2}\frac{d^2\chi}{dr^2} = E\,\chi \qquad r > a$

$\chi = A sen\,(\alpha r) \qquad r < a \qquad \alpha = \lfloor 8m\pi^2(V_0 - |E|)/h^2 \rfloor^{1/2}$

$\chi = Be^{-\beta r} \qquad r > a \qquad \beta = \lfloor 8m\pi^2|E|/h^2 \rfloor^{1/2}$

Igualando las derivadas logarítmicas (1/R) dR/dr de las dos soluciones en r = a , podemos obtener las energías de los estados s. Definimos:

$\xi = \alpha a$ $\qquad \eta = \beta a$ $\qquad \xi\, cotg\, \xi = -\eta$

$\xi^2 + \eta^2 = {u_0}^2 = 8m\,\pi^2 V_0 a^2/h^2$ $\qquad \xi^2 + \eta^2 = {u_0}^2$

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l = 0

$$\alpha = [8m\pi^2(V_0 - |E|)/h^2]^{1/2} \qquad \beta = [8m\pi^2|E|/h^2]^{1/2}$$

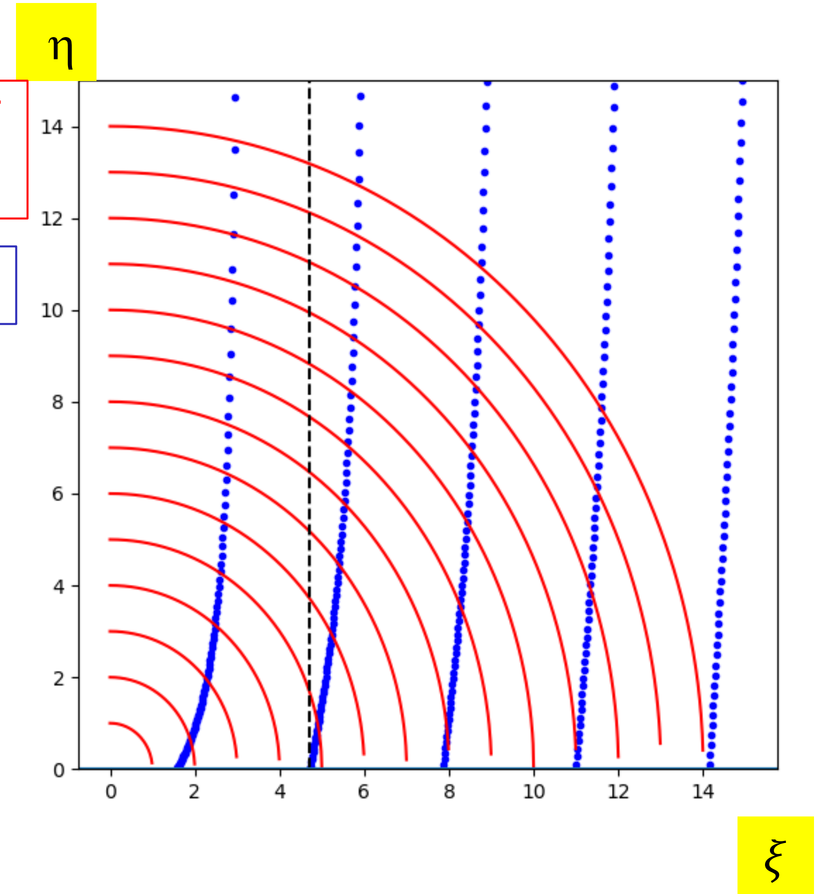
$$\xi\, cotg\, \xi = -\eta \qquad \xi = \alpha\, a$$

$$\xi^2 + \eta^2 = {u_0}^2 \qquad \eta = \beta\, a$$

$$\eta = \sqrt{{u_0}^2 - \xi^2}$$

$$\xi^2 + \eta^2 = {u_0}^2 = 8\mathrm{m}\, \pi^2 V_0 a^2/h^2$$

$$\xi\, cotg\, \xi = -\eta$$



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l = 0

$$\alpha = [8m\pi^2(V_0 - |E|)/h^2]^{1/2} \qquad \beta = [8m\pi^2|E|/h^2]^{1/2}$$

$\xi = \alpha\, a$

$\eta = \beta\, a$

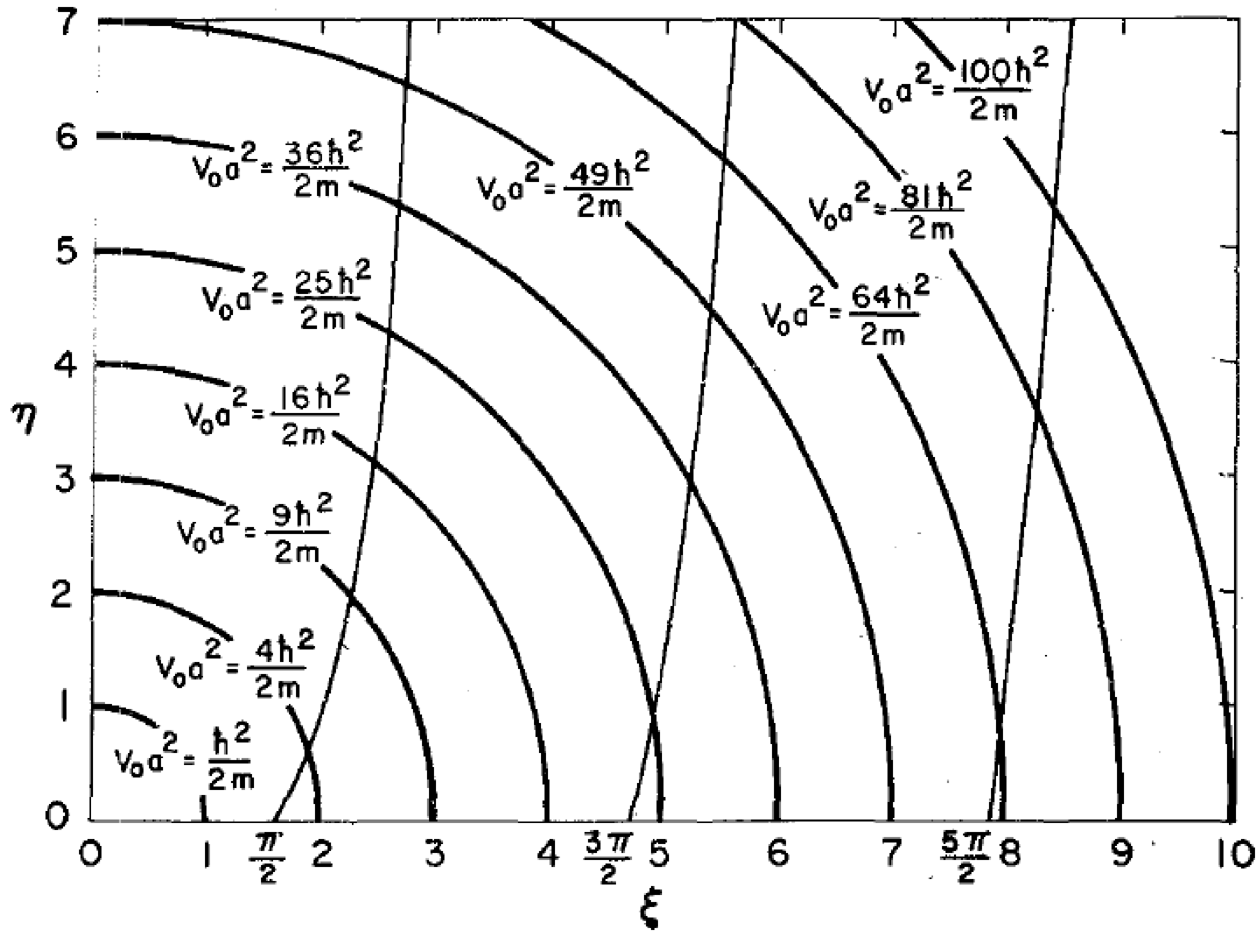

Fig. 2 - Curves of $\eta = -\xi \cot\xi$ and $\xi^2 + \eta^2 = 2mV_0a^2/\hbar^2$.

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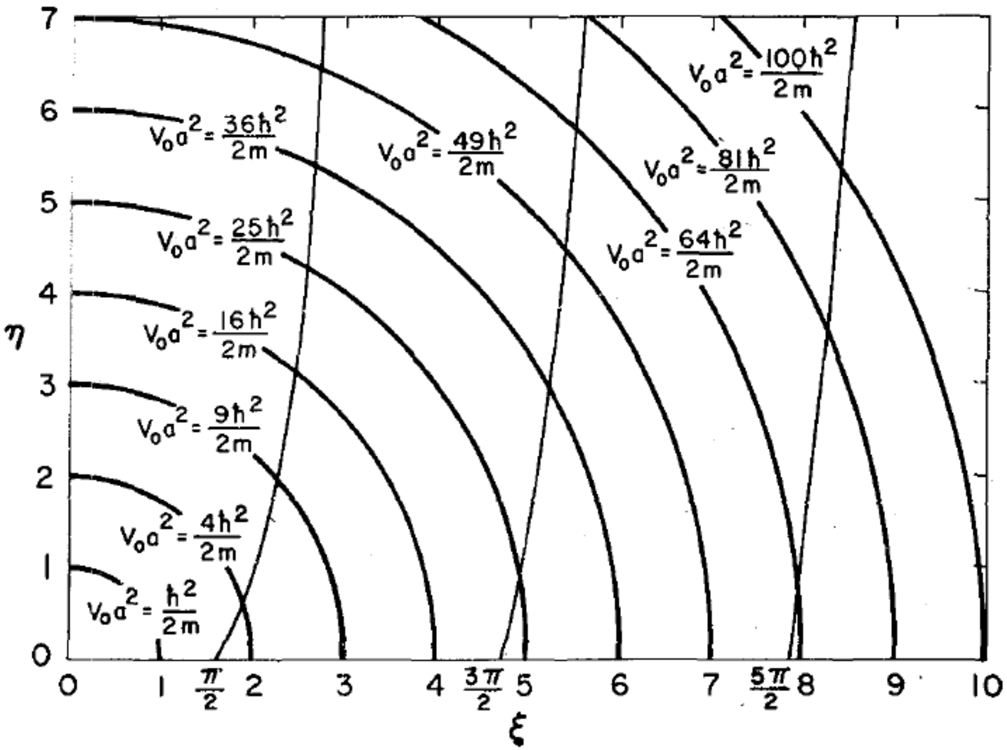
l = 0



no bound s-states if $V_0a^2 \leqslant (\pi^2\hbar^2/8m)$

one bound s-state if $(\pi^2\hbar^2/8m) < V_0a^2 \leqslant (9\pi^2\hbar^2/8m)$

two bound s-state if $(9\pi^2\hbar^2/8m) < V_0a^2 \leqslant (25\pi^2\hbar^2/8m)$

etc.

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$\ell =$ arbitrario

$$\frac{d^2R}{d\rho^2} + \frac{2}{\rho}\frac{dR}{d\rho} + \left[1 - \frac{\ell(\ell+1)}{\rho^2}\right]R = 0$$

$$\rho = \alpha r \quad para\ r < a \quad y\ \rho = i\beta r \quad para\ r > a$$

$\ell =$ 1

$$j_1(\rho) = \frac{sen\ \rho}{\varrho^2} - \frac{cos\rho}{\varrho} \qquad para\ r < a \quad \text{(Bessel esférica)}$$

$$h_1(i\beta r) = i\left(\frac{1}{\beta r} + \frac{1}{\beta^2 r^2}\right)e^{-\beta r} \qquad para\ r > a \quad \text{(Hankel esférica)}$$

Niveles de energía

$$\frac{cotg\xi}{\xi} - \frac{1}{\xi^2} = \frac{1}{\eta} + \frac{1}{\eta^2} \longrightarrow S(\xi)\eta^2 - \eta - 1 = 0$$

$$\xi^2 + \eta^2 = {u_0}^2$$

Pozo de potencial esférico finito

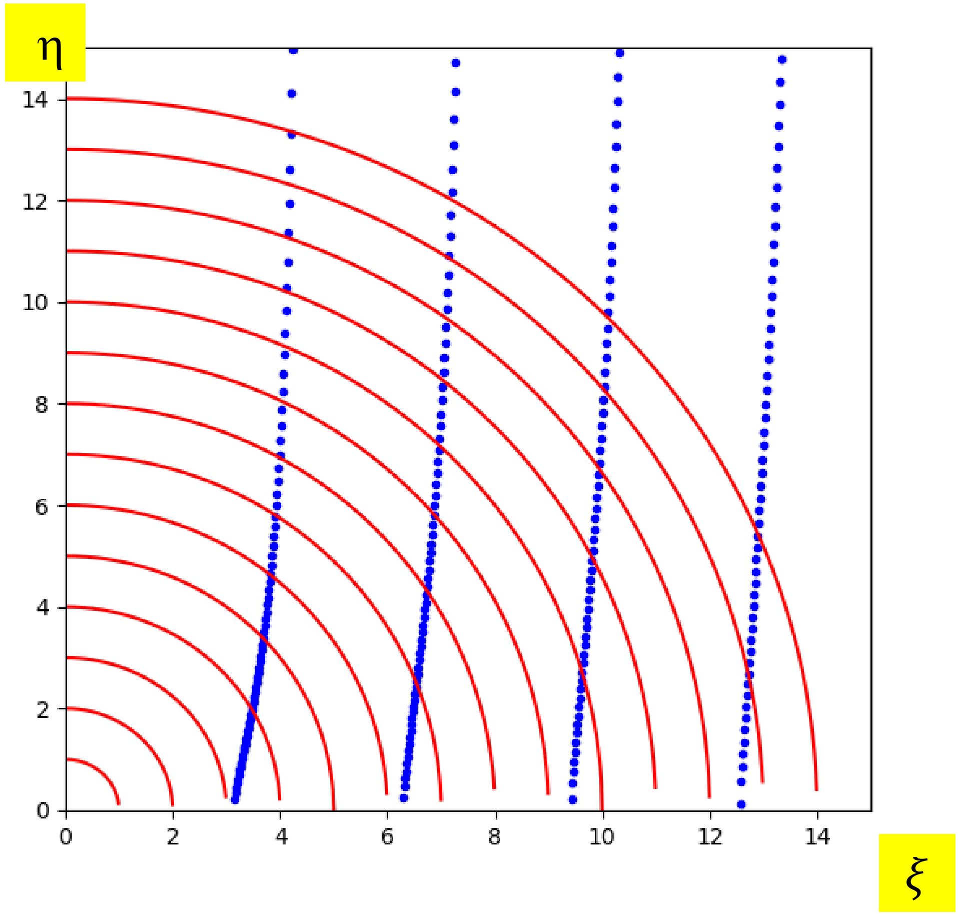
Niveles de energía $\ell = 1$

$$\frac{cotg\xi}{\xi} - \frac{1}{\xi^2} = S(\xi)$$

$$S(\xi)\eta^2 - \eta - 1 = 0$$

$$\eta = \frac{1 + \sqrt{1 + 4S(\xi)}}{2S(\xi)}$$

$$\xi^2 + \eta^2 = {u_0}^2$$



Pozo de potencial esférico finito

$\ell = 1$

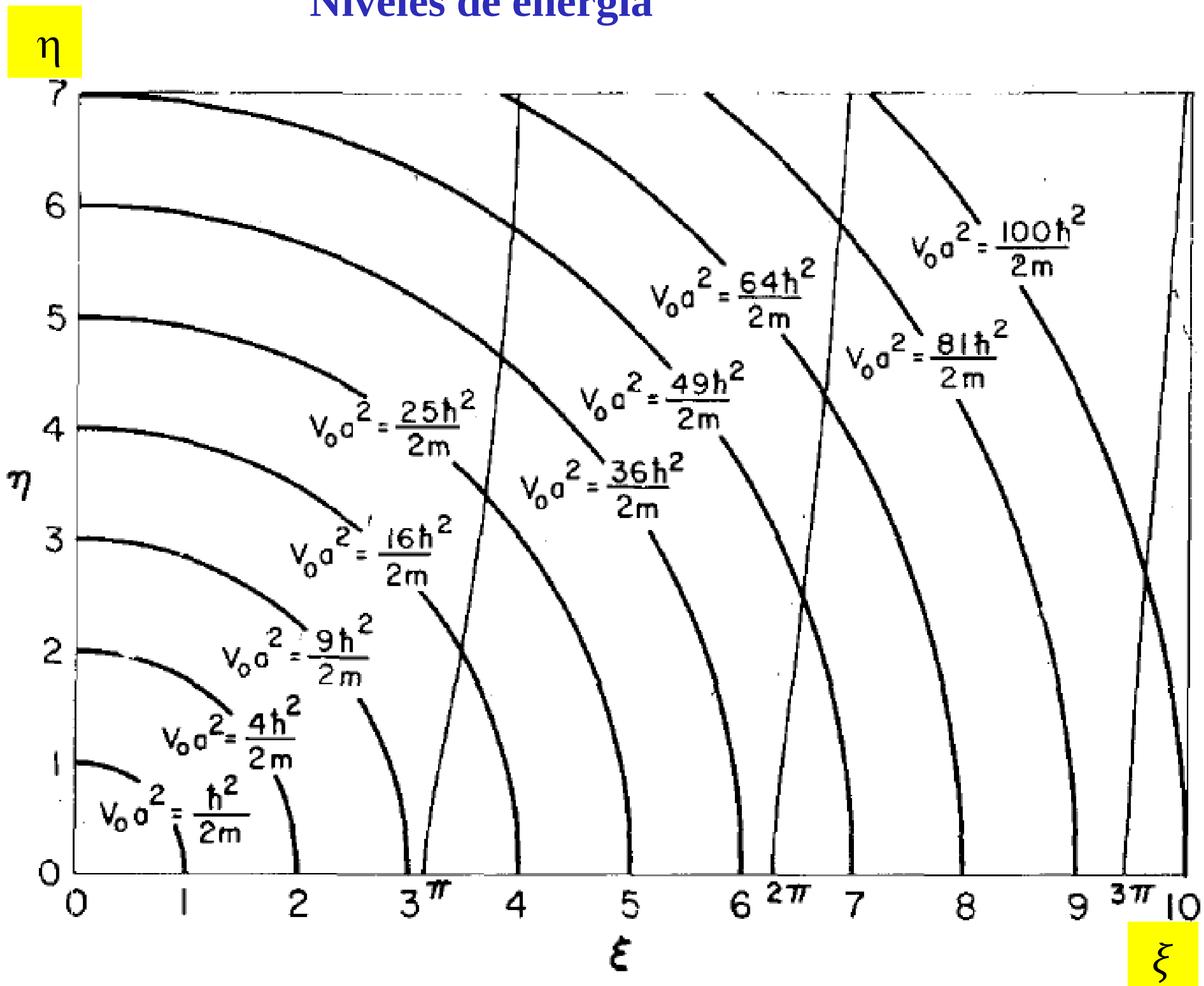
$$\frac{cotg\xi}{\xi} - \frac{1}{\xi^2} = S(\xi)$$

$$S(\xi)\eta^2 - \eta - 1 = 0$$

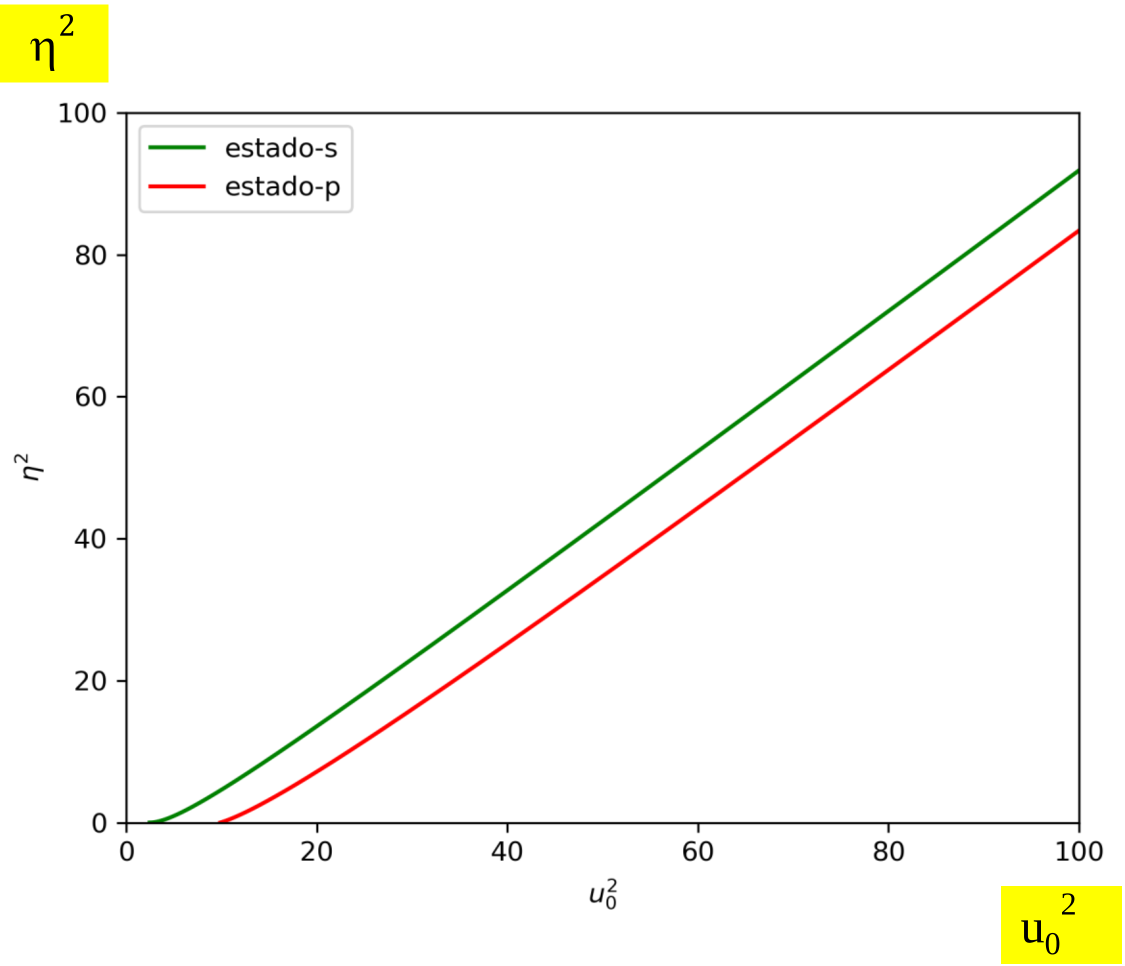
$$\eta = \frac{1 + \sqrt{1 + 4S(\xi)}}{2S(\xi)}$$

$$\xi^2 + \eta^2 = u_0{}^2$$

Niveles de energía



Pozo de potencial esférico finito



Pozo de potencial esférico finito

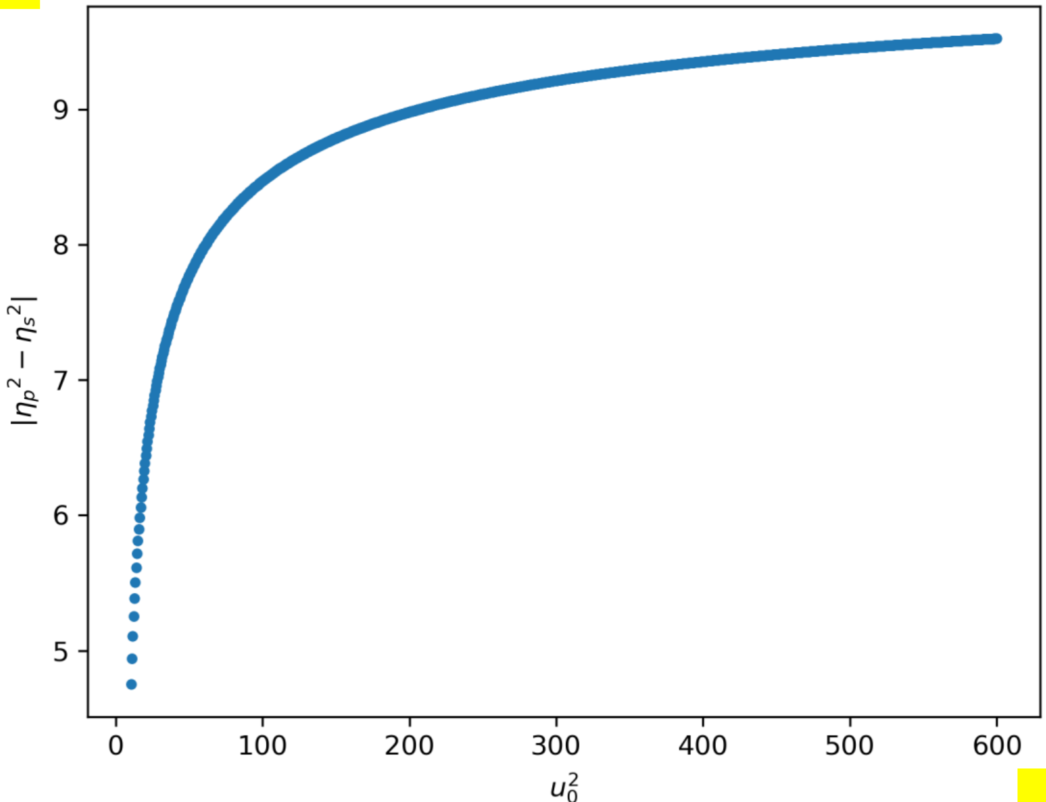
E, V_0 [eV]; R [nm]

$$\Delta\eta^2 = \frac{8m\pi^2}{h^2}|\Delta E|R^2$$

$$\Delta\eta^2 = 26.18|\Delta E|R^2$$

$$u_0^2 = 26.18\, V_0 R^2$$

$\Delta\eta^2$



u_0^2

Pozo infinito

$$\Delta E = \frac{\hbar^2}{2\mu R^2}(z_{1,1}^2 - z_{1,0}^2) \approx 10{,}315\frac{\hbar^2}{2\mu R^2}$$

Pozo de potencial esférico finito

E, V_0 [eV]; a, R [nm]

$$\Delta\eta^2 = \frac{8m\pi^2}{h^2}|\Delta E|R^2$$

$\Delta\eta^2$

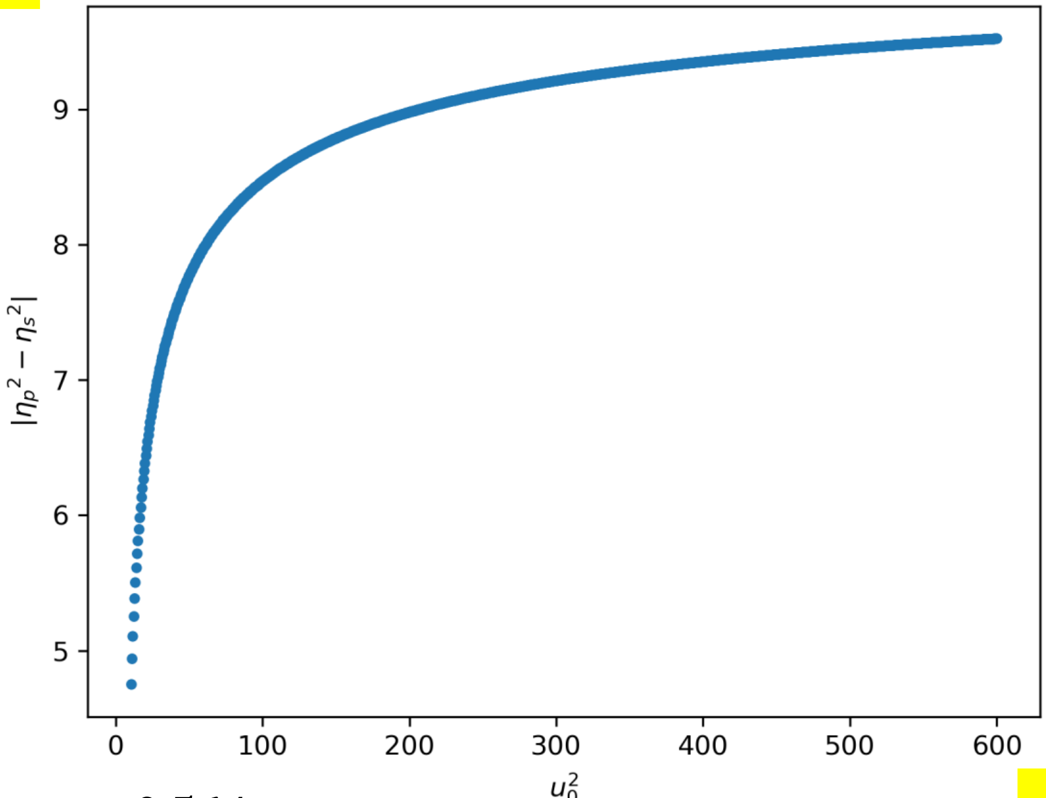
$$\Delta\eta^2 = 26.18\,|\Delta E|R^2$$

$$u_0^2 = 26.18\,V_0 R^2$$

ClNa: 2,746 eV ; a = 0.564 nm

R = a/2

$$\Delta E = E_{1p} - E_{1s} = 2.75\ eV$$



u_0^2

$$\Delta\eta^2 = 26.18 * 2.75 * 0.564 * \frac{0.564}{4} = 5.725$$

$u_0^2 \sim 10$

$V_0 \sim 4.8$ eV

Pozo de potencial esférico finito

E, V_0 [eV]; a, R [nm]

$$\Delta\eta^{\,2} = \frac{8m\pi^2}{h^2}|\Delta E|R^2$$

$$\Delta\eta^{\,2} = 26.18\,|\Delta E|R^2$$

$$u_0^{\,2} = 26.18\,V_0 R^2$$

Para los centros F de interés, es :

$$|\Delta E| = 68\,(10a)^{-1.85}$$

según la ley de Mollwo – Ivey (con «a» en nanómetros , E en eV)

Asumiendo $R = x * a$

$$\Delta\eta^{\,2} = 26.18\,|\Delta E|R^2 = 26.18 * 68\,(10a)^{-1.85} * \,(xa)^2$$

$$\Delta\eta^{\,2} = 25.15\, *\, a^{0.15}\, x^2$$

Para $x = 0.5 \quad y \quad 0.4 \le a \le 0.74 \qquad debe\ ser: \qquad 5.48 \le \Delta\eta^{\,2} \le 6$