Dualidade onda-partícula

Planck-Einstein (1900-1905)

onda eletromagnética (luz) monocromática $\Longrightarrow$ conjunto de partículas não-materiais (fótons)

$$\begin{cases} \lambda \nu = c \text{ (veloc. de fase)} \\ \Psi \sim e^{i(kx - \omega t)} = e^{2\pi i \left(\frac{x}{\lambda} - \nu t\right)} \text{ (função de onda)} \end{cases}$$

(caracteriza o comportamento da luz)

$$\begin{cases} E = \nu h \\ p = \dfrac{h}{\lambda} \end{cases} \Rightarrow E = pc \quad (\lambda \nu = c)$$

de Broglie (1923)

feixe de elétrons $\Longrightarrow$ propriedades ondulatórias

$$\begin{cases} E = \gamma m c^2 \\ p = \gamma m v \end{cases} \Rightarrow p = \frac{E}{c^2} v$$

$$\begin{cases} \nu = \dfrac{E}{h} & (E = \hbar \omega) \\ \lambda = \dfrac{h}{p} & (p = \hbar k) \end{cases} \qquad \begin{cases} \omega = 2\pi\nu \\ \hbar = h/2\pi \\ k = \dfrac{2\pi}{\lambda} \end{cases}$$

relação de L. de Broglie

dualidade onda-partícula

energia de repouso

referencial próprio

$$\nu = \frac{E}{h} = \gamma\left(\frac{mc^2}{h}\right) = \gamma\left(\frac{E_0}{h}\right) = \gamma\,\nu_0$$

no referencial próprio : $\psi \sim e^{-2\pi i \nu_0 t_0}$ $\qquad t_0 = \gamma\left(t - x v/c^2\right)$

$$\sim e^{2\pi i \overset{\nu}{\widetilde{\gamma \nu_0}} \left(x v/c^2 - t\right)} = e^{2\pi i \left(\frac{x}{\lambda} - \nu t\right)} = e^{i(px - Et)/\hbar}$$

$$\lambda = \frac{c^2}{\nu v}$$

$$v_f = \lambda \nu = \frac{c^2}{v} = \left(\frac{c}{v}\right) c > c$$

$$\lambda = \frac{\gamma m c^2}{\gamma m v}\,\frac{1}{\nu} = \frac{E/\nu}{p} = \frac{h}{p} \implies v_f = \frac{E}{p} > c \quad \text{(veloc. de fase)}$$

veloc. de grupo : $v_g = \dfrac{dE}{dp}$

(relativ.) : $E^2 = p^2c^2 + m^2c^4 \implies v_g = c^2 p \left(p^2c^2 + m^2c^4\right)^{-1/2} = c^2 \dfrac{p}{E} = v < c$

(não-relat.) $E = \dfrac{p^2}{2m} \implies v_g = \dfrac{p}{m} = v < c$

Quem caracteriza o comportamento do elétron?

onda plana

$$\psi \sim e^{i(px - Et)/\hbar}$$

- momentum e energia definidos
- extensão infinita

pacote de ondas

peso de cada componente

$$\psi(x,t) \sim \int_{-\infty}^{\infty} a(p)\, e^{i(px - Et)/\hbar}\, dp$$

- não é caracterizado por um único comprimento de onda (momentum) ou frequência (energia)
- dispersão (incerteza) no momentum (Δp) e na energia (ΔE)
- limitação espacial (extensão finita)

$$\psi(x,0) = \frac{1}{\hbar}\int_{-\infty}^{\infty} a(p)\, e^{i\frac{p}{\hbar}x}\, dp \Longrightarrow \int_{-\infty}^{\infty}\psi(x,0)\, e^{-i\frac{p'}{\hbar}x}\, dx = \frac{1}{\hbar}\int_{-\infty}^{\infty} e^{-i\frac{p'}{\hbar}x}\left[\int_{-\infty}^{\infty} a(p)\, e^{i\frac{p}{\hbar}x}\, dp\right] dx$$

$$= \frac{1}{\hbar}\int_{-\infty}^{\infty} a(p)\left[\underbrace{\int_{-\infty}^{\infty} e^{i\frac{(p-p')x}{\hbar}}\, dx}_{2\pi\hbar\,\delta(p-p')}\right] dp = 2\pi\, a(p')$$

$$\Downarrow$$

$$\boxed{a(p) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\psi(x,0)\, e^{-i\frac{p}{\hbar}x}\, dx}$$

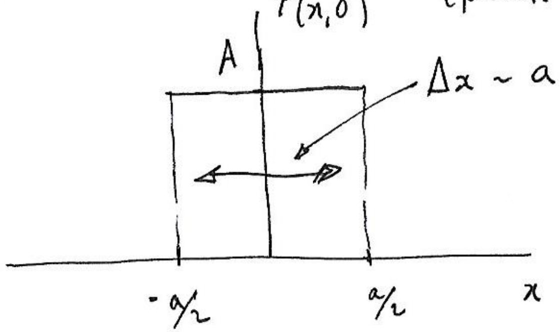
determinado pelo valor inicial (estado inicial)

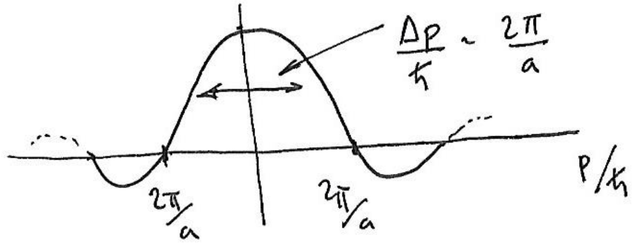
Incerteza na posição x incerteza no momentum

$$a(p) = \frac{A}{2\pi}\int_{-a/2}^{a/2} e^{-i\frac{p}{\hbar}x}\,dx = \frac{A\,i\hbar}{2\pi\,p}\, e^{-i\frac{p}{\hbar}x}\Big|_{-a/2}^{a/2}$$

$$= \frac{A}{\pi}\frac{\hbar}{p}\left[\frac{e^{i\frac{p}{\hbar}\frac{a}{2}} - e^{-i\frac{p}{\hbar}\frac{a}{2}}}{2i}\right]$$

$$a(p) = \frac{A}{\pi}\left(\frac{\operatorname{sen}\frac{p}{\hbar}\frac{a}{2}}{p/\hbar}\right)$$



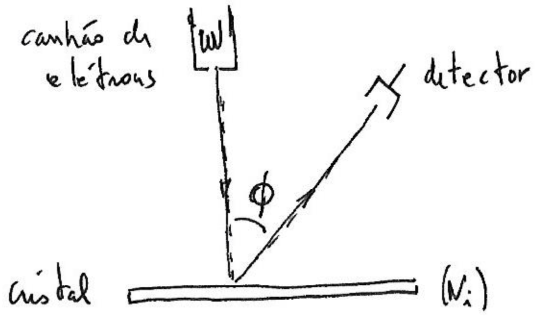


$$\boxed{\Delta p \cdot \Delta x \sim h}$$

Princípio de Incerteza

- $\Delta x \to 0 \ (a \to 0) \Rightarrow \Delta p \to \infty$ { melhor localização / maior incerteza no momentum
- $\Delta x \to \infty \ (a \to \infty) \Rightarrow \Delta p \to 0$ { maior incerteza na localização / menor dispersão no momentum

Experimento de Davison - Germer



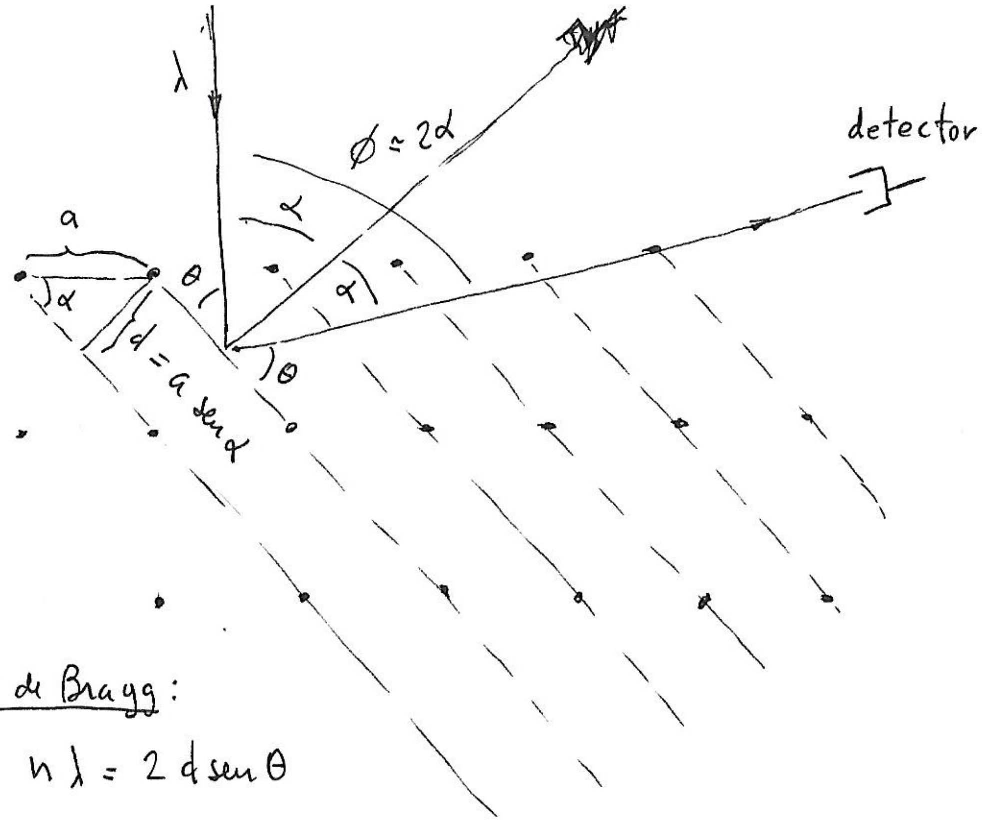
$$\begin{cases} V = 54\,V \text{ (potencial acelerador)} \\ \phi = 50^\circ \text{ (máximo)} \end{cases}$$

de Broglie: $\lambda = \dfrac{h}{p}$

$$\begin{cases} E = eV \text{ (energia dos elétrons)} \\ p = \sqrt{2mE} \end{cases}$$

$$\lambda = \frac{h}{\sqrt{2meV}} = \frac{6,626\times10^{-34}}{\sqrt{2\times 9,1\times10^{-31}\times 1,6\times10^{-19}\times 54}}$$

$$= \frac{6,626\times10^{-34}}{3,965\times10^{-24}} \simeq 1,67\,\text{Å}$$



lei de Bragg:

$$n\lambda = 2d\,\text{sen}\,\theta$$

$$= 2d\cos\alpha$$

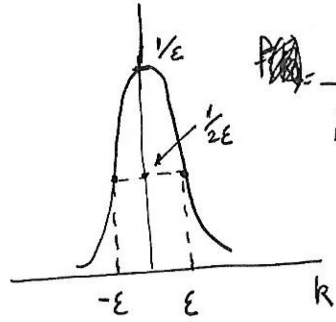
$$= a\,\underbrace{2\,\text{sen}\,\alpha\cos\alpha}_{\text{sen}\,2\alpha} = \boxed{a\,\text{sen}\,\phi = n\lambda}$$

$$\begin{cases} a = 2,15\,\text{Å} \text{ (determinado por raios X)} \\ \phi = 50^\circ \end{cases}$$

$$\lambda = 2,15\times10^{-10}\,\underbrace{\text{sen}(50^\circ)}_{0,766} \simeq 1,65\,\text{Å}$$

Representações para a função delta de Dirac

$$\lim_{\varepsilon\to 0}\frac{1}{\pi}\frac{\varepsilon}{k^2+\varepsilon^2}$$ — apreciável apenas no entorno de $k=0$



$$\frac{\varepsilon}{k^2+\varepsilon^2} \quad (\varepsilon>0)$$ → função par

$$\frac{1}{\pi}\lim_{\varepsilon\to 0}\int_{-\infty}^{\infty} f(k)\frac{\varepsilon}{k^2+\varepsilon^2}\,dk \simeq f(0)\,\frac{2}{\pi}\int_0^{\infty}\frac{1/\varepsilon}{1+(k/\varepsilon)^2}\,dk$$

$$= f(0)\,\frac{2}{\pi}\int_0^{\pi/2} d\theta = f(0)$$

$$\Big\{\, k/\varepsilon = \operatorname{tg}\theta \implies \frac{dk}{d\theta} = \varepsilon\underbrace{\sec^2\theta}_{1+\operatorname{tg}^2\theta}$$

$$\boxed{\frac{1}{\pi}\lim_{\varepsilon\to 0}\frac{\varepsilon}{k^2+\varepsilon^2} = \delta(k)} \quad (\varepsilon>0)$$

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{\pm ikx}\,dk = \frac{1}{2\pi}\lim_{\varepsilon\to 0}\left\{\int_{-\infty}^{0} e^{\pm ikx}e^{\varepsilon k}\,dk + \int_0^{\infty} e^{\pm ikx}e^{-\varepsilon k}\,dk\right\}$$

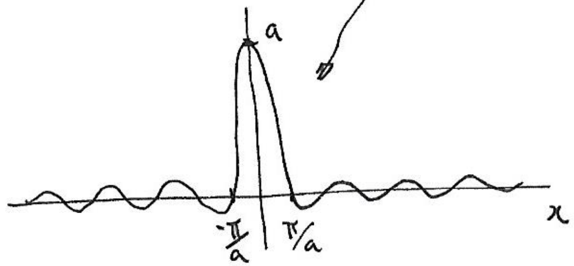
$$= \frac{1}{2\pi}\lim_{\varepsilon\to 0}\left\{\frac{1}{\pm ix+\varepsilon} - \frac{1}{\pm ix-\varepsilon}\right\} = \frac{1}{2\pi}\lim_{\varepsilon\to 0}\left\{\frac{(\pm ix-\varepsilon)-(\pm ix+\varepsilon)}{-x^2-\varepsilon^2}\right\}$$

$$= \frac{1}{\pi}\lim_{\varepsilon\to 0}\frac{\varepsilon}{x^2+\varepsilon^2} = \boxed{\delta(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{\pm ikx}\,dk}$$

$$\boxed{\delta(x) = \frac{1}{\pi}\int_0^{\infty}\cos kx\,dk}$$

$$\frac{1}{\pi}\int_0^{\infty}\cos kx\,dk = \frac{1}{\pi}\lim_{a\to\infty}\int_0^{a}\cos kx\,dk$$

$$\boxed{\delta(x) = \frac{1}{\pi}\lim_{a\to\infty}\frac{\operatorname{sen} ax}{x}}$$



$$\int_{-\infty}^{\infty}\overset{\text{par}}{\delta(ax)}\,f(x)\,dx = \frac{1}{|a|}\int_{-\infty}^{\infty}\delta(\overbrace{|a|x}^{y})\,f(y)\,dy = \frac{f(0)}{|a|}$$

$$\boxed{\delta(ax) = \frac{\delta(x)}{|a|}}$$

Transformada de Fourier

$$f(x) = \underset{\text{cte arbitrária}}{C} \int_{-\infty}^{\infty} F(k)\, e^{\pm ikx}\, dk \quad \text{(superposição de ondas planas)}$$

$$F(k) = \underset{\text{transf. de Fourier}}{T.F.}\, f(x)$$

$$\Downarrow$$

$$\int_{-\infty}^{\infty} f(x)\, e^{\mp ik'x}\, dx = C \int_{-\infty}^{\infty} dk\, F(k) \underbrace{\left[\int_{-\infty}^{\infty} e^{\pm i(k-k')x}\, dx \right]}_{2\pi\delta(k-k')}$$

$$\Downarrow$$

$$\boxed{F(k) = \frac{1}{2\pi C} \int_{-\infty}^{\infty} f(x)\, e^{\mp ikx}\, dx}$$

Escolhas usuais

$C = 1 \qquad C = 1/2\pi$

$C = 1/\sqrt{2\pi}$

Identidade de Parseval (T.F. como transf. unitária)

$$T\,|f(x)|^2 = \frac{1}{2\pi C} \int_{-\infty}^{\infty} f(x)\, f^*(x)\, e^{-ik'x}\, dx = \frac{1}{2\pi C} \int_{-\infty}^{\infty} dx\, f^*(x)\, e^{-ik'x}\, C \int_{-\infty}^{\infty} F(k)\, e^{ikx}\, dk$$

$$= C \int_{-\infty}^{\infty} dk\, F(k) \underbrace{\frac{1}{2\pi C} \int_{-\infty}^{\infty} dx\, f^*(x)\, e^{i(k-k')x}}_{F^*(k-k')} = C \int_{-\infty}^{\infty} dk\, F(k)\, F^*(k-k')$$

P/ $k' = 0$ $\Longrightarrow$ $\displaystyle \frac{1}{2\pi C^2} \int_{-\infty}^{\infty} |f(x)|^2\, dx = \int_{-\infty}^{\infty} |F(k)|^2\, dk$

P/ $C = 1/\sqrt{2\pi}$ $\longrightarrow$ $\begin{cases} \displaystyle\int_{-\infty}^{\infty} |f(x)|^2\, dx = \int_{-\infty}^{\infty} |F(k)|^2\, dk & \text{(identidade de Parseval)} \\ T: f(x) \to F(k) & \text{(transf. linear e unitária)} \end{cases}$