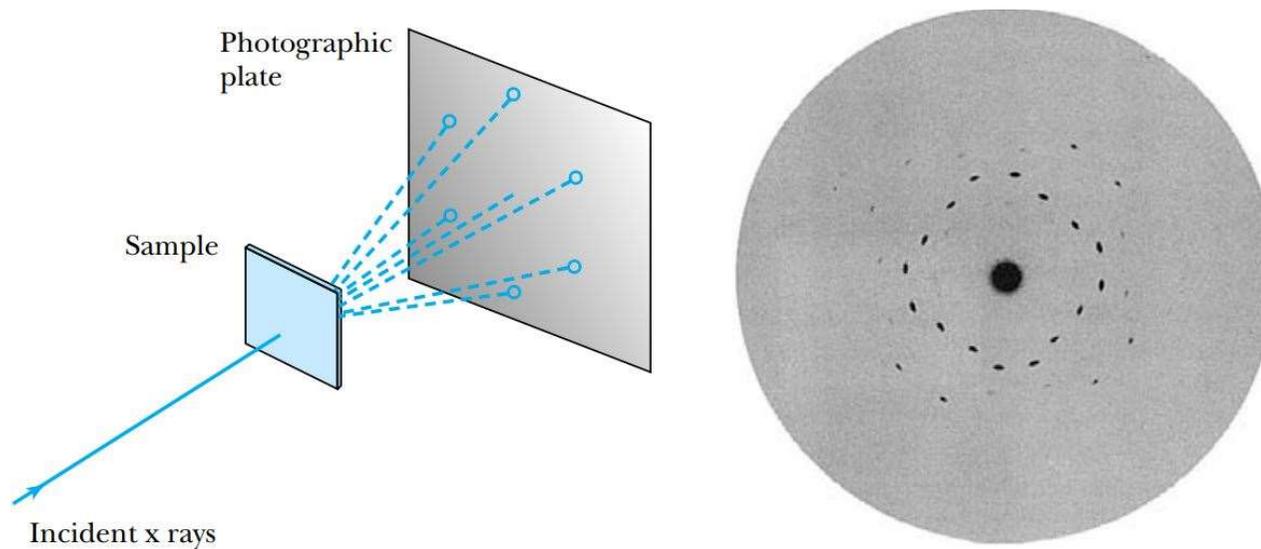
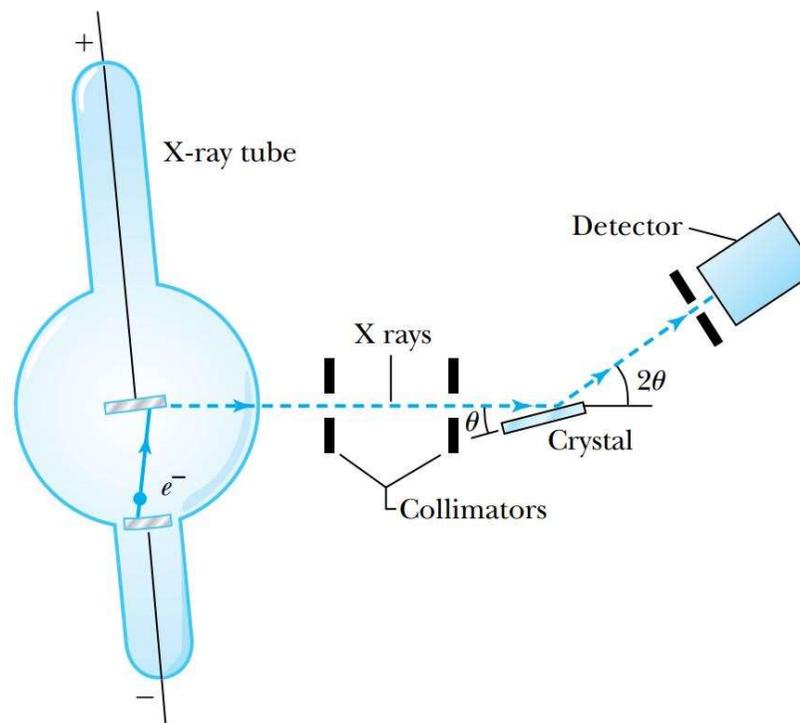


## Chap 5

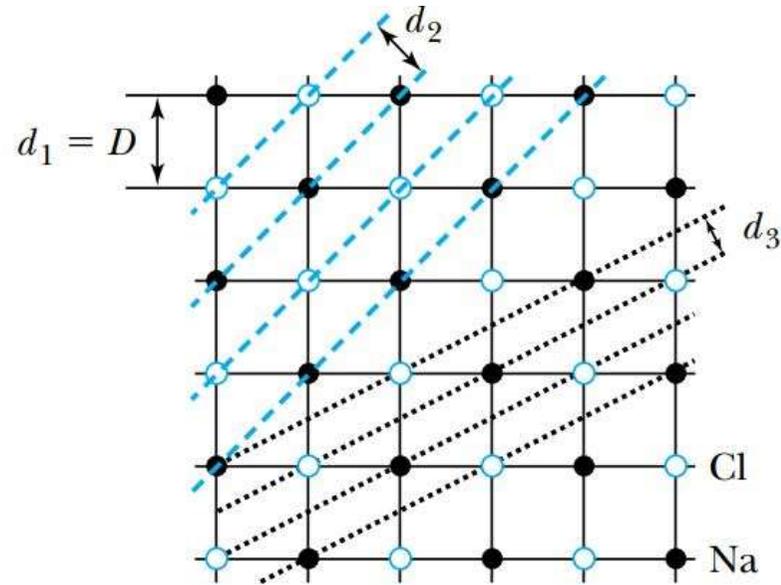
# Wave properties of matter

- X-ray scattering
- De Broglie wave
- Electron scattering
- Phase velocity vs group velocity
- Uncertainty principle
- Wave of probability, Copenhagen interpretation
- Particle in a box > next Chap

# X-ray diffraction by crystal (1912, von Laue)



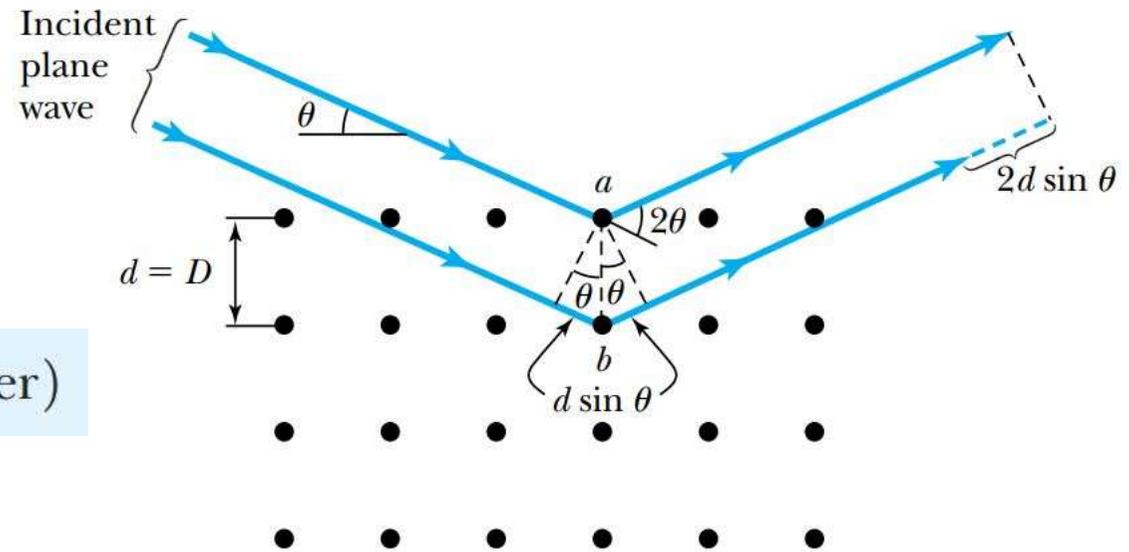
A crystal is a stack of parallel crystal planes  
(with various orientations)



Bragg's law (1912)

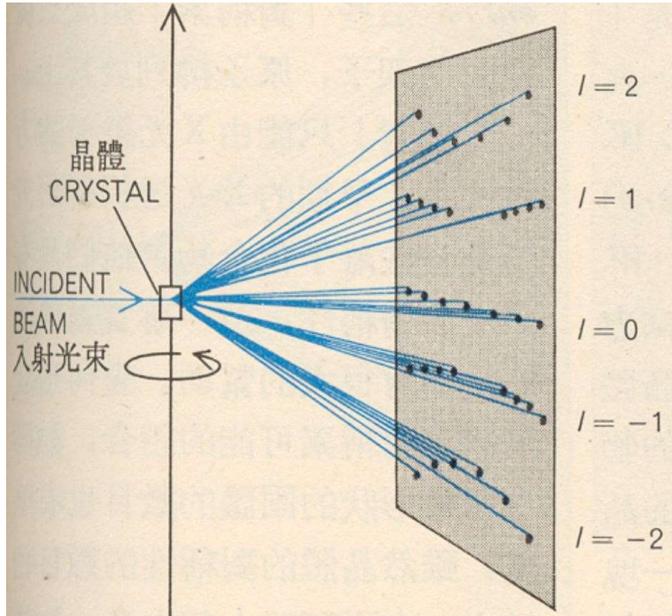
Constructive interference  
from parallel crystal planes

$$n\lambda = 2d \sin \theta \quad (n = \text{integer})$$

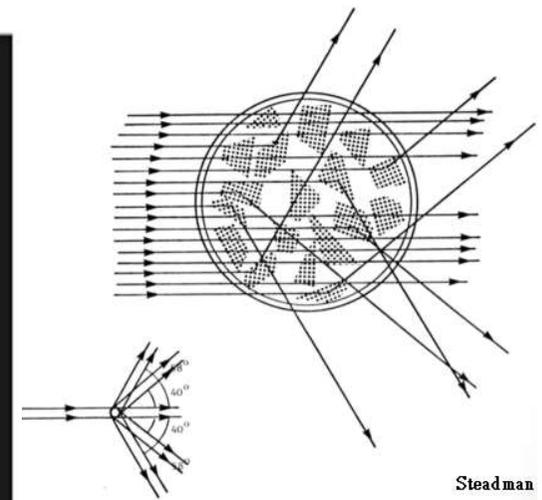
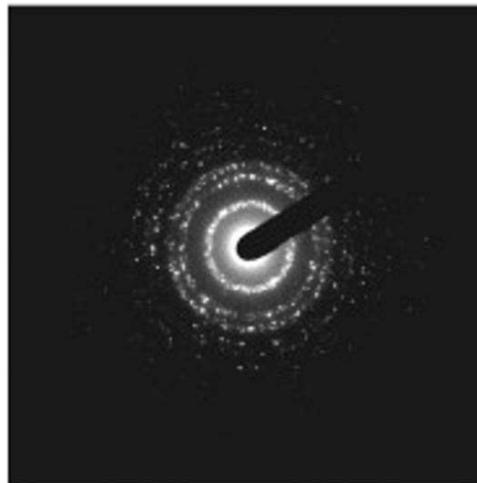
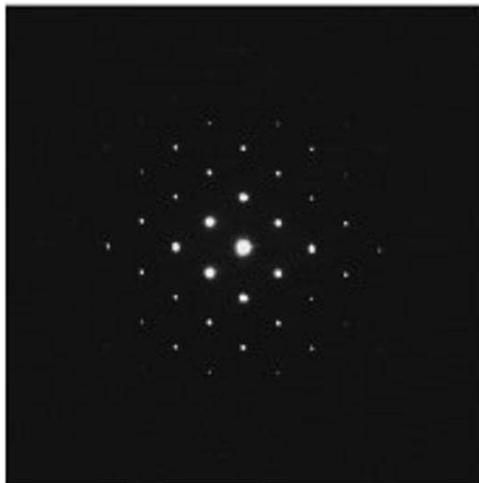
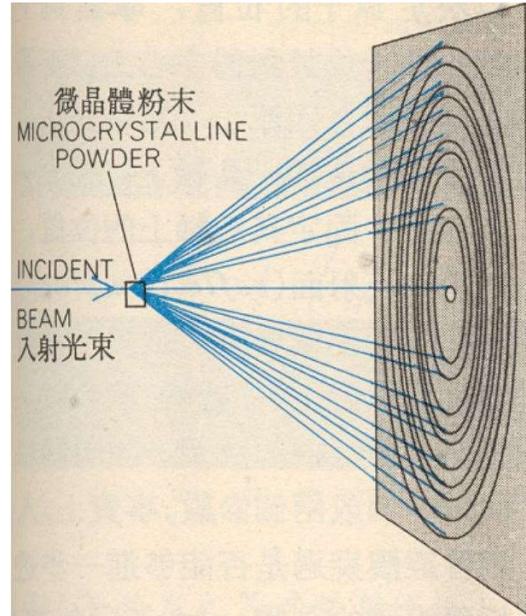


# X-ray diffraction by crystal (1912, von Laue)

- A single crystal



- Polycrystalline powder



4. Example of diffraction patterns: Crystalline Si (left), polycrystalline Si

**Ex 5.1:**

X rays scattered from rock salt (NaCl) are observed to have an intense maximum at an angle of  $20^\circ$  from the incident direction. Assuming  $n = 1$  (from the intensity), what must be the wavelength of the incident radiation?

**Solution**

$$\frac{\text{Number of molecules}}{\text{Volume}} = \frac{N_A \rho}{M}$$

where  $N_A$  is Avogadro's number,  $\rho$  is the density, and  $M$  is the gram-molecular weight. For NaCl,  $\rho = 2.16 \text{ g/cm}^3$  and  $M = 58.5 \text{ g/mol}$ .

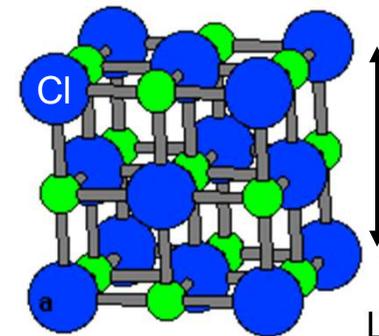
$$\frac{N_A \rho}{M} = \frac{\left(6.02 \times 10^{23} \frac{\text{molecules}}{\text{mol}}\right) \left(2.16 \frac{\text{g}}{\text{cm}^3}\right)}{58.5 \frac{\text{g}}{\text{mol}}} = 4.45 \times 10^{28} \frac{\text{atoms}}{\text{m}^3}$$

fcc: a crystal of cubic structure

$$\frac{1}{d^3} = 4.45 \times 10^{28} \frac{\text{atoms}}{\text{m}^3}$$

$$\rightarrow d = 2.82 \times 10^{-10} \text{ m} = 0.282 \text{ nm}$$

$$\rightarrow \lambda = \frac{2d \sin \theta}{n} = \frac{(2)(0.282 \text{ nm})(\sin 10^\circ)}{1} = 0.098 \text{ nm}$$



Lattice constant  
 $a = 0.564 \text{ nm}$

## De Broglie wave

- De Broglie, while trying to explain diffraction using light-quanta, realized that material particles might have wave property. In his 1924 Ph.D. thesis, he proposed that **just as light has both wave-like and particle-like properties, electrons could also have wave-like properties.**

- For a photon,
$$\left. \begin{array}{l} E = hf \\ E = cp \end{array} \right\} \rightarrow \lambda = \frac{h}{p}.$$

De Broglie extended this relation from photons to all particles.

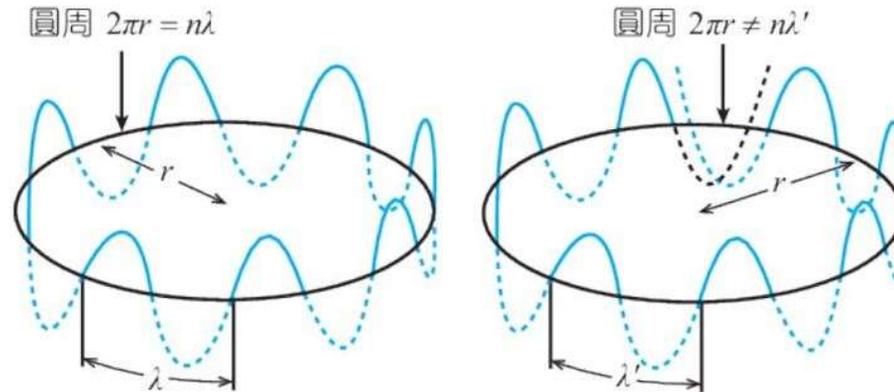
In terms of  $\hbar$ :

$$\begin{array}{l} E = hf = \hbar(2\pi f) = \hbar\omega \\ p = \frac{h}{\lambda} = \hbar\frac{2\pi}{\lambda} = \hbar k \end{array}$$

*“The Sorbonne faculty ... did not know how to evaluate this thesis. ... Langevin... sent a copy of de Broglie’s papers to Einstein. He received a very positive answer; according to Einstein, the paper contained most important discoveries.”*

(From X-rays to quarks)

One initial success: Bohr's mysterious **quantization condition** now can be understood as coming from **standing waves**



- To avoid the discontinuity in wave,  $2\pi r = n\lambda$

$$\lambda = \frac{h}{p} \quad \Rightarrow \quad L = mvr = n\hbar \quad \text{Quantization of angular momentum}$$

- When asked about how to observe it, de Broglie suggested to observe the diffraction of electrons by a crystal

$$\begin{aligned} \lambda &= 2\pi\hbar/p_e = 2\pi\hbar/\sqrt{2m_e E_e} \\ &= 12.26 \times 10^{-8} \text{ cm } [E_e(\text{eV})]^{-1/2} \end{aligned}$$

$$\Rightarrow E_e = 10 \text{ eV}, \lambda \simeq 4 \text{ \AA}$$

# Cavendish Laboratory

## Cavendish Laboratory Nobel Prizes

1904	Physics	Lord Rayleigh *	Density of gases, discovery of argon
1906	Physics	Sir J. J. Thomson	Investigations of electricity in gases
1908	Chemistry	Lord Rutherford *	Element disintegration
1915	Physics	Sir William Lawrence Bragg	X-ray analysis of crystals
1917	Physics	Charles G. Barkla	Secondary x rays
1922	Chemistry	Francis W. Aston	Isotopes discovery
1927	Physics	Charles T. R. Wilson	Cloud chamber
1928	Physics	Sir Owen W. Richardson	Thermionic emission
1935	Physics	Sir James Chadwick	Neutron discovery
1937	Physics	Sir George P. Thomson	Electron diffraction
1947	Physics	Sir Edward V. Appleton *	Upper atmosphere investigations
1948	Physics	Lord Patrick M. S. Blackett	Discoveries in nuclear physics
1951	Physics	Sir John D. Cockcroft and Ernest T. S. Walton	Nuclear transmutation
1962	Physiology or Medicine	Francis H. C. Crick and James D. Watson	DNA discoveries
1962	Chemistry	Max Perutz and Sir John Kendrew	Structures of globular proteins
1973	Physics	Brian D. Josephson	Supercurrent in tunnel barriers
1974	Physics	Sir Martin Ryle and Antony Hewish	Radio astrophysics, pulsars
1977	Physics	Sir Nevill F. Mott	Magnetic and disordered systems
1978	Physics	P. L. Kapitsa *	Low-temperature physics
1982	Chemistry	Sir Aaron Klug	Nucleic acid–protein complexes
2019	Physics	Didler Queloz	Discovery of the first extrasolar planet

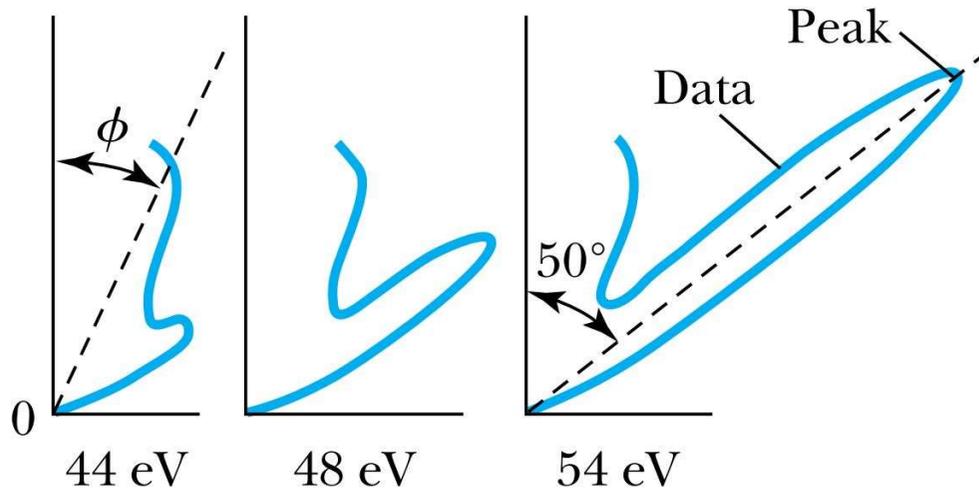
Several physicists fail to observe it, until

1925-27, Davisson and Germer found the evidence of matter wave by accident.

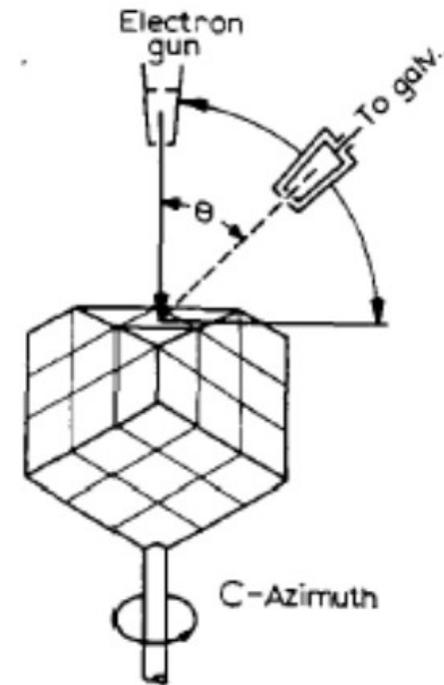
(They did not know about the theory of electron wave).

- They studied the pattern of electron scattering off Ni target in order to determine the electric field inside the atom

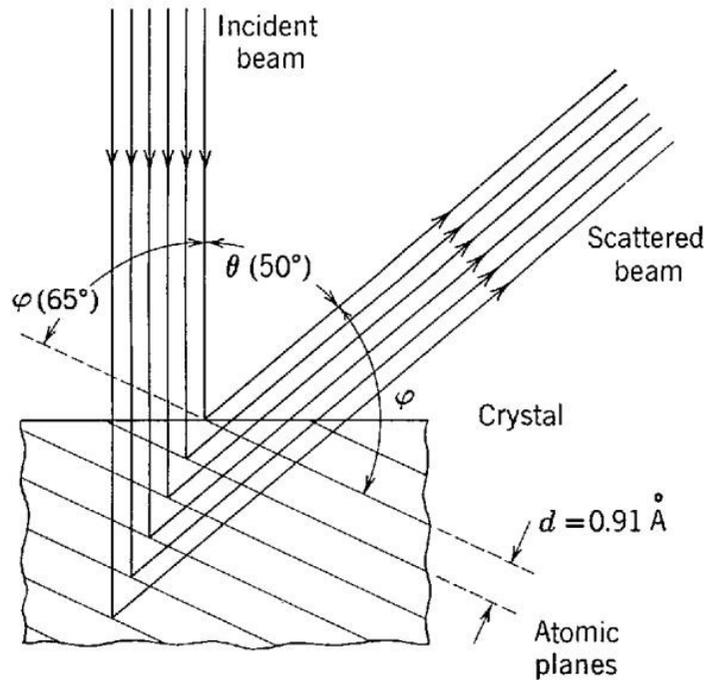
( $E_e=54 \text{ eV}$ ,  $d$  of Ni planes =  $0.91 \text{ \AA}$ )



$$\lambda = 0.167 \text{ nm}$$



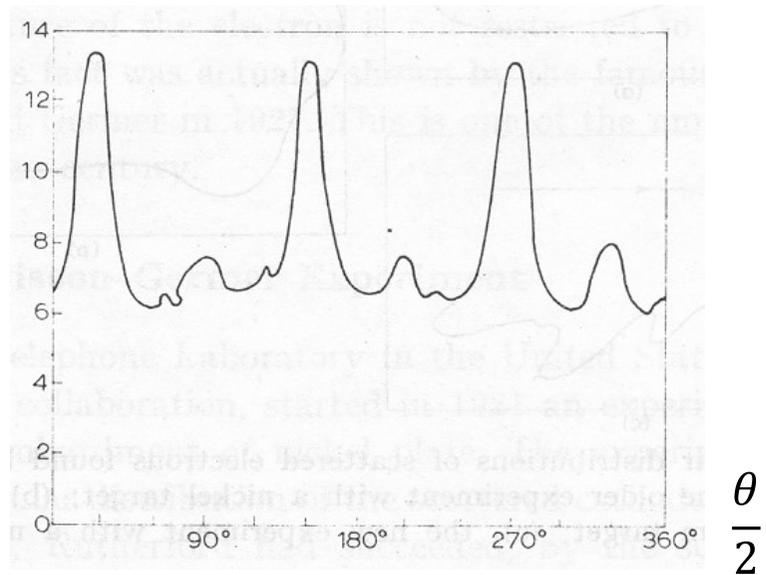
Upon a colleague's (Elasser) advice, they realized that the angular variation of the scattering maybe due to electron wave diffraction.



Eisberg and Resnick

$$n\lambda = 2d \sin \varphi_n$$

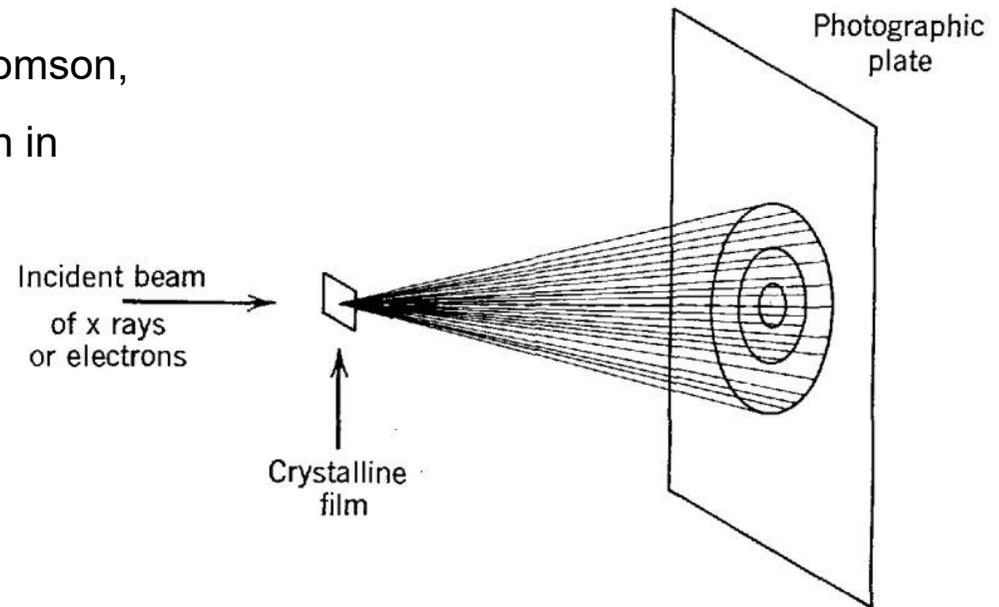
$$\varphi_1 = 65^\circ$$



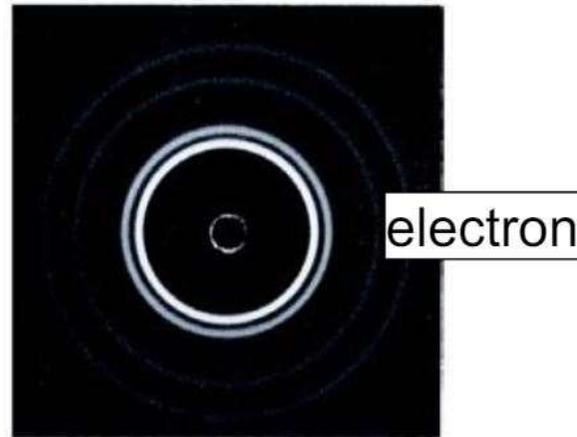
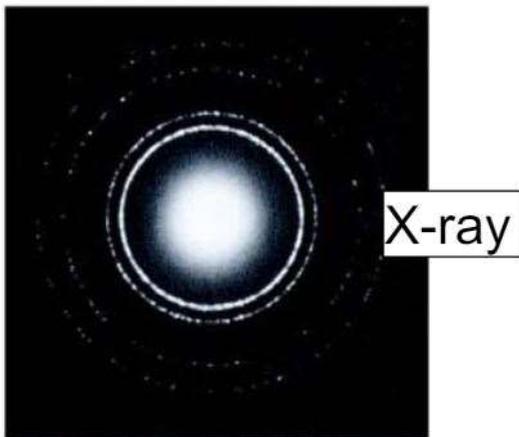
$$\lambda = 2 \times 0.91 \text{ \AA} \times \sin 65^\circ = 1.68 \text{ \AA}$$

Agrees with  $E_e = 54 \text{ eV}$

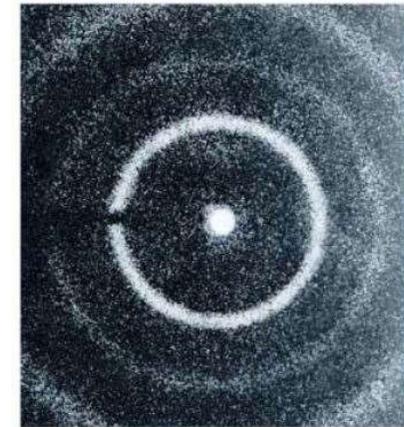
1927, G.P. Thomson, son of J.J. Thomson, saw the effects of electron diffraction in transmission experiments.



Comparison:  
Diffractions of x-ray, electron, neutron



0.07-eV neutrons passing through a polycrystalline sample of iron.

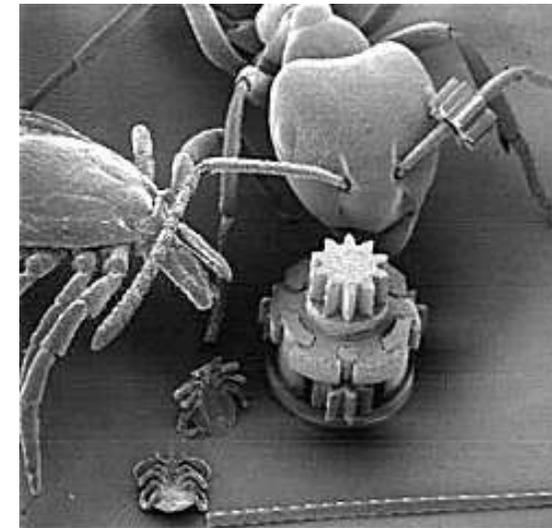
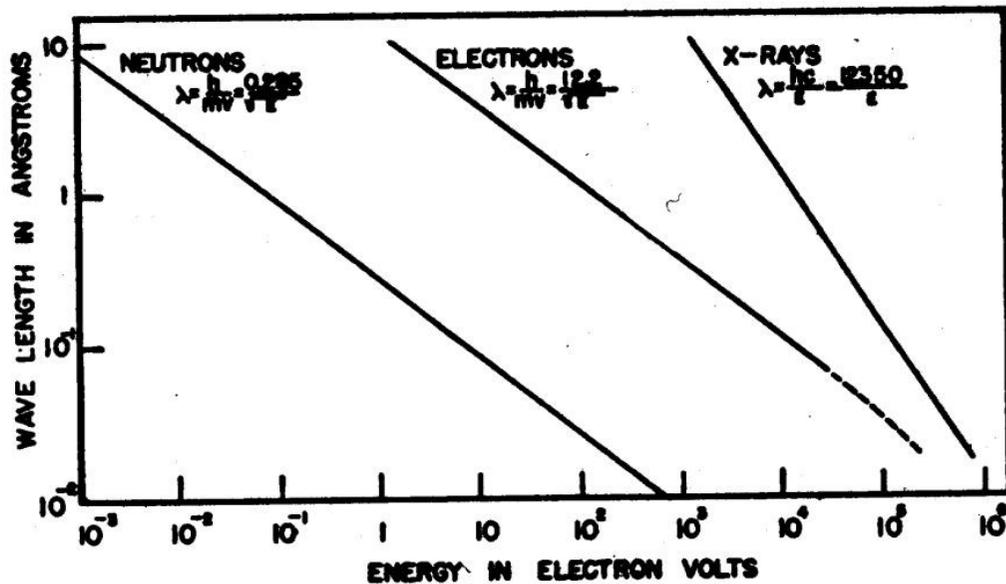


## Electron microscope (Ruska and Knoll 1931)

The ratio of the wavelength of an **electron** to that of a **photon** with the same energy  $E$ :

$$\frac{\lambda_e}{\lambda_\gamma} = \sqrt{\frac{E}{2m_e c^2}}$$

For energies in the range of 10 eV to 10 keV this is very much less than one, giving electron microscopes much better resolution than microscopes using photons of the same energy.



**Ex 5.4:**

In introductory physics, we learned that a particle (ideal gas) in thermal equilibrium with its surroundings has a kinetic energy of  $3kT/2$ . Calculate the de Broglie wavelength for (a) a neutron at room temperature (300 K) and (b) a “cold” neutron at 77 K (liquid nitrogen).

**Solution**

$$\frac{p^2}{2m} = \text{K.E.} = \frac{3}{2}kT$$

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{3mkT}} = \frac{2.52}{T^{1/2}} \text{ nm} \cdot \text{K}^{1/2}$$

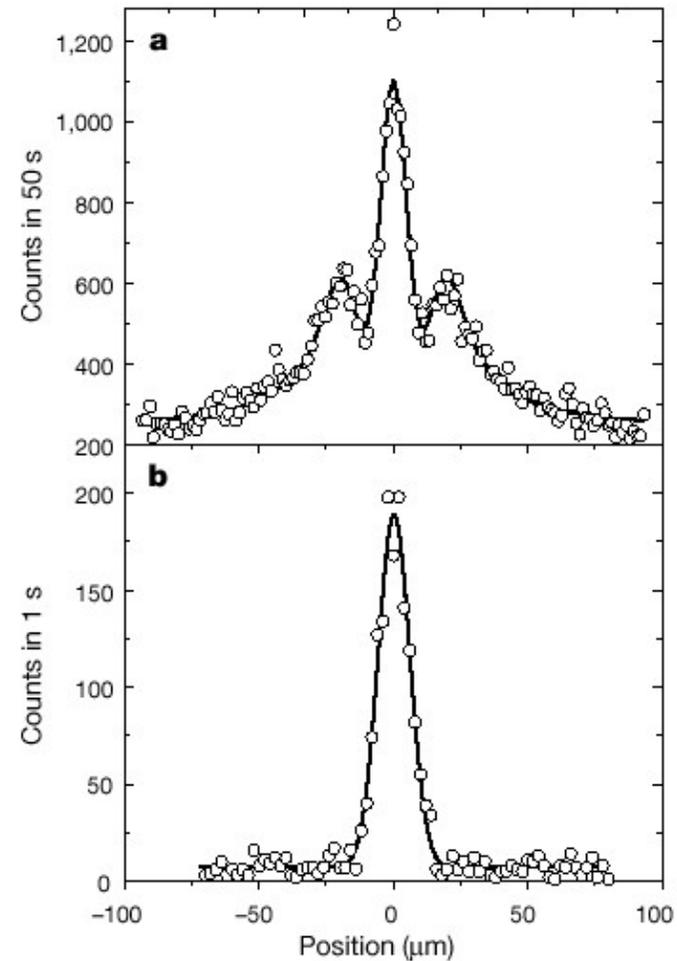
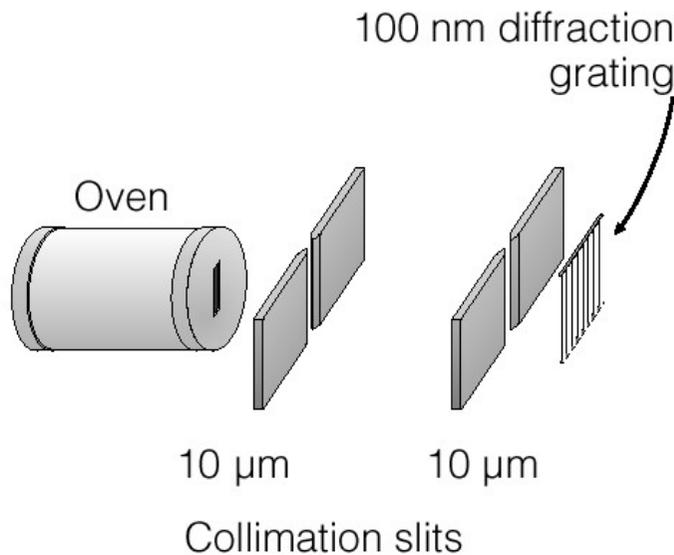
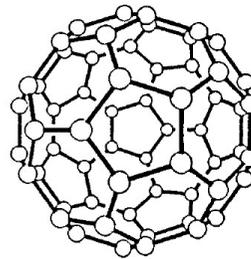
$$\rightarrow \lambda(300 \text{ K}) = \frac{2.52 \text{ nm} \cdot \text{K}^{1/2}}{\sqrt{300 \text{ K}}} = 0.145 \text{ nm}$$

$$\lambda(77 \text{ K}) = \frac{2.52 \text{ nm} \cdot \text{K}^{1/2}}{\sqrt{77 \text{ K}}} = 0.287 \text{ nm}$$

	e- in H atom	<sup>87</sup> Rb atom at 10 nK	baseball
m (kg)	$9.1 \times 10^{-31}$	$1.4 \times 10^{-25}$	0.15
v (m/s)	$2.2 \times 10^6$	0.001	40
$\lambda$ (m)	$3.3 \times 10^{-10}$	$4.7 \times 10^{-6}$	$1.1 \times 10^{-34}$

- 2-slit experiment using C<sub>60</sub> (1999, Zeilinger)

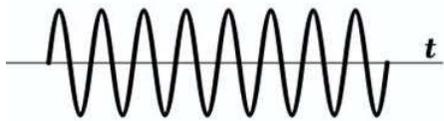
The velocity of 210 m/s corresponds to a de Broglie wavelength for C<sub>60</sub> of 2.5  $\mu\text{m}$ .



- X-ray scattering
- De Broglie wave
- Electron scattering
- Phase velocity vs group velocity
- Uncertainty principle
- Wave of probability, Copenhagen interpretation

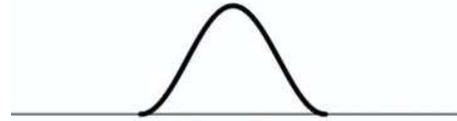
To describe the matter wave, we need to recall some properties of wave

Phase velocity



$$v_p = \frac{\omega}{k}$$

Group velocity



$$v_g = \frac{d\omega}{dk}$$

- The **group velocity** of a wave is the velocity with which the overall envelope propagating through space (wiki).

### Group Velocity / Phase Velocity Animation

$$\begin{aligned}\Psi(x, t) &= \Psi_1(x, t) + \Psi_2(x, t) \\ &= A \cos(k_1 x - \omega_1 t) + A \cos(k_2 x - \omega_2 t) \\ &= 2A \cos\left[\frac{1}{2}(k_1 - k_2)x - \frac{1}{2}(\omega_1 - \omega_2)t\right] \cos\left[\frac{1}{2}(k_1 + k_2)x - \frac{1}{2}(\omega_1 + \omega_2)t\right] \\ &= 2A \cos\left(\frac{\Delta k}{2}x - \frac{\Delta \omega}{2}t\right) \cos(k_{\text{av}}x - \omega_{\text{av}}t) \quad \rightarrow \quad v_g = \frac{d\omega}{dk}\end{aligned}$$

**Ex 5.5:**

Suppose a particle is a wavepacket. Show that the particle velocity is equal to the **group velocity**.

Note: This is not so for the phase velocity

**Solution**

$$u_{\text{gr}} = \frac{d\omega}{dk} = \frac{d(E/\hbar)}{d(p/\hbar)} = \frac{dE}{dp} = \frac{d}{dp} \frac{p^2}{2m} = \frac{2p}{2m} = v$$

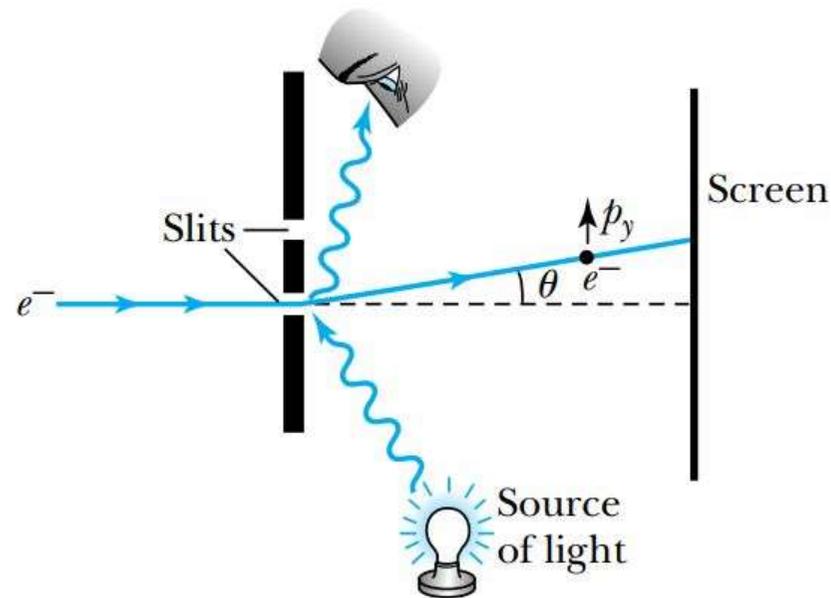
The electrons can interfere even when sent one at a time.

Which slit does the electron pass?

- To determine which slit the electron went through: We shine a light and use a microscope to look at the region. After the electron passes through one of the slits, light bounces off the electron; we observe the reflected light, so we know which slit the electron came through.

need  $\lambda_{ph} < d$

→  $p_{ph} = \frac{h}{\lambda_{ph}} > \frac{h}{d}$



- The momentum of the electrons 
$$p_{\text{el}} = \frac{h}{\lambda_{\text{el}}} \sim \frac{h}{d}.$$
- The momentum of the photons strongly modify the momentum of the electron, thus changing the direction of the electron! **The attempt to identify which slit the electron is passing through will destroy the interference pattern.**

**We can determine the path of electrons, but interference would disappear.**

Particle and wave properties are like 2 sides of a coin.

**Bohr's principle of complementarity:**

It is *not possible* to describe physical observables simultaneously as particles and waves.

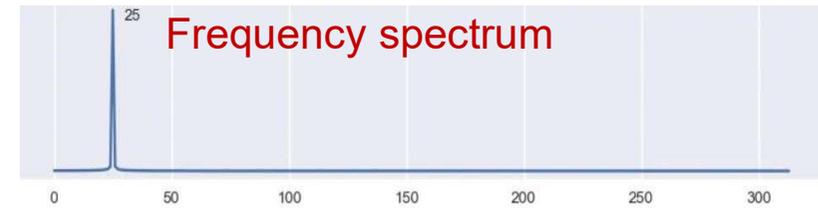
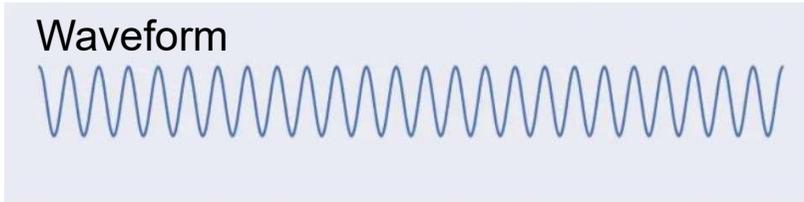
Note: This “principle” does not give you any new information, it just tell you don't bother to figure out this problem.



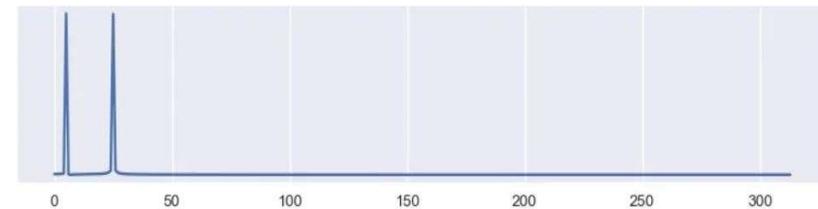
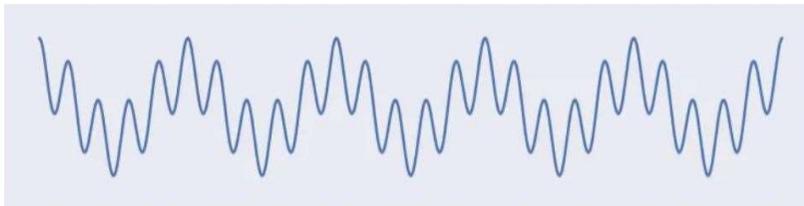
To understand the [uncertainty principle](#), we need to have a deeper look at the properties of wave. This is related to the so called [spectral analysis](#) (or [Fourier analysis](#))

## Spectrum of wave

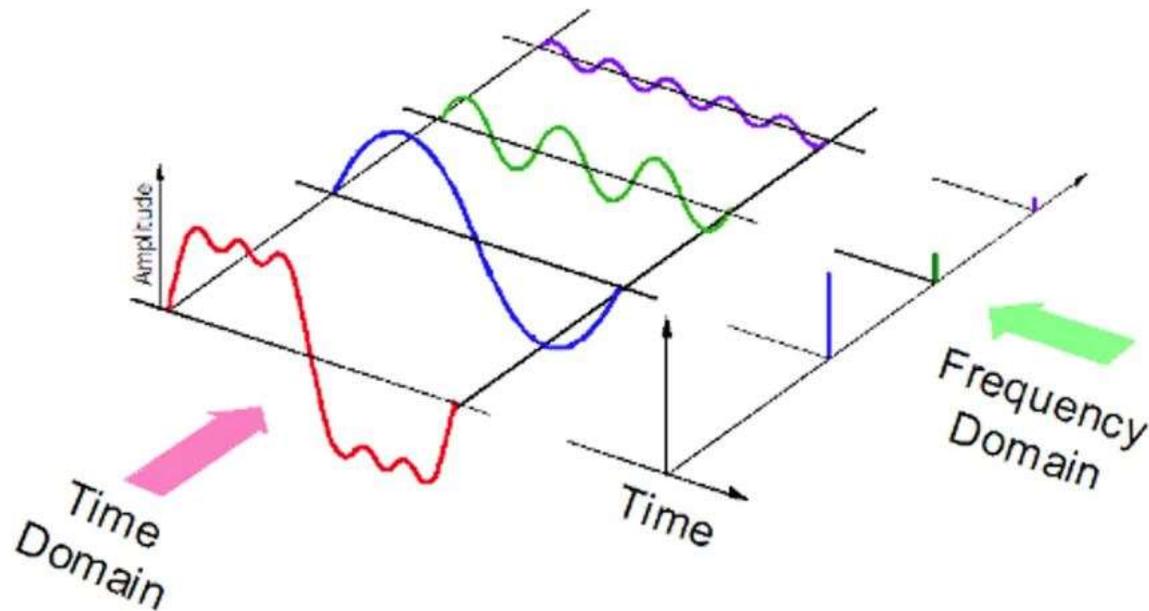
- A wave with 1 freq



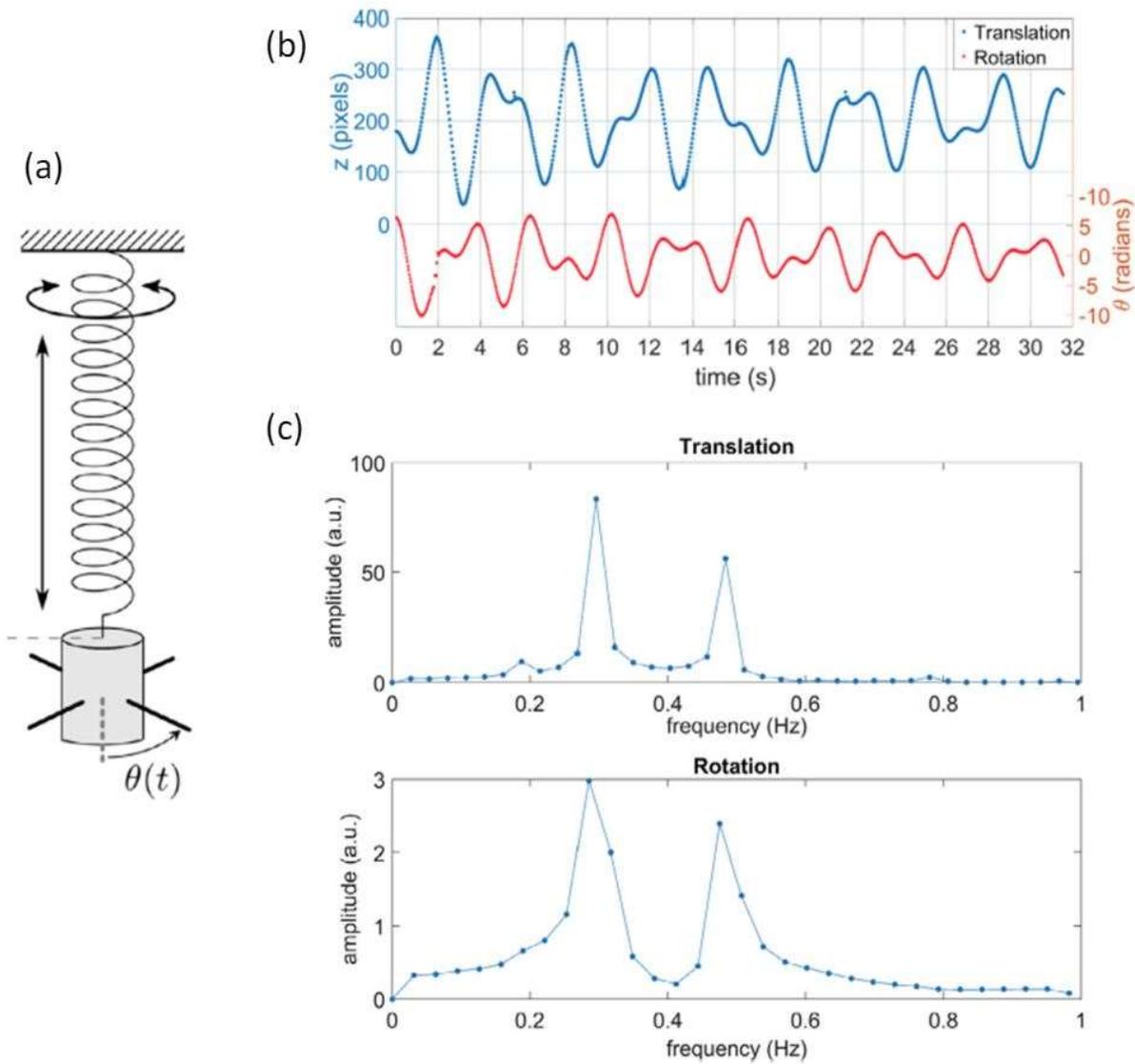
- A wave with 2 freq



- A wave with 3 freq



For example, a [Wilberforce pendulum](#)

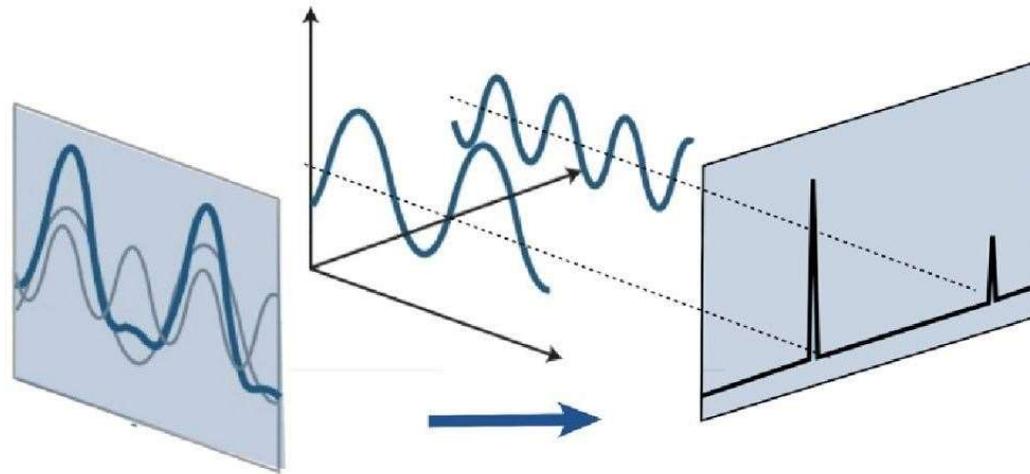


Waveform

Frequency spectrum

Have a try on the [Fourier analysis applet](#)

# Fourier Transform:

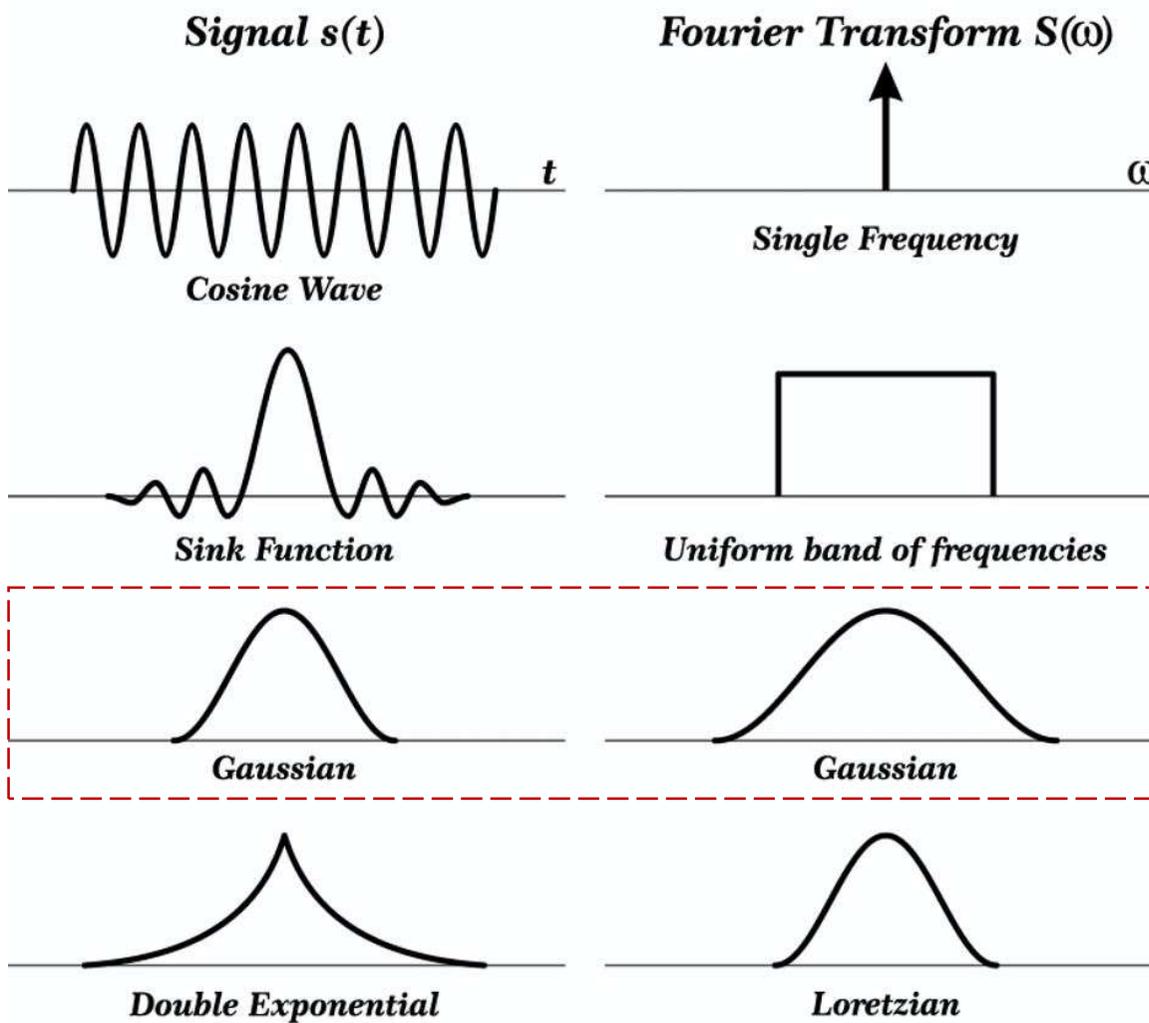


Conjugate variables:  $f(t)$  vs  $f(\omega)$   
or  $f(x)$  vs  $f(k)$

Two different ways to see the same wave

# Spectral analysis (i.e. Fourier analysis)

Waveform (position)  $\longleftrightarrow$  Frequency spectrum (momentum)



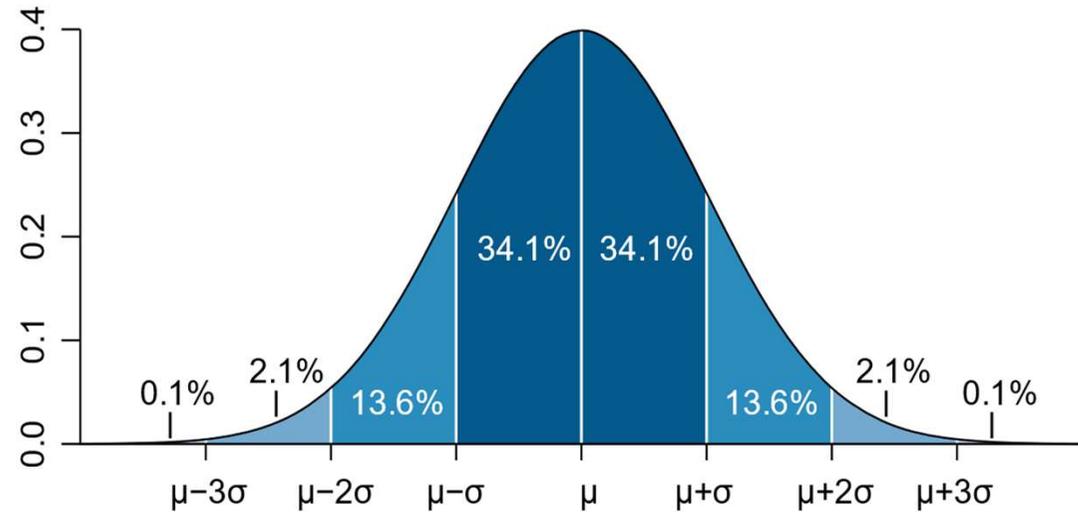
The spectral distribution of a Gaussian wave is also a Gaussian distribution

## Gaussian distribution

$$\psi(x) = Ae^{-(x-x_0)^2/2\sigma^2}$$

### Standard deviation

$$\sigma_x \equiv \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \sigma$$



wiki

➔  $\tilde{\psi}(k) = Be^{-\sigma^2 k^2/2}$

### Standard deviation

$$\sigma_k = \frac{1}{\sigma}$$

- Identify  $\sigma_x, \sigma_k$  with  $\Delta x, \Delta k$  (uncertainties)

➔  $\Delta x \Delta k = 1$

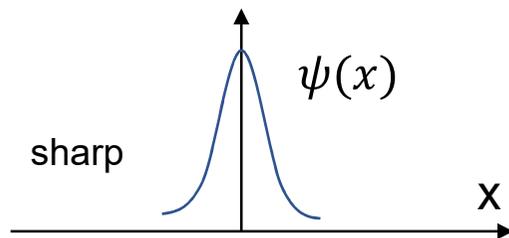
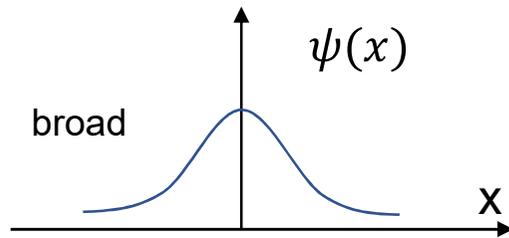
A more detailed calculation gives  $\Delta k \Delta x = 1/2$ .

This is true **only for a Gaussian wavepacket**

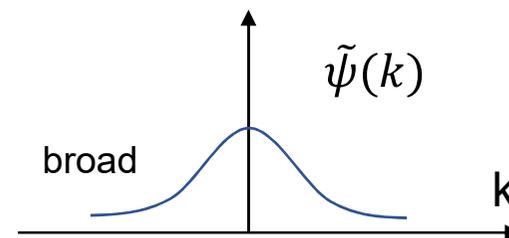
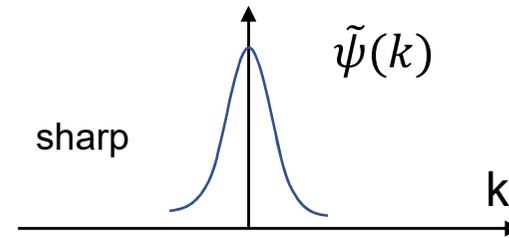
(for others, the product always  $> 1/2$ )

## Uncertainty relation (Heisenberg, 1927)

- Position  $x$



- Momentum  $p$



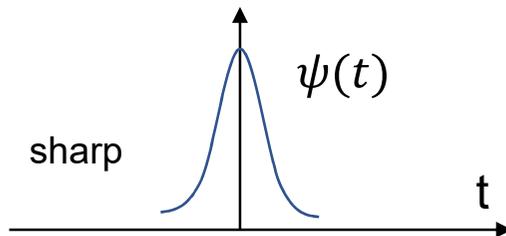
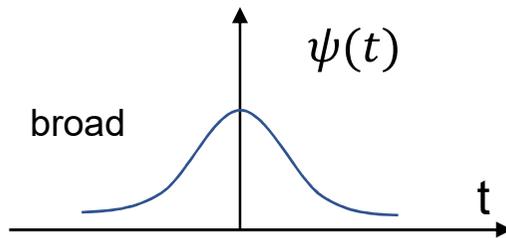
➡ The more localized the position, the more uncertain the momentum, and vice versa. It is impossible to measure simultaneously, with no uncertainty, the precise values of  $p$  and  $x$  for the same particle.

$$\text{Since } \Delta x \Delta k \geq \frac{1}{2} \quad \Rightarrow \quad \Delta x \Delta p \geq \frac{\hbar}{2}$$
$$p = \hbar k$$

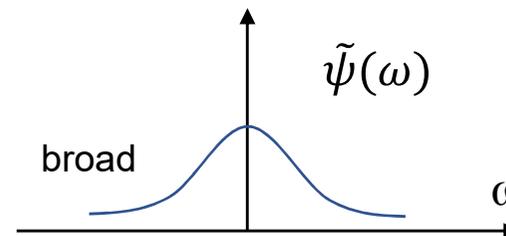
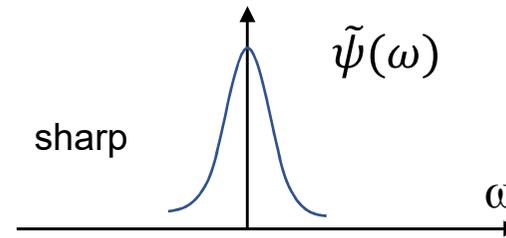
Replace the pair  $(x,p)$  by  $(E,t)$ , then we have

### Uncertainty relation for energy and time

• time  $t$



• energy  $E$



$$\Delta t \Delta \omega \geq \frac{1}{2}, \quad E = \hbar \omega$$

→  $\Delta E \Delta t \geq \frac{\hbar}{2}$

The shorter the state lives, the more uncertain the energy of the state, and vice versa.

A particle that is confined in space cannot have zero kinetic energy

$$k_{\min} = \frac{p_{\min}^2}{2m} \geq \frac{(\Delta p)^2}{2m} \geq \frac{\hbar^2}{2m\ell^2}$$

Examples: **Confinement in atom**

Assume atomic size =  $0.4\text{nm} = \Delta x$

$$\Delta p = \frac{h}{\Delta x} = 1.66 \times 10^{-24} \text{ kg} \cdot \text{m} / \text{s}$$

$$\Delta p = p ; \quad E = \frac{p^2}{2m}$$

For electron:

$$E = \frac{(1.66 \times 10^{-24} \text{ kg} \cdot \text{m} / \text{s})^2}{2(9.11 \times 10^{-31} \text{ kg})(1.6 \times 10^{-19} \text{ J} / \text{eV})}$$

$$E = 9.4 \text{ eV}$$

hyperphys

**Confinement in nucleus**

Nuclear size =  $\frac{1}{20,000} \times 0.4\text{nm} = \Delta x$

$$\Delta p = \frac{h}{\Delta x} = 3.31 \times 10^{-20} \text{ kg} \cdot \text{m} / \text{s}$$

For electron:

$$E = \frac{(3.31 \times 10^{-20} \text{ kg} \cdot \text{m} / \text{s})^2}{2(9.11 \times 10^{-31} \text{ kg})(1.6 \times 10^{-19} \text{ J} / \text{eV})}$$

$$E = 3.77 \times 10^9 \text{ eV} = 3.77 \text{ GeV}$$

For proton, divide by  $m_p / m_e = 1836$

$$E = 2.05 \times 10^6 \text{ eV} = 2.05 \text{ MeV}$$

Energy and time  $\Delta E \Delta t > \frac{\hbar}{2}$

A state that only exists for a short time cannot have a definite energy.

- For example, **excited states** have a finite lifetime. By the time–energy uncertainty principle, they do not have a definite energy. Each time they decay, the energy they release is slightly different. As a result, the spectral line has a finite width called the **natural linewidth**. Fast-decaying states have a broad linewidth, while slow-decaying states have a narrow linewidth.

(wiki)

e.g., for the **first excited state of H**,  $\tau \sim 1.6 \times 10^{-9}$  s

So  $\Delta E \sim 4 \times 10^{-7}$  eV  $\frac{\Delta \lambda}{\lambda} \sim 4 \times 10^{-8}$

Modern instruments are capable of measuring ratios approaching  $10^{-17}$ , or 1 Hz in a frequency of  $10^{17}$  Hz!

- The same effect also makes it difficult to specify **the rest mass of unstable particles**. The faster the particle decays (the shorter its lifetime), the less certain is its mass (the larger the particle's width), wiki

## Uncertainty principle

- The uncertainty relation is a direct consequence of the operator algebra in QM,  $[x, p] = i\hbar$ .
- If we can determine both  $\mathbf{x}$  and  $\mathbf{p}$  accurately, then that means the uncertainty relation is not correct, and the whole mathematical structure of QM would collapse.
- To defend the formalism of QM, Heisenberg, Bohr ... etc say that we **won't and shouldn't** be able to determine both  $\mathbf{x}$  and  $\mathbf{p}$  accurately (uncertainty principle).
- Einstein, Schrödinger ... etc think that it's possible to eliminate the uncertainty. If this can be done, then QM would be like statistical mechanics, and a deeper theory (**hidden variable theory**) is required.
- All of the researches till today support Bohr and Heisenberg's view.

The uncertainty principle contributes to the acceptance of the following **probabilistic view of matter wave**.

# Probability, Wave Functions

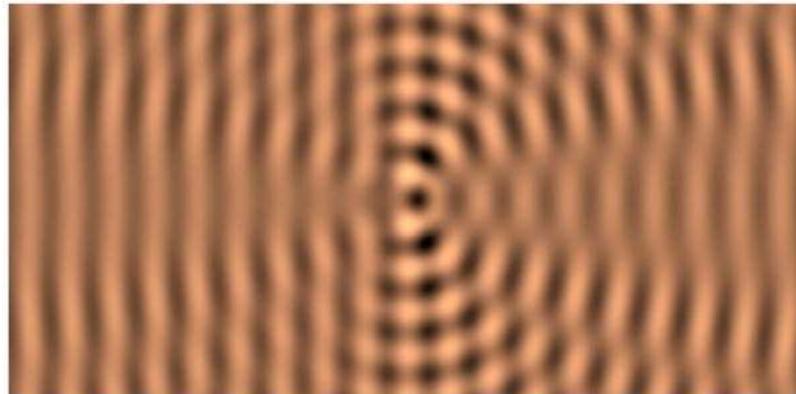
At first, Schrödinger and others thought that wave functions represent particles that are spread out, like pressure disturbances in a fluid — most of the particle is where the wave function is large. This interpretation became untenable with the analysis of scattering in quantum mechanics by Max Born<sup>1</sup> (1882–1970).

Weinberg QM, p.21

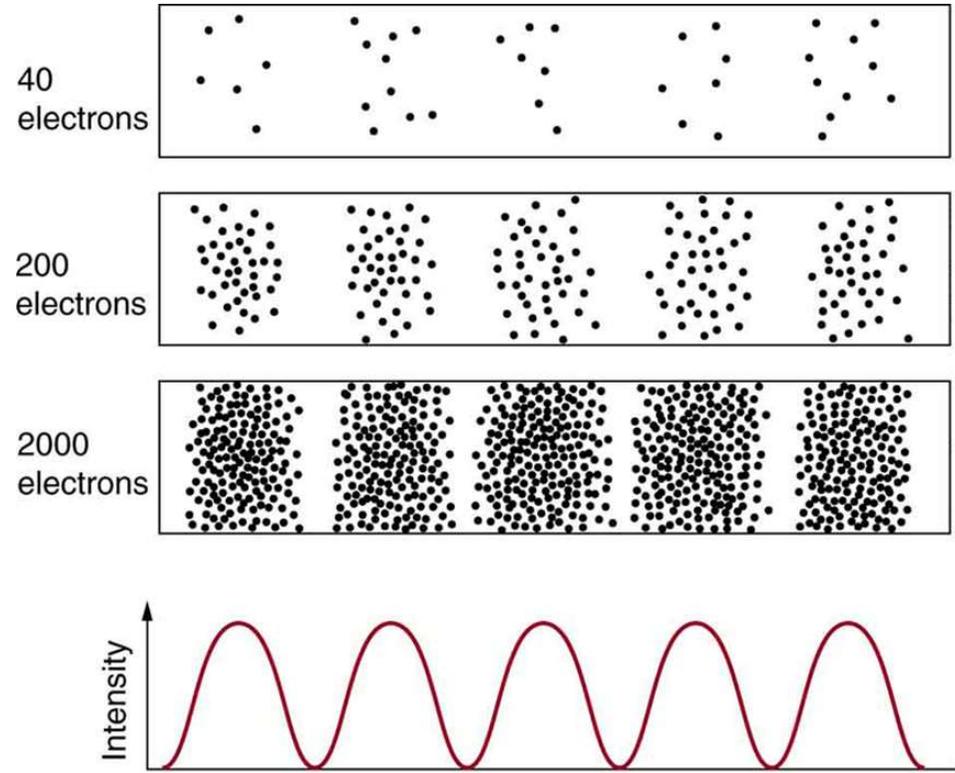
Born studied the quantum scattering of particles.

At low energy, the scattered wave is nearly spherical.

But the actual particle will not spread out evenly.



➔ Born: The matter waves  $\Psi(x,t)$  are waves of probability amplitude



Slightly different terminologies:

- probability amplitude  $\Psi(\vec{r}, t)$
- probability density  $|\Psi(\vec{r}, t)|^2$
- probability  $|\Psi(\vec{r}, t)|^2 d^3v$   
(to find a particle in  $d^3v$ )
- Normalization  $\int d^3v |\Psi(\vec{r}, t)|^2 = 1$

## The Copenhagen Interpretation

- The Copenhagen interpretation is a collection of views about the meaning of quantum mechanics (notoriously opaque). It is the orthodox interpretation of Quantum Mechanics, but there are different versions.
  1. The uncertainty principle of Heisenberg
  2. The complementarity principle of Bohr
  3. The statistical interpretation of Born, based on probabilities determined by the wave function
  4. The **measurement process** itself randomly choose one of the many possibilities allowed by the wave function... and more



The Bohr-Einstein debate (1926 onward)

*“Einstein would not admit that it was, impossible, even in principle, to discover all the partial facts needed for the complete description of a physical process. ‘God does not throw dice’ was a phrase we often heard from his lips in these discussions.*

Physics and beyond, by Heisenberg

Why people like Bohr and Heisenberg strongly believe in uncertainty principle? Because it's a simple and direct consequence of the operator algebra in quantum mechanics. If the uncertainty relation can be brought down, then the whole architecture of quantum mechanics would collapse.

John Bell on Bohr-Einstein debates:

*Bohr was inconsistent, unclear, willfully obscure and **right**.*

*Einstein was consistent, clear, down-to-earth and **wrong**.*