

# Equação de Schrödinger Independente do Tempo via Numerov-Cooley PPGFIS

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# Curvas

- Curva parametrizada:

$$\alpha(t) = (x(t), y(t), z(t)). \quad (1)$$

- Função comprimento:

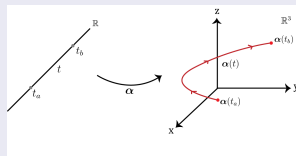
$$s(t) = \int |\alpha'(t)| dt. \quad (2)$$

- Parametrização por comprimento de arco (p.c.a.):

$$\alpha(t(s)), \text{ com } |\alpha'(s)| = 1 \forall s. \quad (3)$$

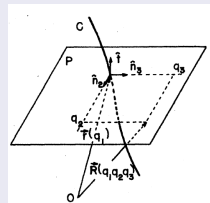
- Curvatura:

$$\kappa(s) = |\alpha''(s)|. \quad (4)$$



R. C. T. da Costa, *Phys. Rev. A* **23**, 1982 (1981)

$$\psi'' + (\varepsilon - \mathcal{V})\psi = 0 \quad (7)$$



## Problema de Valor de Contorno

Temos um problema de valor de contorno,

$$\psi''(x) + P(x)\psi(x) = 0, \quad \psi(x_0) = 0, \psi(x_N) = b. \quad (8)$$

Considere agora o seguinte problema de valor inicial,

$$v''(x) + P(x)v(x) = 0, \quad v(x_0) = 0, v'(x_0) = s. \quad (9)$$

Seja  $w(x) = \theta v(x)$  que atenda  $w(x_N) = b$ . Para isso  $\theta = b/v(x_N)$ . Então,

$$\psi(x) = w(x) = \frac{b}{v(x_N)} v(x). \quad (10)$$

Ainda,

$$\psi_1 = \psi'(x_0)\Delta x + \psi_0. \quad (11)$$

## Numerov

Expandindo usando série de Taylor,

$$\psi(x+\Delta x) = \psi(x) + \psi'(x)\Delta x + \frac{1}{2}\psi''(x)\Delta x^2 + \frac{1}{6}\psi^{(3)}(x)\Delta x^3 + \frac{1}{24}\psi^{(4)}(x)\Delta x^4 + \dots$$

$$\psi(x-\Delta x) = \psi(x) - \psi'(x)\Delta x + \frac{1}{2}\psi''(x)\Delta x^2 - \frac{1}{6}\psi^{(3)}(x)\Delta x^3 + \frac{1}{24}\psi^{(4)}(x)\Delta x^4 + \dots$$

$$\psi(x+\Delta x) + \psi(x-\Delta x) = 2\psi(x) + \psi''(x)\Delta x^2 + \frac{1}{12}\psi^{(4)}(x)\Delta x^4. \quad (12)$$

mas,

$$\psi''(x) = -(V - E)\psi(x) = -P(x)\psi(x), \quad (13)$$

$$\psi^{(4)}(x) = \frac{d^2\psi''(x)}{dx^2} = \frac{\psi''(x+\Delta x) + \psi''(x-\Delta x) - 2\psi''(x)}{\Delta x^2}. \quad (14)$$

## Numerov

Fazendo as substituições,

$$\begin{aligned}\psi(x + \Delta x) \left( 1 + P(x + \Delta x) \frac{\Delta x^2}{12} \right) + \psi(x - \Delta x) \left( 1 + P(x - \Delta x) \frac{\Delta x^2}{12} \right) \\ = 2\psi(x) \left( 1 - 5P(x) \frac{\Delta x^2}{12} \right). \quad (15)\end{aligned}$$

Discretize e defina  $k = \Delta x^2/12$ ,

$$\psi_{j+1} = \frac{2\psi_j(1 - 5kP_j) - \psi_{j-1}(1 + kP_{j-1})}{(1 + kP_{j+1})}. \quad (16)$$

## Matching Method

- Poderíamos chutar  $E$  e resolver a equação de Schrödinger via Numerov até que ela atendesse o contorno em  $x_N$ , porém esse método não é o mais adequado.
- Multiple shooting: resolver indo para direita até  $m$ , resolver indo para esquerda até  $m$  e exigir continuidade da função de onda e de sua derivada nesse ponto.

$$1 \quad \psi_m^r = \psi_m^l \implies \psi = \psi^r = C\psi^l \implies C = \psi_m^r / \psi_m^l$$

$$2 \quad \psi_m^r = \psi_m^l \implies g(E) = \psi_{m+1}^E + \psi_{m-1}^E - 2\psi_m^E = 0$$

## Correção de Cooley

A cada passo faremos correções do tipo

$$E^{k+1} = E^k + \Delta E, \quad (17)$$

Usando teoria de perturbação,

$$\Delta E = E - E_0 = \frac{\langle \psi^{E_0} | H - E_0 | \psi^{E_0} \rangle}{\langle \psi^{E_0} | \psi^{E_0} \rangle}, \quad (18)$$

$$\Delta E = \frac{\psi_m^{E_0*}}{\sum_j |\psi_j^{E_0}|^2} \left[ -\frac{1}{2} \frac{Y_{m+1}^{E_0} + Y_{m-1}^{E_0} - 2Y_m^{E_0}}{\Delta x^2} \right] + (V_m - E_0) \psi_m^{E_0}, \quad (19)$$

onde,

$$Y_m = (1 + kP_m) \psi_m. \quad (20)$$



## Código

```
def numerov(E, V):  
    k = (dx**2)/12          # Numerov Parameter  
    s = s_prime = 1e-6      # Free shooting parameters (inward and backward)  
  
    psi = np.zeros(N)  
    psi[0] = 0.0  
    psi[1] = s  
    psi[-2] = s_prime  
  
    for iteration in range(1000):  
        P = E-V  
  
        # Forward integration to matching point m  
        for i in range(1, N-1):  
            psi[i+1] = (2*psi[i]*(1 - 5*k*P[i]) - psi[i-1]*(1 + k*P[i-1]))/(1 + k*P[i+1])  
            if psi[i] < psi[i-1]:  
                m = i+1  
                psi_out_m = psi[m]  
                break  
  
        # Backward integration to matching point  
        for i in range(N-2, m, -1):  
            psi[i-1] = (2*psi[i]*(1 - 5*k*P[i]) - psi[i+1]*(1 + k*P[i+1]))/(1 + k*P[i-1])  
  
        # Matching for continuity of psi  
        psi[:m] = psi[:m]/psi_out_m  
        psi[m:] = psi[m:]/psi[m]  
  
        # Cooley correction  
        Y = (1+k*P)*psi  
        dE = (psi[m].conj()/np.sum(np.abs(psi)**2))*(-0.5*(Y[m+1]-2*Y[m]+Y[m-1])/(dx**2)+(V[m]-E)*psi[m])  
        E = E + dE  
  
        if np.abs(dE) < 1e-6:  
            print(f'Converged after {iteration+1} steps.')  
            break  
  
        # Normalization  
        A =.simps(psi**2, x)  
        psi = psi/A  
  
    return psi, E
```

## Catenária

Parametrização,

$$\alpha(s) = \left( a \operatorname{arcsinh}(s/a), \sqrt{s^2 + a^2} \right), s \in \mathbb{R}. \quad (21)$$

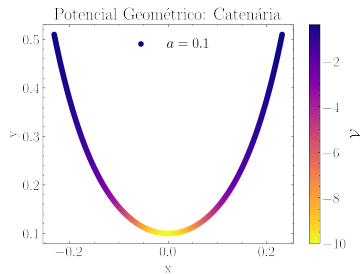
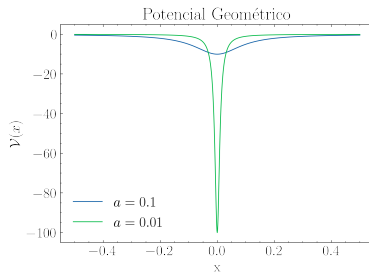
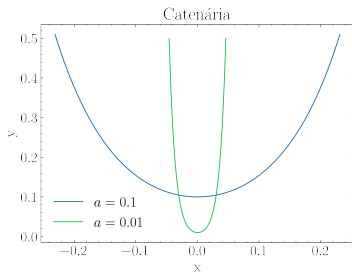
Curvatura,

$$\kappa(s) = \frac{a}{a^2 + s^2}. \quad (22)$$

Equação de Schrödinger,

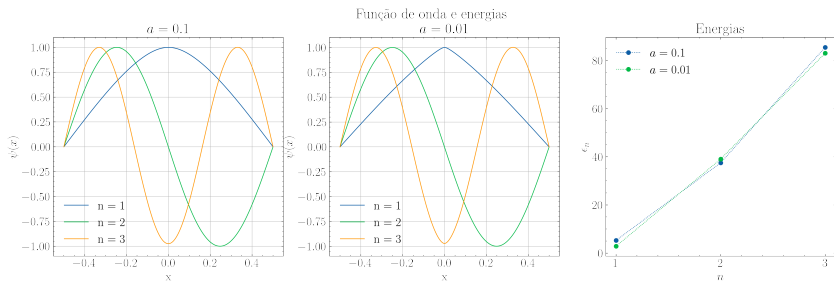
$$\psi'' + \left[ \frac{a^2}{4(a^2 + s^2)^2} + \varepsilon \right] \psi = 0. \quad (23)$$

## Catenária - Curva

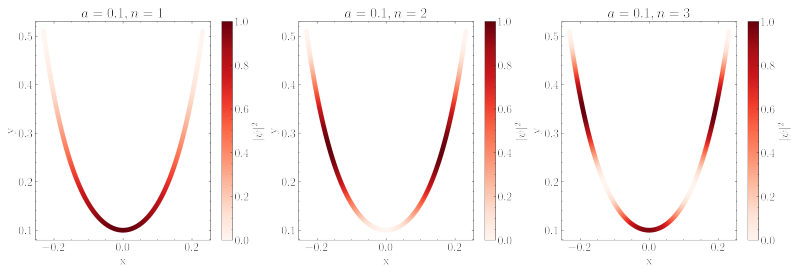


## Catenária - Função de onda e energias

Parâmetros:  $L = 1.0$ ,  $dx = 10^{-3}$ ,  $tol = 10^{-6}$ .



## Catenária - Densidade de probabilidade



## Referências

- CARMO, M. P. do. Geometria diferencial de curvas e superfícies. Sociedade Brasileira de Matemática, 2005.
- COSTA, R. C. T. da. Quantum mechanics of a constrained particle. Physical Review A, v. 23, n. 4, p. 1982–1987, 4 1981.
- IZAAC, J.; WANG, J. Computational Quantum Mechanics. Cham: Springer International Publishing, 2018. (Undergraduate Lecture Notes in Physics).