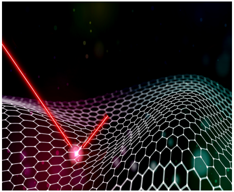
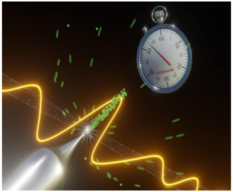
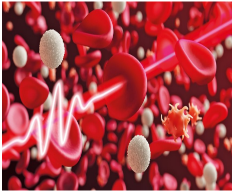
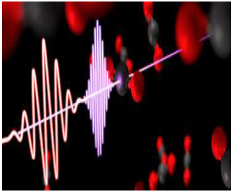
Física del Attosegundo









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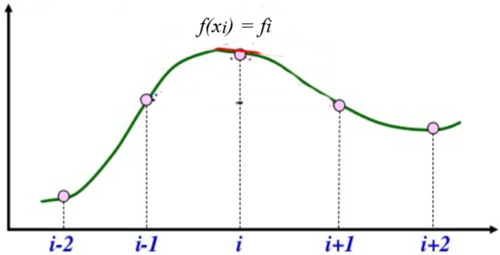
Hamiltoniano Numérico

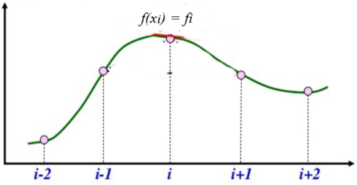
$$f_i = f(x_i)$$

$$\vec{f} = \begin{pmatrix} f_0 \\ f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \end{pmatrix}$$



Operadores

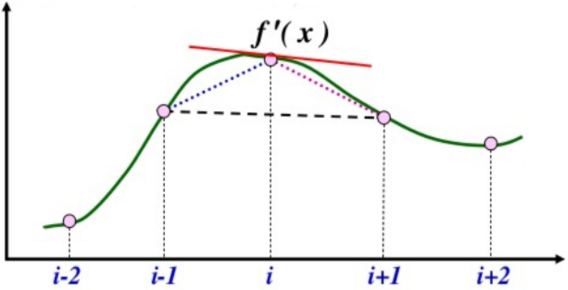
$$\hat{V}(x)\, f(x)$$



$$\mathbf{V} = \begin{pmatrix} V_0 & 0 & 0 & 0 & 0 & 0 \\ 0 & V_1 & 0 & 0 & 0 & 0 \\ 0 & 0 & V_2 & 0 & 0 & 0 \\ 0 & 0 & 0 & V_3 & 0 & 0 \\ 0 & 0 & 0 & 0 & V_4 & 0 \\ 0 & 0 & 0 & 0 & 0 & V_5 \end{pmatrix} \qquad \vec{f} = \begin{pmatrix} f_0 \\ f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \end{pmatrix}$$

$$\mathbf{V}\, \vec{f} = \hat{V}(x)\, f(x)$$

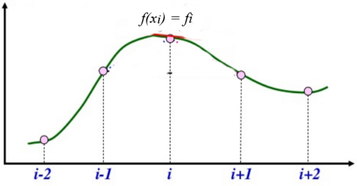
Derivada Numérica



- **Forward difference** $$f'(x) \cong \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i} = \frac{y_{i+1} - y_i}{x_{i+1} - x_i}$$
- **Backward difference** $$f'(x) \cong \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}} = \frac{y_i - y_{i-1}}{x_i - x_{i-1}}$$
- **Central difference** $$f'(x) \cong \frac{f(x_{i+1}) - f(x_{i-1})}{x_{i+1} - x_{i-1}} = \frac{y_{i+1} - y_{i-1}}{x_{i+1} - x_{i-1}}$$

Derivada Numérica: Diferencias Finitas

$$f_i' = \frac{f_{i+1} - f_{i-1}}{2\,\Delta x}$$

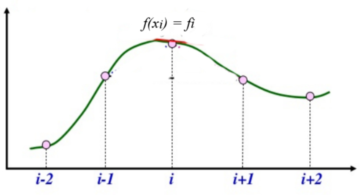


$$\mathbf{D} = \frac{1}{2\,\Delta x}\begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 \end{pmatrix} \qquad \vec{f} = \begin{pmatrix} f_0 \\ f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \end{pmatrix}$$

$$\mathbf{D}\,\vec{f} = \hat{D}\,f(x) = \vec{f}'$$

Derivada Segunda Numérica

$$\begin{aligned} f_i'' &= \frac{f'_{i+1} - f'_i}{\Delta x} = \\ &= \frac{\frac{f_{i+1}-f_i}{\Delta x} - \frac{f_i - f_{i-1}}{\Delta x}}{\Delta x} = \\ &= \frac{f_{i+1} - 2\,f_i + f_{i-1}}{(\Delta x)^2} \end{aligned}$$



$$\mathbf{B} = \frac{1}{(\Delta x)^2} \begin{pmatrix} -2 & 1 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 & 0 \\ 0 & 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & 1 & -2 \end{pmatrix} \qquad \vec{f} = \begin{pmatrix} f_0 \\ f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \end{pmatrix}$$

$$\mathbf{B}\,\vec{f} = \hat{\nabla}^2 f(x) = \vec{f}''$$

Hamiltoniano Numérico

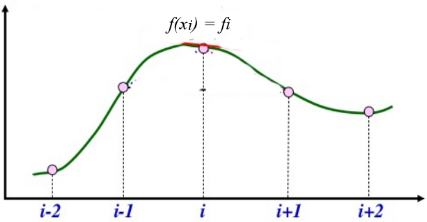
$$\hat{H}\,\varphi(x) \quad = \quad -\frac{1}{2}\frac{d^2\,\varphi(x)}{dx} + V(x)\,\varphi(x)$$

$$\mathbf{H} = \begin{pmatrix} \frac{1}{(\Delta x)^2} + V_0 & -\frac{1}{2(\Delta x)^2} & 0 & 0 & \dots \\ -\frac{1}{2(\Delta x)^2} & \frac{1}{(\Delta x)^2} + V_1 & -\frac{1}{2(\Delta x)^2} & 0 & \dots \\ 0 & -\frac{1}{2(\Delta x)^2} & \frac{1}{(\Delta x)^2} + V_2 & -\frac{1}{2(\Delta x)^2} & \dots \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & -\frac{1}{2(\Delta x)^2} & \frac{1}{(\Delta x)^2} + V_N \end{pmatrix}$$

$$\mathbf{H}\,\vec{f} = \hat{H}\,\varphi(x)$$

Integral Numérica

$$\int_a^b f(x)\,dx \approx \sum_{i=1}^{N} f_i\,\Delta x$$



Otra aproximación (trapecios):

$$\int f(x)\,dx \approx \sum_{i=0}^{N-1} \frac{f_{i+1}+f_i}{2}\,\Delta x = \frac{1}{2} f_0 + \sum_{i=1}^{N-1} f_i + \frac{1}{2} f_N$$

Derivadas con Transformadas de Fourier

Transformada de Fourier

$$\mathcal{F}(k) = \int_{-\infty}^{\infty} f(t)\, e^{-i\, 2\pi\, k\, t}\, dt \tag{1}$$

Antitransformada:

$$f(t) = \int_{-\infty}^{\infty} \mathcal{F}(k)\, e^{i\, 2\pi\, k\, t}\, dk \tag{2}$$

Análisis y Síntesis

Para función periódica de $t \in [-\frac{P}{2}, \frac{P}{2}]$:

$$c_k = \frac{1}{P} \int_{-\frac{P}{2}}^{\frac{P}{2}} f(t)\, e^{-i\, 2\pi\, \frac{k}{P}\, t}\, dt$$

Síntesis:

$$f(t) = \sum_{n=-\infty}^{\infty} c_k\, e^{i\, 2\pi\, \frac{k}{P}\, t}$$

Notación más simple

$$\mathcal{F}[f](k) = \int_{-\infty}^{\infty} f(t)\, e^{-i\,k\,t}\, dt$$

Antitransformada:

$$\mathcal{F}^{-1}[f(t)](k)$$

Derivadas

Derivada de la Transformada:

$$\frac{d}{dk}\mathcal{F}[f](k) = -i\,\mathcal{F}[tf(t)](k)$$

Derivadas

Transformada de la derivada:

$$\mathcal{F}[f'](k) = ik\,\mathcal{F}[f](k)$$

$$\mathcal{F}[f^{(n)}](k) = (ik)^n\,\mathcal{F}[f](k)$$

Derivadas

Transformada de la derivada:

$$\mathcal{F}[f^{(n)}](k) = (ik)^n \, \mathcal{F}[f](k)$$

Receta para derivar $f^{(n)}$:

1. Transformar la función f
2. Multiplicar por $(ik)^n$
3. Antitransformar

Schrödinger en el espacio de momentos

Partícula libre:

$$\hat{H}\,\psi(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x)$$

$$\mathcal{F}[\psi(x)](k) \equiv \phi(k)$$

$$\begin{aligned}\mathcal{F}[\hat{H}\,\psi(x)](k) &= -\frac{\hbar^2}{2m}\,k^2\,\mathcal{F}[\psi(x)] \\ &= -\frac{\hbar^2}{2m}\,k^2\,\phi(k)\end{aligned}$$

Time Dependent Schrödinger Equation

$$i\hbar\frac{d}{dt}\Psi(x,t) = \hat{H}\Psi(x,t)$$

Solución:

$$\Psi(x,\Delta t) = \exp\left[-i\frac{\Delta t}{\hbar}\hat{H}\right]\Psi(x,0)$$

Forma Bestia

$$\Psi(x, \Delta t) = \exp\left[-i\frac{\Delta t}{\hbar}\hat{H}\right]\Psi(x, 0)$$

Podemos hacer:

$$\begin{aligned}\exp\left[-i\frac{\Delta t}{\hbar}\hat{H}\right] &\approx 1 + \left(-i\frac{\Delta t}{\hbar}\right)\hat{H} + \frac{1}{2}\left(-i\frac{\Delta t}{\hbar}\right)^2\hat{H}^2 + \cdots \\ &+ \frac{1}{n!}\left(-i\frac{\Delta t}{\hbar}\right)^n\hat{H}^n\end{aligned}$$

Recomendación: Guardar $\varphi_1 = \hat{H}\Psi$, luego multiplicar $\varphi_2 = \hat{H}\varphi_1 = \hat{H}^2\Psi$, ..., y finalmente, $\varphi_n = \hat{H}\varphi_{n-1}$.

Interludio cuántico: Función de Operadores

$$\begin{aligned}
\hat{A}\,\varphi_n &= a_n\,\varphi_n \\
\hat{A}^2\,\varphi_n &= \hat{A}\,\hat{A}\,\varphi_n = \hat{A}\,a_n\,\varphi_n = a_n\,\hat{A}\,\varphi_n = a_n^2\,\varphi_n \\
\hat{A}^3\,\varphi_n &= \hat{A}\,\hat{A}^2\,\varphi_n = a_n^3\,\varphi_n \\
\ldots &= \ldots \\
\hat{A}^n\,\varphi_n &= a_n^n\,\varphi_n
\end{aligned}$$

Entonces, cualquier función de $\hat{A}$, aplicada a un autovector es

$$f(\hat{A})\,\varphi_n = f(a_n)\,\varphi_n$$

Función de Operadores

Cualquier función de $\hat{A}$, aplicada a un autovector es

$$f(\hat{A})\,\varphi_n = f(a_n)\,\varphi_n$$

Por ejemplo:

$$e^{\hat{A}}\,\varphi_n = e^{a_n}\,\varphi_n$$

Función de Operadores

¿Qué pasa si se aplica esa función de un operador Hermítico a un estado cualquiera (no necesariamente a un autovector)?

$$\begin{aligned} f(\hat{A})\,\psi &= f(\hat{A})\sum_n c_n\,\varphi_n = \sum_n c_n\,f(\hat{A})\,\varphi_n = \\ &= \sum_n c_n\,f(a_n)\,\varphi_n \end{aligned}$$

Por ejemplo:

$$e^{\hat{A}}\,\psi = \sum_n c_n\;e^{a_n}\;\varphi_n$$

Evolución Temporal

Si logramos diagonalizar el Hamiltoniano:

$$\hat{H}\varphi_n(x) = E_n\,\varphi_n(x)$$

entonces podemos escribir cualquier estado inicial como combinación lineal de los estados estacionarios:

$$\Psi(x, t = 0) = \sum_n c_n\,\varphi_n(x)$$

Por lo tanto:

$$\Psi(x, t) = e^{-i\frac{t}{\hbar}\,\hat{H}}\,\Psi(x, 0) = \sum_n e^{-i\frac{t}{\hbar}\,E_n}\,c_n\,\varphi_n(x)$$

Split Operator

$$\Psi(x,\Delta t) = \exp\left[-i\frac{\Delta t}{\hbar}\hat{H}\right]\Psi(x,0)$$

$$\begin{aligned}\hat{H} &= \frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + \hat{V}(x) \equiv \hat{T}(x) + \hat{V}(x) \\ &= \frac{1}{2}\hat{T}(x) + \hat{V}(x) + \frac{1}{2}\hat{T}(x)\end{aligned}$$

$$\exp\left[-i\frac{\Delta t}{\hbar}\hat{H}\right] \approx \exp\left[-i\frac{\Delta t}{2\hbar}\hat{T}\right]\exp\left[-i\frac{\Delta t}{\hbar}\hat{V}\right]\exp\left[-i\frac{\Delta t}{2\hbar}\hat{T}\right] =$$

$$= \exp\left[-i\frac{\Delta t}{2\hbar}\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}\right]\exp\left[-i\frac{\Delta t}{\hbar}V(x)\right]\exp\left[-i\frac{\Delta t}{2\hbar}\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}\right]$$

Split Operator

1. $\mathcal{F}[\psi(x)] \rightarrow \phi(p)$
2. Multiply by $\exp\left[-i\frac{\Delta t}{2\hbar}\frac{k^2}{2m}\right]$
3. $\mathcal{F}^{-1}[\phi(p)] \rightarrow \psi(x)$
4. Multiply by $\exp\left[-i\frac{\Delta t}{\hbar}V(x)\right]$
5. $\mathcal{F}[\psi(x)] \rightarrow \phi(p)$
6. Multiply by $\exp\left[-i\frac{\Delta t}{2\hbar}\frac{k^2}{2m}\right]$
7. $\mathcal{F}^{-1}[\phi(p)] \rightarrow \psi(x)$

Métodos Explícitos

$$i\hbar\frac{d}{dt}\Psi(x,t) = \hat{H}\Psi(x,t)$$

Discretizado se convierte en:

$$i\hbar\frac{\psi_j^{n+1} - \psi_j^n}{\tau} = \hat{H}\psi_j^n$$

y solucionando para ψ_j^{n+1} se puede escribir en forma matricial:

$$\boldsymbol{\psi}^{n+1} = \left(\mathbf{I} - \frac{i\tau}{\hbar}\,\mathbf{H}\right)\boldsymbol{\psi}^n$$

Métodos Explícitos

Interpretación:

$$\boldsymbol{\psi}^{n+1} = \left(\mathbf{I} - \frac{i\tau}{\hbar}\,\mathbf{H}\right)\boldsymbol{\psi}^{n}$$

El primer término de la expansión de Taylor: $e^{-z} \approx 1 - z$.
Este método es inestable.

Métodos Implícitos

Asumimos ahora que el lado derecho está en el futuro:

$$i\hbar \frac{\psi_j^{n+1} - \psi_j^n}{\tau} = \hat{H}\psi_j^{n+1}$$

y solucionando para ψ_j^{n+1} se puede escribir en forma matricial:

$$\left(\mathbf{I} + \frac{i\tau}{\hbar}\,\mathbf{H}\right) \boldsymbol{\psi}^{n+1} = \boldsymbol{\psi}^n$$

$$\boldsymbol{\psi}^{n+1} = \left(\mathbf{I} + \frac{i\tau}{\hbar}\,\mathbf{H}\right)^{-1} \boldsymbol{\psi}^n$$

Métodos Implícitos

Interpretación:

$$\boldsymbol{\psi}^{n+1} = \left(\mathbf{I} + \frac{i\tau}{\hbar} \mathbf{H} \right)^{-1} \boldsymbol{\psi}^{n}$$

Si $z \to 0$, se puede aproximar $(1+z)^{-1} \approx (1-z)$.
Alternativamente: $e^{-z} = \frac{1}{e^z} \approx (1+z)^{-1}$.
Este método es estable, pero menos correcto.
Requiere **inversión** de matrices ($$$).

Método de Crank-Nicolson

Promediamos el lado derecho:

$$i\hbar\frac{\psi_j^{n+1} - \psi_j^n}{\tau} = \hat{H}\,\frac{1}{2}\left(\psi_j^n + \psi_j^{n+1}\right)$$

En notación matricial:

$$\boldsymbol{\psi}^{n+1} - \boldsymbol{\psi}^n = -\frac{i\tau}{2\hbar}\,\mathbf{H}\,\left(\boldsymbol{\psi}^n + \boldsymbol{\psi}^{n+1}\right)$$

$$\left(\mathbf{I} + \frac{i\tau}{2\hbar}\,\mathbf{H}\right)^{-1}\,\boldsymbol{\psi}^{n+1} = \left(\mathbf{I} - \frac{i\tau}{2\hbar}\,\mathbf{H}\right)\,\boldsymbol{\psi}^n$$

Método de Crank-Nicolson

$$\boldsymbol{\psi}^{n+1} = \frac{\left(\mathbf{I} - \frac{i\tau}{2\hbar}\,\mathbf{H}\right)}{\left(\mathbf{I} + \frac{i\tau}{2\hbar}\,\mathbf{H}\right)}\ \boldsymbol{\psi}^{n}$$

Aproximación de Páde: $e^{-z} \approx \frac{1-z}{1+z}$.
Para z compleja: $(e^{-z})^{*} = (e^{-z})^{-1}$.
Por lo tanto, el operador es unitario.