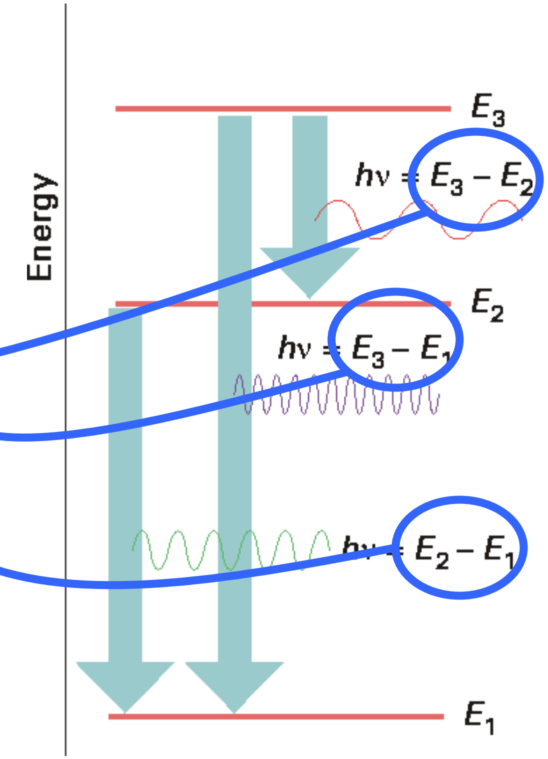
Quantized Energies Explain Atomic and Molecular Emission and Absorption Spectra

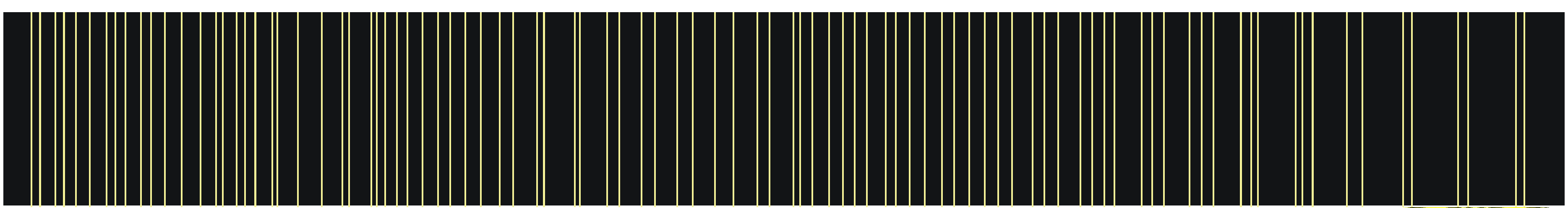
**Emission spectrum of excited mercury:
Spectral lines (projections of slit)**

Frequency (Energy) →



Mercury Lamp!

A molecule (ScF) shows a more complex spectrum (absorption and emission)

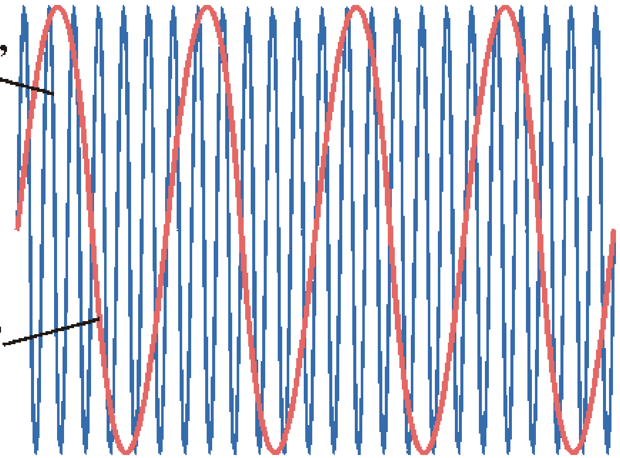


Frequency (Energy) →

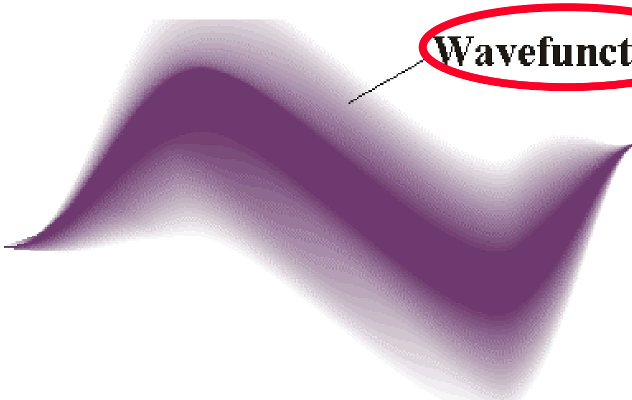
Wave-Particle Dualism: A Particle is Spread Through Space Like a Wave

de Broglie relation:

$$\lambda = \frac{h}{p}$$



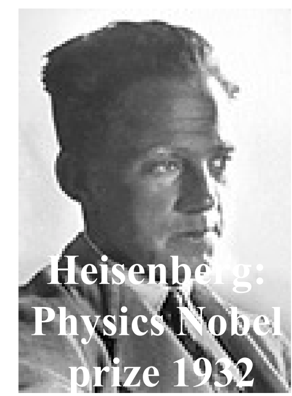
Paradigm shift



Ψ

Fuzziness

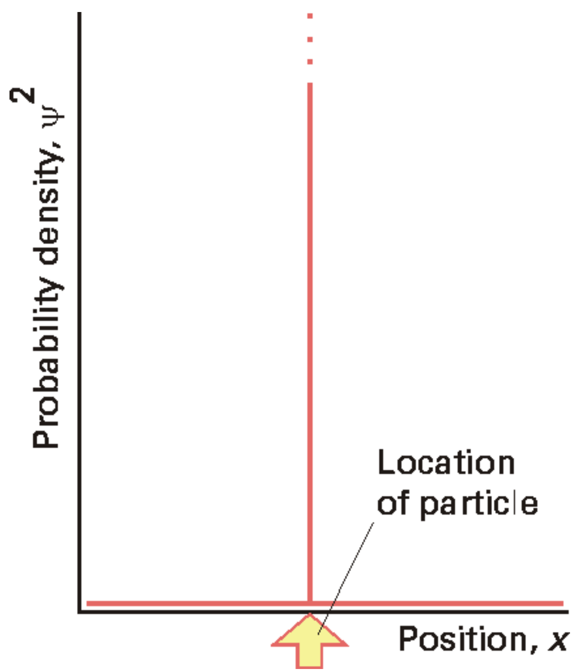
⇒ Heisenberg's uncertainty principle

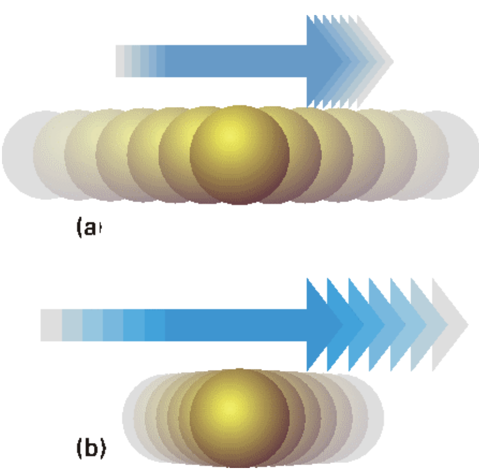


It is impossible to specify simultaneously, with arbitrary precision, both the momentum and the position of a particle

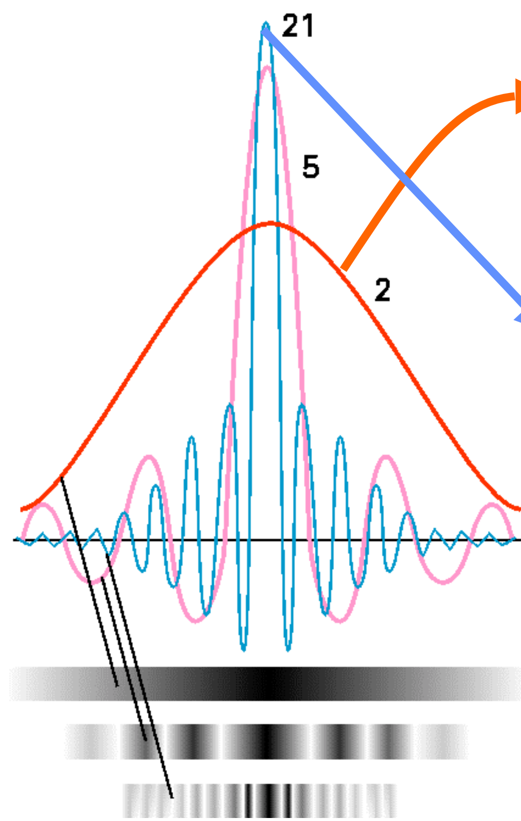
Heisenberg's Uncertainty Principle, less fuzzy

A classical particle





A wave-like particle



A single wave (with defined momentum) has an ill-defined location

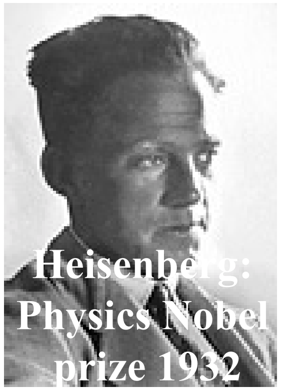
The superposition of many waves (different momenta) to constructively interfere in one position, but destructively in all others, yields a well-defined location, but ill-defined momentum

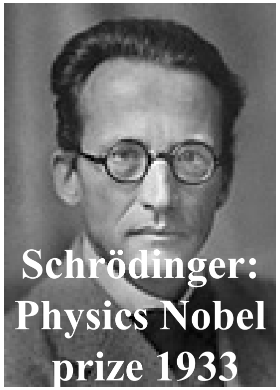
Quantitative (one dimension):

$$\Delta p \Delta x \geq \frac{1}{2}\frac{h}{2\pi} = \frac{1}{2}\hbar$$

Constrained only along the same axis!

Quantum Mechanics: The Schrödinger Equation





Matrix mechanics | Wave mechanics

Quantum mechanics

Differential equation for a one-dimensional wave with amplitude $u(t,x) = \Psi(x)e^{2\pi i \nu t}$:

$$\frac{d^2u}{dx^2} = \frac{1}{\mathrm{v}^2}\frac{d^2u}{dt^2} \quad \Rightarrow \quad \frac{d^2\Psi}{dx^2} + \frac{4\pi^2\nu^2}{\mathrm{v}^2}\Psi = 0$$

time-independent wave function

and

$$E_{total} = E_{kin} + E_{pot} = \frac{1}{2}m\mathrm{v}^2 + V = \frac{p^2}{2m} + V$$

mv = p

$$\Rightarrow \quad p = \sqrt{2m(E-V)}$$

and $\lambda = \frac{h}{p} = \frac{h}{\sqrt{2m(E-V)}} = \frac{\mathrm{v}}{\nu}$

de Broglie relation

$$\Rightarrow \quad -\frac{\hbar^2}{2\mathrm{m}}\frac{d^2\Psi}{dx^2} + V\Psi = E\Psi$$

$$\hat{H}\Psi = E\Psi$$

Hamilton Operator

The Postulates of Quantum Mechanics

1.) The physical state of a particle or system of particles can be described by a wavefunction Ψ(x) or Ψ(x, y, z, t,...)

2.) This wavefunction is a solution to the Schrödinger equation under the specific boundary conditions of the system:

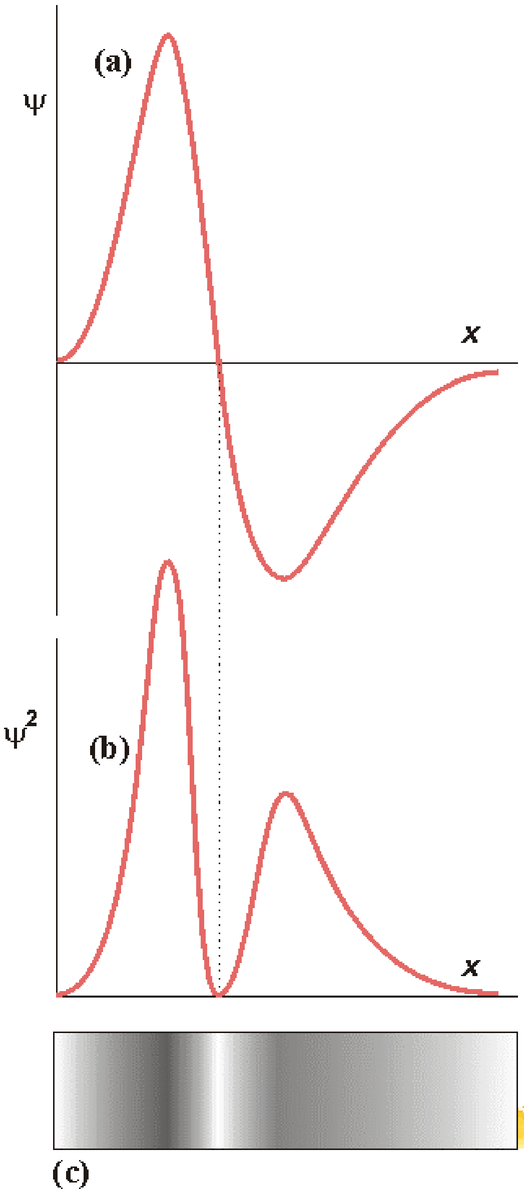
$$\hat{H}\Psi = E\Psi; \quad with\ \hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V \quad and\ \hbar = \frac{h}{2\pi}$$

"Energy Eigenvalue" of the system (discrete!)

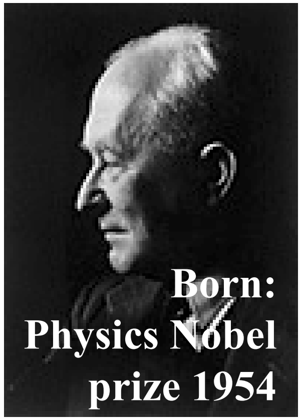
3.) The average value ("expectation value") of any physical property can be calculated from:

$$< F >= \int_{-\infty}^{+\infty} \Psi(x)\,\hat{F}\,\Psi(x)dx \qquad \textbf{e.g.,}\ < x >= \int_{-\infty}^{+\infty} \Psi(x)\,\hat{x}\,\Psi(x)dx$$

The Born Interpretation of the Wavefunction



Statistical (or probabilistic) interpretation of Ψ: "The probability of finding a particle in a small (strictly, infinitesimal) region of space of volume δV is proportional to $\Psi^2 \delta V$, where Ψ is the value of the wavefunction in the region"



Ψ^2 is a probability density

Although Ψ does not have a direct physical interpretation, its square tells us the probability of finding it in a certain region - in accordance with Heisenberg's uncertainty principle