

# **Eletrônica e Fotônica Molecular**

## **parte 1**

**Conceitos básicos da mecânica  
quântica**

# CONTEÚDO

**Modelos e mecanismos de transporte em dispositivos moleculares.**

**Mecanismos de transferência de elétrons.**

**Mecanismos de transferência de energia.**

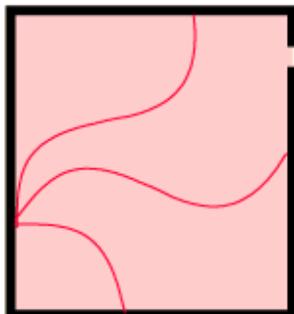
**Interfaces em dispositivos moleculares.**

**Dispositivos e máquinas moleculares.**

**Cristais fotônicos e metamateriais plasmônicos.**

# Max Planck

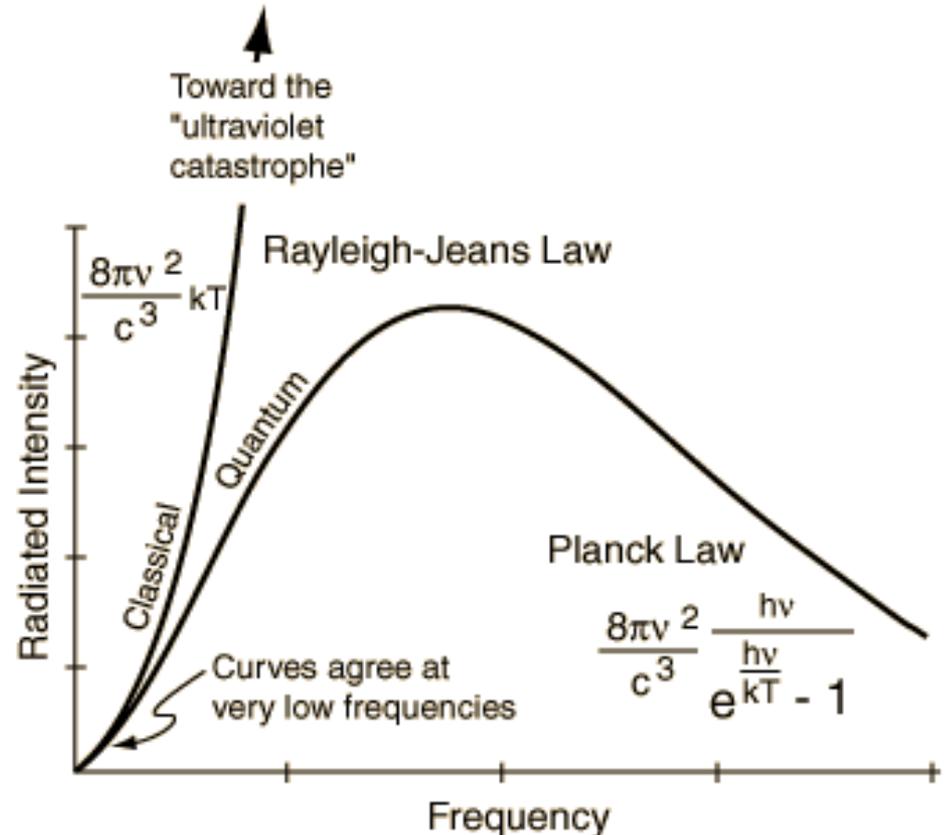
1900 descoberta da teoria quântica  
A partir de modelos totalmente matemáticos: Radiação do corpo negro



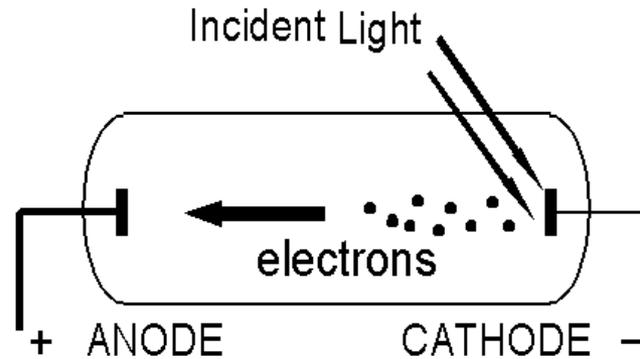
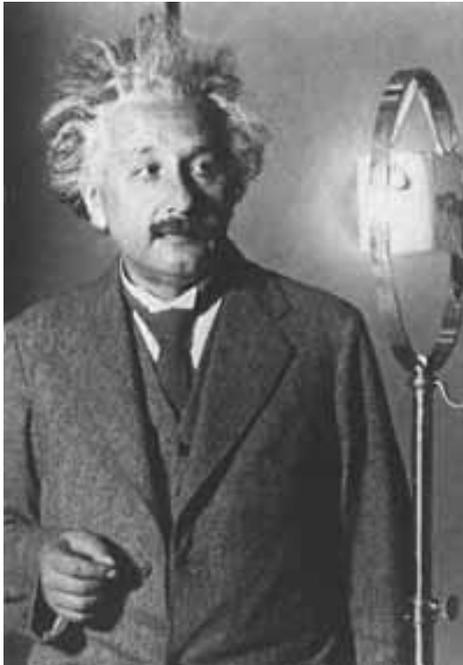
Number of modes per unit frequency per unit volume

$$\frac{8\pi\nu^2}{c^3}$$

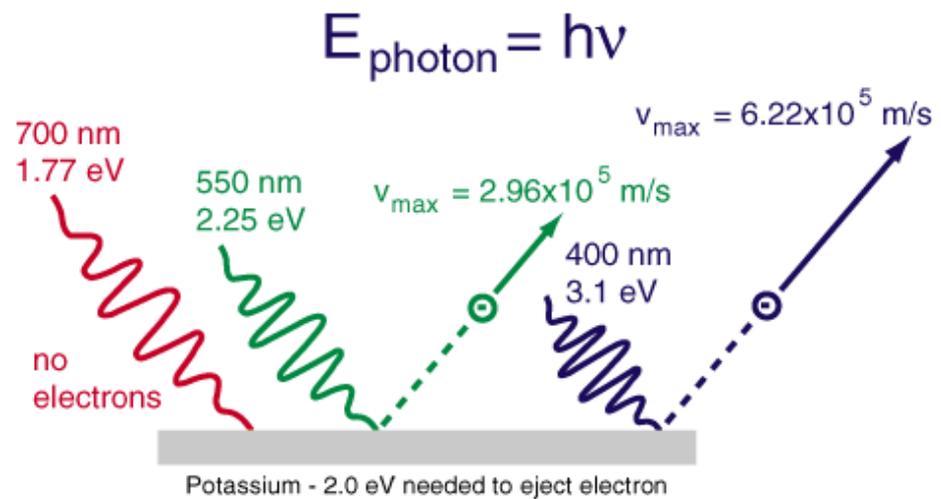
For higher frequencies you can fit more modes into the cavity. For double the frequency, four times as many modes.



# Efeito foto elétrico - Einstein

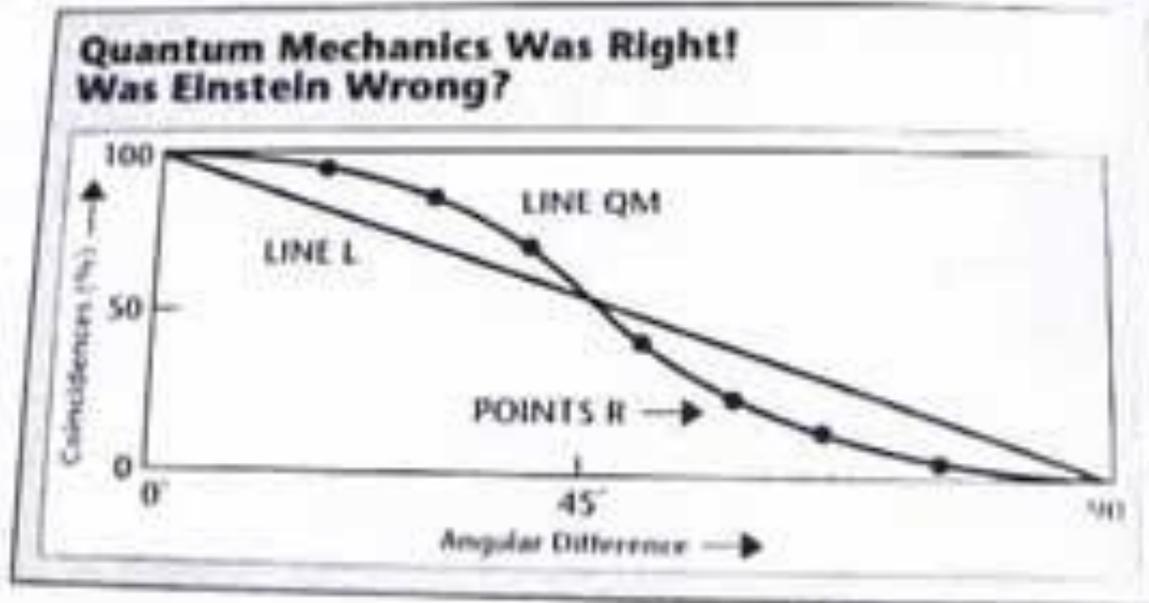
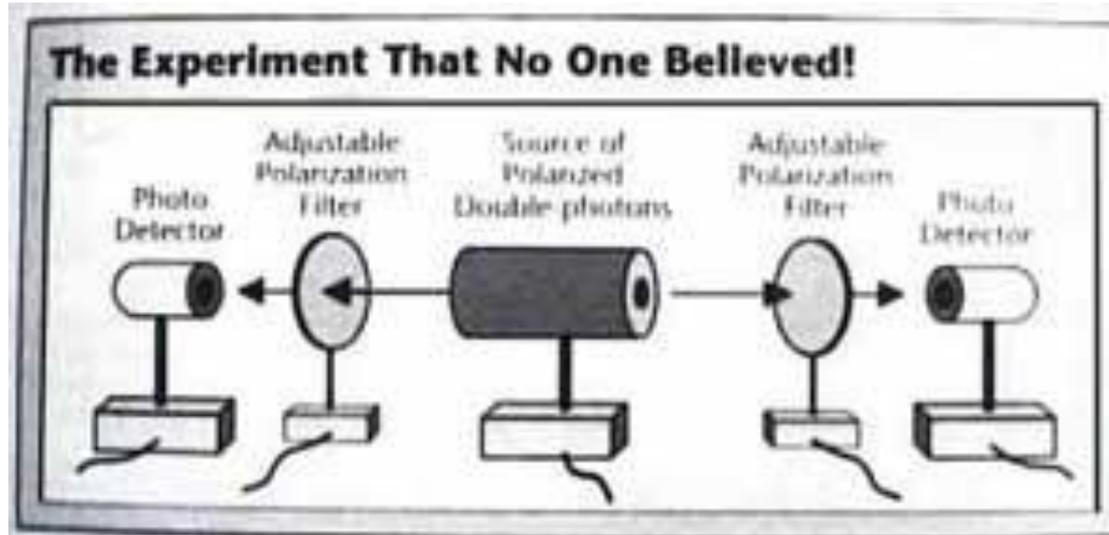


$$E = h\nu$$

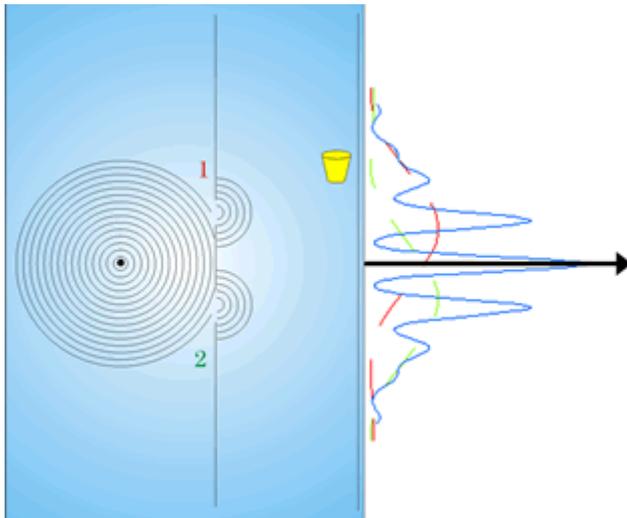
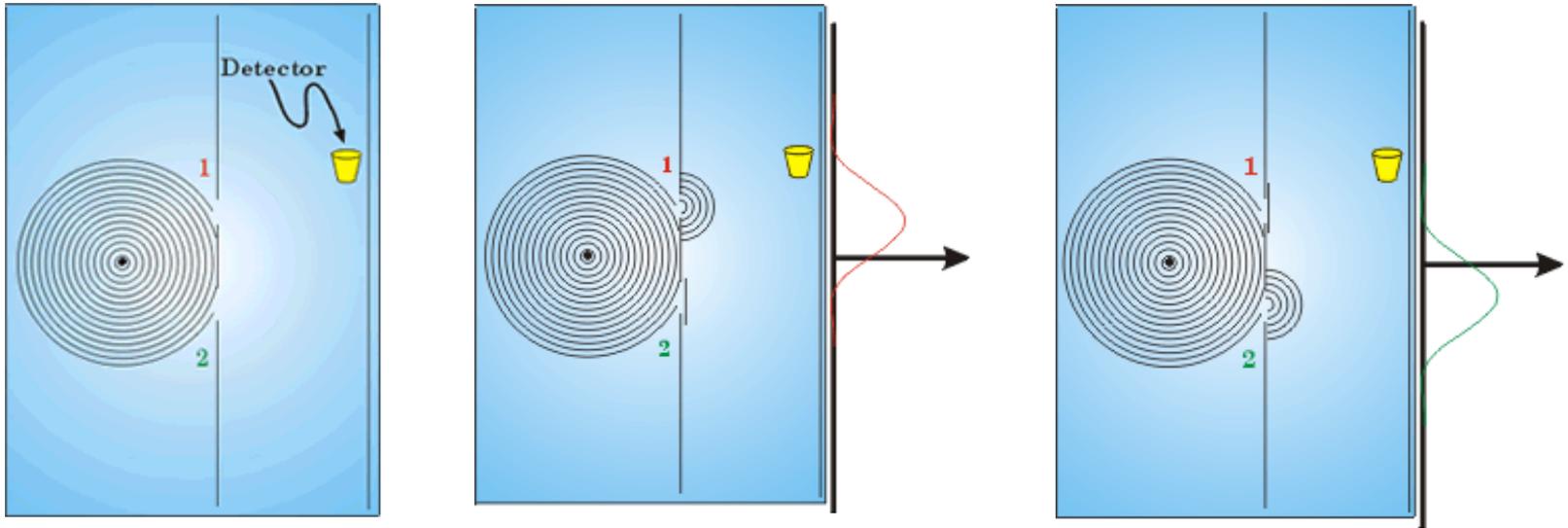


Photoelectric effect

# *Teorema de Bell e o efeito superluminal*



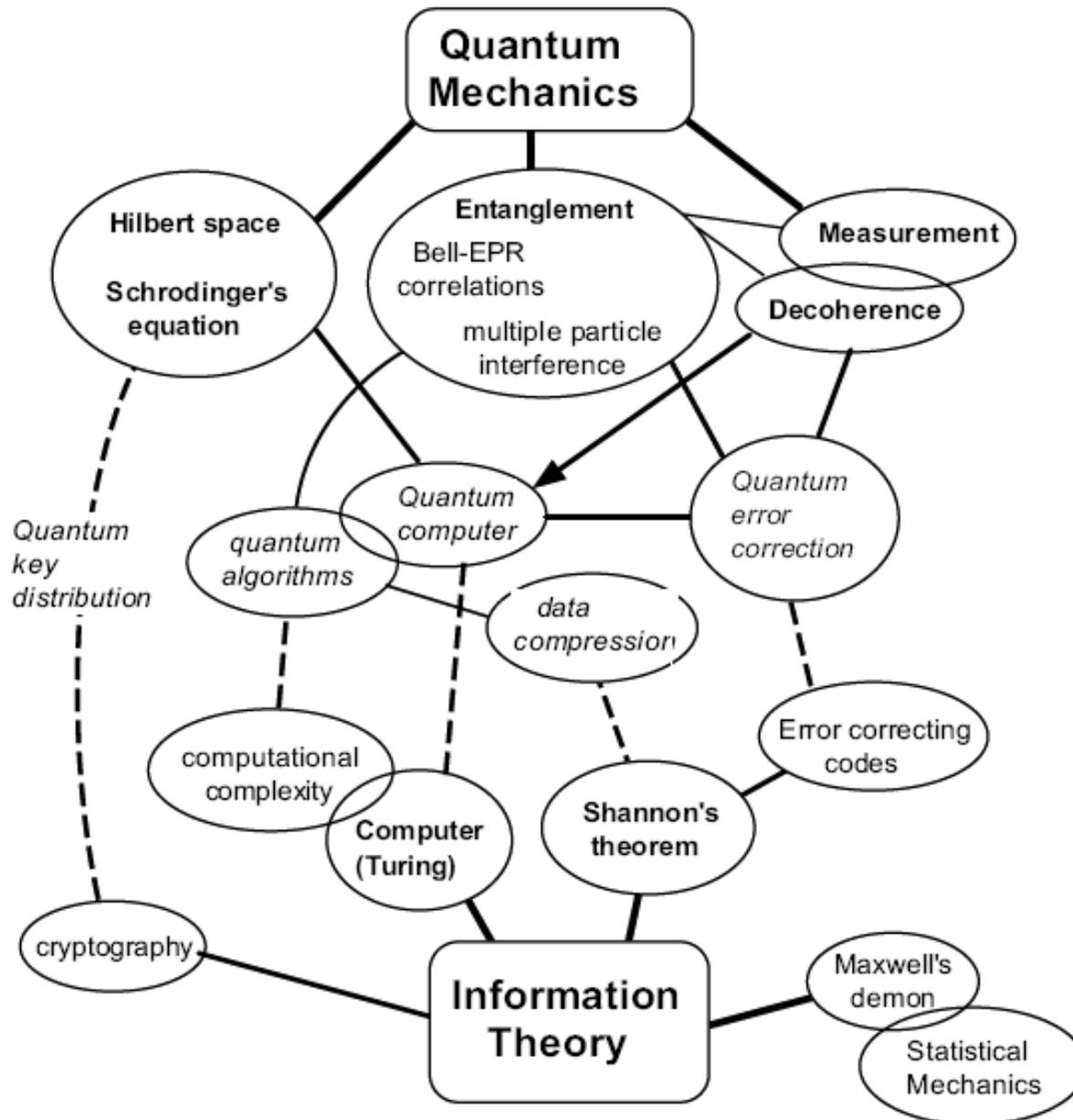
# Efeito de Interferência de ondas



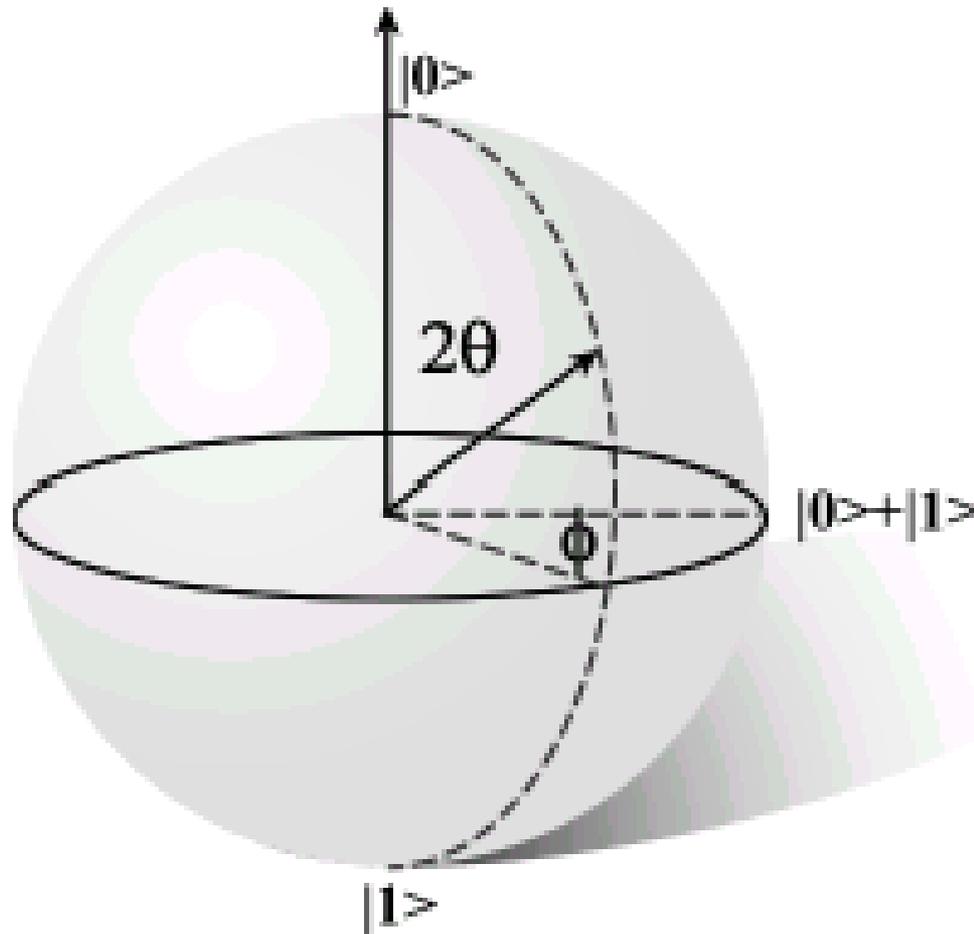
**Mecânica quântica**

**Dualidade: partícula - onda**

# Computação quântica



# Geometric Interpretation of States – Bloch Sphere



$$\cos(\theta)|0\rangle + \sin(\theta)e^{i\phi}|1\rangle$$

- Convenient parameterisation of single-qubit states.
- Orthogonal states are vectors in OPPOSITE directions
- All pure states are on surface of sphere.

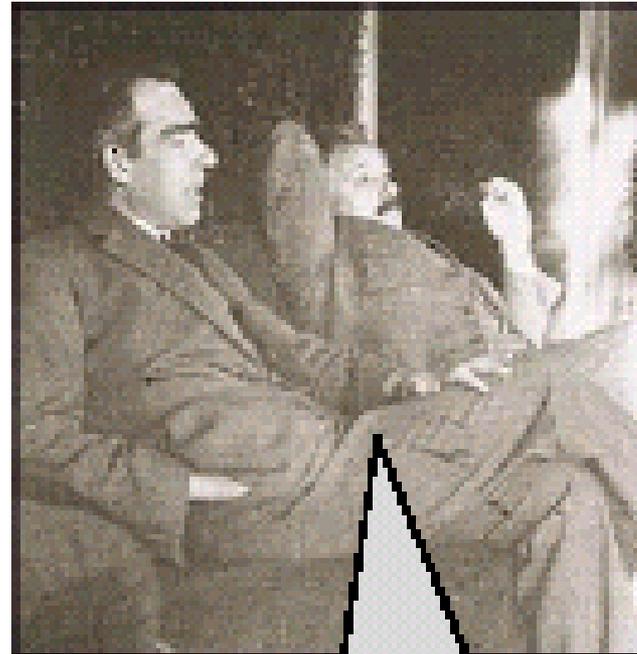
# Logic or Physics?



Why shall I  
accept this  
logically  
impossible  
operation

$\sqrt{NOT}$  ?

Alan Turing



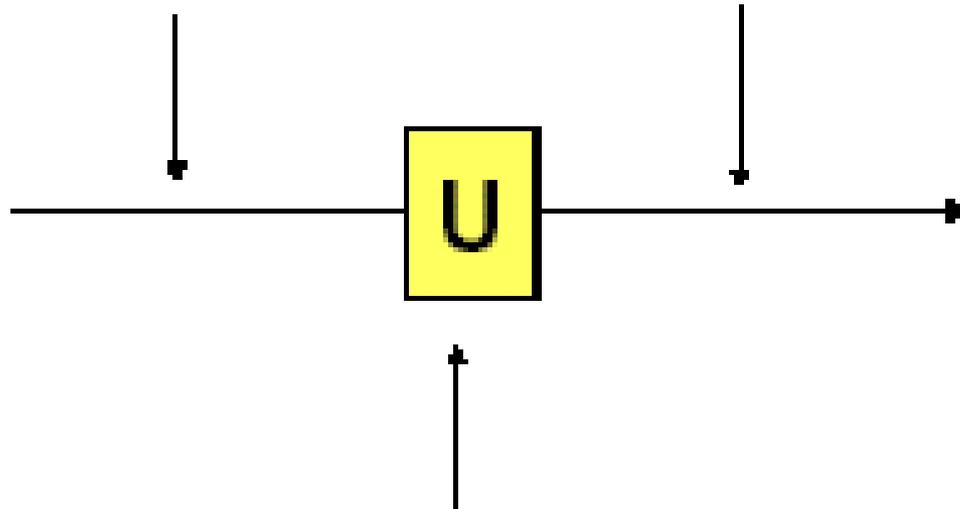
Niels Bohr &  
Albert Einstein

Because its physical  
representation does  
exist in Nature!  
It can be performed!

# Qubits and gates

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A **qubit** is a two-state quantum system; it has a chosen 'computational basis'  $\{|0\rangle, |1\rangle\}$  corresponding to the classical bit values 0 and 1. It can be prepared in a coherent superposition of  $|0\rangle$  and  $|1\rangle$ .



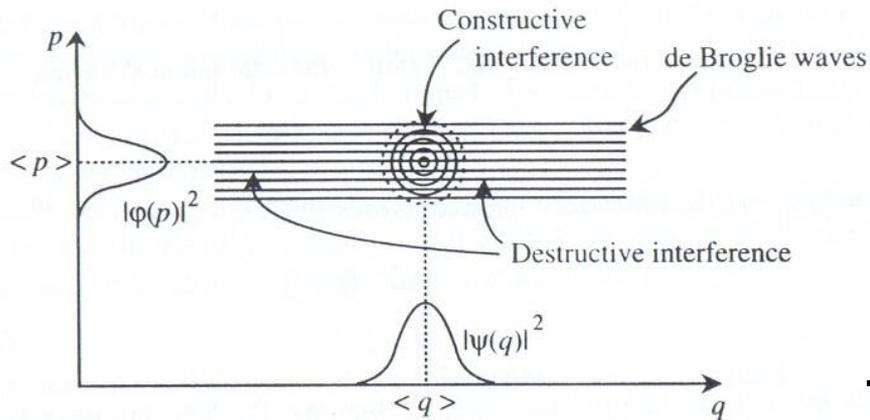
A **quantum logic gate** is an elementary quantum computing device which performs a fixed unitary operation on selected qubits in a fixed period of time.

# Princípios básicos da mecânica quântica

Princípio de incerteza:

$$\Delta p \Delta x \geq \hbar$$

$$\Delta E \Delta t \geq \hbar$$



Evolução temporal do estado quântico:  
Perda de coerência

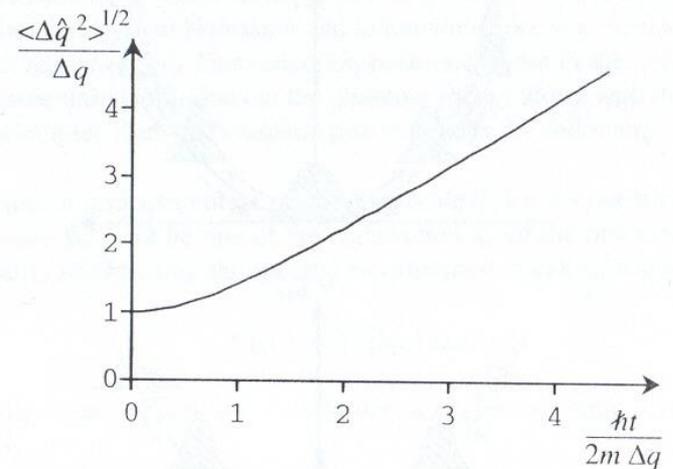
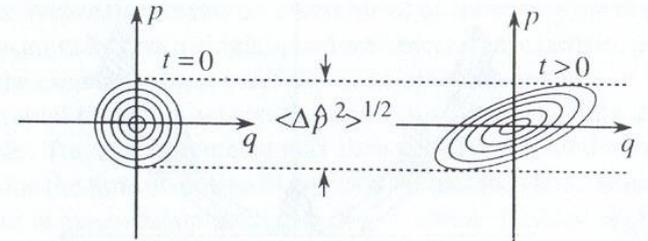


FIGURE 1-2: The quantum diffusion of a free particle.

# Equação de Shrodinger e a função de onda de Shrodinger

$$-i\hbar \frac{\partial}{\partial t} \psi = H\psi = E\psi$$

$$H = \frac{-\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + V(x, y, z)$$

Operador energia  
cinética

Operador energia  
potencial

## Funções de onda de estado estacionário

$$E_n = \langle \psi_n | H | \psi_n \rangle = \int \psi_n^*(x, y, z) H \psi_n(x, y, z) dv$$

Energia media correspondente  
ao n-esimo estado estacionário

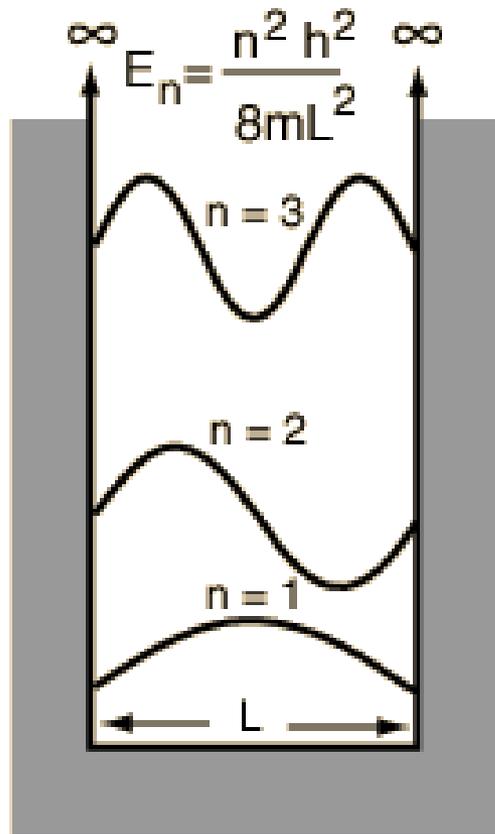
$$|\psi_n|^2 = \psi_n^*(x, y, z) \psi_n(x, y, z)$$

Probabilidade de encontrar a partícula no ponto de  
coordenada (x,y,z) para o e-esimo estado estacionário

$$\langle \psi_n | \psi_n \rangle = \int \psi_n^*(x, y, z) \psi_n(x, y, z) dv = 1$$

Condição de normalização

# Efeito de confinamento quântico



$$\psi_n(x) = C \sin(k_n x) = C \sin\left(\frac{n}{L} x\right), \quad n=1,2,3, \dots$$

$$k_n = \sqrt{\frac{2mE_n}{\hbar^2}}$$

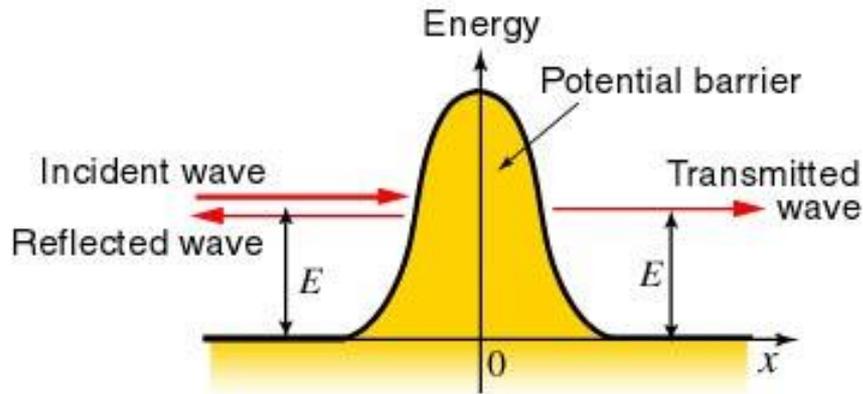
$$E_n = \frac{n^2 \hbar^2}{2mL^2}$$

Níveis “n” quantizados de energia  $\Rightarrow$  níveis discretos

$a_0 =$  Bohr radius = 0.0529 nm

# Efeito de tunelamento

Fig. (D)



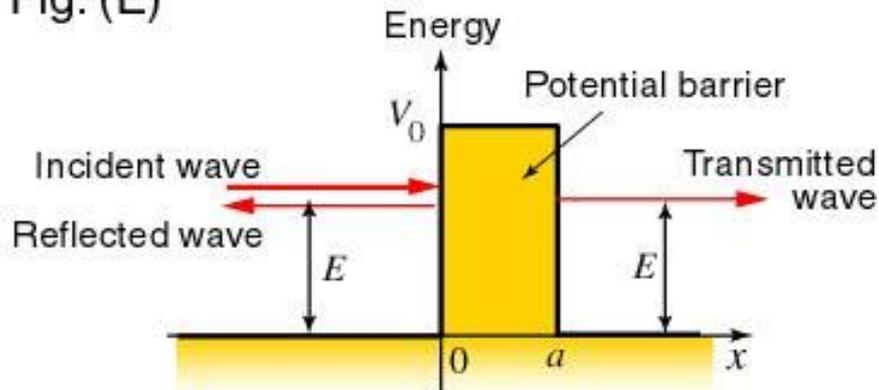
**Função de onda incidente e refletida**

$$\psi(x) = Ae^{ikx} + Be^{-ikx}$$

**Função de onda transmitida**

$$\psi(x) = Ce^{ikx}$$

Fig. (E)



**Coefficiente de tunelamento**

$$T = \frac{|C|^2}{|A|^2} = \left[ 1 + \frac{V_0^2 \sinh(ka)}{4E(V_0 - E)} \right]^{-1}$$

$$k = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

