4 Problema de valores propios:

$$\frac{d^2y}{dx^2} - R(x)\,y = S(x)$$

Condiciones frontera: $y(a) = y_a$ $\quad R(x) \rightarrow$ Real

$y(b) = y_b$ $\quad S(x) \rightarrow$ Término inhomogéneo

Con discretización se llega a:

$$y_{n+1} - 2y_n + y_{n-1} = \left(y_n'' + \frac{h^2}{12} y_n^{IV} \right) h^2 + O(h^6)$$

$$\left(1-\frac{h^2}{12}R_{n+1}\right)y_{n+1}-2\left(1+\frac{5h^2}{12}R_n\right)y_n+\left(1-\frac{h^2}{12}R_{n-1}\right)y_{n-1} = \frac{h^2}{12}(S_{n+1}+10S_n+S_{n-1})+O(h^6). \tag{2.100}$$

a) Definimos $\Delta x = h$ de forma que una función toma valores

$\rightarrow$ Por series de taylor se puede encontrar el valor $y(x+h)$ y $y(x-h)$:

$$y(x+h) = y(x) + y'(x)(\cancel{x}+h-\cancel{x}) + \frac{y''(x)}{2!}(\cancel{x}+h-\cancel{x})^2 + \frac{y'''(x)}{3!}(\cancel{x}+h-\cancel{x})^3 + \frac{y^{IV}(x)}{4!}(\cancel{x}+h-\cancel{x})^4 + \frac{y^{V}(x)}{5!}(\cancel{x}+h-\cancel{x})^5 + O(h^6)$$

$$y(x+h) = y(x) + h\,y'(x) + h^2\frac{y''(x)}{2!} + \frac{h^3\,y'''(x)}{3!} + h^4\frac{y^{IV}(x)}{4!} + h^5\frac{y^{V}(x)}{5!} + O(h^6)$$

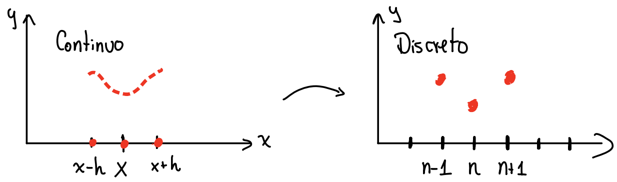
$$y(x-h) = y(x) + y'(x)(\cancel{x}-h-\cancel{x}) + \frac{y''(x)}{2!}(\cancel{x}-h-\cancel{x})^2 + \frac{y'''(x)}{3!}(\cancel{x}-h-\cancel{x})^3 + \frac{y^{IV}(x)}{4!}(\cancel{x}-h-\cancel{x})^4 + \frac{y^{V}(x)}{5!}(\cancel{x}-h-\cancel{x})^5 + O(h^6)$$

$$y(x-h) = y(x) - h\,y'(x) + h^2\frac{y''(x)}{2!} - \frac{h^3\,y'''(x)}{3!} + h^4\frac{y^{IV}(x)}{4!} - h^5\frac{y^{V}(x)}{5!} + O(h^6)$$

$$y(x+h) + y(x-h) = 2y(x) + \frac{2}{2!}h^2 y''(x) + \frac{2}{4!}h^4 y^{IV}(x) + O(h^6)$$

$$y(x+h) - 2y(x) + y(x-h) = \left(y''(x) + \frac{h^2}{12} y^{IV}(x) \right) h^2 + O(h^6)$$

La serie de Taylor se hace sobre un dominio continuo, sin embargo para hallar el algoritmo debemos discretizar el dominio



De forma que la expresión de arriba queda:

$$\boxed{y_{n+1} - 2y_n + y_{n-1} = h^2\left(y''_n + \frac{h^2}{12} y^{IV}_n\right) + O(h^6)} \qquad (1)$$

Por serie de taylor hasta orden $O(h^4)$ se puede dejar $y^{IV}(x)$ en termino de $y''(x)$ para esto sea $u(x) = y''(x)$. Por expansión de Taylor se tiene:

$$u(x+h) - u(x) - h u'(x) = h^2 \frac{u''(x)}{2!} + O(h^4)$$

$$u(x-h) - u(x) + h\, u'(x) = h^2 \frac{u''(x)}{2!} + O(h^4)$$

$$u(x+h) - 2u(x) + u(x-h) + O(h^4) = h^2 u''(x)$$

Que al discretizar queda:

$$u_{n+1} - 2u_n + u_{n-1} + O(h^4) = h^2 u''_n$$

Como $u(x) = y''(x)$ al discretizar $u_n = y''_n$:

$$y''_{n+1} - 2y''_n + y''_{n-1} + O(h^4) = h^2 y^{IV}_n$$

De la ecuación diferencial al discretizar se tiene:

$$y''_n = S_n + R_n y_n$$

De forma que $h^2 y_n^{IV}$ queda:

$$\boxed{h^2 y_n^{IV} = S_{n+1} + R_{n+1} y_{n+1} - 2S_n - 2R_n y_n + S_{n-1} + R_{n-1} y_{n-1}} \quad (2)$$

Usando (2) en (1) y la discretización de la ecuación diferencial:

$$y_{n+1} - 2y_n + y_{n-1} = \frac{12h^2 S_n + 12h^2 R_n y_n}{12}$$

$$+ \frac{h^2 S_{n+1} + h^2 R_{n+1} y_{n+1} - 2h^2 S_n - 2h^2 R_n y_n + h^2 S_{n-1} + h^2 R_{n-1} y_{n-1}}{12} + O(h^6)$$

$$y_{n+1} - 2y_n + y_{n-1} = \frac{h^2 S_{n+1} + 10h^2 S_n + h^2 S_{n-1} + h^2 R_{n+1} y_{n+1} + 10h^2 R_n y_n + h^2 R_{n-1} y_{n-1}}{12} + O(h^6)$$

$$y_{n+1} - 2y_n + y_{n-1} = \frac{h^2}{12}\left(S_{n+1} + 10S_n + S_{n-1}\right) + \frac{h^2}{12}\left(R_{n+1} y_{n+1} + 10h^2 R_n y_n + R_{n-1} y_{n-1}\right) + O(h^6)$$

$$y_{n+1}\left(1 - \frac{h^2 R_{n+1}}{12}\right) - 2y_n\left(1 + \frac{5h^2 R_n}{12}\right) + y_{n-1}\left(1 - \frac{h^2 R_{n-1}}{12}\right) = \frac{h^2}{12}\left(S_{n+1} + 10S_n + S_{n-1}\right) + O(h^6)$$

Esta última ecuación es el algoritmo de Numerov

b) $$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi$$

$$\downarrow$$

$$\frac{d^2\psi}{dx^2} - \underbrace{\left(\frac{2mV(x)}{\hbar^2} - \frac{2mE}{\hbar^2}\right)}_{R(x)}\psi = \underbrace{0}_{S(x)}$$

$R(x)$, $S(x)$ están en el continuo, pasamos al discreto:

$$R_n = \frac{2mV_n}{\hbar^2} - \frac{2mE}{\hbar} = \frac{2m}{\hbar}\left[V_n - E\right]$$

$$S_n = 0$$

Como hacemos $\hbar = 1$, $m = 1$, $w = 1$:

$$R_n = 2(V_n - E)$$
$$S_n = 0$$

El punto c), d) se hacen en python con discretización a través de un linspace y la función potencial (x, w)

e) $y_{n+1}\left(1-\frac{h^2 R_{n+1}}{12}\right) - 2y_n\left(1+\frac{5h^2 R_n}{12}\right) + y_{n-1}\left(1-\frac{h^2 R_{n-1}}{12}\right) = \frac{h^2}{12}\left(S_{n+1}+10S_n+S_{n-1}\right)$

$S_{n+1} = S_n = S_{n-1} = 0$

$$y_{n+1} = \frac{2y_n\left(1+\frac{5h^2 R_n}{12}\right) - y_{n-1}\left(1-\frac{h^2}{12}R_{n-1}\right)}{1-\frac{h^2 R_{n+1}}{12}}$$

Sea $n+1 = K$ $\quad n = K-1 \quad n-1 = K-2$: Pasado del pasado

$$y_K = \frac{2\underbrace{y_{K-1}}_{\text{Pasado}}\left(1+\frac{5h^2 R_{K-1}}{12}\right) - y_{K-2}\left(1-\frac{h^2}{12}R_{K-2}\right)}{1-\frac{h^2 R_K}{12}}$$

Con $\begin{cases} y_0 = 0 \quad y \quad y_1 = 1\times 10^{-5} \\ y(-5) = 0 \quad y(-4.99) = 1\times 10^{-5} \end{cases}$

f) Se halla con la función findEigenvalues

g) Se implementa un ciclo que calcula χ a diferentes energías

h)

i), j) Con las funciones $\begin{cases} \text{phi g, findEigenvalues g} \\ \text{phi r, findEigenvalues r} \end{cases}$

⑥ Coeficientes de Adams-Moulton

$$y_{n+1} = y_n + \frac{h}{12}\left(5f_{n+1} + 8f_n - f_{n-1}\right)$$

Integrar polinomio interpolador

$$\Omega = \left\{ (t_{n-1}, f_{n-1}), (t_n, f_n) \; (t_{n+1}, f_{n+1}) \right\}$$

Hacemos el polinomio interpolador:

$$p_1(t) = \frac{t - t_n}{t_{n-1} - t_n} f_{n-1} + \frac{t - t_{n+1}}{t_n - t_{n+1}} f_n + \frac{t - t_n}{t_{n+1} - t_n} f_{n+1}$$

$\mathcal{L}_i(x)$:

$i = n-1$

$i = n-1$
$j \neq n-1 \qquad j = n, n+1$

$$\frac{(t - t_n)(t - t_{n+1})}{(t_{n-1} - t_n)(t_{n-1} - t_{n+1})} \rightarrow f_{n-1}$$

$i = n$

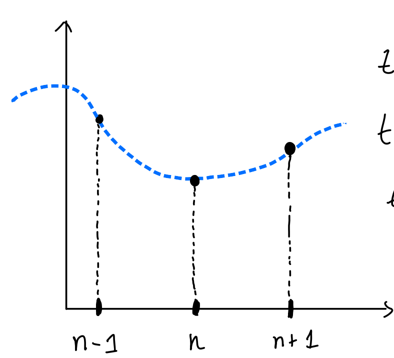
$i = n$
$j \neq n \qquad j = n-1, n+1$

$$\frac{(t - t_{n-1})\;(t - t_{n+1})}{(t_n - t_{n-1})\;(t_n - t_{n+1})} \rightarrow f_n$$

$i = n+1$

$i = n+1$
$j \neq n+1 \qquad j = n, n-1$

$$\frac{(t - t_n)(t - t_{n-1})}{(t_{n+1} - t_n)(t_{n+1} - t_{n-1})} \rightarrow f_{n+1}$$



$t_{n+1} - t_n = h$

$t_{n+1} - t_{n-1} = 2h$

$t_n - t_{n-1} = h$

El polinomio interpolador queda:

$$p(t) = \frac{(t-t_n)(t-t_{n+1})}{\underbrace{(t_{n-1}-t_n)}_{h}\underbrace{(t_{n-1}-t_{n+1})}_{2h}} f_{n-1} + \frac{(t-t_{n-1})(t-t_{n+1})}{\underbrace{(t_n-t_{n-1})}_{h}\underbrace{(t_n-t_{n+1})}_{-h}} f_n + \frac{(t-t_n)(t-t_{n-1})}{\underbrace{(f_{n+1}-t_n)}_{h}\underbrace{(f_{n+1}-t_{n-1})}_{2h}} f_{n+1}$$

Con respecto a $t = t_n$ $\begin{cases} t_{n+1} = h \\ t_{n-1} = -h \end{cases}$

$$p(t) = \left[\frac{t}{h}\right]\left[\frac{-(t-h)}{-2h}\right] f_{n-1} + \left[\frac{t+h}{h}\right]\left[\frac{-(t-h)}{-h}\right] f_n + \left[\frac{t}{h}\right]\left[\frac{t+h}{2h}\right] f_{n+1}$$

Al integrar el método implícito esta dado por:

$$y_{n+1} = y_n + f_{n-1}\int_{t_n}^{t_{n+1}} \mathcal{L}_{n-1}(t)\,dt + f_n \int_{t_n}^{t_{n+1}} \mathcal{L}_n(t)\,dt + f_{n+1}\int_{t_n}^{t_{n+1}} \mathcal{L}_{n+1}(t)\,dt$$

La integración se hace en el notebook de Python